Full wwPDB X-ray Structure Validation Report (i)

Oct 10, 2023 – 12:21 AM EDT

PDB ID	:	5J91
Title	:	Structure of the Wild-type 70S E coli ribosome bound to Tigecycline
Authors	:	Cocozaki, A.; Ferguson, A.
Deposited on	:	2016-04-08
Resolution	:	2.96 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (i)) were used in the production of this report:

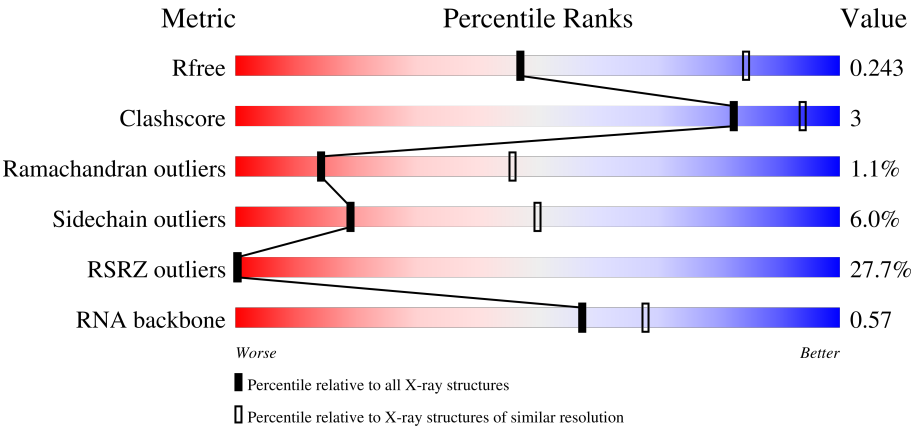
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.96 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3104 (3.00-2.92)
Clashscore	141614	3462 (3.00-2.92)
Ramachandran outliers	138981	3340 (3.00-2.92)
Sidechain outliers	138945	3343 (3.00-2.92)
RSRZ outliers	127900	2986 (3.00-2.92)
RNA backbone	3102	1065 (3.22-2.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	AA	1534	7% 78% 20% .
1	BA	1534	26% 77% 20% .
2	AB	224	32% 88% 11% .
2	BB	224	35% 85% 13% .

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Mol	Chain	Length	Quality of chain
3	AC	206	15% 86% 13%
3	BC	206	56% 83% 17%
4	AD	205	9% 88% 10%
4	BD	205	84% 15%
5	AE	155	8% 81% 17%
5	BE	155	21% 63% 29% 5%
6	AF	106	18% 85% 15%
6	BF	106	14% 70% 24% 6%
7	AG	151	42% 87% 12%
7	BG	151	83% 86% 14%
8	AH	129	7% 81% 19%
8	BH	129	19% 85% 15%
9	AI	127	46% 90% 9%
9	BI	127	61% 90% 9%
10	AJ	99	41% 75% 24%
10	BJ	99	79% 73% 23%
11	AK	117	30% 80% 18%
11	BK	117	28% 74% 22%
12	AL	123	3% 85% 13%
12	BL	123	25% 83% 11% 6%
13	AM	114	50% 80% 17%
13	BM	114	91% 78% 19%
14	AN	100	37% 88% 12%
14	BN	100	75% 88% 12%
15	AO	88	11% 92% 8%

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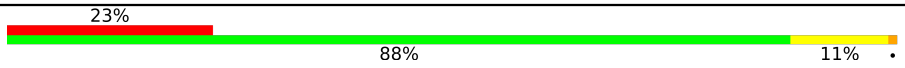
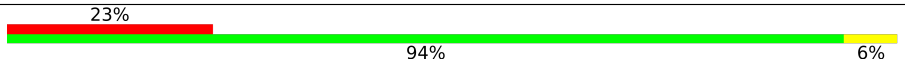
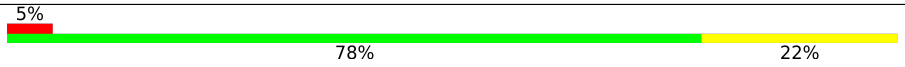
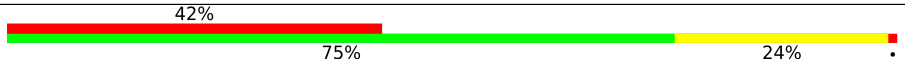
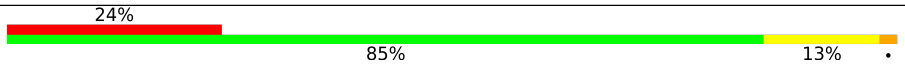
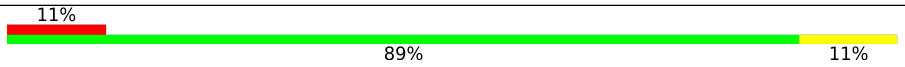
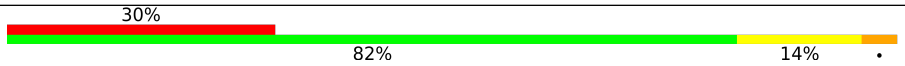
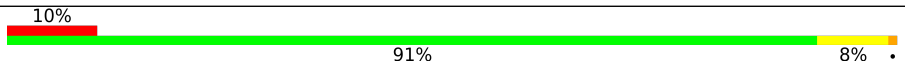
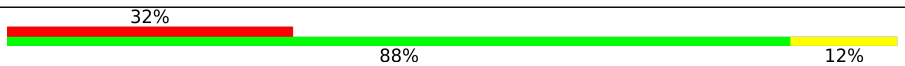
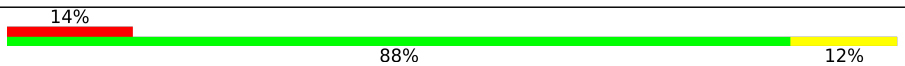
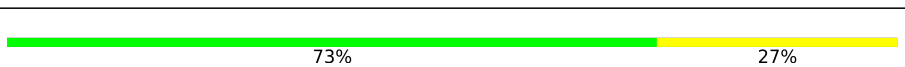
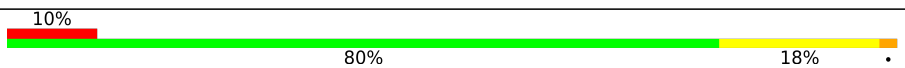
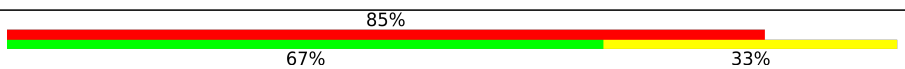
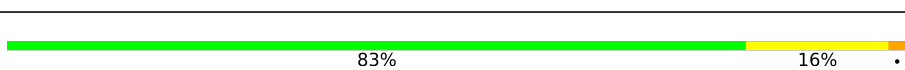
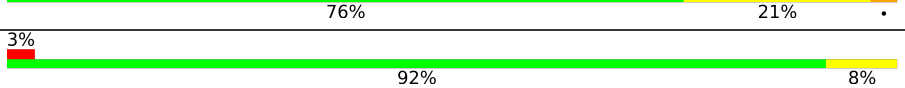
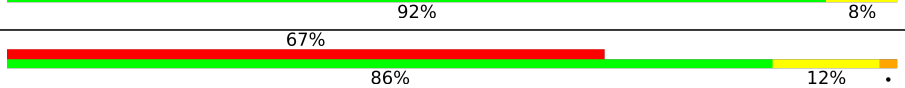
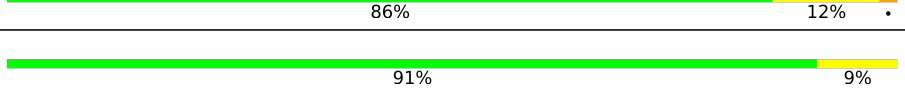
Mol	Chain	Length	Quality of chain
15	BO	88	
16	AP	82	
16	BP	82	
17	AQ	80	
17	BQ	80	
18	AR	55	
18	BR	55	
19	AS	79	
19	BS	79	
20	AT	86	
20	BT	86	
21	AU	56	
21	BU	56	
22	C1	56	
22	D1	56	
23	C2	51	
23	D2	51	
24	C3	46	
24	D3	46	
25	C4	64	
25	D4	64	
26	C5	38	
26	D5	38	
27	C0	58	
27	D0	58	

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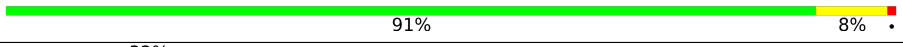
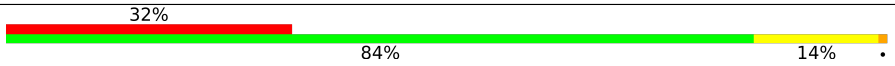
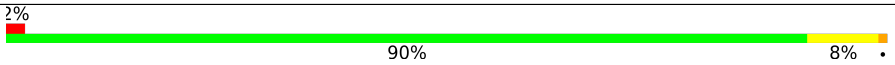
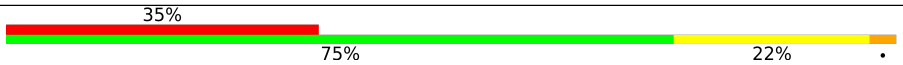
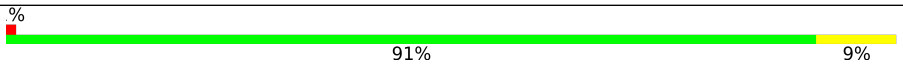
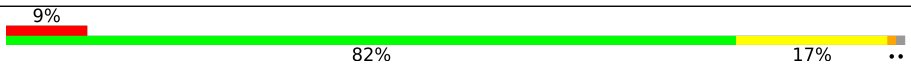
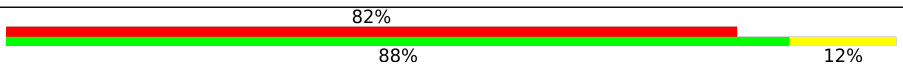
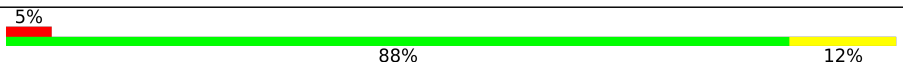
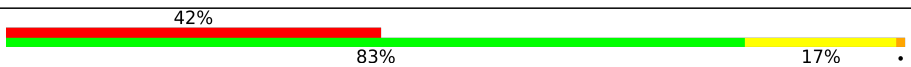
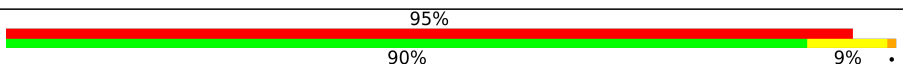
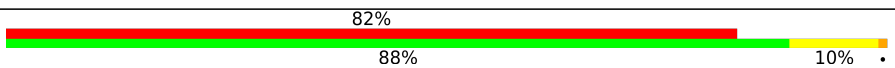
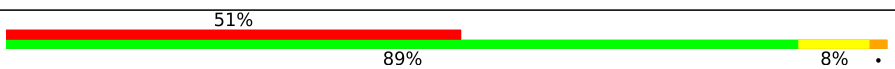
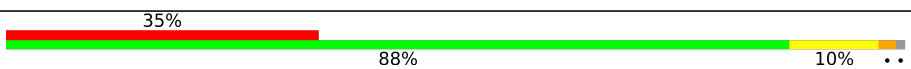
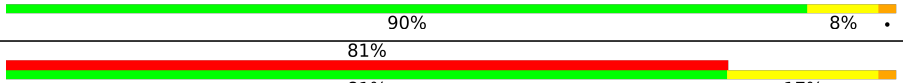
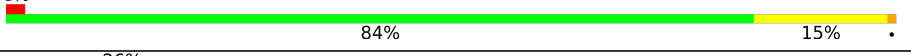
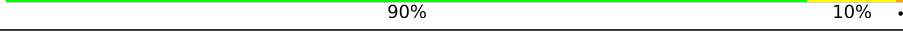
Mol	Chain	Length	Quality of chain
28	CB	120	
28	DB	120	
29	CC	272	
29	DC	272	
30	CD	209	
31	CA	2904	
32	DD	209	
33	CE	201	
33	DE	201	
34	CF	178	
34	DF	178	
35	CG	176	
35	DG	176	
36	CH	149	
36	DH	149	
37	CJ	134	
37	DJ	134	
38	CK	142	
38	DK	142	
39	CL	123	
39	DL	123	
40	CM	144	
40	DM	144	
41	CN	136	
41	DN	136	

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Mol	Chain	Length	Quality of chain
42	CO	125	58% 86% 9%
42	DO	125	% 93% 7%
43	CP	117	74% 86% 11%
43	DP	117	90% 8%
44	CQ	114	57% 89% 11%
44	DQ	114	3% 90% 10%
45	CR	117	61% 89% 11%
45	DR	117	% 93% 6%
46	CS	103	83% 85% 13%
46	DS	103	% 92% 7%
47	CT	110	56% 78% 20%
47	DT	110	86% 14%
48	CU	93	78% 75% 22%
48	DU	93	5% 90% 10%
49	CV	103	85% 83% 15%
49	DV	103	11% 89% 9%
50	CW	94	56% 89% 11%
50	DW	94	91% 9%
51	CX	76	50% 95%
51	DX	76	% 91% 9%
52	CY	77	42% 82% 18%
52	DY	77	% 90% 10%
53	CZ	62	79% 90% 8%
53	DZ	62	10% 94% 6%
54	DI	135	53% 71% 27%

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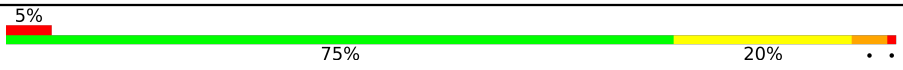
Mol	Chain	Length	Quality of chain
55	DA	2904	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
56	MG	AA	1602	-	-	-	X
56	MG	AA	1603	-	-	-	X
56	MG	AA	1604	-	-	-	X
56	MG	AA	1605	-	-	-	X
56	MG	AA	1606	-	-	-	X
56	MG	AA	1608	-	-	-	X
56	MG	AA	1612	-	-	-	X
56	MG	AA	1613	-	-	-	X
56	MG	AA	1615	-	-	-	X
56	MG	AA	1616	-	-	-	X
56	MG	AA	1618	-	-	-	X
56	MG	AA	1620	-	-	-	X
56	MG	AA	1621	-	-	-	X
56	MG	AA	1622	-	-	-	X
56	MG	AA	1624	-	-	-	X
56	MG	AA	1626	-	-	-	X
56	MG	AA	1627	-	-	-	X
56	MG	AA	1628	-	-	-	X
56	MG	AA	1642	-	-	-	X
56	MG	BA	1623	-	-	-	X
56	MG	BA	1629	-	-	-	X
56	MG	BA	1637	-	-	-	X
56	MG	BA	1638	-	-	-	X
56	MG	BA	1639	-	-	-	X
56	MG	BA	1641	-	-	-	X
56	MG	CA	3003	-	-	-	X
56	MG	CA	3005	-	-	-	X
56	MG	CA	3007	-	-	-	X
56	MG	CA	3010	-	-	-	X
56	MG	CA	3026	-	-	-	X
56	MG	CA	3028	-	-	-	X
56	MG	CA	3032	-	-	-	X
56	MG	CA	3047	-	-	-	X
56	MG	CA	3056	-	-	-	X
56	MG	CA	3068	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
56	MG	CA	3075	-	-	-	X
56	MG	CA	3082	-	-	-	X
56	MG	CA	3090	-	-	-	X
56	MG	CA	3105	-	-	-	X
56	MG	CA	3106	-	-	-	X
56	MG	CA	3108	-	-	-	X
56	MG	CA	3109	-	-	-	X
56	MG	CA	3110	-	-	-	X
56	MG	CA	3111	-	-	-	X
56	MG	CA	3113	-	-	-	X
56	MG	CA	3115	-	-	-	X
56	MG	CA	3121	-	-	-	X
56	MG	CA	3122	-	-	-	X
56	MG	CA	3123	-	-	-	X
56	MG	CA	3124	-	-	-	X
56	MG	CA	3128	-	-	-	X
56	MG	CA	3130	-	-	-	X
56	MG	CA	3131	-	-	-	X
56	MG	CA	3132	-	-	-	X
56	MG	CA	3133	-	-	-	X
56	MG	CA	3134	-	-	-	X
56	MG	CA	3135	-	-	-	X
56	MG	CA	3137	-	-	-	X
56	MG	CA	3139	-	-	-	X
56	MG	CA	3140	-	-	-	X
56	MG	CA	3141	-	-	-	X
56	MG	CA	3142	-	-	-	X
56	MG	CA	3148	-	-	-	X
56	MG	CA	3149	-	-	-	X
56	MG	CA	3154	-	-	-	X
56	MG	DA	3125	-	-	-	X
56	MG	DA	3131	-	-	-	X
56	MG	DA	3143	-	-	-	X
56	MG	DA	3145	-	-	-	X
56	MG	DA	3147	-	-	-	X
56	MG	DA	3155	-	-	-	X
56	MG	DA	3157	-	-	-	X
56	MG	DA	3159	-	-	-	X
56	MG	DA	3161	-	-	-	X
56	MG	DA	3167	-	-	-	X
56	MG	DA	3168	-	-	-	X
56	MG	DA	3171	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
56	MG	DA	3173	-	-	-	X
56	MG	DA	3178	-	-	-	X
56	MG	DA	3179	-	-	-	X
56	MG	DA	3180	-	-	-	X
56	MG	DA	3182	-	-	-	X
56	MG	DB	206	-	-	-	X
56	MG	DB	207	-	-	-	X
57	PG4	DA	3215	-	-	-	X
58	MPD	DA	3203	-	-	-	X
58	MPD	DA	3206	-	-	-	X
58	MPD	DE	302	-	-	-	X
58	MPD	DT	201	-	-	-	X
58	MPD	DT	202	-	-	-	X
59	PUT	AA	1672	-	-	-	X
59	PUT	AA	1673	-	-	-	X
59	PUT	AA	1674	-	-	-	X
59	PUT	AA	1675	-	-	-	X
59	PUT	DA	3218	-	-	-	X
62	PEG	D1	103	-	-	-	X
62	PEG	D3	102	-	-	-	X
62	PEG	DA	3217	-	-	-	X
62	PEG	DP	201	-	-	-	X
62	PEG	DQ	201	-	-	-	X
63	EDO	DA	3004	-	-	-	X
63	EDO	DA	3208	-	-	-	X
63	EDO	DB	210	-	-	-	X
64	PGE	D1	102	-	-	-	X
64	PGE	D3	101	-	-	-	X
69	TRS	DA	3219	-	-	-	X

2 Entry composition

There are 70 unique types of molecules in this entry. The entry contains 295202 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a RNA chain called 16S rRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AA	1534	Total	C	N	O	P	0	0	0
			32930	14694	6041	10661	1534			
1	BA	1533	Total	C	N	O	P	0	0	0
			32908	14684	6036	10655	1533			

- Molecule 2 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	AB	224	Total	C	N	O	S	0	0	0
			1753	1109	315	321	8			
2	BB	224	Total	C	N	O	S	0	0	0
			1753	1109	315	321	8			

- Molecule 3 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	AC	206	Total	C	N	O	S	0	0	0
			1625	1028	305	289	3			
3	BC	206	Total	C	N	O	S	0	0	0
			1625	1028	305	289	3			

- Molecule 4 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	AD	205	Total	C	N	O	S	0	0	0
			1643	1026	315	298	4			
4	BD	205	Total	C	N	O	S	0	0	0
			1643	1026	315	298	4			

- Molecule 5 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	AE	155	Total	C	N	O	S	0	0	0
			1144	711	216	211	6			
5	BE	150	Total	C	N	O	S	0	0	0
			1105	687	211	201	6			

- Molecule 6 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	AF	106	Total	C	N	O	S	0	0	0
			862	545	156	154	7			
6	BF	100	Total	C	N	O	S	0	0	0
			817	515	148	148	6			

- Molecule 7 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	AG	151	Total	C	N	O	S	0	0	0
			1182	735	227	216	4			
7	BG	151	Total	C	N	O	S	0	0	0
			1182	735	227	216	4			

- Molecule 8 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	AH	129	Total	C	N	O	S	0	0	0
			979	616	173	184	6			
8	BH	129	Total	C	N	O	S	0	0	0
			979	616	173	184	6			

- Molecule 9 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	AI	127	Total	C	N	O	S	0	0	0
			1022	634	206	179	3			
9	BI	127	Total	C	N	O	S	0	0	0
			1022	634	206	179	3			

- Molecule 10 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	AJ	99	Total	C	N	O	S	0	0	0
			796	498	152	145	1			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	BJ	98	Total	C	N	O	S	0	0	0
			787	493	150	143	1			

- Molecule 11 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	AK	117	Total	C	N	O	S	0	0	0
			877	540	174	160	3			
11	BK	117	Total	C	N	O	S	0	0	0
			877	540	174	160	3			

- Molecule 12 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	AL	123	Total	C	N	O	S	0	0	0
			957	591	196	165	5			
12	BL	123	Total	C	N	O	S	0	0	0
			957	591	196	165	5			

- Molecule 13 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	AM	114	Total	C	N	O	S	0	0	0
			884	546	178	157	3			
13	BM	114	Total	C	N	O	S	0	0	0
			884	546	178	157	3			

- Molecule 14 is a protein called 30S ribosomal protein S14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	AN	100	Total	C	N	O	S	0	0	0
			805	499	164	139	3			
14	BN	100	Total	C	N	O	S	0	0	0
			805	499	164	139	3			

- Molecule 15 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	AO	88	Total	C	N	O	S	0	0	0
			714	439	144	130	1			
15	BO	88	Total	C	N	O	S	0	0	0
			714	439	144	130	1			

- Molecule 16 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	AP	82	Total	C	N	O	S	0	0	0
			649	406	128	114	1			
16	BP	82	Total	C	N	O	S	0	0	0
			649	406	128	114	1			

- Molecule 17 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	AQ	80	Total	C	N	O	S	0	0	0
			649	411	121	114	3			
17	BQ	80	Total	C	N	O	S	0	0	0
			649	411	121	114	3			

- Molecule 18 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
18	AR	55	Total	C	N	O	0	0	0
			456	288	86	82			
18	BR	55	Total	C	N	O	0	0	0
			456	288	86	82			

- Molecule 19 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	AS	79	Total	C	N	O	S	0	0	0
			638	408	120	108	2			
19	BS	79	Total	C	N	O	S	0	0	0
			638	408	120	108	2			

- Molecule 20 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	AT	86	Total	C	N	O	S	0	0	0
			670	414	138	115	3			
20	BT	85	Total	C	N	O	S	0	0	0
			665	411	137	114	3			

- Molecule 21 is a protein called 30S ribosomal protein S21.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
21	AU	56	Total	C	N	O	S	0	0	0
			465	290	96	78	1			
21	BU	56	Total	C	N	O	S	0	0	0
			465	290	96	78	1			

- Molecule 22 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	C1	56	Total	C	N	O	S	0	0	0
			444	269	94	80	1			
22	D1	56	Total	C	N	O	S	0	0	0
			444	269	94	80	1			

- Molecule 23 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
23	C2	50	Total	C	N	O	0	0	0
			409	263	75	71			
23	D2	51	Total	C	N	O	0	0	0
			414	266	76	72			

- Molecule 24 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	C3	46	Total	C	N	O	S	0	0	0
			377	228	90	57	2			
24	D3	46	Total	C	N	O	S	0	0	0
			377	228	90	57	2			

- Molecule 25 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	C4	64	Total	C	N	O	S	0	0	0
			504	323	105	74	2			
25	D4	64	Total	C	N	O	S	0	0	0
			504	323	105	74	2			

- Molecule 26 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	C5	38	Total	C	N	O	S	0	0	0
			302	185	65	48	4			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	D5	38	Total	C	N	O	S	0	0	0
			302	185	65	48	4			

- Molecule 27 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	C0	58	Total	C	N	O	S	0	0	0
			449	281	87	79	2			
27	D0	58	Total	C	N	O	S	0	2	0
			463	290	90	81	2			

- Molecule 28 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	CB	118	Total	C	N	O	P	0	0	0
			2529	1126	464	821	118			
28	DB	120	Total	C	N	O	P	0	0	0
			2569	1144	468	837	120			

- Molecule 29 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	CC	271	Total	C	N	O	S	0	0	0
			2082	1288	423	364	7			
29	DC	271	Total	C	N	O	S	0	0	0
			2082	1288	423	364	7			

- Molecule 30 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	CD	209	Total	C	N	O	S	0	0	0
			1565	979	288	294	4			

- Molecule 31 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	CA	2898	Total	C	N	O	P	0	0	0
			62229	27768	11448	20115	2898			

- Molecule 32 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	DD	209	Total	C	N	O	S	0	1	0
			1576	986	290	296	4			

- Molecule 33 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
33	CE	201	Total	C	N	O	S	0	0	0
			1552	974	283	290	5			
33	DE	201	Total	C	N	O	S	0	0	0
			1552	974	283	290	5			

- Molecule 34 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
34	CF	177	Total	C	N	O	S	0	0	0
			1410	899	249	256	6			
34	DF	177	Total	C	N	O	S	0	0	0
			1410	899	249	256	6			

- Molecule 35 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
35	CG	176	Total	C	N	O	S	0	0	0
			1323	832	243	246	2			
35	DG	176	Total	C	N	O	S	0	0	0
			1323	832	243	246	2			

- Molecule 36 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
36	CH	149	Total	C	N	O	S	0	0	0
			1110	699	197	213	1			
36	DH	149	Total	C	N	O	S	0	0	0
			1110	699	197	213	1			

- Molecule 37 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
37	CJ	134	Total	C	N	O	S	0	0	0
			979	619	169	185	6			
37	DJ	134	Total	C	N	O	S	0	0	0
			979	619	169	185	6			

- Molecule 38 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
38	CK	142	Total	C	N	O	S	0	0	0
			1129	714	212	199	4			
38	DK	142	Total	C	N	O	S	0	0	0
			1129	714	212	199	4			

- Molecule 39 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
39	CL	122	Total	C	N	O	S	0	0	0
			938	587	180	165	6			
39	DL	123	Total	C	N	O	S	0	0	0
			946	593	181	166	6			

- Molecule 40 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
40	CM	144	Total	C	N	O	S	0	0	0
			1053	654	207	190	2			
40	DM	144	Total	C	N	O	S	0	0	0
			1053	654	207	190	2			

- Molecule 41 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
41	CN	136	Total	C	N	O	S	0	0	0
			1075	686	205	178	6			
41	DN	136	Total	C	N	O	S	0	2	0
			1092	696	211	179	6			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
CN	81	4D4	ARG	conflict	UNP P0ADY7
DN	81	4D4	ARG	conflict	UNP P0ADY7

- Molecule 42 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
42	CO	120	Total	C	N	O	S	0	0	0
			960	593	196	166	5			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
42	DO	125	Total	C	N	O	S	0	0	0
			993	613	202	173	5			

- Molecule 43 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
43	CP	116	Total	C	N	O		0	0	0
			892	552	178	162				
43	DP	117	Total	C	N	O	S	0	0	0
			900	557	179	163	1			

- Molecule 44 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
44	CQ	114	Total	C	N	O	S	0	0	0
			917	574	179	163	1			
44	DQ	114	Total	C	N	O	S	0	0	0
			917	574	179	163	1			

- Molecule 45 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
45	CR	117	Total	C	N	O	0	0	0
			947	604	192	151			
45	DR	117	Total	C	N	O	0	0	0
			947	604	192	151			

- Molecule 46 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
46	CS	103	Total	C	N	O	S	0	0	0
			816	516	153	145	2			
46	DS	103	Total	C	N	O	S	0	0	0
			816	516	153	145	2			

- Molecule 47 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
47	CT	110	Total	C	N	O	S	0	0	0
			857	532	166	156	3			
47	DT	110	Total	C	N	O	S	0	0	0
			857	532	166	156	3			

- Molecule 48 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
48	CU	93	Total	C	N	O	S	0	0	0
			739	466	139	132	2			
48	DU	93	Total	C	N	O	S	0	0	0
			739	466	139	132	2			

- Molecule 49 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
49	CV	102	Total	C	N	O	0	0	0
			779	492	146	141			
49	DV	102	Total	C	N	O	0	0	0
			779	492	146	141			

- Molecule 50 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
50	CW	94	Total	C	N	O	S	0	0	0
			753	479	137	134	3			
50	DW	94	Total	C	N	O	S	0	0	0
			753	479	137	134	3			

- Molecule 51 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
51	CX	75	Total	C	N	O	S	0	0	0
			569	353	113	102	1			
51	DX	76	Total	C	N	O	S	0	1	0
			591	365	121	104	1			

- Molecule 52 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
52	CY	77	Total	C	N	O	S	0	0	0
			625	388	129	106	2			
52	DY	77	Total	C	N	O	S	0	0	0
			625	388	129	106	2			

- Molecule 53 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
53	CZ	62	Total	C	N	O	S	0	0	0
			501	308	98	94	1			
53	DZ	62	Total	C	N	O	S	0	0	0
			501	308	98	94	1			

- Molecule 54 is a protein called 50S ribosomal protein L10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
54	DI	135	Total	C	N	O	S	0	0	0
			1023	649	179	192	3			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
DI	85	VAL	SER	conflict	UNP P0A7J3
DI	86	THR	MET	conflict	UNP P0A7J3

- Molecule 55 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
55	DA	2897	Total	C	N	O	P	0	11	0
			62423	27855	11485	20176	2907			

- Molecule 56 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	AA	71	Total	Mg	0	0
			71	71		
56	BA	43	Total	Mg	0	0
			43	43		
56	CB	3	Total	Mg	0	0
			3	3		
56	CA	156	Total	Mg	0	0
			156	156		
56	DD	2	Total	Mg	0	0
			2	2		
56	DM	1	Total	Mg	0	0
			1	1		
56	DR	2	Total	Mg	0	0
			2	2		
56	DB	9	Total	Mg	0	0
			9	9		

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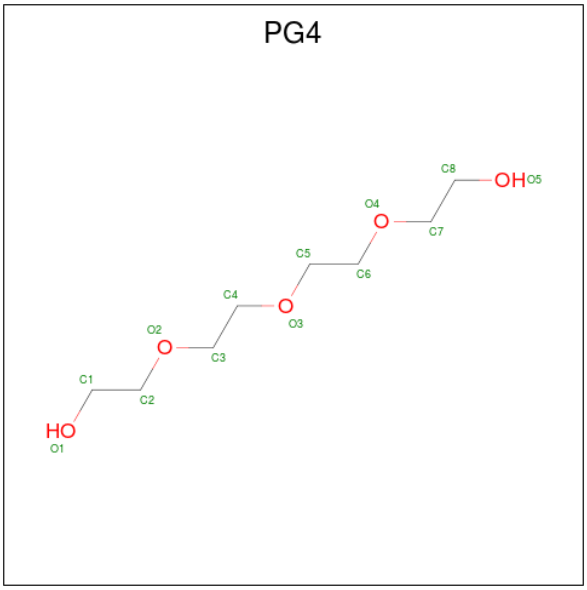
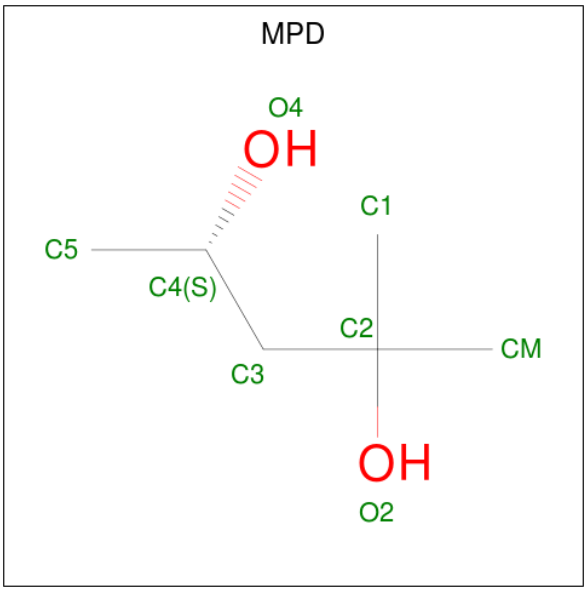
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
56	DA	182	Total Mg 182 182	0	0

- Molecule 57 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: $C_8H_{18}O_5$).



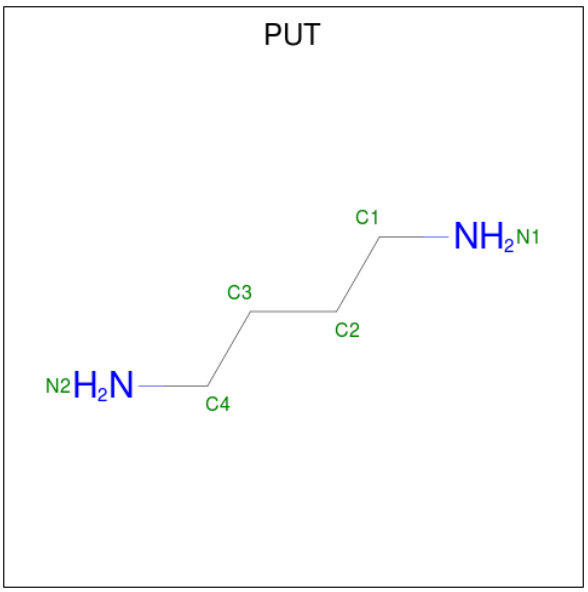
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
57	AA	1	Total C O 13 8 5	0	0
57	BA	1	Total C O 13 8 5	0	0
57	DQ	1	Total C O 13 8 5	0	0
57	DR	1	Total C O 13 8 5	0	0
57	DS	1	Total C O 13 8 5	0	0
57	DA	1	Total C O 13 8 5	0	0
57	DA	1	Total C O 13 8 5	0	0

- Molecule 58 is (4S)-2-METHYL-2,4-PENTANEDIOL (three-letter code: MPD) (formula: $C_6H_{14}O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
58	AA	1	Total	C	O	0	0
			8	6	2		
58	AA	1	Total	C	O	0	0
			8	6	2		
58	DE	1	Total	C	O	0	0
			8	6	2		
58	DE	1	Total	C	O	0	0
			8	6	2		
58	DK	1	Total	C	O	0	0
			8	6	2		
58	DN	1	Total	C	O	0	0
			8	6	2		
58	DS	1	Total	C	O	0	0
			8	6	2		
58	DT	1	Total	C	O	0	0
			8	6	2		
58	DT	1	Total	C	O	0	0
			8	6	2		
58	DA	1	Total	C	O	0	0
			8	6	2		
58	DA	1	Total	C	O	0	0
			8	6	2		
58	DA	1	Total	C	O	0	0
			8	6	2		
58	DA	1	Total	C	O	0	0
			8	6	2		
58	DA	1	Total	C	O	0	0
			8	6	2		

- Molecule 59 is 1,4-DIAMINOBUTANE (three-letter code: PUT) (formula: $C_4H_{12}N_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
59	AA	1	Total C N 6 4 2	0	0
59	AA	1	Total C N 6 4 2	0	0
59	AA	1	Total C N 6 4 2	0	0
59	AA	1	Total C N 6 4 2	0	0
59	DA	1	Total C N 6 4 2	0	0
59	DA	1	Total C N 6 4 2	0	0
59	DA	1	Total C N 6 4 2	0	0
59	DA	1	Total C N 6 4 2	0	0
59	DA	1	Total C N 6 4 2	0	0
59	DA	1	Total C N 6 4 2	0	0
59	DA	1	Total C N 6 4 2	0	0
59	DA	1	Total C N 6 4 2	0	0

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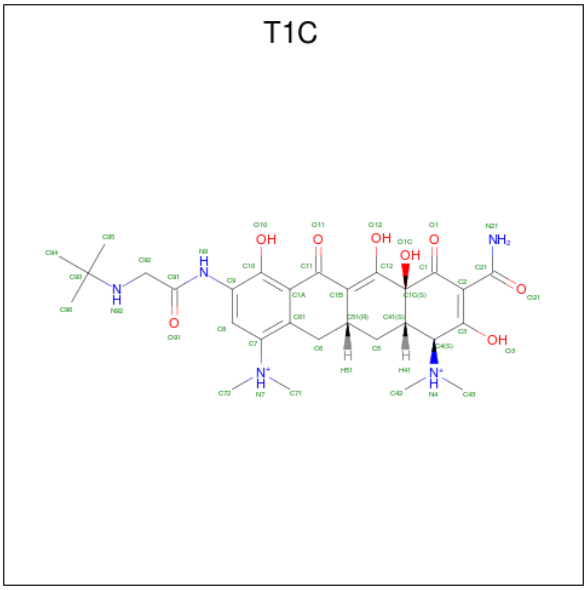
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
59	DA	1	Total C N 6 4 2	0	0
59	DA	1	Total C N 6 4 2	0	0
59	DA	1	Total C N 6 4 2	0	0

- Molecule 60 is TIGECYCLINE (three-letter code: T1C) (formula: $C_{29}H_{41}N_5O_8$).



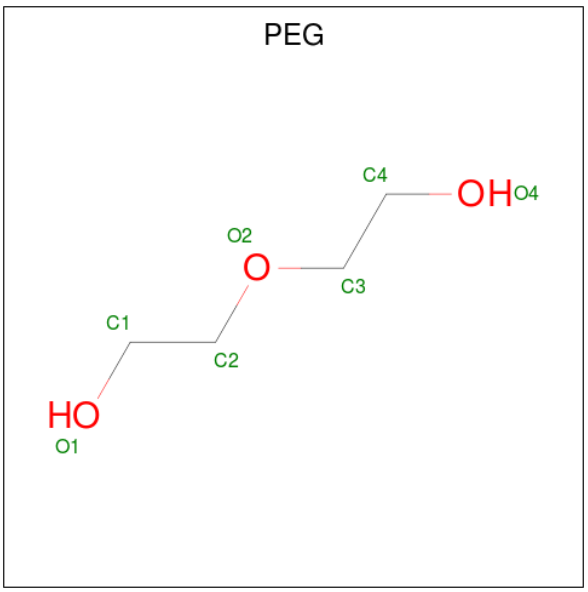
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
60	AA	1	Total C N O 42 29 5 8	0	0
60	BA	1	Total C N O 42 29 5 8	0	0

- Molecule 61 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
61	AB	1	Total Zn 1 1	0	0
61	C5	1	Total Zn 1 1	0	0
61	D5	1	Total Zn 1 1	0	0

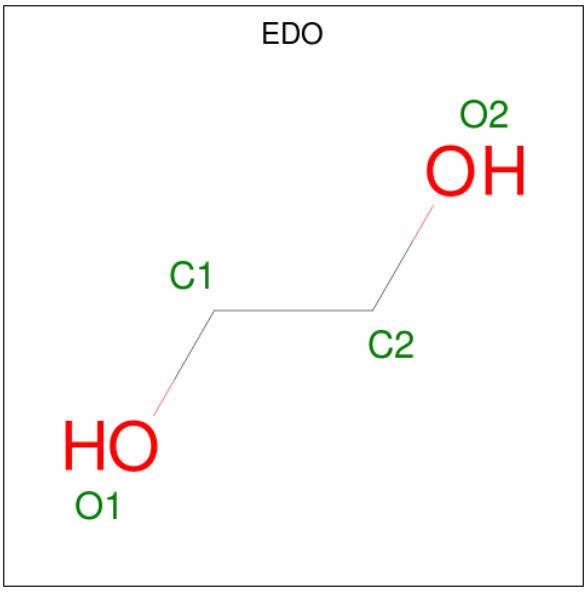
- Molecule 62 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula:

$C_4H_{10}O_3$).



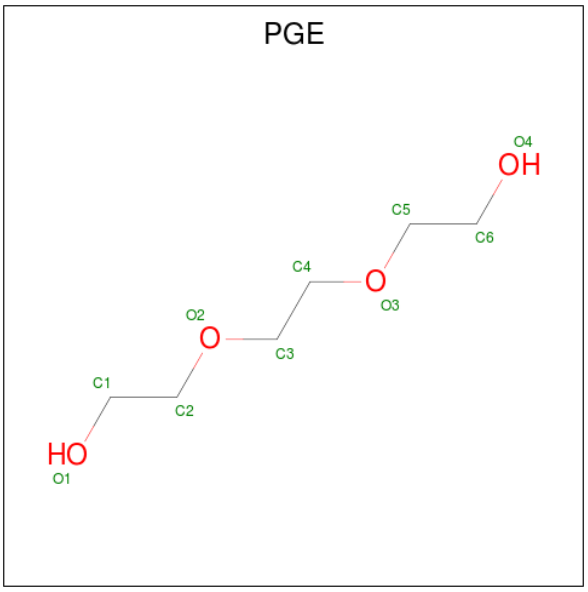
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
62	AL	1	Total C O 7 4 3	0	0
62	D1	1	Total C O 7 4 3	0	0
62	D3	1	Total C O 7 4 3	0	0
62	DL	1	Total C O 7 4 3	0	0
62	DP	1	Total C O 7 4 3	0	0
62	DQ	1	Total C O 7 4 3	0	0
62	DA	1	Total C O 7 4 3	0	0
62	DA	1	Total C O 7 4 3	0	0
62	DA	1	Total C O 7 4 3	0	0
62	DA	1	Total C O 7 4 3	0	0
62	DA	1	Total C O 7 4 3	0	0

- Molecule 63 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



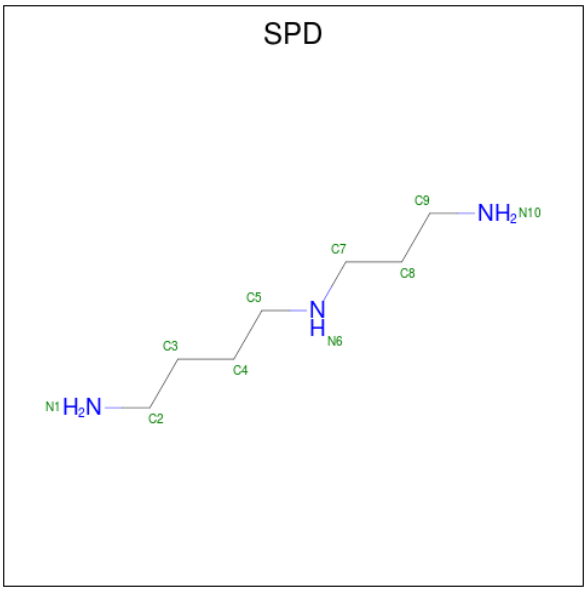
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
63	D1	1	Total	C	O	0	0
			4	2	2		
63	DB	1	Total	C	O	0	0
			4	2	2		
63	DB	1	Total	C	O	0	0
			4	2	2		
63	DA	1	Total	C	O	0	0
			4	2	2		
63	DA	1	Total	C	O	0	0
			4	2	2		
63	DA	1	Total	C	O	0	0
			4	2	2		
63	DA	1	Total	C	O	0	0
			4	2	2		
63	DA	1	Total	C	O	0	0
			4	2	2		
63	DA	1	Total	C	O	0	0
			4	2	2		
63	DA	1	Total	C	O	0	0
			4	2	2		
63	DA	1	Total	C	O	0	0
			4	2	2		
63	DA	1	Total	C	O	0	0
			4	2	2		

- Molecule 64 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: $C_6H_{14}O_4$).



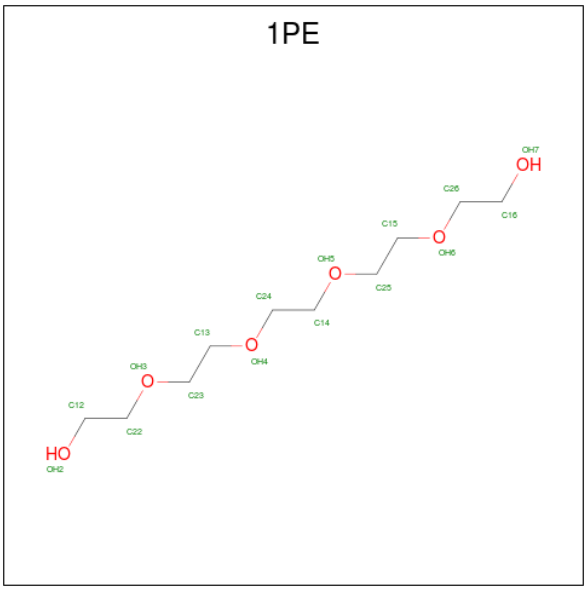
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
64	D1	1	Total C O 10 6 4	0	0
64	D3	1	Total C O 10 6 4	0	0
64	DD	1	Total C O 10 6 4	0	0
64	DS	1	Total C O 10 6 4	0	0
64	DU	1	Total C O 10 6 4	0	0
64	DA	1	Total C O 10 6 4	0	0
64	DA	1	Total C O 10 6 4	0	0
64	DA	1	Total C O 10 6 4	0	0
64	DA	1	Total C O 10 6 4	0	0

- Molecule 65 is SPERMIDINE (three-letter code: SPD) (formula: $C_7H_{19}N_3$).



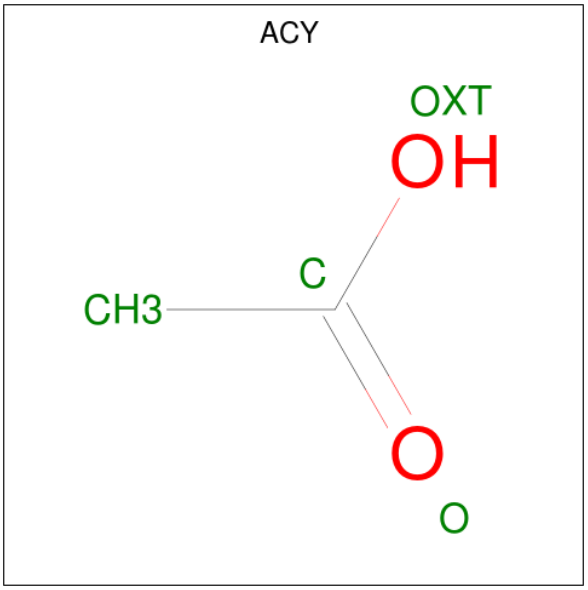
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
65	DA	1	Total C N 10 7 3	0	0
65	DA	1	Total C N 10 7 3	0	0
65	DA	1	Total C N 10 7 3	0	0
65	DA	1	Total C N 10 7 3	0	0

- Molecule 66 is PENTAETHYLENE GLYCOL (three-letter code: 1PE) (formula: $C_{10}H_{22}O_6$).



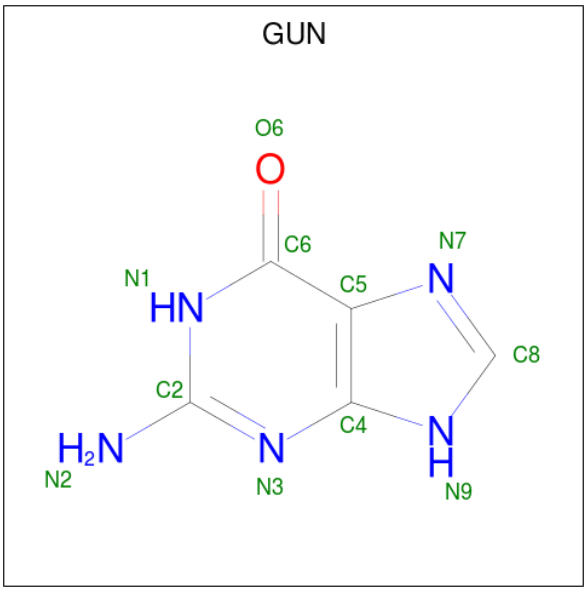
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
66	DA	1	Total C O 16 10 6	0	0
66	DA	1	Total C O 16 10 6	0	0

- Molecule 67 is ACETIC ACID (three-letter code: ACY) (formula: $C_2H_4O_2$).



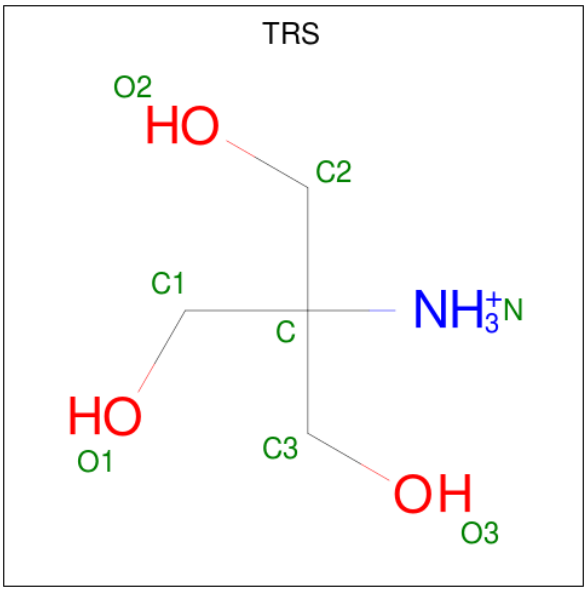
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
67	DA	1	Total C O 4 2 2	0	0
67	DA	1	Total C O 4 2 2	0	0
67	DA	1	Total C O 4 2 2	0	0

- Molecule 68 is GUANINE (three-letter code: GUN) (formula: $C_5H_5N_5O$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
68	DA	1	11	5	5	1	0	0

- Molecule 69 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (three-letter code: TRS) (formula: $C_4H_{12}NO_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
69	DA	1	8	4	1	3	0	0

- Molecule 70 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
70	AA	507	Total O 507 507	0	0
70	AC	4	Total O 4 4	0	0
70	AD	2	Total O 2 2	0	0
70	AE	4	Total O 4 4	0	0
70	AF	1	Total O 1 1	0	0
70	AG	1	Total O 1 1	0	0
70	AH	1	Total O 1 1	0	0
70	AJ	2	Total O 2 2	0	0
70	AK	5	Total O 5 5	0	0
70	AL	8	Total O 8 8	0	0
70	AM	4	Total O 4 4	0	0
70	AN	5	Total O 5 5	0	0
70	AO	2	Total O 2 2	0	0
70	AP	2	Total O 2 2	0	0
70	AR	1	Total O 1 1	0	0
70	AS	1	Total O 1 1	0	0
70	AT	2	Total O 2 2	0	0
70	AU	3	Total O 3 3	0	0
70	C3	3	Total O 3 3	0	0
70	C4	1	Total O 1 1	0	0
70	BA	287	Total O 287 287	0	0
70	BD	13	Total O 13 13	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
70	BE	1	Total O 1 1	0	0
70	BF	1	Total O 1 1	0	0
70	BK	1	Total O 1 1	0	0
70	BL	3	Total O 3 3	0	0
70	BN	2	Total O 2 2	0	0
70	BO	1	Total O 1 1	0	0
70	BP	3	Total O 3 3	0	0
70	BR	1	Total O 1 1	0	0
70	BT	4	Total O 4 4	0	0
70	BU	2	Total O 2 2	0	0
70	D1	42	Total O 42 42	0	0
70	D2	7	Total O 7 7	0	0
70	D3	25	Total O 25 25	0	0
70	D4	32	Total O 32 32	0	0
70	D5	13	Total O 13 13	0	0
70	D0	25	Total O 25 25	0	0
70	CB	13	Total O 13 13	0	0
70	CC	10	Total O 10 10	0	0
70	CD	5	Total O 5 5	0	0
70	CA	694	Total O 694 694	0	0
70	DC	102	Total O 102 102	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
70	DD	105	Total O 105 105	0	0
70	CE	6	Total O 6 6	0	0
70	CL	1	Total O 1 1	0	0
70	CM	3	Total O 3 3	0	0
70	CO	1	Total O 1 1	0	0
70	CU	3	Total O 3 3	0	0
70	CV	1	Total O 1 1	0	0
70	CW	1	Total O 1 1	0	0
70	CY	1	Total O 1 1	0	0
70	DE	63	Total O 63 63	0	0
70	DF	14	Total O 14 14	0	0
70	DG	6	Total O 6 6	0	0
70	DH	2	Total O 2 2	0	0
70	DK	58	Total O 58 58	0	0
70	DL	51	Total O 51 51	0	0
70	DM	60	Total O 60 60	0	0
70	DN	71	Total O 71 71	0	0
70	DO	44	Total O 44 44	0	0
70	DP	35	Total O 35 35	0	0
70	DQ	27	Total O 27 27	0	0
70	DR	64	Total O 64 64	0	0

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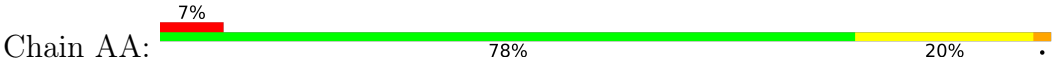
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
70	DS	51	Total O 51 51	0	0
70	DT	70	Total O 70 70	0	0
70	DU	17	Total O 17 17	0	0
70	DV	19	Total O 19 19	0	0
70	DW	31	Total O 31 31	0	0
70	DX	30	Total O 30 30	0	0
70	DY	9	Total O 9 9	0	0
70	DZ	7	Total O 7 7	0	0
70	DB	213	Total O 213 213	0	0
70	DA	4836	Total O 4836 4836	0	0

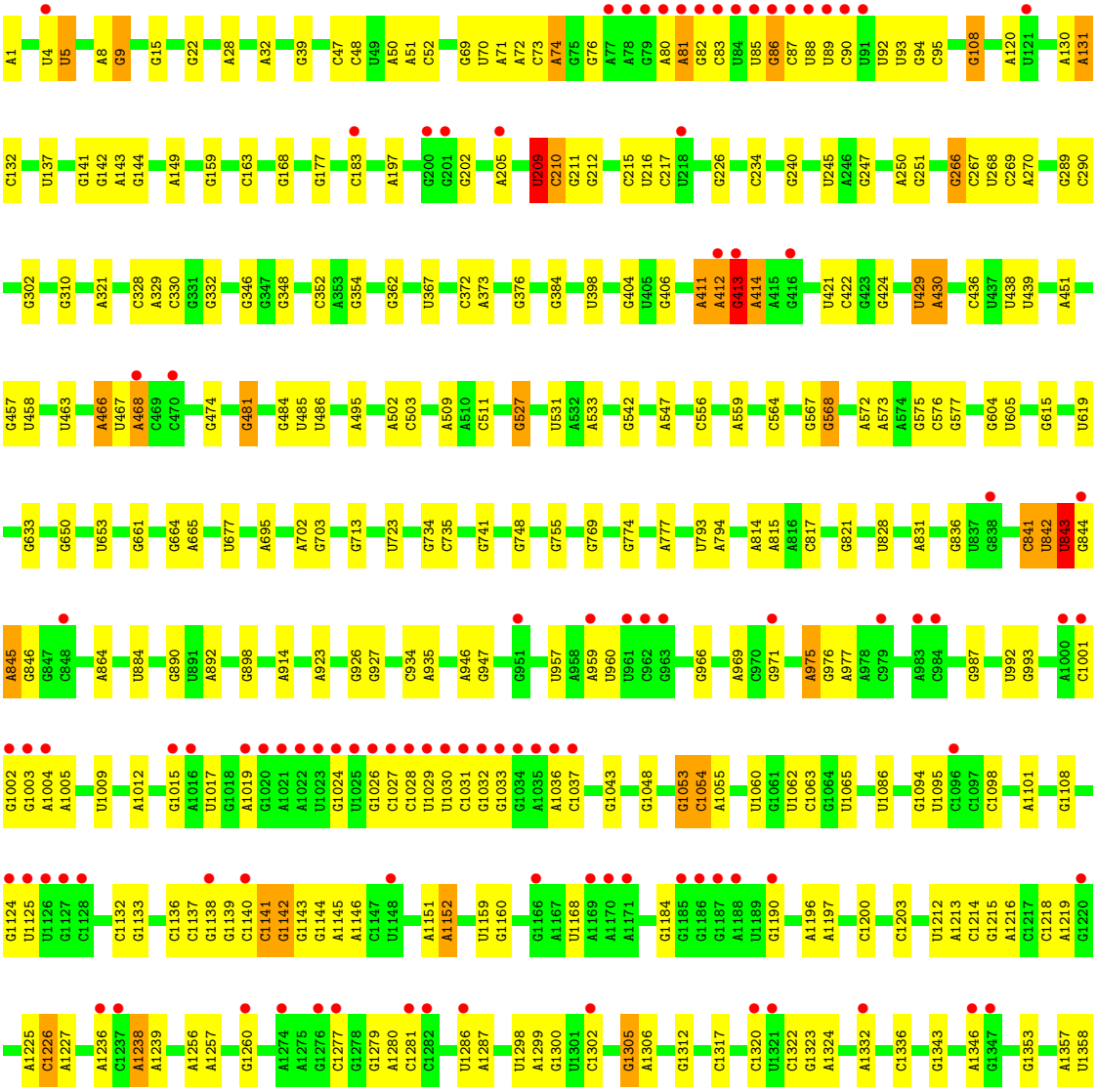
3 Residue-property plots (i)

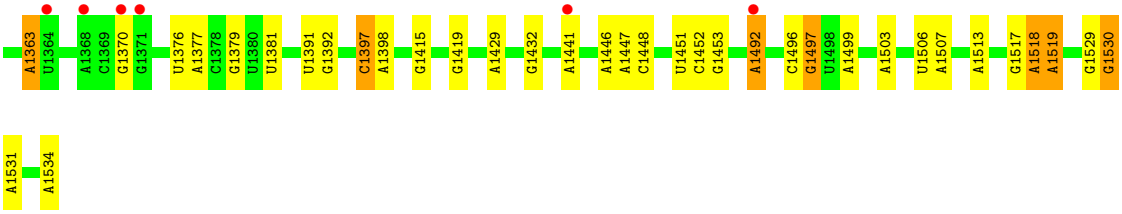
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: 16S rRNA

Chain AA:

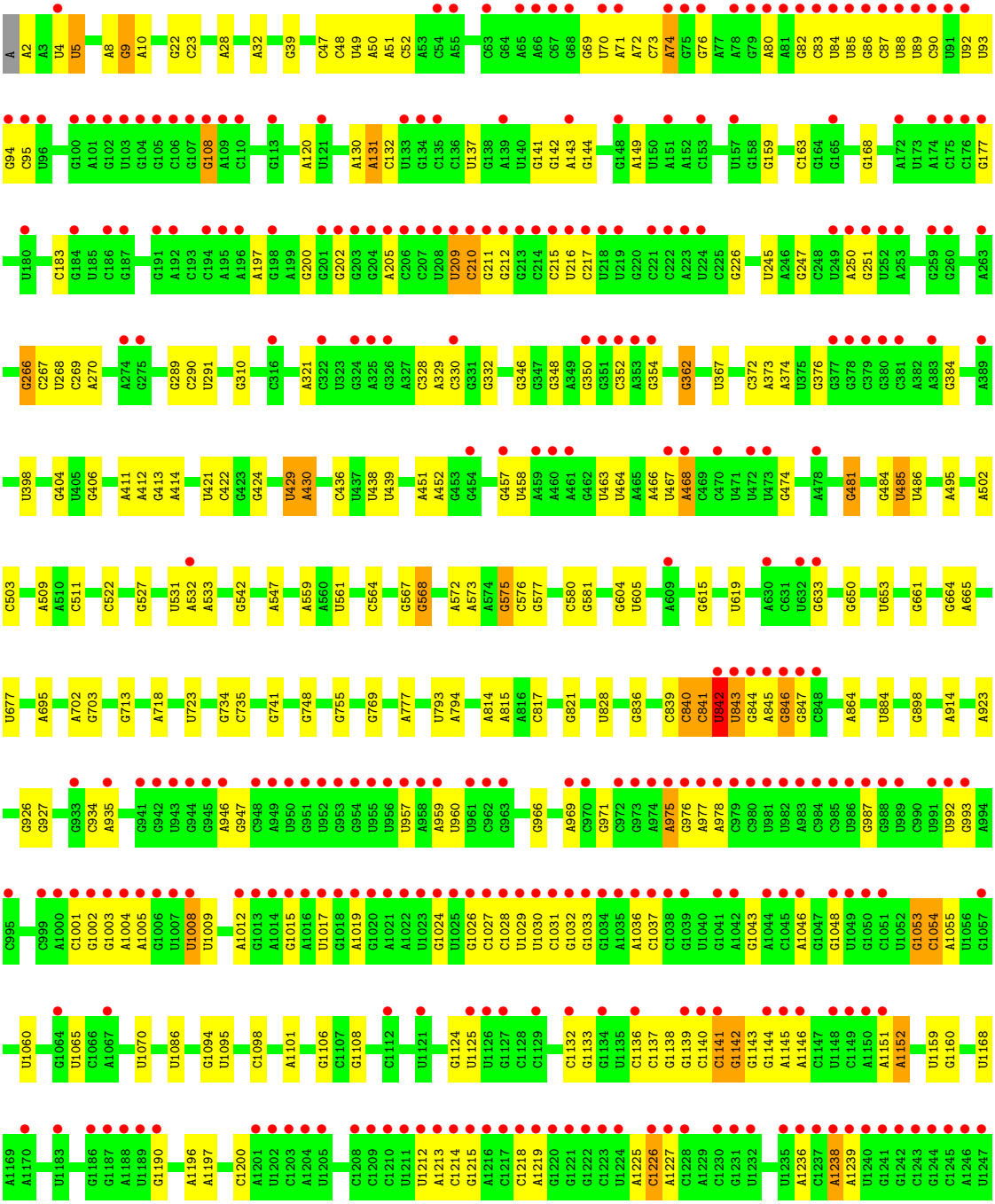


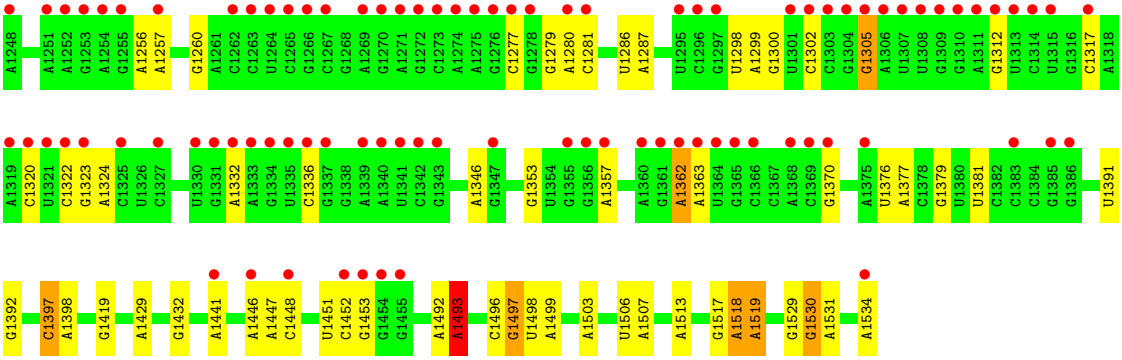




- Molecule 1: 16S rRNA

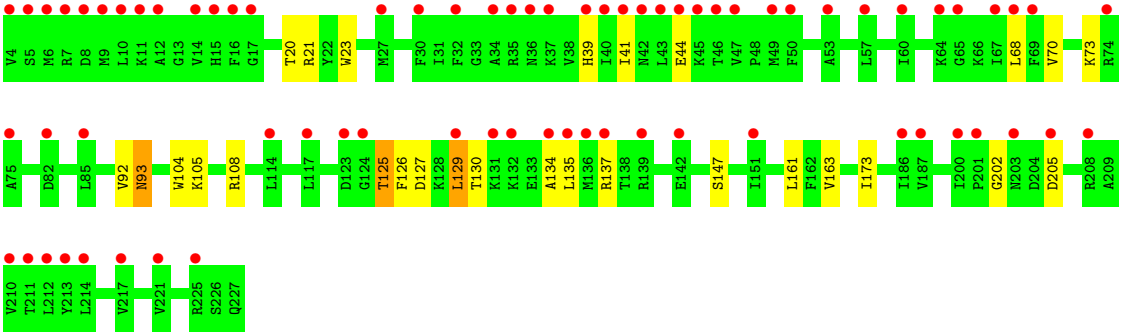
Chain BA:





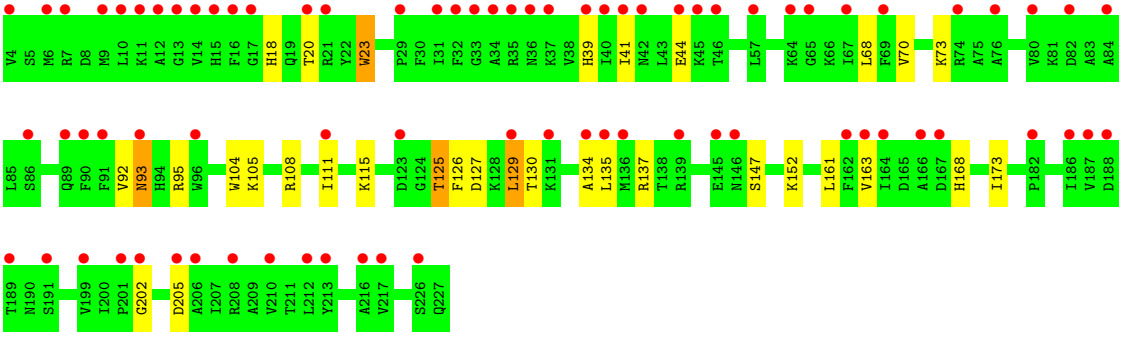
• Molecule 2: 30S ribosomal protein S2

Chain AB:



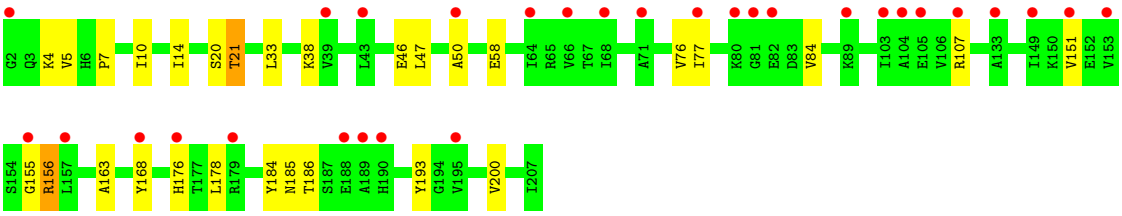
• Molecule 2: 30S ribosomal protein S2

Chain BB:



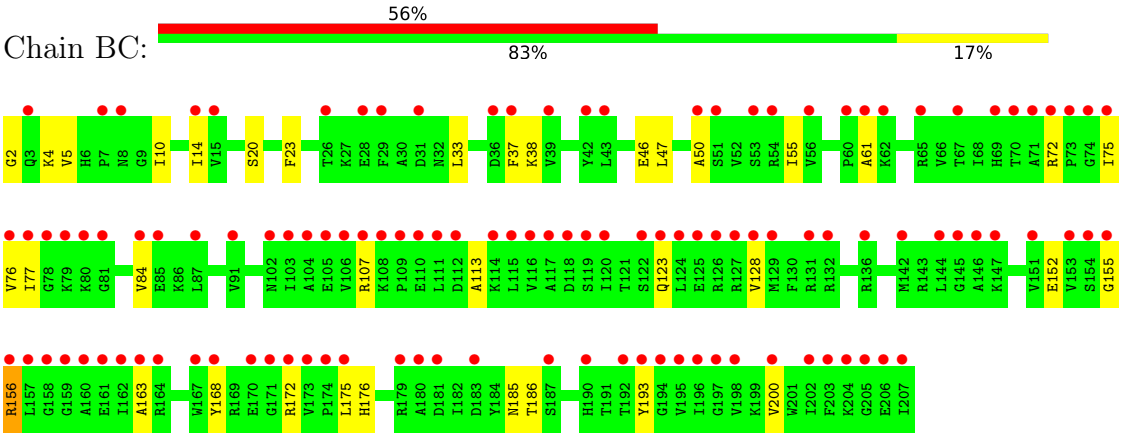
• Molecule 3: 30S ribosomal protein S3

Chain AC:



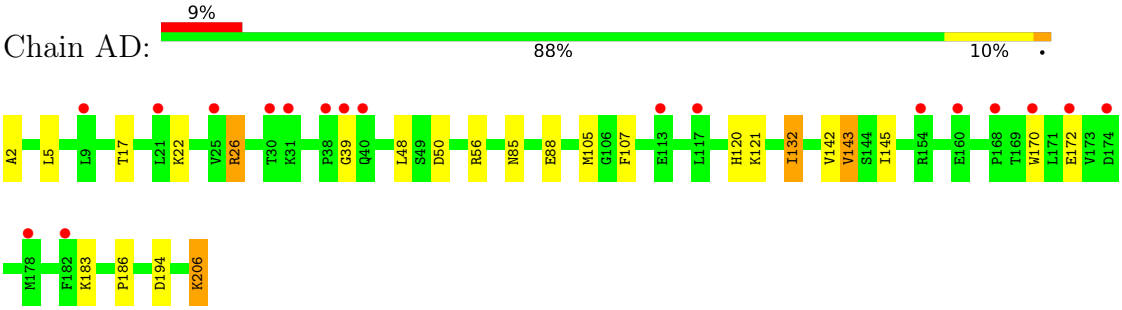
• Molecule 3: 30S ribosomal protein S3

Chain BC:



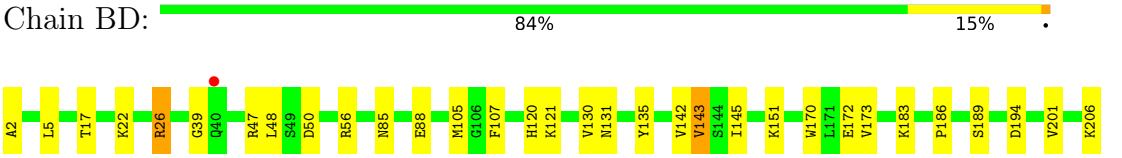
• Molecule 4: 30S ribosomal protein S4

Chain AD:



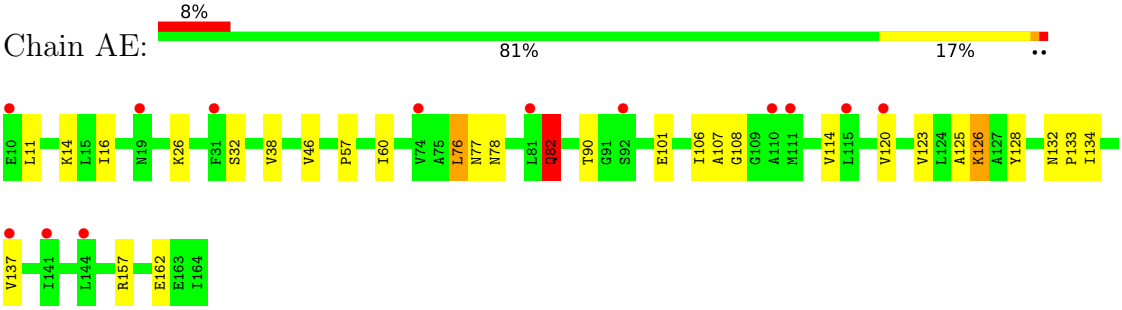
• Molecule 4: 30S ribosomal protein S4

Chain BD:



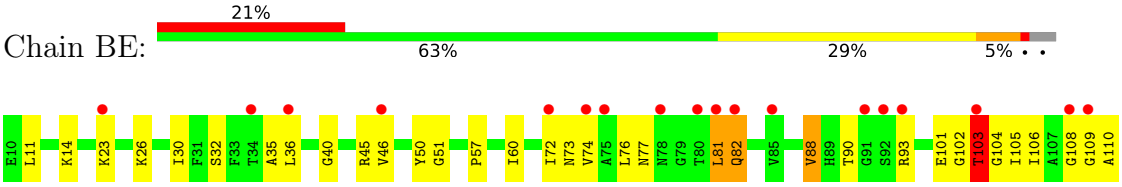
• Molecule 5: 30S ribosomal protein S5

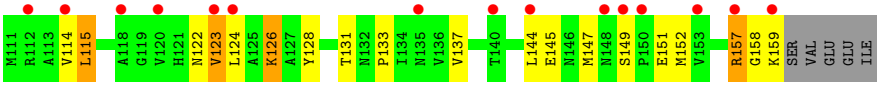
Chain AE:



• Molecule 5: 30S ribosomal protein S5

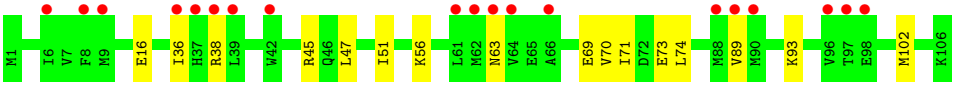
Chain BE:





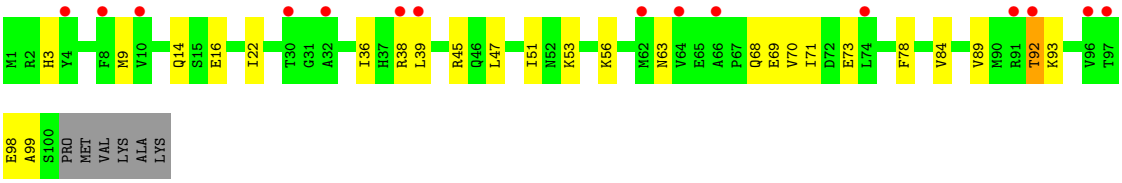
• Molecule 6: 30S ribosomal protein S6

Chain AF:



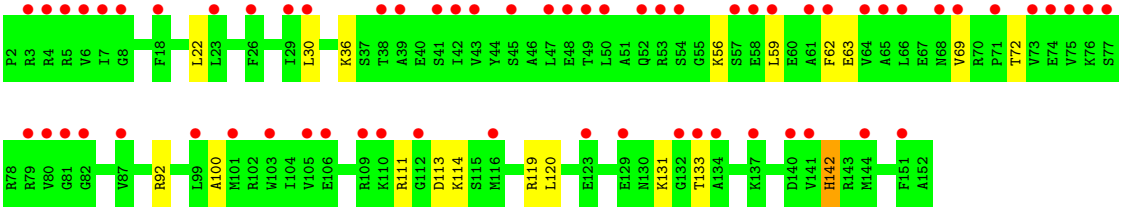
• Molecule 6: 30S ribosomal protein S6

Chain BF:



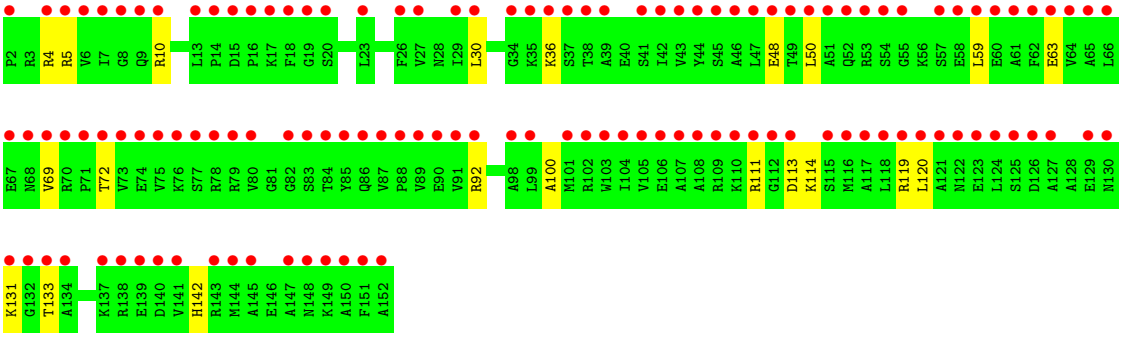
• Molecule 7: 30S ribosomal protein S7

Chain AG:



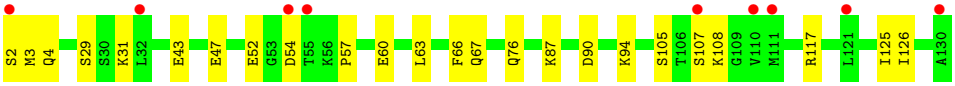
• Molecule 7: 30S ribosomal protein S7

Chain BG:



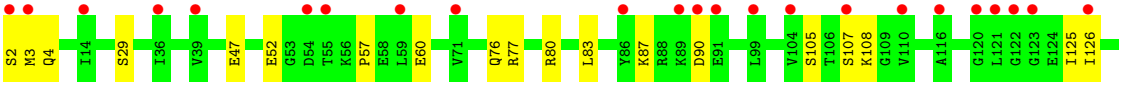
• Molecule 8: 30S ribosomal protein S8

Chain AH:



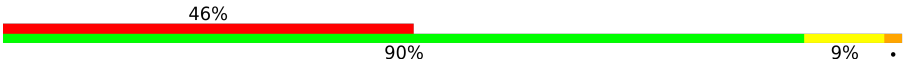
• Molecule 8: 30S ribosomal protein S8

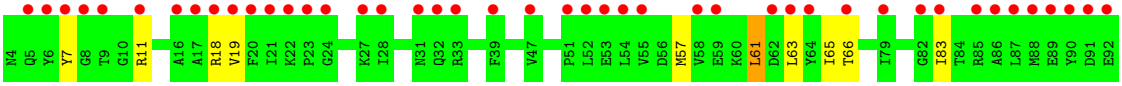
Chain BH:

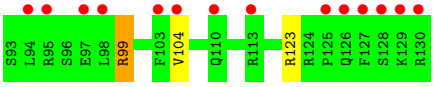


• Molecule 9: 30S ribosomal protein S9

Chain AI:

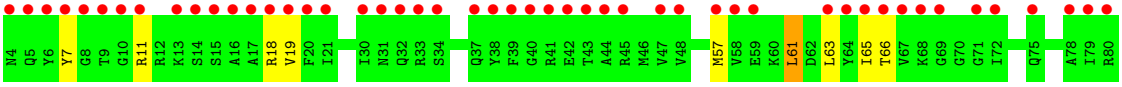


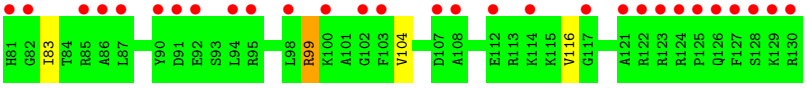




• Molecule 9: 30S ribosomal protein S9

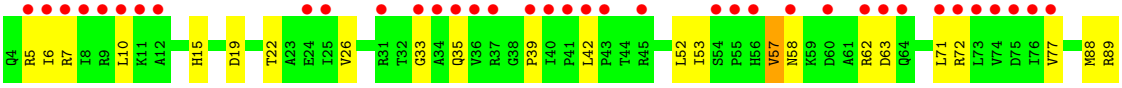
Chain BI:

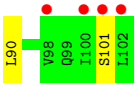




• Molecule 10: 30S ribosomal protein S10

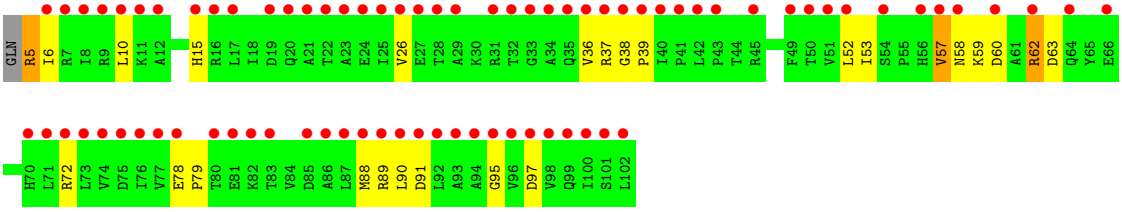
Chain AJ:



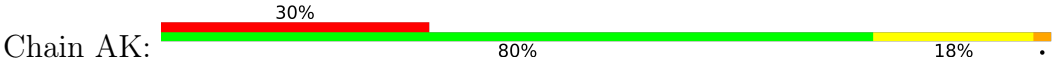


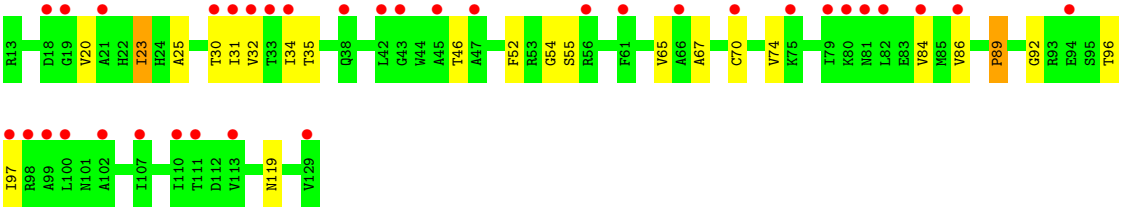
• Molecule 10: 30S ribosomal protein S10

Chain BJ:

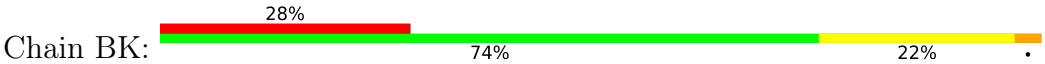


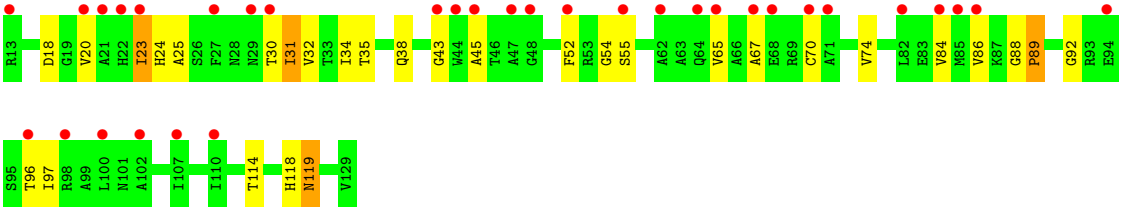
• Molecule 11: 30S ribosomal protein S11



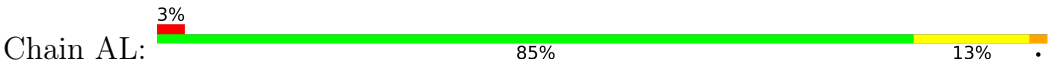


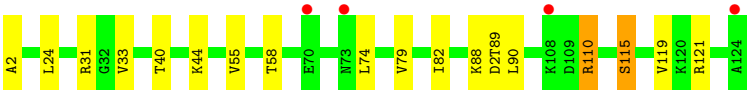
• Molecule 11: 30S ribosomal protein S11



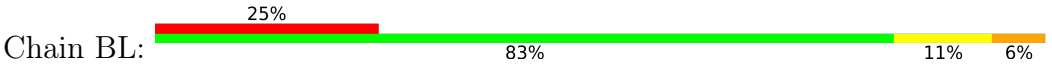


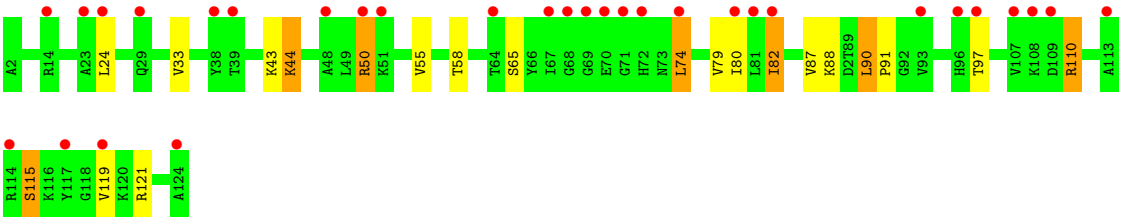
• Molecule 12: 30S ribosomal protein S12





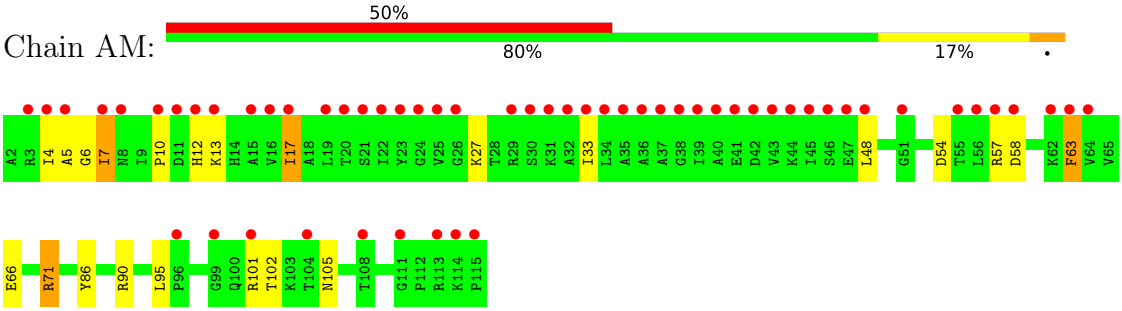
• Molecule 12: 30S ribosomal protein S12





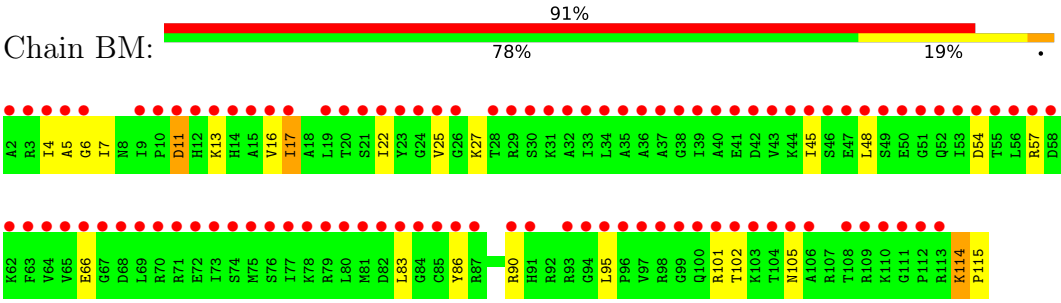
• Molecule 13: 30S ribosomal protein S13

Chain AM:



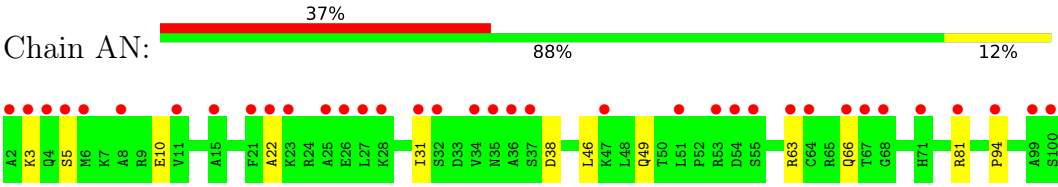
• Molecule 13: 30S ribosomal protein S13

Chain BM:



• Molecule 14: 30S ribosomal protein S14

Chain AN:



• Molecule 14: 30S ribosomal protein S14

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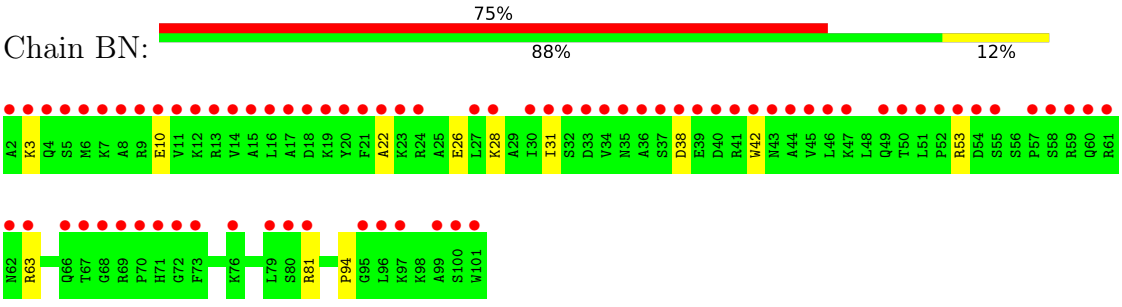
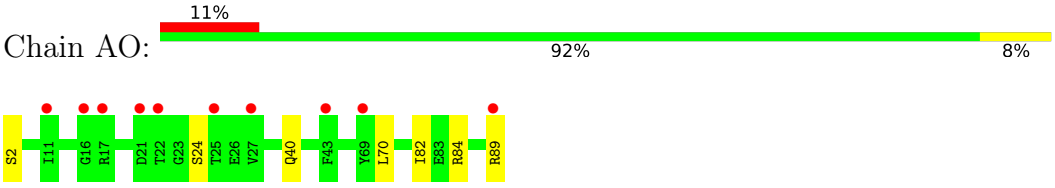


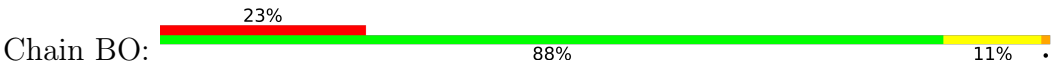
• Molecule 15: 30S ribosomal protein S15

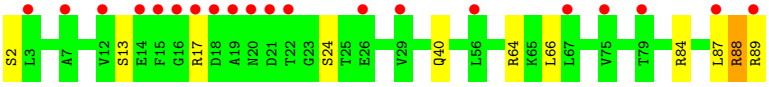
Chain AO:



• Molecule 15: 30S ribosomal protein S15

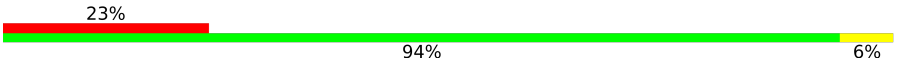
Chain BO:

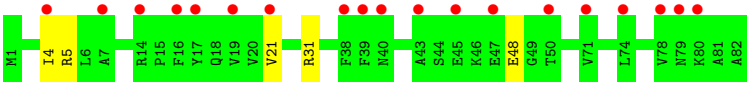




• Molecule 16: 30S ribosomal protein S16

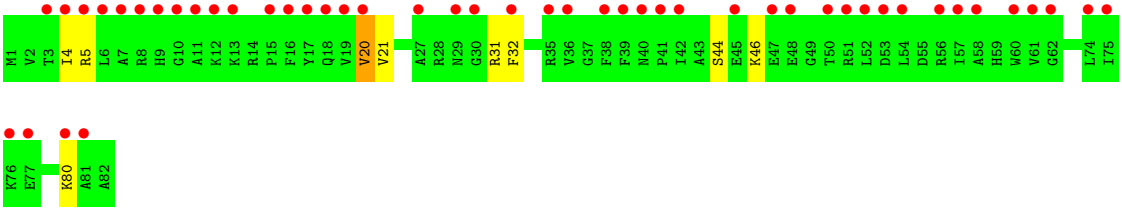
Chain AP:





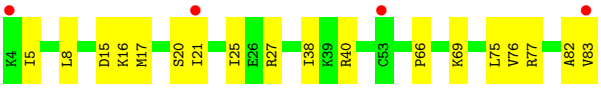
• Molecule 16: 30S ribosomal protein S16

Chain BP:



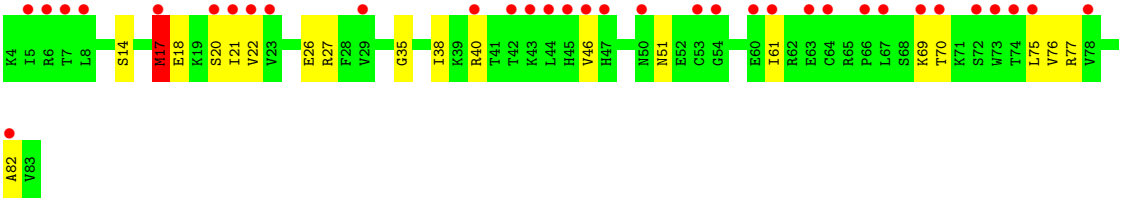
• Molecule 17: 30S ribosomal protein S17

Chain AQ:



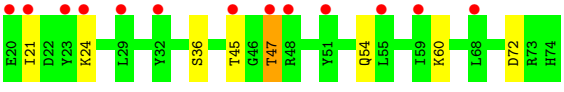
• Molecule 17: 30S ribosomal protein S17

Chain BQ:



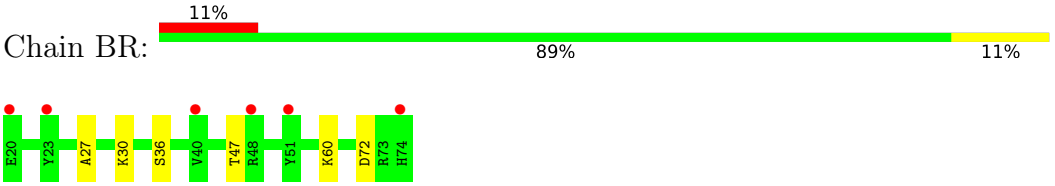
• Molecule 18: 30S ribosomal protein S18

Chain AR:



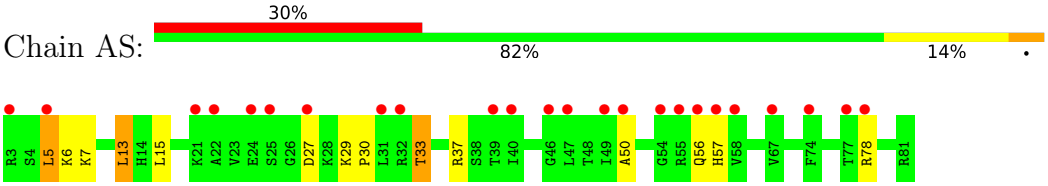
• Molecule 18: 30S ribosomal protein S18

Chain BR:



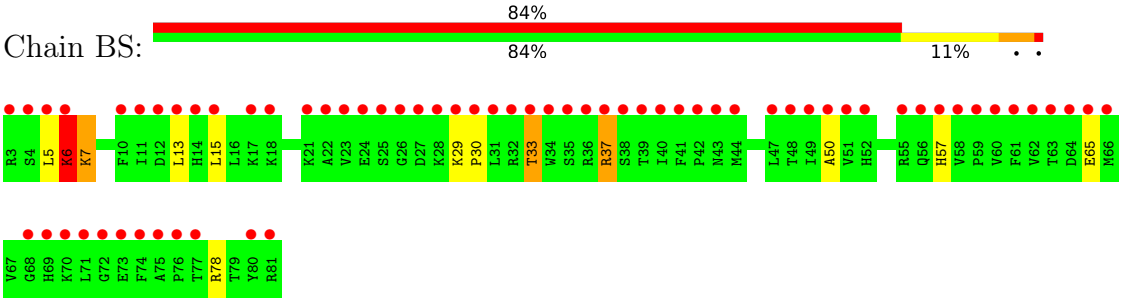
• Molecule 19: 30S ribosomal protein S19

Chain AS:



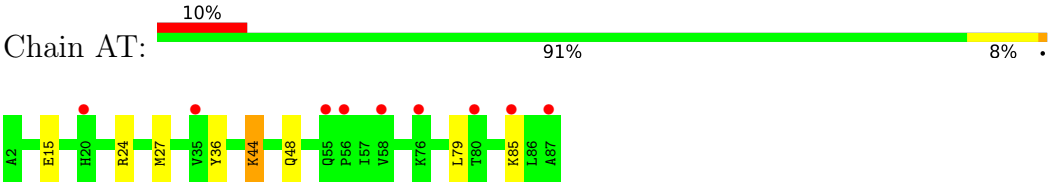
• Molecule 19: 30S ribosomal protein S19

Chain BS:



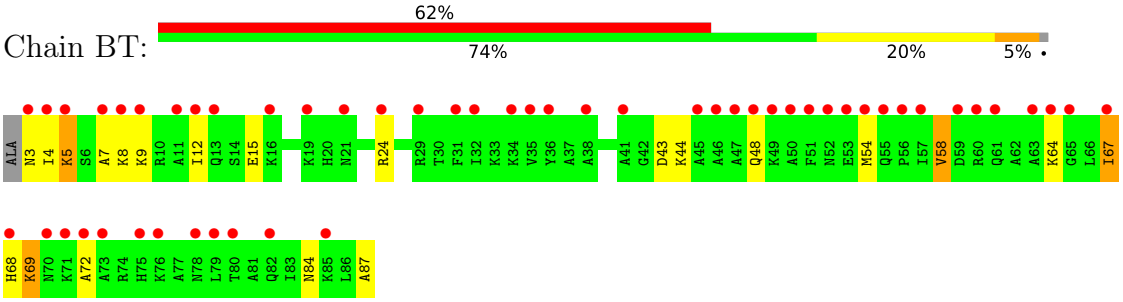
• Molecule 20: 30S ribosomal protein S20

Chain AT:



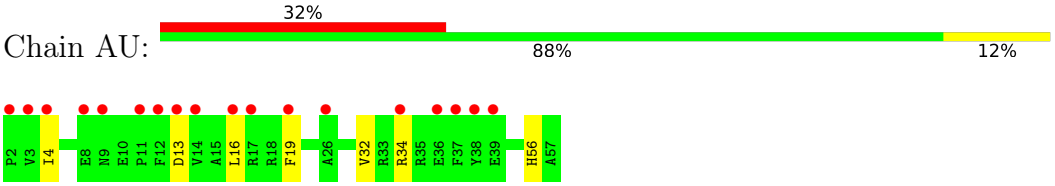
• Molecule 20: 30S ribosomal protein S20

Chain BT:



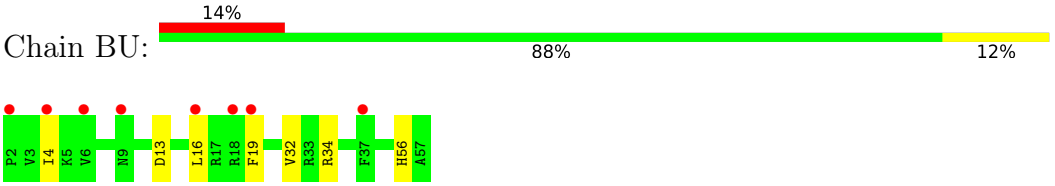
• Molecule 21: 30S ribosomal protein S21

Chain AU:



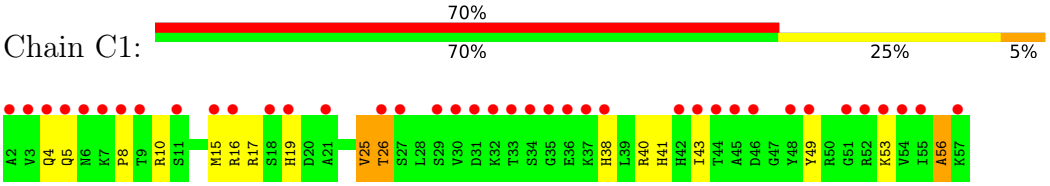
• Molecule 21: 30S ribosomal protein S21

Chain BU:



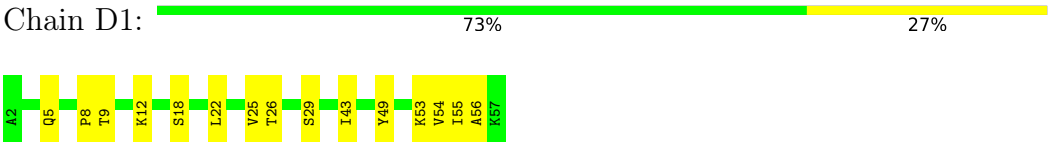
• Molecule 22: 50S ribosomal protein L32

Chain C1:



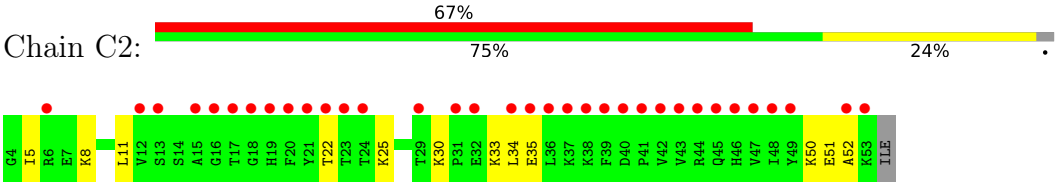
• Molecule 22: 50S ribosomal protein L32

Chain D1:



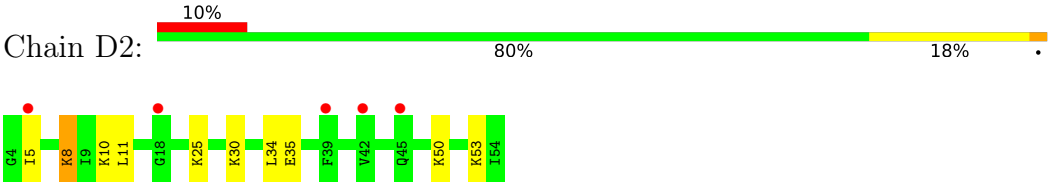
• Molecule 23: 50S ribosomal protein L33

Chain C2:



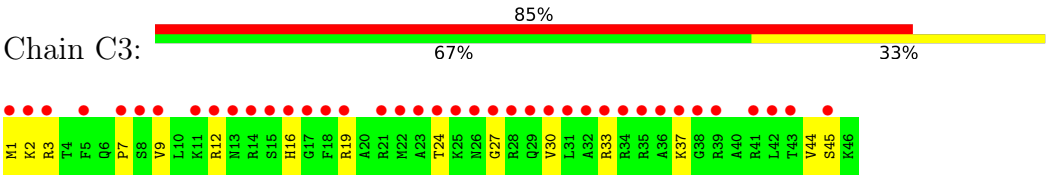
• Molecule 23: 50S ribosomal protein L33

Chain D2:



• Molecule 24: 50S ribosomal protein L34

Chain C3:



• Molecule 24: 50S ribosomal protein L34

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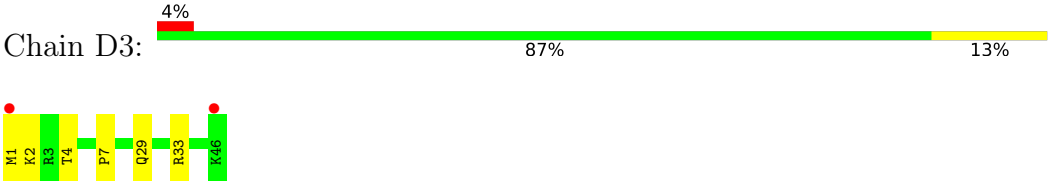
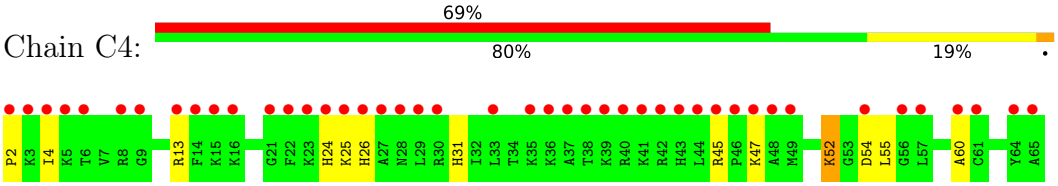


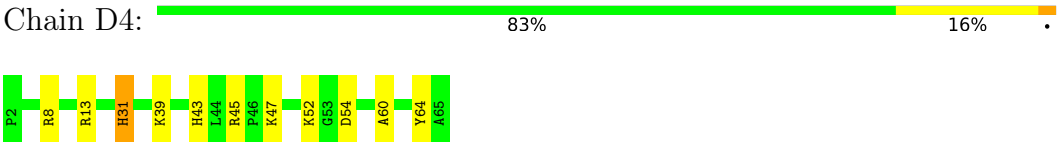
• Molecule 25: 50S ribosomal protein L35

Chain C4:



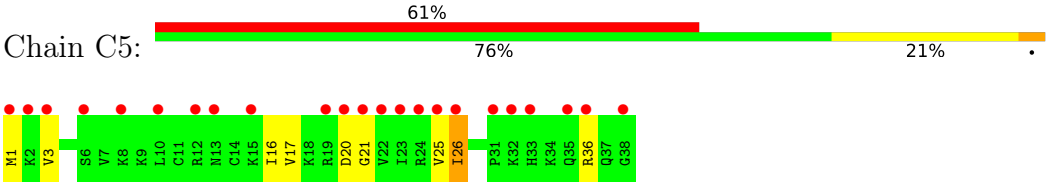
• Molecule 25: 50S ribosomal protein L35

Chain D4:



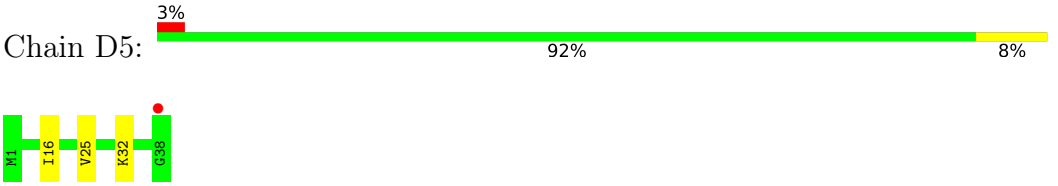
• Molecule 26: 50S ribosomal protein L36

Chain C5:



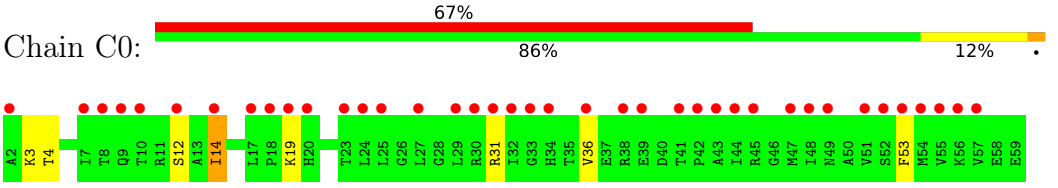
• Molecule 26: 50S ribosomal protein L36

Chain D5:



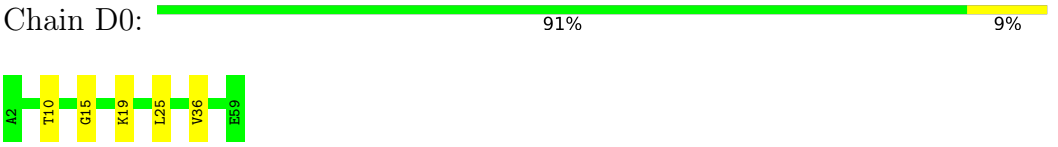
• Molecule 27: 50S ribosomal protein L30

Chain C0:



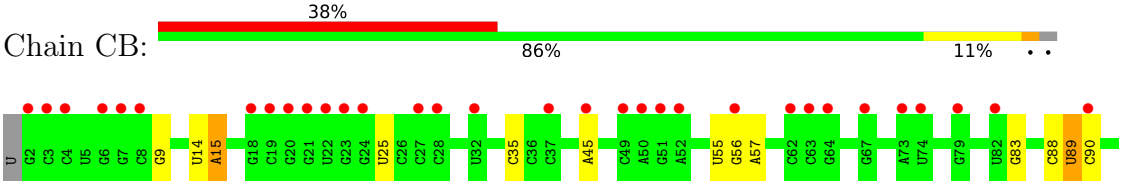
• Molecule 27: 50S ribosomal protein L30

Chain D0:



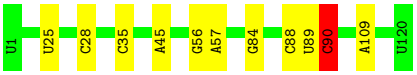
• Molecule 28: 5S rRNA

Chain CB:



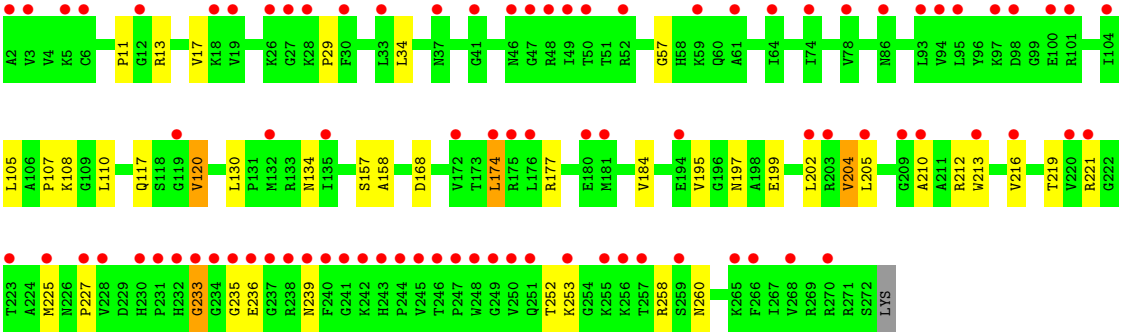
• Molecule 28: 5S rRNA

Chain DB:



• Molecule 29: 50S ribosomal protein L2

Chain CC:



• Molecule 29: 50S ribosomal protein L2

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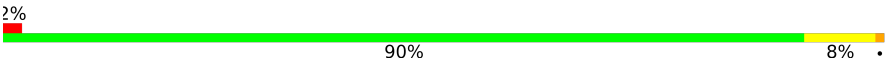
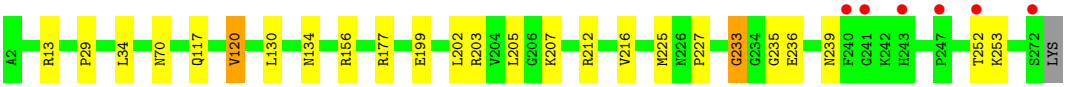
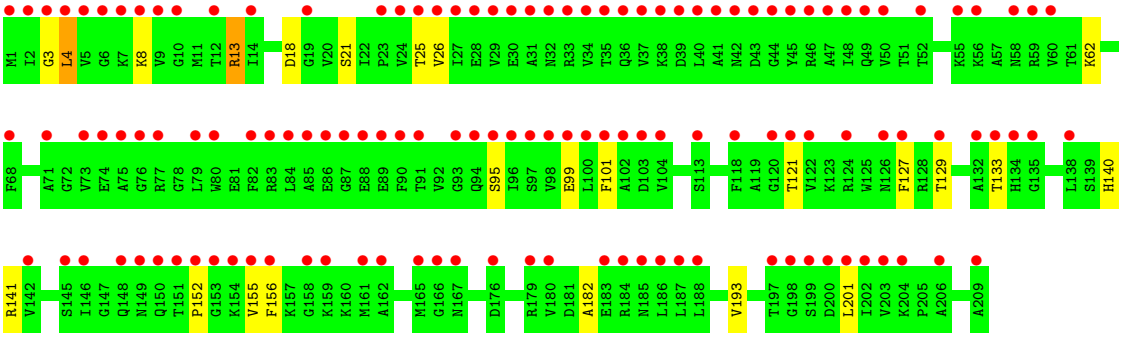




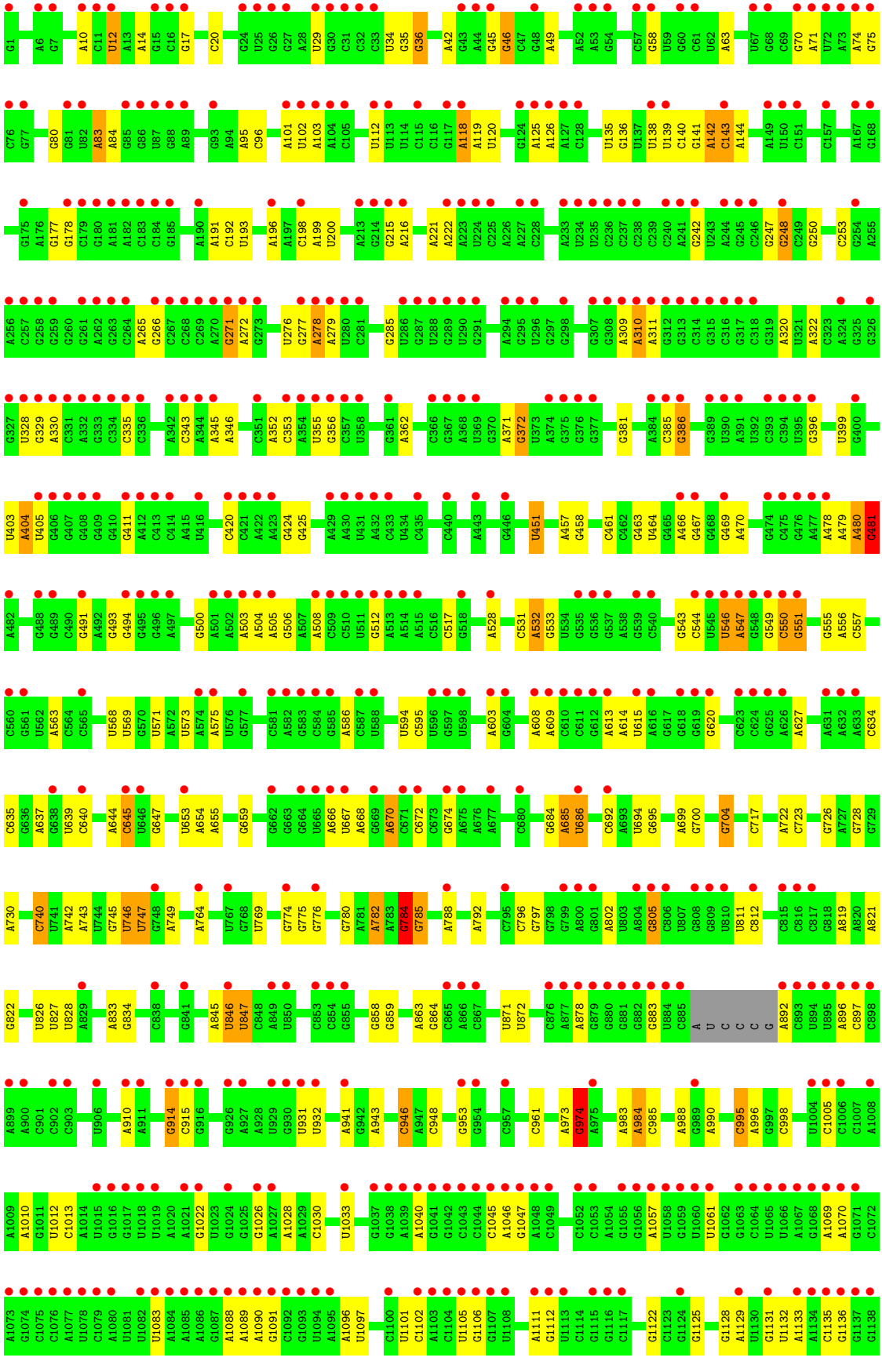
• Molecule 30: 50S ribosomal protein L3

Chain CD:



• Molecule 31: 23S rRNA

Chain CA: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C76 G77 G80 G81 U82 A83 A84 G85 G86 U87 G88 A89 G93 A94 A95 C96 A101 U102 A103 A104 C105 U112 U113 U114 C115 C116 G117 A118 A119 U120 G124 A125 A126 A127 C128 U135 G136 U137 U138 U139 C140 G141 A142 C143 A144 A149 U150 C151 C157 A167 G168
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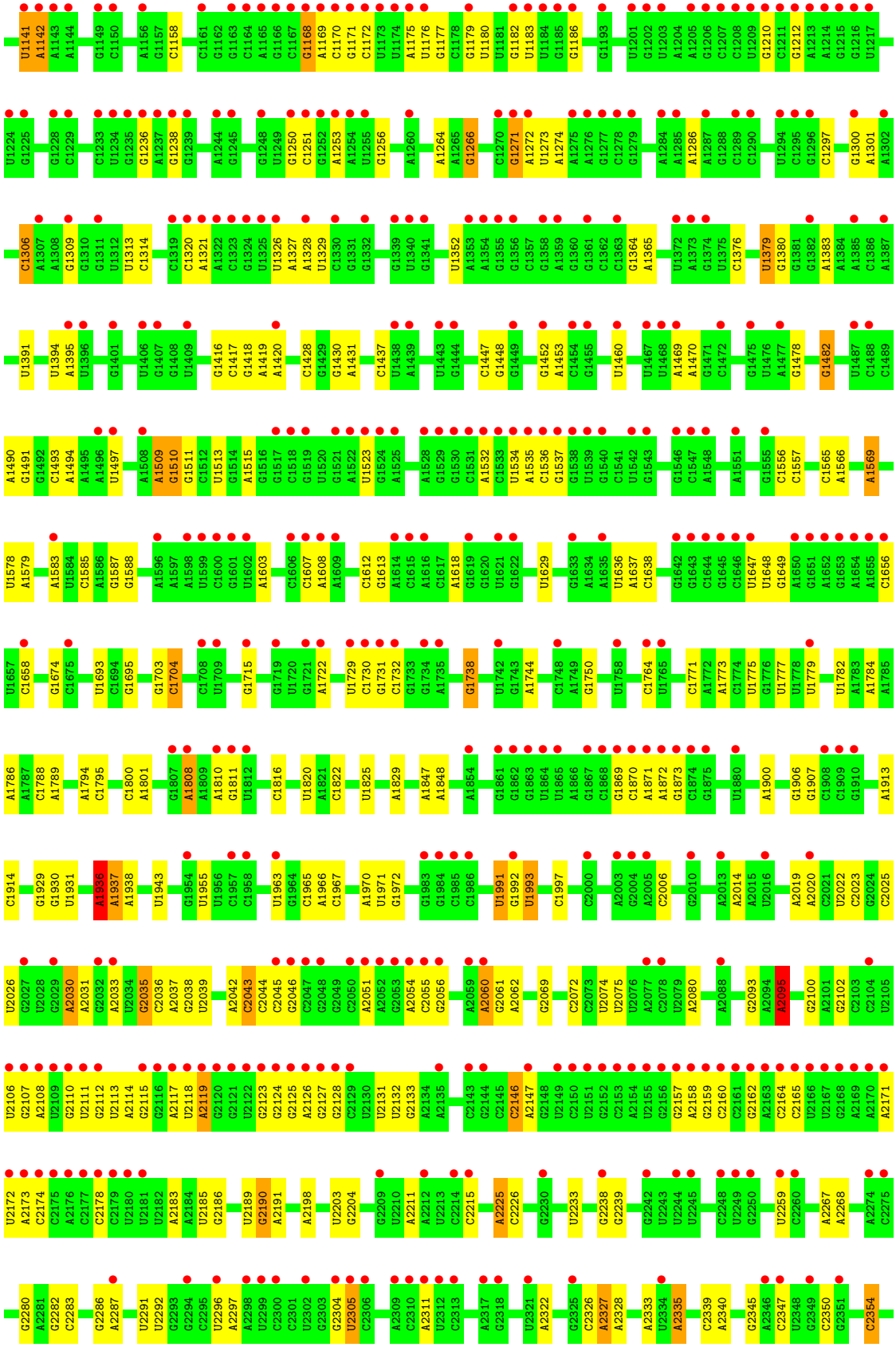
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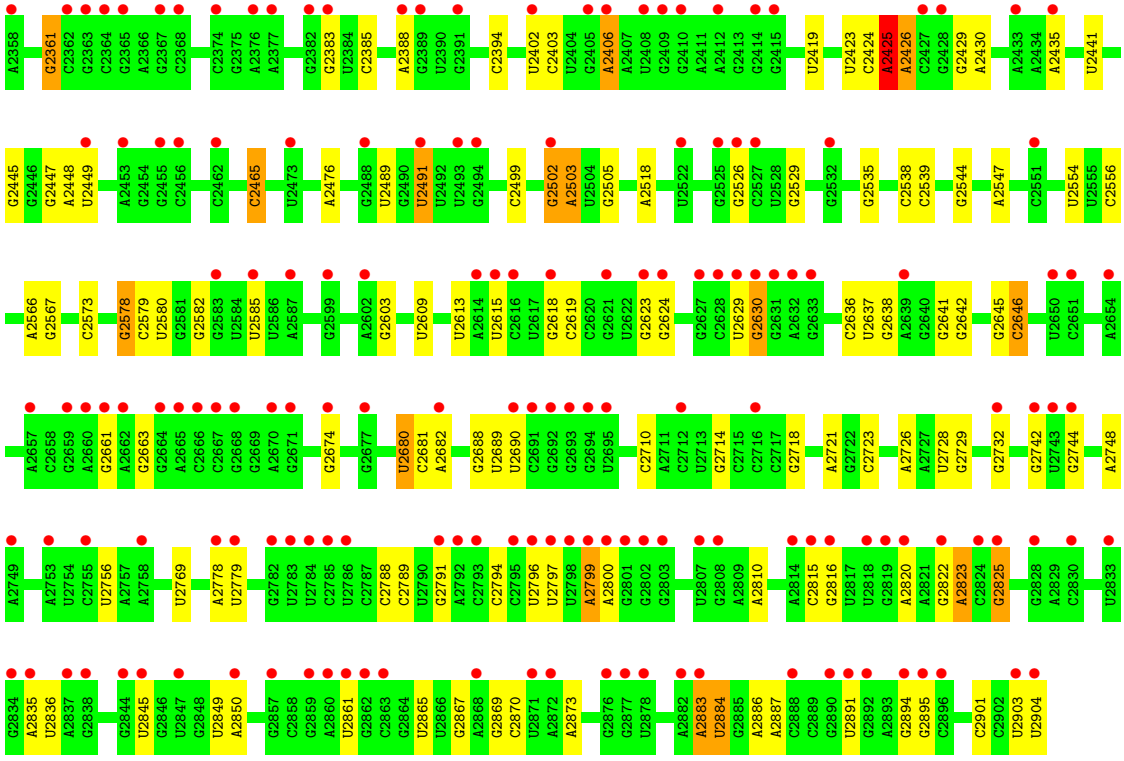
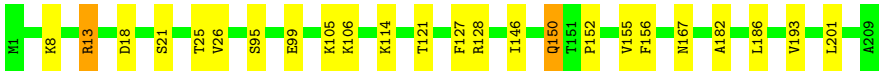


• Molecule 32: 50S ribosomal protein L3

Chain DD:

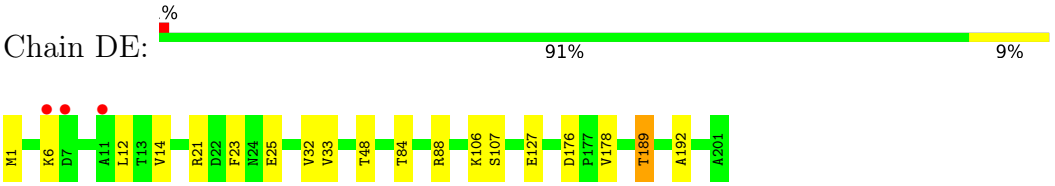


• Molecule 33: 50S ribosomal protein L4

Chain CE:

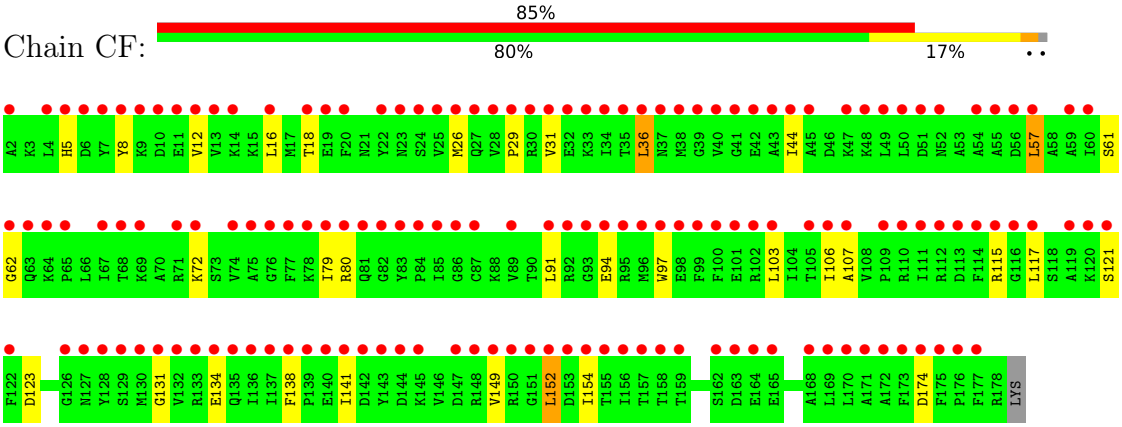
• Molecule 33: 50S ribosomal protein L4

Chain DE:



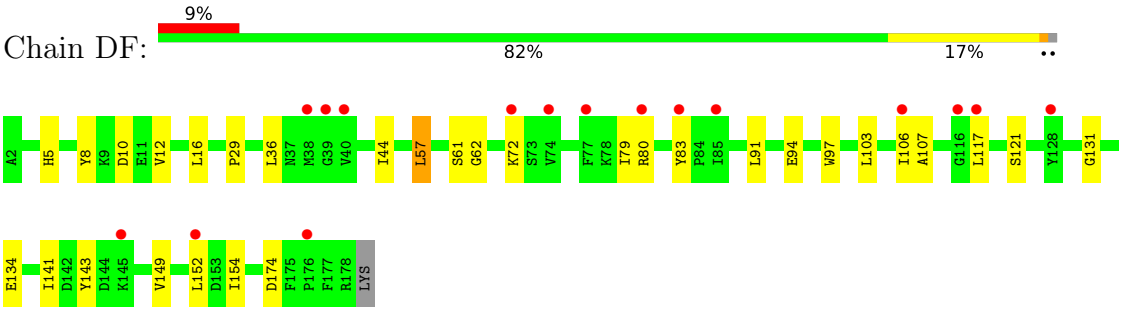
• Molecule 34: 50S ribosomal protein L5

Chain CF:



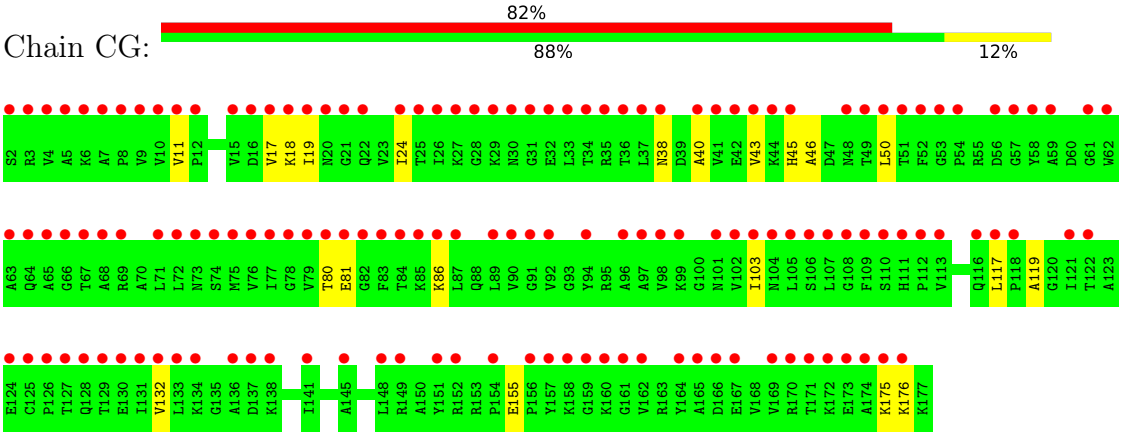
• Molecule 34: 50S ribosomal protein L5

Chain DF:



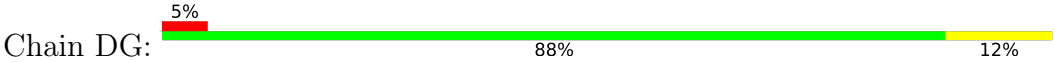
• Molecule 35: 50S ribosomal protein L6

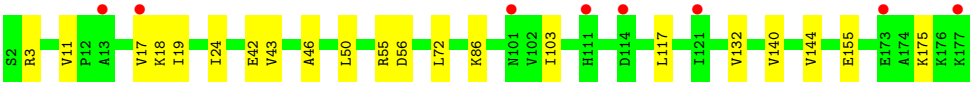
Chain CG:



• Molecule 35: 50S ribosomal protein L6

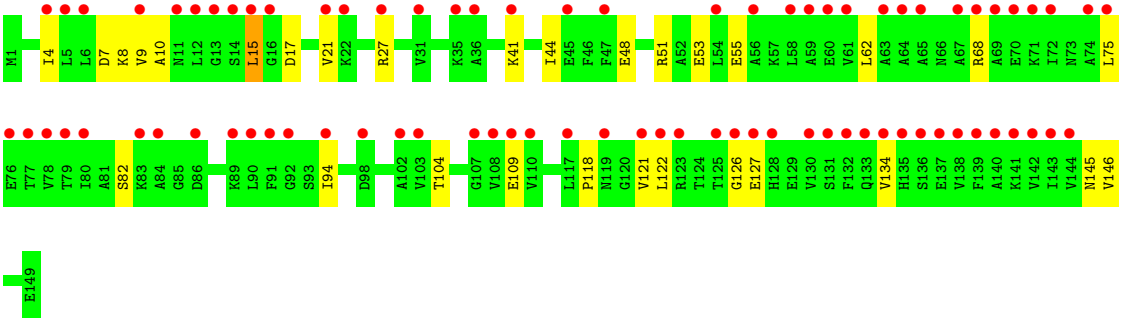
Chain DG:





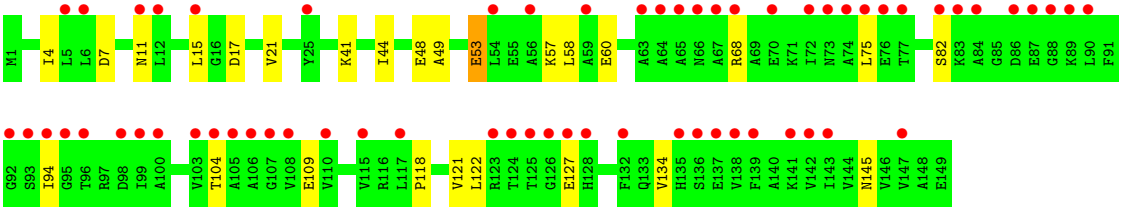
• Molecule 36: 50S ribosomal protein L9

Chain CH:



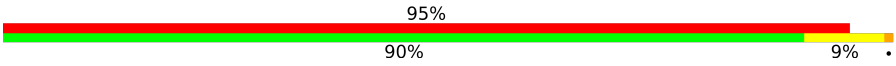
• Molecule 36: 50S ribosomal protein L9

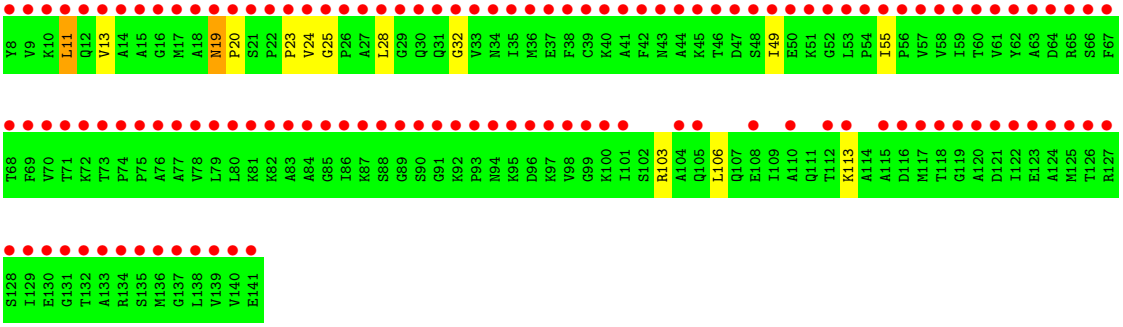
Chain DH:



• Molecule 37: 50S ribosomal protein L11

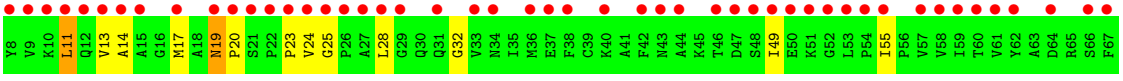
Chain CJ:

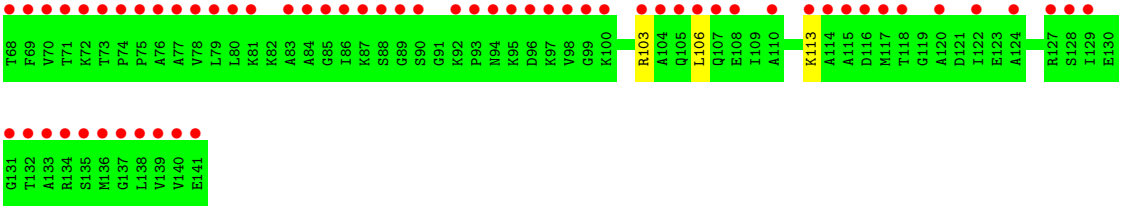




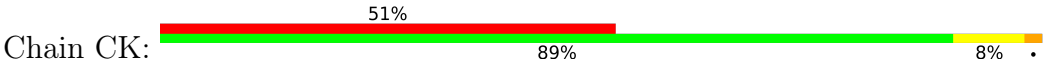
• Molecule 37: 50S ribosomal protein L11

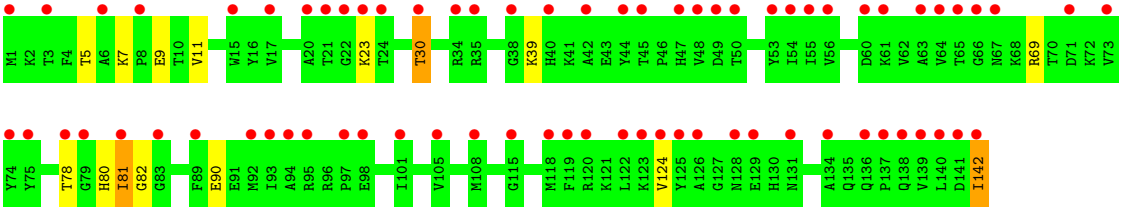
Chain DJ:





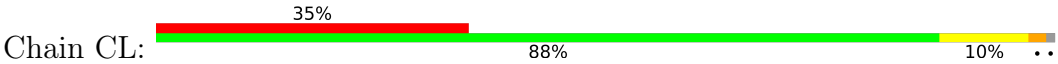
• Molecule 38: 50S ribosomal protein L13

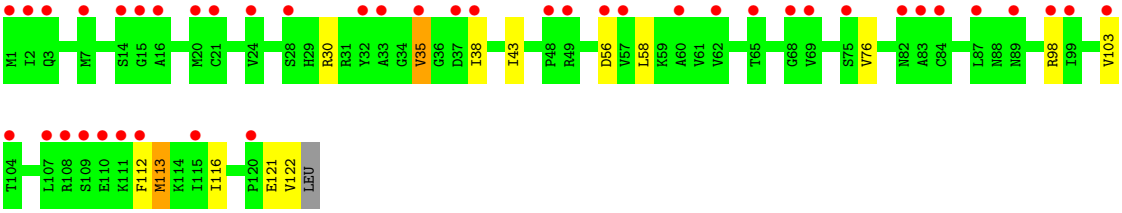




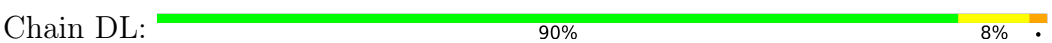
• Molecule 38: 50S ribosomal protein L13

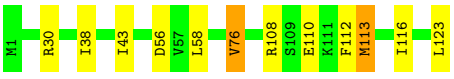
• Molecule 39: 50S ribosomal protein L14



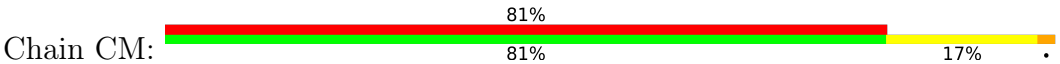


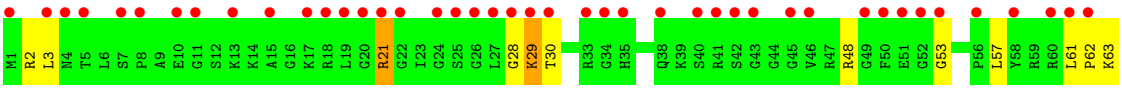
• Molecule 39: 50S ribosomal protein L14

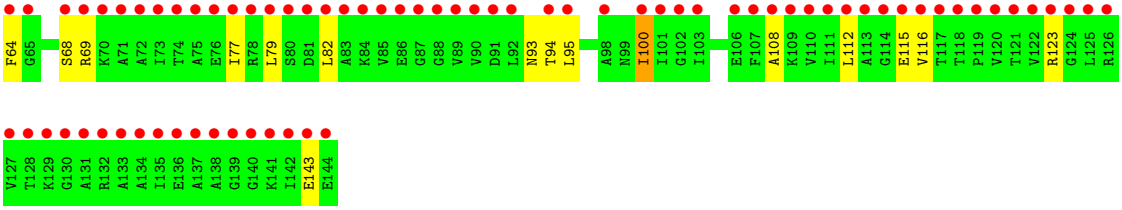




• Molecule 40: 50S ribosomal protein L15

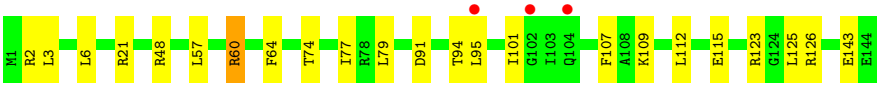






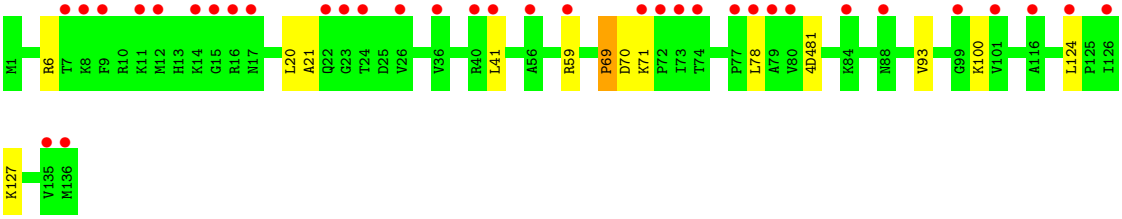
• Molecule 40: 50S ribosomal protein L15

Chain DM:



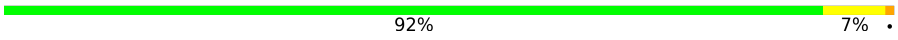
• Molecule 41: 50S ribosomal protein L16

Chain CN:



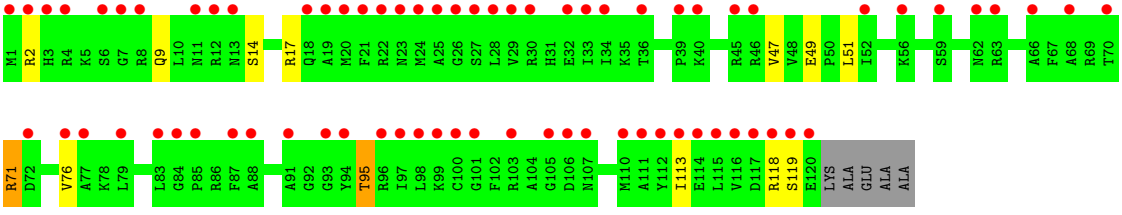
• Molecule 41: 50S ribosomal protein L16

Chain DN:



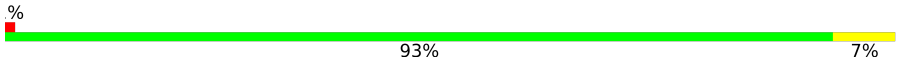
• Molecule 42: 50S ribosomal protein L17

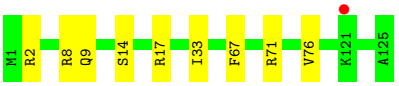
Chain CO:



• Molecule 42: 50S ribosomal protein L17

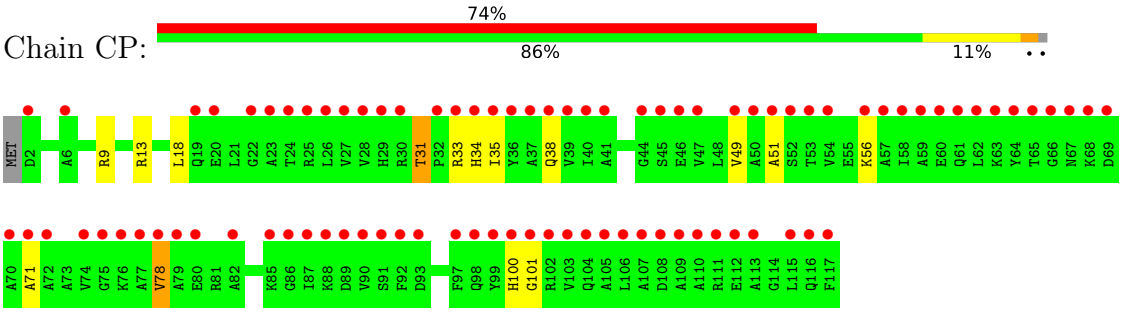
Chain DO:





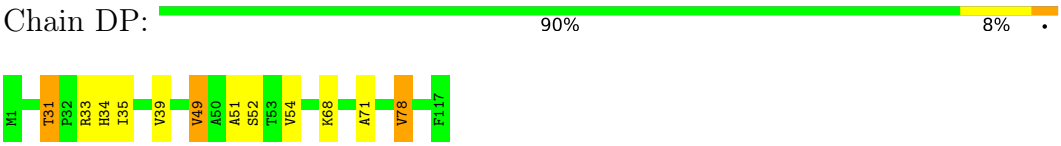
• Molecule 43: 50S ribosomal protein L18

Chain CP:



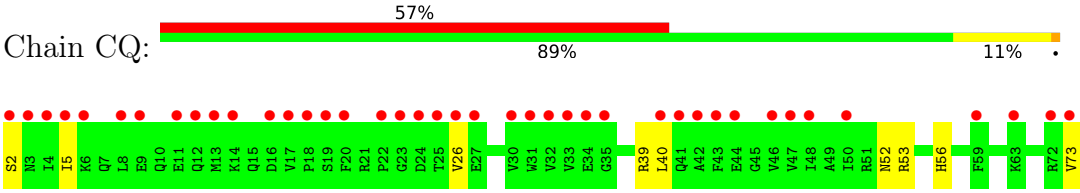
• Molecule 43: 50S ribosomal protein L18

Chain DP:



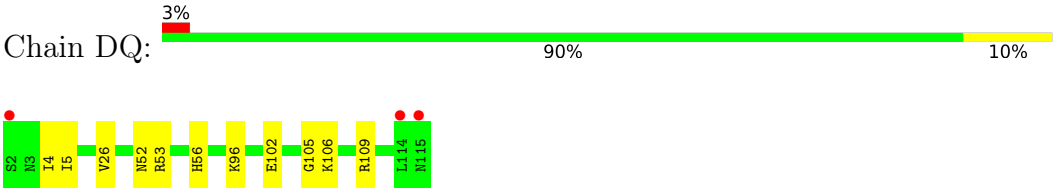
• Molecule 44: 50S ribosomal protein L19

Chain CQ:



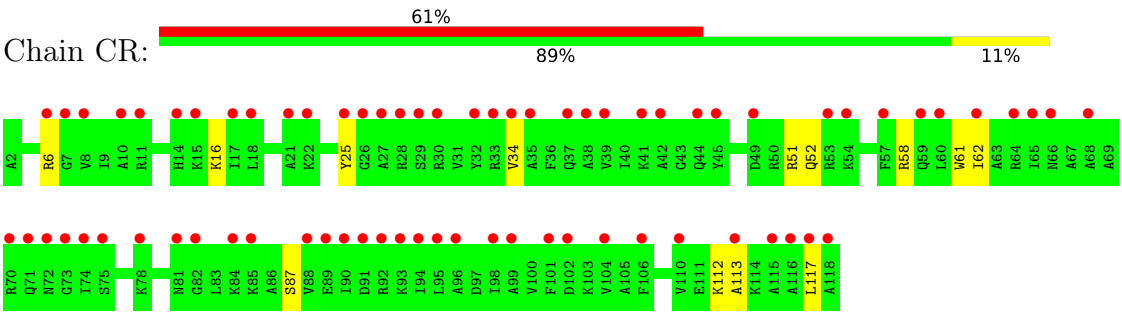
• Molecule 44: 50S ribosomal protein L19

Chain DQ:



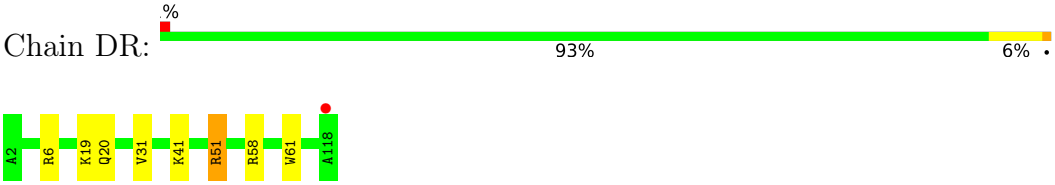
• Molecule 45: 50S ribosomal protein L20

Chain CR:



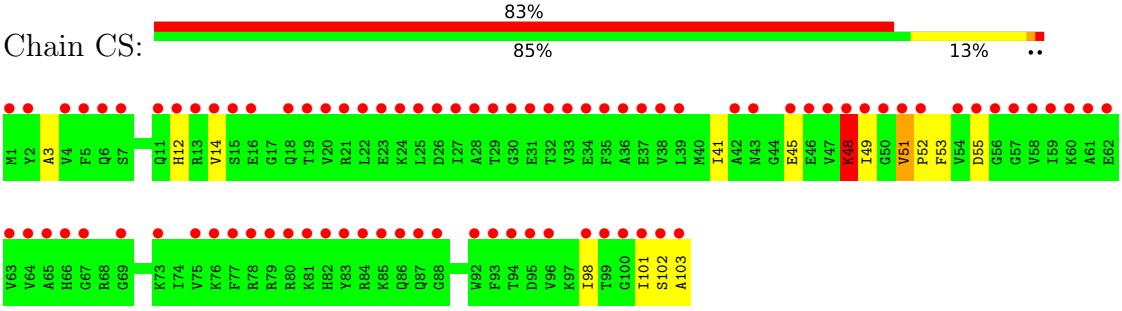
• Molecule 45: 50S ribosomal protein L20

Chain DR:



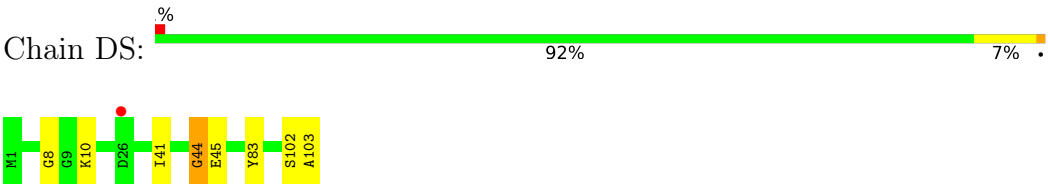
• Molecule 46: 50S ribosomal protein L21

Chain CS:



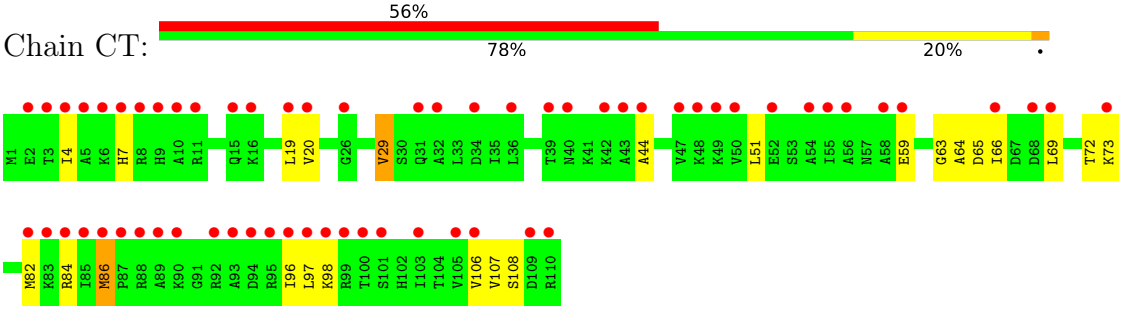
• Molecule 46: 50S ribosomal protein L21

Chain DS:



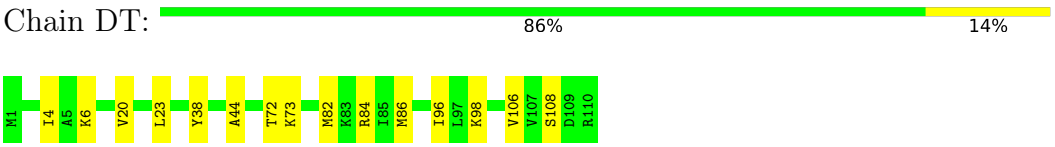
• Molecule 47: 50S ribosomal protein L22

Chain CT:



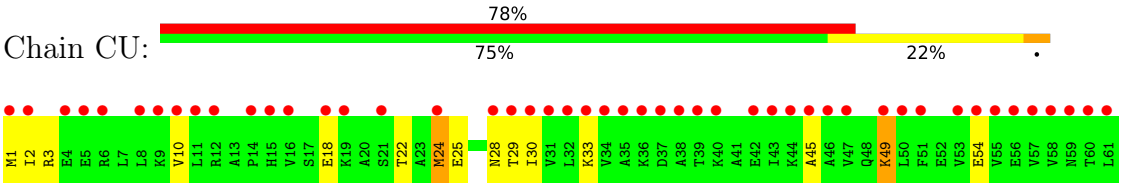
• Molecule 47: 50S ribosomal protein L22

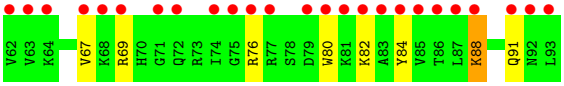
Chain DT:



• Molecule 48: 50S ribosomal protein L23

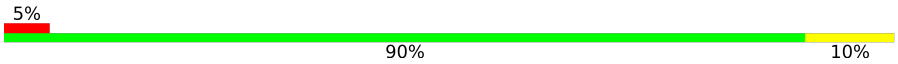
Chain CU:

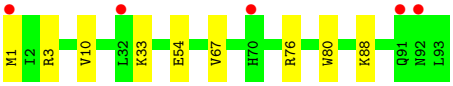




• Molecule 48: 50S ribosomal protein L23

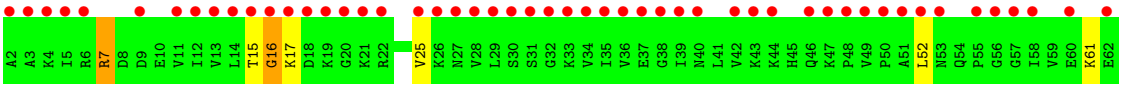
Chain DU:

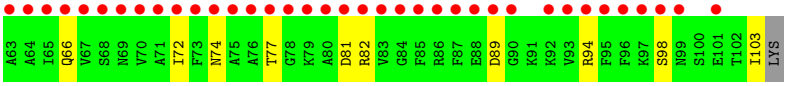




• Molecule 49: 50S ribosomal protein L24

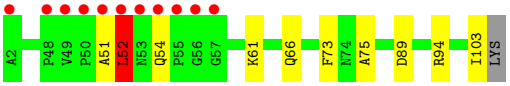
Chain CV:





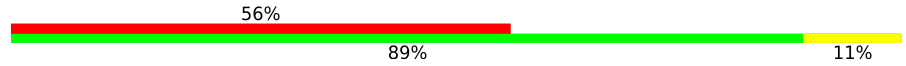
• Molecule 49: 50S ribosomal protein L24

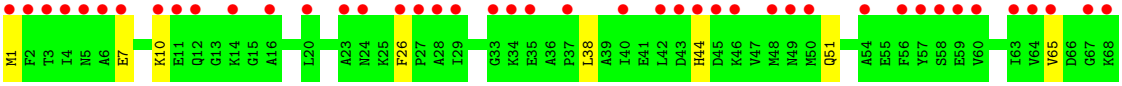
Chain DV:

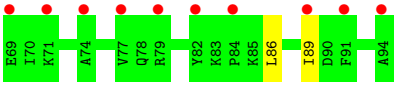


• Molecule 50: 50S ribosomal protein L25

Chain CW:





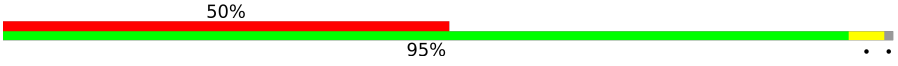


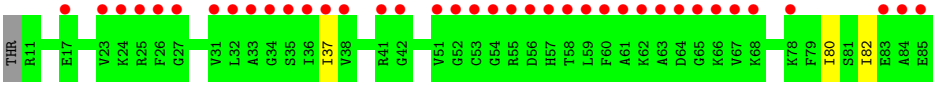
• Molecule 50: 50S ribosomal protein L25

Chain DW:

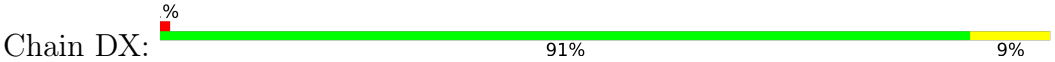
• Molecule 51: 50S ribosomal protein L27

Chain CX:

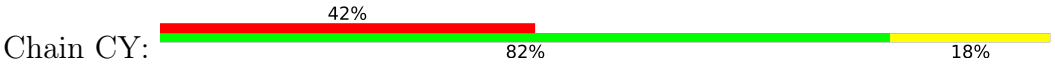


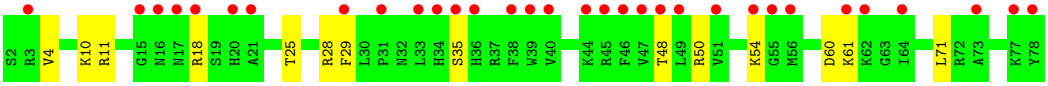


• Molecule 51: 50S ribosomal protein L27



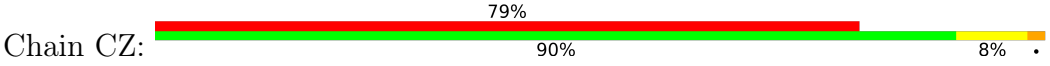
• Molecule 52: 50S ribosomal protein L28

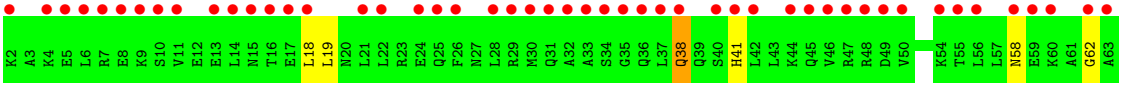




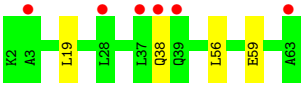
• Molecule 52: 50S ribosomal protein L28

• Molecule 53: 50S ribosomal protein L29

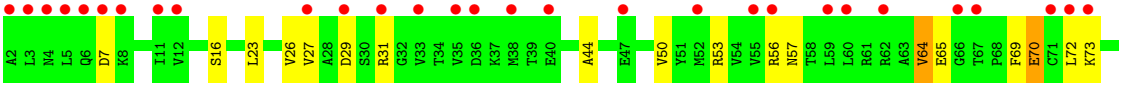


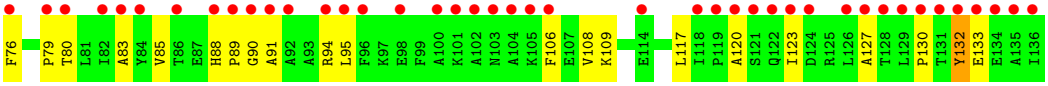


• Molecule 53: 50S ribosomal protein L29



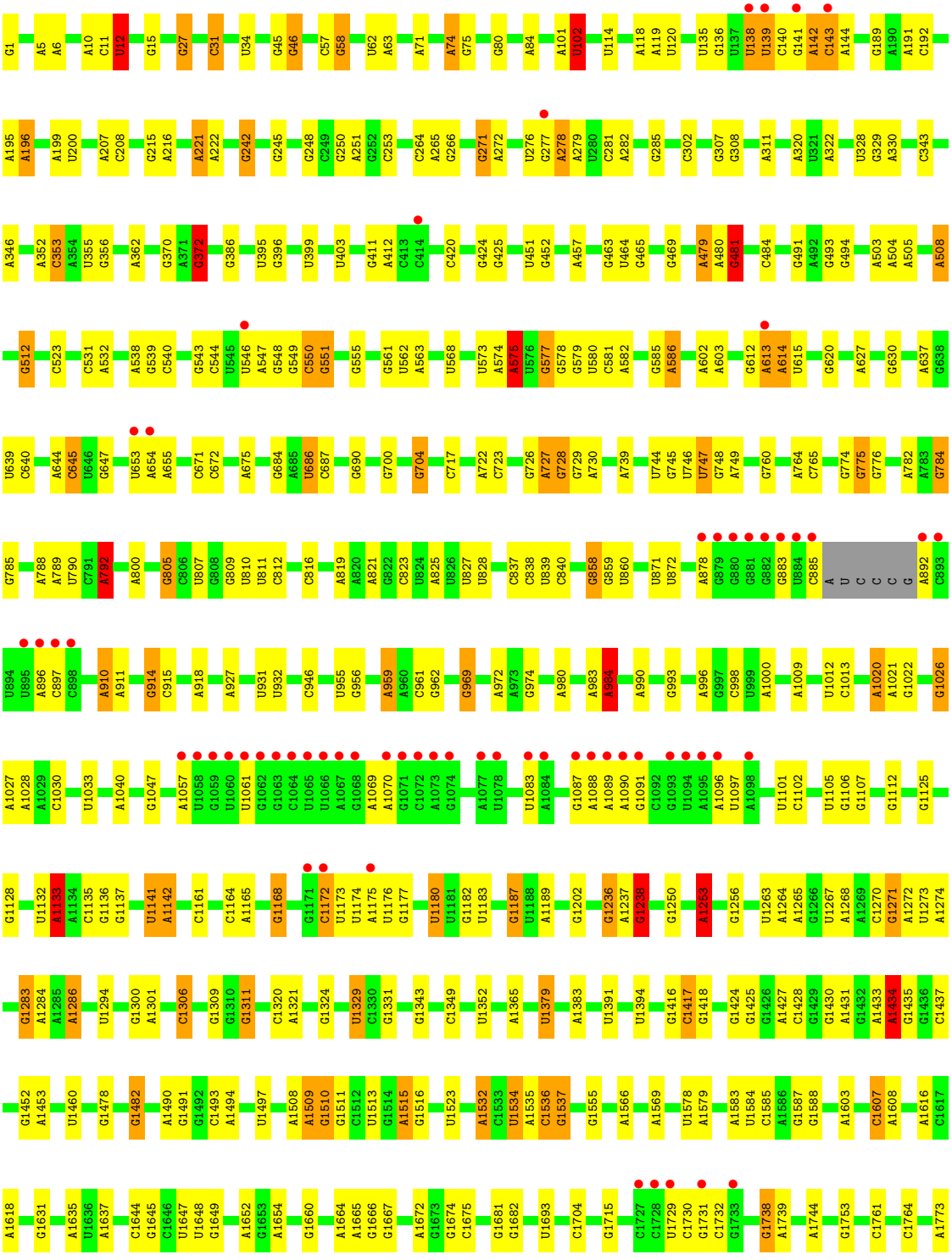
• Molecule 54: 50S ribosomal protein L10

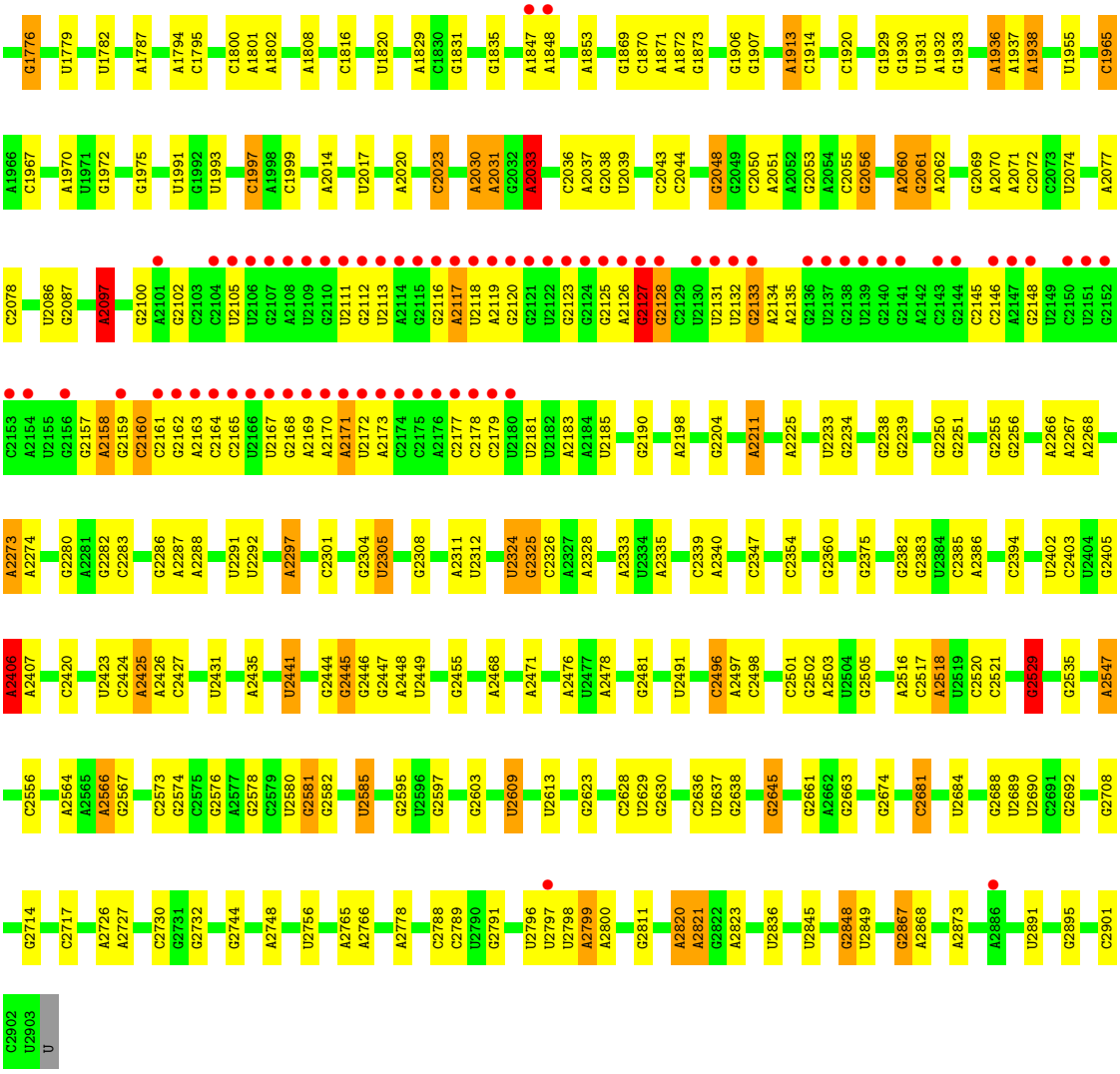




• Molecule 55: 23S rRNA

Chain DA:




G1776 U1779 U1782 A1787 A1794 C1795 C1800 A1801 A1802 A1808 C1816 U1820 A1829 C1830 G1831 G1835 A1847 A1848 A1853 G1869 C1870 A1871 A1872 G1873 G1906 G1907 A1913 C1914 C1920 G1929 G1930 U1931 A1932 G1933 A1936 A1937 A1938 U1955 C1965
A1966 C1967 A1970 U1971 G1972 G1975 U1991 G1992 U1993 C1997 A1998 C1999 A2014 U2017 A2020 C2023 A2030 A2031 G2032 A2033 C2036 A2037 G2038 U2039 C2043 C2044 G2048 G2049 C2050 A2051 A2052 G2053 A2054 C2055 G2056 A2060 G2061 A2062 G2069 A2070 A2071 C2072 C2073 U2074 A2077
C2078 U2086 G2087 A2097 G2100 A2101 G2102 C2103 C2104 U2105 U2106 G2107 A2108 U2109 C2110 U2111 G2112 U2113 A2114 G2115 G2116 A2117 U2118 A2119 G2120 G2121 U2122 G2123 G2124 G2125 A2126 G2127 G2128 C2129 U2130 U2131 U2132 G2133 A2134 A2135 G2136 U2137 G2138 U2139 G2140 G2141 A2142 C2143 G2144 C2145 C2146 A2147 G2148 U2149 C2150 U2151 C2152
C2153 A2154 U2155 G2156 G2157 A2158 G2159 C2160 C2161 G2162 A2163 C2164 C2165 U2166 U2167 G2168 A2169 A2170 A2171 U2172 A2173 C2174 C2175 A2176 C2177 C2178 C2179 U2180 U2181 U2182 A2183 A2184 U2185 G2190 A2198 G2204 A2211 A2225 U2233 G2234 G2238 G2239 G2250 G2251 G2255 G2256 A2266 A2267 A2268
A2273 A2274 G2280 A2281 G2282 C2283 G2286 A2287 A2288 U2291 U2292 A2297 C2301 G2304 U2305 G2308 A2311 U2312 U2324 G2325 C2326 A2327 A2328 A2333 U2334 A2335 C2339 A2340 C2347 C2354 G2360 G2375 G2382 G2383 U2384 C2385 A2386 C2394 U2402 C2403 U2404 G2405
A2406 A2407 C2420 U2423 C2424 A2425 A2426 C2427 U2431 A2435 U2441 G2444 G2445 G2446 G2447 A2448 U2449 G2455 A2468 A2471 A2476 U2477 A2478 G2481 U2491 C2496 A2497 C2498 C2501 G2502 A2503 U2504 G2505 A2516 C2517 A2518 U2519 C2520 C2521 G2529 G2535 A2547
C2556 A2564 A2565 A2566 G2567 C2573 G2574 C2575 G2576 A2577 G2578 C2579 U2580 G2581 G2582 U2585 G2595 U2596 G2597 G2603 U2609 U2613 G2623 C2628 U2629 G2630 C2636 U2637 G2638 G2645 G2661 A2662 G2663 G2674 C2681 U2684 G2688 U2689 U2690 C2691 G2692 G2708
G2714 C2717 A2726 A2727 C2730 G2731 G2732 G2744 A2748 U2756 A2765 A2766 A2778 C2788 C2789 U2790 G2791 U2796 U2797 U2798 A2799 A2800 G2811 A2820 A2821 G2822 A2823 U2836 U2845 G2848 U2849 G2867 A2868 A2873 A2886 U2891 G2895 C2901
C2902 U2903 U

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	212.18Å 434.82Å 624.26Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.51 – 2.96 48.28 – 2.96	Depositor EDS
% Data completeness (in resolution range)	88.6 (48.51-2.96) 88.6 (48.28-2.96)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	21.17 (at 2.96Å)	Xtriage
Refinement program	BUSTER-TNT 2.11.6	Depositor
R, R_{free}	0.208 , 0.221 0.227 , 0.243	Depositor DCC
R_{free} test set	4163 reflections (0.40%)	wwPDB-VP
Wilson B-factor (Å^2)	57.6	Xtriage
Anisotropy	0.403	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.27 , 89.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	295202	wwPDB-VP
Average B, all atoms (Å^2)	123.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.37% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PEG, H2U, GUN, MEQ, PSU, 4D4, MG, MPD, ACY, 1MG, PG4, PGE, TRS, T1C, 4OC, OMC, 2MG, PUT, EDO, 2MA, MA6, 1PE, 6MZ, D2T, OMG, ZN, 3TD, G7M, OMU, 5MU, SPD, 5MC, UR3

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	AA	1.04	9/36593 (0.0%)	0.86	5/57081 (0.0%)
1	BA	1.05	10/36568 (0.0%)	0.86	5/57042 (0.0%)
2	AB	0.48	0/1784	0.65	0/2403
2	BB	0.48	0/1784	0.65	0/2403
3	AC	0.48	0/1652	0.67	0/2225
3	BC	0.47	0/1652	0.67	0/2225
4	AD	0.44	0/1665	0.69	0/2227
4	BD	0.43	0/1665	0.70	0/2227
5	AE	0.48	0/1157	0.77	0/1557
5	BE	0.51	0/1118	0.81	0/1504
6	AF	0.46	0/881	0.69	0/1189
6	BF	0.47	0/835	0.77	0/1128
7	AG	0.45	0/1196	0.61	0/1602
7	BG	0.46	0/1196	0.62	0/1602
8	AH	0.46	0/989	0.71	0/1326
8	BH	0.46	0/989	0.69	0/1326
9	AI	0.44	0/1034	0.66	0/1375
9	BI	0.44	0/1034	0.65	0/1375
10	AJ	0.44	0/806	0.68	0/1089
10	BJ	0.48	0/797	0.71	0/1077
11	AK	0.46	0/893	0.65	0/1205
11	BK	0.45	0/893	0.68	0/1205
12	AL	0.44	0/960	0.74	0/1286
12	BL	0.47	0/960	0.74	0/1286
13	AM	0.51	0/893	0.72	0/1193
13	BM	0.49	0/893	0.72	0/1193
14	AN	0.46	0/817	0.63	0/1088
14	BN	0.44	0/817	0.63	0/1088
15	AO	0.48	0/722	0.60	0/964
15	BO	0.47	0/722	0.63	0/964

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
16	AP	0.48	0/659	0.70	0/884
16	BP	0.50	0/659	0.76	0/884
17	AQ	0.48	0/658	0.73	0/881
17	BQ	0.51	0/658	0.78	0/881
18	AR	0.53	0/463	0.65	0/621
18	BR	0.50	0/463	0.64	0/621
19	AS	0.46	0/653	0.59	0/877
19	BS	0.45	0/653	0.60	0/877
20	AT	0.48	0/676	0.66	0/895
20	BT	0.52	0/671	0.68	0/888
21	AU	0.45	0/472	0.61	0/627
21	BU	0.43	0/472	0.63	0/627
22	C1	0.49	0/450	0.71	0/599
22	D1	0.61	0/450	0.79	0/599
23	C2	0.46	0/416	0.73	0/554
23	D2	0.51	0/421	0.73	0/561
24	C3	0.46	0/380	0.69	0/498
24	D3	0.55	0/380	0.76	0/498
25	C4	0.46	0/513	0.67	0/676
25	D4	0.56	0/513	0.71	0/676
26	C5	0.43	0/303	0.77	0/397
26	D5	0.53	0/303	0.76	0/397
27	C0	0.52	0/453	0.77	0/605
27	D0	0.62	0/467	0.81	0/623
28	CB	0.98	0/2828	0.88	2/4410 (0.0%)
28	DB	1.13	1/2872 (0.0%)	0.90	0/4478
29	CC	0.45	0/2121	0.76	0/2852
29	DC	0.50	0/2121	0.76	1/2852 (0.0%)
30	CD	0.43	0/1586	0.70	0/2134
31	CA	1.07	44/69165 (0.1%)	0.87	17/107896 (0.0%)
32	DD	0.54	0/1576	0.73	0/2119
33	CE	0.45	0/1571	0.72	0/2113
33	DE	0.52	0/1571	0.72	0/2113
34	CF	0.43	0/1434	0.68	0/1926
34	DF	0.46	0/1434	0.70	0/1926
35	CG	0.42	0/1343	0.66	0/1816
35	DG	0.44	0/1343	0.64	0/1816
36	CH	0.48	0/1121	0.68	0/1515
36	DH	0.48	0/1121	0.68	0/1515
37	CJ	0.48	0/993	0.62	0/1341
37	DJ	0.48	0/993	0.61	0/1341
38	CK	0.43	0/1152	0.70	0/1551
38	DK	0.56	0/1152	0.74	0/1551

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
39	CL	0.47	0/947	0.74	0/1268
39	DL	0.54	0/955	0.75	0/1279
40	CM	0.46	0/1062	0.74	1/1413 (0.1%)
40	DM	0.50	0/1062	0.75	1/1413 (0.1%)
41	CN	0.45	0/1081	0.75	1/1443 (0.1%)
41	DN	0.59	0/1092	0.81	0/1457
42	CO	0.46	0/973	0.72	0/1301
42	DO	0.58	0/1006	0.80	0/1345
43	CP	0.43	0/902	0.73	0/1209
43	DP	0.47	0/910	0.73	0/1219
44	CQ	0.41	0/929	0.71	0/1242
44	DQ	0.48	0/929	0.72	0/1242
45	CR	0.48	0/960	0.69	0/1278
45	DR	0.62	0/960	0.76	0/1278
46	CS	0.44	0/829	0.74	0/1107
46	DS	0.55	0/829	0.78	0/1107
47	CT	0.43	0/864	0.74	0/1156
47	DT	0.55	0/864	0.75	0/1156
48	CU	0.44	0/745	0.72	0/994
48	DU	0.48	0/745	0.72	0/994
49	CV	0.44	0/787	0.76	0/1051
49	DV	0.49	0/787	0.77	0/1051
50	CW	0.40	0/766	0.65	0/1025
50	DW	0.50	0/766	0.69	0/1025
51	CX	0.39	0/576	0.65	0/762
51	DX	0.53	0/598	0.73	0/790
52	CY	0.43	0/635	0.73	0/848
52	DY	0.46	0/635	0.72	0/848
53	CZ	0.42	0/502	0.61	0/667
53	DZ	0.43	0/502	0.60	0/667
54	DI	0.51	0/1037	0.74	1/1402 (0.1%)
55	DA	1.27	148/69364 (0.2%)	0.97	26/108207 (0.0%)
All	All	0.98	212/309267 (0.1%)	0.85	60/462210 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	AA	0	3
1	BA	0	4

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Mol	Chain	#Chirality outliers	#Planarity outliers
5	AE	0	1
10	BJ	0	1
31	CA	0	12
55	DA	0	87
All	All	0	108

All (212) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	DA	1020	A	N3-C4	9.93	1.40	1.34
31	CA	1936	A	N9-C4	-9.29	1.32	1.37
31	CA	2095	A	O5'-C5'	-9.00	1.28	1.42
55	DA	539	G	N7-C5	7.77	1.44	1.39
55	DA	12	U	C1'-N1	7.58	1.60	1.48
55	DA	195	A	N9-C4	7.54	1.42	1.37
55	DA	2097	A	O5'-C5'	-7.36	1.31	1.42
55	DA	2050	C	N1-C6	7.35	1.41	1.37
31	CA	769	U	C1'-N1	7.22	1.59	1.48
31	CA	12	U	C1'-N1	7.06	1.59	1.48
55	DA	2585	U	C1'-N1	7.03	1.59	1.48
55	DA	1286	A	N3-C4	7.01	1.39	1.34
31	CA	2425	A	C3'-O3'	6.97	1.51	1.42
55	DA	2060	A	N3-C4	6.87	1.39	1.34
55	DA	2520	C	N1-C6	6.87	1.41	1.37
1	BA	1493	A	C3'-O3'	6.83	1.51	1.42
31	CA	546	U	C1'-N1	6.76	1.58	1.48
55	DA	484	C	C1'-N1	6.76	1.58	1.48
55	DA	1665	A	N7-C5	6.69	1.43	1.39
1	BA	1397	C	N1-C2	6.62	1.46	1.40
55	DA	1787	A	N9-C4	6.58	1.41	1.37
1	BA	5	U	C1'-N1	6.53	1.58	1.48
1	BA	28	A	O5'-C5'	-6.51	1.32	1.42
55	DA	2053	G	C6-N1	6.37	1.44	1.39
55	DA	582	A	N9-C4	6.37	1.41	1.37
55	DA	671	C	C1'-N1	6.33	1.58	1.48
55	DA	1306	C	C1'-N1	6.29	1.58	1.48
31	CA	2225	A	C3'-O3'	6.25	1.50	1.42
55	DA	2547	A	O5'-C5'	-6.23	1.32	1.42
55	DA	998	C	C1'-N1	6.23	1.58	1.48
55	DA	727	A	N3-C4	6.19	1.38	1.34
55	DA	959	A	N3-C4	6.13	1.38	1.34
28	DB	90	C	O5'-C5'	-6.12	1.33	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	AA	28	A	O5'-C5'	-6.11	1.33	1.42
55	DA	2867	G	C3'-O3'	6.10	1.50	1.42
55	DA	372	G	C3'-O3'	6.08	1.50	1.42
55	DA	31	C	N1-C6	6.07	1.40	1.37
55	DA	2547	A	P-O5'	-6.06	1.53	1.59
55	DA	2023	C	N1-C6	6.03	1.40	1.37
55	DA	2521	C	N1-C6	6.01	1.40	1.37
55	DA	1000	A	N3-C4	6.00	1.38	1.34
1	BA	1008	U	O5'-C5'	-6.00	1.33	1.42
55	DA	578	G	N3-C4	5.98	1.39	1.35
55	DA	102	U	N1-C2	5.97	1.44	1.38
55	DA	579	G	C2'-C1'	-5.97	1.46	1.53
55	DA	2717	C	N1-C6	5.96	1.40	1.37
55	DA	1137	G	N3-C4	5.95	1.39	1.35
55	DA	1294	U	O5'-C5'	-5.94	1.33	1.42
55	DA	2297	A	O5'-C5'	-5.93	1.33	1.42
1	AA	1397	C	N1-C6	5.93	1.40	1.37
55	DA	1965	C	C1'-N1	5.92	1.57	1.48
55	DA	972	A	C6-N6	5.90	1.38	1.33
31	CA	253	C	C1'-N1	5.88	1.57	1.48
55	DA	2044	C	N1-C6	5.88	1.40	1.37
55	DA	575	A	N9-C4	5.87	1.41	1.37
1	AA	5	U	C1'-N1	5.86	1.57	1.48
55	DA	969	G	C8-N7	-5.84	1.27	1.30
55	DA	2756	U	C3'-O3'	5.83	1.50	1.42
55	DA	2036	C	N1-C6	5.81	1.40	1.37
55	DA	2518	A	N9-C4	5.80	1.41	1.37
31	CA	1306	C	C1'-N1	5.79	1.57	1.48
55	DA	2447	G	N3-C4	5.79	1.39	1.35
55	DA	2127	G	C3'-O3'	5.79	1.50	1.42
31	CA	2619	C	C1'-N1	5.78	1.57	1.48
55	DA	1635	A	N3-C4	5.77	1.38	1.34
55	DA	1164	C	N1-C6	5.76	1.40	1.37
55	DA	2446	G	N3-C4	5.76	1.39	1.35
31	CA	2579	C	C1'-N1	5.76	1.57	1.48
31	CA	1788	C	C1'-N1	5.74	1.57	1.48
55	DA	984	A	N3-C4	5.70	1.38	1.34
55	DA	2766	A	N9-C4	5.69	1.41	1.37
55	DA	457	A	N3-C4	5.69	1.38	1.34
55	DA	838	C	N1-C6	5.68	1.40	1.37
1	BA	485	U	N1-C2	5.66	1.43	1.38
1	BA	290	C	C1'-N1	5.65	1.57	1.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	DA	821	A	N3-C4	5.65	1.38	1.34
55	DA	1534	U	C1'-N1	5.65	1.57	1.48
55	DA	1311	G	C6-N1	5.63	1.43	1.39
31	CA	1314	C	C1'-N1	5.63	1.57	1.48
55	DA	12	U	N1-C2	5.63	1.43	1.38
55	DA	1267	U	C2-N3	5.63	1.41	1.37
55	DA	744	U	N1-C6	5.60	1.43	1.38
55	DA	2056	G	C6-N1	5.58	1.43	1.39
55	DA	816	C	N1-C6	5.57	1.40	1.37
55	DA	1660	G	O5'-C5'	-5.57	1.33	1.42
55	DA	2426	A	N3-C4	5.57	1.38	1.34
55	DA	823	C	N1-C6	5.56	1.40	1.37
55	DA	990	A	N7-C5	5.55	1.42	1.39
31	CA	1658	C	C1'-N1	5.54	1.57	1.48
55	DA	1920	C	C1'-N1	5.54	1.57	1.48
55	DA	959	A	N9-C4	5.52	1.41	1.37
55	DA	508	A	N3-C4	5.52	1.38	1.34
55	DA	1965	C	C3'-O3'	-5.52	1.34	1.42
55	DA	2425	A	C3'-O3'	5.52	1.49	1.42
55	DA	2576	G	O3'-P	-5.51	1.54	1.61
55	DA	1021	A	N9-C4	5.51	1.41	1.37
55	DA	2821	A	N3-C4	5.51	1.38	1.34
55	DA	2444	G	N7-C5	5.50	1.42	1.39
55	DA	739	A	N3-C4	5.50	1.38	1.34
55	DA	613	A	N9-C4	5.50	1.41	1.37
31	CA	2006	C	C1'-N1	5.49	1.56	1.48
55	DA	196	A	N9-C4	5.48	1.41	1.37
55	DA	809	G	N7-C5	5.48	1.42	1.39
1	BA	575	G	C3'-O3'	5.47	1.49	1.42
55	DA	1265	A	N9-C4	5.46	1.41	1.37
31	CA	2680	U	C3'-O3'	5.46	1.49	1.42
55	DA	2692	G	N3-C4	5.44	1.39	1.35
55	DA	1133	A	O5'-C5'	-5.42	1.34	1.42
31	CA	995	C	O5'-C5'	-5.42	1.34	1.42
31	CA	2146	C	C3'-O3'	5.42	1.49	1.42
55	DA	1189	A	N9-C4	5.42	1.41	1.37
55	DA	12	U	P-O5'	5.41	1.65	1.59
55	DA	561	G	N3-C4	5.41	1.39	1.35
1	AA	1203	C	C1'-N1	5.39	1.56	1.48
31	CA	946	C	C1'-N1	5.39	1.56	1.48
55	DA	810	U	N1-C2	5.39	1.43	1.38
31	CA	2233	U	C1'-N1	5.39	1.56	1.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	CA	2823	A	C3'-O3'	5.38	1.49	1.42
31	CA	480	A	N9-C4	5.36	1.41	1.37
55	DA	469	G	N3-C4	5.36	1.39	1.35
31	CA	404	A	C3'-O3'	5.35	1.49	1.42
31	CA	1825	U	C1'-N1	5.34	1.56	1.48
31	CA	451	U	C1'-N1	5.34	1.56	1.48
31	CA	461	C	C1'-N1	5.34	1.56	1.48
55	DA	819	A	N3-C4	5.34	1.38	1.34
55	DA	2036	C	C1'-N1	5.31	1.56	1.48
55	DA	613	A	C3'-O3'	5.31	1.49	1.42
1	BA	842	U	C3'-O3'	5.30	1.49	1.42
55	DA	2077	A	N3-C4	5.30	1.38	1.34
55	DA	653	U	C1'-N1	5.30	1.56	1.48
31	CA	557	C	C1'-N1	5.30	1.56	1.48
55	DA	1030	C	N1-C6	5.29	1.40	1.37
55	DA	962	G	N3-C4	5.29	1.39	1.35
31	CA	1629	U	C1'-N1	5.29	1.56	1.48
55	DA	271	G	C3'-O3'	5.28	1.49	1.42
31	CA	2723	C	C1'-N1	5.28	1.56	1.48
55	DA	1274	A	N7-C5	-5.26	1.36	1.39
31	CA	653	U	C1'-N1	5.26	1.56	1.48
55	DA	2585	U	N1-C2	5.25	1.43	1.38
55	DA	2730	C	N1-C6	5.24	1.40	1.37
31	CA	198	C	C1'-N1	5.24	1.56	1.48
31	CA	1771	C	C1'-N1	5.22	1.56	1.48
31	CA	2646	C	C1'-N1	5.22	1.56	1.48
55	DA	918	A	N3-C4	5.22	1.38	1.34
55	DA	577	G	N3-C4	5.22	1.39	1.35
1	AA	575	G	C3'-O3'	5.22	1.49	1.42
55	DA	1268	A	N3-C4	5.22	1.38	1.34
55	DA	2288	A	N3-C4	5.22	1.38	1.34
55	DA	195	A	N3-C4	5.21	1.38	1.34
55	DA	1584	U	C1'-N1	5.21	1.56	1.48
55	DA	264	C	N1-C2	5.21	1.45	1.40
55	DA	27	G	C6-N1	5.21	1.43	1.39
1	BA	291	U	C1'-N1	5.21	1.56	1.48
55	DA	2521	C	C1'-N1	5.20	1.56	1.48
55	DA	911	A	N3-C4	5.20	1.38	1.34
55	DA	2901	C	C1'-N1	5.20	1.56	1.48
55	DA	1664	A	N9-C4	5.19	1.41	1.37
55	DA	2211	A	C3'-O3'	5.18	1.49	1.42
55	DA	512	G	N9-C4	5.17	1.42	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	DA	581	C	C1'-N1	5.17	1.56	1.48
1	AA	15	G	N3-C4	5.17	1.39	1.35
31	CA	1971	U	C1'-N1	5.16	1.56	1.48
55	DA	1675	C	N1-C6	5.16	1.40	1.37
55	DA	1776	G	O5'-C5'	-5.16	1.34	1.42
55	DA	1270	C	N1-C6	5.15	1.40	1.37
55	DA	2354	C	O5'-C5'	-5.15	1.34	1.42
55	DA	2033	A	P-O5'	5.15	1.64	1.59
55	DA	353	C	C1'-N1	5.14	1.56	1.48
55	DA	465	G	N3-C4	5.14	1.39	1.35
55	DA	1607	C	N1-C6	5.13	1.40	1.37
55	DA	2273	A	N3-C4	5.13	1.38	1.34
31	CA	2465	C	C1'-N1	5.13	1.56	1.48
31	CA	2756	U	C3'-O3'	5.13	1.49	1.42
55	DA	672	C	N1-C6	5.12	1.40	1.37
55	DA	2581	G	C3'-O3'	5.12	1.49	1.42
55	DA	562	U	N1-C6	5.12	1.42	1.38
55	DA	792	A	N3-C4	5.12	1.38	1.34
55	DA	1704	C	C1'-N1	5.12	1.56	1.48
55	DA	1965	C	O5'-C5'	-5.12	1.34	1.42
55	DA	1020	A	C6-N1	5.12	1.39	1.35
55	DA	2496	C	O5'-C5'	-5.11	1.34	1.42
1	AA	290	C	C1'-N1	5.11	1.56	1.48
31	CA	672	C	C1'-N1	5.11	1.56	1.48
55	DA	2406	A	P-O5'	5.11	1.64	1.59
55	DA	2427	C	N1-C6	5.11	1.40	1.37
55	DA	2471	A	N3-C4	5.10	1.38	1.34
55	DA	585	G	N9-C4	5.09	1.42	1.38
31	CA	2044	C	C1'-N1	5.08	1.56	1.48
55	DA	1999	C	N1-C6	5.08	1.40	1.37
55	DA	2455	G	C3'-O3'	-5.08	1.35	1.42
31	CA	2354	C	C1'-N1	5.08	1.56	1.48
31	CA	2901	C	C1'-N1	5.07	1.56	1.48
31	CA	1704	C	C1'-N1	5.07	1.56	1.48
55	DA	684	G	N3-C4	5.07	1.39	1.35
55	DA	2708	G	N3-C4	5.06	1.39	1.35
55	DA	2301	C	C1'-N1	5.06	1.56	1.48
55	DA	1437	C	O5'-C5'	-5.05	1.34	1.42
1	AA	209	U	C3'-O3'	5.04	1.49	1.42
55	DA	1253	A	O5'-C5'	-5.04	1.34	1.42
55	DA	114	U	C1'-N1	5.04	1.56	1.48
55	DA	1284	A	N3-C4	5.04	1.37	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	CA	692	C	C1'-N1	5.04	1.56	1.48
55	DA	251	A	N3-C4	5.04	1.37	1.34
1	AA	843	U	C1'-N1	5.03	1.56	1.48
55	DA	2585	U	C3'-O3'	5.03	1.49	1.42
55	DA	574	A	O5'-C5'	-5.02	1.34	1.42
55	DA	2061	G	N3-C4	5.02	1.39	1.35
31	CA	20	C	C1'-N1	5.01	1.56	1.48
55	DA	1644	C	C1'-N1	5.01	1.56	1.48
55	DA	1331	G	N3-C4	5.01	1.39	1.35
55	DA	1637	A	N7-C5	5.01	1.42	1.39
31	CA	2215	C	C1'-N1	5.00	1.56	1.48

All (60) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	CB	15	A	O4'-C1'-N9	10.06	116.25	108.20
55	DA	512	G	O4'-C1'-N9	8.55	115.04	108.20
1	AA	413	G	C1'-O4'-C4'	-8.26	103.29	109.90
55	DA	784	G	P-O3'-C3'	7.86	129.13	119.70
41	CN	69	PRO	C-N-CA	7.39	140.18	121.70
55	DA	1936	A	O4'-C1'-N9	7.18	113.94	108.20
1	AA	1	A	OP1-P-OP2	-7.13	108.90	119.60
55	DA	2820	A	P-O3'-C3'	7.09	128.21	119.70
55	DA	892	A	OP1-P-OP2	-7.05	109.03	119.60
54	DI	132	TYR	C-N-CA	7.01	139.24	121.70
31	CA	892	A	OP1-P-OP2	-6.96	109.17	119.60
55	DA	1	G	OP1-P-OP2	-6.87	109.29	119.60
1	BA	1362	A	C1'-O4'-C4'	-6.87	104.40	109.90
31	CA	974	G	N9-C1'-C2'	6.74	122.76	114.00
1	BA	2	A	OP1-P-OP2	-6.72	109.52	119.60
31	CA	271	G	P-O3'-C3'	6.49	127.49	119.70
55	DA	271	G	P-O3'-C3'	6.46	127.45	119.70
1	AA	413	G	O4'-C1'-N9	6.44	113.35	108.20
55	DA	2848	G	O4'-C1'-N9	6.20	113.16	108.20
55	DA	1311	G	O4'-C1'-N9	6.05	113.04	108.20
31	CA	2425	A	P-O3'-C3'	5.92	126.80	119.70
31	CA	451	U	C1'-O4'-C4'	-5.89	105.19	109.90
1	BA	842	U	P-O3'-C3'	5.84	126.71	119.70
31	CA	512	G	O4'-C1'-N9	5.82	112.86	108.20
55	DA	1379	U	P-O3'-C3'	5.81	126.67	119.70
31	CA	784	G	P-O3'-C3'	5.76	126.61	119.70
1	BA	485	U	O4'-C1'-N1	5.76	112.81	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
40	DM	60	ARG	CG-CD-NE	5.73	123.84	111.80
31	CA	1379	U	P-O3'-C3'	5.71	126.55	119.70
55	DA	704	G	O4'-C1'-N9	5.59	112.67	108.20
55	DA	242	G	C3'-C2'-C1'	-5.56	97.05	101.50
55	DA	2406	A	C5'-C4'-O4'	-5.56	102.42	109.10
55	DA	1434	A	O4'-C1'-N9	5.42	112.53	108.20
55	DA	1165	A	O4'-C1'-N9	5.40	112.52	108.20
1	BA	1397	C	C2-N1-C1'	5.39	124.72	118.80
55	DA	27	G	O4'-C1'-N9	5.36	112.49	108.20
29	DC	156	ARG	CB-CG-CD	-5.34	97.71	111.60
31	CA	2225	A	P-O3'-C3'	5.31	126.08	119.70
31	CA	2095	A	C5'-C4'-C3'	-5.28	107.55	116.00
55	DA	2280	G	C4'-C3'-C2'	-5.27	97.33	102.60
31	CA	2035	G	C1'-O4'-C4'	-5.26	105.69	109.90
55	DA	2645	G	O4'-C1'-N9	5.23	112.39	108.20
31	CA	704	G	O4'-C1'-N9	5.20	112.36	108.20
31	CA	2825	G	O4'-C1'-N9	5.19	112.35	108.20
31	CA	242	G	C3'-C2'-C1'	-5.18	97.35	101.50
40	CM	68	SER	C-N-CA	5.18	134.66	121.70
31	CA	2406	A	C5'-C4'-O4'	5.18	115.31	109.10
55	DA	512	G	C1'-O4'-C4'	-5.17	105.76	109.90
55	DA	479	A	C3'-C2'-C1'	-5.17	97.36	101.50
55	DA	807	U	C4'-C3'-C2'	-5.17	97.43	102.60
55	DA	2048	G	C8-N9-C4	-5.15	104.34	106.40
28	CB	89	U	O4'-C1'-N1	5.13	112.31	108.20
55	DA	1238	G	C4'-C3'-C2'	-5.13	97.47	102.60
1	AA	841	C	P-O3'-C3'	5.11	125.83	119.70
1	AA	890	G	C3'-C2'-C1'	-5.08	97.44	101.50
55	DA	1997	C	C4'-C3'-C2'	-5.08	97.52	102.60
31	CA	2447	G	C3'-C2'-C1'	-5.04	97.46	101.50
55	DA	1936	A	C1'-O4'-C4'	-5.03	105.88	109.90
55	DA	2447	G	C3'-C2'-C1'	-5.02	97.48	101.50
31	CA	974	G	C3'-C2'-C1'	-5.01	97.49	101.50

There are no chirality outliers.

All (108) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	AA	1432	G	Sidechain
1	AA	362	G	Sidechain
1	AA	898	G	Sidechain
5	AE	82	GLN	Sidechain

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Mol	Chain	Res	Type	Group
1	BA	1432	G	Sidechain
1	BA	362	G	Sidechain
1	BA	575	G	Sidechain
1	BA	898	G	Sidechain
10	BJ	37	ARG	Mainchain
31	CA	1693	U	Sidechain
31	CA	1777	U	Sidechain
31	CA	1936	A	Sidechain
31	CA	1937	A	Sidechain
31	CA	2267	A	Sidechain
31	CA	2638	G	Sidechain
31	CA	2732	G	Sidechain
31	CA	463	G	Sidechain
31	CA	481	G	Sidechain
31	CA	704	G	Sidechain
31	CA	726	G	Sidechain
31	CA	805	G	Sidechain
55	DA	1009	A	Sidechain
55	DA	1142	A	Sidechain
55	DA	1236	G	Sidechain
55	DA	1253	A	Sidechain
55	DA	1283	G	Sidechain
55	DA	1311	G	Sidechain
55	DA	1324	G	Sidechain
55	DA	1343	G	Sidechain
55	DA	1425	G	Sidechain
55	DA	15	G	Sidechain
55	DA	1631	G	Sidechain
55	DA	1645	G	Sidechain
55	DA	1666	G	Sidechain
55	DA	1667	G	Sidechain
55	DA	1672	A	Sidechain
55	DA	1681	G	Sidechain
55	DA	1682	G	Sidechain
55	DA	1693	U	Sidechain
55	DA	1753	G	Sidechain
55	DA	1761	C	Sidechain
55	DA	1779	U	Sidechain
55	DA	1802	A	Sidechain
55	DA	1938	A	Sidechain
55	DA	2037	A	Sidechain
55	DA	2048	G	Sidechain

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Mol	Chain	Res	Type	Group
55	DA	2074	U	Sidechain
55	DA	2078	C	Sidechain
55	DA	221	A	Sidechain
55	DA	2250	G	Sidechain
55	DA	2266	A	Sidechain
55	DA	2267	A	Sidechain
55	DA	2282	G	Sidechain
55	DA	2328	A	Sidechain
55	DA	2375	G	Sidechain
55	DA	2382	G	Sidechain
55	DA	2405	G	Sidechain
55	DA	2468	A	Sidechain
55	DA	2481	G	Sidechain
55	DA	2497	A	Sidechain
55	DA	250	G	Sidechain
55	DA	2516	A	Sidechain
55	DA	2517	C	Sidechain
55	DA	2529	G	Sidechain
55	DA	2564	A	Sidechain
55	DA	2566	A	Sidechain
55	DA	2581	G	Sidechain
55	DA	2582	G	Sidechain
55	DA	2595	G	Sidechain
55	DA	2597	G	Sidechain
55	DA	2638	G	Sidechain
55	DA	2645	G	Sidechain
55	DA	2688	G	Sidechain
55	DA	27	G	Sidechain
55	DA	2727	A	Sidechain
55	DA	2732	G	Sidechain
55	DA	2848	G	Sidechain
55	DA	307	G	Sidechain
55	DA	308	G	Sidechain
55	DA	395	U	Sidechain
55	DA	452	G	Sidechain
55	DA	463	G	Sidechain
55	DA	464	U	Sidechain
55	DA	481	G	Sidechain
55	DA	512	G	Sidechain
55	DA	555	G	Sidechain
55	DA	575	A	Sidechain
55	DA	577	G	Sidechain

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Mol	Chain	Res	Type	Group
55	DA	58	G	Sidechain
55	DA	630	G	Sidechain
55	DA	675	A	Sidechain
55	DA	690	G	Sidechain
55	DA	700	G	Sidechain
55	DA	704	G	Sidechain
55	DA	726	G	Sidechain
55	DA	727	A	Sidechain
55	DA	728	G	Sidechain
55	DA	748	G	Sidechain
55	DA	774	G	Sidechain
55	DA	775	G	Sidechain
55	DA	800	A	Sidechain
55	DA	805	G	Sidechain
55	DA	858	G	Sidechain
55	DA	910	A	Sidechain
55	DA	956	G	Sidechain
55	DA	959	A	Sidechain
55	DA	980	A	Sidechain
55	DA	984	A	Sidechain

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AA	32930	0	16591	90	0
1	BA	32908	0	16580	97	0
2	AB	1753	0	1780	10	0
2	BB	1753	0	1780	15	0
3	AC	1625	0	1696	14	0
3	BC	1625	0	1696	18	0
4	AD	1643	0	1707	13	0
4	BD	1643	0	1707	17	0
5	AE	1144	0	1185	15	0
5	BE	1105	0	1148	30	0
6	AF	862	0	864	7	0
6	BF	817	0	808	9	0
7	AG	1182	0	1238	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	BG	1182	0	1238	4	0
8	AH	979	0	1031	8	0
8	BH	979	0	1031	4	0
9	AI	1022	0	1070	6	0
9	BI	1022	0	1070	6	0
10	AJ	796	0	836	11	0
10	BJ	787	0	828	10	0
11	AK	877	0	887	14	0
11	BK	877	0	887	17	0
12	AL	957	0	1017	7	0
12	BL	957	0	1017	9	0
13	AM	884	0	941	11	0
13	BM	884	0	941	11	0
14	AN	805	0	844	8	0
14	BN	805	0	844	8	0
15	AO	714	0	734	1	0
15	BO	714	0	734	0	0
16	AP	649	0	666	3	0
16	BP	649	0	666	5	0
17	AQ	649	0	691	6	0
17	BQ	649	0	691	5	0
18	AR	456	0	478	5	0
18	BR	456	0	478	3	0
19	AS	638	0	665	7	0
19	BS	638	0	665	8	0
20	AT	670	0	719	2	0
20	BT	665	0	714	8	0
21	AU	465	0	491	2	0
21	BU	465	0	491	2	0
22	C1	444	0	458	18	0
22	D1	444	0	458	13	0
23	C2	409	0	440	5	0
23	D2	414	0	442	5	0
24	C3	377	0	418	17	0
24	D3	377	0	418	6	0
25	C4	504	0	572	13	0
25	D4	504	0	572	12	0
26	C5	302	0	340	9	0
26	D5	302	0	340	2	0
27	C0	449	0	488	4	0
27	D0	463	0	504	1	0
28	CB	2529	0	1281	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
28	DB	2569	0	1301	5	0
29	CC	2082	0	2154	17	0
29	DC	2082	0	2154	11	0
30	CD	1565	0	1616	16	0
31	CA	62229	0	31318	236	0
32	DD	1576	0	1627	16	0
33	CE	1552	0	1619	14	0
33	DE	1552	0	1619	11	0
34	CF	1410	0	1444	16	0
34	DF	1410	0	1444	12	0
35	CG	1323	0	1371	9	0
35	DG	1323	0	1371	9	0
36	CH	1110	0	1148	8	0
36	DH	1110	0	1148	6	0
37	CJ	979	0	1028	4	0
37	DJ	979	0	1028	5	0
38	CK	1129	0	1162	9	0
38	DK	1129	0	1162	5	0
39	CL	938	0	1012	8	0
39	DL	946	0	1023	6	0
40	CM	1053	0	1129	19	0
40	DM	1053	0	1129	15	0
41	CN	1075	0	1154	5	0
41	DN	1092	0	1177	7	0
42	CO	960	0	1000	5	0
42	DO	993	0	1034	5	0
43	CP	892	0	923	7	0
43	DP	900	0	935	9	0
44	CQ	917	0	962	7	0
44	DQ	917	0	962	7	0
45	CR	947	0	1019	13	0
45	DR	947	0	1019	9	0
46	CS	816	0	839	8	0
46	DS	816	0	839	5	0
47	CT	857	0	922	12	0
47	DT	857	0	922	10	0
48	CU	739	0	807	10	0
48	DU	739	0	807	4	0
49	CV	779	0	831	8	0
49	DV	779	0	831	5	0
50	CW	753	0	780	5	0
50	DW	753	0	780	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
51	CX	569	0	581	1	0
51	DX	591	0	606	5	0
52	CY	625	0	652	8	0
52	DY	625	0	652	4	0
53	CZ	501	0	531	2	0
53	DZ	501	0	531	1	0
54	DI	1023	0	1052	19	0
55	DA	62423	0	31411	173	0
56	AA	71	0	0	0	0
56	BA	43	0	0	0	0
56	CA	156	0	0	0	0
56	CB	3	0	0	0	0
56	DA	182	0	0	0	0
56	DB	9	0	0	0	0
56	DD	2	0	0	0	0
56	DM	1	0	0	0	0
56	DR	2	0	0	0	0
57	AA	13	0	18	1	0
57	BA	13	0	18	0	0
57	DA	26	0	36	2	0
57	DQ	13	0	18	0	0
57	DR	13	0	18	5	0
57	DS	13	0	18	1	0
58	AA	16	0	28	0	0
58	DA	40	0	70	5	0
58	DE	16	0	28	0	0
58	DK	8	0	14	0	0
58	DN	8	0	14	1	0
58	DS	8	0	14	0	0
58	DT	16	0	28	0	0
59	AA	24	0	48	0	0
59	DA	72	0	144	10	0
60	AA	42	0	38	0	0
60	BA	42	0	38	0	0
61	AB	1	0	0	0	0
61	C5	1	0	0	0	0
61	D5	1	0	0	0	0
62	AL	7	0	10	0	0
62	D1	7	0	10	1	0
62	D3	7	0	10	2	0
62	DA	35	0	50	1	0
62	DL	7	0	10	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
62	DP	7	0	10	1	0
62	DQ	7	0	10	0	0
63	D1	4	0	6	0	0
63	DA	36	0	54	2	0
63	DB	8	0	12	1	0
64	D1	10	0	14	2	0
64	D3	10	0	14	0	0
64	DA	40	0	56	5	0
64	DD	10	0	14	2	0
64	DS	10	0	14	0	0
64	DU	10	0	14	1	0
65	DA	40	0	76	4	0
66	DA	32	0	44	0	0
67	DA	12	0	12	0	0
68	DA	11	0	5	0	0
69	DA	8	0	12	1	0
70	AA	507	0	0	0	0
70	AC	4	0	0	0	0
70	AD	2	0	0	0	0
70	AE	4	0	0	0	0
70	AF	1	0	0	0	0
70	AG	1	0	0	0	0
70	AH	1	0	0	0	0
70	AJ	2	0	0	0	0
70	AK	5	0	0	0	0
70	AL	8	0	0	0	0
70	AM	4	0	0	1	0
70	AN	5	0	0	1	0
70	AO	2	0	0	0	0
70	AP	2	0	0	0	0
70	AR	1	0	0	0	0
70	AS	1	0	0	0	0
70	AT	2	0	0	0	0
70	AU	3	0	0	0	0
70	BA	287	0	0	1	0
70	BD	13	0	0	0	0
70	BE	1	0	0	0	0
70	BF	1	0	0	0	0
70	BK	1	0	0	0	0
70	BL	3	0	0	0	0
70	BN	2	0	0	0	0
70	BO	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
70	BP	3	0	0	0	0
70	BR	1	0	0	0	0
70	BT	4	0	0	0	0
70	BU	2	0	0	0	0
70	C3	3	0	0	1	0
70	C4	1	0	0	0	0
70	CA	694	0	0	1	0
70	CB	13	0	0	0	0
70	CC	10	0	0	0	0
70	CD	5	0	0	0	0
70	CE	6	0	0	0	0
70	CL	1	0	0	0	0
70	CM	3	0	0	0	0
70	CO	1	0	0	0	0
70	CU	3	0	0	0	0
70	CV	1	0	0	0	0
70	CW	1	0	0	0	0
70	CY	1	0	0	0	0
70	D0	25	0	0	0	0
70	D1	42	0	0	0	0
70	D2	7	0	0	0	0
70	D3	25	0	0	0	0
70	D4	32	0	0	1	0
70	D5	13	0	0	0	0
70	DA	4836	0	0	8	0
70	DB	213	0	0	0	0
70	DC	102	0	0	0	0
70	DD	105	0	0	1	0
70	DE	63	0	0	0	0
70	DF	14	0	0	0	0
70	DG	6	0	0	0	0
70	DH	2	0	0	0	0
70	DK	58	0	0	0	0
70	DL	51	0	0	0	0
70	DM	60	0	0	0	0
70	DN	71	0	0	0	0
70	DO	44	0	0	0	0
70	DP	35	0	0	0	0
70	DQ	27	0	0	1	0
70	DR	64	0	0	0	0
70	DS	51	0	0	0	0
70	DT	70	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
70	DU	17	0	0	0	0
70	DV	19	0	0	0	0
70	DW	31	0	0	0	0
70	DX	30	0	0	1	0
70	DY	9	0	0	0	0
70	DZ	7	0	0	0	0
All	All	295202	0	194489	1207	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

All (1207) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:C5:3:VAL:HG11	31:CA:2539:C:H5'	1.32	1.05
46:CS:14:VAL:HG21	46:CS:98:ILE:HG13	1.32	1.05
4:BD:85:ASN:HA	5:BE:102:GLY:HA2	1.43	0.99
31:CA:1936:A:H2	31:CA:1943:U:H3	1.01	0.98
48:CU:28:ASN:HD21	48:CU:91:GLN:HB3	1.29	0.96
14:AN:66:GLN:HB2	70:AN:205:HOH:O	1.67	0.95
40:CM:82:LEU:HD11	40:CM:116:VAL:HG23	1.52	0.92
24:C3:7:PRO:HB2	31:CA:1309:G:H4'	1.52	0.91
46:CS:14:VAL:CG2	46:CS:98:ILE:HG13	2.00	0.90
5:AE:77:ASN:HB2	5:AE:82:GLN:NE2	1.86	0.90
40:CM:77:ILE:HD11	40:CM:108:ALA:HB1	1.55	0.89
8:BH:87:LYS:HB2	8:BH:125:ILE:HD11	1.55	0.87
22:C1:4:GLN:HA	31:CA:2615:U:C2	2.10	0.86
5:BE:77:ASN:HB2	5:BE:82:GLN:NE2	1.91	0.86
8:AH:87:LYS:HB2	8:AH:125:ILE:HD11	1.58	0.85
31:CA:2796:U:H3	31:CA:2799:A:H61	1.23	0.85
31:CA:1779:U:H5	31:CA:1784:A:N7	1.74	0.85
31:CA:1005:C:O2'	38:CK:30:THR:HG21	1.78	0.84
55:DA:2796:U:H3	55:DA:2799:A:H61	1.21	0.83
1:BA:1305:G:H21	1:BA:1332:A:H2	1.24	0.83
11:BK:88:GLY:H	11:BK:114:THR:HG22	1.43	0.82
2:BB:23:TRP:HB3	2:BB:39:HIS:CE1	2.14	0.82
1:AA:1305:G:H21	1:AA:1332:A:H2	1.23	0.81
18:AR:21:ILE:HG21	18:AR:54:GLN:HB3	1.61	0.81
31:CA:740:C:H5'	31:CA:1784:A:H3'	1.62	0.81
33:CE:149:ILE:HG12	33:CE:188:MET:HG2	1.62	0.81
12:BL:65:SER:HB2	12:BL:82:ILE:HD11	1.62	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:BM:114:LYS:HB3	13:BM:115:PRO:HD3	1.62	0.80
55:DA:2033:A:H5'	70:DA:4099:HOH:O	1.81	0.80
22:C1:38:HIS:HE1	31:CA:2884:U:O4	1.64	0.80
2:BB:20:THR:HA	2:BB:39:HIS:CE1	2.18	0.79
46:CS:14:VAL:HG21	46:CS:98:ILE:CG1	2.11	0.79
45:DR:20:GLN:CG	57:DR:202:PG4:H42	2.12	0.79
1:BA:9:G:H5'	5:BE:108:GLY:HA3	1.63	0.79
25:C4:60:ALA:O	40:CM:48:ARG:HD2	1.83	0.78
45:DR:20:GLN:HG3	57:DR:202:PG4:H42	1.65	0.78
55:DA:135:U:H3	55:DA:144:A:H61	1.32	0.78
35:CG:24:ILE:HD11	35:CG:43:VAL:HG11	1.66	0.77
35:DG:24:ILE:HD11	35:DG:43:VAL:HG11	1.66	0.77
41:DN:18[A]:ARG:HG2	28:DB:90:C:H5'	1.65	0.77
31:CA:135:U:H3	31:CA:144:A:H61	1.33	0.77
13:BM:22:ILE:HB	13:BM:25:VAL:CG1	2.15	0.77
55:DA:568:U:H1'	55:DA:2030:6MZ:H9C1	1.66	0.77
1:BA:664:G:H22	1:BA:741:G:H1	1.34	0.76
31:CA:568:U:H1'	31:CA:2030:6MZ:H9C1	1.67	0.76
39:CL:38:ILE:HD11	39:CL:112:PHE:HZ	1.49	0.76
13:AM:6:GLY:HA3	13:AM:66:GLU:HG3	1.68	0.75
1:AA:664:G:H22	1:AA:741:G:H1	1.34	0.74
10:AJ:7:ARG:HB3	10:AJ:101:SER:HB2	1.69	0.74
4:AD:107:PHE:HB3	4:AD:145:ILE:HD11	1.70	0.74
4:BD:107:PHE:HB3	4:BD:145:ILE:HD11	1.70	0.74
13:BM:83:LEU:HD21	19:BS:65:GLU:HB2	1.70	0.74
31:CA:528:A:C2	31:CA:2043:C:H4'	2.23	0.73
3:BC:123:GLN:HB3	3:BC:128:VAL:HG21	1.69	0.73
1:AA:842:U:H4'	1:AA:843:U:OP1	1.88	0.73
25:D4:54:ASP:HB3	40:DM:57:LEU:HD22	1.70	0.73
1:BA:522:C:H5	12:BL:50:ARG:HH12	1.37	0.73
13:BM:6:GLY:HA3	13:BM:66:GLU:HG3	1.69	0.73
1:BA:1060:U:C5	3:BC:2:GLY:HA3	2.23	0.73
55:DA:2127:G:H4'	55:DA:2128:G:OP1	1.90	0.72
1:AA:1492:A:H5"	12:AL:44:LYS:HG2	1.72	0.71
24:C3:30:VAL:HG13	31:CA:466:A:H5"	1.72	0.71
39:DL:38:ILE:HD11	39:DL:112:PHE:HZ	1.53	0.71
1:AA:73:C:HO2'	1:AA:74:A:H8	1.38	0.70
1:BA:202:G:HO2'	1:BA:468:A:H8	1.39	0.70
47:CT:86:MET:HB2	47:CT:96:ILE:HD11	1.74	0.70
31:CA:1936:A:H2	31:CA:1943:U:N3	1.83	0.70
55:DA:1913:A:H4'	55:DA:1913:A:OP1	1.90	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
55:DA:2255:G:H21	69:DA:3219:TRS:H12	1.56	0.70
31:CA:846:U:H1'	31:CA:847:U:H5	1.56	0.70
55:DA:2628:C:H5'	59:DA:3195:PUT:H12	1.73	0.69
31:CA:1478:G:H1	31:CA:1513:U:H3	1.39	0.69
54:DI:64:VAL:HG22	54:DI:69:PHE:HB2	1.75	0.69
39:DL:30:ARG:HD2	55:DA:2674:G:H4'	1.74	0.69
24:C3:19:ARG:HG3	31:CA:126:A:O5'	1.94	0.68
55:DA:1478:G:H1	55:DA:1513:U:H3	1.38	0.68
2:BB:23:TRP:HB3	2:BB:39:HIS:HE1	1.56	0.68
34:CF:36:LEU:HD21	34:CF:91:LEU:HD11	1.76	0.68
59:DA:3195:PUT:H11	70:DA:5703:HOH:O	1.94	0.68
4:BD:201:VAL:HG11	5:BE:103:THR:HB	1.76	0.67
11:BK:88:GLY:N	11:BK:114:THR:HG22	2.09	0.67
22:D1:55:ILE:HD12	42:DO:33:ILE:HD11	1.76	0.67
52:CY:4:VAL:HG22	52:CY:11:ARG:HG3	1.75	0.67
49:DV:52:LEU:HB3	49:DV:54:GLN:HB2	1.76	0.67
31:CA:45:G:H5"	31:CA:46:G:H5'	1.76	0.67
31:CA:1250:G:H5"	45:CR:6:ARG:HD3	1.77	0.67
43:DP:39:VAL:HB	43:DP:49:VAL:HG23	1.76	0.67
1:BA:73:C:HO2'	1:BA:74:A:H8	1.42	0.66
27:C0:12:SER:HB3	31:CA:988:A:P	2.35	0.66
1:BA:502:A:OP1	12:BL:115:SER:HB2	1.95	0.66
1:BA:451:A:H2'	70:BA:1701:HOH:O	1.94	0.66
1:AA:202:G:HO2'	1:AA:468:A:H8	1.44	0.66
40:CM:79:LEU:HD11	40:CM:112:LEU:HD12	1.77	0.66
43:DP:31:THR:HG21	28:DB:28:C:OP1	1.97	0.65
55:DA:45:G:H5"	55:DA:46:G:H5'	1.77	0.65
35:CG:80:THR:HG23	35:CG:81:GLU:H	1.60	0.65
30:CD:133:THR:HG22	31:CA:1993:U:H4'	1.78	0.65
26:C5:3:VAL:HG11	31:CA:2539:C:C5'	2.19	0.64
31:CA:974:G:H8	31:CA:990:A:H62	1.46	0.64
1:AA:502:A:OP1	12:AL:115:SER:HB2	1.97	0.64
12:BL:110:ARG:HB2	12:BL:119:VAL:HG21	1.78	0.64
1:AA:412:A:H3'	1:AA:413:G:H5'	1.79	0.64
1:BA:841:C:H3'	1:BA:842:U:C5'	2.27	0.64
31:CA:372:G:H5"	52:CY:61:LYS:HD3	1.78	0.64
34:DF:61:SER:HB2	34:DF:91:LEU:HD21	1.79	0.64
12:BL:43:LYS:HD2	12:BL:91:PRO:HG3	1.79	0.64
24:C3:12:ARG:HD2	24:C3:44:VAL:HG11	1.80	0.64
31:CA:2394:C:H5"	40:CM:63:LYS:HE2	1.80	0.64
22:C1:43:ILE:HG22	22:C1:49:TYR:HB2	1.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:CF:61:SER:HB2	34:CF:91:LEU:HD21	1.80	0.63
29:CC:29:PRO:HG2	29:CC:34:LEU:HD11	1.80	0.63
31:CA:17:G:H4'	45:CR:25:TYR:HE2	1.62	0.63
31:CA:1105:U:H2'	31:CA:1106:G:C8	2.33	0.63
17:BQ:14:SER:HB3	17:BQ:22:VAL:HG12	1.80	0.63
24:D3:7:PRO:HB2	55:DA:1309:G:H4'	1.80	0.63
39:CL:76:VAL:HG12	44:CQ:73:VAL:HB	1.81	0.63
40:DM:77:ILE:HD11	40:DM:101:ILE:CG2	2.29	0.63
55:DA:31:C:O3'	55:DA:1238:G:H5"	1.98	0.63
55:DA:1105:U:H2'	55:DA:1106:G:C8	2.34	0.63
22:C1:15:MET:HB3	31:CA:2045:C:O3'	1.98	0.63
47:CT:82:MET:HB2	47:CT:98:LYS:HB2	1.79	0.63
55:DA:2256:G:H21	57:DA:3193:PG4:H31	1.63	0.63
20:BT:9:LYS:O	20:BT:12:ILE:HG13	1.98	0.62
24:C3:30:VAL:CG1	31:CA:466:A:H5"	2.29	0.62
45:DR:20:GLN:HG2	57:DR:202:PG4:H51	1.81	0.62
55:DA:1482:G:H1'	55:DA:1509:A:H61	1.65	0.62
26:C5:3:VAL:CG1	31:CA:2539:C:H5'	2.20	0.62
31:CA:2728:U:HO2'	31:CA:2729:G:H8	1.47	0.62
29:DC:29:PRO:HG2	29:DC:34:LEU:HD11	1.82	0.62
17:AQ:17:MET:HG2	17:AQ:20:SER:HB2	1.82	0.62
22:C1:8:PRO:HG2	31:CA:1264:A:H5'	1.80	0.62
5:BE:72:ILE:HG12	5:BE:145:GLU:HG3	1.80	0.62
31:CA:328:U:O3'	49:CV:66:GLN:HG3	2.00	0.62
6:BF:38:ARG:HB3	6:BF:63:ASN:HB2	1.80	0.62
1:BA:209:U:H4'	1:BA:210:C:OP2	2.00	0.61
55:DA:788:A:H3'	59:DA:3221:PUT:H41	1.82	0.61
5:AE:77:ASN:HB2	5:AE:82:GLN:HE22	1.62	0.61
6:AF:38:ARG:HB3	6:AF:63:ASN:HB2	1.82	0.61
16:BP:20:VAL:HG13	16:BP:32:PHE:HB2	1.82	0.61
55:DA:1847:A:HO2'	55:DA:1848:A:H8	1.48	0.61
19:BS:6:LYS:HD2	19:BS:7:LYS:H	1.65	0.61
22:D1:43:ILE:HG22	22:D1:49:TYR:HB2	1.83	0.61
64:DD:301:PGE:H12	55:DA:2623:G:OP1	2.01	0.61
2:BB:41:ILE:HD13	2:BB:202:GLY:HA2	1.83	0.61
36:CH:15:LEU:HD22	36:CH:15:LEU:H	1.66	0.61
31:CA:674:G:H1'	33:CE:69:ARG:HD2	1.83	0.61
45:DR:20:GLN:HG2	57:DR:202:PG4:H42	1.81	0.60
12:AL:110:ARG:HB2	12:AL:119:VAL:HG21	1.81	0.60
25:C4:13:ARG:NH1	31:CA:250:G:OP2	2.33	0.60
34:CF:31:VAL:CG1	34:CF:97:TRP:CH2	2.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:DE:48:THR:HG23	33:DE:88:ARG:NH1	2.16	0.60
47:DT:82:MET:HB2	47:DT:98:LYS:HB2	1.82	0.60
29:CC:17:VAL:HB	29:CC:204:VAL:HG13	1.83	0.60
48:DU:80:TRP:HB3	64:DU:101:PGE:H32	1.83	0.60
1:AA:1151:A:HO2'	1:AA:1152:A:H8	1.49	0.60
13:AM:33:ILE:HD11	13:AM:63:PHE:HE1	1.66	0.60
22:C1:25:VAL:HG13	22:C1:26:THR:H	1.67	0.60
1:BA:1323:G:H2'	1:BA:1324:A:C8	2.36	0.60
31:CA:1482:G:H1'	31:CA:1509:A:H61	1.66	0.60
47:CT:59:GLU:HA	47:CT:64:ALA:HA	1.82	0.60
1:BA:843:U:H5"	1:BA:843:U:H6	1.67	0.59
31:CA:528:A:H8	31:CA:528:A:H3'	1.67	0.59
6:AF:16:GLU:HB3	4:BD:189:SER:HA	1.83	0.59
1:BA:9:G:H4'	5:BE:109:GLY:H	1.66	0.59
1:BA:978:A:HO2'	1:BA:1322:C:H5	1.51	0.59
31:CA:1779:U:C5	31:CA:1784:A:N7	2.64	0.59
1:AA:1238:A:H5'	1:AA:1336:C:H41	1.68	0.59
2:AB:41:ILE:HD13	2:AB:202:GLY:HA2	1.83	0.59
1:BA:1141:C:HO2'	1:BA:1142:G:H8	1.51	0.59
5:BE:104:GLY:HA3	5:BE:122:ASN:HA	1.83	0.59
1:AA:1323:G:H2'	1:AA:1324:A:C8	2.38	0.59
31:CA:528:A:H3'	31:CA:528:A:C8	2.38	0.59
22:C1:15:MET:SD	31:CA:2045:C:H5"	2.43	0.59
45:DR:19:LYS:HB3	57:DR:202:PG4:H41	1.85	0.59
1:AA:202:G:H21	1:AA:466:A:H61	1.51	0.59
1:AA:451:A:H61	1:AA:481:G:H5'	1.67	0.59
26:C5:16:ILE:HD13	26:C5:25:VAL:HG22	1.85	0.59
33:DE:33:VAL:HG22	58:DA:3192:MPD:H12	1.84	0.59
31:CA:1847:A:HO2'	31:CA:1848:A:H8	1.48	0.58
31:CA:2728:U:O2'	31:CA:2729:G:H5"	2.04	0.58
13:BM:22:ILE:HB	13:BM:25:VAL:HG12	1.86	0.58
11:AK:34:ILE:HG12	11:AK:70:CYS:SG	2.43	0.58
1:BA:841:C:H3'	1:BA:842:U:H5"	1.86	0.58
55:DA:2128:G:H1	55:DA:2160:C:H42	1.52	0.58
1:BA:946:A:H2'	1:BA:947:G:C8	2.38	0.58
5:BE:133:PRO:O	5:BE:137:VAL:HG12	2.02	0.58
42:CO:49:GLU:OE2	42:CO:95:THR:HG22	2.04	0.58
45:DR:31:VAL:HG13	55:DA:580:U:O3'	2.03	0.58
55:DA:12:U:H2'	55:DA:12:U:O2	2.04	0.58
1:AA:946:A:H2'	1:AA:947:G:C8	2.39	0.58
32:DD:114:LYS:HE2	55:DA:2681:C:OP2	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:CH:41:LYS:HA	36:CH:44:ILE:HG12	1.86	0.58
55:DA:1105:U:H2'	55:DA:1106:G:H8	1.68	0.58
23:C2:35:GLU:HG2	23:C2:50:LYS:HG2	1.86	0.57
19:AS:50:ALA:HB1	19:AS:57:HIS:HB3	1.86	0.57
29:CC:120:VAL:HG12	29:CC:134:ASN:ND2	2.19	0.57
1:BA:209:U:H2'	1:BA:209:U:O2	2.03	0.57
26:D5:16:ILE:HD13	26:D5:25:VAL:HG22	1.86	0.57
18:AR:36:SER:HA	18:AR:72:ASP:HB3	1.87	0.57
7:BG:113:ASP:HB2	7:BG:119:ARG:HG3	1.86	0.57
24:D3:4:THR:HG22	55:DA:687:C:H1'	1.87	0.57
33:DE:189:THR:HG22	33:DE:192:ALA:H	1.69	0.57
31:CA:550:C:H2'	31:CA:551:G:H5"	1.86	0.57
31:CA:1105:U:H2'	31:CA:1106:G:H8	1.68	0.57
1:AA:1492:A:C5'	12:AL:44:LYS:HG2	2.34	0.57
31:CA:310:A:H5"	49:CV:15:THR:HG23	1.86	0.57
31:CA:1703:G:H2'	31:CA:1704:C:C6	2.40	0.57
36:CH:27:ARG:HH11	52:CY:60:ASP:HA	1.70	0.57
1:AA:769:G:H4'	1:AA:1513:A:H4'	1.87	0.57
1:BA:1238:A:H5'	1:BA:1336:C:H41	1.68	0.57
34:CF:36:LEU:HD21	34:CF:91:LEU:CD1	2.34	0.57
40:CM:82:LEU:HD11	40:CM:116:VAL:CG2	2.32	0.57
48:CU:24:MET:HG2	48:CU:29:THR:O	2.05	0.57
40:CM:28:GLY:O	40:CM:29:LYS:O	2.21	0.57
7:AG:113:ASP:HB2	7:AG:119:ARG:HG3	1.86	0.57
47:CT:66:ILE:HA	47:CT:69:LEU:HD22	1.87	0.57
35:DG:42:GLU:HG2	35:DG:55:ARG:HH21	1.68	0.57
36:DH:41:LYS:HA	36:DH:44:ILE:HG12	1.86	0.57
1:AA:81:A:H61	1:AA:86:G:H1	1.53	0.57
1:AA:1141:C:HO2'	1:AA:1142:G:H8	1.52	0.57
29:DC:120:VAL:HG12	29:DC:134:ASN:ND2	2.20	0.57
3:AC:77:ILE:HA	3:AC:84:VAL:HG23	1.87	0.56
7:AG:22:LEU:HD12	7:AG:62:PHE:HE2	1.69	0.56
22:C1:5:GLN:HG3	31:CA:2054:A:C2	2.39	0.56
1:BA:451:A:H61	1:BA:481:G:H5'	1.69	0.56
33:CE:189:THR:HG22	33:CE:192:ALA:H	1.70	0.56
5:BE:77:ASN:HB2	5:BE:82:GLN:HE22	1.68	0.56
31:CA:2095:A:H8	31:CA:2095:A:H5"	1.69	0.56
40:DM:77:ILE:HD11	40:DM:101:ILE:HG21	1.87	0.56
55:DA:62:U:O4'	58:DA:3203:MPD:H31	2.05	0.56
1:AA:8:A:C6	4:AD:206:LYS:HB3	2.40	0.56
1:BA:1012:A:H61	1:BA:1017:U:H3	1.54	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:DD:146:ILE:HD12	32:DD:155:VAL:HG21	1.88	0.56
44:DQ:96:LYS:HE3	70:DQ:306:HOH:O	2.04	0.56
55:DA:550:C:H2'	55:DA:551:G:H5"	1.87	0.56
1:AA:1277:C:HO2'	1:AA:1279:G:H8	1.53	0.56
3:AC:77:ILE:HA	3:AC:84:VAL:CG2	2.36	0.56
31:CA:2304:G:H5'	34:CF:121:SER:HB2	1.87	0.56
11:AK:67:ALA:HB2	11:AK:96:THR:HG23	1.88	0.56
23:D2:35:GLU:HG2	23:D2:50:LYS:HG2	1.86	0.56
22:C1:17:ARG:NH2	31:CA:1266:G:OP2	2.39	0.55
3:BC:77:ILE:HA	3:BC:84:VAL:CG2	2.36	0.55
31:CA:2019:A:H4'	45:CR:34:VAL:HG21	1.87	0.55
41:DN:18[B]:ARG:HG3	28:DB:90:C:H5'	1.89	0.55
1:AA:1012:A:H61	1:AA:1017:U:H3	1.55	0.55
10:AJ:5:ARG:HE	10:AJ:77:VAL:HG22	1.70	0.55
1:BA:1106:G:H5"	3:BC:172:ARG:HG3	1.87	0.55
13:BM:86:TYR:CZ	13:BM:90:ARG:HD2	2.41	0.55
31:CA:457:A:N1	31:CA:470:A:H5"	2.21	0.55
1:BA:619:U:H3	4:BD:131:ASN:HB3	1.71	0.55
19:BS:50:ALA:HB1	19:BS:57:HIS:HB3	1.89	0.55
24:C3:9:VAL:N	31:CA:1309:G:OP1	2.33	0.55
22:D1:8:PRO:HG2	55:DA:1264:A:H5'	1.88	0.55
35:DG:175:LYS:HG3	55:DA:2529:G:H4'	1.88	0.55
55:DA:31:C:O2'	55:DA:1238:G:H5'	2.06	0.55
8:AH:29:SER:HB3	8:AH:57:PRO:HB2	1.88	0.55
5:BE:72:ILE:HG13	5:BE:73:ASN:H	1.72	0.55
1:AA:412:A:H3'	1:AA:413:G:C5'	2.37	0.55
10:AJ:35:GLN:HB2	10:AJ:77:VAL:HB	1.88	0.55
1:BA:1151:A:HO2'	1:BA:1152:A:H8	1.53	0.55
3:BC:77:ILE:HA	3:BC:84:VAL:HG23	1.88	0.55
26:C5:1:MET:HB2	31:CA:2526:G:O2'	2.06	0.55
26:C5:36:ARG:HD3	31:CA:2742:G:OP1	2.07	0.55
4:BD:85:ASN:HB3	4:BD:88:GLU:HB2	1.89	0.55
48:CU:22:THR:HA	48:CU:25:GLU:HG2	1.87	0.55
3:AC:155:GLY:HA2	3:AC:163:ALA:HB1	1.89	0.55
31:CA:2822:G:H2'	31:CA:2823:A:H5"	1.88	0.55
55:DA:2297:A:C8	55:DA:2297:A:H5"	2.42	0.55
25:D4:64:TYR:CE2	55:DA:242:G:H5"	2.42	0.55
13:AM:86:TYR:CZ	13:AM:90:ARG:HD2	2.41	0.54
11:BK:67:ALA:HB2	11:BK:96:THR:HG23	1.88	0.54
11:BK:89:PRO:HG3	21:BU:32:VAL:HG11	1.88	0.54
25:D4:8:ARG:HD3	55:DA:245:G:O6	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:CA:2845:U:H5”	44:CQ:52:ASN:O	2.07	0.54
64:D1:102:PGE:H42	47:DT:23:LEU:HD23	1.89	0.54
16:AP:4:ILE:HG12	16:AP:21:VAL:HG22	1.89	0.54
31:CA:2502:G:H5”	31:CA:2503:2MA:H5”	1.90	0.54
1:BA:108:G:H5”	1:BA:108:G:N3	2.23	0.54
44:DQ:106:LYS:HA	44:DQ:109:ARG:HD3	1.90	0.54
65:DA:3223:SPD:H92	65:DA:3223:SPD:H52	1.90	0.54
11:AK:31:ILE:HG12	11:AK:46:THR:HG22	1.88	0.54
16:BP:4:ILE:HG12	16:BP:21:VAL:HG22	1.90	0.54
45:CR:87:SER:HB3	46:CS:52:PRO:HD3	1.90	0.54
5:AE:76:LEU:HD11	5:AE:120:VAL:HG22	1.90	0.54
26:C5:17:VAL:CG1	26:C5:26:ILE:HD12	2.38	0.54
39:DL:76:VAL:CG2	55:DA:2684:U:H4’	2.37	0.54
1:AA:404:G:N7	4:AD:2:ALA:HB3	2.23	0.54
5:BE:72:ILE:HG13	5:BE:73:ASN:N	2.22	0.54
23:D2:8:LYS:HE3	55:DA:2420:C:H5”	1.89	0.54
13:AM:33:ILE:HD11	13:AM:63:PHE:CE1	2.42	0.54
22:C1:4:GLN:HB3	31:CA:2615:U:H1’	1.90	0.54
10:BJ:5:ARG:HG2	10:BJ:79:PRO:HG3	1.90	0.54
11:BK:52:PHE:HE2	11:BK:65:VAL:HG21	1.73	0.54
1:AA:108:G:N3	1:AA:108:G:H5”	2.22	0.54
5:BE:35:ALA:O	5:BE:50:TYR:O	2.26	0.54
31:CA:1394:U:H4’	31:CA:1603:A:H4’	1.90	0.54
48:DU:67:VAL:HG22	48:DU:76:ARG:HG3	1.90	0.54
1:BA:374:A:OP1	1:BA:452:A:N1	2.41	0.53
1:BA:769:G:H4’	1:BA:1513:A:H4’	1.88	0.53
5:BE:126:LYS:HG2	5:BE:128:TYR:CZ	2.44	0.53
33:CE:149:ILE:HD12	33:CE:172:ALA:HA	1.89	0.53
44:CQ:106:LYS:HA	44:CQ:109:ARG:HD3	1.90	0.53
1:AA:1144:G:H21	1:AA:1146:A:H62	1.56	0.53
4:AD:85:ASN:HB3	4:AD:88:GLU:HB2	1.90	0.53
34:CF:31:VAL:HG11	34:CF:97:TRP:CH2	2.43	0.53
1:AA:209:U:H4’	1:AA:210:C:OP2	2.08	0.53
31:CA:1251:C:OP2	45:CR:6:ARG:HD2	2.09	0.53
1:BA:1144:G:H21	1:BA:1146:A:H62	1.56	0.53
6:BF:45:ARG:O	6:BF:56:LYS:HA	2.08	0.53
12:BL:33:VAL:HG22	12:BL:79:VAL:HG22	1.90	0.53
36:CH:4:ILE:HD11	36:CH:44:ILE:HG22	1.90	0.53
3:BC:5:VAL:HG21	3:BC:10:ILE:HD13	1.91	0.53
2:BB:129:LEU:HD13	2:BB:134:ALA:HB2	1.91	0.53
8:BH:29:SER:HB3	8:BH:57:PRO:HB2	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:AK:52:PHE:HE2	11:AK:65:VAL:HG21	1.73	0.53
54:DI:69:PHE:HB3	54:DI:72:LEU:HD12	1.91	0.53
55:DA:2796:U:H3	55:DA:2799:A:N6	1.97	0.53
1:AA:735:C:H5'	18:AR:60:LYS:HD3	1.91	0.53
10:AJ:42:LEU:HB2	10:AJ:71:LEU:HB3	1.91	0.53
11:AK:89:PRO:HG3	21:AU:32:VAL:HG11	1.90	0.53
6:BF:38:ARG:HH12	6:BF:99:ALA:HB3	1.74	0.53
44:DQ:52:ASN:O	55:DA:2845:U:H5"	2.09	0.53
2:AB:129:LEU:HD13	2:AB:134:ALA:HB2	1.91	0.53
19:AS:29:LYS:HB3	19:AS:30:PRO:HD2	1.91	0.53
10:BJ:26:VAL:HG21	10:BJ:39:PRO:HD3	1.91	0.53
31:CA:1936:A:C2	31:CA:1943:U:N3	2.59	0.53
25:C4:2:PRO:HD2	31:CA:667:U:O2	2.09	0.52
25:C4:47:LYS:NZ	40:CM:64:PHE:CE1	2.77	0.52
3:AC:5:VAL:HG21	3:AC:10:ILE:HD13	1.92	0.52
31:CA:1847:A:O2'	31:CA:1848:A:H8	1.92	0.52
6:AF:45:ARG:O	6:AF:56:LYS:HA	2.08	0.52
3:BC:155:GLY:HA2	3:BC:163:ALA:HB1	1.91	0.52
22:C1:38:HIS:CE1	31:CA:2884:U:O4	2.54	0.52
6:BF:3:HIS:H	6:BF:92:THR:HG23	1.73	0.52
31:CA:2037:A:H2'	31:CA:2038:G:C8	2.44	0.52
31:CA:2796:U:H3	31:CA:2799:A:N6	1.99	0.52
32:DD:128:ARG:HG3	70:DA:7412:HOH:O	2.09	0.52
8:AH:2:SER:HB2	8:AH:4:GLN:HE21	1.75	0.52
13:AM:71:ARG:HH21	34:DF:143:TYR:HB2	1.74	0.52
26:C5:3:VAL:HG12	31:CA:2538:C:O2'	2.10	0.52
31:CA:118:A:N3	31:CA:178:G:H1'	2.25	0.52
43:CP:100:HIS:CD2	43:CP:101:GLY:H	2.28	0.52
35:DG:86:LYS:HG2	35:DG:132:VAL:HG22	1.91	0.52
23:C2:11:LEU:HD21	23:C2:34:LEU:HD23	1.91	0.52
24:C3:33:ARG:NE	31:CA:467:G:OP1	2.36	0.52
31:CA:668:A:H2'	31:CA:670:A:H62	1.75	0.52
31:CA:2297:A:C8	31:CA:2297:A:H5"	2.45	0.52
48:DU:54:GLU:HB3	48:DU:88:LYS:HD2	1.92	0.52
55:DA:74:A:H5"	55:DA:74:A:N3	2.25	0.52
65:DA:3223:SPD:H92	65:DA:3223:SPD:C5	2.40	0.52
1:AA:86:G:H21	1:AA:87:C:H41	1.58	0.52
1:BA:404:G:N7	4:BD:2:ALA:HB3	2.24	0.52
22:C1:41:HIS:HE2	31:CA:2884:U:P	2.32	0.52
6:BF:38:ARG:NH1	6:BF:99:ALA:HB3	2.24	0.52
35:CG:86:LYS:HG2	35:CG:132:VAL:HG22	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:845:A:O4'	1:AA:845:A:P	2.68	0.52
1:AA:1277:C:O2'	1:AA:1279:G:H8	1.93	0.52
22:C1:19:HIS:CE1	31:CA:2624:G:H1'	2.45	0.52
10:BJ:57:VAL:HG22	10:BJ:58:ASN:H	1.75	0.52
33:CE:21:ARG:HD3	33:CE:106:LYS:HB3	1.92	0.52
40:DM:79:LEU:HD11	40:DM:112:LEU:HD12	1.92	0.52
41:DN:81[B]:4D4:H9	55:DA:2496:C:OP2	2.10	0.52
1:AA:1218:C:H2'	1:AA:1219:A:C8	2.45	0.51
10:AJ:26:VAL:HG21	10:AJ:39:PRO:HD3	1.91	0.51
10:AJ:57:VAL:HG22	10:AJ:58:ASN:H	1.76	0.51
11:AK:23:ILE:HD11	11:AK:86:VAL:HG13	1.92	0.51
1:BA:1518:MA6:H103	1:BA:1519:MA6:H102	1.92	0.51
19:BS:29:LYS:HB3	19:BS:30:PRO:HD2	1.93	0.51
31:CA:699:A:H2'	31:CA:700:G:O4'	2.10	0.51
33:DE:21:ARG:HD3	33:DE:106:LYS:HB3	1.91	0.51
29:CC:13:ARG:HD3	31:CA:728:G:H4'	1.92	0.51
43:CP:51:ALA:HB3	43:CP:78:VAL:HG13	1.92	0.51
1:BA:350:G:H5"	20:BT:3:ASN:HD22	1.76	0.51
1:BA:374:A:H5"	1:BA:452:A:N1	2.25	0.51
4:BD:48:LEU:HD21	4:BD:56:ARG:HG3	1.93	0.51
31:CA:17:G:H4'	45:CR:25:TYR:CE2	2.43	0.51
32:DD:25:THR:HG21	32:DD:193:VAL:HG22	1.92	0.51
48:CU:54:GLU:HB3	48:CU:88:LYS:HD2	1.92	0.51
54:DI:44:ALA:HB1	54:DI:95:LEU:HD11	1.91	0.51
11:BK:23:ILE:HD11	11:BK:86:VAL:HG13	1.91	0.51
25:D4:8:ARG:CD	55:DA:245:G:O6	2.59	0.51
31:CA:569:U:H5"	31:CA:821:A:C2	2.46	0.51
55:DA:1853:A:N1	55:DA:2087:G:H1'	2.25	0.51
7:BG:111:ARG:HB3	7:BG:119:ARG:HG2	1.93	0.51
31:CA:532:A:N1	31:CA:2020:A:H1'	2.25	0.51
31:CA:1447:C:H2'	31:CA:1448:G:C8	2.46	0.51
1:AA:1518:MA6:H103	1:AA:1519:MA6:H102	1.92	0.51
1:BA:1218:C:H2'	1:BA:1219:A:C8	2.46	0.51
1:BA:1277:C:O2'	1:BA:1279:G:H8	1.93	0.51
22:D1:22:LEU:HD23	62:D1:103:PEG:H31	1.91	0.51
30:CD:25:THR:HG21	30:CD:193:VAL:HG22	1.93	0.51
31:CA:12:U:H2'	31:CA:12:U:O2	2.11	0.51
47:CT:69:LEU:HG	47:CT:107:VAL:HG22	1.92	0.51
39:DL:38:ILE:HD11	39:DL:112:PHE:CZ	2.42	0.51
11:AK:23:ILE:HG22	11:AK:32:VAL:HG13	1.92	0.51
25:D4:31:HIS:HB2	70:D4:103:HOH:O	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:CD:4:LEU:HD22	30:CD:101:PHE:CE2	2.45	0.51
43:DP:51:ALA:HB3	43:DP:78:VAL:HG13	1.93	0.51
5:AE:126:LYS:HG2	5:AE:128:TYR:CZ	2.46	0.51
31:CA:998:C:OP2	45:CR:58:ARG:NH2	2.44	0.51
31:CA:2025:C:H2'	31:CA:2026:U:C6	2.46	0.51
31:CA:2189:U:H2'	31:CA:2190:G:H8	1.76	0.51
25:D4:60:ALA:O	40:DM:48:ARG:HD2	2.10	0.51
30:CD:129:THR:HG23	30:CD:140:HIS:O	2.11	0.51
55:DA:1847:A:O2'	55:DA:1848:A:H8	1.93	0.51
47:CT:73:LYS:HB2	47:CT:106:VAL:HB	1.92	0.50
36:DH:4:ILE:HD11	36:DH:44:ILE:HG22	1.93	0.50
12:AL:33:VAL:HG22	12:AL:79:VAL:HG22	1.92	0.50
31:CA:784:G:H5'	31:CA:785:G:OP1	2.10	0.50
38:CK:81:ILE:HG23	38:CK:82:GLY:H	1.76	0.50
1:AA:774:G:H21	57:AA:1670:PG4:H51	1.75	0.50
5:BE:106:ILE:HD11	5:BE:124:LEU:HD23	1.93	0.50
11:BK:23:ILE:HG22	11:BK:32:VAL:HG13	1.93	0.50
20:BT:4:ILE:HA	20:BT:8:LYS:HE2	1.93	0.50
31:CA:335:C:H5"	49:CV:82:ARG:HD3	1.93	0.50
34:DF:131:GLY:HA3	55:DA:2305:U:H5"	1.94	0.50
55:DA:1026:G:H2'	55:DA:1027:A:C8	2.45	0.50
24:C3:19:ARG:NH2	31:CA:125:A:OP2	2.41	0.50
48:CU:18:GLU:H	48:CU:18:GLU:CD	2.15	0.50
35:DG:19:ILE:HG12	35:DG:24:ILE:HG12	1.93	0.50
9:BI:19:VAL:HG22	9:BI:65:ILE:HG22	1.92	0.50
1:AA:1358:U:H3	1:AA:1363:A:H62	1.59	0.50
19:AS:15:LEU:HD13	19:AS:33:THR:HG21	1.93	0.50
54:DI:57:ASN:HB3	54:DI:76:PHE:HB3	1.93	0.50
1:BA:1003:G:H21	1:BA:1005:A:H5'	1.77	0.50
17:BQ:17:MET:HB3	17:BQ:20:SER:HB3	1.93	0.50
23:D2:25:LYS:HE2	23:D2:30:LYS:O	2.12	0.50
43:DP:31:THR:HG21	28:DB:28:C:P	2.51	0.50
3:AC:20:SER:HB3	14:AN:94:PRO:HG3	1.92	0.50
18:AR:45:THR:OG1	18:AR:47:THR:HG22	2.12	0.50
8:BH:2:SER:HB2	8:BH:4:GLN:HE21	1.76	0.50
31:CA:1638:C:H5"	31:CA:2710:C:O2'	2.12	0.50
55:DA:1536:C:H4'	55:DA:1537:G:H5"	1.93	0.50
7:AG:111:ARG:HB3	7:AG:119:ARG:HG2	1.93	0.50
11:BK:43:GLY:HA3	11:BK:74:VAL:HG12	1.93	0.50
31:CA:70:G:H5"	31:CA:112:U:O2	2.12	0.50
55:DA:914:G:H5"	55:DA:914:G:H8	1.77	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:AI:19:VAL:HG22	9:AI:65:ILE:HG22	1.93	0.49
1:BA:374:A:H5"	1:BA:452:A:C2	2.47	0.49
1:BA:735:C:H5'	18:BR:60:LYS:HD3	1.93	0.49
9:BI:57:MET:HG3	9:BI:61:LEU:HG	1.93	0.49
30:CD:99:GLU:HG2	30:CD:182:ALA:HB2	1.94	0.49
31:CA:532:A:N3	31:CA:532:A:H2'	2.26	0.49
43:DP:68:LYS:HB3	62:DP:201:PEG:H22	1.93	0.49
7:AG:69:VAL:HG23	7:AG:100:ALA:HB1	1.94	0.49
24:C3:24:THR:HG23	24:C3:27:GLY:H	1.77	0.49
34:CF:44:ILE:HG21	34:CF:79:ILE:HG22	1.94	0.49
55:DA:479:A:N3	55:DA:481:G:H5"	2.26	0.49
3:AC:47:LEU:HB3	3:AC:50:ALA:HB3	1.94	0.49
7:BG:69:VAL:HG23	7:BG:100:ALA:HB1	1.94	0.49
18:BR:36:SER:HA	18:BR:72:ASP:HB3	1.93	0.49
22:D1:9:THR:HG21	55:DA:2020:A:H5'	1.94	0.49
29:CC:210:ALA:HA	29:CC:213:TRP:CE2	2.47	0.49
31:CA:2185:U:H2'	31:CA:2186:G:C8	2.46	0.49
31:CA:2445:2MG:HM21	31:CA:2449:U:O4	2.11	0.49
29:DC:227:PRO:HA	29:DC:233:GLY:HA2	1.95	0.49
41:CN:21:ALA:HB1	41:CN:100:LYS:HG2	1.94	0.49
54:DI:31:ARG:HB2	54:DI:79:PRO:HG2	1.93	0.49
55:DA:1433:A:O2'	55:DA:1434:A:H5'	2.12	0.49
29:CC:227:PRO:HA	29:CC:233:GLY:HA2	1.95	0.49
35:CG:19:ILE:HG12	35:CG:24:ILE:HG12	1.93	0.49
55:DA:2441:U:O2'	65:DA:3223:SPD:H91	2.13	0.49
1:AA:411:A:P	4:AD:26:ARG:HH12	2.36	0.49
11:AK:84:VAL:HG21	11:AK:97:ILE:HG23	1.95	0.49
1:BA:202:G:H1	1:BA:215:C:H42	1.59	0.49
55:DA:789:A:OP1	59:DA:3221:PUT:H12	2.12	0.49
1:BA:76:G:H1	1:BA:93:U:H3	1.61	0.49
3:BC:113:ALA:O	3:BC:200:VAL:HG11	2.12	0.49
31:CA:1587:G:H2'	31:CA:1588:G:H8	1.78	0.49
28:CB:14:U:H2'	28:CB:15:A:H2	1.76	0.49
1:AA:202:G:O2'	1:AA:468:A:H8	1.95	0.49
1:BA:202:G:O2'	1:BA:468:A:H8	1.95	0.49
1:AA:1003:G:H21	1:AA:1005:A:H5'	1.77	0.49
1:BA:840:C:H2'	1:BA:841:C:O4'	2.13	0.49
47:CT:4:ILE:HG12	47:CT:106:VAL:HG22	1.94	0.49
5:AE:107:ALA:HB2	5:AE:125:ALA:HB3	1.94	0.48
11:AK:34:ILE:HB	11:AK:74:VAL:HG11	1.95	0.48
3:BC:20:SER:HB3	14:BN:94:PRO:HG3	1.93	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:BC:47:LEU:HB3	3:BC:50:ALA:HB3	1.95	0.48
31:CA:479:A:N3	31:CA:481:G:H5"	2.28	0.48
31:CA:1182:G:H2'	31:CA:1183:U:O4'	2.13	0.48
32:DD:99:GLU:HG2	32:DD:182:ALA:HB2	1.94	0.48
33:CE:75:SER:O	33:CE:78:TRP:HB2	2.13	0.48
39:CL:43:ILE:HD12	39:CL:56:ASP:HB2	1.94	0.48
28:DB:84:G:H21	63:DB:211:EDO:H11	1.78	0.48
55:DA:837:C:H5	70:DA:6720:HOH:O	1.95	0.48
15:AO:82:ILE:HG21	15:AO:89:ARG:OXT	2.13	0.48
31:CA:2630:G:O4'	31:CA:2894:G:H1'	2.13	0.48
32:DD:13:ARG:NH1	70:DD:401:HOH:O	2.44	0.48
4:AD:48:LEU:HD21	4:AD:56:ARG:HG3	1.94	0.48
2:BB:73:LYS:HD2	2:BB:168:HIS:HD2	1.77	0.48
3:BC:72:ARG:HB3	3:BC:75:ILE:HG22	1.94	0.48
31:CA:2060:A:N6	33:CE:69:ARG:NH2	2.60	0.48
29:CC:177:ARG:HG2	31:CA:1820:U:OP1	2.14	0.48
31:CA:914:G:H8	31:CA:914:G:H5"	1.79	0.48
31:CA:2623:G:H4'	31:CA:2825:G:H8	1.78	0.48
1:BA:975:A:H8	1:BA:1357:A:HO2'	1.61	0.48
35:CG:80:THR:HG23	35:CG:81:GLU:N	2.24	0.48
9:AI:57:MET:HG3	9:AI:61:LEU:HG	1.94	0.48
25:C4:24:HIS:CG	40:CM:61:LEU:HD13	2.49	0.48
1:BA:677:U:H3	1:BA:713:G:H22	1.61	0.48
11:BK:30:THR:HG21	11:BK:92:GLY:HA3	1.96	0.48
28:CB:14:U:H2'	28:CB:15:A:C2	2.49	0.48
31:CA:634:C:H2'	31:CA:635:C:C6	2.49	0.48
43:DP:31:THR:HG22	43:DP:33:ARG:H	1.79	0.48
54:DI:50:VAL:HG13	54:DI:85:VAL:HG22	1.95	0.48
1:AA:413:G:H5"	1:AA:414:A:H5'	1.96	0.48
24:C3:37:LYS:O	31:CA:458:G:H2'	2.13	0.48
25:D4:64:TYR:CZ	55:DA:242:G:H5"	2.49	0.48
1:AA:975:A:H8	1:AA:1357:A:HO2'	1.59	0.48
2:AB:20:THR:HG22	2:AB:39:HIS:CE1	2.48	0.48
11:AK:30:THR:HG21	11:AK:92:GLY:HA3	1.95	0.48
25:C4:54:ASP:HB3	40:CM:57:LEU:HD22	1.95	0.48
31:CA:247:G:H4'	31:CA:386:G:C5	2.49	0.48
39:CL:38:ILE:HD11	39:CL:112:PHE:CZ	2.38	0.48
47:DT:4:ILE:HG12	47:DT:106:VAL:HG22	1.94	0.48
47:DT:72:THR:HG21	47:DT:108:SER:HB3	1.95	0.48
5:AE:38:VAL:HG11	5:AE:114:VAL:HG22	1.96	0.48
23:D2:11:LEU:HD21	23:D2:34:LEU:HD23	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:DM:21:ARG:HA	55:DA:811:U:H2'	1.95	0.48
41:DN:41:LEU:HG	41:DN:96:ILE:HG13	1.96	0.48
7:AG:22:LEU:HD12	7:AG:62:PHE:CE2	2.48	0.48
5:BE:36:LEU:HD21	5:BE:137:VAL:HG11	1.95	0.48
22:D1:55:ILE:HD12	42:DO:33:ILE:CD1	2.44	0.48
32:DD:150[B]:MEQ:HE2	55:DA:2033:A:O5'	2.14	0.48
34:DF:44:ILE:HG21	34:DF:79:ILE:HG22	1.95	0.48
47:DT:73:LYS:HB2	47:DT:106:VAL:HB	1.95	0.48
51:DX:41[A]:ARG:HG3	55:DA:2386:A:N3	2.28	0.48
55:DA:11:C:H2'	55:DA:12:U:H5'	1.95	0.48
1:AA:542:G:H5'	4:AD:39:GLY:HA3	1.96	0.47
24:C3:16:HIS:CD2	31:CA:464:U:HO2'	2.32	0.47
22:D1:25:VAL:HG11	47:DT:38:TYR:HB2	1.96	0.47
34:CF:36:LEU:HB2	34:CF:57:LEU:HD21	1.96	0.47
45:DR:6:ARG:HD3	55:DA:1250:G:H5"	1.95	0.47
55:DA:1172:C:C5	55:DA:1173:U:H1'	2.49	0.47
55:DA:1587:G:H2'	55:DA:1588:G:H8	1.79	0.47
5:AE:133:PRO:O	5:AE:137:VAL:HG13	2.14	0.47
23:C2:25:LYS:HE2	23:C2:30:LYS:O	2.14	0.47
1:BA:542:G:H5'	4:BD:39:GLY:HA3	1.96	0.47
17:BQ:76:VAL:HG12	17:BQ:77:ARG:HG3	1.97	0.47
31:CA:1364:G:P	52:CY:50:ARG:HH22	2.36	0.47
37:CJ:19:ASN:H	37:CJ:20:PRO:HD2	1.80	0.47
55:DA:1975:G:H21	64:DA:3224:PGE:C2	2.27	0.47
1:AA:1055:A:H2'	3:AC:156:ARG:HD2	1.96	0.47
6:AF:38:ARG:HE	6:AF:63:ASN:ND2	2.12	0.47
1:BA:1391:U:H2'	1:BA:1392:G:C8	2.49	0.47
32:DD:8:LYS:HB2	32:DD:201:LEU:HD11	1.96	0.47
39:DL:43:ILE:HD12	39:DL:56:ASP:HB2	1.96	0.47
1:BA:1190:G:H5'	3:BC:176:HIS:NE2	2.29	0.47
32:DD:105:LYS:NZ	32:DD:106:LYS:HE3	2.30	0.47
37:DJ:103:ARG:HA	37:DJ:106:LEU:HD12	1.96	0.47
55:DA:2291:U:H2'	55:DA:2292:U:C6	2.49	0.47
11:BK:84:VAL:HG21	11:BK:97:ILE:HG23	1.97	0.47
31:CA:2185:U:H2'	31:CA:2186:G:H8	1.79	0.47
34:CF:8:TYR:HA	34:CF:12:VAL:HB	1.97	0.47
13:AM:4:ILE:HD12	13:AM:10:PRO:HG2	1.95	0.47
25:C4:25:LYS:HD3	40:CM:62:PRO:HG2	1.97	0.47
31:CA:1141:U:H4'	31:CA:1142:A:O4'	2.15	0.47
52:CY:10:LYS:HE3	52:CY:54:LYS:HG2	1.97	0.47
55:DA:789:A:OP1	59:DA:3221:PUT:C1	2.63	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:269:C:H2'	1:AA:270:A:C8	2.50	0.47
22:D1:5:GLN:O	55:DA:2017:U:H4'	2.15	0.47
30:CD:26:VAL:HG21	44:CQ:5:ILE:HG12	1.97	0.47
31:CA:2030:6MZ:C2	31:CA:2499:C:H5"	2.45	0.47
34:DF:8:TYR:HA	34:DF:12:VAL:HB	1.97	0.47
34:DF:36:LEU:HB2	34:DF:57:LEU:HD21	1.96	0.47
36:DH:49:ALA:O	36:DH:53:GLU:HB3	2.15	0.47
37:DJ:19:ASN:H	37:DJ:20:PRO:HD2	1.80	0.47
43:DP:52:SER:OG	43:DP:54:VAL:HG22	2.14	0.47
49:DV:73:PHE:CE2	49:DV:75:ALA:HA	2.49	0.47
52:DY:10:LYS:HE3	52:DY:54:LYS:HG2	1.97	0.47
55:DA:644:A:H2'	55:DA:645:C:O4'	2.14	0.47
55:DA:1975:G:H21	64:DA:3224:PGE:H2	1.79	0.47
24:C3:3:ARG:HD3	31:CA:1613:G:O2'	2.15	0.47
1:BA:269:C:H2'	1:BA:270:A:C8	2.50	0.47
1:BA:846:G:H2'	1:BA:847:G:H8	1.79	0.47
30:CD:155:VAL:HG21	31:CA:2618:G:H21	1.79	0.47
31:CA:608:A:H2'	31:CA:609:A:C8	2.50	0.47
31:CA:2060:A:N6	33:CE:69:ARG:HH21	2.13	0.47
31:CA:2291:U:H2'	31:CA:2292:U:C6	2.50	0.47
32:DD:186:LEU:HD21	44:DQ:4:ILE:HG21	1.95	0.47
49:CV:74:ASN:HD22	49:CV:77:THR:H	1.63	0.47
1:AA:677:U:H3	1:AA:713:G:H22	1.63	0.47
24:C3:7:PRO:CB	31:CA:1309:G:H4'	2.37	0.47
55:DA:1236:G:N7	59:DA:3189:PUT:H41	2.30	0.47
25:C4:25:LYS:O	40:CM:62:PRO:HD2	2.15	0.47
31:CA:193:U:H5	70:CA:3372:HOH:O	1.98	0.47
31:CA:1936:A:H62	31:CA:1963:U:H3	1.60	0.47
33:CE:1:MET:HG2	33:CE:14:VAL:HG23	1.97	0.47
38:DK:69:ARG:O	38:DK:90:GLU:HB2	2.16	0.47
55:DA:1182:G:H2'	55:DA:1183:U:O4'	2.15	0.47
1:AA:310:G:H5"	16:AP:31:ARG:HB2	1.97	0.46
5:BE:57:PRO:O	5:BE:60:ILE:HG13	2.15	0.46
33:DE:176:ASP:OD2	33:DE:178:VAL:HG12	2.15	0.46
55:DA:749:A:H4'	55:DA:1271:G:N3	2.29	0.46
1:AA:73:C:O2'	1:AA:74:A:H8	1.97	0.46
1:BA:23:C:H5	1:BA:561:U:O4	1.98	0.46
1:BA:1055:A:H2'	3:BC:156:ARG:HD2	1.97	0.46
2:BB:73:LYS:HD2	2:BB:168:HIS:CD2	2.51	0.46
42:CO:47:VAL:O	42:CO:51:LEU:HD23	2.15	0.46
43:CP:31:THR:HG22	43:CP:33:ARG:H	1.79	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:DF:121:SER:HB2	55:DA:2304:G:H5'	1.96	0.46
6:AF:47:LEU:HD13	6:AF:51:ILE:HG12	1.97	0.46
31:CA:309:A:H4'	49:CV:16:GLY:HA2	1.97	0.46
31:CA:846:U:H1'	31:CA:847:U:C5	2.44	0.46
34:CF:103:LEU:HA	34:CF:107:ALA:HB3	1.97	0.46
49:CV:7:ARG:O	49:CV:25:VAL:HB	2.15	0.46
34:DF:103:LEU:HA	34:DF:107:ALA:HB3	1.97	0.46
55:DA:1180:U:H5"	55:DA:1180:U:H6	1.80	0.46
21:AU:4:ILE:HG13	21:AU:19:PHE:HA	1.97	0.46
1:BA:202:G:H21	1:BA:466:A:H61	1.62	0.46
19:BS:15:LEU:HD13	19:BS:33:THR:HG21	1.95	0.46
30:CD:152:PRO:HG3	30:CD:156:PHE:CZ	2.51	0.46
51:DX:39:ARG:NH1	70:DX:101:HOH:O	2.48	0.46
1:AA:76:G:H1	1:AA:93:U:H3	1.62	0.46
64:D1:102:PGE:H4	70:DT:313:HOH:O	2.15	0.46
30:CD:3:GLY:O	30:CD:4:LEU:HD13	2.15	0.46
30:CD:62:LYS:HE2	31:CA:2810:A:H5"	1.98	0.46
30:CD:133:THR:CG2	31:CA:1993:U:H4'	2.45	0.46
31:CA:740:C:H5'	31:CA:1784:A:C3'	2.38	0.46
40:CM:77:ILE:CD1	40:CM:108:ALA:HB1	2.36	0.46
55:DA:57:C:H2'	55:DA:58:G:O4'	2.16	0.46
1:AA:1190:G:H5'	3:AC:176:HIS:NE2	2.31	0.46
1:AA:1391:U:H2'	1:AA:1392:G:C8	2.50	0.46
1:BA:1001:C:H2'	1:BA:1002:G:H8	1.81	0.46
21:BU:4:ILE:HG13	21:BU:19:PHE:HA	1.97	0.46
29:CC:219:THR:O	31:CA:1789:A:H5"	2.15	0.46
31:CA:749:A:H4'	31:CA:1271:G:N3	2.29	0.46
31:CA:1010:A:H5'	45:CR:62:ILE:CG2	2.46	0.46
31:CA:1250:G:C5'	45:CR:6:ARG:HD3	2.44	0.46
44:CQ:114:LEU:HD23	44:CQ:114:LEU:H	1.81	0.46
55:DA:102:U:H2'	55:DA:102:U:O2	2.15	0.46
29:DC:207:LYS:HB2	55:DA:729:G:C6	2.51	0.46
45:CR:58:ARG:HA	45:CR:61:TRP:CE3	2.50	0.46
48:CU:45:ALA:O	48:CU:49:LYS:HG2	2.14	0.46
52:DY:61:LYS:HD3	55:DA:372:G:H5"	1.98	0.46
17:AQ:76:VAL:HG12	17:AQ:77:ARG:HG3	1.97	0.46
23:C2:22:THR:HG21	31:CA:2419:U:H5"	1.98	0.46
1:BA:310:G:H5"	16:BP:31:ARG:HB2	1.97	0.46
1:BA:376:G:H5"	16:BP:5:ARG:HB2	1.97	0.46
1:BA:438:U:H5'	4:BD:120:HIS:HB3	1.97	0.46
24:D3:4:THR:HA	55:DA:687:C:O4'	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:CC:235:GLY:HA3	29:CC:239:ASN:HB2	1.97	0.46
31:CA:948:C:H1'	31:CA:984:A:C8	2.50	0.46
35:CG:80:THR:CG2	35:CG:81:GLU:H	2.27	0.46
40:DM:60:ARG:HD2	55:DA:2360:G:H1'	1.98	0.46
1:AA:216:U:H2'	1:AA:217:C:C6	2.50	0.46
1:BA:1496:C:H2'	1:BA:1497:G:O4'	2.16	0.46
23:D2:10:LYS:HE3	23:D2:53:LYS:O	2.16	0.46
48:CU:67:VAL:HG22	48:CU:76:ARG:HG3	1.98	0.46
1:AA:438:U:H5'	4:AD:120:HIS:HB3	1.98	0.46
1:AA:1054:C:H5"	1:AA:1054:C:H6	1.80	0.46
5:AE:57:PRO:O	5:AE:60:ILE:HG13	2.15	0.46
18:BR:27:ALA:O	18:BR:30:LYS:HG2	2.16	0.46
31:CA:694:U:OP1	31:CA:1569:A:H1'	2.15	0.46
31:CA:833:A:H2'	31:CA:834:G:C8	2.51	0.46
55:DA:722:A:H2'	55:DA:723:C:O4'	2.16	0.46
55:DA:871:U:H2'	55:DA:872:U:C6	2.51	0.46
55:DA:2070:A:H2'	55:DA:2071:A:O4'	2.16	0.46
55:DA:2800:A:C2	55:DA:2895:G:H1'	2.51	0.46
5:AE:16:ILE:HD13	5:AE:137:VAL:HG11	1.97	0.45
1:BA:846:G:H2'	1:BA:847:G:C8	2.51	0.45
9:BI:7:TYR:HE1	9:BI:18:ARG:HB2	1.80	0.45
22:D1:9:THR:CG2	55:DA:2020:A:H5'	2.46	0.45
31:CA:594:U:H2'	31:CA:595:C:C6	2.51	0.45
36:DH:104:THR:HG22	36:DH:109:GLU:HA	1.97	0.45
30:CD:8:LYS:HB2	30:CD:201:LEU:HD11	1.97	0.45
29:DC:177:ARG:HG2	55:DA:1820:U:OP1	2.16	0.45
29:DC:235:GLY:HA3	29:DC:239:ASN:HB2	1.98	0.45
41:CN:69:PRO:O	41:CN:93:VAL:O	2.34	0.45
55:DA:2086:U:H2'	55:DA:2087:G:C8	2.51	0.45
55:DA:2117:A:H61	55:DA:2171:A:H61	1.63	0.45
65:DA:3223:SPD:H82	70:DA:4260:HOH:O	2.16	0.45
10:AJ:52:LEU:HB2	14:AN:81:ARG:HD2	1.99	0.45
1:BA:216:U:H2'	1:BA:217:C:C6	2.51	0.45
1:BA:411:A:P	4:BD:26:ARG:HH12	2.39	0.45
1:BA:1108:G:H5"	3:BC:176:HIS:CE1	2.52	0.45
31:CA:1326:U:H2'	31:CA:1327:A:H8	1.81	0.45
37:CJ:103:ARG:HA	37:CJ:106:LEU:HD12	1.96	0.45
43:CP:31:THR:HG22	43:CP:34:HIS:H	1.81	0.45
33:DE:1:MET:HG2	33:DE:14:VAL:HG23	1.97	0.45
42:DO:9:GLN:O	42:DO:17:ARG:HD3	2.17	0.45
51:DX:37:ILE:HG21	51:DX:80:ILE:HG21	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:DY:7:VAL:HG23	52:DY:51:VAL:HG12	1.98	0.45
55:DA:2628:C:C5'	59:DA:3195:PUT:H12	2.42	0.45
1:AA:845:A:H2'	1:AA:846:G:O4'	2.17	0.45
1:AA:923:A:OP1	5:AE:26:LYS:HG2	2.16	0.45
1:BA:1053:G:N7	1:BA:1200:C:H5"	2.32	0.45
2:BB:163:VAL:HG11	2:BB:173:ILE:HD11	1.99	0.45
31:CA:871:U:H2'	31:CA:872:U:C6	2.51	0.45
32:DD:152:PRO:HG3	32:DD:156:PHE:CZ	2.52	0.45
38:CK:69:ARG:O	38:CK:90:GLU:HB3	2.16	0.45
45:DR:58:ARG:HA	45:DR:61:TRP:CE3	2.51	0.45
55:DA:1133:A:N3	59:DA:3212:PUT:H22	2.32	0.45
1:AA:266:G:H3'	17:AQ:69:LYS:HB2	1.97	0.45
1:AA:376:G:H5"	16:AP:5:ARG:HB2	1.98	0.45
27:D0:15:GLY:HA2	55:DA:969:G:O3'	2.16	0.45
31:CA:2296:U:H5	43:CP:9:ARG:NH2	2.14	0.45
33:DE:32:VAL:HG21	40:DM:6:LEU:HD13	1.99	0.45
55:DA:1509:A:HO2'	55:DA:1510:G:H8	1.64	0.45
2:AB:93:ASN:H	2:AB:93:ASN:HD22	1.65	0.45
1:BA:8:A:H1'	5:BE:108:GLY:HA2	1.97	0.45
31:CA:191:A:H2'	31:CA:192:C:C6	2.51	0.45
31:CA:722:A:H2'	31:CA:723:C:O4'	2.16	0.45
47:CT:84:ARG:HB2	47:CT:96:ILE:HB	1.99	0.45
48:CU:28:ASN:ND2	48:CU:91:GLN:HB3	2.14	0.45
35:DG:103:ILE:HD11	35:DG:117:LEU:HD21	1.99	0.45
1:BA:923:A:OP1	5:BE:26:LYS:HG2	2.17	0.45
31:CA:248:G:H5'	31:CA:250:G:N7	2.31	0.45
31:CA:381:G:OP1	52:CY:18:ARG:HD3	2.16	0.45
31:CA:674:G:H1'	33:CE:69:ARG:HH11	1.82	0.45
31:CA:2544:G:H5'	31:CA:2645:G:C2	2.51	0.45
45:CR:112:LYS:HD3	46:CS:48:LYS:HG3	1.99	0.45
43:DP:35:ILE:HG21	43:DP:71:ALA:HA	1.98	0.45
44:DQ:52:ASN:O	44:DQ:53:ARG:HD3	2.16	0.45
55:DA:136:G:H1	55:DA:143:C:H42	1.65	0.45
55:DA:1168:G:H8	55:DA:1168:G:H5"	1.81	0.45
4:AD:172:GLU:HG2	4:AD:183:LYS:HD2	1.99	0.45
8:AH:105:SER:HB2	8:AH:126:ILE:HD11	1.98	0.45
2:BB:93:ASN:HD22	2:BB:93:ASN:H	1.65	0.45
31:CA:1810:A:H2'	31:CA:1811:G:O4'	2.17	0.45
31:CA:1965:C:H5"	31:CA:1966:A:H2'	1.99	0.45
33:CE:176:ASP:OD2	33:CE:178:VAL:HG12	2.16	0.45
46:CS:49:ILE:HB	46:CS:51:VAL:O	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
55:DA:2609:U:C5	63:DA:3194:EDO:H12	2.52	0.45
1:AA:202:G:H1	1:AA:215:C:H42	1.64	0.45
47:CT:72:THR:HG21	47:CT:108:SER:HB3	1.98	0.45
54:DI:70:GLU:HG2	54:DI:73:LYS:HE3	1.98	0.45
1:AA:1001:C:H2'	1:AA:1002:G:H8	1.82	0.45
25:C4:47:LYS:NZ	40:CM:64:PHE:CD1	2.75	0.45
24:D3:33:ARG:HG3	62:D3:102:PEG:H31	1.99	0.45
31:CA:278:A:N3	31:CA:278:A:H2'	2.32	0.45
31:CA:826:U:O2'	40:CM:53:GLY:HA3	2.17	0.45
31:CA:1775:U:O4	31:CA:1789:A:H2	2.00	0.45
38:DK:7:LYS:O	38:DK:11:VAL:HG23	2.17	0.45
46:DS:8:GLY:HA2	55:DA:1161:C:O2'	2.17	0.45
50:DW:38:LEU:HD21	50:DW:65:VAL:HG11	1.99	0.45
55:DA:355:U:H2'	55:DA:356:G:H8	1.82	0.45
4:BD:172:GLU:HG2	4:BD:183:LYS:HD2	1.99	0.44
31:CA:320:A:H4'	31:CA:322:A:N7	2.32	0.44
31:CA:478:A:H61	31:CA:500:G:H4'	1.81	0.44
29:DC:199:GLU:O	29:DC:202:LEU:HB2	2.17	0.44
55:DA:278:A:N3	55:DA:278:A:H2'	2.32	0.44
55:DA:612:G:H2'	55:DA:614:A:C8	2.52	0.44
55:DA:1283:G:H1'	55:DA:1329:U:O2	2.17	0.44
55:DA:1349:C:O2'	57:DA:3215:PG4:H82	2.16	0.44
9:AI:7:TYR:HE1	9:AI:18:ARG:HB2	1.81	0.44
22:C1:16:ARG:HA	31:CA:2046:G:C5'	2.47	0.44
1:BA:957:U:O2	1:BA:959:A:H8	2.01	0.44
1:BA:1493:A:H1'	31:CA:1913:A:H61	1.82	0.44
2:BB:68:LEU:HD11	2:BB:92:VAL:HG23	2.00	0.44
54:DI:132:TYR:H	54:DI:133:GLU:HB2	1.81	0.44
55:DA:760:G:H4'	55:DA:1776:G:OP1	2.18	0.44
1:AA:957:U:O2	1:AA:959:A:H8	2.01	0.44
1:BA:1054:C:H5"	1:BA:1054:C:H6	1.83	0.44
6:BF:47:LEU:HD13	6:BF:51:ILE:HG12	1.99	0.44
31:CA:639:U:H2'	31:CA:640:C:C6	2.52	0.44
31:CA:1556:C:H2'	31:CA:1557:C:C6	2.52	0.44
31:CA:2641:G:H5"	38:CK:78:THR:HB	1.99	0.44
29:DC:212:ARG:HD2	29:DC:216:VAL:O	2.18	0.44
34:DF:16:LEU:HD13	34:DF:29:PRO:HD2	1.99	0.44
43:DP:31:THR:HG22	43:DP:34:HIS:H	1.80	0.44
1:AA:1053:G:N7	1:AA:1200:C:H5"	2.33	0.44
2:AB:68:LEU:HD11	2:AB:92:VAL:HG23	1.99	0.44
24:C3:2:LYS:NZ	70:C3:101:HOH:O	2.49	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BA:73:C:O2'	1:BA:74:A:H8	1.97	0.44
1:BA:1226:C:H2'	13:BM:102:THR:HB	1.99	0.44
31:CA:811:U:H2'	40:CM:21:ARG:HA	1.99	0.44
51:CX:37:ILE:HG21	51:CX:80:ILE:HG21	1.98	0.44
55:DA:1738:G:HO2'	55:DA:1739:A:H8	1.62	0.44
1:AA:9:G:H5'	5:AE:108:GLY:HA3	1.99	0.44
1:AA:864:A:H4'	5:AE:90:THR:HG23	2.00	0.44
9:AI:99:ARG:HG2	9:AI:104:VAL:HG21	1.99	0.44
13:AM:12:HIS:HB3	70:AM:302:HOH:O	2.17	0.44
22:C1:53:LYS:HE3	22:C1:56:ALA:HA	1.99	0.44
25:C4:4:ILE:HG23	31:CA:666:A:O2'	2.17	0.44
11:BK:84:VAL:HG11	11:BK:97:ILE:HG12	2.00	0.44
14:BN:31:ILE:HG23	14:BN:42:TRP:CZ2	2.53	0.44
20:BT:58:VAL:HG13	20:BT:72:ALA:HB1	1.99	0.44
31:CA:747:5MU:O2	31:CA:2014:A:H1'	2.18	0.44
31:CA:863:A:H2'	31:CA:864:G:C8	2.53	0.44
31:CA:2489:U:HO2'	31:CA:2491:U:H5	1.64	0.44
31:CA:2674:G:H4'	39:CL:30:ARG:HD2	2.00	0.44
29:DC:203:ARG:HH21	29:DC:205:LEU:HD21	1.82	0.44
34:CF:16:LEU:HD13	34:CF:29:PRO:HD2	1.98	0.44
50:CW:38:LEU:HD21	50:CW:65:VAL:HG11	1.98	0.44
33:DE:84:THR:HG21	55:DA:586:A:H5'	1.98	0.44
55:DA:1321:A:C2	64:DA:3216:PGE:H12	2.53	0.44
2:AB:129:LEU:H	2:AB:129:LEU:HG	1.51	0.44
29:DC:13:ARG:HD3	55:DA:728:G:H4'	2.00	0.44
43:CP:35:ILE:HG21	43:CP:71:ALA:HA	1.98	0.44
55:DA:639:U:H2'	55:DA:640:C:C6	2.53	0.44
8:AH:87:LYS:HB2	8:AH:125:ILE:CD1	2.41	0.44
13:AM:17:ILE:HD12	13:AM:17:ILE:H	1.83	0.44
25:C4:13:ARG:NH1	31:CA:250:G:P	2.91	0.44
1:BA:266:G:H3'	17:BQ:69:LYS:HB2	2.00	0.44
31:CA:659:G:H4'	33:CE:95:LYS:HD3	1.99	0.44
36:CH:104:THR:HG22	36:CH:109:GLU:HA	1.98	0.44
54:DI:85:VAL:HG21	54:DI:90:GLY:O	2.17	0.44
55:DA:62:U:H5'	58:DA:3203:MPD:H53	2.00	0.44
55:DA:493:G:H2'	55:DA:494:G:O4'	2.18	0.44
55:DA:1831:G:H1'	64:DA:3224:PGE:H22	1.98	0.44
1:AA:1496:C:H2'	1:AA:1497:G:O4'	2.18	0.44
3:AC:21:THR:HG23	3:AC:58:GLU:HB3	1.99	0.44
11:AK:84:VAL:HG11	11:AK:97:ILE:HG12	1.99	0.44
23:C2:33:LYS:HA	23:C2:52:ALA:HB3	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BA:1060:U:H5	3:BC:2:GLY:HA3	1.81	0.44
29:CC:199:GLU:O	29:CC:202:LEU:HB2	2.18	0.44
31:CA:2051:A:H5'	31:CA:2578:G:O4'	2.18	0.44
38:CK:7:LYS:O	38:CK:11:VAL:HG23	2.17	0.44
37:DJ:11:LEU:HD22	37:DJ:24:VAL:HG23	2.00	0.44
24:C3:7:PRO:HG3	31:CA:1612:C:H5'	2.00	0.44
20:BT:5:LYS:HB3	20:BT:7:ALA:H	1.82	0.44
29:CC:212:ARG:HD2	29:CC:216:VAL:O	2.18	0.44
31:CA:95:A:H4'	53:CZ:38:GLN:O	2.18	0.44
31:CA:528:A:C8	31:CA:528:A:C3'	3.00	0.44
31:CA:1469:A:H2'	31:CA:1470:A:C8	2.53	0.44
31:CA:1808:A:N1	52:CY:28:ARG:HD2	2.33	0.44
46:DS:41:ILE:HD13	46:DS:103:ALA:HA	1.99	0.44
49:DV:94:ARG:HB3	49:DV:103:ILE:HD12	1.99	0.44
17:AQ:8:LEU:HD13	17:AQ:25:ILE:HG13	1.99	0.43
4:BD:85:ASN:HA	5:BE:102:GLY:CA	2.31	0.43
14:BN:10:GLU:HG3	14:BN:63:ARG:HD2	2.00	0.43
30:CD:13:ARG:HD3	30:CD:21:SER:OG	2.18	0.43
31:CA:1274:A:N3	31:CA:1297:C:H1'	2.33	0.43
31:CA:1991:U:H2'	31:CA:1992:G:H5"	2.00	0.43
45:CR:113:ALA:O	45:CR:117:LEU:HD12	2.18	0.43
50:CW:51:GLN:HG2	50:CW:86:LEU:HD11	2.00	0.43
41:DN:42:THR:HG22	41:DN:93:VAL:HG12	1.99	0.43
1:AA:1060:U:H4'	10:AJ:53:ILE:HG23	2.00	0.43
14:AN:10:GLU:HG3	14:AN:63:ARG:HD2	2.00	0.43
14:AN:46:LEU:HA	14:AN:49:GLN:HE21	1.83	0.43
16:BP:20:VAL:CG1	16:BP:32:PHE:HB2	2.47	0.43
31:CA:355:U:H2'	31:CA:356:G:H8	1.83	0.43
34:CF:5:HIS:HB2	34:CF:97:TRP:CD1	2.53	0.43
55:DA:1394:U:H4'	55:DA:1603:A:H4'	2.00	0.43
2:AB:70:VAL:HB	2:AB:163:VAL:HG22	2.00	0.43
2:AB:163:VAL:HG11	2:AB:173:ILE:HD11	2.00	0.43
1:BA:10:A:OP2	5:BE:131:THR:HG21	2.18	0.43
1:BA:1060:U:H4'	10:BJ:53:ILE:HG23	2.00	0.43
6:BF:70:VAL:HA	6:BF:73:GLU:HG2	2.00	0.43
10:BJ:52:LEU:HB2	14:BN:81:ARG:HD2	2.00	0.43
31:CA:532:A:H4'	31:CA:533:G:C8	2.54	0.43
31:CA:2623:G:H4'	31:CA:2825:G:C8	2.53	0.43
31:CA:2688:G:H1'	31:CA:2721:A:N6	2.34	0.43
35:CG:17:VAL:HG11	35:CG:50:LEU:HD21	2.00	0.43
1:AA:604:G:H2'	1:AA:605:U:O4'	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:1226:C:H2'	13:AM:102:THR:HB	2.00	0.43
12:AL:31:ARG:O	12:AL:58:THR:HG23	2.18	0.43
1:BA:1277:C:HO2'	1:BA:1279:G:H8	1.62	0.43
22:D1:53:LYS:HE3	22:D1:56:ALA:HA	2.00	0.43
34:DF:5:HIS:HB2	34:DF:97:TRP:CD1	2.54	0.43
34:DF:80:ARG:HB3	34:DF:83:TYR:CE1	2.53	0.43
55:DA:142:A:H2'	55:DA:143:C:C6	2.53	0.43
55:DA:1424:G:H21	64:DA:3213:PGE:H32	1.84	0.43
55:DA:2031:A:C6	55:DA:2498:OMC:H1'	2.53	0.43
17:AQ:15:ASP:HA	17:AQ:21:ILE:HG22	1.99	0.43
20:AT:44:LYS:H	20:AT:44:LYS:HG3	1.61	0.43
11:BK:24:HIS:HB3	11:BK:31:ILE:HG23	2.00	0.43
13:BM:54:ASP:HA	13:BM:57:ARG:HD2	2.00	0.43
17:BQ:46:VAL:HG11	17:BQ:61:ILE:CG2	2.48	0.43
30:CD:121:THR:HB	30:CD:127:PHE:CD2	2.54	0.43
31:CA:96:C:H4'	53:CZ:41:HIS:CG	2.53	0.43
31:CA:1030:C:OP2	41:CN:127:LYS:HE3	2.19	0.43
37:CJ:11:LEU:HD22	37:CJ:24:VAL:HG23	2.00	0.43
39:CL:103:VAL:O	39:CL:122:VAL:HB	2.18	0.43
42:CO:71:ARG:HG3	42:CO:71:ARG:O	2.19	0.43
49:CV:94:ARG:HB3	49:CV:103:ILE:HD12	1.99	0.43
54:DI:56:ARG:HA	55:DA:1107:G:OP1	2.19	0.43
10:AJ:10:LEU:HB2	10:AJ:72:ARG:HB2	2.00	0.43
3:BC:23:PHE:CD2	10:BJ:97:ASP:HB2	2.54	0.43
8:BH:105:SER:HB2	8:BH:126:ILE:HD11	1.99	0.43
25:D4:13:ARG:HH11	55:DA:2394:C:H5'	1.82	0.43
29:CC:225:MET:O	29:CC:233:GLY:O	2.36	0.43
31:CA:142:A:H2'	31:CA:143:C:C6	2.53	0.43
31:CA:309:A:O3'	49:CV:16:GLY:HA2	2.18	0.43
39:CL:113:MET:O	39:CL:116:ILE:HG13	2.18	0.43
46:DS:44:GLY:O	46:DS:45:GLU:HG2	2.17	0.43
54:DI:50:VAL:HG22	54:DI:85:VAL:HG13	2.00	0.43
55:DA:5:A:H2'	55:DA:6:A:C8	2.53	0.43
55:DA:191:A:H2'	55:DA:192:C:C6	2.53	0.43
55:DA:1028:A:N6	55:DA:1125:G:H2'	2.33	0.43
55:DA:2849:U:H4'	55:DA:2868:A:C2	2.54	0.43
1:BA:502:A:H2'	1:BA:503:C:O4'	2.19	0.43
31:CA:493:G:H2'	31:CA:494:G:O4'	2.18	0.43
31:CA:528:A:C2	31:CA:2042:A:H2'	2.54	0.43
31:CA:2728:U:O2'	31:CA:2729:G:H8	2.01	0.43
45:DR:51:ARG:HH22	55:DA:993:G:P	2.41	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:DU:33:LYS:HG3	48:DU:80:TRP:CE3	2.53	0.43
54:DI:27:VAL:HG13	54:DI:80:THR:HG23	2.00	0.43
55:DA:523:C:H4'	55:DA:540:C:O2	2.19	0.43
3:AC:7:PRO:HD2	3:AC:184:TYR:CD1	2.54	0.43
26:C5:17:VAL:HG12	26:C5:26:ILE:HD12	2.01	0.43
1:BA:1493:A:H8	1:BA:1493:A:OP2	2.01	0.43
4:BD:105:MET:SD	4:BD:143:VAL:HG22	2.59	0.43
31:CA:685:A:H5"	31:CA:774:G:O6	2.19	0.43
31:CA:2636:C:H2'	31:CA:2637:U:C6	2.54	0.43
40:CM:95:LEU:HD22	40:CM:100:ILE:HG12	2.00	0.43
42:CO:9:GLN:O	42:CO:17:ARG:HD3	2.17	0.43
46:CS:3:ALA:HB3	46:CS:101:ILE:HD12	2.01	0.43
34:DF:36:LEU:HD22	34:DF:154:ILE:HG12	2.01	0.43
38:DK:23:LYS:HE2	38:DK:142:ILE:OXT	2.19	0.43
55:DA:1654:A:H1'	55:DA:2823:A:H5'	2.00	0.43
6:AF:70:VAL:HA	6:AF:73:GLU:HG2	2.00	0.43
8:AH:66:PHE:CD2	8:AH:67:GLN:HG2	2.54	0.43
27:C0:53:PHE:CG	28:CB:83:G:H4'	2.54	0.43
1:BA:1152:A:H5'	10:BJ:15:HIS:HB2	2.01	0.43
5:BE:40:GLY:HA2	5:BE:45:ARG:O	2.19	0.43
5:BE:88:VAL:HG12	5:BE:93:ARG:HG2	2.00	0.43
13:BM:90:ARG:HH21	13:BM:95:LEU:HB3	1.84	0.43
31:CA:83:A:H2	31:CA:103:A:N7	2.17	0.43
31:CA:1168:G:H5"	31:CA:1168:G:H8	1.83	0.43
46:DS:83:TYR:CE1	55:DA:1187:G:H5"	2.54	0.43
55:DA:2233:U:H2'	55:DA:2234:G:C8	2.54	0.43
1:AA:892:A:O2'	1:AA:1415:G:H4'	2.19	0.43
1:AA:1062:U:H2'	1:AA:1063:C:C6	2.54	0.43
1:AA:1376:U:H2'	1:AA:1377:A:C8	2.54	0.43
30:CD:13:ARG:HH11	44:CQ:56:HIS:HA	1.84	0.43
31:CA:35:G:H2'	31:CA:36:G:O4'	2.19	0.43
31:CA:1936:A:N6	31:CA:1963:U:H3	2.16	0.43
31:CA:2642:G:H5'	38:CK:80:HIS:CG	2.53	0.43
32:DD:121:THR:HB	32:DD:127:PHE:CD2	2.54	0.43
35:DG:17:VAL:HG11	35:DG:50:LEU:HD21	2.00	0.43
41:DN:21:ALA:HB1	41:DN:100:LYS:HG2	2.00	0.43
46:DS:10:LYS:HE3	57:DS:202:PG4:H21	2.00	0.43
50:DW:51:GLN:HG2	50:DW:86:LEU:HD11	2.01	0.43
54:DI:26:VAL:HB	54:DI:83:ALA:HB3	2.01	0.43
62:DA:3200:PEG:H32	70:DA:3804:HOH:O	2.18	0.43
3:AC:151:VAL:HG12	3:AC:200:VAL:HG22	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:BB:104:TRP:O	2:BB:108:ARG:HB2	2.19	0.42
9:BI:99:ARG:HG2	9:BI:104:VAL:HG21	2.00	0.42
24:D3:29:GLN:HG2	62:D3:102:PEG:H21	2.01	0.42
29:CC:105:LEU:H	29:CC:105:LEU:HD12	1.84	0.42
31:CA:2106:U:H2'	31:CA:2107:G:H8	1.84	0.42
35:CG:103:ILE:HD11	35:CG:117:LEU:HD21	2.01	0.42
55:DA:1101:U:H2'	55:DA:1102:C:C6	2.54	0.42
55:DA:2326:C:H3'	70:DA:7772:HOH:O	2.18	0.42
1:AA:619:U:C2	4:AD:132:ILE:HD11	2.54	0.42
22:C1:4:GLN:CB	31:CA:2615:U:H1'	2.50	0.42
1:BA:978:A:O2'	1:BA:1322:C:H5	2.00	0.42
5:BE:81:LEU:HB3	5:BE:147:MET:SD	2.58	0.42
12:BL:80:ILE:HD12	12:BL:97:THR:HG22	2.01	0.42
31:CA:136:G:H1	31:CA:143:C:H42	1.65	0.42
31:CA:2815:C:H2'	31:CA:2816:G:O4'	2.19	0.42
32:DD:13:ARG:HD3	32:DD:21:SER:OG	2.18	0.42
38:CK:23:LYS:HE3	38:CK:142:ILE:OXT	2.20	0.42
50:DW:26:PHE:CE2	50:DW:44:HIS:HA	2.54	0.42
55:DA:1510:G:H2'	55:DA:1511:G:O4'	2.18	0.42
55:DA:2051:A:H5'	55:DA:2578:G:O4'	2.19	0.42
55:DA:2636:C:H2'	55:DA:2637:U:C6	2.53	0.42
8:AH:94:LYS:HB3	8:AH:117:ARG:HH22	1.84	0.42
5:BE:74:VAL:HG11	5:BE:144:LEU:HB3	2.01	0.42
22:D1:54:VAL:HG23	22:D1:55:ILE:HG12	2.00	0.42
34:CF:36:LEU:HD12	34:CF:154:ILE:HG12	2.01	0.42
48:CU:33:LYS:HG3	48:CU:80:TRP:CE3	2.55	0.42
50:CW:26:PHE:CE1	50:CW:44:HIS:HA	2.54	0.42
33:DE:48:THR:HG23	33:DE:88:ARG:HH12	1.82	0.42
42:DO:8:ARG:HD3	55:DA:1652:A:OP1	2.18	0.42
55:DA:1654:A:C1'	55:DA:2823:A:H5'	2.50	0.42
55:DA:1932:A:H2'	55:DA:1933:G:O4'	2.19	0.42
1:BA:864:A:H4'	5:BE:90:THR:HG23	2.01	0.42
2:BB:70:VAL:HB	2:BB:163:VAL:HG22	2.00	0.42
3:BC:47:LEU:HD22	3:BC:76:VAL:HG22	2.00	0.42
14:BN:28:LYS:HA	14:BN:31:ILE:HG22	2.01	0.42
31:CA:822:G:O6	31:CA:943:A:H2	2.01	0.42
31:CA:2869:G:H2'	31:CA:2870:C:O4'	2.19	0.42
32:DD:167:ASN:O	64:DD:301:PGE:H52	2.20	0.42
46:CS:41:ILE:HD13	46:CS:103:ALA:HA	2.00	0.42
55:DA:189:G:N7	63:DA:3197:EDO:H21	2.35	0.42
1:BA:49:U:O2	1:BA:362:G:H1'	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BA:604:G:H2'	1:BA:605:U:O4'	2.20	0.42
31:CA:1028:A:N6	31:CA:1125:G:H2'	2.34	0.42
31:CA:1430:G:H2'	31:CA:1431:A:O4'	2.19	0.42
31:CA:2060:A:H62	33:CE:69:ARG:NH2	2.18	0.42
39:CL:121:GLU:HG2	39:CL:122:VAL:HG23	2.02	0.42
1:AA:1305:G:HO2'	1:AA:1306:A:H8	1.65	0.42
3:AC:47:LEU:HD22	3:AC:76:VAL:HG22	2.01	0.42
5:AE:132:ASN:OD1	5:AE:134:ILE:HG22	2.20	0.42
2:BB:129:LEU:H	2:BB:129:LEU:HG	1.53	0.42
10:BJ:10:LEU:HB2	10:BJ:72:ARG:HB2	2.00	0.42
11:BK:25:ALA:HA	11:BK:30:THR:HG22	2.01	0.42
13:BM:11:ASP:HA	13:BM:45:ILE:HD13	2.01	0.42
13:BM:17:ILE:H	13:BM:17:ILE:HD12	1.84	0.42
25:D4:47:LYS:HE3	40:DM:64:PHE:CD1	2.55	0.42
38:CK:81:ILE:HG23	38:CK:82:GLY:N	2.35	0.42
42:DO:67:PHE:O	42:DO:71:ARG:HD2	2.20	0.42
55:DA:2445:2MG:HM21	55:DA:2449:H2U:O4	2.20	0.42
1:AA:1530:G:H2'	1:AA:1531:A:C8	2.55	0.42
22:C1:15:MET:O	31:CA:2045:C:O2'	2.31	0.42
27:C0:31:ARG:HD3	31:CA:1158:C:H5"	2.02	0.42
28:CB:55:U:H1'	34:CF:26:MET:HG3	2.01	0.42
29:CC:57:GLY:HA2	29:CC:213:TRP:HA	2.01	0.42
31:CA:686:U:H2'	31:CA:788:A:N1	2.34	0.42
31:CA:1510:G:H2'	31:CA:1511:G:O4'	2.20	0.42
31:CA:2800:A:C2	31:CA:2895:G:H1'	2.54	0.42
29:DC:225:MET:O	29:DC:233:GLY:O	2.38	0.42
34:CF:138:PHE:HE1	34:CF:152:LEU:HD21	1.85	0.42
49:DV:51:ALA:O	49:DV:52:LEU:HB2	2.19	0.42
55:DA:355:U:H2'	55:DA:356:G:C8	2.55	0.42
1:AA:502:A:H2'	1:AA:503:C:O4'	2.19	0.42
5:AE:77:ASN:HB2	5:AE:82:GLN:HE21	1.74	0.42
20:AT:36:TYR:CE2	20:AT:79:LEU:HD21	2.55	0.42
1:BA:1322:C:OP1	1:BA:1322:C:O2	2.37	0.42
5:BE:157:ARG:HG2	5:BE:158:GLY:N	2.35	0.42
31:CA:2305:U:H5"	34:CF:131:GLY:HA3	2.02	0.42
36:CH:68:ARG:HB3	36:CH:134:VAL:HG21	2.02	0.42
47:CT:20:VAL:HG11	47:CT:44:ALA:HA	2.02	0.42
50:CW:86:LEU:HD13	50:CW:89:ILE:HD11	2.01	0.42
55:DA:825:A:H5"	59:DA:3222:PUT:H12	2.02	0.42
55:DA:984:A:N3	55:DA:984:A:H2'	2.34	0.42
1:AA:1322:C:P	19:AS:78:ARG:HH22	2.43	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:AB:104:TRP:O	2:AB:108:ARG:HB2	2.20	0.42
4:AD:105:MET:SD	4:AD:143:VAL:HG22	2.60	0.42
25:C4:26:HIS:HD1	31:CA:2361:G:P	2.43	0.42
1:BA:1530:G:H2'	1:BA:1531:A:C8	2.55	0.42
24:D3:2:LYS:HE2	55:DA:687:C:H5"	2.02	0.42
31:CA:796:C:H2'	31:CA:797:G:C8	2.54	0.42
36:CH:82:SER:HB2	36:CH:94:ILE:HD11	2.02	0.42
41:CN:41:LEU:HD21	41:CN:124:LEU:HD22	2.02	0.42
40:DM:109:LYS:HG2	40:DM:126:ARG:HB2	2.02	0.42
47:DT:6:LYS:HB2	55:DA:494:G:H4'	2.01	0.42
55:DA:747:5MU:O2	55:DA:2014:A:H1'	2.20	0.42
55:DA:1555:G:OP1	59:DA:3218:PUT:H41	2.20	0.42
55:DA:1794:A:H2'	55:DA:1795:C:C6	2.54	0.42
1:AA:1152:A:H5'	10:AJ:15:HIS:HB2	2.02	0.42
1:AA:1298:U:H3	7:AG:114:LYS:HA	1.85	0.42
11:AK:25:ALA:HA	11:AK:30:THR:HG22	2.02	0.42
5:BE:115:LEU:HG	5:BE:123:VAL:HG21	2.01	0.42
31:CA:1101:U:H2'	31:CA:1102:C:C6	2.54	0.42
32:DD:13:ARG:HH11	44:DQ:56:HIS:HA	1.85	0.42
33:CE:178:VAL:HG23	40:CM:3:LEU:HD21	2.02	0.42
50:CW:26:PHE:HE1	50:CW:44:HIS:HA	1.85	0.42
38:DK:7:LYS:HG2	55:DA:538:A:H4'	2.02	0.42
55:DA:320:A:H4'	55:DA:322:A:N7	2.35	0.42
55:DA:2406:A:H5'	55:DA:2406:A:C8	2.55	0.42
7:AG:72:THR:HG22	7:AG:142:HIS:CE1	2.55	0.41
24:C3:16:HIS:CD2	31:CA:464:U:O2'	2.73	0.41
1:BA:1048:G:H4'	14:BN:3:LYS:HE2	2.02	0.41
25:D4:39:LYS:O	25:D4:43:HIS:HD2	2.03	0.41
31:CA:2074:U:H2'	31:CA:2075:U:C6	2.55	0.41
31:CA:2425:A:H4'	31:CA:2426:A:O5'	2.20	0.41
3:AC:156:ARG:HD3	3:AC:193:TYR:O	2.20	0.41
19:AS:30:PRO:HB2	19:AS:50:ALA:HB2	2.03	0.41
11:BK:45:ALA:HB3	11:BK:70:CYS:HB2	2.02	0.41
25:D4:8:ARG:HG3	55:DA:253:C:N4	2.36	0.41
44:CQ:52:ASN:O	44:CQ:53:ARG:HD3	2.20	0.41
48:CU:82:LYS:HD3	48:CU:84:TYR:CE1	2.55	0.41
55:DA:136:G:H1	55:DA:143:C:N4	2.18	0.41
1:AA:131:A:H2'	1:AA:132:C:C6	2.56	0.41
1:AA:302:G:O2'	1:AA:556:C:H5"	2.20	0.41
1:AA:1048:G:H4'	14:AN:3:LYS:HE2	2.01	0.41
1:AA:1108:G:H5"	3:AC:176:HIS:ND1	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:BN:31:ILE:HG23	14:BN:42:TRP:HZ2	1.85	0.41
20:BT:67:ILE:O	20:BT:68:HIS:HB2	2.20	0.41
31:CA:136:G:H1	31:CA:143:C:N4	2.19	0.41
31:CA:2339:C:H2'	31:CA:2340:A:C8	2.56	0.41
32:DD:26:VAL:HG21	44:DQ:5:ILE:HG12	2.02	0.41
55:DA:686:U:H2'	55:DA:788:A:N1	2.35	0.41
55:DA:1430:G:H2'	55:DA:1431:A:O4'	2.20	0.41
5:BE:23:LYS:HB3	5:BE:30:ILE:HG23	2.02	0.41
29:CC:221:ARG:NH1	31:CA:1789:A:OP2	2.53	0.41
31:CA:355:U:H2'	31:CA:356:G:C8	2.56	0.41
31:CA:742:A:H2'	31:CA:743:A:C8	2.55	0.41
31:CA:1794:A:H2'	31:CA:1795:C:C6	2.56	0.41
31:CA:2043:C:H5"	31:CA:2043:C:C6	2.55	0.41
31:CA:2106:U:H2'	31:CA:2107:G:C8	2.55	0.41
40:CM:123:ARG:HG3	40:CM:143:GLU:HG3	2.03	0.41
41:CN:71:LYS:HB3	41:CN:93:VAL:O	2.21	0.41
54:DI:94:ARG:HG2	54:DI:127:ALA:HA	2.02	0.41
55:DA:1202:G:H1'	58:DA:3192:MPD:HM1	2.02	0.41
55:DA:1418:G:H2'	55:DA:1579:A:N6	2.35	0.41
27:C0:14:ILE:HG21	31:CA:988:A:C6	2.56	0.41
1:BA:131:A:H2'	1:BA:132:C:C6	2.56	0.41
1:BA:429:U:H1'	1:BA:430:A:H5"	2.03	0.41
4:BD:130:VAL:HG11	4:BD:135:TYR:CG	2.55	0.41
11:BK:20:VAL:HB	11:BK:35:THR:HG23	2.02	0.41
31:CA:2114:A:N6	31:CA:2119:A:H62	2.18	0.41
36:DH:82:SER:HB2	36:DH:94:ILE:HD11	2.02	0.41
47:DT:20:VAL:HG11	47:DT:44:ALA:HA	2.03	0.41
55:DA:602:A:C6	58:DA:3190:MPD:H31	2.56	0.41
55:DA:792:A:N3	55:DA:2072:C:O2'	2.48	0.41
55:DA:1417:C:H5'	55:DA:1588:G:H1'	2.01	0.41
1:AA:429:U:H1'	1:AA:430:A:H5"	2.02	0.41
1:AA:1343:G:O2'	9:AI:123:ARG:HD2	2.20	0.41
13:AM:54:ASP:HA	13:AM:57:ARG:HD2	2.02	0.41
1:BA:1298:U:H3	7:BG:114:LYS:HA	1.86	0.41
14:BN:53:ARG:HH21	19:BS:37:ARG:HH22	1.69	0.41
29:CC:174:LEU:CD2	29:CC:184:VAL:HB	2.50	0.41
31:CA:2788:C:H2'	31:CA:2789:C:C6	2.55	0.41
47:CT:29:VAL:HG22	47:CT:51:LEU:HD11	2.02	0.41
52:DY:29:PHE:HB3	55:DA:396:G:H1'	2.02	0.41
55:DA:2128:G:H1	55:DA:2160:C:N4	2.18	0.41
55:DA:2324:U:H3'	55:DA:2325:G:H5"	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:439:U:H5”	4:AD:121:LYS:HD2	2.02	0.41
4:AD:170:TRP:CD2	4:AD:186:PRO:HB3	2.56	0.41
6:AF:102:MET:CE	18:AR:24:LYS:HB3	2.50	0.41
12:BL:87:VAL:HG11	12:BL:90:LEU:HD22	2.02	0.41
20:BT:44:LYS:HB3	20:BT:87:ALA:HB2	2.03	0.41
30:CD:141:ARG:HB2	31:CA:1656:C:H5”	2.01	0.41
31:CA:2095:A:H5”	31:CA:2095:A:C8	2.54	0.41
42:CO:95:THR:HG21	42:CO:113:ILE:HD11	2.02	0.41
47:CT:69:LEU:HG	47:CT:107:VAL:CG2	2.51	0.41
51:DX:41[B]:ARG:HD3	51:DX:41[B]:ARG:HA	1.94	0.41
55:DA:138:U:H5’	55:DA:139:U:H5’	2.03	0.41
55:DA:2038:G:H2’	55:DA:2039:U:O4’	2.21	0.41
9:AI:19:VAL:HG11	9:AI:83:ILE:HA	2.03	0.41
1:BA:1376:U:H2’	1:BA:1377:A:C8	2.55	0.41
4:BD:170:TRP:CD2	4:BD:186:PRO:HB3	2.56	0.41
5:BE:77:ASN:HB2	5:BE:82:GLN:HE21	1.79	0.41
5:BE:82:GLN:HG2	5:BE:149:SER:HA	2.01	0.41
19:BS:30:PRO:HB2	19:BS:50:ALA:HB2	2.02	0.41
25:D4:13:ARG:NH1	55:DA:2394:C:H5’	2.36	0.41
31:CA:1722:A:N6	31:CA:1738:G:H1’	2.36	0.41
31:CA:2038:G:H2’	31:CA:2039:U:O4’	2.21	0.41
33:DE:23:PHE:HE2	33:DE:25:GLU:HG3	1.86	0.41
35:DG:140:VAL:O	35:DG:144:VAL:HG23	2.20	0.41
51:DX:38:VAL:HG12	51:DX:59:LEU:HB2	2.02	0.41
55:DA:1020:A:C2	55:DA:1141:U:C2	3.08	0.41
55:DA:1515:A:H2’	55:DA:1516:G:O4’	2.20	0.41
55:DA:2097:A:H8	55:DA:2097:A:H5”	1.85	0.41
5:AE:157:ARG:CD	8:AH:43:GLU:O	2.69	0.41
11:AK:20:VAL:HB	11:AK:35:THR:HG23	2.03	0.41
19:AS:5:LEU:H	19:AS:5:LEU:HG	1.75	0.41
1:BA:216:U:H4’	1:BA:464:U:H4’	2.02	0.41
1:BA:567:G:H2’	1:BA:568:G:O4’	2.20	0.41
1:BA:841:C:H3’	1:BA:842:U:C4’	2.51	0.41
9:BI:19:VAL:HG11	9:BI:83:ILE:HA	2.03	0.41
29:CC:107:PRO:HD2	29:CC:110:LEU:HD22	2.03	0.41
31:CA:396:G:H1’	52:CY:29:PHE:HB3	2.01	0.41
31:CA:547:A:H2’	31:CA:547:A:N3	2.36	0.41
31:CA:1636:U:H2’	31:CA:1637:A:C8	2.55	0.41
33:DE:178:VAL:HG23	40:DM:3:LEU:HD21	2.01	0.41
36:DH:68:ARG:HB3	36:DH:134:VAL:HG21	2.03	0.41
54:DI:29:ASP:HB3	54:DI:106:PHE:HB2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:831:A:H5”	2:AB:21:ARG:HD3	2.03	0.41
1:AA:1141:C:O2’	1:AA:1142:G:H8	2.03	0.41
1:AA:1216:A:H5”	14:AN:5:SER:HB3	2.02	0.41
13:AM:90:ARG:HH21	13:AM:95:LEU:HB3	1.85	0.41
1:BA:439:U:H5”	4:BD:121:LYS:HD2	2.02	0.41
11:BK:34:ILE:HG12	11:BK:70:CYS:SG	2.60	0.41
20:BT:69:LYS:H	20:BT:69:LYS:HG3	1.60	0.41
31:CA:29:U:H6	31:CA:29:U:O5’	2.02	0.41
31:CA:2335:A:OP1	43:CP:13:ARG:HD2	2.21	0.41
37:CJ:49:ILE:HG13	37:CJ:55:ILE:HD13	2.03	0.41
38:DK:9:GLU:HG2	70:DA:3412:HOH:O	2.21	0.41
40:DM:74:THR:HG23	40:DM:107:PHE:HB2	2.02	0.41
40:DM:123:ARG:HG3	40:DM:143:GLU:HG3	2.02	0.41
41:DN:89:VAL:CG1	58:DN:201:MPD:HM3	2.50	0.41
54:DI:23:LEU:HD13	54:DI:89:PRO:HD3	2.03	0.41
55:DA:207:A:H2’	55:DA:208:C:O4’	2.20	0.41
55:DA:281:C:H2’	55:DA:282:A:C8	2.56	0.41
55:DA:2133:G:H21	55:DA:2158:A:N6	2.18	0.41
10:AJ:19:ASP:HA	10:AJ:22:THR:HB	2.03	0.40
22:C1:49:TYR:OH	31:CA:2883:A:OP1	2.34	0.40
1:BA:718:A:H5’	11:BK:119:ASN:HB2	2.03	0.40
1:BA:1108:G:H5”	3:BC:176:HIS:ND1	2.36	0.40
6:BF:22:ILE:HG23	6:BF:39:LEU:HD11	2.02	0.40
22:D1:8:PRO:HD2	55:DA:1263:U:O2’	2.22	0.40
31:CA:780:G:H2’	31:CA:782:A:N7	2.36	0.40
35:CG:38:ASN:HD22	35:CG:40:ALA:HB3	1.86	0.40
35:DG:50:LEU:HD13	35:DG:72:LEU:HD23	2.02	0.40
37:DJ:14:ALA:HB3	37:DJ:17:MET:HB2	2.03	0.40
40:DM:77:ILE:CD1	40:DM:101:ILE:CG2	2.97	0.40
54:DI:132:TYR:N	54:DI:133:GLU:HB2	2.35	0.40
55:DA:839:U:H2’	55:DA:840:C:C6	2.56	0.40
55:DA:1306:C:H6	55:DA:1306:C:H5”	1.85	0.40
55:DA:2273:A:H2’	55:DA:2274:A:C8	2.55	0.40
1:AA:568:G:O6	12:AL:2:ALA:HB2	2.21	0.40
1:AA:842:U:H5”	2:BB:115:LYS:HD3	2.03	0.40
10:BJ:59:LYS:HD2	10:BJ:60:ASP:OD1	2.21	0.40
47:DT:84:ARG:HB2	47:DT:96:ILE:HB	2.02	0.40
54:DI:65:GLU:HA	54:DI:70:GLU:HG3	2.02	0.40
54:DI:120:ALA:HA	54:DI:123:ILE:HD11	2.03	0.40
55:DA:1532:A:H5”	55:DA:1532:A:H8	1.85	0.40
1:AA:268:U:H2’	1:AA:269:C:C6	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:AK:31:ILE:HG12	11:AK:46:THR:CG2	2.51	0.40
14:AN:46:LEU:HD22	19:AS:13:LEU:HG	2.02	0.40
25:C4:52:LYS:HA	25:C4:55:LEU:HD12	2.03	0.40
1:BA:1322:C:P	19:BS:78:ARG:HH22	2.43	0.40
9:BI:116:VAL:HG21	10:BJ:62:ARG:HD3	2.04	0.40
22:D1:12:LYS:HD2	22:D1:12:LYS:HA	1.86	0.40
31:CA:1418:G:H2'	31:CA:1579:A:N6	2.36	0.40
31:CA:2190:G:H2'	31:CA:2191:A:C8	2.57	0.40
39:DL:113:MET:O	39:DL:116:ILE:HG13	2.19	0.40
40:DM:95:LEU:HD11	40:DM:125:LEU:HD21	2.03	0.40
47:DT:72:THR:CG2	47:DT:108:SER:HB3	2.52	0.40
53:DZ:56:LEU:HA	53:DZ:59:GLU:HG2	2.04	0.40
1:AA:234:C:H4'	17:AQ:66:PRO:HG3	2.03	0.40
1:AA:567:G:H2'	1:AA:568:G:O4'	2.21	0.40
1:BA:268:U:H2'	1:BA:269:C:C6	2.56	0.40
2:BB:111:ILE:HD12	2:BB:152:LYS:HA	2.04	0.40
26:D5:32:LYS:HG2	55:DA:2478:A:H5'	2.03	0.40
31:CA:1131:G:OP1	38:CK:82:GLY:HA2	2.21	0.40
31:CA:1306:C:H5"	31:CA:1306:C:H6	1.86	0.40
36:CH:126:GLY:H	36:CH:146:VAL:HB	1.87	0.40
45:CR:58:ARG:HH11	45:CR:62:ILE:HD11	1.86	0.40
55:DA:2788:C:H2'	55:DA:2789:C:C6	2.57	0.40
24:C3:37:LYS:NZ	31:CA:469:G:O6	2.53	0.40
1:BA:580:C:H2'	1:BA:581:G:O4'	2.21	0.40
6:BF:78:PHE:HA	6:BF:84:VAL:HG11	2.04	0.40
12:BL:74:LEU:HD21	12:BL:80:ILE:HG21	2.03	0.40
31:CA:644:A:H2'	31:CA:645:C:O4'	2.22	0.40
31:CA:1101:U:H2'	31:CA:1102:C:H6	1.87	0.40
31:CA:2327:A:H2'	31:CA:2328:A:C8	2.57	0.40
37:DJ:49:ILE:HG13	37:DJ:55:ILE:HD13	2.03	0.40
49:DV:66:GLN:HG3	55:DA:328:U:O3'	2.22	0.40
55:DA:2339:C:H2'	55:DA:2340:A:C8	2.57	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries

of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	AB	222/224 (99%)	210 (95%)	9 (4%)	3 (1%)	11	39
2	BB	222/224 (99%)	211 (95%)	7 (3%)	4 (2%)	8	33
3	AC	204/206 (99%)	192 (94%)	11 (5%)	1 (0%)	29	64
3	BC	204/206 (99%)	194 (95%)	8 (4%)	2 (1%)	15	48
4	AD	203/205 (99%)	198 (98%)	5 (2%)	0	100	100
4	BD	203/205 (99%)	198 (98%)	5 (2%)	0	100	100
5	AE	153/155 (99%)	147 (96%)	5 (3%)	1 (1%)	22	56
5	BE	148/155 (96%)	132 (89%)	12 (8%)	4 (3%)	5	23
6	AF	104/106 (98%)	101 (97%)	3 (3%)	0	100	100
6	BF	98/106 (92%)	91 (93%)	5 (5%)	2 (2%)	7	30
7	AG	149/151 (99%)	137 (92%)	11 (7%)	1 (1%)	22	56
7	BG	149/151 (99%)	140 (94%)	9 (6%)	0	100	100
8	AH	127/129 (98%)	120 (94%)	7 (6%)	0	100	100
8	BH	127/129 (98%)	119 (94%)	8 (6%)	0	100	100
9	AI	125/127 (98%)	110 (88%)	15 (12%)	0	100	100
9	BI	125/127 (98%)	110 (88%)	15 (12%)	0	100	100
10	AJ	97/99 (98%)	88 (91%)	7 (7%)	2 (2%)	7	29
10	BJ	96/99 (97%)	77 (80%)	14 (15%)	5 (5%)	2	9
11	AK	115/117 (98%)	107 (93%)	6 (5%)	2 (2%)	9	34
11	BK	115/117 (98%)	104 (90%)	9 (8%)	2 (2%)	9	34
12	AL	120/123 (98%)	115 (96%)	5 (4%)	0	100	100
12	BL	120/123 (98%)	114 (95%)	5 (4%)	1 (1%)	19	53
13	AM	112/114 (98%)	103 (92%)	6 (5%)	3 (3%)	5	23
13	BM	112/114 (98%)	102 (91%)	5 (4%)	5 (4%)	2	12
14	AN	98/100 (98%)	88 (90%)	8 (8%)	2 (2%)	7	30
14	BN	98/100 (98%)	90 (92%)	6 (6%)	2 (2%)	7	30
15	AO	86/88 (98%)	84 (98%)	2 (2%)	0	100	100
15	BO	86/88 (98%)	83 (96%)	2 (2%)	1 (1%)	13	43
16	AP	80/82 (98%)	74 (92%)	6 (8%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
16	BP	80/82 (98%)	70 (88%)	8 (10%)	2 (2%)	5 25
17	AQ	78/80 (98%)	70 (90%)	7 (9%)	1 (1%)	12 41
17	BQ	78/80 (98%)	68 (87%)	5 (6%)	5 (6%)	1 5
18	AR	53/55 (96%)	53 (100%)	0	0	100 100
18	BR	53/55 (96%)	50 (94%)	3 (6%)	0	100 100
19	AS	77/79 (98%)	70 (91%)	6 (8%)	1 (1%)	12 41
19	BS	77/79 (98%)	68 (88%)	7 (9%)	2 (3%)	5 24
20	AT	84/86 (98%)	83 (99%)	1 (1%)	0	100 100
20	BT	83/86 (96%)	79 (95%)	3 (4%)	1 (1%)	13 43
21	AU	54/56 (96%)	53 (98%)	1 (2%)	0	100 100
21	BU	54/56 (96%)	53 (98%)	1 (2%)	0	100 100
22	C1	54/56 (96%)	47 (87%)	4 (7%)	3 (6%)	2 8
22	D1	54/56 (96%)	51 (94%)	3 (6%)	0	100 100
23	C2	48/51 (94%)	44 (92%)	2 (4%)	2 (4%)	3 13
23	D2	49/51 (96%)	48 (98%)	1 (2%)	0	100 100
24	C3	44/46 (96%)	41 (93%)	2 (4%)	1 (2%)	6 27
24	D3	44/46 (96%)	43 (98%)	1 (2%)	0	100 100
25	C4	62/64 (97%)	60 (97%)	2 (3%)	0	100 100
25	D4	62/64 (97%)	60 (97%)	2 (3%)	0	100 100
26	C5	36/38 (95%)	34 (94%)	1 (3%)	1 (3%)	5 22
26	D5	36/38 (95%)	36 (100%)	0	0	100 100
27	C0	56/58 (97%)	54 (96%)	0	2 (4%)	3 16
27	D0	57/58 (98%)	56 (98%)	1 (2%)	0	100 100
29	CC	269/272 (99%)	252 (94%)	12 (4%)	5 (2%)	8 32
29	DC	269/272 (99%)	257 (96%)	10 (4%)	2 (1%)	22 56
30	CD	207/209 (99%)	201 (97%)	6 (3%)	0	100 100
32	DD	206/209 (99%)	202 (98%)	4 (2%)	0	100 100
33	CE	199/201 (99%)	191 (96%)	5 (2%)	3 (2%)	10 38
33	DE	199/201 (99%)	194 (98%)	4 (2%)	1 (0%)	29 64
34	CF	175/178 (98%)	168 (96%)	6 (3%)	1 (1%)	25 60
34	DF	175/178 (98%)	169 (97%)	5 (3%)	1 (1%)	25 60

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
35	CG	174/176 (99%)	162 (93%)	7 (4%)	5 (3%)	4 21
35	DG	174/176 (99%)	165 (95%)	8 (5%)	1 (1%)	25 60
36	CH	147/149 (99%)	136 (92%)	6 (4%)	5 (3%)	3 17
36	DH	147/149 (99%)	138 (94%)	6 (4%)	3 (2%)	7 30
37	CJ	132/134 (98%)	125 (95%)	3 (2%)	4 (3%)	4 20
37	DJ	132/134 (98%)	125 (95%)	3 (2%)	4 (3%)	4 20
38	CK	140/142 (99%)	135 (96%)	4 (3%)	1 (1%)	22 56
38	DK	140/142 (99%)	137 (98%)	2 (1%)	1 (1%)	22 56
39	CL	120/123 (98%)	112 (93%)	7 (6%)	1 (1%)	19 53
39	DL	121/123 (98%)	117 (97%)	3 (2%)	1 (1%)	19 53
40	CM	142/144 (99%)	132 (93%)	7 (5%)	3 (2%)	7 29
40	DM	142/144 (99%)	136 (96%)	6 (4%)	0	100 100
41	CN	133/136 (98%)	125 (94%)	7 (5%)	1 (1%)	19 53
41	DN	134/136 (98%)	129 (96%)	5 (4%)	0	100 100
42	CO	118/125 (94%)	111 (94%)	5 (4%)	2 (2%)	9 34
42	DO	123/125 (98%)	116 (94%)	7 (6%)	0	100 100
43	CP	114/117 (97%)	110 (96%)	4 (4%)	0	100 100
43	DP	115/117 (98%)	112 (97%)	3 (3%)	0	100 100
44	CQ	112/114 (98%)	107 (96%)	5 (4%)	0	100 100
44	DQ	112/114 (98%)	107 (96%)	4 (4%)	1 (1%)	17 51
45	CR	115/117 (98%)	113 (98%)	2 (2%)	0	100 100
45	DR	115/117 (98%)	114 (99%)	1 (1%)	0	100 100
46	CS	101/103 (98%)	93 (92%)	5 (5%)	3 (3%)	4 20
46	DS	101/103 (98%)	98 (97%)	2 (2%)	1 (1%)	15 48
47	CT	108/110 (98%)	101 (94%)	5 (5%)	2 (2%)	8 32
47	DT	108/110 (98%)	106 (98%)	2 (2%)	0	100 100
48	CU	91/93 (98%)	86 (94%)	4 (4%)	1 (1%)	14 46
48	DU	91/93 (98%)	85 (93%)	6 (7%)	0	100 100
49	CV	100/103 (97%)	91 (91%)	4 (4%)	5 (5%)	2 10
49	DV	100/103 (97%)	96 (96%)	2 (2%)	2 (2%)	7 30
50	CW	92/94 (98%)	91 (99%)	1 (1%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
50	DW	92/94 (98%)	91 (99%)	1 (1%)	0	100 100
51	CX	73/76 (96%)	72 (99%)	1 (1%)	0	100 100
51	DX	75/76 (99%)	74 (99%)	1 (1%)	0	100 100
52	CY	75/77 (97%)	74 (99%)	1 (1%)	0	100 100
52	DY	75/77 (97%)	74 (99%)	1 (1%)	0	100 100
53	CZ	60/62 (97%)	58 (97%)	1 (2%)	1 (2%)	9 34
53	DZ	60/62 (97%)	59 (98%)	1 (2%)	0	100 100
54	DI	133/135 (98%)	114 (86%)	13 (10%)	6 (4%)	2 12
All	All	11407/11635 (98%)	10791 (95%)	485 (4%)	131 (1%)	14 46

All (131) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	AB	126	PHE
3	AC	156	ARG
13	AM	5	ALA
22	C1	25	VAL
2	BB	126	PHE
3	BC	156	ARG
5	BE	51	GLY
10	BJ	38	GLY
10	BJ	91	ASP
13	BM	7	ILE
16	BP	80	LYS
20	BT	5	LYS
29	CC	158	ALA
29	CC	197	ASN
33	CE	83	VAL
35	CG	119	ALA
35	CG	175	LYS
35	CG	176	LYS
36	CH	10	ALA
37	CJ	19	ASN
38	CK	81	ILE
39	CL	35	VAL
40	CM	29	LYS
41	CN	70	ASP
42	CO	118	ARG
48	CU	88	LYS

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Mol	Chain	Res	Type
49	CV	7	ARG
37	DJ	19	ASN
49	DV	52	LEU
10	AJ	57	VAL
13	AM	105	ASN
14	AN	38	ASP
17	AQ	82	ALA
22	C1	56	ALA
23	C2	5	ILE
23	C2	51	GLU
27	C0	4	THR
27	C0	14	ILE
3	BC	61	ALA
5	BE	110	ALA
6	BF	92	THR
6	BF	98	GLU
10	BJ	57	VAL
12	BL	44	LYS
13	BM	5	ALA
13	BM	105	ASN
13	BM	114	LYS
17	BQ	70	THR
17	BQ	82	ALA
19	BS	6	LYS
29	CC	233	GLY
29	CC	253	LYS
29	DC	233	GLY
29	DC	253	LYS
33	CE	82	GLY
35	CG	46	ALA
37	CJ	25	GLY
40	CM	69	ARG
49	CV	16	GLY
49	CV	17	LYS
35	DG	46	ALA
37	DJ	25	GLY
2	AB	125	THR
2	AB	127	ASP
7	AG	56	LYS
11	AK	54	GLY
11	AK	89	PRO
13	AM	7	ILE

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Mol	Chain	Res	Type
22	C1	26	THR
24	C3	45	SER
2	BB	125	THR
2	BB	127	ASP
5	BE	103	THR
10	BJ	95	GLY
11	BK	54	GLY
11	BK	89	PRO
14	BN	38	ASP
15	BO	88	ARG
17	BQ	17	MET
17	BQ	18	GLU
19	BS	5	LEU
29	CC	108	LYS
33	CE	6	LYS
36	CH	118	PRO
49	CV	89	ASP
33	DE	6	LYS
36	DH	118	PRO
39	DL	108	ARG
46	DS	44	GLY
49	DV	89	ASP
54	DI	70	GLU
54	DI	91	ALA
54	DI	109	LYS
54	DI	130	PRO
5	AE	162	GLU
5	BE	105	ILE
10	BJ	36	VAL
13	BM	4	ILE
36	CH	9	VAL
40	CM	30	THR
42	CO	119	SER
46	CS	55	ASP
47	CT	63	GLY
36	DH	11	ASN
54	DI	88	HIS
19	AS	6	LYS
2	BB	95	ARG
14	BN	22	ALA
36	CH	8	LYS
36	CH	122	LEU

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Mol	Chain	Res	Type
37	CJ	23	PRO
46	CS	48	LYS
46	CS	53	PHE
36	DH	122	LEU
37	DJ	23	PRO
44	DQ	105	GLY
54	DI	108	VAL
14	AN	22	ALA
16	BP	44	SER
35	CG	45	HIS
47	CT	65	ASP
49	CV	52	LEU
53	CZ	62	GLY
38	DK	83	GLY
26	C5	21	GLY
34	CF	62	GLY
37	CJ	32	GLY
34	DF	62	GLY
37	DJ	32	GLY
17	BQ	35	GLY
10	AJ	33	GLY

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	AB	186/186 (100%)	173 (93%)	13 (7%)	15 43
2	BB	186/186 (100%)	173 (93%)	13 (7%)	15 43
3	AC	170/170 (100%)	159 (94%)	11 (6%)	17 46
3	BC	170/170 (100%)	156 (92%)	14 (8%)	11 36
4	AD	172/172 (100%)	162 (94%)	10 (6%)	20 51
4	BD	172/172 (100%)	160 (93%)	12 (7%)	15 43
5	AE	118/118 (100%)	107 (91%)	11 (9%)	9 30
5	BE	113/118 (96%)	95 (84%)	18 (16%)	2 10

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
6	AF	92/92 (100%)	86 (94%)	6 (6%)	17 46
6	BF	87/92 (95%)	77 (88%)	10 (12%)	5 21
7	AG	124/124 (100%)	115 (93%)	9 (7%)	14 41
7	BG	124/124 (100%)	109 (88%)	15 (12%)	5 19
8	AH	104/104 (100%)	93 (89%)	11 (11%)	6 24
8	BH	104/104 (100%)	93 (89%)	11 (11%)	6 24
9	AI	105/105 (100%)	100 (95%)	5 (5%)	25 59
9	BI	105/105 (100%)	100 (95%)	5 (5%)	25 59
10	AJ	87/87 (100%)	81 (93%)	6 (7%)	15 44
10	BJ	86/87 (99%)	78 (91%)	8 (9%)	9 30
11	AK	90/90 (100%)	87 (97%)	3 (3%)	38 70
11	BK	90/90 (100%)	83 (92%)	7 (8%)	12 38
12	AL	102/102 (100%)	92 (90%)	10 (10%)	8 27
12	BL	102/102 (100%)	90 (88%)	12 (12%)	5 20
13	AM	92/92 (100%)	83 (90%)	9 (10%)	8 27
13	BM	92/92 (100%)	85 (92%)	7 (8%)	13 39
14	AN	83/83 (100%)	82 (99%)	1 (1%)	71 88
14	BN	83/83 (100%)	82 (99%)	1 (1%)	71 88
15	AO	76/76 (100%)	71 (93%)	5 (7%)	16 46
15	BO	76/76 (100%)	65 (86%)	11 (14%)	3 13
16	AP	65/65 (100%)	64 (98%)	1 (2%)	65 85
16	BP	65/65 (100%)	63 (97%)	2 (3%)	40 71
17	AQ	74/74 (100%)	67 (90%)	7 (10%)	8 29
17	BQ	74/74 (100%)	66 (89%)	8 (11%)	6 23
18	AR	48/48 (100%)	47 (98%)	1 (2%)	53 80
18	BR	48/48 (100%)	47 (98%)	1 (2%)	53 80
19	AS	70/70 (100%)	63 (90%)	7 (10%)	7 26
19	BS	70/70 (100%)	65 (93%)	5 (7%)	14 43
20	AT	65/65 (100%)	59 (91%)	6 (9%)	9 30
20	BT	65/65 (100%)	55 (85%)	10 (15%)	2 11
21	AU	48/48 (100%)	44 (92%)	4 (8%)	11 35

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
21	BU	48/48 (100%)	44 (92%)	4 (8%)	11 35
22	C1	47/47 (100%)	45 (96%)	2 (4%)	29 62
22	D1	47/47 (100%)	44 (94%)	3 (6%)	17 47
23	C2	45/46 (98%)	44 (98%)	1 (2%)	52 79
23	D2	45/46 (98%)	43 (96%)	2 (4%)	28 62
24	C3	38/38 (100%)	37 (97%)	1 (3%)	46 75
24	D3	38/38 (100%)	37 (97%)	1 (3%)	46 75
25	C4	51/51 (100%)	48 (94%)	3 (6%)	19 50
25	D4	51/51 (100%)	48 (94%)	3 (6%)	19 50
26	C5	34/34 (100%)	32 (94%)	2 (6%)	19 50
26	D5	34/34 (100%)	34 (100%)	0	100 100
27	C0	48/48 (100%)	45 (94%)	3 (6%)	18 48
27	D0	49/48 (102%)	45 (92%)	4 (8%)	11 36
29	CC	216/217 (100%)	202 (94%)	14 (6%)	17 46
29	DC	216/217 (100%)	210 (97%)	6 (3%)	43 74
30	CD	164/164 (100%)	160 (98%)	4 (2%)	49 77
32	DD	163/163 (100%)	160 (98%)	3 (2%)	59 82
33	CE	165/165 (100%)	152 (92%)	13 (8%)	12 37
33	DE	165/165 (100%)	161 (98%)	4 (2%)	49 77
34	CF	148/149 (99%)	133 (90%)	15 (10%)	7 26
34	DF	148/149 (99%)	137 (93%)	11 (7%)	13 41
35	CG	137/137 (100%)	134 (98%)	3 (2%)	52 79
35	DG	137/137 (100%)	132 (96%)	5 (4%)	35 67
36	CH	114/114 (100%)	101 (89%)	13 (11%)	5 21
36	DH	114/114 (100%)	101 (89%)	13 (11%)	5 21
37	CJ	104/104 (100%)	100 (96%)	4 (4%)	33 66
37	DJ	104/104 (100%)	100 (96%)	4 (4%)	33 66
38	CK	116/116 (100%)	110 (95%)	6 (5%)	23 56
38	DK	116/116 (100%)	114 (98%)	2 (2%)	60 83
39	CL	103/104 (99%)	99 (96%)	4 (4%)	32 65
39	DL	104/104 (100%)	99 (95%)	5 (5%)	25 59

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
40	CM	103/103 (100%)	97 (94%)	6 (6%)	20 51
40	DM	103/103 (100%)	99 (96%)	4 (4%)	32 65
41	CN	108/108 (100%)	104 (96%)	4 (4%)	34 66
41	DN	109/108 (101%)	106 (97%)	3 (3%)	43 74
42	CO	100/102 (98%)	95 (95%)	5 (5%)	24 57
42	DO	102/102 (100%)	99 (97%)	3 (3%)	42 73
43	CP	86/87 (99%)	80 (93%)	6 (7%)	15 43
43	DP	87/87 (100%)	84 (97%)	3 (3%)	37 69
44	CQ	99/99 (100%)	93 (94%)	6 (6%)	18 49
44	DQ	99/99 (100%)	97 (98%)	2 (2%)	55 80
45	CR	89/89 (100%)	86 (97%)	3 (3%)	37 69
45	DR	89/89 (100%)	87 (98%)	2 (2%)	52 79
46	CS	84/84 (100%)	79 (94%)	5 (6%)	19 50
46	DS	84/84 (100%)	83 (99%)	1 (1%)	71 88
47	CT	93/93 (100%)	88 (95%)	5 (5%)	22 54
47	DT	93/93 (100%)	92 (99%)	1 (1%)	73 89
48	CU	80/80 (100%)	72 (90%)	8 (10%)	7 26
48	DU	80/80 (100%)	77 (96%)	3 (4%)	33 66
49	CV	83/84 (99%)	79 (95%)	4 (5%)	25 59
49	DV	83/84 (99%)	81 (98%)	2 (2%)	49 77
50	CW	78/78 (100%)	75 (96%)	3 (4%)	33 66
50	DW	78/78 (100%)	76 (97%)	2 (3%)	46 75
51	CX	56/58 (97%)	55 (98%)	1 (2%)	59 82
51	DX	58/58 (100%)	57 (98%)	1 (2%)	60 83
52	CY	67/67 (100%)	63 (94%)	4 (6%)	19 50
52	DY	67/67 (100%)	65 (97%)	2 (3%)	41 72
53	CZ	54/54 (100%)	50 (93%)	4 (7%)	13 41
53	DZ	54/54 (100%)	52 (96%)	2 (4%)	34 66
54	DI	103/103 (100%)	98 (95%)	5 (5%)	25 58
All	All	9461/9484 (100%)	8897 (94%)	564 (6%)	19 50

All (564) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	AB	23	TRP
2	AB	44	GLU
2	AB	73	LYS
2	AB	93	ASN
2	AB	105	LYS
2	AB	125	THR
2	AB	129	LEU
2	AB	130	THR
2	AB	135	LEU
2	AB	137	ARG
2	AB	147	SER
2	AB	161	LEU
2	AB	205	ASP
3	AC	4	LYS
3	AC	14	ILE
3	AC	21	THR
3	AC	33	LEU
3	AC	38	LYS
3	AC	46	GLU
3	AC	107	ARG
3	AC	168	TYR
3	AC	178	LEU
3	AC	185	ASN
3	AC	186	THR
4	AD	5	LEU
4	AD	17	THR
4	AD	22	LYS
4	AD	26	ARG
4	AD	50	ASP
4	AD	132	ILE
4	AD	142	VAL
4	AD	143	VAL
4	AD	194	ASP
4	AD	206	LYS
5	AE	11	LEU
5	AE	14	LYS
5	AE	32	SER
5	AE	46	VAL
5	AE	76	LEU
5	AE	78	ASN
5	AE	82	GLN
5	AE	101	GLU
5	AE	106	ILE

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Mol	Chain	Res	Type
5	AE	123	VAL
5	AE	126	LYS
6	AF	36	ILE
6	AF	69	GLU
6	AF	71	ILE
6	AF	74	LEU
6	AF	89	VAL
6	AF	93	LYS
7	AG	30	LEU
7	AG	36	LYS
7	AG	59	LEU
7	AG	63	GLU
7	AG	92	ARG
7	AG	120	LEU
7	AG	131	LYS
7	AG	133	THR
7	AG	142	HIS
8	AH	3	MET
8	AH	31	LYS
8	AH	47	GLU
8	AH	52	GLU
8	AH	54	ASP
8	AH	60	GLU
8	AH	63	LEU
8	AH	76	GLN
8	AH	90	ASP
8	AH	107	SER
8	AH	108	LYS
9	AI	11	ARG
9	AI	61	LEU
9	AI	63	LEU
9	AI	66	THR
9	AI	99	ARG
10	AJ	6	ILE
10	AJ	62	ARG
10	AJ	63	ASP
10	AJ	88	MET
10	AJ	89	ARG
10	AJ	90	LEU
11	AK	23	ILE
11	AK	55	SER
11	AK	119	ASN

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Mol	Chain	Res	Type
12	AL	24	LEU
12	AL	40	THR
12	AL	55	VAL
12	AL	74	LEU
12	AL	82	ILE
12	AL	88	LYS
12	AL	90	LEU
12	AL	110	ARG
12	AL	115	SER
12	AL	121	ARG
13	AM	7	ILE
13	AM	13	LYS
13	AM	17	ILE
13	AM	27	LYS
13	AM	48	LEU
13	AM	58	ASP
13	AM	63	PHE
13	AM	71	ARG
13	AM	101	ARG
14	AN	31	ILE
15	AO	2	SER
15	AO	24	SER
15	AO	40	GLN
15	AO	70	LEU
15	AO	84	ARG
16	AP	48	GLU
17	AQ	5	ILE
17	AQ	16	LYS
17	AQ	27	ARG
17	AQ	38	ILE
17	AQ	40	ARG
17	AQ	75	LEU
17	AQ	83	VAL
18	AR	47	THR
19	AS	5	LEU
19	AS	7	LYS
19	AS	13	LEU
19	AS	27	ASP
19	AS	33	THR
19	AS	37	ARG
19	AS	56	GLN
20	AT	15	GLU

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Mol	Chain	Res	Type
20	AT	24	ARG
20	AT	27	MET
20	AT	44	LYS
20	AT	48	GLN
20	AT	85	LYS
21	AU	13	ASP
21	AU	16	LEU
21	AU	34	ARG
21	AU	56	HIS
22	C1	10	ARG
22	C1	40	ARG
23	C2	8	LYS
24	C3	1	MET
25	C4	31	HIS
25	C4	45	ARG
25	C4	52	LYS
26	C5	20	ASP
26	C5	26	ILE
27	C0	3	LYS
27	C0	19	LYS
27	C0	36	VAL
2	BB	18	HIS
2	BB	23	TRP
2	BB	44	GLU
2	BB	93	ASN
2	BB	105	LYS
2	BB	125	THR
2	BB	129	LEU
2	BB	130	THR
2	BB	135	LEU
2	BB	137	ARG
2	BB	147	SER
2	BB	161	LEU
2	BB	205	ASP
3	BC	4	LYS
3	BC	14	ILE
3	BC	33	LEU
3	BC	37	PHE
3	BC	38	LYS
3	BC	46	GLU
3	BC	55	ILE
3	BC	107	ARG

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Mol	Chain	Res	Type
3	BC	152	GLU
3	BC	168	TYR
3	BC	175	LEU
3	BC	185	ASN
3	BC	186	THR
3	BC	193	TYR
4	BD	5	LEU
4	BD	17	THR
4	BD	22	LYS
4	BD	26	ARG
4	BD	47	ARG
4	BD	50	ASP
4	BD	142	VAL
4	BD	143	VAL
4	BD	151	LYS
4	BD	173	VAL
4	BD	194	ASP
4	BD	206	LYS
5	BE	11	LEU
5	BE	14	LYS
5	BE	32	SER
5	BE	46	VAL
5	BE	76	LEU
5	BE	81	LEU
5	BE	82	GLN
5	BE	88	VAL
5	BE	101	GLU
5	BE	103	THR
5	BE	114	VAL
5	BE	115	LEU
5	BE	123	VAL
5	BE	126	LYS
5	BE	151	GLU
5	BE	152	MET
5	BE	157	ARG
5	BE	159	LYS
6	BF	9	MET
6	BF	14	GLN
6	BF	16	GLU
6	BF	36	ILE
6	BF	53	LYS
6	BF	68	GLN

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Mol	Chain	Res	Type
6	BF	69	GLU
6	BF	71	ILE
6	BF	89	VAL
6	BF	93	LYS
7	BG	4	ARG
7	BG	5	ARG
7	BG	10	ARG
7	BG	30	LEU
7	BG	36	LYS
7	BG	48	GLU
7	BG	50	LEU
7	BG	59	LEU
7	BG	63	GLU
7	BG	72	THR
7	BG	92	ARG
7	BG	120	LEU
7	BG	131	LYS
7	BG	133	THR
7	BG	142	HIS
8	BH	3	MET
8	BH	47	GLU
8	BH	52	GLU
8	BH	60	GLU
8	BH	76	GLN
8	BH	77	ARG
8	BH	80	ARG
8	BH	83	LEU
8	BH	90	ASP
8	BH	107	SER
8	BH	108	LYS
9	BI	11	ARG
9	BI	61	LEU
9	BI	63	LEU
9	BI	66	THR
9	BI	99	ARG
10	BJ	5	ARG
10	BJ	6	ILE
10	BJ	62	ARG
10	BJ	63	ASP
10	BJ	78	GLU
10	BJ	88	MET
10	BJ	89	ARG

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Mol	Chain	Res	Type
10	BJ	90	LEU
11	BK	18	ASP
11	BK	23	ILE
11	BK	31	ILE
11	BK	38	GLN
11	BK	55	SER
11	BK	118	HIS
11	BK	119	ASN
12	BL	24	LEU
12	BL	44	LYS
12	BL	50	ARG
12	BL	55	VAL
12	BL	58	THR
12	BL	74	LEU
12	BL	82	ILE
12	BL	88	LYS
12	BL	90	LEU
12	BL	110	ARG
12	BL	115	SER
12	BL	121	ARG
13	BM	11	ASP
13	BM	13	LYS
13	BM	16	VAL
13	BM	17	ILE
13	BM	27	LYS
13	BM	48	LEU
13	BM	101	ARG
14	BN	26	GLU
15	BO	2	SER
15	BO	13	SER
15	BO	17	ARG
15	BO	24	SER
15	BO	40	GLN
15	BO	64	ARG
15	BO	66	LEU
15	BO	84	ARG
15	BO	87	LEU
15	BO	88	ARG
15	BO	89	ARG
16	BP	20	VAL
16	BP	46	LYS
17	BQ	17	MET

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Mol	Chain	Res	Type
17	BQ	21	ILE
17	BQ	26	GLU
17	BQ	27	ARG
17	BQ	38	ILE
17	BQ	40	ARG
17	BQ	51	ASN
17	BQ	75	LEU
18	BR	47	THR
19	BS	6	LYS
19	BS	7	LYS
19	BS	13	LEU
19	BS	33	THR
19	BS	37	ARG
20	BT	15	GLU
20	BT	24	ARG
20	BT	43	ASP
20	BT	48	GLN
20	BT	54	MET
20	BT	58	VAL
20	BT	64	LYS
20	BT	67	ILE
20	BT	69	LYS
20	BT	84	ASN
21	BU	13	ASP
21	BU	16	LEU
21	BU	34	ARG
21	BU	56	HIS
22	D1	18	SER
22	D1	26	THR
22	D1	29	SER
23	D2	5	ILE
23	D2	8	LYS
24	D3	1	MET
25	D4	31	HIS
25	D4	45	ARG
25	D4	52	LYS
27	D0	10	THR
27	D0	19	LYS
27	D0	25	LEU
27	D0	36	VAL
29	CC	11	PRO
29	CC	117	GLN

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Mol	Chain	Res	Type
29	CC	120	VAL
29	CC	130	LEU
29	CC	157	SER
29	CC	168	ASP
29	CC	174	LEU
29	CC	195	VAL
29	CC	204	VAL
29	CC	205	LEU
29	CC	236	GLU
29	CC	252	THR
29	CC	258	ARG
29	CC	260	ASN
30	CD	4	LEU
30	CD	13	ARG
30	CD	18	ASP
30	CD	95	SER
29	DC	70	ASN
29	DC	117	GLN
29	DC	120	VAL
29	DC	130	LEU
29	DC	236	GLU
29	DC	252	THR
32	DD	13	ARG
32	DD	18	ASP
32	DD	95	SER
33	CE	7	ASP
33	CE	12	LEU
33	CE	25	GLU
33	CE	44	ARG
33	CE	72	SER
33	CE	78	TRP
33	CE	83	VAL
33	CE	107	SER
33	CE	122	GLU
33	CE	127	GLU
33	CE	149	ILE
33	CE	152	GLU
33	CE	189	THR
34	CF	18	THR
34	CF	36	LEU
34	CF	57	LEU
34	CF	72	LYS

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Mol	Chain	Res	Type
34	CF	80	ARG
34	CF	94	GLU
34	CF	106	ILE
34	CF	115	ARG
34	CF	117	LEU
34	CF	123	ASP
34	CF	134	GLU
34	CF	141	ILE
34	CF	149	VAL
34	CF	152	LEU
34	CF	174	ASP
35	CG	11	VAL
35	CG	18	LYS
35	CG	155	GLU
36	CH	7	ASP
36	CH	15	LEU
36	CH	17	ASP
36	CH	21	VAL
36	CH	48	GLU
36	CH	51	ARG
36	CH	53	GLU
36	CH	55	GLU
36	CH	62	LEU
36	CH	75	LEU
36	CH	121	VAL
36	CH	127	GLU
36	CH	145	ASN
37	CJ	11	LEU
37	CJ	13	VAL
37	CJ	28	LEU
37	CJ	113	LYS
38	CK	5	THR
38	CK	9	GLU
38	CK	30	THR
38	CK	39	LYS
38	CK	124	VAL
38	CK	142	ILE
39	CL	35	VAL
39	CL	58	LEU
39	CL	98	ARG
39	CL	113	MET
40	CM	2	ARG

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Mol	Chain	Res	Type
40	CM	21	ARG
40	CM	93	ASN
40	CM	94	THR
40	CM	100	ILE
40	CM	115	GLU
41	CN	6	ARG
41	CN	20	LEU
41	CN	59	ARG
41	CN	78	LEU
42	CO	2	ARG
42	CO	14	SER
42	CO	71	ARG
42	CO	76	VAL
42	CO	95	THR
43	CP	18	LEU
43	CP	31	THR
43	CP	38	GLN
43	CP	49	VAL
43	CP	56	LYS
43	CP	78	VAL
44	CQ	2	SER
44	CQ	26	VAL
44	CQ	39	ARG
44	CQ	40	LEU
44	CQ	102	GLU
44	CQ	114	LEU
45	CR	16	LYS
45	CR	51	ARG
45	CR	52	GLN
46	CS	12	HIS
46	CS	45	GLU
46	CS	48	LYS
46	CS	51	VAL
46	CS	102	SER
47	CT	7	HIS
47	CT	19	LEU
47	CT	29	VAL
47	CT	86	MET
47	CT	97	LEU
48	CU	1	MET
48	CU	2	ILE
48	CU	3	ARG

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Mol	Chain	Res	Type
48	CU	10	VAL
48	CU	24	MET
48	CU	30	ILE
48	CU	49	LYS
48	CU	69	ARG
49	CV	61	LYS
49	CV	72	ILE
49	CV	81	ASP
49	CV	98	SER
50	CW	1	MET
50	CW	7	GLU
50	CW	10	LYS
51	CX	82	ILE
52	CY	25	THR
52	CY	35	SER
52	CY	48	THR
52	CY	71	LEU
53	CZ	18	LEU
53	CZ	19	LEU
53	CZ	38	GLN
53	CZ	58	ASN
33	DE	12	LEU
33	DE	107	SER
33	DE	127	GLU
33	DE	189	THR
34	DF	10	ASP
34	DF	57	LEU
34	DF	72	LYS
34	DF	94	GLU
34	DF	106	ILE
34	DF	117	LEU
34	DF	134	GLU
34	DF	141	ILE
34	DF	149	VAL
34	DF	152	LEU
34	DF	174	ASP
35	DG	3	ARG
35	DG	11	VAL
35	DG	18	LYS
35	DG	56	ASP
35	DG	155	GLU
36	DH	7	ASP

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Mol	Chain	Res	Type
36	DH	15	LEU
36	DH	17	ASP
36	DH	21	VAL
36	DH	48	GLU
36	DH	53	GLU
36	DH	57	LYS
36	DH	58	LEU
36	DH	60	GLU
36	DH	75	LEU
36	DH	121	VAL
36	DH	127	GLU
36	DH	145	ASN
37	DJ	11	LEU
37	DJ	13	VAL
37	DJ	28	LEU
37	DJ	113	LYS
38	DK	124	VAL
38	DK	142	ILE
39	DL	58	LEU
39	DL	76	VAL
39	DL	110	GLU
39	DL	113	MET
39	DL	123	LEU
40	DM	2	ARG
40	DM	91	ASP
40	DM	94	THR
40	DM	115	GLU
41	DN	58	LYS
41	DN	59	ARG
41	DN	100	LYS
42	DO	2	ARG
42	DO	14	SER
42	DO	76	VAL
43	DP	31	THR
43	DP	49	VAL
43	DP	78	VAL
44	DQ	26	VAL
44	DQ	102	GLU
45	DR	41	LYS
45	DR	51	ARG
46	DS	102	SER
47	DT	86	MET

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Mol	Chain	Res	Type
48	DU	1	MET
48	DU	3	ARG
48	DU	10	VAL
49	DV	52	LEU
49	DV	61	LYS
50	DW	7	GLU
50	DW	53	LYS
51	DX	82	ILE
52	DY	25	THR
52	DY	35	SER
53	DZ	19	LEU
53	DZ	38	GLN
54	DI	7	ASP
54	DI	16	SER
54	DI	53	ARG
54	DI	64	VAL
54	DI	117	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (43) such sidechains are listed below:

Mol	Chain	Res	Type
2	AB	18	HIS
2	AB	93	ASN
2	AB	94	HIS
2	AB	120	GLN
4	AD	136	GLN
5	AE	89	HIS
6	AF	63	ASN
7	AG	97	ASN
7	AG	142	HIS
8	AH	4	GLN
10	AJ	58	ASN
20	AT	48	GLN
20	AT	78	ASN
22	C1	6	ASN
22	C1	38	HIS
2	BB	39	HIS
2	BB	93	ASN
2	BB	94	HIS
2	BB	120	GLN
2	BB	168	HIS
4	BD	131	ASN

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Mol	Chain	Res	Type
5	BE	70	ASN
5	BE	89	HIS
5	BE	122	ASN
7	BG	97	ASN
8	BH	4	GLN
8	BH	38	ASN
17	BQ	51	ASN
20	BT	3	ASN
24	D3	26	ASN
25	D4	43	HIS
29	CC	142	HIS
29	DC	142	HIS
33	CE	115	GLN
35	CG	38	ASN
38	CK	138	GLN
43	CP	100	HIS
48	CU	28	ASN
49	CV	74	ASN
51	CX	57	HIS
53	CZ	45	GLN
49	DV	54	GLN
54	DI	122	GLN

5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	1530/1534 (99%)	239 (15%)	27 (1%)
1	BA	1529/1534 (99%)	246 (16%)	28 (1%)
28	CB	117/120 (97%)	11 (9%)	0
28	DB	119/120 (99%)	9 (7%)	0
31	CA	2892/2904 (99%)	426 (14%)	72 (2%)
55	DA	2880/2904 (99%)	367 (12%)	57 (1%)
All	All	9067/9116 (99%)	1298 (14%)	184 (2%)

All (1298) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	4	U
1	AA	5	U
1	AA	9	G
1	AA	22	G

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Mol	Chain	Res	Type
1	AA	32	A
1	AA	39	G
1	AA	47	C
1	AA	48	C
1	AA	50	A
1	AA	51	A
1	AA	52	C
1	AA	69	G
1	AA	71	A
1	AA	72	A
1	AA	74	A
1	AA	80	A
1	AA	81	A
1	AA	82	G
1	AA	83	C
1	AA	85	U
1	AA	86	G
1	AA	88	U
1	AA	89	U
1	AA	90	C
1	AA	92	U
1	AA	94	G
1	AA	95	C
1	AA	108	G
1	AA	120	A
1	AA	130	A
1	AA	131	A
1	AA	137	U
1	AA	141	G
1	AA	142	G
1	AA	143	A
1	AA	144	G
1	AA	149	A
1	AA	159	G
1	AA	163	C
1	AA	168	G
1	AA	177	G
1	AA	183	C
1	AA	197	A
1	AA	205	A
1	AA	210	C
1	AA	211	G

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Mol	Chain	Res	Type
1	AA	212	G
1	AA	226	G
1	AA	240	G
1	AA	245	U
1	AA	247	G
1	AA	250	A
1	AA	251	G
1	AA	266	G
1	AA	267	C
1	AA	289	G
1	AA	321	A
1	AA	328	C
1	AA	329	A
1	AA	330	C
1	AA	332	G
1	AA	346	G
1	AA	348	G
1	AA	352	C
1	AA	354	G
1	AA	367	U
1	AA	372	C
1	AA	373	A
1	AA	384	G
1	AA	398	U
1	AA	406	G
1	AA	411	A
1	AA	412	A
1	AA	413	G
1	AA	414	A
1	AA	421	U
1	AA	422	C
1	AA	424	G
1	AA	429	U
1	AA	430	A
1	AA	436	C
1	AA	457	G
1	AA	458	U
1	AA	463	U
1	AA	466	A
1	AA	467	U
1	AA	468	A
1	AA	474	G

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Mol	Chain	Res	Type
1	AA	481	G
1	AA	484	G
1	AA	486	U
1	AA	495	A
1	AA	509	A
1	AA	511	C
1	AA	527	G7M
1	AA	531	U
1	AA	533	A
1	AA	547	A
1	AA	559	A
1	AA	564	C
1	AA	568	G
1	AA	572	A
1	AA	573	A
1	AA	576	C
1	AA	577	G
1	AA	615	G
1	AA	633	G
1	AA	650	G
1	AA	653	U
1	AA	661	G
1	AA	665	A
1	AA	695	A
1	AA	702	A
1	AA	703	G
1	AA	723	U
1	AA	734	G
1	AA	748	G
1	AA	755	G
1	AA	777	A
1	AA	793	U
1	AA	794	A
1	AA	814	A
1	AA	815	A
1	AA	817	C
1	AA	821	G
1	AA	828	U
1	AA	836	G
1	AA	841	C
1	AA	842	U
1	AA	843	U

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Mol	Chain	Res	Type
1	AA	844	G
1	AA	845	A
1	AA	914	A
1	AA	926	G
1	AA	927	G
1	AA	934	C
1	AA	935	A
1	AA	960	U
1	AA	966	2MG
1	AA	969	A
1	AA	971	G
1	AA	975	A
1	AA	976	G
1	AA	977	A
1	AA	987	G
1	AA	993	G
1	AA	1004	A
1	AA	1009	U
1	AA	1015	G
1	AA	1019	A
1	AA	1024	G
1	AA	1026	G
1	AA	1027	C
1	AA	1028	C
1	AA	1029	U
1	AA	1030	U
1	AA	1031	C
1	AA	1032	G
1	AA	1033	G
1	AA	1036	A
1	AA	1037	C
1	AA	1043	G
1	AA	1053	G
1	AA	1054	C
1	AA	1065	U
1	AA	1086	U
1	AA	1094	G
1	AA	1095	U
1	AA	1098	C
1	AA	1101	A
1	AA	1124	G
1	AA	1125	U

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Mol	Chain	Res	Type
1	AA	1132	C
1	AA	1133	G
1	AA	1136	C
1	AA	1137	C
1	AA	1138	G
1	AA	1139	G
1	AA	1140	C
1	AA	1141	C
1	AA	1142	G
1	AA	1143	G
1	AA	1145	A
1	AA	1152	A
1	AA	1159	U
1	AA	1160	G
1	AA	1168	U
1	AA	1184	G
1	AA	1196	A
1	AA	1197	A
1	AA	1212	U
1	AA	1213	A
1	AA	1214	C
1	AA	1215	G
1	AA	1225	A
1	AA	1226	C
1	AA	1227	A
1	AA	1236	A
1	AA	1238	A
1	AA	1239	A
1	AA	1256	A
1	AA	1257	A
1	AA	1260	G
1	AA	1280	A
1	AA	1281	C
1	AA	1286	U
1	AA	1287	A
1	AA	1300	G
1	AA	1302	C
1	AA	1305	G
1	AA	1312	G
1	AA	1317	C
1	AA	1320	C
1	AA	1346	A

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Mol	Chain	Res	Type
1	AA	1353	G
1	AA	1363	A
1	AA	1370	G
1	AA	1379	G
1	AA	1381	U
1	AA	1398	A
1	AA	1419	G
1	AA	1429	A
1	AA	1441	A
1	AA	1446	A
1	AA	1447	A
1	AA	1448	C
1	AA	1451	U
1	AA	1452	C
1	AA	1453	G
1	AA	1492	A
1	AA	1497	G
1	AA	1499	A
1	AA	1503	A
1	AA	1506	U
1	AA	1507	A
1	AA	1517	G
1	AA	1529	G
1	AA	1530	G
1	AA	1534	A
1	BA	4	U
1	BA	5	U
1	BA	9	G
1	BA	22	G
1	BA	32	A
1	BA	39	G
1	BA	47	C
1	BA	48	C
1	BA	50	A
1	BA	51	A
1	BA	52	C
1	BA	69	G
1	BA	71	A
1	BA	72	A
1	BA	74	A
1	BA	80	A
1	BA	82	G

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Mol	Chain	Res	Type
1	BA	83	C
1	BA	84	U
1	BA	85	U
1	BA	86	G
1	BA	87	C
1	BA	88	U
1	BA	89	U
1	BA	90	C
1	BA	92	U
1	BA	94	G
1	BA	95	C
1	BA	108	G
1	BA	120	A
1	BA	130	A
1	BA	131	A
1	BA	137	U
1	BA	141	G
1	BA	142	G
1	BA	143	A
1	BA	144	G
1	BA	149	A
1	BA	159	G
1	BA	163	C
1	BA	168	G
1	BA	177	G
1	BA	183	C
1	BA	197	A
1	BA	200	G
1	BA	205	A
1	BA	210	C
1	BA	211	G
1	BA	212	G
1	BA	226	G
1	BA	245	U
1	BA	247	G
1	BA	250	A
1	BA	251	G
1	BA	266	G
1	BA	267	C
1	BA	289	G
1	BA	321	A
1	BA	328	C

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Mol	Chain	Res	Type
1	BA	329	A
1	BA	330	C
1	BA	332	G
1	BA	346	G
1	BA	348	G
1	BA	352	C
1	BA	354	G
1	BA	367	U
1	BA	372	C
1	BA	373	A
1	BA	384	G
1	BA	398	U
1	BA	406	G
1	BA	412	A
1	BA	413	G
1	BA	414	A
1	BA	421	U
1	BA	422	C
1	BA	424	G
1	BA	429	U
1	BA	430	A
1	BA	436	C
1	BA	457	G
1	BA	458	U
1	BA	463	U
1	BA	467	U
1	BA	468	A
1	BA	474	G
1	BA	481	G
1	BA	484	G
1	BA	486	U
1	BA	495	A
1	BA	509	A
1	BA	511	C
1	BA	527	G7M
1	BA	531	U
1	BA	532	A
1	BA	533	A
1	BA	547	A
1	BA	559	A
1	BA	564	C
1	BA	568	G

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Mol	Chain	Res	Type
1	BA	572	A
1	BA	573	A
1	BA	576	C
1	BA	577	G
1	BA	615	G
1	BA	633	G
1	BA	650	G
1	BA	653	U
1	BA	661	G
1	BA	665	A
1	BA	695	A
1	BA	702	A
1	BA	703	G
1	BA	723	U
1	BA	734	G
1	BA	748	G
1	BA	755	G
1	BA	777	A
1	BA	793	U
1	BA	794	A
1	BA	814	A
1	BA	815	A
1	BA	817	C
1	BA	821	G
1	BA	828	U
1	BA	836	G
1	BA	839	C
1	BA	840	C
1	BA	841	C
1	BA	842	U
1	BA	843	U
1	BA	844	G
1	BA	845	A
1	BA	846	G
1	BA	914	A
1	BA	926	G
1	BA	927	G
1	BA	934	C
1	BA	935	A
1	BA	960	U
1	BA	966	2MG
1	BA	969	A

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Mol	Chain	Res	Type
1	BA	971	G
1	BA	975	A
1	BA	976	G
1	BA	977	A
1	BA	987	G
1	BA	993	G
1	BA	1004	A
1	BA	1008	U
1	BA	1009	U
1	BA	1015	G
1	BA	1019	A
1	BA	1024	G
1	BA	1026	G
1	BA	1027	C
1	BA	1028	C
1	BA	1029	U
1	BA	1030	U
1	BA	1031	C
1	BA	1032	G
1	BA	1033	G
1	BA	1036	A
1	BA	1037	C
1	BA	1043	G
1	BA	1046	A
1	BA	1053	G
1	BA	1054	C
1	BA	1065	U
1	BA	1070	U
1	BA	1086	U
1	BA	1094	G
1	BA	1095	U
1	BA	1098	C
1	BA	1101	A
1	BA	1124	G
1	BA	1125	U
1	BA	1132	C
1	BA	1133	G
1	BA	1136	C
1	BA	1137	C
1	BA	1138	G
1	BA	1139	G
1	BA	1140	C

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Mol	Chain	Res	Type
1	BA	1141	C
1	BA	1142	G
1	BA	1143	G
1	BA	1145	A
1	BA	1152	A
1	BA	1159	U
1	BA	1160	G
1	BA	1168	U
1	BA	1196	A
1	BA	1197	A
1	BA	1212	U
1	BA	1213	A
1	BA	1214	C
1	BA	1215	G
1	BA	1225	A
1	BA	1226	C
1	BA	1227	A
1	BA	1236	A
1	BA	1238	A
1	BA	1239	A
1	BA	1256	A
1	BA	1257	A
1	BA	1260	G
1	BA	1280	A
1	BA	1281	C
1	BA	1286	U
1	BA	1287	A
1	BA	1300	G
1	BA	1302	C
1	BA	1305	G
1	BA	1312	G
1	BA	1317	C
1	BA	1320	C
1	BA	1346	A
1	BA	1353	G
1	BA	1362	A
1	BA	1363	A
1	BA	1370	G
1	BA	1379	G
1	BA	1381	U
1	BA	1398	A
1	BA	1419	G

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Mol	Chain	Res	Type
1	BA	1429	A
1	BA	1441	A
1	BA	1446	A
1	BA	1447	A
1	BA	1448	C
1	BA	1451	U
1	BA	1452	C
1	BA	1453	G
1	BA	1492	A
1	BA	1493	A
1	BA	1497	G
1	BA	1499	A
1	BA	1503	A
1	BA	1506	U
1	BA	1507	A
1	BA	1517	G
1	BA	1529	G
1	BA	1530	G
1	BA	1534	A
28	CB	9	G
28	CB	25	U
28	CB	35	C
28	CB	45	A
28	CB	56	G
28	CB	57	A
28	CB	88	C
28	CB	89	U
28	CB	90	C
28	CB	99	A
28	CB	109	A
31	CA	10	A
31	CA	14	A
31	CA	34	U
31	CA	36	G
31	CA	42	A
31	CA	46	G
31	CA	49	A
31	CA	58	G
31	CA	63	A
31	CA	71	A
31	CA	74	A
31	CA	75	G

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Mol	Chain	Res	Type
31	CA	80	G
31	CA	83	A
31	CA	84	A
31	CA	101	A
31	CA	102	U
31	CA	118	A
31	CA	119	A
31	CA	120	U
31	CA	138	U
31	CA	139	U
31	CA	140	C
31	CA	141	G
31	CA	142	A
31	CA	143	C
31	CA	196	A
31	CA	199	A
31	CA	200	U
31	CA	215	G
31	CA	216	A
31	CA	221	A
31	CA	222	A
31	CA	248	G
31	CA	265	A
31	CA	266	G
31	CA	272	A
31	CA	276	U
31	CA	277	G
31	CA	278	A
31	CA	279	A
31	CA	285	G
31	CA	311	A
31	CA	329	G
31	CA	330	A
31	CA	343	C
31	CA	346	A
31	CA	352	A
31	CA	353	C
31	CA	362	A
31	CA	371	A
31	CA	372	G
31	CA	385	C
31	CA	386	G

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Mol	Chain	Res	Type
31	CA	399	U
31	CA	404	A
31	CA	405	U
31	CA	411	G
31	CA	420	C
31	CA	424	G
31	CA	425	G
31	CA	451	U
31	CA	480	A
31	CA	481	G
31	CA	491	G
31	CA	503	A
31	CA	504	A
31	CA	505	A
31	CA	508	A
31	CA	517	C
31	CA	531	C
31	CA	532	A
31	CA	543	G
31	CA	544	C
31	CA	546	U
31	CA	547	A
31	CA	549	G
31	CA	550	C
31	CA	551	G
31	CA	555	G
31	CA	556	A
31	CA	563	A
31	CA	571	U
31	CA	573	U
31	CA	575	A
31	CA	586	A
31	CA	603	A
31	CA	613	A
31	CA	614	A
31	CA	615	U
31	CA	627	A
31	CA	637	A
31	CA	645	C
31	CA	647	G
31	CA	654	A
31	CA	655	A

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Mol	Chain	Res	Type
31	CA	670	A
31	CA	684	G
31	CA	685	A
31	CA	686	U
31	CA	695	G
31	CA	717	C
31	CA	730	A
31	CA	740	C
31	CA	746	PSU
31	CA	747	5MU
31	CA	775	G
31	CA	776	G
31	CA	782	A
31	CA	784	G
31	CA	785	G
31	CA	792	A
31	CA	802	A
31	CA	805	G
31	CA	812	C
31	CA	819	A
31	CA	827	U
31	CA	828	U
31	CA	845	A
31	CA	846	U
31	CA	847	U
31	CA	858	G
31	CA	859	G
31	CA	878	A
31	CA	883	G
31	CA	896	A
31	CA	897	C
31	CA	910	A
31	CA	914	G
31	CA	915	C
31	CA	931	U
31	CA	932	U
31	CA	941	A
31	CA	946	C
31	CA	953	G
31	CA	961	C
31	CA	974	G
31	CA	983	A

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Mol	Chain	Res	Type
31	CA	984	A
31	CA	985	C
31	CA	995	C
31	CA	996	A
31	CA	1012	U
31	CA	1013	C
31	CA	1022	G
31	CA	1026	G
31	CA	1033	U
31	CA	1040	A
31	CA	1045	C
31	CA	1046	A
31	CA	1047	G
31	CA	1057	A
31	CA	1061	U
31	CA	1070	A
31	CA	1083	U
31	CA	1088	A
31	CA	1089	A
31	CA	1090	A
31	CA	1091	G
31	CA	1096	A
31	CA	1097	U
31	CA	1111	A
31	CA	1112	G
31	CA	1122	G
31	CA	1128	G
31	CA	1129	A
31	CA	1132	U
31	CA	1133	A
31	CA	1135	C
31	CA	1136	G
31	CA	1142	A
31	CA	1168	G
31	CA	1169	A
31	CA	1170	C
31	CA	1171	G
31	CA	1172	C
31	CA	1175	A
31	CA	1176	U
31	CA	1177	G
31	CA	1179	G

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Mol	Chain	Res	Type
31	CA	1180	U
31	CA	1186	G
31	CA	1210	G
31	CA	1212	G
31	CA	1236	G
31	CA	1238	G
31	CA	1253	A
31	CA	1256	G
31	CA	1266	G
31	CA	1271	G
31	CA	1272	A
31	CA	1273	U
31	CA	1300	G
31	CA	1301	A
31	CA	1313	U
31	CA	1320	C
31	CA	1321	A
31	CA	1328	A
31	CA	1352	U
31	CA	1365	A
31	CA	1376	C
31	CA	1379	U
31	CA	1380	G
31	CA	1383	A
31	CA	1391	U
31	CA	1395	A
31	CA	1416	G
31	CA	1417	C
31	CA	1419	A
31	CA	1420	A
31	CA	1428	C
31	CA	1437	C
31	CA	1452	G
31	CA	1453	A
31	CA	1460	U
31	CA	1482	G
31	CA	1490	A
31	CA	1491	G
31	CA	1493	C
31	CA	1494	A
31	CA	1497	U
31	CA	1509	A

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Mol	Chain	Res	Type
31	CA	1510	G
31	CA	1515	A
31	CA	1523	U
31	CA	1532	A
31	CA	1534	U
31	CA	1535	A
31	CA	1536	C
31	CA	1537	G
31	CA	1565	C
31	CA	1566	A
31	CA	1569	A
31	CA	1578	U
31	CA	1583	A
31	CA	1585	C
31	CA	1607	C
31	CA	1608	A
31	CA	1647	U
31	CA	1648	U
31	CA	1649	G
31	CA	1674	G
31	CA	1695	G
31	CA	1715	G
31	CA	1729	U
31	CA	1730	C
31	CA	1731	G
31	CA	1732	C
31	CA	1738	G
31	CA	1744	A
31	CA	1750	G
31	CA	1764	C
31	CA	1773	A
31	CA	1782	U
31	CA	1800	C
31	CA	1801	A
31	CA	1808	A
31	CA	1816	C
31	CA	1822	C
31	CA	1829	A
31	CA	1869	G
31	CA	1870	C
31	CA	1871	A
31	CA	1872	A

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Mol	Chain	Res	Type
31	CA	1873	G
31	CA	1900	A
31	CA	1906	G
31	CA	1907	G
31	CA	1914	C
31	CA	1929	G
31	CA	1930	G
31	CA	1931	U
31	CA	1937	A
31	CA	1938	A
31	CA	1955	U
31	CA	1967	C
31	CA	1970	A
31	CA	1972	G
31	CA	1991	U
31	CA	1993	U
31	CA	1997	C
31	CA	2022	U
31	CA	2023	C
31	CA	2031	A
31	CA	2033	A
31	CA	2036	C
31	CA	2043	C
31	CA	2055	C
31	CA	2056	G
31	CA	2060	A
31	CA	2061	G
31	CA	2062	A
31	CA	2069	G7M
31	CA	2072	C
31	CA	2080	A
31	CA	2093	G
31	CA	2095	A
31	CA	2100	G
31	CA	2102	G
31	CA	2108	A
31	CA	2110	G
31	CA	2111	U
31	CA	2112	G
31	CA	2113	U
31	CA	2115	G
31	CA	2117	A

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Mol	Chain	Res	Type
31	CA	2118	U
31	CA	2119	A
31	CA	2123	G
31	CA	2124	G
31	CA	2125	G
31	CA	2126	A
31	CA	2127	G
31	CA	2128	G
31	CA	2131	U
31	CA	2132	U
31	CA	2133	G
31	CA	2146	C
31	CA	2147	A
31	CA	2157	G
31	CA	2158	A
31	CA	2159	G
31	CA	2160	C
31	CA	2162	G
31	CA	2164	C
31	CA	2165	C
31	CA	2171	A
31	CA	2172	U
31	CA	2173	A
31	CA	2174	C
31	CA	2178	C
31	CA	2183	A
31	CA	2190	G
31	CA	2198	A
31	CA	2203	U
31	CA	2204	G
31	CA	2211	A
31	CA	2225	A
31	CA	2226	C
31	CA	2238	G
31	CA	2239	G
31	CA	2259	U
31	CA	2268	A
31	CA	2280	G
31	CA	2283	C
31	CA	2287	A
31	CA	2305	U
31	CA	2311	A

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Mol	Chain	Res	Type
31	CA	2322	A
31	CA	2326	C
31	CA	2327	A
31	CA	2333	A
31	CA	2335	A
31	CA	2345	G
31	CA	2347	C
31	CA	2350	C
31	CA	2354	C
31	CA	2361	G
31	CA	2383	G
31	CA	2385	C
31	CA	2388	A
31	CA	2402	U
31	CA	2403	C
31	CA	2406	A
31	CA	2423	U
31	CA	2424	C
31	CA	2425	A
31	CA	2426	A
31	CA	2429	G
31	CA	2430	A
31	CA	2435	A
31	CA	2441	U
31	CA	2448	A
31	CA	2465	C
31	CA	2476	A
31	CA	2491	U
31	CA	2502	G
31	CA	2505	G
31	CA	2518	A
31	CA	2529	G
31	CA	2535	G
31	CA	2547	A
31	CA	2554	U
31	CA	2556	C
31	CA	2566	A
31	CA	2567	G
31	CA	2573	C
31	CA	2578	G
31	CA	2582	G
31	CA	2585	U

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Mol	Chain	Res	Type
31	CA	2603	G
31	CA	2609	U
31	CA	2613	U
31	CA	2629	U
31	CA	2630	G
31	CA	2646	C
31	CA	2661	G
31	CA	2663	G
31	CA	2681	C
31	CA	2682	A
31	CA	2689	U
31	CA	2690	U
31	CA	2714	G
31	CA	2718	G
31	CA	2726	A
31	CA	2744	G
31	CA	2748	A
31	CA	2769	U
31	CA	2778	A
31	CA	2791	G
31	CA	2794	C
31	CA	2799	A
31	CA	2820	A
31	CA	2835	A
31	CA	2836	U
31	CA	2850	A
31	CA	2861	U
31	CA	2865	U
31	CA	2867	G
31	CA	2883	A
31	CA	2884	U
31	CA	2886	A
31	CA	2887	A
31	CA	2891	U
31	CA	2903	U
31	CA	2904	U
28	DB	25	U
28	DB	35	C
28	DB	45	A
28	DB	56	G
28	DB	57	A
28	DB	88	C

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Mol	Chain	Res	Type
28	DB	89	U
28	DB	90	C
28	DB	109	A
55	DA	10	A
55	DA	12	U
55	DA	34	U
55	DA	46	G
55	DA	63	A
55	DA	71	A
55	DA	74	A
55	DA	75	G
55	DA	80	G
55	DA	84	A
55	DA	101	A
55	DA	102	U
55	DA	118	A
55	DA	119	A
55	DA	120	U
55	DA	138	U
55	DA	139	U
55	DA	140	C
55	DA	141	G
55	DA	142	A
55	DA	143	C
55	DA	196	A
55	DA	199	A
55	DA	200	U
55	DA	215	G
55	DA	216	A
55	DA	221	A
55	DA	222	A
55	DA	248	G
55	DA	265	A
55	DA	266	G
55	DA	272	A
55	DA	276	U
55	DA	277	G
55	DA	278	A
55	DA	279	A
55	DA	285	G
55	DA	302	C
55	DA	311	A

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Mol	Chain	Res	Type
55	DA	329	G
55	DA	330	A
55	DA	343	C
55	DA	346	A
55	DA	352	A
55	DA	353	C
55	DA	362	A
55	DA	370	G
55	DA	372	G
55	DA	386	G
55	DA	399	U
55	DA	411	G
55	DA	412	A
55	DA	420	C
55	DA	424	G
55	DA	425	G
55	DA	451	U
55	DA	480	A
55	DA	481	G
55	DA	491	G
55	DA	504	A
55	DA	505	A
55	DA	508	A
55	DA	531	C
55	DA	532	A
55	DA	543	G
55	DA	544	C
55	DA	546	U
55	DA	547	A
55	DA	548	G
55	DA	549	G
55	DA	550	C
55	DA	551	G
55	DA	563	A
55	DA	573	U
55	DA	575	A
55	DA	586	A
55	DA	603	A
55	DA	613	A
55	DA	614	A
55	DA	615	U
55	DA	627	A

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Mol	Chain	Res	Type
55	DA	637	A
55	DA	645	C
55	DA	647	G
55	DA	654	A
55	DA	655	A
55	DA	686	U
55	DA	717	C
55	DA	730	A
55	DA	747	5MU
55	DA	764	A
55	DA	765	C
55	DA	775	G
55	DA	776	G
55	DA	782	A
55	DA	784	G
55	DA	785	G
55	DA	790	U
55	DA	792	A
55	DA	805	G
55	DA	812	C
55	DA	827	U
55	DA	828	U
55	DA	858	G
55	DA	859	G
55	DA	860	U
55	DA	878	A
55	DA	883	G
55	DA	885	C
55	DA	896	A
55	DA	897	C
55	DA	910	A
55	DA	914	G
55	DA	915	C
55	DA	927	A
55	DA	931	U
55	DA	932	U
55	DA	946	C
55	DA	961	C
55	DA	974	G
55	DA	983	A
55	DA	996	A
55	DA	1012	U

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Mol	Chain	Res	Type
55	DA	1013	C
55	DA	1022	G
55	DA	1026	G
55	DA	1033	U
55	DA	1040	A
55	DA	1047	G
55	DA	1057	A
55	DA	1061	U
55	DA	1070	A
55	DA	1083	U
55	DA	1088	A
55	DA	1089	A
55	DA	1090	A
55	DA	1091	G
55	DA	1096	A
55	DA	1097	U
55	DA	1112	G
55	DA	1132	U
55	DA	1133	A
55	DA	1135	C
55	DA	1136	G
55	DA	1142	A
55	DA	1168	G
55	DA	1172	C
55	DA	1174	U
55	DA	1175	A
55	DA	1176	U
55	DA	1177	G
55	DA	1180	U
55	DA	1187	G
55	DA	1237	A
55	DA	1238	G
55	DA	1253	A
55	DA	1256	G
55	DA	1271	G
55	DA	1272	A
55	DA	1273	U
55	DA	1300	G
55	DA	1301	A
55	DA	1329	U
55	DA	1352	U
55	DA	1365	A

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Mol	Chain	Res	Type
55	DA	1379	U
55	DA	1383	A
55	DA	1391	U
55	DA	1416	G
55	DA	1417	C
55	DA	1427	A
55	DA	1428	C
55	DA	1434	A
55	DA	1435	G
55	DA	1452	G
55	DA	1453	A
55	DA	1460	U
55	DA	1482	G
55	DA	1490	A
55	DA	1491	G
55	DA	1493	C
55	DA	1494	A
55	DA	1497	U
55	DA	1508	A
55	DA	1509	A
55	DA	1510	G
55	DA	1515	A
55	DA	1523	U
55	DA	1532	A
55	DA	1534	U
55	DA	1535	A
55	DA	1536	C
55	DA	1537	G
55	DA	1566	A
55	DA	1569	A
55	DA	1578	U
55	DA	1583	A
55	DA	1585	C
55	DA	1607	C
55	DA	1608	A
55	DA	1616	A
55	DA	1647	U
55	DA	1648	U
55	DA	1649	G
55	DA	1674	G
55	DA	1715	G
55	DA	1729	U

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Mol	Chain	Res	Type
55	DA	1730	C
55	DA	1731	G
55	DA	1732	C
55	DA	1738	G
55	DA	1744	A
55	DA	1764	C
55	DA	1773	A
55	DA	1782	U
55	DA	1800	C
55	DA	1801	A
55	DA	1808	A
55	DA	1816	C
55	DA	1829	A
55	DA	1869	G
55	DA	1870	C
55	DA	1871	A
55	DA	1872	A
55	DA	1873	G
55	DA	1906	G
55	DA	1907	G
55	DA	1913	A
55	DA	1914	C
55	DA	1929	G
55	DA	1930	G
55	DA	1931	U
55	DA	1937	A
55	DA	1938	A
55	DA	1955	U
55	DA	1965	C
55	DA	1967	C
55	DA	1970	A
55	DA	1972	G
55	DA	1991	U
55	DA	1993	U
55	DA	1997	C
55	DA	2023	C
55	DA	2031	A
55	DA	2033	A
55	DA	2043	C
55	DA	2055	C
55	DA	2056	G
55	DA	2060	A

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Mol	Chain	Res	Type
55	DA	2061	G
55	DA	2062	A
55	DA	2069	G7M
55	DA	2097	A
55	DA	2100	G
55	DA	2102	G
55	DA	2105	U
55	DA	2111	U
55	DA	2112	G
55	DA	2113	U
55	DA	2116	G
55	DA	2117	A
55	DA	2118	U
55	DA	2119	A
55	DA	2120	G
55	DA	2123	G
55	DA	2125	G
55	DA	2126	A
55	DA	2128	G
55	DA	2131	U
55	DA	2132	U
55	DA	2133	G
55	DA	2134	A
55	DA	2135	A
55	DA	2145	C
55	DA	2146	C
55	DA	2148	G
55	DA	2158	A
55	DA	2159	G
55	DA	2160	C
55	DA	2161	C
55	DA	2162	G
55	DA	2163	A
55	DA	2164	C
55	DA	2165	C
55	DA	2167	U
55	DA	2168	G
55	DA	2169	A
55	DA	2170	A
55	DA	2171	A
55	DA	2172	U
55	DA	2173	A

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Mol	Chain	Res	Type
55	DA	2177	C
55	DA	2178	C
55	DA	2179	C
55	DA	2181	U
55	DA	2183	A
55	DA	2185	U
55	DA	2190	G
55	DA	2198	A
55	DA	2204	G
55	DA	2211	A
55	DA	2225	A
55	DA	2238	G
55	DA	2239	G
55	DA	2268	A
55	DA	2283	C
55	DA	2286	G
55	DA	2287	A
55	DA	2305	U
55	DA	2308	G
55	DA	2312	U
55	DA	2324	U
55	DA	2325	G
55	DA	2333	A
55	DA	2335	A
55	DA	2347	C
55	DA	2383	G
55	DA	2385	C
55	DA	2402	U
55	DA	2403	C
55	DA	2406	A
55	DA	2407	A
55	DA	2423	U
55	DA	2424	C
55	DA	2425	A
55	DA	2431	U
55	DA	2435	A
55	DA	2441	U
55	DA	2448	A
55	DA	2476	A
55	DA	2491	U
55	DA	2502	G
55	DA	2505	G

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Mol	Chain	Res	Type
55	DA	2518	A
55	DA	2529	G
55	DA	2535	G
55	DA	2547	A
55	DA	2556	C
55	DA	2566	A
55	DA	2567	G
55	DA	2573	C
55	DA	2574	G
55	DA	2585	U
55	DA	2603	G
55	DA	2609	U
55	DA	2613	U
55	DA	2629	U
55	DA	2630	G
55	DA	2661	G
55	DA	2663	G
55	DA	2689	U
55	DA	2690	U
55	DA	2714	G
55	DA	2726	A
55	DA	2744	G
55	DA	2748	A
55	DA	2765	A
55	DA	2778	A
55	DA	2791	G
55	DA	2798	U
55	DA	2799	A
55	DA	2811	G
55	DA	2820	A
55	DA	2821	A
55	DA	2836	U
55	DA	2867	G
55	DA	2891	U

All (184) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	AA	5	U
1	AA	70	U
1	AA	88	U
1	AA	89	U

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Mol	Chain	Res	Type
1	AA	209	U
1	AA	413	G
1	AA	429	U
1	AA	485	U
1	AA	576	C
1	AA	653	U
1	AA	702	A
1	AA	793	U
1	AA	841	C
1	AA	842	U
1	AA	884	U
1	AA	992	U
1	AA	1086	U
1	AA	1137	C
1	AA	1139	G
1	AA	1140	C
1	AA	1141	C
1	AA	1225	A
1	AA	1281	C
1	AA	1299	A
1	AA	1397	C
1	AA	1447	A
1	AA	1452	C
1	BA	5	U
1	BA	70	U
1	BA	86	G
1	BA	89	U
1	BA	209	U
1	BA	429	U
1	BA	485	U
1	BA	576	C
1	BA	653	U
1	BA	702	A
1	BA	793	U
1	BA	842	U
1	BA	844	G
1	BA	884	U
1	BA	992	U
1	BA	1008	U
1	BA	1086	U
1	BA	1137	C
1	BA	1139	G

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Mol	Chain	Res	Type
1	BA	1140	C
1	BA	1141	C
1	BA	1225	A
1	BA	1281	C
1	BA	1299	A
1	BA	1362	A
1	BA	1397	C
1	BA	1447	A
1	BA	1452	C
31	CA	83	A
31	CA	101	A
31	CA	138	U
31	CA	141	G
31	CA	177	G
31	CA	196	A
31	CA	199	A
31	CA	221	A
31	CA	271	G
31	CA	278	A
31	CA	310	A
31	CA	345	A
31	CA	403	U
31	CA	404	A
31	CA	451	U
31	CA	503	A
31	CA	506	G
31	CA	555	G
31	CA	620	G
31	CA	764	A
31	CA	784	G
31	CA	846	U
31	CA	973	A
31	CA	984	A
31	CA	1045	C
31	CA	1046	A
31	CA	1061	U
31	CA	1069	A
31	CA	1070	A
31	CA	1088	A
31	CA	1089	A
31	CA	1128	G
31	CA	1141	U

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Mol	Chain	Res	Type
31	CA	1253	A
31	CA	1286	A
31	CA	1300	G
31	CA	1320	C
31	CA	1329	U
31	CA	1379	U
31	CA	1452	G
31	CA	1490	A
31	CA	1497	U
31	CA	1509	A
31	CA	1535	A
31	CA	1536	C
31	CA	1607	C
31	CA	1647	U
31	CA	1730	C
31	CA	1786	A
31	CA	1870	C
31	CA	1871	A
31	CA	2035	G
31	CA	2095	A
31	CA	2119	A
31	CA	2126	A
31	CA	2146	C
31	CA	2157	G
31	CA	2164	C
31	CA	2225	A
31	CA	2282	G
31	CA	2286	G
31	CA	2326	C
31	CA	2423	U
31	CA	2425	A
31	CA	2430	A
31	CA	2680	U
31	CA	2681	C
31	CA	2778	A
31	CA	2779	U
31	CA	2797	U
31	CA	2849	U
31	CA	2873	A
55	DA	138	U
55	DA	141	G
55	DA	199	A

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Mol	Chain	Res	Type
55	DA	271	G
55	DA	278	A
55	DA	370	G
55	DA	403	U
55	DA	503	A
55	DA	620	G
55	DA	764	A
55	DA	784	G
55	DA	859	G
55	DA	961	C
55	DA	984	A
55	DA	1061	U
55	DA	1069	A
55	DA	1070	A
55	DA	1087	G
55	DA	1088	A
55	DA	1089	A
55	DA	1128	G
55	DA	1141	U
55	DA	1142	A
55	DA	1175	A
55	DA	1253	A
55	DA	1286	A
55	DA	1300	G
55	DA	1320	C
55	DA	1490	A
55	DA	1497	U
55	DA	1509	A
55	DA	1535	A
55	DA	1607	C
55	DA	1647	U
55	DA	1730	C
55	DA	1870	C
55	DA	1871	A
55	DA	1936	A
55	DA	2097	A
55	DA	2119	A
55	DA	2127	G
55	DA	2146	C
55	DA	2157	G
55	DA	2158	A
55	DA	2164	C

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Mol	Chain	Res	Type
55	DA	2172	U
55	DA	2286	G
55	DA	2311	A
55	DA	2324	U
55	DA	2406	A
55	DA	2423	U
55	DA	2501	C
55	DA	2585	U
55	DA	2681	C
55	DA	2797	U
55	DA	2798	U
55	DA	2873	A

5.4 Non-standard residues in protein, DNA, RNA chains (i)

75 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
1	2MG	BA	1516	1	18,26,27	0.78	0	16,38,41	0.64	0
55	6MZ	DA	2030	55	18,25,26	0.88	1 (5%)	16,36,39	0.92	1 (6%)
55	5MU	DA	747	55	19,22,23	0.51	0	28,32,35	0.43	0
1	MA6	AA	1518	1	19,26,27	0.86	0	18,38,41	0.93	1 (5%)
31	PSU	CA	746	56,31	18,21,22	0.63	1 (5%)	22,30,33	0.44	0
55	H2U	DA	2449	55	18,21,22	0.47	0	21,30,33	0.50	0
41	4D4	CN	81	41	9,11,12	2.00	2 (22%)	8,13,15	2.39	2 (25%)
31	PSU	CA	2504	31	18,21,22	0.48	0	22,30,33	0.46	0
31	PSU	CA	2580	31	18,21,22	0.47	0	22,30,33	0.68	1 (4%)
1	G7M	AA	527	1	20,26,27	0.85	0	17,39,42	0.86	1 (5%)
55	PSU	DA	1911	55	18,21,22	0.32	0	22,30,33	0.38	0
55	3TD	DA	1915	55	18,22,23	0.50	0	22,32,35	0.52	0
55	PSU	DA	2457	55	18,21,22	0.45	0	22,30,33	0.42	0
31	2MG	CA	2445	31	18,26,27	0.94	0	16,38,41	0.59	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
55	2MG	DA	2445	55	18,26,27	0.88	1 (5%)	16,38,41	0.80	1 (6%)
31	2MA	CA	2503	31	17,25,26	0.79	1 (5%)	17,37,40	0.47	0
1	5MC	AA	967	1	18,22,23	0.30	0	26,32,35	0.37	0
1	UR3	AA	1498	1	19,22,23	0.31	0	26,32,35	0.36	0
32	MEQ	DD	150[A]	32	8,9,10	0.58	0	5,10,12	0.45	0
1	5MC	BA	967	1	18,22,23	0.30	0	26,32,35	0.37	0
55	PSU	DA	746	56,55	18,21,22	1.01	2 (11%)	22,30,33	0.49	0
1	PSU	AA	516	1,56	18,21,22	0.29	0	22,30,33	0.45	0
31	5MU	CA	747	31	19,22,23	0.39	0	28,32,35	0.38	0
31	G7M	CA	2069	31	20,26,27	0.52	0	17,39,42	0.41	0
1	2MG	AA	966	1	18,26,27	0.76	0	16,38,41	0.53	0
1	2MG	BA	966	1	18,26,27	0.76	0	16,38,41	0.50	0
1	4OC	AA	1402	1	20,23,24	0.33	0	26,32,35	0.51	0
1	MA6	BA	1518	1	19,26,27	0.86	0	18,38,41	0.96	1 (5%)
31	PSU	CA	955	31	18,21,22	0.31	0	22,30,33	0.51	0
31	5MC	CA	1962	31	18,22,23	0.28	0	26,32,35	0.35	0
31	PSU	CA	2605	31	18,21,22	0.35	0	22,30,33	0.55	0
55	1MG	DA	745	55	18,26,27	1.09	1 (5%)	19,39,42	0.62	1 (5%)
31	OMG	CA	2251	31	18,26,27	0.77	0	19,38,41	0.58	0
55	PSU	DA	955	55	18,21,22	0.67	1 (5%)	22,30,33	0.62	0
55	OMU	DA	2552	55	19,22,23	0.38	0	26,31,34	0.36	0
1	G7M	BA	527	1	20,26,27	0.87	0	17,39,42	0.75	0
1	PSU	BA	516	1	18,21,22	0.44	0	22,30,33	0.45	0
1	2MG	AA	1516	1	18,26,27	0.84	0	16,38,41	0.63	0
31	PSU	CA	1911	31	18,21,22	0.31	0	22,30,33	0.40	0
55	G7M	DA	2069	55	20,26,27	0.65	0	17,39,42	0.56	0
55	PSU	DA	2504	55	18,21,22	0.71	0	22,30,33	0.44	0
41	4D4	DN	81[B]	-	9,11,12	1.42	1 (11%)	8,13,15	2.41	2 (25%)
1	5MC	AA	1407	1	18,22,23	0.37	0	26,32,35	0.46	0
1	5MC	BA	1407	1	18,22,23	0.36	0	26,32,35	0.44	0
55	2MA	DA	2503	56,55	17,25,26	0.81	1 (5%)	17,37,40	0.51	0
55	2MG	DA	1835	55	18,26,27	0.82	1 (5%)	16,38,41	0.63	0
31	6MZ	CA	1618	31	18,25,26	0.84	0	16,36,39	1.12	2 (12%)
55	OMG	DA	2251	55	18,26,27	0.89	1 (5%)	19,38,41	0.63	0
55	PSU	DA	2604	55	18,21,22	0.61	0	22,30,33	0.63	0
31	OMC	CA	2498	56,31	19,22,23	0.51	0	26,31,34	0.47	0
55	6MZ	DA	1618	55	18,25,26	0.90	0	16,36,39	1.80	2 (12%)
55	PSU	DA	1917	55	18,21,22	0.44	0	22,30,33	0.49	0
31	1MG	CA	745	31	18,26,27	0.81	1 (5%)	19,39,42	0.42	0
1	MA6	BA	1519	1	19,26,27	0.73	0	18,38,41	1.31	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
31	OMU	CA	2552	31	19,22,23	0.32	0	26,31,34	0.30	0
55	PSU	DA	2580	55	18,21,22	0.81	1 (5%)	22,30,33	0.68	0
1	4OC	BA	1402	1	20,23,24	0.45	0	26,32,35	0.51	0
1	UR3	BA	1498	1	19,22,23	0.51	0	26,32,35	0.70	1 (3%)
12	D2T	BL	89	12	7,9,10	0.75	0	6,11,13	0.65	0
31	6MZ	CA	2030	31	18,25,26	0.84	0	16,36,39	0.96	2 (12%)
1	MA6	AA	1519	1	19,26,27	0.75	0	18,38,41	1.33	1 (5%)
32	MEQ	DD	150[B]	32	8,9,10	2.22	1 (12%)	5,10,12	1.71	1 (20%)
55	5MU	DA	1939	55	19,22,23	0.37	0	28,32,35	0.40	0
12	D2T	AL	89	12	7,9,10	1.33	1 (14%)	6,11,13	0.67	0
31	3TD	CA	1915	31	18,22,23	0.49	0	22,32,35	0.50	0
31	PSU	CA	2457	31	18,21,22	0.52	0	22,30,33	0.46	0
55	5MC	DA	1962	55	18,22,23	0.50	0	26,32,35	0.46	0
55	PSU	DA	2605	55	18,21,22	0.45	0	22,30,33	0.55	0
31	2MG	CA	1835	31	18,26,27	0.91	0	16,38,41	0.50	0
31	PSU	CA	1917	31	18,21,22	0.35	0	22,30,33	0.44	0
41	4D4	DN	81[A]	-	9,11,12	2.14	2 (22%)	8,13,15	2.19	2 (25%)
1	2MG	BA	1207	1	18,26,27	0.76	0	16,38,41	0.55	0
55	OMC	DA	2498	56,55	19,22,23	0.39	0	26,31,34	0.57	0
31	5MU	CA	1939	31	19,22,23	0.53	0	28,32,35	0.42	0
1	2MG	AA	1207	1	18,26,27	0.77	0	16,38,41	0.58	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	2MG	BA	1516	1	-	0/5/27/28	0/3/3/3
55	6MZ	DA	2030	55	-	2/5/27/28	0/3/3/3
55	5MU	DA	747	55	-	0/7/25/26	0/2/2/2
1	MA6	AA	1518	1	-	0/7/29/30	0/3/3/3
31	PSU	CA	746	56,31	-	1/7/25/26	0/2/2/2
55	H2U	DA	2449	55	-	1/7/38/39	0/2/2/2
41	4D4	CN	81	41	-	1/11/12/14	-
31	PSU	CA	2504	31	-	1/7/25/26	0/2/2/2
31	PSU	CA	2580	31	-	0/7/25/26	0/2/2/2
1	G7M	AA	527	1	-	2/3/25/26	0/3/3/3
55	PSU	DA	1911	55	-	0/7/25/26	0/2/2/2
55	3TD	DA	1915	55	-	0/7/25/26	0/2/2/2
55	PSU	DA	2457	55	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	2MG	CA	2445	31	-	0/5/27/28	0/3/3/3
55	2MG	DA	2445	55	-	0/5/27/28	0/3/3/3
31	2MA	CA	2503	31	-	2/3/25/26	0/3/3/3
1	5MC	AA	967	1	-	0/7/25/26	0/2/2/2
1	UR3	AA	1498	1	-	0/7/25/26	0/2/2/2
32	MEQ	DD	150[A]	32	-	3/8/9/11	-
1	5MC	BA	967	1	-	0/7/25/26	0/2/2/2
55	PSU	DA	746	56,55	-	1/7/25/26	0/2/2/2
1	PSU	AA	516	1,56	-	0/7/25/26	0/2/2/2
31	5MU	CA	747	31	-	0/7/25/26	0/2/2/2
31	G7M	CA	2069	31	-	2/3/25/26	0/3/3/3
1	2MG	AA	966	1	-	0/5/27/28	0/3/3/3
1	2MG	BA	966	1	-	0/5/27/28	0/3/3/3
1	4OC	AA	1402	1	-	0/9/29/30	0/2/2/2
1	MA6	BA	1518	1	-	0/7/29/30	0/3/3/3
31	PSU	CA	955	31	-	0/7/25/26	0/2/2/2
31	5MC	CA	1962	31	-	0/7/25/26	0/2/2/2
31	PSU	CA	2605	31	-	0/7/25/26	0/2/2/2
55	1MG	DA	745	55	-	0/3/25/26	0/3/3/3
31	OMG	CA	2251	31	-	1/5/27/28	0/3/3/3
55	PSU	DA	955	55	-	0/7/25/26	0/2/2/2
55	OMU	DA	2552	55	-	1/9/27/28	0/2/2/2
1	G7M	BA	527	1	-	2/3/25/26	0/3/3/3
1	PSU	BA	516	1	-	0/7/25/26	0/2/2/2
1	2MG	AA	1516	1	-	0/5/27/28	0/3/3/3
31	PSU	CA	1911	31	-	0/7/25/26	0/2/2/2
55	G7M	DA	2069	55	-	2/3/25/26	0/3/3/3
55	PSU	DA	2504	55	-	1/7/25/26	0/2/2/2
41	4D4	DN	81[B]	-	-	2/11/12/14	-
1	5MC	AA	1407	1	-	0/7/25/26	0/2/2/2
1	5MC	BA	1407	1	-	0/7/25/26	0/2/2/2
55	2MA	DA	2503	56,55	-	2/3/25/26	0/3/3/3
55	2MG	DA	1835	55	-	2/5/27/28	0/3/3/3
31	6MZ	CA	1618	31	-	0/5/27/28	0/3/3/3
55	OMG	DA	2251	55	-	1/5/27/28	0/3/3/3
55	PSU	DA	2604	55	-	0/7/25/26	0/2/2/2
31	OMC	CA	2498	56,31	-	0/9/27/28	0/2/2/2
55	6MZ	DA	1618	55	-	0/5/27/28	0/3/3/3
55	PSU	DA	1917	55	-	0/7/25/26	0/2/2/2
31	1MG	CA	745	31	-	0/3/25/26	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	MA6	BA	1519	1	-	1/7/29/30	0/3/3/3
31	OMU	CA	2552	31	-	1/9/27/28	0/2/2/2
55	PSU	DA	2580	55	-	0/7/25/26	0/2/2/2
1	4OC	BA	1402	1	-	0/9/29/30	0/2/2/2
1	UR3	BA	1498	1	-	0/7/25/26	0/2/2/2
12	D2T	BL	89	12	-	4/7/12/14	-
31	6MZ	CA	2030	31	-	1/5/27/28	0/3/3/3
1	MA6	AA	1519	1	-	1/7/29/30	0/3/3/3
32	MEQ	DD	150[B]	32	-	4/8/9/11	-
55	5MU	DA	1939	55	-	0/7/25/26	0/2/2/2
12	D2T	AL	89	12	-	2/7/12/14	-
31	3TD	CA	1915	31	-	0/7/25/26	0/2/2/2
31	PSU	CA	2457	31	-	0/7/25/26	0/2/2/2
55	5MC	DA	1962	55	-	2/7/25/26	0/2/2/2
55	PSU	DA	2605	55	-	0/7/25/26	0/2/2/2
31	2MG	CA	1835	31	-	2/5/27/28	0/3/3/3
31	PSU	CA	1917	31	-	0/7/25/26	0/2/2/2
41	4D4	DN	81[A]	-	-	0/11/12/14	-
1	2MG	BA	1207	1	-	0/5/27/28	0/3/3/3
55	OMC	DA	2498	56,55	-	0/9/27/28	0/2/2/2
31	5MU	CA	1939	31	-	0/7/25/26	0/2/2/2
1	2MG	AA	1207	1	-	0/5/27/28	0/3/3/3

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	DD	150[B]	MEQ	CB-CA	6.11	1.61	1.53
41	DN	81[A]	4D4	CZ-NE	5.93	1.45	1.33
41	CN	81	4D4	CZ-NE	5.45	1.44	1.33
41	DN	81[B]	4D4	CZ-NE	3.76	1.40	1.33
12	AL	89	D2T	CB-SB	2.80	1.85	1.82
55	DA	745	1MG	C8-N7	-2.77	1.30	1.35
55	DA	746	PSU	O4'-C1'	-2.76	1.40	1.43
55	DA	746	PSU	C2'-C1'	-2.65	1.50	1.53
55	DA	2580	PSU	O4'-C1'	-2.54	1.40	1.43
55	DA	2251	OMG	C5-C6	-2.35	1.42	1.47
31	CA	746	PSU	O4'-C1'	-2.33	1.40	1.43
41	DN	81[A]	4D4	CZ-NH1	2.18	1.43	1.34
55	DA	1835	2MG	C8-N7	-2.14	1.31	1.35
41	CN	81	4D4	CZ-NH1	2.14	1.43	1.34
55	DA	955	PSU	C2'-C1'	-2.14	1.51	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	DA	2030	6MZ	O5'-C5'	-2.12	1.39	1.44
55	DA	2445	2MG	O3'-C3'	-2.11	1.38	1.43
55	DA	2503	2MA	C8-N7	-2.10	1.31	1.35
31	CA	2503	2MA	C8-N7	-2.09	1.31	1.35
31	CA	745	1MG	C8-N7	-2.06	1.31	1.35

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
55	DA	1618	6MZ	C9-N6-C6	6.56	128.52	122.87
41	CN	81	4D4	NE-CZ-NH2	5.63	130.60	120.70
41	DN	81[B]	4D4	NE-CZ-NH2	5.50	130.36	120.70
41	DN	81[A]	4D4	NE-CZ-NH2	5.14	129.72	120.70
1	AA	1519	MA6	N1-C6-N6	-4.73	112.08	117.06
1	BA	1519	MA6	N1-C6-N6	-4.62	112.19	117.06
32	DD	150[B]	MEQ	CB-CG-CD	3.81	121.54	113.04
41	DN	81[B]	4D4	NH1-CZ-NE	-3.70	110.65	119.19
41	CN	81	4D4	NH1-CZ-NE	-3.27	111.64	119.19
31	CA	1618	6MZ	C9-N6-C6	3.27	125.69	122.87
41	DN	81[A]	4D4	NH1-CZ-NE	-2.76	112.83	119.19
1	BA	1498	UR3	C4-N3-C2	-2.66	122.06	124.56
1	BA	1518	MA6	N1-C6-N6	-2.58	114.34	117.06
31	CA	1618	6MZ	C2-N1-C6	2.38	118.63	116.59
31	CA	2030	6MZ	C2-N1-C6	2.38	118.63	116.59
55	DA	2030	6MZ	C2-N1-C6	2.38	118.63	116.59
31	CA	2030	6MZ	C9-N6-C6	2.36	124.91	122.87
1	AA	527	G7M	O4'-C1'-C2'	-2.35	103.49	106.93
55	DA	2445	2MG	O6-C6-C5	2.28	128.82	124.37
1	AA	1518	MA6	N1-C6-N6	-2.20	114.74	117.06
55	DA	1618	6MZ	C2-N1-C6	2.15	118.43	116.59
55	DA	745	1MG	O4'-C4'-C3'	-2.09	100.97	105.11
31	CA	2580	PSU	O4'-C1'-C2'	2.06	108.06	105.14

There are no chirality outliers.

All (48) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	AA	527	G7M	O4'-C4'-C5'-O5'
1	AA	527	G7M	C3'-C4'-C5'-O5'
12	AL	89	D2T	SB-CB-CG-OD2
1	BA	527	G7M	O4'-C4'-C5'-O5'
1	BA	527	G7M	C3'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
12	BL	89	D2T	CG-CB-SB-CB1
12	BL	89	D2T	CA-CB-CG-OD1
12	BL	89	D2T	CA-CB-CG-OD2
31	CA	2251	OMG	C1'-C2'-O2'-CM2
32	DD	150[B]	MEQ	N-CA-CB-CG
55	DA	2030	6MZ	O4'-C4'-C5'-O5'
41	DN	81[B]	4D4	CA-CB-CG-CD
32	DD	150[A]	MEQ	OE1-CD-CG-CB
32	DD	150[A]	MEQ	NE2-CD-CG-CB
55	DA	2030	6MZ	C3'-C4'-C5'-O5'
41	DN	81[B]	4D4	OB-CB-CG-CD
32	DD	150[A]	MEQ	CA-CB-CG-CD
32	DD	150[B]	MEQ	C-CA-CB-CG
31	CA	1835	2MG	O4'-C4'-C5'-O5'
12	AL	89	D2T	CG-CB-SB-CB1
55	DA	2069	G7M	C4'-C5'-O5'-P
31	CA	2030	6MZ	O4'-C4'-C5'-O5'
1	AA	1519	MA6	C5-C6-N6-C9
1	BA	1519	MA6	C5-C6-N6-C9
31	CA	1835	2MG	C3'-C4'-C5'-O5'
55	DA	1835	2MG	O4'-C4'-C5'-O5'
32	DD	150[B]	MEQ	CA-CB-CG-CD
31	CA	2069	G7M	C4'-C5'-O5'-P
55	DA	2503	2MA	C4'-C5'-O5'-P
55	DA	1835	2MG	C3'-C4'-C5'-O5'
32	DD	150[B]	MEQ	OE1-CD-NE2-CE
31	CA	2503	2MA	C4'-C5'-O5'-P
41	CN	81	4D4	CG-CD-NE-CZ
12	BL	89	D2T	SB-CB-CG-OD2
31	CA	2504	PSU	O4'-C4'-C5'-O5'
55	DA	2251	OMG	C1'-C2'-O2'-CM2
31	CA	2552	OMU	C3'-C2'-O2'-CM2
55	DA	1962	5MC	O4'-C1'-N1-C6
31	CA	746	PSU	O4'-C1'-C5-C6
55	DA	746	PSU	O4'-C1'-C5-C6
55	DA	2069	G7M	O4'-C4'-C5'-O5'
55	DA	2552	OMU	C3'-C2'-O2'-CM2
31	CA	2069	G7M	O4'-C4'-C5'-O5'
31	CA	2503	2MA	O4'-C4'-C5'-O5'
55	DA	2503	2MA	O4'-C4'-C5'-O5'
55	DA	2504	PSU	O4'-C4'-C5'-O5'
55	DA	1962	5MC	C2'-C1'-N1-C6

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Mol	Chain	Res	Type	Atoms
55	DA	2449	H2U	C4'-C5'-O5'-P

There are no ring outliers.

15 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
55	DA	2030	6MZ	1	0
55	DA	747	5MU	1	0
1	AA	1518	MA6	1	0
55	DA	2449	H2U	1	0
31	CA	2445	2MG	1	0
55	DA	2445	2MG	1	0
31	CA	2503	2MA	1	0
31	CA	747	5MU	1	0
1	BA	1518	MA6	1	0
41	DN	81[B]	4D4	1	0
1	BA	1519	MA6	1	0
31	CA	2030	6MZ	2	0
1	AA	1519	MA6	1	0
32	DD	150[B]	MEQ	1	0
55	DA	2498	OMC	1	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 554 ligands modelled in this entry, 472 are monoatomic - leaving 82 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
63	EDO	DA	3003	-	3,3,3	0.77	0	2,2,2	0.11	0
63	EDO	D1	101	-	3,3,3	0.68	0	2,2,2	0.15	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
59	PUT	DA	3002	-	5,5,5	0.19	0	4,4,4	0.09	0
63	EDO	DB	210	-	3,3,3	0.61	0	2,2,2	0.22	0
69	TRS	DA	3219	-	7,7,7	0.29	0	9,9,9	0.29	0
59	PUT	DA	3218	-	5,5,5	0.14	0	4,4,4	0.12	0
58	MPD	DA	3206	-	7,7,7	1.05	1 (14%)	9,10,10	0.54	0
59	PUT	DA	3220	-	5,5,5	0.19	0	4,4,4	0.13	0
58	MPD	AA	1671	-	7,7,7	0.72	0	9,10,10	0.45	0
62	PEG	D3	102	-	6,6,6	0.33	0	5,5,5	0.25	0
62	PEG	DA	3200	-	6,6,6	0.51	0	5,5,5	0.28	0
64	PGE	DS	201	-	9,9,9	0.48	0	8,8,8	0.49	0
63	EDO	DA	3001	-	3,3,3	0.86	0	2,2,2	0.10	0
64	PGE	DA	3216	-	9,9,9	0.13	0	8,8,8	0.25	0
58	MPD	DA	3209	-	7,7,7	0.72	0	9,10,10	0.39	0
65	SPD	DA	3223	-	9,9,9	0.18	0	8,8,8	0.67	0
62	PEG	DA	3226	-	6,6,6	0.42	0	5,5,5	0.28	0
59	PUT	DA	3222	-	5,5,5	0.29	0	4,4,4	0.30	0
58	MPD	AA	1676	-	7,7,7	0.62	0	9,10,10	0.42	0
57	PG4	DQ	202	-	12,12,12	0.15	0	11,11,11	0.16	0
59	PUT	DA	3184	-	5,5,5	0.24	0	4,4,4	0.16	0
63	EDO	DA	3207	-	3,3,3	0.72	0	2,2,2	0.16	0
58	MPD	DA	3190	-	7,7,7	0.49	0	9,10,10	0.47	0
59	PUT	DA	3212	-	5,5,5	0.37	0	4,4,4	0.31	0
59	PUT	DA	3211	-	5,5,5	0.31	0	4,4,4	0.16	0
59	PUT	DA	3188	-	5,5,5	0.43	0	4,4,4	0.27	0
59	PUT	DA	3204	-	5,5,5	0.35	0	4,4,4	0.28	0
63	EDO	DA	3197	-	3,3,3	0.65	0	2,2,2	0.22	0
66	1PE	DA	3185	-	15,15,15	0.16	0	14,14,14	0.16	0
64	PGE	D1	102	-	9,9,9	0.30	0	8,8,8	0.30	0
59	PUT	DA	3195	-	5,5,5	0.32	0	4,4,4	0.51	0
58	MPD	DT	202	-	7,7,7	0.84	0	9,10,10	0.43	0
64	PGE	D3	101	-	9,9,9	0.29	0	8,8,8	0.23	0
62	PEG	AL	201	-	6,6,6	0.25	0	5,5,5	0.13	0
66	1PE	DA	3202	-	15,15,15	0.35	0	14,14,14	0.40	0
60	T1C	BA	1643	56	44,45,45	0.99	3 (6%)	53,72,72	1.41	2 (3%)
67	ACY	DA	3201	-	3,3,3	0.95	0	3,3,3	0.99	0
64	PGE	DD	301	-	9,9,9	0.29	0	8,8,8	0.33	0
62	PEG	D1	103	-	6,6,6	0.42	0	5,5,5	0.15	0
62	PEG	DA	3199	-	6,6,6	0.30	0	5,5,5	0.21	0
57	PG4	DS	202	-	12,12,12	0.47	0	11,11,11	0.43	0
63	EDO	DA	3214	-	3,3,3	0.68	0	2,2,2	0.23	0
58	MPD	DE	301	-	7,7,7	0.87	0	9,10,10	0.78	0
58	MPD	DA	3203	-	7,7,7	0.92	0	9,10,10	0.65	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
64	PGE	DU	101	-	9,9,9	0.25	0	8,8,8	0.38	0
57	PG4	DA	3215	-	12,12,12	0.17	0	11,11,11	0.13	0
57	PG4	BA	1642	-	12,12,12	0.20	0	11,11,11	0.22	0
67	ACY	DA	3196	-	3,3,3	1.39	1 (33%)	3,3,3	0.91	0
67	ACY	DA	3191	-	3,3,3	0.98	0	3,3,3	0.97	0
59	PUT	DA	3189	-	5,5,5	0.47	0	4,4,4	0.42	0
58	MPD	DT	201	-	7,7,7	0.63	0	9,10,10	0.20	0
62	PEG	DP	201	-	6,6,6	0.29	0	5,5,5	0.17	0
57	PG4	DA	3193	-	12,12,12	0.30	0	11,11,11	0.43	0
59	PUT	DA	3221	-	5,5,5	0.45	0	4,4,4	0.62	0
59	PUT	AA	1674	-	5,5,5	0.16	0	4,4,4	0.15	0
63	EDO	DA	3004	-	3,3,3	0.74	0	2,2,2	0.12	0
63	EDO	DB	211	-	3,3,3	0.61	0	2,2,2	0.17	0
64	PGE	DA	3186	-	9,9,9	0.35	0	8,8,8	0.56	0
62	PEG	DL	201	-	6,6,6	0.13	0	5,5,5	0.12	0
64	PGE	DA	3224	-	9,9,9	0.24	0	8,8,8	0.18	0
58	MPD	DS	203	-	7,7,7	0.42	0	9,10,10	0.69	0
65	SPD	DA	3205	-	9,9,9	0.24	0	8,8,8	0.18	0
63	EDO	DA	3198	-	3,3,3	0.68	0	2,2,2	0.38	0
62	PEG	DA	3217	-	6,6,6	0.29	0	5,5,5	0.09	0
58	MPD	DE	302	-	7,7,7	0.93	1 (14%)	9,10,10	0.47	0
62	PEG	DQ	201	-	6,6,6	0.21	0	5,5,5	0.15	0
58	MPD	DN	201	-	7,7,7	1.12	1 (14%)	9,10,10	0.60	0
64	PGE	DA	3213	-	9,9,9	0.16	0	8,8,8	0.18	0
68	GUN	DA	3210	-	7,12,12	0.72	0	8,17,17	0.80	0
63	EDO	DA	3194	-	3,3,3	0.66	0	2,2,2	0.07	0
57	PG4	AA	1670	-	12,12,12	0.27	0	11,11,11	0.41	0
62	PEG	DA	3225	-	6,6,6	0.49	0	5,5,5	0.27	0
59	PUT	AA	1672	-	5,5,5	0.22	0	4,4,4	0.18	0
60	T1C	AA	1677	56	44,45,45	1.01	4 (9%)	53,72,72	1.43	3 (5%)
65	SPD	DA	3187	-	9,9,9	0.17	0	8,8,8	0.42	0
65	SPD	DA	3183	-	9,9,9	0.13	0	8,8,8	0.20	0
63	EDO	DA	3208	-	3,3,3	0.59	0	2,2,2	0.30	0
57	PG4	DR	202	-	12,12,12	0.43	0	11,11,11	0.54	0
58	MPD	DK	201	-	7,7,7	0.76	0	9,10,10	0.26	0
58	MPD	DA	3192	-	7,7,7	0.71	0	9,10,10	0.81	0
59	PUT	AA	1675	-	5,5,5	0.21	0	4,4,4	0.22	0
59	PUT	AA	1673	-	5,5,5	0.16	0	4,4,4	0.15	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns.

'-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
63	EDO	DA	3003	-	-	0/1/1/1	-
63	EDO	D1	101	-	-	0/1/1/1	-
59	PUT	DA	3002	-	-	0/3/3/3	-
63	EDO	DB	210	-	-	0/1/1/1	-
69	TRS	DA	3219	-	-	0/9/9/9	-
59	PUT	DA	3218	-	-	0/3/3/3	-
58	MPD	DA	3206	-	-	1/5/5/5	-
59	PUT	DA	3220	-	-	0/3/3/3	-
58	MPD	AA	1671	-	-	1/5/5/5	-
62	PEG	D3	102	-	-	2/4/4/4	-
62	PEG	DA	3200	-	-	3/4/4/4	-
64	PGE	DS	201	-	-	3/7/7/7	-
63	EDO	DA	3001	-	-	1/1/1/1	-
64	PGE	DA	3216	-	-	4/7/7/7	-
58	MPD	DA	3209	-	-	1/5/5/5	-
65	SPD	DA	3223	-	-	4/7/7/7	-
62	PEG	DA	3226	-	-	0/4/4/4	-
59	PUT	DA	3222	-	-	1/3/3/3	-
58	MPD	AA	1676	-	-	2/5/5/5	-
57	PG4	DQ	202	-	-	1/10/10/10	-
59	PUT	DA	3184	-	-	0/3/3/3	-
63	EDO	DA	3207	-	-	0/1/1/1	-
58	MPD	DA	3190	-	-	2/5/5/5	-
59	PUT	DA	3212	-	-	1/3/3/3	-
59	PUT	DA	3211	-	-	0/3/3/3	-
59	PUT	DA	3188	-	-	0/3/3/3	-
59	PUT	DA	3204	-	-	1/3/3/3	-
63	EDO	DA	3197	-	-	0/1/1/1	-
66	1PE	DA	3185	-	-	5/13/13/13	-
64	PGE	D1	102	-	-	4/7/7/7	-
59	PUT	DA	3195	-	-	1/3/3/3	-
58	MPD	DT	202	-	-	2/5/5/5	-
64	PGE	D3	101	-	-	2/7/7/7	-
62	PEG	AL	201	-	-	2/4/4/4	-
66	1PE	DA	3202	-	-	8/13/13/13	-
60	T1C	BA	1643	56	-	11/22/80/80	0/4/4/4
64	PGE	DD	301	-	-	4/7/7/7	-
62	PEG	D1	103	-	-	1/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
62	PEG	DA	3199	-	-	3/4/4/4	-
57	PG4	DS	202	-	-	2/10/10/10	-
63	EDO	DA	3214	-	-	0/1/1/1	-
58	MPD	DE	301	-	-	5/5/5/5	-
58	MPD	DA	3203	-	-	1/5/5/5	-
64	PGE	DU	101	-	-	4/7/7/7	-
57	PG4	DA	3215	-	-	4/10/10/10	-
57	PG4	BA	1642	-	-	0/10/10/10	-
59	PUT	DA	3189	-	-	0/3/3/3	-
58	MPD	DT	201	-	-	2/5/5/5	-
62	PEG	DP	201	-	-	2/4/4/4	-
57	PG4	DA	3193	-	-	8/10/10/10	-
59	PUT	DA	3221	-	-	1/3/3/3	-
59	PUT	AA	1674	-	-	0/3/3/3	-
63	EDO	DA	3004	-	-	0/1/1/1	-
63	EDO	DB	211	-	-	0/1/1/1	-
64	PGE	DA	3186	-	-	4/7/7/7	-
62	PEG	DL	201	-	-	2/4/4/4	-
64	PGE	DA	3224	-	-	4/7/7/7	-
58	MPD	DS	203	-	-	0/5/5/5	-
65	SPD	DA	3205	-	-	5/7/7/7	-
63	EDO	DA	3198	-	-	1/1/1/1	-
62	PEG	DA	3217	-	-	3/4/4/4	-
58	MPD	DE	302	-	-	2/5/5/5	-
62	PEG	DQ	201	-	-	2/4/4/4	-
58	MPD	DN	201	-	-	4/5/5/5	-
64	PGE	DA	3213	-	-	2/7/7/7	-
68	GUN	DA	3210	-	-	-	0/2/2/2
63	EDO	DA	3194	-	-	1/1/1/1	-
57	PG4	AA	1670	-	-	4/10/10/10	-
62	PEG	DA	3225	-	-	2/4/4/4	-
59	PUT	AA	1672	-	-	0/3/3/3	-
60	T1C	AA	1677	56	-	8/22/80/80	0/4/4/4
65	SPD	DA	3187	-	-	0/7/7/7	-
65	SPD	DA	3183	-	-	1/7/7/7	-
63	EDO	DA	3208	-	-	0/1/1/1	-
57	PG4	DR	202	-	-	6/10/10/10	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
58	MPD	DK	201	-	-	2/5/5/5	-
58	MPD	DA	3192	-	-	2/5/5/5	-
59	PUT	AA	1675	-	-	1/3/3/3	-
59	PUT	AA	1673	-	-	0/3/3/3	-

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
60	BA	1643	T1C	C4-C3	3.26	1.58	1.51
60	AA	1677	T1C	C4-C3	2.87	1.57	1.51
60	BA	1643	T1C	C7-N7	2.61	1.49	1.42
60	AA	1677	T1C	C7-C61	2.58	1.43	1.40
58	DN	201	MPD	C3-C2	2.57	1.60	1.53
60	AA	1677	T1C	C7-N7	2.54	1.49	1.42
60	BA	1643	T1C	C7-C61	2.48	1.43	1.40
58	DA	3206	MPD	C3-C2	2.41	1.60	1.53
58	DE	302	MPD	C3-C2	2.20	1.59	1.53
67	DA	3196	ACY	OXT-C	2.10	1.40	1.30
60	AA	1677	T1C	C4-N4	2.03	1.51	1.47

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
60	BA	1643	T1C	C92-N92-C93	6.96	124.57	115.84
60	AA	1677	T1C	C92-N92-C93	6.83	124.40	115.84
60	BA	1643	T1C	C8-C9-C10	-4.64	115.88	120.49
60	AA	1677	T1C	C8-C9-C10	-4.18	116.33	120.49
60	AA	1677	T1C	C6-C61-C1A	2.44	122.38	118.09

There are no chirality outliers.

All (156) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
58	AA	1676	MPD	C2-C3-C4-O4
58	DE	301	MPD	C1-C2-C3-C4
58	DE	301	MPD	O2-C2-C3-C4
58	DE	301	MPD	C2-C3-C4-O4
58	DN	201	MPD	CM-C2-C3-C4
58	DT	202	MPD	C2-C3-C4-C5
58	DA	3190	MPD	C2-C3-C4-O4
58	DA	3190	MPD	C2-C3-C4-C5

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Mol	Chain	Res	Type	Atoms
60	AA	1677	T1C	C95-C93-N92-C92
60	AA	1677	T1C	C96-C93-N92-C92
60	BA	1643	T1C	C1-C2-C21-O21
60	BA	1643	T1C	C1-C2-C21-N21
57	DR	202	PG4	O3-C5-C6-O4
66	DA	3202	1PE	OH6-C15-C25-OH5
64	DA	3213	PGE	O2-C3-C4-O3
65	DA	3205	SPD	C3-C4-C5-N6
60	AA	1677	T1C	C94-C93-N92-C92
57	DA	3193	PG4	O3-C5-C6-O4
57	DR	202	PG4	O2-C3-C4-O3
66	DA	3202	1PE	OH4-C13-C23-OH3
57	DS	202	PG4	O4-C7-C8-O5
64	DA	3186	PGE	O3-C5-C6-O4
66	DA	3185	1PE	OH2-C12-C22-OH3
57	DQ	202	PG4	O1-C1-C2-O2
64	DU	101	PGE	O3-C5-C6-O4
60	BA	1643	T1C	C92-C91-N9-C9
59	DA	3195	PUT	C1-C2-C3-C4
64	DS	201	PGE	O3-C5-C6-O4
63	DA	3194	EDO	O1-C1-C2-O2
65	DA	3205	SPD	C4-C5-N6-C7
65	DA	3205	SPD	C8-C7-N6-C5
62	D1	103	PEG	O2-C3-C4-O4
62	DL	201	PEG	O2-C3-C4-O4
62	DA	3199	PEG	O2-C3-C4-O4
62	DA	3200	PEG	O2-C3-C4-O4
64	DA	3186	PGE	O1-C1-C2-O2
64	DA	3224	PGE	O3-C5-C6-O4
66	DA	3202	1PE	OH2-C12-C22-OH3
59	DA	3204	PUT	C1-C2-C3-C4
65	DA	3205	SPD	C2-C3-C4-C5
60	BA	1643	T1C	O91-C91-N9-C9
64	DD	301	PGE	O2-C3-C4-O3
64	DA	3224	PGE	O1-C1-C2-O2
59	DA	3222	PUT	C1-C2-C3-C4
57	DR	202	PG4	C5-C6-O4-C7
62	DA	3217	PEG	O2-C3-C4-O4
59	DA	3212	PUT	C1-C2-C3-C4
64	DU	101	PGE	O1-C1-C2-O2
58	DN	201	MPD	O2-C2-C3-C4
65	DA	3223	SPD	C4-C5-N6-C7

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Mol	Chain	Res	Type	Atoms
62	DA	3199	PEG	O1-C1-C2-O2
64	DD	301	PGE	O3-C5-C6-O4
57	DR	202	PG4	C6-C5-O3-C4
57	DA	3193	PG4	C1-C2-O2-C3
62	DL	201	PEG	C4-C3-O2-C2
62	DP	201	PEG	C1-C2-O2-C3
57	AA	1670	PG4	C4-C3-O2-C2
64	D3	101	PGE	C3-C4-O3-C5
57	DA	3215	PG4	C3-C4-O3-C5
66	DA	3185	1PE	C12-C22-OH3-C23
62	AL	201	PEG	C1-C2-O2-C3
60	AA	1677	T1C	C91-C92-N92-C93
60	BA	1643	T1C	C91-C92-N92-C93
57	DA	3215	PG4	C1-C2-O2-C3
57	AA	1670	PG4	C3-C4-O3-C5
62	DA	3199	PEG	C1-C2-O2-C3
62	DA	3200	PEG	C1-C2-O2-C3
66	DA	3202	1PE	C16-C26-OH6-C15
57	DA	3193	PG4	C4-C3-O2-C2
62	DA	3225	PEG	C1-C2-O2-C3
64	DA	3213	PGE	C4-C3-O2-C2
62	DA	3225	PEG	C4-C3-O2-C2
62	DA	3217	PEG	O1-C1-C2-O2
66	DA	3185	1PE	C16-C26-OH6-C15
57	AA	1670	PG4	C5-C6-O4-C7
57	DA	3215	PG4	C8-C7-O4-C6
62	DP	201	PEG	C4-C3-O2-C2
66	DA	3202	1PE	C12-C22-OH3-C23
64	DD	301	PGE	C4-C3-O2-C2
57	DR	202	PG4	C4-C3-O2-C2
60	BA	1643	T1C	O91-C91-C92-N92
58	DA	3192	MPD	C2-C3-C4-C5
60	BA	1643	T1C	C3-C2-C21-N21
66	DA	3185	1PE	C24-C14-OH5-C25
57	AA	1670	PG4	O1-C1-C2-O2
63	DA	3001	EDO	O1-C1-C2-O2
62	DA	3200	PEG	C4-C3-O2-C2
60	BA	1643	T1C	C3-C2-C21-O21
64	DA	3216	PGE	C3-C4-O3-C5
62	DA	3217	PEG	C1-C2-O2-C3
58	DE	302	MPD	C2-C3-C4-O4
58	DA	3192	MPD	C2-C3-C4-O4

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Mol	Chain	Res	Type	Atoms
64	DA	3224	PGE	C1-C2-O2-C3
58	DE	301	MPD	CM-C2-C3-C4
58	DN	201	MPD	C1-C2-C3-C4
58	DT	201	MPD	C1-C2-C3-C4
64	DA	3216	PGE	C4-C3-O2-C2
59	AA	1675	PUT	C1-C2-C3-C4
64	DA	3224	PGE	C3-C4-O3-C5
60	AA	1677	T1C	O91-C91-N9-C9
57	DA	3193	PG4	C3-C4-O3-C5
65	DA	3223	SPD	C3-C4-C5-N6
59	DA	3221	PUT	C1-C2-C3-C4
57	DR	202	PG4	C3-C4-O3-C5
65	DA	3205	SPD	N6-C7-C8-C9
62	AL	201	PEG	C4-C3-O2-C2
63	DA	3198	EDO	O1-C1-C2-O2
60	BA	1643	T1C	N9-C91-C92-N92
64	D1	102	PGE	O3-C5-C6-O4
64	DA	3186	PGE	C3-C4-O3-C5
66	DA	3202	1PE	C15-C25-OH5-C14
64	D1	102	PGE	C3-C4-O3-C5
57	DA	3193	PG4	C6-C5-O3-C4
64	D1	102	PGE	C4-C3-O2-C2
64	DS	201	PGE	C6-C5-O3-C4
64	DU	101	PGE	C6-C5-O3-C4
64	DA	3186	PGE	C4-C3-O2-C2
57	DS	202	PG4	O2-C3-C4-O3
57	DA	3193	PG4	C8-C7-O4-C6
64	DD	301	PGE	C3-C4-O3-C5
64	DA	3216	PGE	C1-C2-O2-C3
62	D3	102	PEG	C1-C2-O2-C3
58	DT	201	MPD	O2-C2-C3-C4
57	DA	3193	PG4	O4-C7-C8-O5
64	DU	101	PGE	O2-C3-C4-O3
65	DA	3183	SPD	C8-C7-N6-C5
66	DA	3185	1PE	C13-C23-OH3-C22
60	AA	1677	T1C	C92-C91-N9-C9
57	DA	3193	PG4	O2-C3-C4-O3
65	DA	3223	SPD	C8-C7-N6-C5
64	DA	3216	PGE	O2-C3-C4-O3
64	D3	101	PGE	C4-C3-O2-C2
65	DA	3223	SPD	C7-C8-C9-N10
57	DA	3215	PG4	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
62	DQ	201	PEG	O1-C1-C2-O2
60	AA	1677	T1C	C61-C7-N7-C72
64	DS	201	PGE	O2-C3-C4-O3
64	D1	102	PGE	O2-C3-C4-O3
62	D3	102	PEG	O1-C1-C2-O2
60	BA	1643	T1C	C61-C7-N7-C71
58	AA	1676	MPD	C2-C3-C4-C5
58	DE	301	MPD	C2-C3-C4-C5
58	DE	302	MPD	C2-C3-C4-C5
58	DK	201	MPD	C2-C3-C4-C5
58	DA	3203	MPD	C2-C3-C4-C5
58	DA	3206	MPD	C2-C3-C4-C5
60	AA	1677	T1C	C61-C7-N7-C71
66	DA	3202	1PE	OH5-C14-C24-OH4
62	DQ	201	PEG	C1-C2-O2-C3
60	BA	1643	T1C	C61-C7-N7-C72
58	AA	1671	MPD	C2-C3-C4-O4
58	DK	201	MPD	C2-C3-C4-O4
58	DN	201	MPD	C2-C3-C4-O4
58	DT	202	MPD	C2-C3-C4-O4
58	DA	3209	MPD	C2-C3-C4-O4
66	DA	3202	1PE	C14-C24-OH4-C13

There are no ring outliers.

30 monomers are involved in 48 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
69	DA	3219	TRS	1	0
59	DA	3218	PUT	1	0
62	D3	102	PEG	2	0
62	DA	3200	PEG	1	0
64	DA	3216	PGE	1	0
65	DA	3223	SPD	4	0
59	DA	3222	PUT	1	0
58	DA	3190	MPD	1	0
59	DA	3212	PUT	1	0
63	DA	3197	EDO	1	0
64	D1	102	PGE	2	0
59	DA	3195	PUT	3	0
64	DD	301	PGE	2	0
62	D1	103	PEG	1	0
57	DS	202	PG4	1	0

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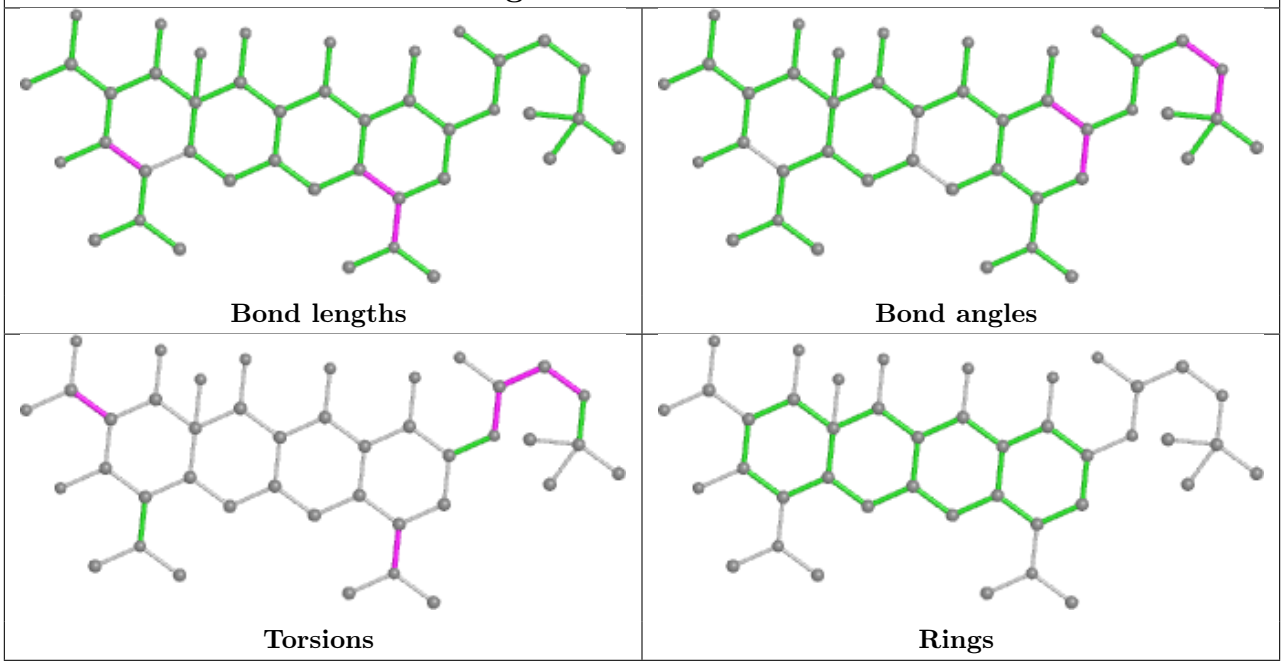
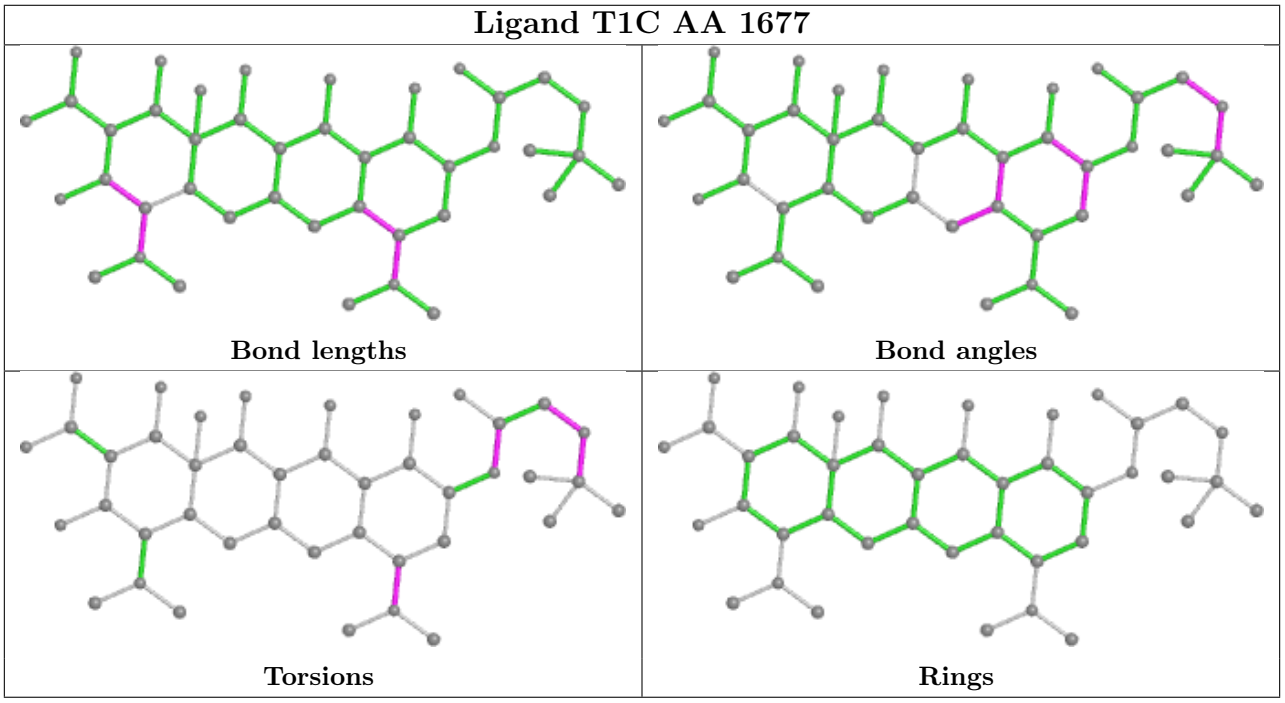
Mol	Chain	Res	Type	Clashes	Symm-Clashes
58	DA	3203	MPD	2	0
64	DU	101	PGE	1	0
57	DA	3215	PG4	1	0
59	DA	3189	PUT	1	0
62	DP	201	PEG	1	0
57	DA	3193	PG4	1	0
59	DA	3221	PUT	3	0
63	DB	211	EDO	1	0
64	DA	3224	PGE	3	0
58	DN	201	MPD	1	0
64	DA	3213	PGE	1	0
63	DA	3194	EDO	1	0
57	AA	1670	PG4	1	0
57	DR	202	PG4	5	0
58	DA	3192	MPD	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand T1C BA 1643



Ligand T1C AA 1677



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	AA	1523/1534 (99%)	0.70	105 (6%) 16 10	46, 105, 241, 293	0
1	BA	1522/1534 (99%)	1.53	397 (26%) 0 0	61, 140, 279, 284	0
2	AB	224/224 (100%)	1.62	72 (32%) 0 0	83, 127, 202, 270	0
2	BB	224/224 (100%)	1.76	78 (34%) 0 0	99, 144, 211, 261	0
3	AC	206/206 (100%)	0.82	30 (14%) 2 1	80, 108, 141, 163	0
3	BC	206/206 (100%)	2.64	116 (56%) 0 0	115, 151, 190, 231	0
4	AD	205/205 (100%)	0.62	18 (8%) 10 5	64, 103, 131, 154	0
4	BD	205/205 (100%)	0.20	1 (0%) 91 81	61, 81, 107, 131	0
5	AE	155/155 (100%)	0.77	13 (8%) 11 6	67, 91, 133, 169	0
5	BE	150/155 (96%)	1.17	33 (22%) 0 0	77, 97, 144, 227	0
6	AF	106/106 (100%)	0.83	19 (17%) 1 1	82, 105, 128, 142	0
6	BF	100/106 (94%)	0.97	15 (15%) 2 1	86, 121, 146, 154	0
7	AG	151/151 (100%)	2.15	64 (42%) 0 0	107, 137, 166, 179	0
7	BG	151/151 (100%)	5.30	125 (82%) 0 0	147, 202, 218, 228	0
8	AH	129/129 (100%)	0.64	9 (6%) 16 9	71, 91, 118, 136	0
8	BH	129/129 (100%)	1.02	24 (18%) 1 0	91, 116, 150, 168	0
9	AI	127/127 (100%)	2.31	58 (45%) 0 0	96, 132, 169, 200	0
9	BI	127/127 (100%)	3.78	78 (61%) 0 0	138, 176, 209, 229	0
10	AJ	99/99 (100%)	2.03	41 (41%) 0 0	94, 121, 153, 168	0
10	BJ	98/99 (98%)	4.86	78 (79%) 0 0	141, 171, 197, 207	0
11	AK	117/117 (100%)	1.61	35 (29%) 0 0	68, 112, 147, 163	0
11	BK	117/117 (100%)	1.47	33 (28%) 0 0	83, 116, 148, 168	0
12	AL	122/123 (99%)	0.60	4 (3%) 46 30	55, 72, 104, 132	0
12	BL	122/123 (99%)	1.39	31 (25%) 0 0	79, 97, 118, 142	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
13	AM	114/114 (100%)	2.48	57 (50%) 0 0	106, 131, 182, 202	0
13	BM	114/114 (100%)	5.54	104 (91%) 0 0	203, 237, 245, 249	0
14	AN	100/100 (100%)	1.81	37 (37%) 0 0	90, 117, 206, 215	0
14	BN	100/100 (100%)	3.85	75 (75%) 0 0	132, 181, 239, 250	0
15	AO	88/88 (100%)	0.69	10 (11%) 5 3	72, 94, 112, 132	0
15	BO	88/88 (100%)	1.25	20 (22%) 0 0	79, 112, 132, 150	0
16	AP	82/82 (100%)	1.27	19 (23%) 0 0	67, 86, 121, 139	0
16	BP	82/82 (100%)	2.79	48 (58%) 0 0	94, 111, 157, 166	0
17	AQ	80/80 (100%)	0.65	4 (5%) 28 18	70, 86, 119, 143	0
17	BQ	80/80 (100%)	2.17	34 (42%) 0 0	100, 128, 151, 156	0
18	AR	55/55 (100%)	1.21	13 (23%) 0 0	79, 99, 135, 164	0
18	BR	55/55 (100%)	1.07	6 (10%) 5 3	80, 96, 129, 157	0
19	AS	79/79 (100%)	1.56	24 (30%) 0 0	103, 119, 156, 164	0
19	BS	79/79 (100%)	5.06	66 (83%) 0 0	215, 232, 243, 251	0
20	AT	86/86 (100%)	1.04	9 (10%) 6 4	70, 85, 120, 133	0
20	BT	85/86 (98%)	3.27	53 (62%) 0 0	108, 128, 165, 179	0
21	AU	56/56 (100%)	1.59	18 (32%) 0 0	83, 123, 159, 172	0
21	BU	56/56 (100%)	1.01	8 (14%) 2 1	80, 106, 149, 160	0
22	C1	56/56 (100%)	3.35	39 (69%) 0 0	110, 150, 178, 195	0
22	D1	56/56 (100%)	0.59	0 100 100	26, 46, 71, 102	0
23	C2	50/51 (98%)	3.69	34 (68%) 0 0	133, 148, 161, 183	0
23	D2	51/51 (100%)	0.72	5 (9%) 7 4	55, 69, 95, 110	0
24	C3	46/46 (100%)	4.62	39 (84%) 0 0	108, 117, 127, 138	0
24	D3	46/46 (100%)	0.61	2 (4%) 35 22	38, 46, 61, 104	0
25	C4	64/64 (100%)	3.11	44 (68%) 0 0	112, 130, 142, 148	0
25	D4	64/64 (100%)	0.57	0 100 100	36, 44, 53, 68	0
26	C5	38/38 (100%)	2.71	23 (60%) 0 0	108, 122, 133, 143	0
26	D5	38/38 (100%)	0.64	1 (2%) 56 39	43, 54, 68, 91	0
27	C0	58/58 (100%)	3.36	39 (67%) 0 0	104, 121, 140, 143	0
27	D0	58/58 (100%)	0.52	0 100 100	33, 40, 60, 72	0
28	CB	118/120 (98%)	1.71	45 (38%) 0 0	140, 195, 250, 254	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
28	DB	120/120 (100%)	0.30	0 100 100	33, 60, 99, 143	0
29	CC	271/272 (99%)	1.49	88 (32%) 0 0	88, 119, 152, 165	0
29	DC	271/272 (99%)	0.30	6 (2%) 62 45	31, 57, 83, 96	0
30	CD	209/209 (100%)	3.00	130 (62%) 0 0	103, 134, 170, 190	0
31	CA	2876/2904 (99%)	1.90	1023 (35%) 0 0	73, 178, 274, 295	0
32	DD	208/209 (99%)	0.16	0 100 100	22, 41, 69, 91	0
33	CE	201/201 (100%)	3.31	140 (69%) 0 0	119, 167, 201, 218	0
33	DE	201/201 (100%)	0.38	3 (1%) 73 57	31, 59, 101, 141	0
34	CF	177/178 (99%)	4.96	152 (85%) 0 0	204, 217, 226, 233	0
34	DF	177/178 (99%)	0.68	16 (9%) 9 5	58, 84, 125, 138	0
35	CG	176/176 (100%)	4.32	144 (81%) 0 0	140, 181, 219, 228	0
35	DG	176/176 (100%)	0.34	8 (4%) 33 21	49, 73, 99, 128	0
36	CH	149/149 (100%)	2.34	80 (53%) 0 0	86, 156, 175, 183	0
36	DH	149/149 (100%)	2.10	63 (42%) 0 0	79, 157, 193, 208	0
37	CJ	134/134 (100%)	7.53	127 (94%) 0 0	236, 253, 264, 272	0
37	DJ	134/134 (100%)	5.79	110 (82%) 0 0	204, 229, 238, 246	0
38	CK	142/142 (100%)	2.31	72 (50%) 0 0	105, 129, 168, 221	0
38	DK	142/142 (100%)	0.11	0 100 100	25, 37, 61, 75	0
39	CL	122/123 (99%)	1.70	43 (35%) 0 0	95, 116, 149, 167	0
39	DL	123/123 (100%)	0.09	0 100 100	30, 46, 71, 109	0
40	CM	144/144 (100%)	4.11	116 (80%) 0 0	113, 163, 214, 236	0
40	DM	144/144 (100%)	0.32	3 (2%) 63 46	21, 58, 88, 117	0
41	CN	135/136 (99%)	1.38	35 (25%) 0 0	98, 119, 150, 189	0
41	DN	135/136 (99%)	-0.02	0 100 100	28, 43, 69, 88	0
42	CO	120/125 (96%)	2.71	72 (60%) 0 0	110, 132, 155, 186	0
42	DO	125/125 (100%)	0.22	1 (0%) 86 73	29, 39, 68, 111	0
43	CP	116/117 (99%)	3.84	87 (75%) 0 0	147, 171, 185, 189	0
43	DP	117/117 (100%)	0.28	0 100 100	47, 60, 87, 97	0
44	CQ	114/114 (100%)	2.53	65 (57%) 0 0	108, 126, 156, 172	0
44	DQ	114/114 (100%)	0.14	3 (2%) 56 39	34, 52, 82, 114	0
45	CR	117/117 (100%)	2.82	71 (60%) 0 0	98, 138, 174, 199	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
45	DR	117/117 (100%)	0.29	1 (0%) 84 71	23, 33, 48, 70	0
46	CS	103/103 (100%)	4.11	85 (82%) 0 0	114, 143, 185, 201	0
46	DS	103/103 (100%)	0.13	1 (0%) 82 68	26, 45, 71, 93	0
47	CT	110/110 (100%)	2.50	62 (56%) 0 0	109, 137, 180, 193	0
47	DT	110/110 (100%)	0.10	0 100 100	21, 36, 60, 118	0
48	CU	93/93 (100%)	3.96	73 (78%) 0 0	131, 156, 184, 194	0
48	DU	93/93 (100%)	0.63	5 (5%) 25 16	37, 60, 114, 130	0
49	CV	102/103 (99%)	5.48	88 (86%) 0 0	119, 167, 203, 213	0
49	DV	102/103 (99%)	0.55	11 (10%) 5 3	47, 64, 112, 144	0
50	CW	94/94 (100%)	2.59	53 (56%) 0 0	125, 145, 165, 170	0
50	DW	94/94 (100%)	0.06	0 100 100	38, 56, 80, 92	0
51	CX	75/76 (98%)	2.94	38 (50%) 0 0	111, 134, 148, 178	0
51	DX	76/76 (100%)	0.09	1 (1%) 77 61	31, 45, 69, 107	0
52	CY	77/77 (100%)	1.91	32 (41%) 0 0	103, 122, 147, 168	0
52	DY	77/77 (100%)	0.30	1 (1%) 77 61	37, 59, 92, 108	0
53	CZ	62/62 (100%)	4.42	49 (79%) 0 0	134, 171, 184, 195	0
53	DZ	62/62 (100%)	0.77	6 (9%) 7 4	52, 75, 111, 132	0
54	DI	135/135 (100%)	2.40	71 (52%) 0 0	82, 158, 202, 211	1 (0%)
55	DA	2873/2904 (98%)	0.64	135 (4%) 31 20	22, 48, 215, 300	0
All	All	20634/20751 (99%)	1.61	5723 (27%) 0 0	21, 116, 247, 300	1 (0%)

All (5723) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
37	DJ	54	PRO	42.4
9	BI	128	SER	22.8
37	CJ	13	VAL	22.8
37	DJ	76	ALA	22.6
37	DJ	55	ILE	21.9
37	CJ	69	PHE	21.1
37	CJ	76	ALA	21.0
37	DJ	53	LEU	21.0
37	CJ	14	ALA	18.4
34	CF	128	TYR	18.2
37	CJ	11	LEU	18.0

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Mol	Chain	Res	Type	RSRZ
37	CJ	12	GLN	17.9
37	DJ	114	ALA	17.9
9	BI	16	ALA	17.0
51	CX	54	GLY	16.4
37	DJ	79	LEU	16.2
9	BI	31	ASN	16.1
10	BJ	41	PRO	16.1
49	CV	80	ALA	16.0
49	CV	31	SER	15.6
9	AI	130	ARG	15.5
31	CA	2172	U	15.3
10	BJ	74	VAL	15.2
10	BJ	8	ILE	15.1
7	BG	62	PHE	14.9
37	CJ	54	PRO	14.8
55	DA	2120	G	14.7
7	BG	65	ALA	14.7
40	CM	114	GLY	14.6
49	CV	20	GLY	14.6
20	BT	4	ILE	14.6
34	CF	85	ILE	14.6
37	DJ	80	LEU	14.5
37	CJ	138	LEU	14.5
13	BM	45	ILE	14.2
46	CS	96	VAL	14.0
1	BA	211	G	14.0
31	CA	1067	A	13.9
49	CV	13	VAL	13.9
37	CJ	57	VAL	13.8
9	BI	130	ARG	13.8
37	DJ	96	ASP	13.7
37	CJ	55	ILE	13.7
7	BG	52	GLN	13.6
37	DJ	135	SER	13.6
10	BJ	42	LEU	13.5
10	BJ	73	LEU	13.5
33	CE	55	SER	13.5
37	DJ	78	VAL	13.4
19	BS	48	THR	13.3
37	CJ	80	LEU	13.3
40	CM	80	SER	13.2
31	CA	1068	G	13.2

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Mol	Chain	Res	Type	RSRZ
34	CF	156	ILE	13.1
19	BS	66	MET	13.1
37	CJ	82	LYS	13.1
14	BN	60	GLN	13.0
9	BI	17	ALA	13.0
37	DJ	13	VAL	13.0
37	CJ	17	MET	13.0
53	CZ	45	GLN	12.9
37	CJ	129	ILE	12.9
7	BG	49	THR	12.9
49	CV	36	VAL	12.9
24	C3	1	MET	12.8
7	BG	111	ARG	12.7
37	CJ	99	GLY	12.7
1	BA	1307	U	12.7
37	DJ	88	SER	12.6
54	DI	131	THR	12.6
37	CJ	20	PRO	12.6
33	CE	172	ALA	12.5
34	CF	76	GLY	12.5
37	CJ	56	PRO	12.5
19	BS	29	LYS	12.4
30	CD	4	LEU	12.4
37	CJ	21	SER	12.4
34	CF	157	THR	12.4
37	DJ	67	PHE	12.4
48	CU	83	ALA	12.3
30	CD	6	GLY	12.3
13	BM	105	ASN	12.3
1	BA	1302	C	12.3
7	BG	42	ILE	12.2
48	CU	43	ILE	12.2
1	BA	1242	G	12.2
34	CF	40	VAL	12.2
1	BA	983	A	12.2
1	AA	86	G	12.2
40	CM	101	ILE	12.1
53	CZ	32	ALA	12.1
13	BM	46	SER	12.1
46	CS	50	GLY	12.1
13	BM	10	PRO	12.1
7	BG	133	THR	12.1

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Mol	Chain	Res	Type	RSRZ
22	C1	5	GLN	12.1
49	CV	33	LYS	12.0
48	CU	60	THR	12.0
7	BG	75	VAL	12.0
35	CG	32	GLU	12.0
37	CJ	23	PRO	11.9
48	CU	59	ASN	11.9
31	CA	2174	C	11.8
1	BA	1024	G	11.8
1	BA	1030	U	11.8
9	BI	67	VAL	11.8
35	CG	40	ALA	11.7
46	CS	27	ILE	11.7
35	CG	108	GLY	11.7
55	DA	2163	A	11.6
1	BA	1020	G	11.6
7	BG	116	MET	11.5
37	CJ	42	PHE	11.5
37	CJ	139	VAL	11.5
49	CV	39	ILE	11.4
23	C2	24	THR	11.4
37	CJ	51	LYS	11.3
34	CF	154	ILE	11.3
9	BI	126	GLN	11.3
37	CJ	59	ILE	11.3
37	CJ	126	THR	11.2
13	BM	95	LEU	11.2
46	CS	32	THR	11.2
13	BM	84	GLY	11.2
40	CM	81	ASP	11.1
49	CV	78	GLY	11.1
31	CA	2126	A	11.1
31	CA	931	U	11.1
31	CA	2110	G	11.1
1	AA	1030	U	11.1
40	CM	100	ILE	11.1
34	CF	97	TRP	11.1
31	CA	331	C	11.1
13	BM	32	ALA	11.0
7	BG	134	ALA	11.0
37	CJ	38	PHE	10.9
1	BA	209	U	10.9

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Mol	Chain	Res	Type	RSRZ
13	BM	22	ILE	10.9
35	CG	33	LEU	10.9
34	CF	65	PRO	10.8
50	CW	57	TYR	10.8
31	CA	1537	G	10.8
14	BN	4	GLN	10.8
1	BA	1022	A	10.7
40	CM	79	LEU	10.7
37	CJ	120	ALA	10.7
37	CJ	121	ASP	10.7
13	BM	23	TYR	10.7
40	CM	92	LEU	10.6
37	CJ	97	LYS	10.6
20	BT	3	ASN	10.6
23	C2	47	VAL	10.6
37	DJ	12	GLN	10.6
30	CD	26	VAL	10.5
53	CZ	15	ASN	10.5
37	CJ	132	THR	10.5
14	BN	36	ALA	10.5
37	CJ	78	VAL	10.5
7	BG	43	VAL	10.4
35	CG	103	ILE	10.4
1	BA	1021	A	10.4
22	C1	3	VAL	10.4
49	CV	50	PRO	10.4
49	CV	35	ILE	10.4
37	CJ	22	PRO	10.3
37	DJ	23	PRO	10.3
35	CG	148	LEU	10.3
34	CF	106	ILE	10.3
43	CP	117	PHE	10.3
37	DJ	24	VAL	10.2
31	CA	1103	A	10.2
37	CJ	130	GLU	10.2
35	CG	105	LEU	10.2
37	DJ	138	LEU	10.2
9	BI	11	ARG	10.2
35	CG	157	TYR	10.2
35	CG	62	TRP	10.1
37	CJ	68	THR	10.1
1	BA	1025	U	10.1

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Mol	Chain	Res	Type	RSRZ
7	BG	73	VAL	10.1
23	C2	21	TYR	10.0
34	CF	155	THR	10.0
3	BC	196	ILE	10.0
37	CJ	43	ASN	10.0
37	CJ	94	ASN	10.0
7	BG	103	TRP	9.9
31	CA	1087	G	9.9
54	DI	128	THR	9.9
19	BS	14	HIS	9.9
31	CA	2125	G	9.9
55	DA	2121	G	9.9
34	CF	35	THR	9.9
24	C3	42	LEU	9.9
7	BG	91	VAL	9.9
10	BJ	26	VAL	9.9
37	CJ	87	LYS	9.8
7	BG	66	LEU	9.8
37	CJ	96	ASP	9.8
22	C1	2	ALA	9.8
13	BM	83	LEU	9.8
13	BM	5	ALA	9.8
31	CA	1084	A	9.8
34	CF	86	GLY	9.8
1	BA	1016	A	9.8
7	BG	77	SER	9.8
30	CD	10	GLY	9.7
7	BG	69	VAL	9.7
37	CJ	98	VAL	9.7
7	BG	151	PHE	9.7
34	CF	129	SER	9.7
1	BA	1305	G	9.7
13	BM	33	ILE	9.6
19	BS	49	ILE	9.6
37	CJ	89	GLY	9.6
40	CM	82	LEU	9.6
22	C1	6	ASN	9.6
9	AI	20	PHE	9.6
19	BS	38	SER	9.6
1	BA	204	G	9.6
10	BJ	40	ILE	9.5
44	CQ	85	SER	9.5

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Mol	Chain	Res	Type	RSRZ
13	BM	39	ILE	9.5
24	C3	35	ARG	9.5
31	CA	1086	A	9.5
49	CV	87	PHE	9.4
9	BI	32	GLN	9.4
13	BM	96	PRO	9.4
37	DJ	94	ASN	9.4
37	CJ	61	VAL	9.3
51	CX	53	CYS	9.3
1	AA	87	C	9.3
34	CF	105	THR	9.3
53	CZ	29	ARG	9.3
13	BM	19	LEU	9.3
37	CJ	28	LEU	9.3
43	CP	40	ILE	9.3
3	BC	155	GLY	9.3
16	BP	57	ILE	9.3
37	DJ	36	MET	9.3
1	BA	1274	A	9.2
43	CP	64	TYR	9.2
19	BS	28	LYS	9.2
1	BA	1222	G	9.2
10	BJ	90	LEU	9.2
46	CS	88	GLY	9.2
43	CP	63	LYS	9.1
10	BJ	87	LEU	9.1
18	BR	20	GLU	9.1
49	CV	19	LYS	9.1
55	DA	2124	G	9.1
37	DJ	133	ALA	9.1
7	BG	112	GLY	9.1
1	BA	985	C	9.1
7	BG	46	ALA	9.1
14	BN	72	GLY	9.1
7	BG	71	PRO	9.1
10	BJ	76	ILE	9.1
3	BC	197	GLY	9.1
31	CA	329	G	9.1
34	CF	117	LEU	9.1
46	CS	63	VAL	9.1
31	CA	2666	C	9.0
37	CJ	71	THR	9.0

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Mol	Chain	Res	Type	RSRZ
7	BG	137	LYS	9.0
3	BC	193	TYR	9.0
20	BT	60	ARG	9.0
31	CA	613	A	9.0
24	C3	17	GLY	9.0
31	CA	1066	U	9.0
19	BS	31	LEU	9.0
55	DA	2110	G	9.0
48	CU	47	VAL	9.0
9	BI	66	THR	8.9
46	CS	20	VAL	8.9
49	CV	3	ALA	8.9
1	BA	1032	G	8.9
49	CV	75	ALA	8.9
34	CF	131	GLY	8.9
53	CZ	17	GLU	8.9
37	CJ	90	SER	8.9
7	BG	53	ARG	8.8
13	BM	48	LEU	8.8
49	CV	14	LEU	8.8
34	CF	153	ASP	8.8
49	CV	79	LYS	8.8
49	CV	29	LEU	8.8
19	BS	63	THR	8.8
48	CU	72	GLN	8.8
16	BP	17	TYR	8.8
1	BA	958	A	8.8
49	CV	89	ASP	8.8
29	CC	241	GLY	8.8
9	BI	18	ARG	8.8
40	CM	89	VAL	8.8
29	CC	239	ASN	8.8
37	DJ	69	PHE	8.7
48	CU	55	VAL	8.7
1	BA	1271	A	8.7
27	C0	56	LYS	8.7
37	DJ	116	ASP	8.7
1	BA	1243	C	8.7
31	CA	2665	A	8.7
34	CF	126	GLY	8.7
31	CA	1175	A	8.7
10	BJ	72	ARG	8.7

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Mol	Chain	Res	Type	RSRZ
40	CM	78	ARG	8.7
37	CJ	75	PRO	8.7
37	CJ	60	THR	8.7
34	CF	23	ASN	8.6
33	CE	33	VAL	8.6
7	BG	45	SER	8.6
10	BJ	77	VAL	8.6
24	C3	18	PHE	8.6
37	CJ	47	ASP	8.6
13	AM	30	SER	8.6
34	CF	132	VAL	8.6
37	DJ	89	GLY	8.6
13	BM	64	VAL	8.6
1	BA	1026	G	8.6
34	CF	176	PRO	8.6
33	CE	143	LEU	8.6
34	CF	95	ARG	8.6
37	DJ	115	ALA	8.6
31	CA	1211	C	8.6
49	CV	98	SER	8.6
48	CU	10	VAL	8.5
19	BS	37	ARG	8.5
10	BJ	12	ALA	8.5
24	C3	7	PRO	8.5
37	DJ	59	ILE	8.5
34	CF	130	MET	8.5
7	BG	148	ASN	8.5
3	BC	71	ALA	8.5
54	DI	130	PRO	8.5
14	AN	21	PHE	8.5
34	CF	147	ASP	8.5
31	CA	1083	U	8.5
49	CV	32	GLY	8.5
1	BA	1296	C	8.5
14	BN	20	TYR	8.5
3	BC	195	VAL	8.4
7	BG	17	LYS	8.4
37	CJ	9	VAL	8.4
7	BG	106	GLU	8.4
31	CA	2123	G	8.4
9	AI	21	ILE	8.4
13	BM	40	ALA	8.4

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Mol	Chain	Res	Type	RSRZ
37	DJ	20	PRO	8.4
37	DJ	68	THR	8.4
35	CG	52	PHE	8.4
9	BI	68	LYS	8.4
23	C2	36	LEU	8.4
45	CR	106	PHE	8.3
35	CG	43	VAL	8.3
19	BS	60	VAL	8.3
1	BA	948	C	8.3
7	BG	79	ARG	8.3
17	BQ	70	THR	8.3
1	BA	984	C	8.3
1	BA	942	G	8.3
34	CF	144	ASP	8.3
7	BG	132	GLY	8.3
50	CW	94	ALA	8.3
10	BJ	7	ARG	8.3
43	CP	99	TYR	8.3
19	BS	5	LEU	8.3
7	BG	39	ALA	8.3
13	BM	2	ALA	8.3
24	C3	30	VAL	8.3
49	CV	48	PRO	8.3
48	CU	42	GLU	8.3
53	CZ	33	ALA	8.3
10	BJ	86	ALA	8.2
49	CV	81	ASP	8.2
35	CG	172	LYS	8.2
19	BS	24	GLU	8.2
7	BG	4	ARG	8.2
51	CX	33	ALA	8.2
43	CP	24	THR	8.2
48	CU	15	HIS	8.2
19	BS	32	ARG	8.2
34	CF	80	ARG	8.2
33	CE	104	ALA	8.2
9	BI	40	GLY	8.2
33	CE	173	THR	8.2
7	BG	109	ARG	8.2
14	BN	35	ASN	8.2
37	DJ	137	GLY	8.2
42	CO	111	ALA	8.1

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Mol	Chain	Res	Type	RSRZ
31	CA	1085	A	8.1
31	CA	75	G	8.1
7	BG	141	VAL	8.1
9	BI	127	PHE	8.1
40	CM	20	GLY	8.1
40	CM	71	ALA	8.1
43	CP	51	ALA	8.1
10	BJ	94	ALA	8.1
3	BC	119	SER	8.1
1	BA	1241	G	8.1
23	C2	52	ALA	8.1
35	CG	151	TYR	8.1
44	CQ	84	ILE	8.1
37	CJ	83	ALA	8.0
2	BB	34	ALA	8.0
55	DA	2125	G	8.0
13	BM	55	THR	8.0
35	CG	171	THR	8.0
19	BS	74	PHE	8.0
11	BK	47	ALA	8.0
37	CJ	133	ALA	8.0
2	AB	14	VAL	8.0
24	C3	36	ALA	8.0
55	DA	2174	C	8.0
35	CG	111	HIS	8.0
19	BS	76	PRO	8.0
55	DA	896	A	8.0
55	DA	1067	A	8.0
10	BJ	71	LEU	7.9
42	CO	28	LEU	7.9
55	DA	2116	G	7.9
2	AB	6	MET	7.9
16	BP	80	LYS	7.9
33	CE	23	PHE	7.9
2	AB	136	MET	7.9
48	CU	61	LEU	7.9
33	CE	150	THR	7.9
37	CJ	33	VAL	7.9
14	AN	31	ILE	7.9
7	BG	144	MET	7.9
48	CU	46	ALA	7.9
1	BA	1017	U	7.9

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Mol	Chain	Res	Type	RSRZ
7	BG	54	SER	7.9
24	C3	33	ARG	7.9
1	BA	82	G	7.9
31	CA	330	A	7.9
19	BS	39	THR	7.9
40	CM	8	PRO	7.9
49	CV	88	GLU	7.9
1	AA	1031	C	7.9
20	BT	72	ALA	7.9
14	AN	23	LYS	7.9
40	CM	130	GLY	7.8
1	BA	80	A	7.8
31	CA	2124	G	7.8
31	CA	1078	U	7.8
34	CF	31	VAL	7.8
13	AM	33	ILE	7.8
43	CP	54	VAL	7.8
1	AA	1032	G	7.8
9	BI	14	SER	7.8
13	BM	47	GLU	7.8
36	DH	137	GLU	7.8
16	BP	52	LEU	7.8
35	CG	169	VAL	7.8
40	CM	120	VAL	7.8
22	C1	4	GLN	7.8
37	CJ	119	GLY	7.8
3	BC	198	VAL	7.7
33	CE	47	LYS	7.7
35	CG	26	ILE	7.7
45	CR	74	ILE	7.7
55	DA	138	U	7.7
33	CE	201	ALA	7.7
24	C3	27	GLY	7.7
40	CM	10	GLU	7.7
37	CJ	31	GLN	7.7
31	CA	1167	C	7.7
13	BM	85	CYS	7.7
7	BG	41	SER	7.7
30	CD	186	LEU	7.7
36	CH	140	ALA	7.7
13	AM	43	VAL	7.7
55	DA	2175	C	7.7

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Mol	Chain	Res	Type	RSRZ
10	BJ	75	ASP	7.6
43	CP	65	THR	7.7
13	BM	25	VAL	7.6
34	CF	93	GLY	7.6
51	CX	63	ALA	7.6
1	BA	1031	C	7.6
10	BJ	22	THR	7.6
50	CW	6	ALA	7.6
10	BJ	95	GLY	7.6
13	BM	29	ARG	7.6
14	BN	54	ASP	7.6
7	BG	87	VAL	7.6
34	CF	34	ILE	7.6
7	AG	62	PHE	7.6
29	CC	27	GLY	7.6
37	CJ	29	GLY	7.6
31	CA	2171	A	7.6
1	BA	1028	C	7.6
16	BP	41	PRO	7.6
7	BG	15	ASP	7.6
35	CG	106	SER	7.5
3	BC	192	THR	7.5
14	BN	2	ALA	7.5
2	AB	135	LEU	7.5
36	CH	11	ASN	7.5
9	BI	44	ALA	7.5
31	CA	1069	A	7.5
34	CF	113	ASP	7.5
9	BI	64	TYR	7.5
37	DJ	66	SER	7.5
40	CM	77	ILE	7.5
43	CP	38	GLN	7.5
46	CS	59	ILE	7.5
35	CG	2	SER	7.5
43	CP	29	HIS	7.5
40	CM	102	GLY	7.5
37	CJ	24	VAL	7.5
42	CO	116	VAL	7.5
35	CG	83	PHE	7.5
2	BB	135	LEU	7.5
53	CZ	14	LEU	7.5
1	BA	949	A	7.5

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Mol	Chain	Res	Type	RSRZ
25	C4	43	HIS	7.5
31	CA	2802	G	7.5
33	CE	119	ILE	7.5
34	CF	152	LEU	7.5
55	DA	2172	U	7.4
7	BG	105	VAL	7.4
55	DA	1065	U	7.4
1	BA	953	G	7.4
1	BA	1314	C	7.4
31	CA	2402	U	7.4
25	C4	37	ALA	7.4
47	CT	5	ALA	7.4
34	CF	28	VAL	7.4
53	CZ	49	ASP	7.4
31	CA	1077	A	7.4
37	CJ	73	THR	7.4
37	CJ	74	PRO	7.4
1	BA	1275	A	7.4
31	CA	2163	A	7.4
37	DJ	134	ARG	7.4
20	BT	79	LEU	7.4
13	BM	24	GLY	7.4
1	BA	959	A	7.4
26	C5	10	LEU	7.4
34	CF	83	TYR	7.4
55	DA	1172	C	7.4
31	CA	312	G	7.3
49	CV	83	VAL	7.3
19	BS	30	PRO	7.3
53	CZ	37	LEU	7.3
53	CZ	59	GLU	7.3
29	CC	233	GLY	7.3
31	CA	2173	A	7.3
1	AA	88	U	7.3
41	CN	136	MET	7.3
34	CF	39	GLY	7.3
33	CE	144	GLU	7.3
31	CA	1065	U	7.3
33	CE	164	LEU	7.3
37	DJ	84	ALA	7.3
40	CM	142	ILE	7.3
47	CT	84	ARG	7.3

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Mol	Chain	Res	Type	RSRZ
31	CA	1075	C	7.3
34	CF	151	GLY	7.3
33	CE	200	LEU	7.3
46	CS	103	ALA	7.3
13	BM	101	ARG	7.3
27	C0	29	LEU	7.3
10	BJ	101	SER	7.3
1	BA	94	G	7.3
1	BA	1050	G	7.3
31	CA	289	G	7.3
49	CV	52	LEU	7.2
31	CA	2300	C	7.2
31	CA	2891	U	7.2
2	BB	14	VAL	7.2
10	BJ	10	LEU	7.2
14	BN	68	GLY	7.2
24	C3	32	ALA	7.2
37	CJ	86	ILE	7.2
49	CV	30	SER	7.2
35	CG	10	VAL	7.2
34	CF	173	PHE	7.2
46	CS	35	PHE	7.2
31	CA	2169	A	7.2
38	CK	22	GLY	7.2
3	BC	156	ARG	7.2
9	BI	5	GLN	7.2
48	CU	8	LEU	7.2
55	DA	2118	U	7.2
49	CV	5	ILE	7.2
1	BA	1218	C	7.2
35	CG	86	LYS	7.2
9	BI	4	ASN	7.2
7	BG	16	PRO	7.2
53	CZ	31	GLN	7.2
43	CP	115	LEU	7.2
31	CA	878	A	7.2
50	CW	27	PRO	7.2
48	CU	87	LEU	7.2
53	CZ	42	LEU	7.2
7	BG	150	ALA	7.2
26	C5	32	LYS	7.2
37	CJ	95	LYS	7.2

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Mol	Chain	Res	Type	RSRZ
31	CA	1057	A	7.2
37	CJ	85	GLY	7.1
34	CF	102	ARG	7.1
37	CJ	18	ALA	7.1
55	DA	2111	U	7.1
1	BA	954	G	7.1
19	BS	61	PHE	7.1
37	DJ	28	LEU	7.1
46	CS	14	VAL	7.1
39	CL	110	GLU	7.1
10	BJ	91	ASP	7.1
7	BG	108	ALA	7.1
49	CV	12	ILE	7.1
49	CV	77	THR	7.1
31	CA	2175	C	7.1
7	BG	129	GLU	7.1
44	CQ	97	LEU	7.1
37	DJ	77	ALA	7.1
1	AA	81	A	7.1
1	BA	1303	C	7.1
49	CV	26	LYS	7.1
10	AJ	6	ILE	7.1
37	DJ	52	GLY	7.1
31	CA	2127	G	7.1
43	CP	108	ASP	7.1
23	C2	37	LYS	7.1
53	CZ	41	HIS	7.1
31	CA	2797	U	7.1
44	CQ	95	ALA	7.1
23	C2	23	THR	7.1
37	DJ	87	LYS	7.1
25	C4	28	ASN	7.0
40	CM	28	GLY	7.0
34	CF	174	ASP	7.0
31	CA	2121	G	7.0
43	CP	39	VAL	7.0
55	DA	2178	C	7.0
51	CX	52	GLY	7.0
3	BC	79	LYS	7.0
33	CE	183	PHE	7.0
37	CJ	8	TYR	7.0
10	BJ	11	LYS	7.0

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Mol	Chain	Res	Type	RSRZ
7	BG	18	PHE	7.0
7	BG	47	LEU	7.0
20	BT	75	HIS	7.0
35	CG	9	VAL	7.0
55	DA	2167	U	7.0
1	BA	203	G	7.0
40	CM	90	VAL	7.0
55	DA	2166	U	7.0
10	AJ	42	LEU	7.0
3	BC	159	GLY	7.0
19	BS	80	TYR	7.0
34	CF	158	THR	7.0
7	BG	48	GLU	7.0
14	BN	61	ARG	7.0
10	BJ	98	VAL	6.9
13	BM	109	ARG	6.9
14	BN	53	ARG	6.9
13	BM	94	GLY	6.9
27	C0	24	LEU	6.9
19	BS	41	PHE	6.9
31	CA	1536	C	6.9
31	CA	2667	C	6.9
46	CS	98	ILE	6.9
33	CE	118	LEU	6.9
48	CU	57	VAL	6.9
37	CJ	93	PRO	6.9
37	CJ	50	GLU	6.9
1	BA	79	G	6.9
30	CD	44	GLY	6.9
37	CJ	113	LYS	6.9
49	CV	38	GLY	6.9
1	BA	1304	G	6.9
31	CA	549	G	6.9
31	CA	1185	G	6.9
34	CF	121	SER	6.9
54	DI	2	ALA	6.9
13	BM	28	THR	6.9
35	CG	30	ASN	6.9
31	CA	1095	A	6.9
31	CA	2170	A	6.9
26	C5	38	GLY	6.9
54	DI	134	GLU	6.9

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Mol	Chain	Res	Type	RSRZ
31	CA	316	C	6.8
34	CF	175	PHE	6.8
31	CA	1168	G	6.8
30	CD	8	LYS	6.8
30	CD	38	LYS	6.8
9	AI	90	TYR	6.8
31	CA	2119	A	6.8
49	CV	28	VAL	6.8
16	BP	60	TRP	6.8
40	CM	75	ALA	6.8
31	CA	2120	G	6.8
35	CG	45	HIS	6.8
27	C0	43	ALA	6.8
31	CA	2168	G	6.8
37	CJ	62	TYR	6.8
25	C4	4	ILE	6.8
33	CE	24	ASN	6.8
1	BA	1023	U	6.8
31	CA	1210	G	6.8
37	CJ	44	ALA	6.8
55	DA	2176	A	6.8
13	AM	19	LEU	6.8
2	BB	186	ILE	6.8
34	CF	75	ALA	6.8
46	CS	28	ALA	6.8
31	CA	311	A	6.8
35	CG	41	VAL	6.8
46	CS	101	ILE	6.8
33	CE	75	SER	6.8
43	CP	107	ALA	6.8
7	BG	30	LEU	6.8
47	CT	97	LEU	6.8
55	DA	2123	G	6.8
2	AB	123	ASP	6.8
19	BS	72	GLY	6.8
20	BT	56	PRO	6.8
30	CD	166	GLY	6.8
35	CG	92	VAL	6.8
34	CF	107	ALA	6.7
37	CJ	123	GLU	6.7
31	CA	12	U	6.7
31	CA	1076	C	6.7

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Mol	Chain	Res	Type	RSRZ
31	CA	1104	C	6.7
36	DH	66	ASN	6.7
13	BM	51	GLY	6.7
2	BB	201	PRO	6.7
47	CT	86	MET	6.7
14	BN	16	LEU	6.7
3	BC	53	SER	6.7
1	BA	1217	C	6.7
9	BI	7	TYR	6.7
13	BM	31	LYS	6.7
25	C4	40	ARG	6.7
31	CA	356	G	6.7
13	BM	56	LEU	6.7
46	CS	78	ARG	6.7
13	BM	63	PHE	6.7
31	CA	877	A	6.7
55	DA	2127	G	6.7
13	BM	6	GLY	6.7
49	DV	56	GLY	6.7
20	BT	76	LYS	6.7
30	CD	96	ILE	6.7
10	BJ	102	LEU	6.7
11	AK	82	LEU	6.7
35	CG	84	THR	6.7
10	BJ	6	ILE	6.7
10	BJ	9	ARG	6.7
31	CA	1105	U	6.7
7	BG	107	ALA	6.7
31	CA	267	C	6.7
46	CS	87	GLN	6.7
53	CZ	22	LEU	6.7
23	C2	49	TYR	6.7
14	BN	31	ILE	6.7
53	CZ	40	SER	6.7
10	AJ	74	VAL	6.7
9	AI	129	LYS	6.7
7	BG	101	MET	6.6
42	CO	24	MET	6.6
42	CO	120	GLU	6.6
31	CA	2108	A	6.6
35	CG	112	PRO	6.6
1	BA	1049	U	6.6

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Mol	Chain	Res	Type	RSRZ
49	CV	69	ASN	6.6
10	BJ	82	LYS	6.6
14	BN	52	PRO	6.6
35	CG	69	ARG	6.6
44	CQ	110	ILE	6.6
35	CG	51	THR	6.6
34	CF	55	ALA	6.6
1	BA	1004	A	6.6
31	CA	1535	A	6.6
13	BM	12	HIS	6.6
19	BS	40	ILE	6.6
43	CP	103	VAL	6.6
13	BM	35	ALA	6.6
2	BB	35	ARG	6.6
3	BC	154	SER	6.6
20	BT	24	ARG	6.6
31	CA	2128	G	6.6
21	AU	2	PRO	6.6
30	CD	154	LYS	6.6
40	CM	85	VAL	6.6
1	BA	1331	G	6.6
31	CA	846	U	6.6
35	CG	102	VAL	6.6
42	CO	29	VAL	6.6
37	DJ	99	GLY	6.6
1	BA	1236	A	6.6
37	DJ	73	THR	6.5
37	DJ	22	PRO	6.5
54	DI	121	SER	6.5
7	AG	4	ARG	6.5
43	CP	25	ARG	6.5
14	BN	27	LEU	6.5
17	BQ	45	HIS	6.5
7	BG	123	GLU	6.5
37	DJ	14	ALA	6.5
9	BI	9	THR	6.5
33	CE	54	GLY	6.5
49	CV	95	PHE	6.5
9	BI	38	TYR	6.5
35	CG	58	TYR	6.5
53	CZ	24	GLU	6.5
9	AI	17	ALA	6.5

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Mol	Chain	Res	Type	RSRZ
1	AA	1026	G	6.5
38	CK	35	ARG	6.5
36	CH	136	SER	6.5
37	CJ	122	ILE	6.5
37	CJ	131	GLY	6.5
35	CG	7	ALA	6.5
1	BA	1018	G	6.5
13	BM	21	SER	6.5
31	CA	1169	A	6.5
36	CH	132	PHE	6.5
13	BM	79	ARG	6.5
16	BP	81	ALA	6.5
45	CR	90	ILE	6.5
1	BA	989	U	6.5
8	BH	55	THR	6.5
27	C0	23	THR	6.5
31	CA	1082	U	6.5
30	CD	201	LEU	6.5
31	CA	1213	A	6.5
54	DI	132	TYR	6.5
1	BA	85	U	6.5
47	CT	105	VAL	6.5
9	AI	128	SER	6.5
7	BG	8	GLY	6.5
51	CX	26	PHE	6.5
3	BC	43	LEU	6.5
31	CA	2161	C	6.5
25	C4	41	LYS	6.4
31	CA	409	G	6.5
35	CG	27	LYS	6.4
10	BJ	25	ILE	6.4
10	BJ	100	ILE	6.4
51	CX	59	LEU	6.4
37	CJ	84	ALA	6.4
19	BS	12	ASP	6.4
49	CV	40	ASN	6.4
37	CJ	77	ALA	6.4
7	BG	38	THR	6.4
10	BJ	38	GLY	6.4
1	BA	78	A	6.4
33	CE	193	VAL	6.4
34	CF	84	PRO	6.4

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Mol	Chain	Res	Type	RSRZ
7	BG	115	SER	6.4
27	C0	8	THR	6.4
34	CF	136	ILE	6.4
47	CT	47	VAL	6.4
1	BA	1276	G	6.4
17	BQ	73	TRP	6.4
31	CA	2803	G	6.4
34	CF	41	GLY	6.4
55	DA	1062	G	6.4
37	DJ	11	LEU	6.4
31	CA	1870	C	6.4
13	BM	108	THR	6.4
55	DA	1064	C	6.4
24	C3	31	LEU	6.4
27	C0	34	HIS	6.4
43	CP	46	GLU	6.4
54	DI	96	PHE	6.3
31	CA	885	C	6.3
37	CJ	79	LEU	6.3
2	BB	12	ALA	6.3
12	AL	124	ALA	6.3
13	BM	98	ARG	6.3
25	C4	36	LYS	6.3
34	CF	69	LYS	6.3
7	BG	145	ALA	6.3
34	CF	122	PHE	6.3
15	BO	17	ARG	6.3
37	CJ	58	VAL	6.3
31	CA	1094	U	6.3
14	BN	22	ALA	6.3
33	CE	128	ALA	6.3
43	CP	92	PHE	6.3
14	AN	47	LYS	6.3
35	CG	17	VAL	6.3
35	CG	107	LEU	6.3
22	C1	46	ASP	6.3
35	CG	80	THR	6.3
44	CQ	22	PRO	6.3
49	CV	4	LYS	6.3
30	CD	77	ARG	6.3
45	CR	98	ILE	6.3
7	AG	66	LEU	6.3

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Mol	Chain	Res	Type	RSRZ
31	CA	81	G	6.3
31	CA	1238	G	6.3
30	CD	97	SER	6.3
40	CM	113	ALA	6.3
13	BM	93	ARG	6.3
37	DJ	19	ASN	6.3
37	CJ	67	PHE	6.3
7	AG	42	ILE	6.3
37	CJ	46	THR	6.3
37	CJ	81	LYS	6.3
1	AA	844	G	6.3
37	CJ	32	GLY	6.2
43	CP	66	GLY	6.2
2	AB	74	ARG	6.2
1	BA	1321	U	6.2
13	BM	36	ALA	6.2
43	CP	52	SER	6.2
13	BM	103	LYS	6.2
13	BM	65	VAL	6.2
31	CA	930	G	6.2
31	CA	1107	G	6.2
37	CJ	70	VAL	6.2
1	AA	85	U	6.2
36	CH	72	ILE	6.2
34	CF	92	ARG	6.2
42	CO	118	ARG	6.2
43	CP	27	VAL	6.2
9	AI	6	TYR	6.2
31	CA	2860	A	6.2
34	CF	143	TYR	6.2
40	CM	88	GLY	6.2
10	BJ	80	THR	6.2
50	CW	89	ILE	6.2
7	BG	35	LYS	6.2
30	CD	74	GLU	6.2
34	CF	94	GLU	6.2
35	CG	174	ALA	6.2
53	CZ	56	LEU	6.2
19	BS	21	LYS	6.2
37	CJ	19	ASN	6.2
51	CX	62	LYS	6.2
40	CM	126	ARG	6.2

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Mol	Chain	Res	Type	RSRZ
7	BG	72	THR	6.2
2	BB	67	ILE	6.2
53	CZ	18	LEU	6.2
37	DJ	74	PRO	6.1
2	BB	20	THR	6.1
33	CE	154	ASP	6.1
44	CQ	27	GLU	6.1
14	BN	8	ALA	6.1
40	CM	19	LEU	6.1
40	CM	117	THR	6.1
13	AM	99	GLY	6.1
13	BM	99	GLY	6.1
24	C3	28	ARG	6.1
49	CV	25	VAL	6.1
20	BT	34	LYS	6.1
33	CE	89	PRO	6.1
55	DA	883	G	6.1
55	DA	884	U	6.1
34	CF	60	ILE	6.1
10	AJ	35	GLN	6.1
13	BM	43	VAL	6.1
1	BA	1270	G	6.1
13	BM	30	SER	6.1
37	DJ	117	MET	6.1
38	CK	93	ILE	6.1
51	CX	32	LEU	6.1
13	BM	41	GLU	6.1
34	CF	164	GLU	6.1
2	BB	21	ARG	6.1
13	BM	54	ASP	6.1
31	CA	344	A	6.1
7	BG	50	LEU	6.1
31	CA	1106	G	6.1
37	CJ	30	GLN	6.1
40	CM	135	ILE	6.1
7	AG	79	ARG	6.1
40	CM	107	PHE	6.1
45	CR	73	GLY	6.1
14	BN	18	ASP	6.1
18	BR	51	TYR	6.1
55	DA	2122	U	6.1
1	BA	1005	A	6.1

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Mol	Chain	Res	Type	RSRZ
23	C2	43	VAL	6.1
24	C3	26	ASN	6.0
7	BG	58	GLU	6.0
1	BA	1019	A	6.0
29	CC	234	GLY	6.0
36	CH	130	VAL	6.0
37	DJ	98	VAL	6.0
10	AJ	73	LEU	6.0
33	CE	131	THR	6.0
43	CP	41	ALA	6.0
30	CD	9	VAL	6.0
49	CV	6	ARG	6.0
20	BT	63	ALA	6.0
2	BB	40	ILE	6.0
29	CC	242	LYS	6.0
43	CP	106	LEU	6.0
10	BJ	21	ALA	6.0
16	BP	54	LEU	6.0
49	CV	51	ALA	6.0
31	CA	476	G	6.0
43	CP	87	ILE	6.0
29	CC	245	VAL	6.0
1	BA	1280	A	6.0
1	BA	1306	A	6.0
31	CA	345	A	6.0
7	BG	99	LEU	6.0
23	C2	45	GLN	6.0
40	CM	133	ALA	6.0
43	CP	105	ALA	6.0
46	CS	22	LEU	6.0
35	CG	82	GLY	6.0
16	BP	20	VAL	6.0
27	C0	55	VAL	6.0
31	CA	2892	G	6.0
1	BA	208	U	6.0
22	C1	35	GLY	6.0
43	CP	78	VAL	6.0
54	DI	38	MET	6.0
31	CA	2107	G	6.0
45	CR	29	SER	6.0
46	CS	18	GLN	6.0
31	CA	1217	U	6.0

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Mol	Chain	Res	Type	RSRZ
31	CA	1088	A	6.0
19	BS	77	THR	6.0
37	CJ	118	THR	6.0
37	CJ	53	LEU	6.0
25	C4	61	CYS	6.0
9	BI	90	TYR	6.0
19	BS	52	HIS	6.0
14	BN	55	SER	5.9
16	BP	16	PHE	5.9
1	BA	1201	A	5.9
22	C1	34	SER	5.9
29	CC	244	PRO	5.9
3	BC	126	ARG	5.9
44	CQ	9	GLU	5.9
10	AJ	75	ASP	5.9
35	CG	8	PRO	5.9
38	CK	119	PHE	5.9
31	CA	2118	U	5.9
35	CG	152	ARG	5.9
23	C2	18	GLY	5.9
43	CP	62	LEU	5.9
23	C2	15	ALA	5.9
23	C2	53	LYS	5.9
1	BA	950	U	5.9
7	AG	109	ARG	5.9
31	CA	2150	C	5.9
48	CU	85	VAL	5.9
46	CS	55	ASP	5.9
35	CG	31	GLY	5.9
46	CS	61	ALA	5.9
17	BQ	63	GLU	5.9
45	CR	33	ARG	5.9
30	CD	82	PHE	5.9
37	CJ	27	ALA	5.9
55	DA	2115	G	5.9
34	CF	165	GLU	5.9
45	CR	71	GLN	5.9
51	CX	55	ARG	5.9
20	BT	73	ALA	5.9
15	BO	89	ARG	5.9
37	DJ	38	PHE	5.9
46	CS	31	GLU	5.9

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Mol	Chain	Res	Type	RSRZ
52	CY	78	TYR	5.8
19	BS	6	LYS	5.8
1	BA	1235	U	5.8
10	BJ	89	ARG	5.8
11	BK	55	SER	5.8
37	CJ	91	GLY	5.8
10	BJ	19	ASP	5.8
54	DI	129	LEU	5.8
19	BS	27	ASP	5.8
33	CE	138	LEU	5.8
52	CY	49	LEU	5.8
7	BG	152	ALA	5.8
31	CA	896	A	5.8
31	CA	1215	G	5.8
37	CJ	41	ALA	5.8
37	DJ	85	GLY	5.8
47	CT	101	SER	5.8
34	CF	170	LEU	5.8
13	BM	86	TYR	5.8
30	CD	185	ASN	5.8
31	CA	1064	C	5.8
36	DH	74	ALA	5.8
37	DJ	100	LYS	5.8
35	CG	4	VAL	5.8
30	CD	76	GLY	5.8
17	BQ	17	MET	5.8
49	CV	73	PHE	5.8
2	AB	131	LYS	5.8
2	BB	187	VAL	5.8
46	CS	62	GLU	5.8
2	AB	46	THR	5.8
25	C4	27	ALA	5.8
47	CT	43	ALA	5.8
41	CN	16	ARG	5.8
20	BT	49	LYS	5.8
55	DA	1068	G	5.8
9	AI	104	VAL	5.8
13	AM	16	VAL	5.8
36	CH	15	LEU	5.8
1	BA	196	A	5.8
14	BN	37	SER	5.8
37	CJ	135	SER	5.8

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Mol	Chain	Res	Type	RSRZ
9	AI	19	VAL	5.8
25	C4	2	PRO	5.8
51	CX	60	PHE	5.8
46	CS	49	ILE	5.7
31	CA	2162	G	5.7
55	DA	879	G	5.7
7	BG	60	GLU	5.7
35	CG	121	ILE	5.7
29	CC	249	GLY	5.7
39	CL	68	GLY	5.7
49	CV	64	ALA	5.7
30	CD	30	GLU	5.7
44	CQ	8	LEU	5.7
31	CA	1049	C	5.7
45	CR	91	ASP	5.7
2	AB	4	VAL	5.7
35	CG	162	VAL	5.7
44	CQ	115	ASN	5.7
7	BG	88	PRO	5.7
35	CG	35	ARG	5.7
35	CG	56	ASP	5.7
55	DA	2165	C	5.7
35	CG	110	SER	5.7
42	CO	119	SER	5.7
48	CU	34	VAL	5.7
49	CV	70	VAL	5.7
1	BA	1240	U	5.7
43	CP	26	LEU	5.7
37	CJ	125	MET	5.7
48	CU	1	MET	5.7
50	CW	1	MET	5.7
1	BA	213	G	5.7
34	CF	135	GLN	5.7
3	BC	106	VAL	5.7
1	BA	1126	U	5.7
9	BI	81	HIS	5.7
35	CG	104	ASN	5.7
37	DJ	71	THR	5.7
31	CA	1214	A	5.7
34	CF	110	ARG	5.7
37	DJ	50	GLU	5.7
33	CE	178	VAL	5.7

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Mol	Chain	Res	Type	RSRZ
43	CP	67	ASN	5.7
7	BG	140	ASP	5.7
47	CT	82	MET	5.7
49	CV	71	ALA	5.7
33	CE	98	LYS	5.7
35	CG	78	GLY	5.7
36	DH	70	GLU	5.7
51	CX	61	ALA	5.7
37	CJ	45	LYS	5.7
53	CZ	11	VAL	5.7
1	BA	1029	U	5.7
1	BA	987	G	5.7
30	CD	3	GLY	5.7
31	CA	317	G	5.7
34	CF	79	ILE	5.6
35	CG	54	PRO	5.7
37	CJ	124	ALA	5.6
37	DJ	110	ALA	5.6
31	CA	646	U	5.6
31	CA	1174	U	5.6
25	C4	64	TYR	5.6
9	BI	125	PRO	5.6
10	BJ	39	PRO	5.6
27	C0	9	GLN	5.6
30	CD	43	ASP	5.6
34	CF	43	ALA	5.6
31	CA	514	A	5.6
13	AM	64	VAL	5.6
37	DJ	103	ARG	5.6
24	C3	37	LYS	5.6
30	CD	200	ASP	5.6
35	CG	67	THR	5.6
55	DA	2109	U	5.6
1	BA	90	C	5.6
31	CA	1606	C	5.6
13	BM	14	HIS	5.6
31	CA	1046	A	5.6
13	BM	76	SER	5.6
27	C0	27	LEU	5.6
50	CW	42	LEU	5.6
7	BG	83	SER	5.6
34	CF	32	GLU	5.6

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Mol	Chain	Res	Type	RSRZ
11	AK	19	GLY	5.6
36	DH	94	ILE	5.6
45	CR	6	ARG	5.6
47	CT	103	ILE	5.6
1	AA	82	G	5.6
31	CA	2628	C	5.6
49	DV	53	ASN	5.6
37	CJ	15	ALA	5.6
1	BA	81	A	5.6
29	CC	240	PHE	5.6
19	BS	71	LEU	5.6
31	CA	355	U	5.6
19	BS	59	PRO	5.6
45	CR	118	ALA	5.6
1	BA	202	G	5.6
25	C4	22	PHE	5.6
30	CD	203	VAL	5.6
30	CD	151	THR	5.6
33	CE	101	TYR	5.5
36	DH	63	ALA	5.5
37	DJ	27	ALA	5.5
7	BG	76	LYS	5.5
31	CA	1872	A	5.5
33	CE	17	THR	5.5
46	CS	94	THR	5.5
24	C3	16	HIS	5.5
1	BA	1237	C	5.5
35	CG	117	LEU	5.5
31	CA	546	U	5.5
44	CQ	12	GLN	5.5
31	CA	45	G	5.5
42	CO	56	LYS	5.5
34	CF	99	PHE	5.5
7	AG	82	GLY	5.5
9	BI	15	SER	5.5
22	C1	27	SER	5.5
1	BA	102	G	5.5
31	CA	1089	A	5.5
9	BI	58	VAL	5.5
30	CD	5	VAL	5.5
36	CH	142	VAL	5.5
38	CK	139	VAL	5.5

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Mol	Chain	Res	Type	RSRZ
1	AA	1027	C	5.5
7	BG	5	ARG	5.5
29	CC	48	ARG	5.5
10	BJ	93	ALA	5.5
33	CE	142	ALA	5.5
1	BA	1221	G	5.5
3	BC	76	VAL	5.5
10	BJ	27	GLU	5.5
31	CA	1212	G	5.5
31	CA	328	U	5.5
1	BA	1333	A	5.5
55	DA	1077	A	5.5
31	CA	291	G	5.5
37	CJ	128	SER	5.5
27	C0	48	ILE	5.5
35	CG	57	GLY	5.5
51	CX	56	ASP	5.5
3	BC	39	VAL	5.5
7	BG	118	LEU	5.5
14	BN	11	VAL	5.5
14	BN	45	VAL	5.5
37	DJ	8	TYR	5.5
7	BG	130	ASN	5.5
34	CF	37	ASN	5.5
41	CN	17	ASN	5.5
49	CV	66	GLN	5.5
55	DA	1098	A	5.5
1	BA	4	U	5.5
9	BI	30	ILE	5.5
49	CV	18	ASP	5.5
40	CM	131	ALA	5.5
53	CZ	47	ARG	5.5
42	CO	62	ASN	5.5
31	CA	1048	A	5.5
13	BM	74	SER	5.5
31	CA	879	G	5.5
31	CA	1518	C	5.5
48	CU	35	ALA	5.4
3	BC	111	LEU	5.4
30	CD	180	VAL	5.4
14	BN	49	GLN	5.4
2	BB	37	LYS	5.4

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Mol	Chain	Res	Type	RSRZ
10	BJ	99	GLN	5.4
38	CK	97	PRO	5.4
3	BC	206	GLU	5.4
3	BC	120	ILE	5.4
10	AJ	76	ILE	5.4
40	CM	45	GLY	5.4
34	CF	77	PHE	5.4
31	CA	74	A	5.4
1	BA	844	G	5.4
31	CA	327	G	5.4
37	CJ	52	GLY	5.4
35	CG	109	PHE	5.4
36	DH	139	PHE	5.4
39	CL	37	ASP	5.4
13	AM	32	ALA	5.4
7	BG	89	VAL	5.4
34	CF	74	VAL	5.4
30	CD	46	ARG	5.4
31	CA	2801	G	5.4
2	BB	82	ASP	5.4
45	CR	99	ALA	5.4
1	BA	974	A	5.4
19	AS	55	ARG	5.4
23	C2	44	ARG	5.4
42	CO	63	ARG	5.4
1	BA	1245	C	5.4
1	BA	1273	C	5.4
31	CA	183	C	5.4
9	BI	10	GLY	5.4
34	CF	18	THR	5.4
50	CW	29	ILE	5.4
1	BA	955	U	5.4
51	CX	57	HIS	5.4
46	CS	25	LEU	5.4
31	CA	626	A	5.4
31	CA	892	A	5.4
9	AI	127	PHE	5.4
27	C0	7	ILE	5.4
54	DI	84	TYR	5.4
10	BJ	81	GLU	5.4
30	CD	41	ALA	5.4
35	CG	160	LYS	5.4

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Mol	Chain	Res	Type	RSRZ
31	CA	548	G	5.4
36	DH	138	VAL	5.4
48	CU	58	VAL	5.4
7	BG	119	ARG	5.4
13	AM	44	LYS	5.4
23	C2	46	HIS	5.4
49	CV	43	LYS	5.4
33	CE	197	GLU	5.4
12	BL	124	ALA	5.4
13	AM	5	ALA	5.4
35	CG	132	VAL	5.3
43	CP	110	ALA	5.4
55	DA	882	G	5.3
31	CA	335	C	5.3
45	CR	81	ASN	5.3
37	CJ	136	MET	5.3
1	BA	1015	G	5.3
1	BA	1244	G	5.3
43	CP	69	ASP	5.3
7	AG	69	VAL	5.3
49	CV	49	VAL	5.3
19	BS	68	GLY	5.3
9	BI	20	PHE	5.3
1	AA	1020	G	5.3
1	BA	988	G	5.3
1	BA	1297	G	5.3
14	BN	43	ASN	5.3
31	CA	1873	G	5.3
14	BN	5	SER	5.3
35	CG	131	ILE	5.3
1	BA	1148	U	5.3
55	DA	1061	U	5.3
34	CF	25	VAL	5.3
37	DJ	43	ASN	5.3
37	DJ	48	SER	5.3
27	C0	44	ILE	5.3
31	CA	1216	G	5.3
10	BJ	37	ARG	5.3
33	CE	72	SER	5.3
19	BS	58	VAL	5.3
30	CD	31	ALA	5.3
37	DJ	104	ALA	5.3

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Mol	Chain	Res	Type	RSRZ
31	CA	420	C	5.3
27	C0	10	THR	5.3
38	CK	142	ILE	5.3
14	BN	6	MET	5.3
20	BT	53	GLU	5.3
10	BJ	85	ASP	5.3
46	CS	33	VAL	5.3
16	BP	42	ILE	5.2
9	AI	5	GLN	5.2
31	CA	268	C	5.2
34	CF	26	MET	5.2
36	CH	133	GLN	5.2
49	CV	15	THR	5.2
55	DA	2106	U	5.2
31	CA	1171	G	5.2
34	CF	177	PHE	5.2
35	CG	161	GLY	5.2
31	CA	138	U	5.2
23	C2	39	PHE	5.2
37	DJ	10	LYS	5.2
50	CW	69	GLU	5.2
13	BM	77	ILE	5.2
55	DA	2168	G	5.2
30	CD	153	GLY	5.2
15	AO	17	ARG	5.2
7	BG	110	LYS	5.2
7	BG	113	ASP	5.2
35	CG	59	ALA	5.2
37	DJ	132	THR	5.2
46	CS	54	VAL	5.2
52	CY	35	SER	5.2
3	BC	77	ILE	5.2
9	BI	8	GLY	5.2
13	BM	34	LEU	5.2
33	CE	88	ARG	5.2
43	CP	30	ARG	5.2
31	CA	1271	G	5.2
48	CU	36	LYS	5.2
7	BG	80	VAL	5.2
34	CF	119	ALA	5.2
36	CH	74	ALA	5.2
40	CM	115	GLU	5.2

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Mol	Chain	Res	Type	RSRZ
47	CT	85	ILE	5.2
1	BA	101	A	5.2
13	AM	11	ASP	5.2
31	CA	2651	C	5.2
6	AF	61	LEU	5.2
17	BQ	50	ASN	5.2
42	CO	83	LEU	5.2
13	BM	58	ASP	5.2
31	CA	1166	G	5.2
51	CX	58	THR	5.2
35	CG	81	GLU	5.2
20	BT	38	ALA	5.2
1	BA	1336	C	5.2
33	CE	48	THR	5.2
13	AM	7	ILE	5.2
44	CQ	4	ILE	5.2
12	BL	70	GLU	5.2
40	CM	35	HIS	5.2
24	C3	34	ARG	5.2
48	CU	37	ASP	5.2
1	BA	977	A	5.1
31	CA	893	C	5.1
37	DJ	131	GLY	5.1
7	BG	131	LYS	5.1
9	BI	41	ARG	5.1
31	CA	408	G	5.1
31	CA	1047	G	5.1
13	AM	4	ILE	5.1
1	BA	207	C	5.1
37	DJ	51	LYS	5.1
14	BN	58	SER	5.1
34	CF	4	LEU	5.1
19	BS	50	ALA	5.1
39	CL	33	ALA	5.1
50	CW	91	PHE	5.1
21	AU	11	PRO	5.1
30	CD	152	PRO	5.1
13	BM	113	ARG	5.1
13	BM	104	THR	5.1
27	C0	53	PHE	5.1
54	DI	124	ASP	5.1
49	CV	84	GLY	5.1

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Mol	Chain	Res	Type	RSRZ
7	BG	102	ARG	5.1
34	CF	67	ILE	5.1
3	BC	124	LEU	5.1
53	CZ	21	LEU	5.1
34	CF	68	THR	5.1
46	CS	83	TYR	5.1
34	CF	56	ASP	5.1
48	CU	24	MET	5.1
46	CS	100	GLY	5.1
34	CF	91	LEU	5.1
7	AG	151	PHE	5.1
33	CE	124	PHE	5.1
26	C5	20	ASP	5.1
48	CU	16	VAL	5.1
48	CU	84	TYR	5.1
9	BI	37	GLN	5.1
14	BN	13	ARG	5.1
34	CF	81	GLN	5.1
3	BC	103	ILE	5.1
53	CZ	28	LEU	5.1
1	BA	1312	G	5.1
36	DH	132	PHE	5.1
51	CX	83	GLU	5.1
30	CD	133	THR	5.1
31	CA	2177	C	5.1
40	CM	74	THR	5.1
45	CR	113	ALA	5.1
52	CY	34	HIS	5.1
20	BT	64	LYS	5.1
34	CF	172	ALA	5.1
33	CE	73	ILE	5.1
17	BQ	44	LEU	5.1
7	AG	53	ARG	5.1
22	C1	36	GLU	5.1
49	CV	76	ALA	5.1
37	DJ	106	LEU	5.0
31	CA	501	A	5.0
9	BI	103	PHE	5.0
20	BT	50	ALA	5.0
16	BP	50	THR	5.0
7	BG	68	ASN	5.0
14	BN	9	ARG	5.0

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Mol	Chain	Res	Type	RSRZ
35	CG	141	ILE	5.0
37	DJ	42	PHE	5.0
44	CQ	74	PHE	5.0
7	BG	82	GLY	5.0
33	CE	11	ALA	5.0
36	DH	65	ALA	5.0
19	BS	57	HIS	5.0
14	BN	30	ILE	5.0
37	DJ	49	ILE	5.0
37	DJ	60	THR	5.0
1	BA	1309	G	5.0
2	BB	9	MET	5.0
53	CZ	63	ALA	5.0
43	CP	88	LYS	5.0
47	CT	6	LYS	5.0
52	CY	45	ARG	5.0
53	CZ	54	LYS	5.0
13	BM	4	ILE	5.0
1	BA	222	C	5.0
13	AM	25	VAL	5.0
51	CX	25	ARG	5.0
34	CF	38	MET	5.0
31	CA	332	A	5.0
31	CA	513	A	5.0
24	C3	12	ARG	5.0
10	BJ	34	ALA	5.0
30	CD	47	ALA	5.0
36	CH	67	ALA	5.0
40	CM	108	ALA	5.0
40	CM	144	GLU	5.0
43	CP	93	ASP	5.0
31	CA	2904	U	5.0
55	DA	654	A	5.0
3	BC	73	PRO	5.0
16	BP	39	PHE	5.0
38	CK	128	ASN	5.0
42	CO	36	THR	5.0
48	CU	75	GLY	5.0
1	BA	83	C	5.0
1	AA	1025	U	5.0
1	BA	1034	G	5.0
7	AG	5	ARG	5.0

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Mol	Chain	Res	Type	RSRZ
8	AH	2	SER	5.0
19	BS	25	SER	5.0
19	BS	42	PRO	5.0
51	CX	34	GLY	5.0
35	CG	25	THR	5.0
1	BA	962	C	5.0
7	AG	134	ALA	5.0
14	BN	33	ASP	5.0
13	BM	81	MET	5.0
9	AI	32	GLN	5.0
11	AK	81	ASN	5.0
11	BK	21	ALA	5.0
20	BT	46	ALA	5.0
44	CQ	111	LYS	5.0
31	CA	369	U	5.0
48	CU	12	ARG	5.0
54	DI	40	GLU	4.9
38	CK	136	GLN	4.9
13	AM	36	ALA	4.9
3	BC	107	ARG	4.9
13	BM	11	ASP	4.9
33	CE	157	LEU	4.9
53	CZ	6	LEU	4.9
33	CE	32	VAL	4.9
19	AS	39	THR	4.9
30	CD	25	THR	4.9
46	CS	26	ASP	4.9
55	DA	2141	G	4.9
48	CU	2	ILE	4.9
14	BN	24	ARG	4.9
30	CD	199	SER	4.9
30	CD	48	ILE	4.9
31	CA	103	A	4.9
36	CH	58	LEU	4.9
42	CO	93	GLY	4.9
31	CA	1056	G	4.9
2	BB	39	HIS	4.9
27	C0	42	PRO	4.9
7	AG	59	LEU	4.9
31	CA	431	U	4.9
55	DA	1094	U	4.9
31	CA	1235	G	4.9

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Mol	Chain	Res	Type	RSRZ
7	AG	58	GLU	4.9
9	BI	92	GLU	4.9
10	AJ	36	VAL	4.9
17	BQ	78	VAL	4.9
22	C1	55	ILE	4.9
43	CP	58	ILE	4.9
2	AB	139	ARG	4.9
31	CA	357	C	4.9
37	CJ	92	LYS	4.9
17	BQ	46	VAL	4.9
27	C0	2	ALA	4.9
14	BN	32	SER	4.9
45	CR	26	GLY	4.9
50	CW	58	SER	4.9
44	CQ	59	PHE	4.9
45	CR	94	ILE	4.9
49	CV	47	LYS	4.9
55	DA	885	C	4.9
38	CK	47	HIS	4.9
14	BN	40	ASP	4.9
41	CN	79	ALA	4.9
31	CA	1863	G	4.9
31	CA	2808	G	4.9
34	CF	30	ARG	4.9
13	AM	45	ILE	4.9
13	BM	80	LEU	4.9
31	CA	2180	U	4.9
37	CJ	88	SER	4.9
9	AI	55	VAL	4.9
48	CU	31	VAL	4.9
31	CA	262	A	4.9
55	DA	892	A	4.9
3	BC	144	LEU	4.9
37	DJ	113	LYS	4.9
31	CA	2106	U	4.9
11	BK	64	GLN	4.8
53	CZ	36	GLN	4.8
19	BS	34	TRP	4.8
3	BC	42	TYR	4.8
31	CA	2800	A	4.8
35	CG	77	ILE	4.8
31	CA	1234	U	4.8

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Mol	Chain	Res	Type	RSRZ
34	CF	42	GLU	4.8
17	BQ	6	ARG	4.8
31	CA	882	G	4.8
35	CG	127	THR	4.8
33	CE	186	VAL	4.8
1	BA	1209	C	4.8
3	BC	80	LYS	4.8
34	CF	47	LYS	4.8
49	CV	82	ARG	4.8
30	CD	35	THR	4.8
36	DH	107	GLY	4.8
16	BP	9	HIS	4.8
30	CD	132	ALA	4.8
37	CJ	37	GLU	4.8
47	CT	4	ILE	4.8
37	DJ	40	LYS	4.8
40	CM	132	ARG	4.8
36	DH	96	THR	4.8
43	CP	59	ALA	4.8
9	AI	22	LYS	4.8
30	CD	45	TYR	4.8
10	AJ	7	ARG	4.8
30	CD	101	PHE	4.8
41	CN	72	PRO	4.8
52	CY	46	PHE	4.8
18	AR	51	TYR	4.8
20	BT	67	ILE	4.8
27	C0	32	ILE	4.8
31	CA	895	U	4.8
55	DA	1066	U	4.8
7	BG	122	ASN	4.8
1	BA	1219	A	4.8
31	CA	505	A	4.8
31	CA	343	C	4.8
31	CA	1547	C	4.8
7	AG	106	GLU	4.8
46	CS	13	ARG	4.8
6	BF	39	LEU	4.8
34	CF	8	TYR	4.8
35	CG	175	LYS	4.8
40	CM	70	LYS	4.8
31	CA	336	C	4.8

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Mol	Chain	Res	Type	RSRZ
19	BS	55	ARG	4.8
2	AB	210	VAL	4.8
16	BP	19	VAL	4.8
41	CN	80	VAL	4.8
3	BC	203	PHE	4.8
13	AM	40	ALA	4.8
13	BM	61	ALA	4.8
13	BM	52	GLN	4.8
16	BP	53	ASP	4.8
36	DH	56	ALA	4.8
37	DJ	75	PRO	4.8
1	BA	1340	A	4.8
31	CA	101	A	4.8
55	DA	2126	A	4.8
1	BA	1341	U	4.8
55	DA	2132	U	4.8
30	CD	83	ARG	4.7
30	CD	60	VAL	4.7
9	BI	107	ASP	4.7
31	CA	315	G	4.7
34	CF	10	ASP	4.7
9	BI	43	THR	4.7
38	CK	21	THR	4.7
40	CM	21	ARG	4.7
14	BN	34	VAL	4.7
47	CT	83	LYS	4.7
54	DI	101	LYS	4.7
35	CG	94	TYR	4.7
41	CN	41	LEU	4.7
55	DA	2177	C	4.7
2	AB	44	GLU	4.7
7	AG	65	ALA	4.7
10	BJ	35	GLN	4.7
54	DI	114	GLU	4.7
1	BA	1231	G	4.7
31	CA	2627	G	4.7
31	CA	2877	G	4.7
1	AA	1022	A	4.7
1	BA	1534	A	4.7
7	BG	78	ARG	4.7
19	BS	3	ARG	4.7
36	CH	137	GLU	4.7

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Mol	Chain	Res	Type	RSRZ
45	CR	38	ALA	4.7
45	CR	95	LEU	4.7
29	CC	232	HIS	4.7
11	BK	30	THR	4.7
25	C4	14	PHE	4.7
31	CA	214	G	4.7
40	CM	76	GLU	4.7
13	BM	13	LYS	4.7
20	BT	8	LYS	4.7
48	CU	81	LYS	4.7
11	AK	43	GLY	4.7
30	CD	1	MET	4.7
30	CD	90	PHE	4.7
36	DH	125	THR	4.7
10	BJ	92	LEU	4.7
30	CD	187	LEU	4.7
1	BA	1033	G	4.7
7	AG	7	ILE	4.7
55	DA	1089	A	4.7
55	DA	2117	A	4.7
2	BB	32	PHE	4.7
26	C5	1	MET	4.7
39	CL	111	LYS	4.7
2	BB	10	LEU	4.7
13	BM	69	LEU	4.7
36	DH	124	THR	4.7
35	CG	24	ILE	4.7
40	CM	72	ALA	4.7
7	AG	68	ASN	4.7
36	CH	135	HIS	4.7
40	CM	127	VAL	4.7
43	CP	53	THR	4.7
33	CE	22	ASP	4.7
14	AN	100	SER	4.7
31	CA	318	C	4.7
51	CX	23	VAL	4.6
13	AM	26	GLY	4.6
13	BM	70	ARG	4.6
1	BA	981	U	4.6
31	CA	2122	U	4.6
49	CV	55	PRO	4.6
43	CP	97	PHE	4.6

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Mol	Chain	Res	Type	RSRZ
39	CL	3	GLN	4.6
44	CQ	13	MET	4.6
48	CU	62	VAL	4.6
21	AU	16	LEU	4.6
43	CP	36	TYR	4.6
1	BA	1224	U	4.6
24	C3	22	MET	4.6
30	CD	29	VAL	4.6
31	CA	1868	C	4.6
55	DA	2164	C	4.6
35	CG	6	LYS	4.6
54	DI	94	ARG	4.6
31	CA	1530	G	4.6
51	CX	42	GLY	4.6
55	DA	1063	G	4.6
47	CT	94	ASP	4.6
22	C1	44	THR	4.6
14	BN	21	PHE	4.6
33	CE	177	PRO	4.6
35	CG	126	PRO	4.6
34	CF	150	ARG	4.6
43	CP	33	ARG	4.6
7	BG	63	GLU	4.6
33	CE	127	GLU	4.6
36	DH	87	GLU	4.6
37	DJ	37	GLU	4.6
39	CL	38	ILE	4.6
1	BA	205	A	4.6
1	BA	946	A	4.6
31	CA	313	G	4.6
24	C3	43	THR	4.6
33	CE	43	THR	4.6
31	CA	1534	U	4.6
35	CG	75	MET	4.6
36	DH	136	SER	4.6
43	CP	49	VAL	4.6
2	BB	33	GLY	4.6
13	BM	50	GLU	4.6
45	CR	7	GLY	4.6
38	CK	55	ILE	4.6
47	CT	92	ARG	4.6
1	BA	68	G	4.6

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Mol	Chain	Res	Type	RSRZ
1	BA	951	G	4.6
20	BT	31	PHE	4.6
31	CA	880	G	4.6
31	CA	1074	G	4.6
43	CP	104	GLN	4.6
33	CE	134	LEU	4.6
49	CV	11	VAL	4.6
22	C1	15	MET	4.6
50	CW	48	MET	4.6
1	BA	972	C	4.6
7	BG	98	ALA	4.6
43	CP	109	ALA	4.6
45	CR	17	ILE	4.6
31	CA	44	A	4.6
25	C4	38	THR	4.6
31	CA	850	U	4.6
2	AB	117	LEU	4.6
3	BC	109	PRO	4.6
17	BQ	8	LEU	4.6
31	CA	88	G	4.6
50	CW	67	GLY	4.6
7	AG	54	SER	4.6
27	C0	12	SER	4.6
33	CE	15	SER	4.6
2	BB	16	PHE	4.6
36	CH	61	VAL	4.6
53	CZ	35	GLY	4.6
33	CE	199	MET	4.6
31	CA	2630	G	4.6
13	BM	42	ASP	4.6
1	BA	1027	C	4.6
45	CR	37	GLN	4.6
55	DA	1060	U	4.6
29	CC	47	GLY	4.6
25	C4	46	PRO	4.5
38	CK	42	ALA	4.5
40	CM	137	ALA	4.5
35	CG	44	LYS	4.5
55	DA	881	G	4.5
7	AG	26	PHE	4.5
3	BC	78	GLY	4.5
33	CE	42	GLY	4.5

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Mol	Chain	Res	Type	RSRZ
39	CL	69	VAL	4.5
21	AU	9	ASN	4.5
38	CK	137	PRO	4.5
33	CE	100	MET	4.5
43	CP	56	LYS	4.5
31	CA	2116	G	4.5
1	BA	89	U	4.5
30	CD	73	VAL	4.5
40	CM	121	THR	4.5
42	CO	114	GLU	4.5
48	DU	1	MET	4.5
1	AA	78	A	4.5
37	CJ	64	ASP	4.5
26	C5	33	HIS	4.5
33	CE	103	GLY	4.5
7	AG	6	VAL	4.5
31	CA	1059	G	4.5
47	CT	48	LYS	4.5
37	DJ	107	GLN	4.5
31	CA	1061	U	4.5
31	CA	281	C	4.5
49	CV	42	VAL	4.5
31	CA	1407	G	4.5
54	DI	135	ALA	4.5
11	AK	18	ASP	4.5
48	CU	76	ARG	4.5
34	CF	100	PHE	4.5
9	AI	63	LEU	4.5
35	CG	76	VAL	4.5
31	CA	314	C	4.5
55	DA	2161	C	4.5
47	CT	54	ALA	4.5
17	BQ	72	SER	4.5
40	CM	122	VAL	4.5
54	DI	133	GLU	4.5
13	AM	39	ILE	4.5
13	AM	115	PRO	4.5
19	BS	44	MET	4.5
14	BN	73	PHE	4.5
1	BA	941	G	4.5
13	AM	48	LEU	4.5
33	CE	180	LEU	4.5

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Mol	Chain	Res	Type	RSRZ
19	BS	11	ILE	4.5
54	DI	136	ILE	4.5
31	CA	876	C	4.5
31	CA	2178	C	4.5
7	AG	8	GLY	4.5
16	AP	16	PHE	4.5
40	CM	124	GLY	4.5
5	BE	140	THR	4.5
9	BI	98	LEU	4.5
26	C5	19	ARG	4.5
37	DJ	127	ARG	4.5
38	CK	40	HIS	4.5
15	BO	19	ALA	4.4
31	CA	1233	C	4.4
16	BP	51	ARG	4.4
16	BP	56	ARG	4.4
1	BA	1125	U	4.4
37	DJ	33	VAL	4.4
2	BB	206	ALA	4.4
49	CV	63	ALA	4.4
7	BG	90	GLU	4.4
27	C0	39	GLU	4.4
37	CJ	25	GLY	4.4
38	CK	98	GLU	4.4
31	CA	816	C	4.4
33	CE	49	ARG	4.4
37	DJ	92	LYS	4.4
55	DA	897	C	4.4
34	CF	49	LEU	4.4
1	BA	842	U	4.4
7	AG	141	VAL	4.4
31	CA	2181	U	4.4
35	CG	129	THR	4.4
50	CW	64	VAL	4.4
9	BI	79	ILE	4.4
41	CN	73	ILE	4.4
7	AG	52	GLN	4.4
7	BG	86	GLN	4.4
43	CP	32	PRO	4.4
31	CA	1093	G	4.4
31	CA	1984	G	4.4
10	BJ	96	VAL	4.4

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Mol	Chain	Res	Type	RSRZ
35	CG	113	VAL	4.4
42	CO	76	VAL	4.4
49	CV	67	VAL	4.4
2	BB	213	TYR	4.4
10	BJ	32	THR	4.4
34	CF	14	LYS	4.4
49	CV	21	LYS	4.4
2	AB	9	MET	4.4
40	CM	91	ASP	4.4
1	BA	1003	G	4.4
12	BL	81	LEU	4.4
35	CG	38	ASN	4.4
36	CH	110	VAL	4.4
2	AB	7	ARG	4.4
30	CD	184	ARG	4.4
34	CF	11	GLU	4.4
34	CF	112	ARG	4.4
51	CX	37	ILE	4.4
34	CF	27	GLN	4.4
13	BM	75	MET	4.4
51	CX	64	ASP	4.4
14	BN	63	ARG	4.4
26	C5	12	ARG	4.4
31	CA	413	C	4.4
37	CJ	127	ARG	4.4
36	CH	94	ILE	4.4
42	CO	113	ILE	4.4
40	CM	7	SER	4.4
46	CS	15	SER	4.4
13	BM	62	LYS	4.4
19	AS	56	GLN	4.4
20	BT	9	LYS	4.4
35	CG	166	ASP	4.4
1	AA	1001	C	4.4
11	AK	97	ILE	4.4
33	CE	175	ILE	4.4
8	BH	130	ALA	4.4
13	BM	49	SER	4.4
35	CG	156	PRO	4.4
46	CS	29	THR	4.4
35	CG	48	ASN	4.4
17	BQ	21	ILE	4.4

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Mol	Chain	Res	Type	RSRZ
49	CV	72	ILE	4.4
14	AN	25	ALA	4.3
51	CX	41	ARG	4.3
33	CE	122	GLU	4.3
51	CX	85	GLU	4.3
8	AH	121	LEU	4.3
30	CD	84	LEU	4.3
45	CR	117	LEU	4.3
30	CD	55	LYS	4.3
3	BC	102	ASN	4.3
7	BG	9	GLN	4.3
34	CF	101	GLU	4.3
55	DA	893	C	4.3
7	BG	44	TYR	4.3
9	BI	129	LYS	4.3
9	BI	48	VAL	4.3
31	CA	2799	A	4.3
31	CA	1015	U	4.3
46	CS	6	GLN	4.3
20	BT	68	HIS	4.3
34	CF	22	TYR	4.3
42	CO	94	TYR	4.3
40	CM	139	GLY	4.3
1	BA	1239	A	4.3
15	BO	15	PHE	4.3
9	AI	59	GLU	4.3
19	BS	56	GLN	4.3
31	CA	1090	A	4.3
31	CA	124	G	4.3
31	CA	2693	G	4.3
37	DJ	97	LYS	4.3
54	DI	72	LEU	4.3
19	BS	23	VAL	4.3
30	CD	50	VAL	4.3
40	CM	30	THR	4.3
52	CY	47	VAL	4.3
31	CA	2657	A	4.3
14	BN	71	HIS	4.3
33	CE	147	LEU	4.3
1	BA	1281	C	4.3
13	BM	111	GLY	4.3
31	CA	1079	C	4.3

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Mol	Chain	Res	Type	RSRZ
23	C2	22	THR	4.3
49	DV	52	LEU	4.3
12	BL	108	LYS	4.3
25	C4	35	LYS	4.3
28	CB	24	G	4.3
31	CA	2668	G	4.3
31	CA	2164	C	4.3
40	CM	119	PRO	4.3
11	BK	110	ILE	4.3
40	CM	38	GLN	4.3
44	CQ	50	ILE	4.3
34	CF	171	ALA	4.3
45	CR	30	ARG	4.3
2	AB	37	LYS	4.3
20	BT	59	ASP	4.3
42	CO	79	LEU	4.3
2	AB	27	MET	4.3
9	AI	89	GLU	4.3
14	BN	10	GLU	4.3
37	CJ	16	GLY	4.3
41	CN	12	MET	4.3
1	AA	1033	G	4.3
1	BA	1013	G	4.3
1	BA	1310	G	4.3
31	CA	1112	G	4.3
31	CA	1279	G	4.3
33	CE	121	VAL	4.3
1	BA	1007	U	4.3
19	BS	43	ASN	4.3
46	CS	60	LYS	4.3
49	CV	2	ALA	4.3
7	BG	120	LEU	4.3
19	BS	65	GLU	4.3
27	C0	25	LEU	4.3
31	CA	1073	A	4.3
31	CA	1548	A	4.3
38	CK	118	MET	4.3
49	DV	49	VAL	4.3
2	BB	164	ILE	4.3
31	CA	475	C	4.3
1	BA	1272	G	4.3
31	CA	280	U	4.3

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Mol	Chain	Res	Type	RSRZ
36	DH	89	LYS	4.3
55	DA	2105	U	4.3
3	BC	112	ASP	4.2
54	DI	3	LEU	4.2
33	CE	28	VAL	4.2
1	BA	1150	A	4.2
45	CR	101	PHE	4.2
49	CV	85	PHE	4.2
25	C4	45	ARG	4.2
16	AP	47	GLU	4.2
17	BQ	74	THR	4.2
20	AT	80	THR	4.2
34	CF	114	PHE	4.2
36	CH	139	PHE	4.2
37	CJ	36	MET	4.2
11	AK	110	ILE	4.2
20	BT	36	TYR	4.2
22	C1	8	PRO	4.2
40	CM	50	PHE	4.2
50	CW	2	PHE	4.2
55	DA	2146	C	4.2
19	BS	13	LEU	4.2
49	CV	56	GLY	4.2
2	BB	131	LYS	4.2
16	AP	39	PHE	4.2
37	DJ	57	VAL	4.2
1	BA	952	U	4.2
31	CA	884	U	4.2
1	BA	250	A	4.2
1	BA	1035	A	4.2
3	BC	50	ALA	4.2
11	BK	67	ALA	4.2
10	AJ	102	LEU	4.2
25	C4	25	LYS	4.2
28	CB	63	C	4.2
13	BM	90	ARG	4.2
13	BM	102	THR	4.2
47	CT	95	ARG	4.2
24	C3	13	ASN	4.2
5	BE	120	VAL	4.2
15	BO	75	VAL	4.2
31	CA	180	G	4.2

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Mol	Chain	Res	Type	RSRZ
35	CG	125	CYS	4.2
9	AI	97	GLU	4.2
9	BI	21	ILE	4.2
45	CR	25	TYR	4.2
48	CU	33	LYS	4.2
1	AA	1000	A	4.2
1	BA	1230	C	4.2
9	BI	94	LEU	4.2
30	CD	39	ASP	4.2
31	CA	1874	C	4.2
6	BF	97	THR	4.2
24	C3	5	PHE	4.2
40	CM	5	THR	4.2
37	CJ	117	MET	4.2
6	AF	37	HIS	4.2
31	CA	1444	G	4.2
49	DV	51	ALA	4.2
7	AG	23	LEU	4.2
34	CF	36	LEU	4.2
15	BO	21	ASP	4.2
33	CE	126	VAL	4.2
37	DJ	81	LYS	4.2
42	CO	1	MET	4.2
48	CU	44	LYS	4.2
19	AS	49	ILE	4.2
34	CF	29	PRO	4.2
44	CQ	5	ILE	4.2
31	CA	810	U	4.2
35	CG	21	GLY	4.2
31	CA	2032	G	4.2
37	CJ	115	ALA	4.2
40	CM	83	ALA	4.2
43	CP	70	ALA	4.2
13	BM	44	LYS	4.2
33	CE	140	ASP	4.2
31	CA	2165	C	4.2
1	AA	1036	A	4.2
5	BE	80	THR	4.2
54	DI	123	ILE	4.2
13	AM	35	ALA	4.2
3	BC	108	LYS	4.2
45	CR	18	LEU	4.2

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Mol	Chain	Res	Type	RSRZ
14	AN	37	SER	4.2
1	AA	1277	C	4.2
10	AJ	45	ARG	4.2
33	CE	196	VAL	4.2
9	AI	88	MET	4.2
46	CS	82	HIS	4.2
1	AA	89	U	4.2
35	CG	173	GLU	4.1
46	CS	46	GLU	4.1
38	CK	141	ASP	4.1
9	BI	33	ARG	4.1
1	AA	1037	C	4.1
36	DH	99	ILE	4.1
37	CJ	34	ASN	4.1
38	CK	54	ILE	4.1
49	CV	65	ILE	4.1
13	AM	34	LEU	4.1
9	AI	39	PHE	4.1
46	CS	92	TRP	4.1
54	DI	106	PHE	4.1
40	CM	84	LYS	4.1
1	BA	1001	C	4.1
8	BH	122	GLY	4.1
31	CA	638	G	4.1
31	CA	1531	C	4.1
31	CA	1533	C	4.1
14	BN	39	GLU	4.1
12	BL	50	ARG	4.1
53	CZ	48	ARG	4.1
55	DA	2171	A	4.1
34	CF	64	LYS	4.1
4	AD	39	GLY	4.1
46	CS	30	GLY	4.1
39	CL	89	ASN	4.1
1	BA	1210	C	4.1
7	AG	50	LEU	4.1
30	CD	59	ARG	4.1
31	CA	2111	U	4.1
43	CP	102	ARG	4.1
44	CQ	72	ARG	4.1
48	CU	80	TRP	4.1
37	CJ	137	GLY	4.1

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Mol	Chain	Res	Type	RSRZ
11	BK	68	GLU	4.1
21	AU	36	GLU	4.1
46	CS	37	GLU	4.1
7	AG	110	LYS	4.1
28	CB	22	U	4.1
30	CD	121	THR	4.1
31	CA	799	G	4.1
31	CA	477	A	4.1
31	CA	1142	A	4.1
9	BI	117	GLY	4.1
13	BM	53	ILE	4.1
36	DH	127	GLU	4.1
37	CJ	35	ILE	4.1
54	DI	66	GLY	4.1
13	AM	13	LYS	4.1
14	BN	47	LYS	4.1
2	AB	214	LEU	4.1
8	BH	121	LEU	4.1
31	CA	1325	U	4.1
34	CF	139	PRO	4.1
36	DH	67	ALA	4.1
2	AB	16	PHE	4.1
7	AG	49	THR	4.1
7	BG	26	PHE	4.1
8	BH	90	ASP	4.1
33	CE	176	ASP	4.1
13	BM	38	GLY	4.1
17	BQ	23	VAL	4.1
19	BS	81	ARG	4.1
31	CA	1041	G	4.1
35	CG	90	VAL	4.1
34	CF	141	ILE	4.1
45	CR	65	ILE	4.1
45	CR	92	ARG	4.1
2	AB	132	LYS	4.1
30	CD	95	SER	4.1
37	CJ	66	SER	4.1
9	BI	121	ALA	4.1
43	CP	61	GLN	4.1
45	CR	35	ALA	4.1
3	BC	118	ASP	4.1
3	BC	179	ARG	4.1

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Mol	Chain	Res	Type	RSRZ
3	BC	204	LYS	4.1
35	CG	158	LYS	4.1
49	CV	62	GLU	4.1
7	AG	64	VAL	4.1
11	AK	84	VAL	4.1
30	CD	80	TRP	4.1
33	CE	10	SER	4.1
1	BA	982	U	4.1
33	CE	50	ALA	4.1
46	CS	24	LYS	4.1
22	C1	51	GLY	4.1
31	CA	1044	C	4.1
31	CA	1732	C	4.1
17	BQ	61	ILE	4.1
1	BA	945	G	4.1
1	BA	1048	G	4.1
31	CA	85	G	4.1
31	CA	2835	A	4.1
40	CM	138	ALA	4.1
44	CQ	91	ALA	4.1
55	DA	277	G	4.1
19	BS	26	GLY	4.0
33	CE	35	TYR	4.0
46	CS	51	VAL	4.0
6	AF	36	ILE	4.0
10	AJ	8	ILE	4.0
9	BI	124	ARG	4.0
11	AK	100	LEU	4.0
29	CC	101	ARG	4.0
36	CH	122	LEU	4.0
41	CN	78	LEU	4.0
41	CN	116	ALA	4.0
43	CP	60	GLU	4.0
47	CT	99	ARG	4.0
31	CA	1018	U	4.0
31	CA	2167	U	4.0
1	AA	412	A	4.0
31	CA	866	A	4.0
31	CA	801	G	4.0
33	CE	171	ASP	4.0
40	CM	52	GLY	4.0
42	CO	101	GLY	4.0

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Mol	Chain	Res	Type	RSRZ
36	CH	134	VAL	4.0
28	CB	37	C	4.0
28	CB	97	C	4.0
33	CE	12	LEU	4.0
35	CG	73	ASN	4.0
49	CV	27	ASN	4.0
3	BC	200	VAL	4.0
48	CU	30	ILE	4.0
1	BA	1226	C	4.0
3	BC	172	ARG	4.0
2	AB	10	LEU	4.0
31	CA	545	U	4.0
23	C2	31	PRO	4.0
50	CW	37	PRO	4.0
2	AB	36	ASN	4.0
13	BM	16	VAL	4.0
44	CQ	26	VAL	4.0
31	CA	2872	A	4.0
1	AA	1276	G	4.0
42	CO	20	MET	4.0
7	BG	51	ALA	4.0
30	CD	75	ALA	4.0
31	CA	290	U	4.0
33	CE	76	PRO	4.0
33	CE	67	ARG	4.0
49	CV	22	ARG	4.0
53	CZ	5	GLU	4.0
1	BA	460	A	4.0
15	AO	69	TYR	4.0
55	DA	1847	A	4.0
14	AN	27	LEU	4.0
7	AG	116	MET	4.0
3	BC	194	GLY	4.0
33	CE	64	GLY	4.0
37	CJ	104	ALA	4.0
50	CW	28	ALA	4.0
31	CA	224	U	4.0
16	AP	4	ILE	4.0
22	C1	37	LYS	4.0
45	CR	45	TYR	4.0
31	CA	603	A	4.0
14	BN	15	ALA	4.0

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Mol	Chain	Res	Type	RSRZ
22	C1	33	THR	4.0
43	CP	22	GLY	4.0
31	CA	1406	U	4.0
1	BA	1127	G	4.0
31	CA	361	G	4.0
35	CG	154	PRO	4.0
1	BA	174	A	4.0
11	AK	21	ALA	4.0
19	BS	75	ALA	4.0
23	C2	29	THR	4.0
31	CA	222	A	4.0
31	CA	1143	A	4.0
55	DA	2114	A	4.0
34	CF	98	GLU	4.0
13	AM	31	LYS	4.0
14	BN	3	LYS	4.0
1	BA	1041	G	4.0
31	CA	2367	G	4.0
31	CA	2383	G	4.0
34	CF	149	VAL	4.0
36	DH	142	VAL	4.0
44	CQ	92	VAL	4.0
45	CR	39	VAL	4.0
2	AB	85	LEU	4.0
54	DI	88	HIS	4.0
36	DH	123	ARG	4.0
40	CM	34	GLY	4.0
29	CC	225	MET	4.0
33	CE	135	ALA	4.0
38	CK	94	ALA	4.0
7	AG	48	GLU	4.0
1	BA	194	C	3.9
1	BA	1038	C	3.9
14	BN	50	THR	3.9
22	C1	26	THR	3.9
31	CA	2833	U	3.9
36	CH	127	GLU	4.0
47	CT	16	LYS	3.9
7	AG	105	VAL	3.9
49	DV	55	PRO	3.9
1	BA	976	G	3.9
2	BB	212	LEU	3.9

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Mol	Chain	Res	Type	RSRZ
31	CA	259	G	3.9
31	CA	1202	G	3.9
31	CA	2819	G	3.9
35	CG	91	GLY	3.9
2	AB	49	MET	3.9
13	BM	106	ALA	3.9
33	CE	26	ALA	3.9
47	CT	98	LYS	3.9
23	C2	40	ASP	3.9
35	CG	49	THR	3.9
31	CA	2176	A	3.9
37	DJ	61	VAL	3.9
49	CV	94	ARG	3.9
13	BM	100	GLN	3.9
7	BG	23	LEU	3.9
34	CF	127	ASN	3.9
37	DJ	21	SER	3.9
40	CM	3	LEU	3.9
43	CP	101	GLY	3.9
48	CU	82	LYS	3.9
2	BB	134	ALA	3.9
31	CA	989	G	3.9
31	CA	2895	G	3.9
35	CG	96	ALA	3.9
46	CS	1	MET	3.9
3	BC	56	VAL	3.9
14	BN	59	ARG	3.9
17	BQ	5	ILE	3.9
36	CH	108	VAL	3.9
31	CA	76	C	3.9
46	CS	99	THR	3.9
9	AI	16	ALA	3.9
44	CQ	99	TYR	3.9
1	BA	944	G	3.9
31	CA	1017	G	3.9
9	AI	51	PRO	3.9
14	BN	7	LYS	3.9
20	BT	35	VAL	3.9
1	BA	1277	C	3.9
35	CG	50	LEU	3.9
1	AA	1004	A	3.9
31	CA	213	A	3.9

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Mol	Chain	Res	Type	RSRZ
38	CK	23	LYS	3.9
29	CC	172	VAL	3.9
31	CA	1731	G	3.9
55	DA	2128	G	3.9
29	CC	236	GLU	3.9
36	CH	70	GLU	3.9
48	CU	56	GLU	3.9
1	BA	175	C	3.9
3	BC	171	GLY	3.9
2	AB	42	ASN	3.9
20	BT	45	ALA	3.9
31	CA	423	A	3.9
49	CV	86	ARG	3.9
52	CY	18	ARG	3.9
55	DA	2119	A	3.9
3	BC	116	VAL	3.9
8	BH	110	VAL	3.9
21	AU	13	ASP	3.9
34	CF	12	VAL	3.9
1	BA	1253	G	3.9
27	C0	41	THR	3.9
30	CD	188	LEU	3.9
31	CA	805	G	3.9
3	BC	117	ALA	3.9
20	AT	87	ALA	3.9
53	DZ	63	ALA	3.9
1	BA	325	A	3.9
30	CD	86	GLU	3.9
50	CW	45	ASP	3.9
30	CD	68	PHE	3.9
39	CL	48	PRO	3.9
3	BC	54	ARG	3.9
36	CH	68	ARG	3.9
42	CO	107	ASN	3.9
55	DA	2162	G	3.9
16	BP	58	ALA	3.9
19	BS	22	ALA	3.9
3	BC	122	SER	3.9
50	CW	7	GLU	3.9
1	BA	1254	A	3.9
27	C0	57	VAL	3.9
34	CF	142	ASP	3.9

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Mol	Chain	Res	Type	RSRZ
13	AM	24	GLY	3.9
40	CM	65	GLY	3.9
48	CU	71	GLY	3.9
36	CH	77	THR	3.9
2	AB	12	ALA	3.9
7	BG	121	ALA	3.9
16	AP	45	GLU	3.9
35	CG	20	ASN	3.9
20	BT	5	LYS	3.8
2	AB	41	ILE	3.8
49	DV	54	GLN	3.8
31	CA	2309	A	3.8
35	CG	167	GLU	3.8
1	BA	1214	C	3.8
31	CA	2129	C	3.8
53	CZ	44	LYS	3.8
3	BC	127	ARG	3.8
6	AF	62	MET	3.8
7	BG	57	SER	3.8
14	AN	5	SER	3.8
24	C3	14	ARG	3.8
45	CR	14	HIS	3.8
26	C5	25	VAL	3.8
1	BA	108	G	3.8
10	BJ	33	GLY	3.8
51	CX	51	VAL	3.8
31	CA	308	G	3.8
35	CG	37	LEU	3.8
1	AA	80	A	3.8
31	CA	1395	A	3.8
7	BG	149	LYS	3.8
34	CF	120	LYS	3.8
7	BG	84	THR	3.8
38	CK	78	THR	3.8
1	BA	1364	U	3.8
31	CA	1043	C	3.8
30	CD	2	ILE	3.8
38	CK	60	ASP	3.8
7	BG	59	LEU	3.8
1	AA	1002	G	3.8
1	BA	165	G	3.8
28	CB	23	G	3.8

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Mol	Chain	Res	Type	RSRZ
46	CS	52	PRO	3.8
1	AA	1019	A	3.8
40	CM	118	THR	3.8
31	CA	1599	U	3.8
31	CA	2491	U	3.8
26	C5	2	LYS	3.8
10	AJ	39	PRO	3.8
31	CA	1341	G	3.8
31	CA	2876	G	3.8
7	BG	127	ALA	3.8
16	AP	43	ALA	3.8
30	CD	42	ASN	3.8
36	DH	11	ASN	3.8
38	CK	1	MET	3.8
38	CK	64	VAL	3.8
47	CT	40	ASN	3.8
2	AB	30	PHE	3.8
41	CN	84	LYS	3.8
3	AC	168	TYR	3.8
14	BN	69	ARG	3.8
10	BJ	23	ALA	3.8
1	AA	1024	G	3.8
31	CA	1524	G	3.8
33	CE	168	ASP	3.8
46	CS	19	THR	3.8
46	CS	64	VAL	3.8
31	CA	2045	C	3.8
37	DJ	124	ALA	3.8
2	BB	89	GLN	3.8
30	CD	49	GLN	3.8
2	BB	36	ASN	3.8
3	BC	181	ASP	3.8
10	AJ	10	LEU	3.8
28	CB	51	G	3.8
28	CB	98	G	3.8
30	CD	149	ASN	3.8
33	CE	148	ILE	3.8
37	CJ	116	ASP	3.8
38	CK	17	VAL	3.8
31	CA	474	G	3.8
1	BA	1267	C	3.8
31	CA	228	C	3.8

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Mol	Chain	Res	Type	RSRZ
35	CG	66	GLY	3.8
11	BK	65	VAL	3.8
33	CE	14	VAL	3.8
37	CJ	134	ARG	3.8
36	CH	143	ILE	3.8
1	BA	1002	G	3.8
22	C1	57	LYS	3.8
31	CA	412	A	3.8
55	DA	2133	G	3.8
1	BA	1265	C	3.8
2	BB	44	GLU	3.8
10	AJ	5	ARG	3.8
30	CD	206	ALA	3.8
35	CG	68	ALA	3.8
53	CZ	25	GLN	3.8
44	CQ	86	VAL	3.8
51	CX	38	VAL	3.8
54	DI	55	VAL	3.8
2	AB	8	ASP	3.7
25	C4	15	LYS	3.7
20	BT	70	ASN	3.7
31	CA	233	A	3.7
31	CA	1328	A	3.7
1	BA	100	G	3.7
7	AG	39	ALA	3.7
10	BJ	20	GLN	3.7
16	BP	77	GLU	3.7
31	CA	295	G	3.7
31	CA	377	G	3.7
31	CA	611	C	3.7
31	CA	2890	G	3.7
45	CR	42	ALA	3.7
53	CZ	8	GLU	3.7
49	CV	93	VAL	3.7
33	CE	188	MET	3.7
7	BG	85	TYR	3.7
33	CE	13	THR	3.7
37	CJ	112	THR	3.7
38	CK	95	ARG	3.7
44	CQ	93	ARG	3.7
37	CJ	26	PRO	3.7
38	CK	66	GLY	3.7

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Mol	Chain	Res	Type	RSRZ
1	BA	172	A	3.7
13	BM	37	ALA	3.7
31	CA	270	A	3.7
37	DJ	83	ALA	3.7
40	CM	15	ALA	3.7
40	CM	141	LYS	3.7
46	CS	42	ALA	3.7
38	CK	89	PHE	3.7
55	DA	880	G	3.7
45	CR	8	VAL	3.7
46	CS	58	VAL	3.7
25	C4	26	HIS	3.7
45	CR	64	ARG	3.7
26	C5	8	LYS	3.7
29	CC	5	LYS	3.7
37	CJ	100	LYS	3.7
38	CK	53	TYR	3.7
22	C1	18	SER	3.7
30	CD	102	ALA	3.7
33	CE	37	ALA	3.7
42	CO	6	SER	3.7
1	BA	1320	C	3.7
31	CA	680	C	3.7
36	CH	91	PHE	3.7
2	BB	31	ILE	3.7
7	BG	104	ILE	3.7
17	BQ	29	VAL	3.7
37	DJ	58	VAL	3.7
31	CA	1653	G	3.7
33	CE	7	ASP	3.7
43	CP	89	ASP	3.7
47	CT	11	ARG	3.7
22	C1	19	HIS	3.7
53	CZ	58	ASN	3.7
42	CO	7	GLY	3.7
13	AM	56	LEU	3.7
31	CA	1289	C	3.7
31	CA	2614	A	3.7
31	CA	495	G	3.7
31	CA	1245	G	3.7
46	CS	12	HIS	3.7
52	CY	20	HIS	3.7

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Mol	Chain	Res	Type	RSRZ
7	BG	61	ALA	3.7
13	AM	15	ALA	3.7
46	CS	36	ALA	3.7
2	AB	186	ILE	3.7
2	BB	41	ILE	3.7
10	AJ	77	VAL	3.7
13	BM	3	ARG	3.7
33	CE	179	SER	3.7
37	DJ	128	SER	3.7
13	BM	97	VAL	3.7
14	BN	12	LYS	3.7
50	CW	79	ARG	3.7
9	BI	91	ASP	3.7
10	BJ	24	GLU	3.7
15	BO	26	GLU	3.7
28	CB	19	C	3.7
40	CM	95	LEU	3.7
2	BB	6	MET	3.7
11	BK	85	MET	3.7
33	DE	7	ASP	3.7
55	DA	2147	A	3.7
1	BA	212	G	3.7
29	CC	251	GLN	3.7
13	AM	10	PRO	3.7
2	AB	47	VAL	3.7
14	BN	51	LEU	3.7
30	CD	34	VAL	3.7
35	CG	74	SER	3.7
36	CH	14	SER	3.7
46	CS	45	GLU	3.7
1	BA	121	U	3.7
1	BA	1132	C	3.7
1	BA	1313	U	3.7
42	CO	117	ASP	3.7
5	BE	91	GLY	3.7
14	BN	62	ASN	3.7
15	BO	20	ASN	3.7
33	CE	30	GLN	3.7
18	BR	48	ARG	3.7
27	C0	20	HIS	3.7
39	CL	21	CYS	3.7
12	BL	117	TYR	3.7

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Mol	Chain	Res	Type	RSRZ
14	BN	99	ALA	3.7
31	CA	117	G	3.7
8	BH	2	SER	3.7
38	CK	140	LEU	3.7
48	CU	29	THR	3.7
46	CS	95	ASP	3.7
1	BA	1037	C	3.7
31	CA	1045	C	3.7
31	CA	1278	C	3.7
9	BI	39	PHE	3.7
19	BS	69	HIS	3.7
33	CE	190	ALA	3.7
47	CT	7	HIS	3.7
47	CT	44	ALA	3.7
33	CE	129	PRO	3.7
9	BI	19	VAL	3.7
30	CD	100	LEU	3.7
42	CO	52	ILE	3.7
6	AF	97	THR	3.7
20	BT	80	THR	3.7
31	CA	1236	G	3.7
14	AN	66	GLN	3.6
31	CA	353	C	3.6
4	AD	113	GLU	3.6
2	AB	134	ALA	3.6
10	AJ	34	ALA	3.6
19	AS	57	HIS	3.6
26	C5	13	ASN	3.6
31	CA	53	A	3.6
16	BP	36	VAL	3.6
21	AU	3	VAL	3.6
35	CG	133	LEU	3.6
54	DI	126	LEU	3.6
2	BB	123	ASP	3.6
31	CA	2796	U	3.6
10	BJ	88	MET	3.6
31	CA	30	G	3.6
7	AG	18	PHE	3.6
3	BC	160	ALA	3.6
9	AI	83	ILE	3.6
18	AR	23	TYR	3.6
31	CA	666	A	3.6

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Mol	Chain	Res	Type	RSRZ
40	CM	27	LEU	3.6
45	CR	34	VAL	3.6
54	DI	59	LEU	3.6
55	DA	2108	A	3.6
10	BJ	97	ASP	3.6
3	BC	70	THR	3.6
31	CA	2629	U	3.6
35	CG	22	GLN	3.6
1	BA	1266	G	3.6
1	BA	63	C	3.6
1	BA	210	C	3.6
16	BP	38	PHE	3.6
54	DI	104	ALA	3.6
9	AI	94	LEU	3.6
14	AN	101	TRP	3.6
11	BK	86	VAL	3.6
40	CM	18	ARG	3.6
46	CS	75	VAL	3.6
2	BB	13	GLY	3.6
42	CO	105	GLY	3.6
1	BA	1036	A	3.6
44	CQ	24	ASP	3.6
34	CF	96	MET	3.6
36	CH	109	GLU	3.6
47	CT	3	THR	3.6
42	CO	103	ARG	3.6
39	CL	99	ILE	3.6
31	CA	1060	U	3.6
31	CA	1608	A	3.6
2	AB	5	SER	3.6
24	C3	24	THR	3.6
37	CJ	48	SER	3.6
11	AK	66	ALA	3.6
2	AB	15	HIS	3.6
2	AB	221	VAL	3.6
22	C1	42	HIS	3.6
28	CB	110	C	3.6
30	CD	27	ILE	3.6
33	CE	77	ILE	3.6
36	CH	89	LYS	3.6
40	CM	62	PRO	3.6
1	AA	121	U	3.6

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Mol	Chain	Res	Type	RSRZ
31	CA	1647	U	3.6
31	CA	2305	U	3.6
35	CG	128	GLN	3.6
13	BM	57	ARG	3.6
29	CC	30	PHE	3.6
31	CA	2117	A	3.6
9	AI	87	LEU	3.6
1	AA	1281	C	3.6
7	AG	74	GLU	3.6
13	BM	66	GLU	3.6
13	BM	67	GLY	3.6
37	DJ	93	PRO	3.6
17	BQ	53	CYS	3.6
31	CA	512	G	3.6
31	CA	619	G	3.6
31	CA	1309	G	3.6
1	BA	195	A	3.6
30	CD	91	THR	3.6
31	CA	2792	A	3.6
33	CE	34	ALA	3.6
35	CG	5	ALA	3.6
37	CJ	49	ILE	3.6
40	CM	106	GLU	3.6
1	BA	980	C	3.6
10	AJ	55	PRO	3.6
31	CA	565	C	3.6
31	CA	1207	C	3.6
31	CA	1320	C	3.6
11	AK	56	ARG	3.6
31	CA	2109	U	3.6
34	CF	7	TYR	3.6
36	CH	27	ARG	3.6
1	AA	1015	G	3.6
1	BA	1006	G	3.6
4	AD	21	LEU	3.6
14	AN	67	THR	3.6
33	CE	36	ALA	3.6
43	CP	20	GLU	3.6
14	BN	79	LEU	3.6
11	AK	129	VAL	3.6
31	CA	849	A	3.6
33	CE	4	VAL	3.6

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Mol	Chain	Res	Type	RSRZ
38	CK	56	VAL	3.6
40	CM	116	VAL	3.6
2	BB	139	ARG	3.6
48	CU	28	ASN	3.6
33	CE	132	LYS	3.5
33	CE	16	GLU	3.5
1	BA	1323	G	3.5
1	BA	1347	G	3.5
6	AF	39	LEU	3.5
7	BG	37	SER	3.5
12	BL	69	GLY	3.5
31	CA	7	G	3.5
31	CA	1475	G	3.5
36	DH	126	GLY	3.5
13	BM	73	ILE	3.5
37	CJ	101	ILE	3.5
37	DJ	129	ILE	3.5
10	BJ	15	HIS	3.5
34	DF	176	PRO	3.5
1	BA	986	U	3.5
31	CA	11	C	3.5
31	CA	2364	C	3.5
4	AD	117	LEU	3.5
18	AR	48	ARG	3.5
30	CD	146	ILE	3.5
10	BJ	28	THR	3.5
55	DA	1059	G	3.5
1	BA	216	U	3.5
31	CA	767	U	3.5
36	CH	128	HIS	3.5
42	CO	11	ASN	3.5
1	BA	1325	C	3.5
31	CA	2047	C	3.5
36	CH	60	GLU	3.5
3	BC	129	MET	3.5
2	BB	7	ARG	3.5
34	CF	62	GLY	3.5
46	CS	79	ARG	3.5
19	BS	4	SER	3.5
39	CL	2	ILE	3.5
41	CN	126	ILE	3.5
28	CB	21	G	3.5

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Mol	Chain	Res	Type	RSRZ
31	CA	2502	G	3.5
1	BA	957	U	3.5
31	CA	1201	U	3.5
31	CA	2654	A	3.5
1	BA	1327	C	3.5
2	BB	11	LYS	3.5
14	BN	23	LYS	3.5
13	BM	15	ALA	3.5
36	DH	105	ALA	3.5
7	BG	74	GLU	3.5
11	AK	111	THR	3.5
13	AM	42	ASP	3.5
2	AB	32	PHE	3.5
7	BG	2	PRO	3.5
44	CQ	43	PHE	3.5
45	CR	57	PHE	3.5
46	CS	81	LYS	3.5
28	CB	117	G	3.5
1	BA	979	C	3.5
1	BA	1208	C	3.5
16	AP	71	VAL	3.5
43	CP	28	VAL	3.5
16	BP	45	GLU	3.5
50	CW	12	GLN	3.5
19	BS	35	SER	3.5
34	DF	80	ARG	3.5
43	CP	111	ARG	3.5
45	CR	102	ASP	3.5
1	BA	1295	U	3.5
14	BN	70	PRO	3.5
55	DA	546	U	3.5
48	DU	92	ASN	3.5
1	BA	223	A	3.5
25	C4	29	LEU	3.5
31	CA	508	A	3.5
43	CP	82	ALA	3.5
54	DI	120	ALA	3.5
3	AC	195	VAL	3.5
19	BS	51	VAL	3.5
35	DG	17	VAL	3.5
4	AD	31	LYS	3.5
20	BT	71	LYS	3.5

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Mol	Chain	Res	Type	RSRZ
49	CV	92	LYS	3.5
7	AG	57	SER	3.5
37	DJ	90	SER	3.5
20	BT	51	PHE	3.5
27	C0	17	LEU	3.5
7	AG	43	VAL	3.5
22	C1	32	LYS	3.5
34	CF	137	ILE	3.5
35	CG	79	VAL	3.5
35	CG	130	GLU	3.5
50	CW	63	ILE	3.5
1	BA	1252	A	3.5
31	CA	422	A	3.5
31	CA	808	G	3.5
31	CA	1026	G	3.5
7	BG	125	SER	3.5
30	CD	156	PHE	3.5
34	CF	24	SER	3.5
40	CM	42	SER	3.5
9	AI	24	GLY	3.5
31	CA	1864	U	3.5
40	CM	26	GLY	3.5
41	CN	99	GLY	3.5
47	CT	87	PRO	3.5
36	DH	77	THR	3.5
9	AI	31	ASN	3.5
9	AI	85	ARG	3.5
16	BP	11	ALA	3.5
33	CE	21	ARG	3.5
35	CG	136	ALA	3.5
46	CS	39	LEU	3.5
27	C0	14	ILE	3.5
48	CU	6	ARG	3.5
31	CA	406	G	3.5
31	CA	881	G	3.5
31	CA	1322	A	3.5
31	CA	1551	A	3.5
31	CA	1734	G	3.5
10	AJ	33	GLY	3.4
1	BA	956	U	3.4
10	AJ	43	PRO	3.4
31	CA	2783	U	3.4

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Mol	Chain	Res	Type	RSRZ
37	CJ	39	CYS	3.4
37	DJ	46	THR	3.4
45	CR	11	ARG	3.4
11	AK	47	ALA	3.4
30	CD	36	GLN	3.4
34	DF	74	VAL	3.4
36	DH	108	VAL	3.4
54	DI	36	ASP	3.4
1	BA	88	U	3.4
1	BA	473	U	3.4
2	AB	225	ARG	3.4
31	CA	407	G	3.4
31	CA	1869	G	3.4
31	CA	2861	U	3.4
34	CF	133	ARG	3.4
44	CQ	11	GLU	3.4
47	CT	39	THR	3.4
2	AB	213	TYR	3.4
30	CD	98	VAL	3.4
53	CZ	38	GLN	3.4
36	DH	95	GLY	3.4
44	CQ	35	GLY	3.4
1	AA	1029	U	3.4
1	BA	1330	U	3.4
1	BA	975	A	3.4
9	AI	54	LEU	3.4
12	BL	24	LEU	3.4
36	CH	75	LEU	3.4
1	BA	1356	G	3.4
31	CA	1332	G	3.4
31	CA	1622	G	3.4
47	CT	9	HIS	3.4
40	CM	128	THR	3.4
55	DA	1093	G	3.4
5	BE	123	VAL	3.4
36	CH	141	LYS	3.4
36	CH	144	VAL	3.4
29	DC	240	PHE	3.4
7	BG	70	ARG	3.4
12	BL	114	ARG	3.4
40	CM	140	GLY	3.4
50	CW	11	GLU	3.4

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Mol	Chain	Res	Type	RSRZ
50	CW	43	ASP	3.4
1	AA	83	C	3.4
1	BA	206	C	3.4
31	CA	405	U	3.4
31	CA	817	C	3.4
31	CA	126	A	3.4
31	CA	478	A	3.4
33	CE	63	LYS	3.4
30	CD	167	ASN	3.4
31	CA	539	G	3.4
31	CA	1875	G	3.4
31	CA	2238	G	3.4
31	CA	2405	G	3.4
13	AM	57	ARG	3.4
13	BM	71	ARG	3.4
40	CM	24	GLY	3.4
42	CO	2	ARG	3.4
48	CU	4	GLU	3.4
28	CB	118	C	3.4
47	CT	49	LYS	3.4
2	BB	166	ALA	3.4
5	AE	111	MET	3.4
40	CM	1	MET	3.4
45	DR	118	ALA	3.4
37	CJ	140	VAL	3.4
12	BL	71	GLY	3.4
45	CR	82	GLY	3.4
31	CA	1250	G	3.4
14	BN	97	LYS	3.4
31	CA	2650	U	3.4
2	BB	208	ARG	3.4
21	AU	17	ARG	3.4
26	C5	36	ARG	3.4
29	CC	235	GLY	3.4
31	CA	309	A	3.4
38	CK	65	THR	3.4
48	CU	68	LYS	3.4
2	AB	35	ARG	3.4
7	BG	117	ALA	3.4
13	BM	60	VAL	3.4
39	CL	103	VAL	3.4
41	CN	36	VAL	3.4

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Mol	Chain	Res	Type	RSRZ
44	CQ	30	VAL	3.4
54	DI	47	GLU	3.4
5	BE	109	GLY	3.4
33	CE	151	GLY	3.4
14	BN	67	THR	3.4
31	CA	1609	A	3.4
1	BA	1308	U	3.4
7	BG	143	ARG	3.4
31	CA	1539	U	3.4
36	CH	117	LEU	3.4
2	BB	145	GLU	3.4
7	AG	123	GLU	3.4
30	CD	28	GLU	3.4
5	BE	23	LYS	3.4
5	BE	46	VAL	3.4
24	C3	11	LYS	3.4
31	CA	334	C	3.4
31	CA	510	C	3.4
34	CF	33	LYS	3.4
34	CF	59	ALA	3.4
37	CJ	72	LYS	3.4
38	CK	105	VAL	3.4
13	AM	23	TYR	3.4
1	BA	969	A	3.3
3	BC	167	TRP	3.4
29	CC	213	TRP	3.4
31	CA	241	A	3.3
31	CA	279	A	3.3
38	CK	34	ARG	3.3
1	BA	1247	U	3.3
5	BE	36	LEU	3.3
17	BQ	69	LYS	3.3
49	CV	44	LYS	3.3
11	AK	102	ALA	3.3
13	BM	112	PRO	3.3
35	CG	65	ALA	3.3
37	CJ	110	ALA	3.3
43	CP	44	GLY	3.3
7	AG	41	SER	3.3
31	CA	1042	G	3.3
31	CA	2310	C	3.3
6	AF	63	ASN	3.3

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Mol	Chain	Res	Type	RSRZ
10	AJ	37	ARG	3.3
51	CX	68	LYS	3.3
1	BA	218	U	3.3
1	BA	532	A	3.3
1	BA	1014	A	3.3
31	CA	911	A	3.3
55	DA	1070	A	3.3
55	DA	1088	A	3.3
11	BK	45	ALA	3.3
14	AN	99	ALA	3.3
45	CR	27	ALA	3.3
37	DJ	136	MET	3.3
39	CL	35	VAL	3.3
39	CL	83	ALA	3.3
39	CL	112	PHE	3.3
3	BC	164	ARG	3.3
29	CC	230	HIS	3.3
31	CA	1052	C	3.3
1	BA	1039	G	3.3
1	BA	1187	G	3.3
1	BA	1334	G	3.3
14	AN	54	ASP	3.3
31	CA	266	G	3.3
31	CA	2159	G	3.3
36	DH	86	ASP	3.3
20	BT	13	GLN	3.3
33	CE	182	ALA	3.3
34	CF	138	PHE	3.3
15	AO	89	ARG	3.3
35	CG	99	LYS	3.3
3	BC	170	GLU	3.3
31	CA	2691	C	3.3
1	BA	275	G	3.3
1	BA	847	G	3.3
1	BA	1139	G	3.3
55	DA	141	G	3.3
1	BA	1211	U	3.3
11	BK	43	GLY	3.3
2	AB	69	PHE	3.3
30	CD	162	ALA	3.3
41	CN	11	LYS	3.3
17	BQ	64	CYS	3.3

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Mol	Chain	Res	Type	RSRZ
40	CM	143	GLU	3.3
46	CS	7	SER	3.3
1	BA	87	C	3.3
31	CA	57	C	3.3
31	CA	1607	C	3.3
31	CA	150	U	3.3
31	CA	1880	U	3.3
1	AA	1034	G	3.3
1	BA	1454	G	3.3
31	CA	914	G	3.3
36	CH	83	LYS	3.3
33	CE	158	PHE	3.3
36	DH	143	ILE	3.3
40	CM	13	LYS	3.3
42	CO	84	GLY	3.3
47	CT	8	ARG	3.3
12	BL	23	ALA	3.3
48	CU	67	VAL	3.3
53	CZ	13	GLU	3.3
2	BB	15	HIS	3.3
7	AG	140	ASP	3.3
15	BO	18	ASP	3.3
33	CE	165	HIS	3.3
43	CP	34	HIS	3.3
1	AA	1028	C	3.3
11	AK	42	LEU	3.3
35	CG	116	GLN	3.3
30	CD	204	LYS	3.3
40	CM	129	LYS	3.3
44	CQ	101	ARG	3.3
49	CV	97	LYS	3.3
53	CZ	2	LYS	3.3
3	AC	155	GLY	3.3
7	BG	55	GLY	3.3
31	CA	139	U	3.3
30	CD	197	THR	3.3
44	CQ	33	VAL	3.3
1	BA	933	G	3.3
31	CA	271	G	3.3
31	CA	2455	G	3.3
1	BA	978	A	3.3
3	BC	190	HIS	3.3

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Mol	Chain	Res	Type	RSRZ
9	BI	85	ARG	3.3
9	BI	95	ARG	3.3
24	C3	41	ARG	3.3
31	CA	31	C	3.3
15	BO	12	VAL	3.3
34	CF	134	GLU	3.3
45	CR	68	ALA	3.3
49	CV	101	GLU	3.3
50	CW	50	MET	3.3
25	C4	3	LYS	3.3
31	CA	1022	G	3.3
31	CA	1277	G	3.3
10	AJ	31	ARG	3.3
25	C4	44	LEU	3.3
34	CF	169	LEU	3.3
40	CM	61	LEU	3.3
25	C4	9	GLY	3.3
31	CA	515	A	3.3
31	CA	2412	A	3.3
1	BA	153	C	3.3
1	BA	186	C	3.3
1	BA	330	C	3.3
10	AJ	25	ILE	3.3
49	CV	60	GLU	3.3
17	AQ	53	CYS	3.3
23	C2	12	VAL	3.3
37	DJ	70	VAL	3.3
8	BH	89	LYS	3.3
35	CG	138	LYS	3.3
10	BJ	45	ARG	3.3
3	BC	145	GLY	3.3
36	DH	92	GLY	3.3
44	CQ	40	LEU	3.3
48	CU	32	LEU	3.3
3	AC	82	GLU	3.2
3	BC	37	PHE	3.2
21	AU	4	ILE	3.2
31	CA	1173	U	3.2
37	DJ	34	ASN	3.2
31	CA	421	C	3.2
31	CA	1205	A	3.2
55	DA	613	A	3.2

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Mol	Chain	Res	Type	RSRZ
55	DA	1057	A	3.2
46	CS	38	VAL	3.2
13	AM	101	ARG	3.2
3	BC	26	THR	3.2
3	BC	85	GLU	3.2
34	DF	39	GLY	3.2
1	BA	86	G	3.2
7	BG	7	ILE	3.2
28	CB	56	G	3.2
30	CD	202	ILE	3.2
31	CA	894	U	3.2
31	CA	1326	U	3.2
31	CA	2152	G	3.2
37	DJ	62	TYR	3.2
48	CU	92	ASN	3.2
11	AK	99	ALA	3.2
12	BL	93	VAL	3.2
25	C4	42	ARG	3.2
31	CA	1373	A	3.2
31	CA	1600	C	3.2
31	CA	1764	C	3.2
31	CA	1986	C	3.2
36	CH	123	ARG	3.2
36	DH	147	VAL	3.2
41	CN	40	ARG	3.2
7	BG	14	PRO	3.2
10	BJ	43	PRO	3.2
21	BU	16	LEU	3.2
42	CO	100	CYS	3.2
47	CT	2	GLU	3.2
52	CY	44	LYS	3.2
33	CE	102	ARG	3.2
48	CU	74	ILE	3.2
11	AK	32	VAL	3.2
39	CL	24	VAL	3.2
31	CA	1730	C	3.2
31	CA	2004	G	3.2
31	CA	2525	G	3.2
31	CA	2862	G	3.2
1	AA	1332	A	3.2
53	DZ	39	GLN	3.2
2	AB	211	THR	3.2

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Mol	Chain	Res	Type	RSRZ
3	BC	183	ASP	3.2
5	BE	103	THR	3.2
52	CY	48	THR	3.2
10	AJ	56	HIS	3.2
23	C2	20	PHE	3.2
31	CA	2807	U	3.2
36	DH	135	HIS	3.2
24	C3	15	SER	3.2
38	CK	15	TRP	3.2
43	CP	90	VAL	3.2
1	BA	1355	G	3.2
31	CA	1239	G	3.2
31	CA	2363	G	3.2
38	CK	92	MET	3.2
19	AS	27	ASP	3.2
31	CA	1253	A	3.2
21	AU	19	PHE	3.2
36	DH	128	HIS	3.2
2	BB	210	VAL	3.2
9	AI	64	TYR	3.2
16	AP	17	TYR	3.2
36	CH	65	ALA	3.2
45	CR	10	ALA	3.2
45	CR	93	LYS	3.2
25	C4	49	MET	3.2
30	CD	148	GLN	3.2
46	CS	34	GLU	3.2
54	DI	98	GLU	3.2
27	C0	33	GLY	3.2
28	CB	4	C	3.2
28	CB	49	C	3.2
53	CZ	30	MET	3.2
1	AA	79	G	3.2
1	AA	1170	A	3.2
1	BA	1269	A	3.2
1	BA	1362	A	3.2
31	CA	182	A	3.2
31	CA	1133	A	3.2
31	CA	1285	A	3.2
31	CA	1538	G	3.2
31	CA	1643	G	3.2
31	CA	2732	G	3.2

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Mol	Chain	Res	Type	RSRZ
50	CW	56	PHE	3.2
55	DA	2170	A	3.2
2	AB	60	ILE	3.2
30	CD	14	ILE	3.2
50	CW	68	LYS	3.2
52	CY	77	LYS	3.2
2	BB	199	VAL	3.2
31	CA	596	U	3.2
31	CA	929	U	3.2
55	DA	2131	U	3.2
3	AC	105	GLU	3.2
7	AG	77	SER	3.2
49	CV	53	ASN	3.2
33	CE	56	GLY	3.2
1	AA	984	C	3.2
1	BA	999	C	3.2
31	CA	550	C	3.2
31	CA	1172	C	3.2
35	CG	16	ASP	3.2
39	CL	56	ASP	3.2
46	CS	93	PHE	3.2
53	CZ	60	LYS	3.2
1	AA	1127	G	3.2
1	BA	91	U	3.2
31	CA	375	G	3.2
31	CA	535	G	3.2
31	CA	1596	A	3.2
41	CN	24	THR	3.2
51	CX	36	ILE	3.2
30	CD	88	GLU	3.2
35	CG	63	ALA	3.2
47	CT	56	ALA	3.2
13	AM	29	ARG	3.2
24	C3	21	ARG	3.2
33	CE	62	GLN	3.2
43	CP	75	GLY	3.2
44	CQ	3	ASN	3.2
48	CU	69	ARG	3.2
5	BE	144	LEU	3.2
25	C4	57	LEU	3.2
37	DJ	95	LYS	3.2
50	CW	71	LYS	3.2

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Mol	Chain	Res	Type	RSRZ
52	CY	54	LYS	3.2
1	BA	1141	C	3.2
20	BT	12	ILE	3.2
43	CP	35	ILE	3.2
54	DI	11	ILE	3.2
11	AK	45	ALA	3.2
17	BQ	42	THR	3.2
31	CA	29	U	3.2
36	CH	78	VAL	3.2
41	CN	74	THR	3.2
23	C2	19	HIS	3.2
47	CT	110	ARG	3.2
16	BP	10	GLY	3.2
44	DQ	2	SER	3.2
36	DH	90	LEU	3.2
44	CQ	31	TRP	3.2
1	BA	1262	C	3.2
1	BA	1263	C	3.2
31	CA	2260	C	3.2
38	CK	81	ILE	3.1
30	CD	179	ARG	3.1
11	BK	102	ALA	3.1
38	CK	124	VAL	3.1
42	CO	91	ALA	3.1
45	CR	110	VAL	3.1
35	CG	176	LYS	3.1
46	CS	76	LYS	3.1
1	BA	1145	A	3.1
24	C3	8	SER	3.1
31	CA	1037	G	3.1
31	CA	2782	G	3.1
36	CH	6	LEU	3.1
39	CL	109	SER	3.1
21	BU	2	PRO	3.1
44	CQ	16	ASP	3.1
1	BA	1317	C	3.1
1	BA	1383	C	3.1
31	CA	2815	C	3.1
2	AB	53	ALA	3.1
21	AU	26	ALA	3.1
33	CE	8	ALA	3.1
35	CG	145	ALA	3.1

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Mol	Chain	Res	Type	RSRZ
36	CH	9	VAL	3.1
43	CP	50	ALA	3.1
13	AM	38	GLY	3.1
25	C4	24	HIS	3.1
48	CU	91	GLN	3.1
1	BA	1151	A	3.1
3	AC	43	LEU	3.1
16	AP	74	LEU	3.1
20	BT	21	ASN	3.1
31	CA	2639	A	3.1
42	CO	23	ASN	3.1
4	AD	154	ARG	3.1
31	CA	597	G	3.1
31	CA	2410	G	3.1
34	CF	51	ASP	3.1
43	CP	2	ASP	3.1
12	AL	108	LYS	3.1
53	CZ	4	LYS	3.1
13	AM	17	ILE	3.1
10	BJ	36	VAL	3.1
29	CC	237	GLY	3.1
31	CA	587	C	3.1
36	CH	63	ALA	3.1
43	CP	74	VAL	3.1
34	DF	83	TYR	3.1
38	CK	125	TYR	3.1
41	CN	88	ASN	3.1
54	DI	5	LEU	3.1
1	BA	1000	A	3.1
49	CV	9	ASP	3.1
1	BA	1144	G	3.1
1	BA	1215	G	3.1
5	AE	137	VAL	3.1
7	AG	61	ALA	3.1
44	CQ	42	ALA	3.1
1	AA	1282	C	3.1
45	CR	44	GLN	3.1
34	CF	5	HIS	3.1
14	AN	63	ARG	3.1
36	CH	90	LEU	3.1
34	CF	163	ASP	3.1
46	CS	43	ASN	3.1

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Mol	Chain	Res	Type	RSRZ
13	BM	9	ILE	3.1
31	CA	1525	A	3.1
55	DA	1175	A	3.1
11	AK	86	VAL	3.1
1	BA	177	G	3.1
12	BL	113	ALA	3.1
12	BL	119	VAL	3.1
31	CA	1138	G	3.1
31	CA	2786	U	3.1
41	CN	56	ALA	3.1
55	DA	2140	G	3.1
1	BA	1342	C	3.1
45	CR	89	GLU	3.1
4	AD	30	THR	3.1
18	AR	55	LEU	3.1
14	BN	57	PRO	3.1
42	CO	39	PRO	3.1
13	BM	78	LYS	3.1
21	AU	14	VAL	3.1
25	C4	39	LYS	3.1
26	D5	38	GLY	3.1
31	CA	2814	A	3.1
31	CA	288	U	3.1
31	CA	2245	U	3.1
40	CM	134	ALA	3.1
44	CQ	73	VAL	3.1
53	CZ	7	ARG	3.1
7	BG	124	LEU	3.1
31	CA	1024	G	3.1
31	CA	1071	G	3.1
31	CA	1517	G	3.1
31	CA	2325	G	3.1
43	CP	100	HIS	3.1
12	BL	97	THR	3.1
37	DJ	118	THR	3.1
13	AM	21	SER	3.1
30	CD	7	LYS	3.1
34	CF	44	ILE	3.1
37	DJ	86	ILE	3.1
53	CZ	10	SER	3.1
2	AB	208	ARG	3.1
44	CQ	23	GLY	3.1

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Mol	Chain	Res	Type	RSRZ
7	BG	64	VAL	3.1
20	BT	48	GLN	3.1
22	C1	54	VAL	3.1
1	AA	84	U	3.1
1	BA	96	U	3.1
31	CA	615	U	3.1
31	CA	1260	A	3.1
31	CA	1321	A	3.1
36	DH	15	LEU	3.1
31	CA	61	C	3.1
31	CA	1092	C	3.1
31	CA	2313	C	3.1
1	BA	963	G	3.1
1	BA	993	G	3.1
9	BI	6	TYR	3.1
31	CA	2115	G	3.1
34	CF	9	LYS	3.1
12	BL	67	ILE	3.1
38	CK	67	ASN	3.1
42	CO	96	ARG	3.1
6	BF	10	VAL	3.1
30	CD	94	GLN	3.1
14	BN	17	ALA	3.1
42	CO	25	ALA	3.1
1	AA	1492	A	3.1
1	BA	1368	A	3.1
21	AU	37	PHE	3.1
28	CB	119	A	3.1
29	CC	26	LYS	3.1
31	CA	2346	A	3.1
40	CM	64	PHE	3.1
46	CS	5	PHE	3.1
55	DA	878	A	3.1
55	DA	2169	A	3.1
1	BA	1149	C	3.1
1	BA	1322	C	3.1
3	BC	72	ARG	3.1
16	BP	35	ARG	3.1
23	C2	6	ARG	3.1
28	CB	27	C	3.1
31	CA	1319	C	3.1
35	CG	3	ARG	3.1

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Mol	Chain	Res	Type	RSRZ
1	BA	354	G	3.1
28	CB	20	G	3.1
31	CA	1016	G	3.1
31	CA	1225	G	3.1
31	CA	2526	G	3.1
55	DA	2156	G	3.1
2	BB	217	VAL	3.0
3	BC	180	ALA	3.0
31	CA	1108	U	3.0
30	CD	118	PHE	3.0
36	CH	47	PHE	3.0
1	BA	1204	A	3.0
22	C1	16	ARG	3.0
31	CA	2052	A	3.0
31	CA	2311	A	3.0
2	AB	40	ILE	3.0
10	AJ	100	ILE	3.0
31	CA	544	C	3.0
13	AM	96	PRO	3.0
38	CK	138	GLN	3.0
7	AG	73	VAL	3.0
1	BA	1370	G	3.0
19	BS	18	LYS	3.0
44	CQ	17	VAL	3.0
9	AI	95	ARG	3.0
21	BU	19	PHE	3.0
3	AC	190	HIS	3.0
31	CA	1532	A	3.0
36	CH	16	GLY	3.0
36	DH	88	GLY	3.0
9	BI	75	GLN	3.0
31	CA	151	C	3.0
31	CA	1958	C	3.0
43	CP	47	VAL	3.0
5	BE	75	ALA	3.0
9	BI	86	ALA	3.0
54	DI	80	THR	3.0
31	CA	1438	U	3.0
31	CA	2299	U	3.0
1	AA	1187	G	3.0
28	CB	7	G	3.0
3	BC	36	ASP	3.0

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Mol	Chain	Res	Type	RSRZ
7	BG	6	VAL	3.0
31	CA	257	C	3.0
31	CA	443	A	3.0
31	CA	2632	A	3.0
39	CL	32	TYR	3.0
41	CN	77	PRO	3.0
12	BL	48	ALA	3.0
25	C4	8	ARG	3.0
36	CH	36	ALA	3.0
36	DH	100	ALA	3.0
45	CR	53	ARG	3.0
51	CX	84	ALA	3.0
31	CA	1460	U	3.0
2	AB	129	LEU	3.0
50	CW	46	LYS	3.0
1	BA	378	G	3.0
31	CA	376	G	3.0
31	CA	748	G	3.0
9	AI	79	ILE	3.0
14	BN	66	GLN	3.0
30	CD	134	HIS	3.0
14	BN	41	ARG	3.0
21	BU	6	VAL	3.0
36	DH	25	TYR	3.0
1	BA	352	C	3.0
31	CA	502	A	3.0
31	CA	902	C	3.0
36	DH	64	ALA	3.0
38	CK	126	ALA	3.0
47	CT	93	ALA	3.0
1	BA	1008	U	3.0
10	BJ	83	THR	3.0
19	BS	73	GLU	3.0
36	DH	12	LEU	3.0
37	DJ	31	GLN	3.0
37	DJ	47	ASP	3.0
3	BC	132	ARG	3.0
10	BJ	56	HIS	3.0
40	DM	104	GLN	3.0
53	DZ	38	GLN	3.0
31	CA	1228	G	3.0
31	CA	1252	G	3.0

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Mol	Chain	Res	Type	RSRZ
42	CO	46	ARG	3.0
3	AC	39	VAL	3.0
11	BK	84	VAL	3.0
5	AE	19	ASN	3.0
29	CC	37	ASN	3.0
31	CA	236	C	3.0
31	CA	2248	C	3.0
31	CA	2616	C	3.0
37	CJ	108	GLU	3.0
31	CA	504	A	3.0
31	CA	2660	A	3.0
53	CZ	55	THR	3.0
54	DI	67	THR	3.0
42	CO	26	GLY	3.0
9	AI	62	ASP	3.0
30	CD	150	GLN	3.0
40	CM	41	ARG	3.0
43	CP	98	GLN	3.0
46	CS	84	ARG	3.0
3	AC	66	VAL	3.0
44	CQ	34	GLU	3.0
51	CX	67	VAL	3.0
1	BA	104	G	3.0
31	CA	1186	G	3.0
31	CA	2112	G	3.0
31	CA	184	C	3.0
15	BO	22	THR	3.0
29	CC	223	THR	3.0
31	CA	310	A	3.0
9	BI	123	ARG	3.0
29	CC	28	LYS	3.0
49	CV	17	LYS	3.0
12	AL	70	GLU	3.0
29	CC	243	HIS	3.0
40	CM	110	VAL	3.0
3	BC	104	ALA	3.0
7	AG	71	PRO	3.0
1	BA	1220	G	3.0
16	BP	40	ASN	3.0
18	AR	29	LEU	3.0
31	CA	245	G	3.0
31	CA	411	G	3.0

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Mol	Chain	Res	Type	RSRZ
1	BA	176	C	3.0
1	BA	470	C	3.0
7	AG	132	GLY	3.0
31	CA	1983	G	3.0
31	CA	2633	G	3.0
31	CA	540	C	3.0
25	C4	47	LYS	3.0
39	CL	65	THR	3.0
1	AA	77	A	3.0
31	CA	272	A	3.0
31	CA	609	A	3.0
31	CA	1652	A	3.0
31	CA	2453	A	3.0
13	BM	17	ILE	3.0
42	CO	33	ILE	3.0
6	AF	96	VAL	3.0
30	CD	155	VAL	3.0
37	DJ	140	VAL	3.0
43	CP	79	ALA	2.9
44	CQ	108	ALA	2.9
50	CW	26	PHE	2.9
1	BA	1212	U	2.9
31	CA	1224	U	2.9
36	CH	13	GLY	2.9
44	CQ	109	ARG	2.9
20	BT	16	LYS	2.9
52	CY	55	GLY	2.9
1	BA	1337	G	2.9
7	AG	133	THR	2.9
13	AM	46	SER	2.9
31	CA	494	G	2.9
31	CA	1295	C	2.9
31	CA	1529	G	2.9
3	AC	68	ILE	2.9
18	AR	20	GLU	2.9
45	CR	59	GLN	2.9
1	BA	468	A	2.9
16	AP	21	VAL	2.9
49	CV	34	VAL	2.9
9	BI	122	ARG	2.9
24	C3	23	ALA	2.9
34	CF	20	PHE	2.9

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Mol	Chain	Res	Type	RSRZ
42	CO	66	ALA	2.9
46	CS	66	HIS	2.9
54	DI	127	ALA	2.9
1	AA	1023	U	2.9
1	BA	632	U	2.9
11	AK	80	LYS	2.9
19	AS	47	LEU	2.9
29	CC	97	LYS	2.9
31	CA	665	U	2.9
44	CQ	100	LEU	2.9
42	CO	112	TYR	2.9
49	CV	90	GLY	2.9
35	CG	64	GLN	2.9
1	BA	54	C	2.9
1	BA	1129	C	2.9
13	AM	20	THR	2.9
13	BM	82	ASP	2.9
22	C1	11	SER	2.9
31	CA	2078	C	2.9
31	CA	2896	C	2.9
31	CA	2365	G	2.9
1	BA	1248	A	2.9
1	BA	1339	A	2.9
36	DH	110	VAL	2.9
50	CW	77	VAL	2.9
22	C1	45	ALA	2.9
3	BC	158	GLY	2.9
7	AG	47	LEU	2.9
31	CA	1468	U	2.9
34	CF	109	PRO	2.9
36	CH	107	GLY	2.9
38	CK	79	GLY	2.9
30	CD	183	GLU	2.9
14	BN	19	LYS	2.9
22	C1	53	LYS	2.9
31	CA	2362	C	2.9
37	CJ	65	ARG	2.9
42	CO	45	ARG	2.9
45	CR	70	ARG	2.9
36	DH	103	VAL	2.9
1	AA	963	G	2.9
1	BA	198	G	2.9

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Mol	Chain	Res	Type	RSRZ
6	BF	8	PHE	2.9
9	BI	63	LEU	2.9
13	AM	37	ALA	2.9
34	CF	168	ALA	2.9
31	CA	1616	A	2.9
31	CA	2158	A	2.9
31	CA	1113	U	2.9
49	DV	48	PRO	2.9
7	BG	139	GLU	2.9
34	CF	19	GLU	2.9
33	CE	99	LYS	2.9
43	CP	68	LYS	2.9
9	AI	28	ILE	2.9
24	C3	39	ARG	2.9
39	CL	49	ARG	2.9
49	CV	58	ILE	2.9
1	BA	1369	C	2.9
30	CD	24	VAL	2.9
31	CA	1985	C	2.9
31	CA	2000	C	2.9
36	CH	21	VAL	2.9
34	CF	45	ALA	2.9
48	CU	45	ALA	2.9
54	DI	76	PHE	2.9
19	BS	47	LEU	2.9
36	CH	126	GLY	2.9
1	BA	1205	U	2.9
9	AI	92	GLU	2.9
29	CC	227	PRO	2.9
31	CA	1237	A	2.9
31	CA	1244	A	2.9
31	CA	2694	G	2.9
54	DI	119	PRO	2.9
1	AA	1021	A	2.9
31	CA	71	A	2.9
55	DA	2107	G	2.9
16	BP	18	GLN	2.9
40	CM	29	LYS	2.9
49	CV	46	GLN	2.9
52	CY	61	LYS	2.9
10	BJ	16	ARG	2.9
29	CC	270	ARG	2.9

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Mol	Chain	Res	Type	RSRZ
7	BG	29	ILE	2.9
7	BG	27	VAL	2.9
19	BS	33	THR	2.9
26	C5	3	VAL	2.9
31	CA	32	C	2.9
31	CA	815	C	2.9
35	CG	159	GLY	2.9
36	CH	125	THR	2.9
48	CU	21	SER	2.9
3	BC	157	LEU	2.9
5	BE	108	GLY	2.9
50	CW	3	THR	2.9
17	BQ	67	LEU	2.9
29	CC	210	ALA	2.9
50	CW	74	ALA	2.9
52	CY	15	GLY	2.9
31	CA	2878	U	2.9
55	DA	1058	U	2.9
9	AI	33	ARG	2.9
1	BA	105	G	2.9
1	BA	134	G	2.9
1	BA	1363	A	2.9
1	BA	1375	A	2.9
28	CB	96	G	2.9
31	CA	326	G	2.9
31	CA	612	G	2.9
31	CA	941	A	2.9
31	CA	1583	A	2.9
31	CA	1862	G	2.9
5	BE	78	ASN	2.9
29	CC	46	ASN	2.9
47	CT	66	ILE	2.9
2	BB	80	VAL	2.9
14	AN	32	SER	2.9
1	AA	1320	C	2.9
1	BA	1140	C	2.9
3	AC	189	ALA	2.9
24	D3	46	LYS	2.9
26	C5	21	GLY	2.9
33	CE	2	GLU	2.9
42	CO	21	PHE	2.9
30	CD	56	LYS	2.9

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Mol	Chain	Res	Type	RSRZ
30	CD	138	LEU	2.9
36	DH	6	LEU	2.9
38	CK	20	ALA	2.9
40	CM	87	GLY	2.9
42	CO	70	THR	2.9
1	AA	1125	U	2.9
31	CA	598	U	2.9
31	CA	1729	U	2.9
55	DA	2113	U	2.9
31	CA	127	A	2.9
40	CM	111	ILE	2.9
31	CA	2157	G	2.9
55	DA	1090	A	2.9
7	AG	137	LYS	2.9
13	AM	114	LYS	2.9
9	AI	82	GLY	2.9
17	AQ	83	VAL	2.9
21	AU	39	GLU	2.9
10	AJ	12	ALA	2.9
38	CK	108	MET	2.9
47	CT	58	ALA	2.9
51	CX	35	SER	2.9
6	AF	42	TRP	2.9
31	CA	2050	C	2.9
29	DC	243	HIS	2.9
31	CA	1542	U	2.9
14	BN	76	LYS	2.9
17	AQ	4	LYS	2.9
2	BB	93	ASN	2.9
35	CG	124	GLU	2.9
50	CW	5	ASN	2.9
30	CD	135	GLY	2.9
31	CA	196	A	2.9
1	BA	201	G	2.9
1	BA	1361	G	2.9
3	BC	65	ARG	2.9
7	BG	13	LEU	2.9
11	AK	98	ARG	2.9
31	CA	2358	A	2.9
41	CN	101	VAL	2.9
31	CA	70	G	2.9
31	CA	86	G	2.9

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Mol	Chain	Res	Type	RSRZ
31	CA	883	G	2.9
31	CA	1521	G	2.9
31	CA	1100	C	2.8
31	CA	1176	U	2.8
31	CA	1523	U	2.8
31	CA	2903	U	2.8
50	CW	84	PRO	2.8
55	DA	2180	U	2.8
10	BJ	70	HIS	2.8
21	AU	8	GLU	2.8
36	CH	4	ILE	2.8
5	BE	148	ASN	2.8
10	BJ	31	ARG	2.8
34	CF	13	VAL	2.8
35	CG	15	VAL	2.8
42	CO	12	ARG	2.8
1	AA	959	A	2.8
31	CA	2778	A	2.8
40	CM	112	LEU	2.8
1	BA	1264	U	2.8
1	BA	1343	G	2.8
10	AJ	101	SER	2.8
20	AT	55	GLN	2.8
39	CL	28	SER	2.8
31	CA	653	U	2.8
31	CA	2847	U	2.8
40	CM	109	LYS	2.8
46	CS	11	GLN	2.8
1	AA	1302	C	2.8
34	CF	87	CYS	2.8
55	DA	2153	C	2.8
18	AR	59	ILE	2.8
21	BU	4	ILE	2.8
7	BG	126	ASP	2.8
9	AI	18	ARG	2.8
3	BC	74	GLY	2.8
15	AO	21	ASP	2.8
33	CE	96	VAL	2.8
44	CQ	32	VAL	2.8
54	DI	35	VAL	2.8
2	AB	57	LEU	2.8
2	BB	84	ALA	2.8

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Mol	Chain	Res	Type	RSRZ
33	CE	153	LEU	2.8
16	BP	12	LYS	2.8
36	DH	141	LYS	2.8
1	AA	1441	A	2.8
1	BA	1227	A	2.8
1	AA	1148	U	2.8
31	CA	2149	U	2.8
36	DH	82	SER	2.8
17	BQ	60	GLU	2.8
29	CC	231	PRO	2.8
6	BF	38	ARG	2.8
11	BK	98	ARG	2.8
31	CA	77	G	2.8
31	CA	215	G	2.8
31	CA	261	G	2.8
42	CO	85	PRO	2.8
44	CQ	25	THR	2.8
38	CK	75	TYR	2.8
48	CU	79	ASP	2.8
24	C3	9	VAL	2.8
5	BE	124	LEU	2.8
46	CS	48	LYS	2.8
6	AF	66	ALA	2.8
20	BT	11	ALA	2.8
45	CR	116	ALA	2.8
1	BA	263	A	2.8
9	BI	45	ARG	2.8
27	C0	45	ARG	2.8
31	CA	2302	U	2.8
31	CA	616	A	2.8
10	BJ	50	THR	2.8
12	BL	82	ILE	2.8
13	AM	104	THR	2.8
50	CW	40	ILE	2.8
51	DX	10	THR	2.8
21	AU	12	PHE	2.8
31	CA	623	C	2.8
31	CA	273	G	2.8
31	CA	561	G	2.8
53	CZ	9	LYS	2.8
10	BJ	51	VAL	2.8
33	CE	60	TRP	2.8

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Mol	Chain	Res	Type	RSRZ
14	AN	36	ALA	2.8
25	C4	60	ALA	2.8
38	CK	131	ASN	2.8
29	CC	238	ARG	2.8
35	CG	42	GLU	2.8
1	AA	1286	U	2.8
1	BA	961	U	2.8
3	BC	51	SER	2.8
16	BP	15	PRO	2.8
19	AS	25	SER	2.8
34	CF	72	LYS	2.8
25	C4	21	GLY	2.8
31	CA	6	A	2.8
31	CA	1275	A	2.8
31	CA	2147	A	2.8
34	CF	82	GLY	2.8
1	BA	1228	C	2.8
2	AB	82	ASP	2.8
30	CD	176	ASP	2.8
31	CA	128	C	2.8
31	CA	1909	C	2.8
45	CR	49	ASP	2.8
14	BN	46	LEU	2.8
38	CK	74	TYR	2.8
31	CA	168	G	2.8
31	CA	307	G	2.8
31	CA	367	G	2.8
31	CA	2621	G	2.8
55	DA	2159	G	2.8
20	BT	61	GLN	2.8
23	D2	45	GLN	2.8
46	CS	21	ARG	2.8
52	CY	56	MET	2.8
22	C1	7	LYS	2.8
20	BT	32	ILE	2.8
41	CN	23	GLY	2.8
46	CS	102	SER	2.8
1	BA	1044	A	2.8
1	BA	1238	A	2.8
8	AH	54	ASP	2.8
11	AK	33	THR	2.8
3	BC	87	LEU	2.8

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Mol	Chain	Res	Type	RSRZ
21	AU	38	TYR	2.8
31	CA	1135	C	2.8
31	CA	2830	C	2.8
36	CH	138	VAL	2.8
45	CR	88	VAL	2.8
3	AC	104	ALA	2.8
33	CE	39	ALA	2.8
40	CM	4	ASN	2.8
43	CP	77	ALA	2.8
31	CA	1807	G	2.8
31	CA	2816	G	2.8
31	CA	87	U	2.8
2	BB	91	PHE	2.8
11	AK	34	ILE	2.8
40	CM	25	SER	2.8
3	BC	69	HIS	2.8
10	AJ	98	VAL	2.8
23	C2	35	GLU	2.8
25	C4	6	THR	2.8
34	CF	71	ARG	2.8
30	CD	71	ALA	2.8
31	CA	264	C	2.8
31	CA	368	A	2.8
31	CA	1080	A	2.8
31	CA	1420	A	2.8
31	CA	2716	C	2.8
50	CW	10	LYS	2.8
42	CO	77	ALA	2.8
43	CP	37	ALA	2.8
45	CR	96	ALA	2.8
7	AG	103	TRP	2.8
20	BT	52	ASN	2.8
3	AC	81	GLY	2.8
9	BI	69	GLY	2.8
31	CA	178	G	2.8
31	CA	235	U	2.8
31	CA	551	G	2.8
31	CA	1324	G	2.8
31	CA	2677	G	2.8
11	AK	31	ILE	2.8
35	CG	12	PRO	2.8
35	CG	19	ILE	2.8

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Mol	Chain	Res	Type	RSRZ
47	CT	55	ILE	2.8
47	CT	96	ILE	2.8
3	BC	161	GLU	2.8
16	BP	76	LYS	2.8
37	DJ	108	GLU	2.8
46	CS	23	GLU	2.8
50	CW	14	LYS	2.8
51	CX	66	LYS	2.8
18	BR	40	VAL	2.8
54	DI	33	VAL	2.8
25	C4	65	ALA	2.8
33	CE	195	GLN	2.8
31	CA	240	C	2.8
31	CA	440	C	2.8
31	CA	1871	A	2.7
31	CA	2179	C	2.8
12	AL	73	ASN	2.7
31	CA	2376	A	2.7
31	CA	2749	A	2.7
34	DF	38	MET	2.7
3	BC	205	GLY	2.7
3	AC	103	ILE	2.7
5	AE	10	GLU	2.7
29	CC	18	LYS	2.7
33	CE	114	ARG	2.7
34	DF	77	PHE	2.7
44	CQ	103	ARG	2.7
1	BA	1186	G	2.7
1	BA	1278	G	2.7
31	CA	93	G	2.7
31	CA	488	G	2.7
31	CA	1063	G	2.7
54	DI	29	ASP	2.7
27	C0	36	VAL	2.7
30	CD	37	VAL	2.7
47	CT	69	LEU	2.7
42	CO	18	GLN	2.7
5	BE	118	ALA	2.7
1	AA	962	C	2.7
27	C0	54	MET	2.7
31	CA	394	C	2.7
31	CA	854	C	2.7

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Mol	Chain	Res	Type	RSRZ
31	CA	867	C	2.7
31	CA	1330	C	2.7
31	CA	244	A	2.7
31	CA	1111	A	2.7
4	AD	160	GLU	2.7
31	CA	1340	U	2.7
31	CA	1467	U	2.7
31	CA	2334	U	2.7
34	CF	6	ASP	2.7
38	CK	71	ASP	2.7
47	CT	68	ASP	2.7
54	DI	7	ASP	2.7
15	BO	29	VAL	2.7
3	BC	123	GLN	2.7
5	BE	149	SER	2.7
6	AF	89	VAL	2.7
30	CD	145	SER	2.7
54	DI	27	VAL	2.7
1	BA	377	G	2.7
1	BA	1057	G	2.7
31	CA	263	G	2.7
31	CA	333	G	2.7
31	CA	1311	G	2.7
22	C1	48	TYR	2.7
40	CM	98	ALA	2.7
52	CY	21	ALA	2.7
13	AM	51	GLY	2.7
31	CA	1658	C	2.7
31	CA	1708	C	2.7
40	CM	11	GLY	2.7
1	BA	157	U	2.7
1	BA	109	A	2.7
2	BB	69	PHE	2.7
13	AM	63	PHE	2.7
31	CA	390	U	2.7
31	CA	1004	U	2.7
31	CA	2259	U	2.7
31	CA	52	A	2.7
22	C1	30	VAL	2.7
29	CC	202	LEU	2.7
42	CO	115	LEU	2.7
46	CS	4	VAL	2.7

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Mol	Chain	Res	Type	RSRZ
3	BC	147	LYS	2.7
25	C4	23	LYS	2.7
37	DJ	72	LYS	2.7
42	CO	59	SER	2.7
38	CK	134	ALA	2.7
43	CP	85	LYS	2.7
19	AS	78	ARG	2.7
40	CM	123	ARG	2.7
2	BB	46	THR	2.7
7	AG	144	MET	2.7
30	CD	19	GLY	2.7
31	CA	26	G	2.7
31	CA	43	G	2.7
31	CA	248	G	2.7
31	CA	1633	G	2.7
39	CL	15	GLY	2.7
55	DA	1087	G	2.7
55	DA	2148	G	2.7
1	BA	1136	C	2.7
20	BT	78	ASN	2.7
31	CA	584	C	2.7
31	CA	1963	U	2.7
31	CA	2793	C	2.7
45	CR	66	ASN	2.7
9	BI	65	ILE	2.7
1	BA	478	A	2.7
5	BE	150	PRO	2.7
31	CA	227	A	2.7
31	CA	256	A	2.7
9	AI	58	VAL	2.7
23	C2	42	VAL	2.7
35	CG	85	LYS	2.7
36	CH	12	LEU	2.7
41	CN	26	VAL	2.7
7	BG	10	ARG	2.7
10	AJ	62	ARG	2.7
25	C4	30	ARG	2.7
44	CQ	2	SER	2.7
16	BP	62	GLY	2.7
46	CS	56	GLY	2.7
1	BA	943	U	2.7
2	BB	42	ASN	2.7

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Mol	Chain	Res	Type	RSRZ
28	CB	102	G	2.7
31	CA	102	U	2.7
31	CA	1183	U	2.7
31	CA	2618	G	2.7
55	DA	1078	U	2.7
1	BA	71	A	2.7
11	BK	44	TRP	2.7
16	BP	5	ARG	2.7
35	CG	71	LEU	2.7
28	CB	50	A	2.7
55	DA	1848	A	2.7
2	AB	142	GLU	2.7
8	BH	123	GLY	2.7
9	BI	34	SER	2.7
10	BJ	54	SER	2.7
33	CE	107	SER	2.7
40	CM	136	GLU	2.7
35	CG	28	GLY	2.7
37	DJ	25	GLY	2.7
45	CR	75	SER	2.7
3	BC	202	ILE	2.7
27	C0	19	LYS	2.7
29	CC	86	ASN	2.7
30	CD	32	ASN	2.7
30	CD	126	ASN	2.7
31	CA	113	U	2.7
35	CG	36	THR	2.7
35	CG	122	THR	2.7
45	CR	78	LYS	2.7
33	CE	156	ASN	2.7
1	BA	191	G	2.7
31	CA	536	G	2.7
31	CA	953	G	2.7
14	BN	14	VAL	2.7
1	AA	1035	A	2.7
1	BA	1188	A	2.7
10	BJ	29	ALA	2.7
20	BT	7	ALA	2.7
31	CA	1070	A	2.7
31	CA	1635	A	2.7
36	DH	106	ALA	2.7
37	DJ	29	GLY	2.7

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Mol	Chain	Res	Type	RSRZ
43	CP	57	ALA	2.7
55	DA	2173	A	2.7
29	CC	6	CYS	2.7
40	CM	40	SER	2.7
1	AA	1126	U	2.7
1	BA	992	U	2.7
20	BT	57	ILE	2.7
31	CA	511	U	2.7
31	CA	932	U	2.7
38	CK	50	THR	2.7
42	CO	30	ARG	2.7
48	CU	86	THR	2.7
3	BC	105	GLU	2.7
9	AI	47	VAL	2.7
31	CA	640	C	2.7
31	CA	1117	C	2.7
31	CA	1251	C	2.7
36	DH	117	LEU	2.7
28	CB	116	G	2.7
31	CA	841	G	2.7
31	CA	1137	G	2.7
31	CA	1193	G	2.7
16	BP	27	ALA	2.7
20	AT	76	LYS	2.7
30	CD	198	GLY	2.7
40	CM	22	GLY	2.7
46	CS	69	GLY	2.7
48	CU	9	LYS	2.7
50	CW	54	ALA	2.7
17	BQ	20	SER	2.7
26	C5	6	SER	2.7
31	CA	1272	A	2.7
31	CA	1496	A	2.7
40	CM	68	SER	2.7
3	BC	168	TYR	2.7
4	AD	178	MET	2.7
10	AJ	9	ARG	2.7
19	AS	32	ARG	2.7
29	CC	266	PHE	2.7
1	BA	92	U	2.7
16	BP	4	ILE	2.7
31	CA	72	U	2.7

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Mol	Chain	Res	Type	RSRZ
31	CA	2166	U	2.7
29	CC	180	GLU	2.7
29	CC	246	THR	2.7
2	BB	163	VAL	2.7
3	BC	91	VAL	2.7
4	AD	174	ASP	2.7
3	AC	89	LYS	2.7
14	AN	3	LYS	2.7
29	CC	3	VAL	2.7
34	DF	40	VAL	2.7
42	CO	106	ASP	2.7
48	CU	50	LEU	2.7
44	CQ	94	LYS	2.7
14	BN	95	GLY	2.7
41	CN	15	GLY	2.7
35	CG	97	ALA	2.7
14	AN	53	ARG	2.7
20	BT	29	ARG	2.7
45	CR	28	ARG	2.7
27	C0	52	SER	2.6
36	CH	131	SER	2.6
31	CA	89	A	2.6
31	CA	1614	A	2.6
39	CL	1	MET	2.6
40	CM	73	ILE	2.6
40	CM	103	ILE	2.6
16	BP	47	GLU	2.6
9	AI	98	LEU	2.6
13	AM	8	ASN	2.6
18	AR	47	THR	2.6
29	CC	228	VAL	2.6
29	CC	257	THR	2.6
38	CK	3	THR	2.6
39	CL	84	CYS	2.6
44	DQ	115	ASN	2.6
2	AB	65	GLY	2.6
31	CA	237	C	2.6
31	CA	610	C	2.6
11	BK	13	ARG	2.6
24	C3	3	ARG	2.6
33	CE	161	ALA	2.6
34	CF	54	ALA	2.6

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Mol	Chain	Res	Type	RSRZ
46	CS	80	ARG	2.6
11	AK	61	PHE	2.6
29	CC	74	ILE	2.6
31	CA	2743	U	2.6
37	CJ	10	LYS	2.6
54	DI	118	ILE	2.6
1	AA	1171	A	2.6
1	BA	1257	A	2.6
2	AB	114	LEU	2.6
8	BH	99	LEU	2.6
31	CA	216	A	2.6
34	DF	117	LEU	2.6
43	CP	19	GLN	2.6
8	AH	110	VAL	2.6
14	BN	38	ASP	2.6
15	AO	27	VAL	2.6
27	C0	51	VAL	2.6
9	AI	9	THR	2.6
9	AI	66	THR	2.6
3	BC	7	PRO	2.6
29	CC	203	ARG	2.6
3	AC	50	ALA	2.6
31	CA	1454	C	2.6
31	CA	1615	C	2.6
55	DA	898	C	2.6
55	DA	1072	C	2.6
3	BC	110	GLU	2.6
13	AM	41	GLU	2.6
14	BN	28	LYS	2.6
18	AR	24	LYS	2.6
26	C5	15	LYS	2.6
43	CP	76	LYS	2.6
50	CW	44	HIS	2.6
1	BA	1121	U	2.6
3	BC	75	ILE	2.6
6	AF	88	MET	2.6
23	D2	5	ILE	2.6
31	CA	1141	U	2.6
31	CA	2871	U	2.6
55	DA	895	U	2.6
10	AJ	71	LEU	2.6
31	CA	277	G	2.6

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Mol	Chain	Res	Type	RSRZ
31	CA	1715	G	2.6
31	CA	2859	G	2.6
1	BA	845	A	2.6
1	BA	1357	A	2.6
10	BJ	57	VAL	2.6
16	BP	30	GLY	2.6
19	AS	67	VAL	2.6
31	CA	631	A	2.6
31	CA	633	A	2.6
31	CA	1134	A	2.6
42	CO	8	ARG	2.6
9	AI	23	PRO	2.6
23	C2	41	PRO	2.6
39	CL	16	ALA	2.6
31	CA	269	C	2.6
31	CA	1323	C	2.6
46	CS	77	PHE	2.6
8	BH	36	ILE	2.6
1	BA	252	U	2.6
4	AD	170	TRP	2.6
5	AE	115	LEU	2.6
16	BP	74	LEU	2.6
33	CE	79	ARG	2.6
2	AB	17	GLY	2.6
29	CC	98	ASP	2.6
29	CC	250	VAL	2.6
30	CD	87	GLY	2.6
31	CA	583	G	2.6
31	CA	608	A	2.6
31	CA	1021	A	2.6
31	CA	1179	G	2.6
31	CA	2003	A	2.6
42	CO	40	LYS	2.6
55	DA	2154	A	2.6
3	AC	133	ALA	2.6
37	DJ	44	ALA	2.6
42	CO	68	ALA	2.6
50	CW	35	GLU	2.6
31	CA	2275	C	2.6
55	DA	2143	C	2.6
17	BQ	47	HIS	2.6
36	CH	80	ILE	2.6

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Mol	Chain	Res	Type	RSRZ
36	DH	72	ILE	2.6
1	BA	1189	U	2.6
1	BA	1301	U	2.6
3	AC	107	ARG	2.6
37	DJ	17	MET	2.6
11	AK	70	CYS	2.6
8	BH	120	GLY	2.6
14	BN	80	SER	2.6
16	BP	6	LEU	2.6
50	CW	20	LEU	2.6
35	CG	53	GLY	2.6
10	AJ	60	ASP	2.6
42	CO	72	ASP	2.6
29	CC	2	ALA	2.6
33	CE	198	GLU	2.6
44	CQ	18	PRO	2.6
51	CX	17	GLU	2.6
1	BA	609	A	2.6
1	BA	1213	A	2.6
11	AK	30	THR	2.6
31	CA	528	A	2.6
31	CA	1354	A	2.6
31	CA	1867	G	2.6
33	CE	65	THR	2.6
53	CZ	16	THR	2.6
55	DA	1731	G	2.6
5	BE	112	ARG	2.6
35	CG	149	ARG	2.6
1	BA	1223	C	2.6
50	CW	4	ILE	2.6
1	BA	103	U	2.6
7	AG	30	LEU	2.6
31	CA	906	U	2.6
31	CA	2690	U	2.6
35	CG	18	LYS	2.6
36	CH	41	LYS	2.6
41	CN	14	LYS	2.6
3	BC	31	ASP	2.6
22	C1	29	SER	2.6
29	CC	194	GLU	2.6
48	CU	54	GLU	2.6
10	AJ	58	ASN	2.6

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Mol	Chain	Res	Type	RSRZ
19	AS	74	PHE	2.6
43	CP	6	ALA	2.6
43	CP	71	ALA	2.6
47	CT	10	ALA	2.6
48	CU	14	PRO	2.6
13	AM	3	ARG	2.6
16	BP	3	THR	2.6
40	CM	60	ARG	2.6
1	AA	1166	G	2.6
1	BA	148	G	2.6
1	BA	1146	A	2.6
31	CA	10	A	2.6
24	C3	29	GLN	2.6
28	CB	2	G	2.6
31	CA	68	G	2.6
31	CA	389	G	2.6
31	CA	1124	G	2.6
45	CR	85	LYS	2.6
29	DC	241	GLY	2.6
31	CA	667	U	2.6
31	CA	1443	U	2.6
40	CM	53	GLY	2.6
6	BF	96	VAL	2.6
8	BH	86	TYR	2.6
9	BI	42	GLU	2.6
13	BM	68	ASP	2.6
29	DC	272	SER	2.6
30	CD	89	GLU	2.6
30	CD	113	SER	2.6
33	CE	116	ASP	2.6
34	CF	162	SER	2.6
35	CG	137	ASP	2.6
17	BQ	82	ALA	2.6
33	CE	61	ARG	2.6
35	CG	170	ARG	2.6
3	AC	64	ILE	2.6
34	CF	159	THR	2.6
1	BA	935	A	2.6
1	BA	1441	A	2.6
29	CC	181	MET	2.6
30	CD	158	GLY	2.6
31	CA	1276	A	2.6

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Mol	Chain	Res	Type	RSRZ
31	CA	2151	U	2.6
34	DF	152	LEU	2.6
44	CQ	114	LEU	2.6
1	AA	1347	G	2.6
1	BA	107	G	2.6
1	BA	187	G	2.6
31	CA	1	G	2.6
31	CA	1270	C	2.6
31	CA	2242	G	2.6
31	CA	2791	G	2.6
7	AG	87	VAL	2.6
16	AP	78	VAL	2.6
37	CJ	141	GLU	2.6
50	CW	60	VAL	2.6
27	C0	31	ARG	2.6
39	CL	108	ARG	2.6
44	CQ	19	SER	2.6
46	CS	2	TYR	2.6
48	CU	49	LYS	2.6
52	CY	39	TRP	2.6
11	AK	107	ILE	2.5
13	AM	111	GLY	2.5
19	AS	54	GLY	2.5
29	CC	12	GLY	2.5
1	BA	139	A	2.5
1	BA	135	C	2.5
7	BG	36	LYS	2.5
23	C2	38	LYS	2.5
31	CA	246	C	2.5
41	CN	71	LYS	2.5
1	BA	1255	G	2.5
31	CA	27	G	2.5
31	CA	386	G	2.5
31	CA	2053	G	2.5
31	CA	2857	G	2.5
48	CU	77	ARG	2.5
2	BB	191	SER	2.5
24	C3	45	SER	2.5
25	C4	48	ALA	2.5
17	BQ	66	PRO	2.5
47	CT	15	GLN	2.5
17	BQ	54	GLY	2.5

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Mol	Chain	Res	Type	RSRZ
30	CD	120	GLY	2.5
34	CF	50	LEU	2.5
40	CM	51	GLU	2.5
9	BI	13	LYS	2.5
29	DC	252	THR	2.5
41	CN	124	LEU	2.5
5	AE	120	VAL	2.5
10	BJ	62	ARG	2.5
26	C5	24	ARG	2.5
34	CF	89	VAL	2.5
42	CO	22	ARG	2.5
2	BB	205	ASP	2.5
1	AA	1140	C	2.5
31	CA	581	C	2.5
31	CA	624	C	2.5
31	CA	975	A	2.5
31	CA	1722	A	2.5
31	CA	2054	A	2.5
31	CA	2212	A	2.5
1	BA	351	G	2.5
1	BA	1190	G	2.5
2	BB	216	ALA	2.5
31	CA	489	G	2.5
31	CA	1543	G	2.5
31	CA	1811	G	2.5
31	CA	2046	G	2.5
31	CA	2844	G	2.5
52	CY	73	ALA	2.5
11	AK	75	LYS	2.5
13	AM	62	LYS	2.5
34	CF	78	LYS	2.5
2	AB	212	LEU	2.5
7	AG	99	LEU	2.5
8	AH	32	LEU	2.5
36	CH	5	LEU	2.5
48	CU	93	LEU	2.5
1	BA	84	U	2.5
55	DA	2130	U	2.5
12	BL	72	HIS	2.5
12	BL	107	VAL	2.5
23	D2	42	VAL	2.5
1	BA	379	C	2.5

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Mol	Chain	Res	Type	RSRZ
1	BA	461	A	2.5
1	BA	1045	C	2.5
31	CA	198	C	2.5
31	CA	1008	A	2.5
31	CA	1053	C	2.5
31	CA	1208	C	2.5
31	CA	2274	A	2.5
36	DH	84	ALA	2.5
38	CK	63	ALA	2.5
10	BJ	66	GLU	2.5
20	BT	82	GLN	2.5
20	BT	85	LYS	2.5
36	CH	22	LYS	2.5
37	CJ	40	LYS	2.5
1	AA	1260	G	2.5
1	BA	326	G	2.5
1	BA	380	G	2.5
23	C2	48	ILE	2.5
31	CA	467	G	2.5
31	CA	537	G	2.5
31	CA	1361	G	2.5
33	CE	170	ARG	2.5
40	CM	49	GLY	2.5
55	DA	1071	G	2.5
7	AG	75	VAL	2.5
15	AO	22	THR	2.5
30	CD	52	THR	2.5
30	CD	104	VAL	2.5
52	CY	36	HIS	2.5
2	BB	64	LYS	2.5
1	AA	1128	C	2.5
30	CD	99	GLU	2.5
1	AA	205	A	2.5
1	BA	1311	A	2.5
14	AN	4	GLN	2.5
26	C5	35	GLN	2.5
28	CB	62	C	2.5
31	CA	838	C	2.5
31	CA	1170	C	2.5
31	CA	2374	C	2.5
36	CH	102	ALA	2.5
37	DJ	15	ALA	2.5

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Mol	Chain	Res	Type	RSRZ
38	CK	129	GLU	2.5
50	CW	16	ALA	2.5
2	BB	182	PRO	2.5
7	BG	19	GLY	2.5
27	C0	30	ARG	2.5
31	CA	374	A	2.5
31	CA	482	A	2.5
31	CA	800	A	2.5
2	AB	43	LEU	2.5
19	AS	5	LEU	2.5
1	BA	251	G	2.5
31	CA	618	G	2.5
31	CA	1055	G	2.5
31	CA	1058	U	2.5
31	CA	1619	G	2.5
5	BE	114	VAL	2.5
38	CK	48	VAL	2.5
13	AM	58	ASP	2.5
30	CD	103	ASP	2.5
33	CE	84	THR	2.5
44	CQ	20	PHE	2.5
4	AD	172	GLU	2.5
9	BI	108	ALA	2.5
11	BK	71	ALA	2.5
13	BM	59	GLU	2.5
14	AN	22	ALA	2.5
30	CD	33	ARG	2.5
50	CW	23	ALA	2.5
1	BA	381	C	2.5
9	AI	8	GLY	2.5
2	AB	67	ILE	2.5
14	AN	55	SER	2.5
23	C2	16	GLY	2.5
29	CC	49	ILE	2.5
29	CC	259	SER	2.5
36	CH	92	GLY	2.5
55	DA	2179	C	2.5
2	BB	57	LEU	2.5
2	BB	129	LEU	2.5
31	CA	2287	A	2.5
42	CO	98	LEU	2.5
1	AA	4	U	2.5

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Mol	Chain	Res	Type	RSRZ
31	CA	2321	U	2.5
39	CL	57	VAL	2.5
44	CQ	47	VAL	2.5
1	AA	971	G	2.5
2	AB	50	PHE	2.5
31	CA	491	G	2.5
31	CA	776	G	2.5
31	CA	1038	G	2.5
7	BG	92	ARG	2.5
34	CF	140	GLU	2.5
38	CK	120	ARG	2.5
35	CG	165	ALA	2.5
5	AE	92	SER	2.5
9	AI	125	PRO	2.5
13	AM	22	ILE	2.5
14	BN	100	SER	2.5
30	CD	40	LEU	2.5
31	CA	2527	C	2.5
35	CG	89	LEU	2.5
51	CX	24	LYS	2.5
1	AA	1016	A	2.5
31	CA	429	A	2.5
31	CA	1039	A	2.5
31	CA	1165	A	2.5
31	CA	1522	A	2.5
3	BC	84	VAL	2.5
3	BC	128	VAL	2.5
10	BJ	49	PHE	2.5
44	CQ	44	GLU	2.5
48	CU	18	GLU	2.5
14	BN	101	TRP	2.5
2	BB	189	THR	2.5
28	CB	79	G	2.5
31	CA	48	G	2.5
31	CA	54	G	2.5
31	CA	242	G	2.5
31	CA	1182	G	2.5
31	CA	1296	G	2.5
31	CA	1645	G	2.5
37	CJ	105	GLN	2.5
37	DJ	120	ALA	2.5
44	CQ	41	GLN	2.5

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Mol	Chain	Res	Type	RSRZ
49	CV	16	GLY	2.5
55	DA	2138	G	2.5
12	BL	80	ILE	2.5
16	AP	80	LYS	2.5
29	CC	59	LYS	2.5
34	CF	103	LEU	2.5
34	CF	111	ILE	2.5
37	DJ	122	ILE	2.5
1	BA	215	C	2.5
1	BA	1112	C	2.5
31	CA	2427	C	2.5
39	CL	75	SER	2.5
53	DZ	28	LEU	2.5
3	BC	8	ASN	2.5
2	AB	187	VAL	2.5
8	BH	91	GLU	2.5
19	BS	36	ARG	2.5
33	CE	187	VAL	2.5
36	DH	76	GLU	2.5
54	DI	4	ASN	2.5
30	CD	122	VAL	2.5
1	AA	1368	A	2.5
31	CA	294	A	2.5
31	CA	1654	A	2.5
31	CA	2837	A	2.5
2	AB	64	LYS	2.5
16	BP	13	LYS	2.5
34	CF	145	LYS	2.5
38	CK	24	THR	2.5
42	CO	99	LYS	2.5
47	CT	100	THR	2.5
3	BC	207	ILE	2.5
31	CA	1131	G	2.5
55	DA	2152	G	2.5
2	BB	29	PRO	2.4
1	BA	848	C	2.4
23	C2	32	GLU	2.4
1	BA	467	U	2.4
16	BP	29	ASN	2.4
21	BU	9	ASN	2.4
28	CB	3	C	2.4
31	CA	645	C	2.4

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Mol	Chain	Res	Type	RSRZ
31	CA	2462	C	2.4
40	CM	33	ARG	2.4
55	DA	1727	C	2.4
38	CK	73	VAL	2.4
39	CL	7	MET	2.4
55	DA	2137	U	2.4
1	BA	55	A	2.4
10	AJ	11	LYS	2.4
28	CB	45	A	2.4
31	CA	104	A	2.4
31	CA	432	A	2.4
3	AC	71	ALA	2.4
9	AI	126	GLN	2.4
15	BO	79	THR	2.4
48	CU	39	THR	2.4
17	BQ	75	LEU	2.4
47	CT	19	LEU	2.4
52	CY	64	ILE	2.4
1	AA	1138	G	2.4
31	CA	2414	G	2.4
53	CZ	34	SER	2.4
8	BH	71	VAL	2.4
28	CB	82	U	2.4
30	CD	142	VAL	2.4
31	CA	435	C	2.4
31	CA	1779	U	2.4
31	CA	2347	C	2.4
35	CG	101	ASN	2.4
35	DG	177	LYS	2.4
46	CS	73	LYS	2.4
14	AN	8	ALA	2.4
20	BT	55	GLN	2.4
34	CF	116	GLY	2.4
50	CW	33	GLY	2.4
2	AB	39	HIS	2.4
31	CA	190	A	2.4
31	CA	342	A	2.4
31	CA	2298	A	2.4
31	CA	2602	A	2.4
31	CA	2820	A	2.4
36	CH	76	GLU	2.4
54	DI	31	ARG	2.4

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Mol	Chain	Res	Type	RSRZ
10	BJ	17	LEU	2.4
14	BN	42	TRP	2.4
36	DH	5	LEU	2.4
45	CR	32	TYR	2.4
9	BI	114	LYS	2.4
44	CQ	14	LYS	2.4
3	BC	151	VAL	2.4
8	AH	111	MET	2.4
31	CA	358	U	2.4
33	CE	169	VAL	2.4
52	CY	51	VAL	2.4
55	DA	2151	U	2.4
7	BG	34	GLY	2.4
25	C4	54	ASP	2.4
31	CA	1091	G	2.4
31	CA	1540	G	2.4
31	CA	2742	G	2.4
33	CE	90	GLN	2.4
51	CX	65	GLY	2.4
43	CP	23	ALA	2.4
43	CP	72	ALA	2.4
15	BO	14	GLU	2.4
29	CC	100	GLU	2.4
1	AA	1169	A	2.4
1	AA	1236	A	2.4
1	BA	459	A	2.4
1	BA	1042	A	2.4
2	AB	45	LYS	2.4
29	CC	33	LEU	2.4
31	CA	575	A	2.4
31	CA	1284	A	2.4
31	CA	1302	A	2.4
31	CA	1359	A	2.4
42	CO	97	ILE	2.4
45	CR	54	LYS	2.4
17	BQ	7	THR	2.4
3	BC	60	PRO	2.4
22	C1	49	TYR	2.4
44	CQ	76	THR	2.4
37	DJ	9	VAL	2.4
3	BC	187	SER	2.4
31	CA	112	U	2.4

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Mol	Chain	Res	Type	RSRZ
31	CA	2296	U	2.4
10	BJ	60	ASP	2.4
9	BI	80	ARG	2.4
19	AS	3	ARG	2.4
30	CD	124	ARG	2.4
31	CA	115	C	2.4
31	CA	433	C	2.4
31	CA	853	C	2.4
31	CA	1102	C	2.4
54	DI	122	GLN	2.4
31	CA	2318	G	2.4
31	CA	2391	G	2.4
31	CA	2623	G	2.4
19	BS	17	LYS	2.4
8	BH	59	LEU	2.4
33	CE	29	HIS	2.4
33	CE	108	ILE	2.4
19	AS	77	THR	2.4
31	CA	167	A	2.4
2	BB	162	PHE	2.4
4	AD	38	PRO	2.4
31	CA	1528	A	2.4
4	AD	182	PHE	2.4
29	CC	248	TRP	2.4
37	DJ	26	PRO	2.4
47	CT	20	VAL	2.4
48	CU	51	PHE	2.4
50	CW	65	VAL	2.4
20	BT	65	GLY	2.4
28	CB	32	U	2.4
28	CB	74	U	2.4
31	CA	686	U	2.4
30	CD	161	MET	2.4
13	AM	47	GLU	2.4
24	C3	2	LYS	2.4
47	CT	90	LYS	2.4
50	CW	34	LYS	2.4
1	BA	67	C	2.4
30	CD	209	ALA	2.4
1	AA	413	G	2.4
23	C2	34	LEU	2.4
26	C5	23	ILE	2.4

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Mol	Chain	Res	Type	RSRZ
31	CA	674	G	2.4
31	CA	1358	G	2.4
31	CA	2250	G	2.4
31	CA	2838	G	2.4
1	BA	143	A	2.4
1	BA	1046	A	2.4
9	BI	82	GLY	2.4
30	CD	129	THR	2.4
31	CA	675	A	2.4
31	CA	829	A	2.4
31	CA	1254	A	2.4
31	CA	2882	A	2.4
33	CE	53	THR	2.4
35	CG	11	VAL	2.4
38	CK	8	PRO	2.4
39	CL	120	PRO	2.4
54	DI	12	VAL	2.4
31	CA	1487	U	2.4
31	CA	2473	U	2.4
44	CQ	6	LYS	2.4
55	DA	139	U	2.4
49	CV	99	ASN	2.4
31	CA	2795	C	2.4
6	BF	74	LEU	2.4
29	CC	104	ILE	2.4
29	CC	135	ILE	2.4
30	CD	79	LEU	2.4
34	DF	85	ILE	2.4
44	CQ	48	ILE	2.4
1	AA	1185	G	2.4
1	BA	76	G	2.4
31	CA	496	G	2.4
31	CA	1355	G	2.4
31	CA	2744	G	2.4
39	CL	62	VAL	2.4
46	CS	47	VAL	2.4
51	CX	78	LYS	2.4
1	BA	1202	U	2.4
31	CA	1709	U	2.4
50	CW	59	GLU	2.4
55	DA	1729	U	2.4
28	CB	52	A	2.4

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Mol	Chain	Res	Type	RSRZ
31	CA	1144	A	2.4
31	CA	1477	A	2.4
31	CA	1810	A	2.4
31	CA	2868	A	2.4
55	DA	1073	A	2.4
8	BH	116	ALA	2.4
14	AN	2	ALA	2.4
16	AP	79	ASN	2.4
22	C1	21	ALA	2.4
33	CE	86	ALA	2.4
52	CY	17	ASN	2.4
1	AA	470	C	2.4
1	AA	1237	C	2.4
6	AF	6	ILE	2.4
31	CA	16	C	2.4
29	CC	265	LYS	2.4
30	CD	159	LYS	2.4
48	DU	70	HIS	2.4
16	BP	61	VAL	2.4
46	CS	16	GLU	2.4
35	CG	164	TYR	2.4
53	CZ	46	VAL	2.4
1	BA	224	U	2.4
28	CB	64	G	2.4
31	CA	1396	U	2.4
31	CA	1651	G	2.4
2	BB	136	MET	2.4
7	AG	45	SER	2.4
20	BT	47	ALA	2.4
28	CB	99	A	2.4
31	CA	788	A	2.4
31	CA	1129	A	2.4
31	CA	1385	A	2.4
36	CH	119	ASN	2.4
3	BC	115	LEU	2.4
6	AF	38	ARG	2.4
11	BK	23	ILE	2.4
13	AM	113	ARG	2.4
24	C3	25	LYS	2.4
25	C4	5	LYS	2.4
33	CE	105	LEU	2.4
3	AC	151	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
15	AO	16	GLY	2.3
53	CZ	26	PHE	2.3
27	C0	47	MET	2.3
2	BB	76	ALA	2.3
31	CA	1546	G	2.3
35	CG	29	LYS	2.3
5	BE	92	SER	2.3
43	CP	45	SER	2.3
1	BA	151	A	2.3
2	BB	111	ILE	2.3
3	AC	77	ILE	2.3
3	BC	14	ILE	2.3
47	CT	36	LEU	2.3
48	CU	11	LEU	2.3
49	CV	74	ASN	2.3
31	CA	1650	A	2.3
31	CA	1735	A	2.3
13	BM	72	GLU	2.3
18	BR	74	HIS	2.3
31	CA	179	C	2.3
31	CA	2368	C	2.3
31	CA	2863	C	2.3
38	CK	38	GLY	2.3
38	CK	83	GLY	2.3
3	BC	173	VAL	2.3
8	BH	104	VAL	2.3
1	BA	843	U	2.3
1	BA	1183	U	2.3
12	BL	38	TYR	2.3
19	AS	21	LYS	2.3
31	CA	1184	U	2.3
2	BB	74	ARG	2.3
7	AG	3	ARG	2.3
20	BT	54	MET	2.3
9	BI	87	LEU	2.3
10	AJ	54	SER	2.3
28	CB	67	G	2.3
31	CA	1136	G	2.3
33	CE	78	TRP	2.3
47	CT	52	GLU	2.3
48	CU	5	GLU	2.3
52	CY	16	ASN	2.3

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Mol	Chain	Res	Type	RSRZ
1	AA	468	A	2.3
1	BA	1360	A	2.3
1	AA	90	C	2.3
1	BA	110	C	2.3
3	AC	176	HIS	2.3
4	AD	40	GLN	2.3
11	AK	38	GLN	2.3
17	BQ	22	VAL	2.3
20	AT	20	HIS	2.3
28	CB	28	C	2.3
29	CC	19	VAL	2.3
31	CA	957	C	2.3
41	CN	8	LYS	2.3
44	CQ	63	LYS	2.3
47	CT	42	LYS	2.3
54	DI	105	LYS	2.3
2	AB	137	ARG	2.3
3	BC	136	ARG	2.3
31	CA	395	U	2.3
35	CG	118	PRO	2.3
38	CK	49	ASP	2.3
52	CY	3	ARG	2.3
36	DH	59	ALA	2.3
9	AI	52	LEU	2.3
22	C1	9	THR	2.3
29	CC	95	LEU	2.3
37	DJ	141	GLU	2.3
40	DM	95	LEU	2.3
6	AF	8	PHE	2.3
1	AA	201	G	2.3
1	AA	1003	G	2.3
14	AN	28	LYS	2.3
20	AT	85	LYS	2.3
1	AA	1188	A	2.3
4	AD	25	VAL	2.3
31	CA	547	A	2.3
31	CA	1040	A	2.3
31	CA	1116	G	2.3
31	CA	1455	G	2.3
1	BA	221	C	2.3
28	CB	90	C	2.3
29	CC	52	ARG	2.3

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Mol	Chain	Res	Type	RSRZ
31	CA	1646	C	2.3
31	CA	2215	C	2.3
33	CE	40	ARG	2.3
54	DI	6	GLN	2.3
31	CA	393	C	2.3
6	AF	9	MET	2.3
7	AG	101	MET	2.3
18	AR	32	TYR	2.3
3	BC	175	LEU	2.3
5	BE	81	LEU	2.3
9	BI	72	ILE	2.3
18	AR	21	ILE	2.3
44	DQ	114	LEU	2.3
2	BB	90	PHE	2.3
11	BK	29	ASN	2.3
35	CG	134	LYS	2.3
35	DG	101	ASN	2.3
42	CO	13	ASN	2.3
50	CW	24	ASN	2.3
1	BA	75	G	2.3
1	BA	1453	G	2.3
31	CA	254	G	2.3
31	CA	446	G	2.3
31	CA	466	A	2.3
31	CA	503	A	2.3
31	CA	577	G	2.3
31	CA	671	C	2.3
31	CA	1163	G	2.3
31	CA	1721	G	2.3
31	CA	1861	G	2.3
31	CA	2154	A	2.3
31	CA	2599	G	2.3
31	CA	2822	G	2.3
3	BC	28	GLU	2.3
9	AI	53	GLU	2.3
9	AI	91	ASP	2.3
6	AF	90	MET	2.3
11	BK	100	LEU	2.3
5	BE	135	ASN	2.3
5	BE	157	ARG	2.3
17	BQ	40	ARG	2.3
29	CC	50	THR	2.3

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Mol	Chain	Res	Type	RSRZ
40	DM	102	GLY	2.3
41	CN	7	THR	2.3
8	BH	107	SER	2.3
42	CO	27	SER	2.3
40	CM	46	VAL	2.3
1	BA	1232	U	2.3
30	CD	23	PRO	2.3
55	DA	2797	U	2.3
31	CA	125	A	2.3
31	CA	324	A	2.3
31	CA	1401	G	2.3
31	CA	1449	G	2.3
31	CA	1655	A	2.3
31	CA	1719	G	2.3
31	CA	2230	G	2.3
31	CA	2488	G	2.3
31	CA	2753	A	2.3
31	CA	2883	A	2.3
11	BK	70	CYS	2.3
19	AS	22	ALA	2.3
11	BK	107	ILE	2.3
29	CC	93	LEU	2.3
36	CH	56	ALA	2.3
36	CH	69	ALA	2.3
14	BN	81	ARG	2.3
47	CT	88	ARG	2.3
5	AE	31	PHE	2.3
54	DI	90	GLY	2.3
5	BE	82	GLN	2.3
34	CF	63	GLN	2.3
36	CH	31	VAL	2.3
33	CE	74	LYS	2.3
43	CP	80	GLU	2.3
31	CA	67	U	2.3
31	CA	1765	U	2.3
31	CA	1865	U	2.3
31	CA	2784	U	2.3
1	BA	322	C	2.3
1	BA	1366	C	2.3
31	CA	865	C	2.3
38	CK	6	ALA	2.3
48	DU	32	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
54	DI	102	ALA	2.3
1	BA	973	G	2.3
1	BA	1365	G	2.3
2	BB	202	GLY	2.3
3	BC	81	GLY	2.3
30	CD	93	GLY	2.3
31	CA	1439	A	2.3
31	CA	2317	A	2.3
31	CA	2894	G	2.3
6	BF	92	THR	2.3
12	BL	29	GLN	2.3
14	AN	35	ASN	2.3
45	CR	72	ASN	2.3
48	CU	19	LYS	2.3
35	CG	98	VAL	2.3
36	CH	103	VAL	2.3
50	CW	49	ASN	2.3
52	CY	40	VAL	2.3
10	AJ	72	ARG	2.3
31	CA	2585	U	2.3
31	CA	2615	U	2.3
31	CA	2818	U	2.3
33	CE	69	ARG	2.3
2	AB	68	LEU	2.3
3	BC	146	ALA	2.3
5	AE	110	ALA	2.3
14	AN	15	ALA	2.3
15	BO	3	LEU	2.3
19	BS	15	LEU	2.3
35	CG	61	GLY	2.3
36	CH	64	ALA	2.3
38	CK	115	GLY	2.3
54	DI	91	ALA	2.3
54	DI	100	ALA	2.3
3	AC	149	ILE	2.3
31	CA	1488	C	2.3
1	BA	274	A	2.3
1	BA	1067	A	2.3
9	AI	27	LYS	2.3
19	BS	70	LYS	2.3
31	CA	73	A	2.3
31	CA	677	A	2.3

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Mol	Chain	Res	Type	RSRZ
31	CA	1156	A	2.3
31	CA	1469	A	2.3
31	CA	2758	A	2.3
33	CE	85	PHE	2.3
33	DE	6	LYS	2.3
45	CR	22	LYS	2.3
48	CU	88	LYS	2.3
55	DA	1084	A	2.3
1	AA	951	G	2.3
1	AA	1190	G	2.3
1	AA	1370	G	2.3
3	BC	125	GLU	2.3
9	AI	110	GLN	2.3
31	CA	2056	G	2.3
49	CV	37	GLU	2.3
11	BK	20	VAL	2.2
12	BL	64	THR	2.2
26	C5	22	VAL	2.2
5	BE	93	ARG	2.2
21	BU	18	ARG	2.2
36	DH	98	ASP	2.2
2	BB	45	LYS	2.2
6	BF	66	ALA	2.2
19	AS	31	LEU	2.2
29	CC	41	GLY	2.2
29	CC	247	PRO	2.2
34	CF	16	LEU	2.2
34	DF	72	LYS	2.2
44	CQ	96	LYS	2.2
45	CR	21	ALA	2.2
3	BC	29	PHE	2.2
11	BK	27	PHE	2.2
29	CC	64	ILE	2.2
54	DI	52	MET	2.2
54	DI	73	LYS	2.2
7	AG	129	GLU	2.2
31	CA	414	C	2.2
1	BA	389	A	2.2
11	AK	113	VAL	2.2
31	CA	149	A	2.2
31	CA	1508	A	2.2
31	CA	2060	A	2.2

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Mol	Chain	Res	Type	RSRZ
31	CA	2088	A	2.2
16	AP	14	ARG	2.2
30	CD	58	ASN	2.2
33	CE	120	VAL	2.2
31	CA	1248	G	2.2
31	CA	1910	G	2.2
31	CA	2294	G	2.2
31	CA	2631	G	2.2
31	CA	2671	G	2.2
49	CV	68	SER	2.2
1	BA	249	U	2.2
1	BA	1315	U	2.2
4	AD	9	LEU	2.2
11	BK	62	ALA	2.2
12	BL	96	HIS	2.2
38	CK	123	LYS	2.2
19	AS	50	ALA	2.2
39	CL	107	LEU	2.2
54	DI	92	ALA	2.2
10	AJ	40	ILE	2.2
23	D2	39	PHE	2.2
33	CE	141	MET	2.2
39	CL	115	ILE	2.2
9	AI	7	TYR	2.2
33	CE	51	GLU	2.2
31	CA	143	C	2.2
31	CA	385	C	2.2
31	CA	1161	C	2.2
33	CE	41	GLN	2.2
46	CS	86	GLN	2.2
2	AB	217	VAL	2.2
5	BE	153	VAL	2.2
36	DH	68	ARG	2.2
1	BA	1170	A	2.2
5	BE	159	LYS	2.2
9	BI	100	LYS	2.2
31	CA	900	A	2.2
31	CA	2033	A	2.2
31	CA	2077	A	2.2
36	DH	73	ASN	2.2
39	CL	82	ASN	2.2
45	CR	41	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
38	CK	45	THR	2.2
1	BA	113	G	2.2
1	BA	457	G	2.2
1	BA	1385	G	2.2
31	CA	185	G	2.2
31	CA	469	G	2.2
31	CA	1203	U	2.2
31	CA	2522	U	2.2
55	DA	2139	U	2.2
2	AB	151	ILE	2.2
2	AB	200	ILE	2.2
6	BF	32	ALA	2.2
9	BI	112	GLU	2.2
47	CT	32	ALA	2.2
15	AO	43	PHE	2.2
16	BP	32	PHE	2.2
21	BU	37	PHE	2.2
42	CO	87	PHE	2.2
52	CY	31	PRO	2.2
14	AN	81	ARG	2.2
43	CP	116	GLN	2.2
1	BA	995	C	2.2
19	AS	58	VAL	2.2
31	CA	509	C	2.2
31	CA	672	C	2.2
31	CA	903	C	2.2
16	AP	40	ASN	2.2
1	BA	630	A	2.2
9	BI	71	GLY	2.2
12	BL	109	ASP	2.2
9	BI	59	GLU	2.2
10	BJ	52	LEU	2.2
13	AM	55	THR	2.2
31	CA	927	A	2.2
31	CA	2059	A	2.2
34	DF	116	GLY	2.2
47	CT	34	ASP	2.2
55	DA	1095	A	2.2
14	AN	26	GLU	2.2
15	BO	67	LEU	2.2
29	CC	176	LEU	2.2
34	CF	2	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
35	DG	13	ALA	2.2
36	CH	54	LEU	2.2
40	CM	125	LEU	2.2
3	BC	174	PRO	2.2
14	AN	71	HIS	2.2
27	C0	18	PRO	2.2
1	BA	1455	G	2.2
31	CA	60	G	2.2
31	CA	1115	G	2.2
31	CA	1382	G	2.2
31	CA	2389	G	2.2
31	CA	2532	G	2.2
31	CA	2624	G	2.2
54	DI	62	ARG	2.2
55	DA	2112	G	2.2
44	CQ	98	TYR	2.2
7	AG	80	VAL	2.2
9	BI	47	VAL	2.2
14	AN	11	VAL	2.2
31	CA	238	C	2.2
31	CA	1229	C	2.2
41	CN	135	VAL	2.2
12	BL	68	GLY	2.2
19	AS	24	GLU	2.2
40	CM	43	GLY	2.2
46	CS	57	GLY	2.2
46	CS	67	GLY	2.2
47	CT	26	GLY	2.2
28	CB	111	U	2.2
31	CA	1019	U	2.2
31	CA	1027	A	2.2
31	CA	2020	A	2.2
34	CF	57	LEU	2.2
53	DZ	37	LEU	2.2
54	DI	60	LEU	2.2
55	DA	1083	U	2.2
1	BA	65	A	2.2
1	BA	1319	A	2.2
17	AQ	21	ILE	2.2
27	C0	38	ARG	2.2
30	CD	127	PHE	2.2
40	CM	56	PRO	2.2

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Mol	Chain	Res	Type	RSRZ
42	CO	19	ALA	2.2
54	DI	56	ARG	2.2
55	DA	2101	A	2.2
14	AN	6	MET	2.2
35	DG	111	HIS	2.2
37	DJ	105	GLN	2.2
45	CR	84	LYS	2.2
54	DI	79	PRO	2.2
1	BA	350	G	2.2
6	BF	4	TYR	2.2
31	CA	1374	G	2.2
31	CA	2209	G	2.2
50	CW	82	TYR	2.2
47	CT	50	VAL	2.2
1	BA	214	C	2.2
1	BA	1203	C	2.2
1	BA	1452	C	2.2
6	AF	98	GLU	2.2
14	AN	64	CYS	2.2
7	AG	112	GLY	2.2
31	CA	692	C	2.2
31	CA	1748	C	2.2
33	CE	174	GLY	2.2
44	CQ	112	GLU	2.2
1	BA	180	U	2.2
3	BC	131	ARG	2.2
7	AG	76	LYS	2.2
15	BO	56	LEU	2.2
16	BP	8	ARG	2.2
34	CF	52	ASN	2.2
35	DG	114	ASP	2.2
36	CH	86	ASP	2.2
40	CM	69	ARG	2.2
55	DA	653	U	2.2
37	CJ	63	ALA	2.2
40	CM	94	THR	2.2
48	CU	38	ALA	2.2
53	DZ	3	ALA	2.2
1	BA	353	A	2.2
1	BA	1332	A	2.2
24	D3	1	MET	2.2
31	CA	223	A	2.2

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Mol	Chain	Res	Type	RSRZ
31	CA	430	A	2.2
31	CA	574	A	2.2
31	CA	1287	A	2.2
42	CO	110	MET	2.2
55	DA	2886[A]	A	2.2
14	AN	34	VAL	2.2
20	AT	35	VAL	2.2
29	CC	78	VAL	2.2
37	DJ	139	VAL	2.2
48	CU	53	VAL	2.2
2	AB	124	GLY	2.2
1	BA	106	C	2.2
1	BA	217	C	2.2
13	BM	87	ARG	2.2
29	CC	119	GLY	2.2
31	CA	400	G	2.2
31	CA	1206	G	2.2
31	CA	2828	G	2.2
43	CP	112	GLU	2.2
31	CA	157	C	2.2
31	CA	1957	C	2.2
47	CT	73	LYS	2.2
54	DI	8	LYS	2.2
20	BT	41	ALA	2.2
31	CA	1621	U	2.2
41	CN	9	PHE	2.2
3	BC	142	MET	2.2
29	DC	247	PRO	2.2
36	DH	93	SER	2.2
43	CP	91	SER	2.2
1	BA	1446	A	2.2
31	CA	354	A	2.2
31	CA	2435	A	2.2
31	CA	2662	A	2.2
3	BC	15	VAL	2.2
19	BS	62	VAL	2.2
29	CC	268	VAL	2.2
12	BL	14	ARG	2.2
34	DF	145	LYS	2.2
46	CS	85	LYS	2.2
23	D2	18	GLY	2.2
49	DV	57	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
1	AA	183	C	2.2
14	BN	96	LEU	2.2
1	AA	1321	U	2.2
1	AA	1371	G	2.2
1	BA	219	U	2.2
1	BA	1051	C	2.2
1	BA	1134	G	2.2
1	BA	1448	C	2.2
2	AB	203	ASN	2.2
2	BB	146	ASN	2.2
28	CB	114	C	2.2
31	CA	33	C	2.2
31	CA	518	G	2.2
31	CA	625	G	2.2
31	CA	1005	C	2.2
31	CA	1472	C	2.2
31	CA	1519	G	2.2
31	CA	1675	C	2.2
31	CA	1992	G	2.2
31	CA	2016	U	2.2
31	CA	2055	C	2.2
31	CA	2144	G	2.2
31	CA	2493	U	2.2
31	CA	2661	G	2.2
55	DA	414	C	2.2
55	DA	1171	G	2.2
55	DA	1733	G	2.2
55	DA	2144	G	2.2
8	BH	126	ILE	2.2
15	AO	11	ILE	2.2
33	DE	11	ALA	2.2
33	CE	136	GLN	2.2
49	DV	50	PRO	2.2
13	AM	108	THR	2.2
3	AC	80	LYS	2.2
11	AK	94	GLU	2.2
16	BP	48	GLU	2.2
34	CF	48	LYS	2.2
36	CH	71	LYS	2.2
40	CM	86	GLU	2.2
42	DO	121	LYS	2.2
1	AA	1346	A	2.2

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Mol	Chain	Res	Type	RSRZ
1	BA	383	A	2.2
3	BC	153	VAL	2.2
31	CA	1353	A	2.2
31	CA	1808	A	2.2
31	CA	2406	A	2.2
51	CX	31	VAL	2.2
12	BL	74	LEU	2.1
1	BA	472	U	2.1
1	BA	1335	U	2.1
31	CA	105	C	2.1
31	CA	234	U	2.1
31	CA	915	C	2.1
31	CA	1812	U	2.1
49	CV	96	PHE	2.1
3	BC	114	LYS	2.1
8	BH	3	MET	2.1
29	CC	255	LYS	2.1
31	CA	2494	G	2.1
31	CA	2692	G	2.1
36	CH	35	LYS	2.1
48	CU	64	LYS	2.1
55	DA	1091	G	2.1
13	AM	12	HIS	2.1
18	AR	45	THR	2.1
29	CC	221	ARG	2.1
36	CH	45	GLU	2.1
36	DH	104	THR	2.1
39	CL	104	THR	2.1
18	BR	23	TYR	2.1
1	BA	253	A	2.1
1	BA	1012	A	2.1
31	CA	1307	A	2.1
31	CA	1854	A	2.1
31	CA	2388	A	2.1
2	BB	167	ASP	2.1
1	AA	1364	U	2.1
31	CA	286	U	2.1
31	CA	296	U	2.1
31	CA	1209	U	2.1
31	CA	1294	U	2.1
31	CA	2408	U	2.1
2	BB	96	TRP	2.1

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Mol	Chain	Res	Type	RSRZ
47	CT	89	ALA	2.1
3	AC	188	GLU	2.1
22	C1	52	ARG	2.1
31	CA	1006	C	2.1
26	C5	31	PRO	2.1
1	BA	324	G	2.1
2	BB	86	SER	2.1
2	BB	226	SER	2.1
28	CB	6	G	2.1
28	CB	18	G	2.1
31	CA	15	G	2.1
31	CA	1149	G	2.1
31	CA	2349	G	2.1
31	CA	2415	G	2.1
31	CA	2583	G	2.1
55	DA	1074	G	2.1
3	AC	153	VAL	2.1
7	AG	38	THR	2.1
11	BK	48	GLY	2.1
15	AO	25	THR	2.1
29	CC	94	VAL	2.1
38	CK	30	THR	2.1
48	CU	63	VAL	2.1
53	CZ	50	VAL	2.1
2	BB	188	ASP	2.1
13	BM	110	LYS	2.1
25	C4	33	LEU	2.1
54	DI	71	CYS	2.1
31	CA	391	A	2.1
31	CA	2377	A	2.1
3	BC	163	ALA	2.1
24	C3	19	ARG	2.1
25	C4	13	ARG	2.1
31	CA	1409	U	2.1
31	CA	1742	U	2.1
31	CA	2155	U	2.1
33	CE	44	ARG	2.1
35	DG	173	GLU	2.1
42	CO	32	GLU	2.1
43	CP	113	ALA	2.1
27	C0	49	ASN	2.1
31	CA	897	C	2.1

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Mol	Chain	Res	Type	RSRZ
31	CA	1150	C	2.1
2	BB	65	GLY	2.1
7	BG	20	SER	2.1
20	AT	58	VAL	2.1
25	C4	56	GLY	2.1
1	BA	454	G	2.1
31	CA	855	G	2.1
31	CA	954	G	2.1
31	CA	2010	G	2.1
31	CA	2029	G	2.1
31	CA	2428	G	2.1
31	CA	2659	G	2.1
52	CY	62	LYS	2.1
54	DI	86	THR	2.1
45	CR	60	LEU	2.1
52	CY	29	PHE	2.1
52	CY	33	LEU	2.1
2	AB	205	ASP	2.1
7	BG	67	GLU	2.1
19	BS	64	ASP	2.1
1	BA	66	A	2.1
8	AH	130	ALA	2.1
31	CA	1372	U	2.1
31	CA	2798	U	2.1
33	CE	149	ILE	2.1
34	DF	106	ILE	2.1
31	CA	1387	A	2.1
46	CS	65	ALA	2.1
54	DI	103	ASN	2.1
1	BA	316	C	2.1
3	BC	62	LYS	2.1
14	AN	68	GLY	2.1
20	BT	19	LYS	2.1
29	CC	253	LYS	2.1
31	CA	806	C	2.1
31	CA	1644	C	2.1
31	CA	2456	C	2.1
36	CH	121	VAL	2.1
49	CV	57	GLY	2.1
3	BC	67	THR	2.1
8	AH	55	THR	2.1
9	AI	11	ARG	2.1

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Mol	Chain	Res	Type	RSRZ
29	CC	205	LEU	2.1
1	BA	1386	G	2.1
10	BJ	78	GLU	2.1
33	CE	19	PHE	2.1
34	DF	128	TYR	2.1
3	BC	3	GLN	2.1
10	BJ	64	GLN	2.1
22	C1	31	ASP	2.1
28	CB	100	G	2.1
31	CA	24	G	2.1
31	CA	258	G	2.1
31	CA	604	G	2.1
31	CA	2027	G	2.1
31	CA	2409	G	2.1
31	CA	2834	G	2.1
47	CT	59	GLU	2.1
2	AB	34	ALA	2.1
9	AI	86	ALA	2.1
29	CC	61	ALA	2.1
31	CA	25	U	2.1
31	CA	1255	U	2.1
31	CA	2312	U	2.1
36	CH	59	ALA	2.1
1	BA	1246	A	2.1
1	BA	1251	A	2.1
3	AC	2	GLY	2.1
19	AS	46	GLY	2.1
31	CA	278	A	2.1
31	CA	764	A	2.1
31	CA	2005	A	2.1
31	CA	2051	A	2.1
51	CX	27	GLY	2.1
1	AA	1096	C	2.1
11	BK	22	HIS	2.1
31	CA	366	C	2.1
31	CA	898	C	2.1
31	CA	1164	C	2.1
31	CA	2214	C	2.1
31	CA	2824	C	2.1
55	DA	143	C	2.1
42	CO	4	ARG	2.1
19	BS	10	PHE	2.1

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Mol	Chain	Res	Type	RSRZ
23	C2	17	THR	2.1
35	CG	87	LEU	2.1
52	CY	38	PHE	2.1
4	BD	40	GLN	2.1
41	CN	22	GLN	2.1
5	AE	141	ILE	2.1
7	AG	29	ILE	2.1
15	BO	7	ALA	2.1
19	AS	40	ILE	2.1
1	AA	838	G	2.1
1	AA	1186	G	2.1
2	AB	11	LYS	2.1
29	CC	256	LYS	2.1
31	CA	2449	U	2.1
42	CO	88	ALA	2.1
54	DI	83	ALA	2.1
31	CA	396	G	2.1
31	CA	620	G	2.1
31	CA	809	G	2.1
31	CA	1300	G	2.1
31	CA	1555	G	2.1
31	CA	1601	G	2.1
31	CA	2351	G	2.1
55	DA	2136	G	2.1
13	BM	26	GLY	2.1
8	BH	39	VAL	2.1
29	CC	220	VAL	2.1
31	CA	632	A	2.1
31	CA	2013	A	2.1
39	CL	20	MET	2.1
45	CR	104	VAL	2.1
54	DI	89	PRO	2.1
10	AJ	24	GLU	2.1
31	CA	351	C	2.1
31	CA	1656	C	2.1
31	CA	2153	C	2.1
31	CA	2755	C	2.1
31	CA	2888	C	2.1
55	DA	1728	C	2.1
5	AE	144	LEU	2.1
25	C4	16	LYS	2.1
38	CK	61	LYS	2.1

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Mol	Chain	Res	Type	RSRZ
47	CT	31	GLN	2.1
47	CT	109	ASP	2.1
48	DU	91	GLN	2.1
1	AA	218	U	2.1
7	BG	147	ALA	2.1
30	CD	85	ALA	2.1
31	CA	2845	U	2.1
36	CH	84	ALA	2.1
38	CK	101	ILE	2.1
39	CL	60	ALA	2.1
42	CO	34	ILE	2.1
49	DV	2	ALA	2.1
1	AA	200	G	2.1
1	BA	184	G	2.1
1	BA	633	G	2.1
7	BG	138	ARG	2.1
2	AB	201	PRO	2.1
6	AF	64	VAL	2.1
29	CC	132	MET	2.1
31	CA	585	G	2.1
31	CA	664	G	2.1
31	CA	774	G	2.1
31	CA	926	G	2.1
31	CA	1339	G	2.1
31	CA	2304	G	2.1
31	CA	2382	G	2.1
31	CA	2674	G	2.1
31	CA	2825	G	2.1
29	CC	174	LEU	2.1
31	CA	497	A	2.1
31	CA	795	C	2.1
31	CA	910	A	2.1
31	CA	2143	C	2.1
31	CA	2433	A	2.1
36	DH	54	LEU	2.1
52	DY	77	LYS	2.1
55	DA	2150	C	2.1
1	AA	961	U	2.1
2	AB	75	ALA	2.1
9	BI	78	ALA	2.1
11	AK	79	ILE	2.1
14	BN	44	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
22	C1	43	ILE	2.1
26	C5	26	ILE	2.1
33	CE	181	ILE	2.1
35	DG	121	ILE	2.1
36	CH	98	ASP	2.1
46	DS	26	ASP	2.1
30	CD	12	THR	2.1
36	CH	79	THR	2.1
2	BB	17	GLY	2.1
21	AU	34	ARG	2.1
41	CN	59	ARG	2.1
53	CZ	62	GLY	2.1
2	BB	4	VAL	2.1
10	BJ	58	ASN	2.1
29	CC	216	VAL	2.1
30	CD	165	MET	2.1
1	AA	1124	G	2.1
1	AA	1220	G	2.1
1	BA	1064	G	2.1
31	CA	1356	G	2.1
31	CA	1452	G	2.1
15	BO	87	LEU	2.0
36	DH	75	LEU	2.0
1	AA	979	C	2.0
1	BA	74	A	2.0
1	BA	970	C	2.0
31	CA	181	A	2.0
31	CA	582	A	2.0
31	CA	812	C	2.0
31	CA	1908	C	2.0
31	CA	2682	A	2.0
31	CA	2712	C	2.0
1	BA	70	U	2.0
3	BC	61	ALA	2.0
6	BF	91	ARG	2.0
7	AG	81	GLY	2.0
9	BI	102	GLY	2.0
13	BM	20	THR	2.0
16	BP	7	ALA	2.0
45	CR	62	ILE	2.0
24	C3	38	GLY	2.0
31	CA	588	U	2.0

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Mol	Chain	Res	Type	RSRZ
31	CA	1602	U	2.0
31	CA	1758	U	2.0
35	CG	34	THR	2.0
11	BK	94	GLU	2.0
17	BQ	43	LYS	2.0
45	CR	15	LYS	2.0
6	BF	62	MET	2.0
14	AN	94	PRO	2.0
20	AT	56	PRO	2.0
36	DH	115	VAL	2.0
11	BK	52	PHE	2.0
54	DI	95	LEU	2.0
13	BM	91	HIS	2.0
3	AC	179	ARG	2.0
23	C2	13	SER	2.0
31	CA	175	G	2.0
31	CA	298	G	2.0
1	AA	983	A	2.0
1	BA	95	C	2.0
8	AH	107	SER	2.0
10	AJ	63	ASP	2.0
1	BA	192	A	2.0
1	BA	1216	A	2.0
29	CC	209	GLY	2.0
31	CA	384	A	2.0
31	CA	560	C	2.0
31	CA	662	G	2.0
31	CA	669	G	2.0
31	CA	804	A	2.0
31	CA	1363	C	2.0
31	CA	2048	G	2.0
31	CA	1598	A	2.0
31	CA	2160	C	2.0
37	DJ	64	ASP	2.0
31	CA	2670	A	2.0
31	CA	2850	A	2.0
31	CA	2249	U	2.0
33	CE	87	ALA	2.0
54	DI	82	ILE	2.0
38	CK	44	TYR	2.0
40	CM	58	TYR	2.0
43	CP	86	GLY	2.0

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Mol	Chain	Res	Type	RSRZ
5	BE	34	THR	2.0
5	BE	74	VAL	2.0
5	BE	85	VAL	2.0
16	AP	19	VAL	2.0
47	CT	106	VAL	2.0
5	AE	81	LEU	2.0
9	AI	103	PHE	2.0
11	BK	82	LEU	2.0
38	CK	122	LEU	2.0
3	BC	162	ILE	2.0
8	BH	14	ILE	2.0
40	CM	17	LYS	2.0
48	CU	40	LYS	2.0
1	AA	91	U	2.0
1	AA	848	C	2.0
1	BA	133	U	2.0
1	BA	259	G	2.0
1	BA	260	G	2.0
28	CB	73	A	2.0
31	CA	17	G	2.0
31	CA	58	G	2.0
31	CA	416	U	2.0
31	CA	1033	U	2.0
31	CA	1497	U	2.0
31	CA	1642	G	2.0
31	CA	2104	C	2.0
31	CA	2244	U	2.0
31	CA	2306	C	2.0
31	CA	2551	C	2.0
31	CA	2664	G	2.0
31	CA	2695	U	2.0
31	CA	2785	C	2.0
45	CR	115	ALA	2.0
55	DA	2104	C	2.0
31	CA	118	A	2.0
31	CA	899	A	2.0
55	DA	1096	A	2.0
12	BL	39	THR	2.0
6	BF	64	VAL	2.0
44	CQ	46	VAL	2.0
3	AC	157	LEU	2.0
4	AD	168	PRO	2.0

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Mol	Chain	Res	Type	RSRZ
10	AJ	41	PRO	2.0
14	AN	51	LEU	2.0
18	AR	68	LEU	2.0
29	CC	175	ARG	2.0
34	CF	115	ARG	2.0
35	CG	72	LEU	2.0
36	DH	83	LYS	2.0
5	BE	72	ILE	2.0
8	BH	54	ASP	2.0
15	BO	16	GLY	2.0
16	BP	75	ILE	2.0
22	C1	38	HIS	2.0
42	CO	3	HIS	2.0
16	AP	7	ALA	2.0
1	BA	991	U	2.0
28	CB	8	C	2.0
31	CA	82	U	2.0
31	CA	1290	C	2.0
31	CA	2779	U	2.0
39	CL	14	SER	2.0
31	CA	225	C	2.0
1	AA	416	G	2.0
1	AA	1274	A	2.0
1	BA	846	G	2.0
5	AE	74	VAL	2.0
6	BF	30	THR	2.0
9	AI	113	ARG	2.0
11	BK	96	THR	2.0
16	AP	50	THR	2.0
31	CA	287	G	2.0
31	CA	916	G	2.0
31	CA	1954	G	2.0
31	CA	2135	A	2.0
31	CA	2156	G	2.0
31	CA	2587	A	2.0
9	BI	57	MET	2.0
12	BL	51	LYS	2.0
16	AP	38	PHE	2.0
34	CF	148	ARG	2.0
39	CL	98	ARG	2.0
10	AJ	64	GLN	2.0
39	CL	87	LEU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
1	5MC	BA	967	21/22	0.67	0.39	153,164,167,167	0
1	2MG	BA	966	24/25	0.75	0.36	153,160,171,171	0
1	2MG	BA	1207	24/25	0.80	0.29	158,161,165,168	0
31	PSU	CA	1917	20/21	0.81	0.21	119,125,134,135	0
31	2MA	CA	2503	23/24	0.83	0.26	110,115,118,118	0
31	6MZ	CA	2030	23/24	0.85	0.24	108,114,116,117	0
1	PSU	BA	516	20/21	0.85	0.16	88,99,102,104	0
31	OMU	CA	2552	21/22	0.85	0.45	91,96,100,101	0
31	PSU	CA	1911	20/21	0.86	0.24	123,137,138,139	0
31	3TD	CA	1915	21/22	0.86	0.28	150,155,157,157	0
31	PSU	CA	2504	20/21	0.86	0.25	98,108,110,111	0
31	PSU	CA	955	20/21	0.86	0.26	107,112,115,115	0
31	PSU	CA	746	20/21	0.87	0.25	120,123,126,127	0
31	G7M	CA	2069	24/25	0.87	0.26	109,112,115,116	0
31	2MG	CA	2445	24/25	0.87	0.31	105,110,112,113	0
31	PSU	CA	2580	20/21	0.87	0.22	102,105,109,109	0
31	5MU	CA	747	21/22	0.88	0.28	126,128,130,131	0
1	5MC	AA	967	21/22	0.88	0.20	90,106,107,108	0
1	2MG	BA	1516	24/25	0.89	0.21	82,90,99,100	0
31	OMG	CA	2251	24/25	0.89	0.26	90,95,100,101	0
1	5MC	BA	1407	21/22	0.89	0.21	100,109,114,117	0
31	PSU	CA	2457	20/21	0.89	0.25	106,107,108,109	0
31	1MG	CA	745	24/25	0.90	0.25	106,113,118,121	0
41	4D4	CN	81	12/13	0.90	0.34	112,122,143,143	0
12	D2T	BL	89	10/11	0.91	0.28	86,88,94,95	0
31	6MZ	CA	1618	23/24	0.91	0.30	136,143,148,149	0
1	2MG	AA	966	24/25	0.91	0.19	95,98,107,108	0
1	2MG	AA	1207	24/25	0.91	0.16	114,118,121,124	0
55	PSU	DA	1911	20/21	0.91	0.18	78,88,91,91	0
55	3TD	DA	1915	21/22	0.91	0.22	103,106,112,113	0
12	D2T	AL	89	10/11	0.91	0.27	66,71,78,78	0
31	OMC	CA	2498	21/22	0.92	0.28	97,102,104,106	0
31	PSU	CA	2605	20/21	0.92	0.22	82,84,86,87	0
31	2MG	CA	1835	24/25	0.92	0.18	74,76,78,78	0
1	UR3	BA	1498	21/22	0.92	0.18	89,93,97,98	0
1	MA6	BA	1518	24/25	0.92	0.25	84,88,95,96	0
31	5MU	CA	1939	21/22	0.93	0.19	75,79,81,82	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
31	5MC	CA	1962	21/22	0.93	0.16	72,78,79,82	0
1	4OC	BA	1402	22/23	0.93	0.17	78,81,84,85	0
1	MA6	BA	1519	24/25	0.93	0.26	84,87,91,92	0
55	PSU	DA	1917	20/21	0.94	0.17	74,82,90,90	0
1	PSU	AA	516	20/21	0.94	0.16	88,92,97,97	0
1	UR3	AA	1498	21/22	0.95	0.19	64,68,72,73	0
1	MA6	AA	1519	24/25	0.96	0.19	61,62,70,71	0
32	MEQ	DD	150[A]	10/11	0.96	0.24	14,23,32,32	10
32	MEQ	DD	150[B]	10/11	0.96	0.24	27,32,45,50	10
55	2MG	DA	1835	24/25	0.96	0.23	49,55,56,56	0
1	4OC	AA	1402	22/23	0.96	0.18	61,68,72,73	0
1	G7M	AA	527	24/25	0.96	0.17	63,67,73,74	0
1	G7M	BA	527	24/25	0.96	0.15	75,80,83,84	0
55	5MC	DA	1962	21/22	0.96	0.23	43,46,50,52	0
1	2MG	AA	1516	24/25	0.96	0.17	58,61,62,63	0
41	4D4	DN	81[A]	12/13	0.96	0.24	33,38,53,55	9
41	4D4	DN	81[B]	12/13	0.96	0.24	27,32,34,35	9
1	MA6	AA	1518	24/25	0.97	0.16	60,61,62,64	0
1	5MC	AA	1407	21/22	0.97	0.15	60,61,63,64	0
55	PSU	DA	2604	20/21	0.97	0.19	37,42,54,55	0
55	5MU	DA	1939	21/22	0.98	0.22	35,38,40,43	0
55	PSU	DA	2605	20/21	0.98	0.19	35,41,43,44	0
55	OMG	DA	2251	24/25	0.98	0.21	29,33,35,39	0
55	PSU	DA	2504	20/21	0.98	0.21	33,41,49,52	0
55	OMU	DA	2552	21/22	0.98	0.22	33,37,39,43	0
55	2MG	DA	2445	24/25	0.99	0.21	25,29,33,34	0
55	H2U	DA	2449	20/21	0.99	0.22	27,30,36,39	0
55	PSU	DA	2457	20/21	0.99	0.19	25,29,31,35	0
55	OMC	DA	2498	21/22	0.99	0.21	20,27,31,37	0
55	2MA	DA	2503	23/24	0.99	0.20	33,36,39,43	0
55	5MU	DA	747	21/22	0.99	0.20	28,31,37,38	0
55	PSU	DA	955	20/21	0.99	0.21	27,28,32,35	0
55	PSU	DA	2580	20/21	0.99	0.21	25,30,33,35	0
55	6MZ	DA	1618	23/24	0.99	0.20	25,30,32,35	0
55	1MG	DA	745	24/25	0.99	0.21	28,31,33,38	0
55	6MZ	DA	2030	23/24	0.99	0.22	24,28,32,39	0
55	G7M	DA	2069	24/25	0.99	0.20	26,35,36,37	0
55	PSU	DA	746	20/21	0.99	0.19	28,32,36,38	0

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	CA	3140	1/1	-0.34	0.60	147,147,147,147	0
56	MG	AA	1622	1/1	-0.17	1.84	130,130,130,130	0
56	MG	CA	3033	1/1	-0.13	0.30	200,200,200,200	0
56	MG	CA	3038	1/1	-0.04	0.22	268,268,268,268	0
56	MG	CA	3123	1/1	-0.03	0.99	188,188,188,188	0
56	MG	CA	3077	1/1	0.00	0.48	252,252,252,252	0
56	MG	CA	3142	1/1	0.03	0.56	133,133,133,133	0
56	MG	AA	1626	1/1	0.05	1.41	111,111,111,111	0
56	MG	CA	3156	1/1	0.09	0.18	246,246,246,246	0
56	MG	CA	3149	1/1	0.10	1.20	92,92,92,92	0
56	MG	CA	3104	1/1	0.13	0.32	263,263,263,263	0
56	MG	CA	3028	1/1	0.14	0.73	283,283,283,283	0
56	MG	DA	3180	1/1	0.14	1.27	97,97,97,97	0
56	MG	CA	3130	1/1	0.17	1.11	141,141,141,141	0
56	MG	CA	3139	1/1	0.19	1.21	139,139,139,139	0
56	MG	CA	3061	1/1	0.20	0.21	274,274,274,274	0
56	MG	CA	3141	1/1	0.20	0.60	109,109,109,109	0
56	MG	AA	1603	1/1	0.21	1.09	119,119,119,119	0
56	MG	CA	3146	1/1	0.25	0.38	247,247,247,247	0
56	MG	AA	1604	1/1	0.26	0.85	82,82,82,82	0
56	MG	DA	3168	1/1	0.27	0.48	108,108,108,108	0
56	MG	AA	1642	1/1	0.27	0.51	165,165,165,165	0
56	MG	BA	1630	1/1	0.29	0.14	221,221,221,221	0
56	MG	AA	1628	1/1	0.29	0.95	142,142,142,142	0
56	MG	CA	3113	1/1	0.30	0.78	94,94,94,94	0
56	MG	DA	3131	1/1	0.32	0.76	87,87,87,87	0
56	MG	DA	3138	1/1	0.33	0.39	89,89,89,89	0
56	MG	CA	3110	1/1	0.34	0.83	188,188,188,188	0
56	MG	CA	3003	1/1	0.35	2.62	284,284,284,284	0
56	MG	AA	1614	1/1	0.35	0.20	131,131,131,131	0
56	MG	CA	3056	1/1	0.35	0.72	100,100,100,100	0
56	MG	DA	3179	1/1	0.35	0.48	102,102,102,102	0
56	MG	CA	3124	1/1	0.35	0.53	202,202,202,202	0
56	MG	CA	3002	1/1	0.37	0.31	259,259,259,259	0
56	MG	DA	3145	1/1	0.40	0.76	101,101,101,101	0
56	MG	CA	3005	1/1	0.44	1.15	253,253,253,253	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	CA	3133	1/1	0.45	0.63	140,140,140,140	0
56	MG	AA	1606	1/1	0.46	0.49	120,120,120,120	0
62	PEG	DQ	201	7/7	0.47	1.03	107,109,110,110	0
56	MG	DB	207	1/1	0.48	0.77	105,105,105,105	0
56	MG	CA	3092	1/1	0.50	0.23	202,202,202,202	0
56	MG	DA	3163	1/1	0.50	0.36	84,84,84,84	0
56	MG	AA	1616	1/1	0.51	0.93	88,88,88,88	0
56	MG	CA	3039	1/1	0.52	0.36	153,153,153,153	0
56	MG	BA	1629	1/1	0.52	0.58	157,157,157,157	0
56	MG	CA	3068	1/1	0.53	0.43	253,253,253,253	0
56	MG	DA	3130	1/1	0.53	0.36	87,87,87,87	0
56	MG	CA	3134	1/1	0.54	0.52	204,204,204,204	0
56	MG	CA	3097	1/1	0.54	0.16	125,125,125,125	0
56	MG	DA	3178	1/1	0.55	0.67	101,101,101,101	0
56	MG	DB	206	1/1	0.56	0.47	102,102,102,102	0
56	MG	CA	3075	1/1	0.57	1.37	253,253,253,253	0
56	MG	AA	1605	1/1	0.58	0.71	99,99,99,99	0
56	MG	CA	3154	1/1	0.58	0.45	155,155,155,155	0
56	MG	DA	3182	1/1	0.58	0.54	73,73,73,73	0
56	MG	CA	3047	1/1	0.58	1.53	240,240,240,240	0
56	MG	CA	3090	1/1	0.59	0.57	215,215,215,215	0
56	MG	CA	3131	1/1	0.59	0.57	111,111,111,111	0
56	MG	CA	3054	1/1	0.59	0.21	140,140,140,140	0
56	MG	BA	1638	1/1	0.59	0.93	110,110,110,110	0
56	MG	BA	1641	1/1	0.59	0.97	140,140,140,140	0
56	MG	CA	3126	1/1	0.61	0.38	136,136,136,136	0
56	MG	DA	3147	1/1	0.61	0.42	89,89,89,89	0
56	MG	CA	3122	1/1	0.61	0.77	136,136,136,136	0
56	MG	CA	3034	1/1	0.62	0.17	256,256,256,256	0
56	MG	DA	3134	1/1	0.62	0.37	78,78,78,78	0
56	MG	CA	3132	1/1	0.62	0.75	152,152,152,152	0
56	MG	AA	1627	1/1	0.62	0.56	99,99,99,99	0
56	MG	CA	3071	1/1	0.62	0.20	207,207,207,207	0
56	MG	BA	1639	1/1	0.62	0.63	106,106,106,106	0
56	MG	AA	1661	1/1	0.63	0.33	190,190,190,190	0
56	MG	CA	3027	1/1	0.63	0.31	137,137,137,137	0
56	MG	AA	1624	1/1	0.63	0.80	93,93,93,93	0
56	MG	CA	3115	1/1	0.63	0.46	108,108,108,108	0
56	MG	AA	1632	1/1	0.64	0.08	124,124,124,124	0
59	PUT	AA	1675	6/6	0.64	0.62	90,92,93,93	0
56	MG	AA	1602	1/1	0.64	0.55	88,88,88,88	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	CA	3135	1/1	0.65	0.54	104,104,104,104	0
56	MG	CA	3018	1/1	0.65	0.16	133,133,133,133	0
56	MG	AA	1612	1/1	0.65	0.73	81,81,81,81	0
56	MG	BA	1637	1/1	0.65	0.59	93,93,93,93	0
56	MG	CA	3079	1/1	0.65	0.16	143,143,143,143	0
56	MG	AA	1621	1/1	0.66	0.45	83,83,83,83	0
56	MG	AA	1608	1/1	0.66	0.50	119,119,119,119	0
56	MG	CA	3007	1/1	0.66	0.46	257,257,257,257	0
56	MG	CA	3031	1/1	0.67	0.23	127,127,127,127	0
56	MG	CA	3078	1/1	0.67	0.19	195,195,195,195	0
56	MG	BA	1623	1/1	0.67	1.44	235,235,235,235	0
56	MG	AA	1615	1/1	0.67	0.55	90,90,90,90	0
56	MG	BA	1624	1/1	0.68	0.26	275,275,275,275	0
56	MG	CA	3108	1/1	0.68	0.52	109,109,109,109	0
56	MG	AA	1617	1/1	0.68	0.36	98,98,98,98	0
56	MG	CA	3105	1/1	0.69	0.41	254,254,254,254	0
56	MG	CA	3129	1/1	0.69	0.23	141,141,141,141	0
56	MG	CA	3076	1/1	0.69	0.21	213,213,213,213	0
56	MG	DA	3157	1/1	0.69	0.53	73,73,73,73	0
56	MG	CB	203	1/1	0.70	0.10	155,155,155,155	0
56	MG	CA	3013	1/1	0.70	0.18	135,135,135,135	0
56	MG	BA	1604	1/1	0.70	0.19	182,182,182,182	0
64	PGE	D1	102	10/10	0.70	0.59	95,96,100,100	0
65	SPD	DA	3205	10/10	0.70	0.38	75,81,84,85	0
56	MG	DA	3125	1/1	0.71	0.42	83,83,83,83	0
62	PEG	DA	3217	7/7	0.71	0.55	89,93,98,99	0
56	MG	BA	1626	1/1	0.71	0.32	111,111,111,111	0
56	MG	AA	1613	1/1	0.71	1.50	85,85,85,85	0
58	MPD	DT	201	8/8	0.72	0.41	73,82,84,86	0
59	PUT	AA	1672	6/6	0.72	0.66	110,112,114,114	0
59	PUT	AA	1674	6/6	0.72	0.72	98,99,100,100	0
56	MG	CA	3137	1/1	0.72	0.59	168,168,168,168	0
56	MG	CA	3014	1/1	0.72	0.18	262,262,262,262	0
56	MG	BA	1606	1/1	0.72	0.21	251,251,251,251	0
56	MG	CA	3099	1/1	0.72	0.28	235,235,235,235	0
56	MG	AA	1611	1/1	0.72	0.25	113,113,113,113	0
56	MG	DA	3161	1/1	0.73	0.43	78,78,78,78	0
58	MPD	DT	202	8/8	0.73	0.41	87,88,89,91	0
56	MG	BA	1608	1/1	0.73	0.13	122,122,122,122	0
56	MG	DA	3167	1/1	0.73	0.40	75,75,75,75	0
56	MG	CA	3032	1/1	0.73	0.53	269,269,269,269	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	CA	3055	1/1	0.73	0.10	195,195,195,195	0
56	MG	CA	3106	1/1	0.73	0.60	103,103,103,103	0
56	MG	DA	3155	1/1	0.73	0.57	74,74,74,74	0
56	MG	CA	3121	1/1	0.73	0.50	101,101,101,101	0
56	MG	CA	3049	1/1	0.74	0.24	100,100,100,100	0
56	MG	AA	1618	1/1	0.74	0.83	91,91,91,91	0
56	MG	CA	3016	1/1	0.74	0.34	148,148,148,148	0
56	MG	CA	3060	1/1	0.75	0.38	242,242,242,242	0
62	PEG	D3	102	7/7	0.75	1.24	72,74,83,84	0
56	MG	BA	1614	1/1	0.75	0.17	147,147,147,147	0
56	MG	DA	3159	1/1	0.75	0.44	80,80,80,80	0
63	EDO	DA	3208	4/4	0.75	0.48	98,99,100,101	0
56	MG	AA	1679	1/1	0.75	0.25	189,189,189,189	0
56	MG	CA	3111	1/1	0.75	1.00	159,159,159,159	0
56	MG	CA	3109	1/1	0.76	0.58	93,93,93,93	0
56	MG	AA	1620	1/1	0.76	0.46	83,83,83,83	0
56	MG	BA	1625	1/1	0.76	0.39	274,274,274,274	0
56	MG	CA	3151	1/1	0.76	0.36	84,84,84,84	0
57	PG4	DA	3215	13/13	0.76	0.43	95,103,104,104	0
58	MPD	DE	302	8/8	0.76	0.57	96,97,98,98	0
62	PEG	DA	3225	7/7	0.76	0.39	62,65,70,70	0
63	EDO	DA	3004	4/4	0.76	0.45	107,107,108,109	0
56	MG	DA	3136	1/1	0.76	0.12	92,92,92,92	0
56	MG	DA	3170	1/1	0.76	0.39	73,73,73,73	0
64	PGE	D3	101	10/10	0.76	0.66	87,88,88,88	0
58	MPD	DA	3203	8/8	0.76	0.75	96,99,102,104	0
69	TRS	DA	3219	8/8	0.76	0.56	98,99,102,104	0
56	MG	CA	3010	1/1	0.77	0.52	231,231,231,231	0
56	MG	AA	1663	1/1	0.77	0.19	110,110,110,110	0
59	PUT	DA	3218	6/6	0.77	0.42	75,77,80,81	0
62	PEG	D1	103	7/7	0.77	0.47	56,60,61,62	0
56	MG	CA	3148	1/1	0.77	0.79	86,86,86,86	1
56	MG	CA	3001	1/1	0.77	0.38	299,299,299,299	0
67	ACY	DA	3196	4/4	0.77	0.32	75,79,79,80	0
68	GUN	DA	3210	11/11	0.77	0.38	71,73,74,74	0
56	MG	CB	201	1/1	0.77	0.10	166,166,166,166	0
56	MG	DA	3126	1/1	0.78	0.37	76,76,76,76	0
59	PUT	AA	1673	6/6	0.78	0.49	125,126,127,128	0
56	MG	CA	3006	1/1	0.78	0.19	227,227,227,227	0
64	PGE	DA	3224	10/10	0.78	0.34	74,81,83,83	0
57	PG4	AA	1670	13/13	0.78	0.30	80,92,101,102	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	CA	3120	1/1	0.78	0.25	195,195,195,195	0
63	EDO	DB	210	4/4	0.78	0.43	85,85,85,86	0
60	T1C	BA	1643	42/42	0.78	0.23	169,175,185,185	0
56	MG	CA	3026	1/1	0.79	1.03	197,197,197,197	0
56	MG	CA	3145	1/1	0.79	0.38	75,75,75,75	0
56	MG	CA	3093	1/1	0.79	0.23	123,123,123,123	0
59	PUT	DA	3211	6/6	0.79	0.34	65,66,72,74	0
56	MG	DA	3171	1/1	0.79	0.57	82,82,82,82	0
56	MG	DA	3173	1/1	0.79	0.56	81,81,81,81	0
56	MG	CA	3082	1/1	0.79	0.45	160,160,160,160	0
56	MG	CA	3128	1/1	0.79	0.42	87,87,87,87	0
62	PEG	DP	201	7/7	0.79	0.53	94,94,99,100	0
58	MPD	DA	3206	8/8	0.79	0.51	89,93,94,94	0
56	MG	CA	3063	1/1	0.79	0.24	207,207,207,207	0
56	MG	CA	3069	1/1	0.80	0.21	115,115,115,115	0
62	PEG	DA	3200	7/7	0.80	0.51	55,58,65,65	0
56	MG	CA	3107	1/1	0.80	0.72	106,106,106,106	0
58	MPD	DE	301	8/8	0.80	0.61	102,104,107,109	0
56	MG	CA	3065	1/1	0.80	0.25	122,122,122,122	0
56	MG	DA	3143	1/1	0.80	0.46	95,95,95,95	0
56	MG	BA	1631	1/1	0.80	0.07	71,71,71,71	0
56	MG	CA	3044	1/1	0.81	0.18	84,84,84,84	0
56	MG	CA	3057	1/1	0.81	0.16	132,132,132,132	0
56	MG	AA	1625	1/1	0.81	0.30	78,78,78,78	0
56	MG	CA	3083	1/1	0.81	0.34	241,241,241,241	0
56	MG	CA	3009	1/1	0.81	0.16	248,248,248,248	0
56	MG	CA	3147	1/1	0.81	0.40	91,91,91,91	1
57	PG4	BA	1642	13/13	0.81	0.42	96,102,107,107	0
56	MG	BA	1603	1/1	0.81	0.70	261,261,261,261	0
56	MG	AA	1655	1/1	0.81	0.16	115,115,115,115	0
59	PUT	DA	3189	6/6	0.81	0.38	47,48,49,49	0
56	MG	AA	1644	1/1	0.82	0.14	94,94,94,94	0
56	MG	DA	3153	1/1	0.82	0.33	100,100,100,100	0
56	MG	CA	3119	1/1	0.82	0.72	134,134,134,134	0
59	PUT	DA	3195	6/6	0.82	0.54	51,53,62,65	0
59	PUT	DA	3204	6/6	0.82	0.43	66,66,70,71	0
58	MPD	DK	201	8/8	0.82	0.27	93,94,95,95	0
56	MG	CA	3008	1/1	0.82	0.10	179,179,179,179	0
56	MG	BA	1618	1/1	0.82	0.19	106,106,106,106	0
61	ZN	C5	101	1/1	0.82	0.06	148,148,148,148	0
56	MG	BA	1622	1/1	0.82	0.12	95,95,95,95	0
56	MG	CA	3023	1/1	0.82	0.14	150,150,150,150	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	CA	3112	1/1	0.82	0.33	110,110,110,110	0
56	MG	CA	3067	1/1	0.82	0.44	289,289,289,289	0
56	MG	DA	3133	1/1	0.83	0.41	78,78,78,78	0
56	MG	DA	3181	1/1	0.83	0.70	91,91,91,91	0
56	MG	CA	3155	1/1	0.83	0.31	204,204,204,204	0
56	MG	CA	3066	1/1	0.83	0.14	125,125,125,125	0
56	MG	CA	3048	1/1	0.83	0.17	107,107,107,107	0
57	PG4	DQ	202	13/13	0.83	0.30	64,66,71,72	0
56	MG	AA	1659	1/1	0.83	0.09	97,97,97,97	0
56	MG	DA	3123	1/1	0.83	0.51	77,77,77,77	0
56	MG	BA	1627	1/1	0.83	0.78	129,129,129,129	0
59	PUT	DA	3212	6/6	0.83	0.45	55,57,64,66	0
56	MG	AA	1654	1/1	0.83	0.49	252,252,252,252	0
58	MPD	DN	201	8/8	0.83	0.41	87,89,92,93	0
56	MG	DA	3176	1/1	0.83	0.32	93,93,93,93	0
56	MG	CA	3072	1/1	0.83	0.88	272,272,272,272	0
56	MG	CA	3022	1/1	0.83	0.70	188,188,188,188	0
56	MG	DA	3151	1/1	0.84	0.10	58,58,58,58	0
56	MG	DA	3124	1/1	0.84	0.38	114,114,114,114	0
63	EDO	DA	3194	4/4	0.84	0.30	51,56,59,60	0
56	MG	BA	1612	1/1	0.84	0.26	137,137,137,137	0
56	MG	AA	1640	1/1	0.84	0.13	62,62,62,62	0
56	MG	DA	3172	1/1	0.84	0.37	89,89,89,89	0
64	PGE	DS	201	10/10	0.84	0.37	56,66,68,69	0
56	MG	CA	3059	1/1	0.84	0.36	147,147,147,147	0
56	MG	DA	3112	1/1	0.84	0.44	293,293,293,293	0
66	1PE	DA	3202	16/16	0.84	0.37	60,63,65,65	0
57	PG4	DR	202	13/13	0.84	0.46	61,63,75,75	0
67	ACY	DA	3201	4/4	0.84	0.33	60,64,64,66	0
56	MG	BA	1610	1/1	0.84	0.08	109,109,109,109	0
63	EDO	D1	101	4/4	0.84	0.34	67,67,68,68	0
62	PEG	AL	201	7/7	0.85	0.39	74,78,85,85	0
56	MG	AA	1657	1/1	0.85	0.47	162,162,162,162	0
56	MG	DA	3169	1/1	0.85	0.33	73,73,73,73	0
56	MG	CA	3080	1/1	0.85	0.35	186,186,186,186	0
56	MG	BA	1601	1/1	0.85	0.17	95,95,95,95	0
56	MG	CA	3058	1/1	0.85	0.41	135,135,135,135	0
58	MPD	DA	3190	8/8	0.85	0.34	91,92,93,94	0
56	MG	AA	1639	1/1	0.85	0.09	132,132,132,132	0
56	MG	DD	303	1/1	0.85	0.36	66,66,66,66	0
56	MG	CA	3125	1/1	0.85	0.27	141,141,141,141	0
56	MG	AA	1665	1/1	0.85	0.43	168,168,168,168	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	DA	3007	1/1	0.85	0.12	112,112,112,112	0
56	MG	DA	3063	1/1	0.85	0.13	222,222,222,222	0
63	EDO	DA	3214	4/4	0.85	0.31	77,78,79,79	0
59	PUT	DA	3184	6/6	0.85	0.37	42,48,50,51	0
56	MG	DA	3065	1/1	0.85	0.16	71,71,71,71	0
56	MG	CA	3050	1/1	0.85	0.13	91,91,91,91	0
64	PGE	DA	3213	10/10	0.85	0.48	84,86,90,90	0
56	MG	CA	3051	1/1	0.85	0.12	109,109,109,109	0
65	SPD	DA	3183	10/10	0.85	0.44	57,63,66,66	0
56	MG	CA	3098	1/1	0.85	0.13	110,110,110,110	0
56	MG	CB	202	1/1	0.85	0.12	139,139,139,139	0
57	PG4	DA	3193	13/13	0.85	0.87	63,65,76,77	0
59	PUT	DA	3220	6/6	0.85	0.36	92,92,94,95	0
56	MG	CA	3040	1/1	0.85	0.09	126,126,126,126	0
56	MG	DA	3128	1/1	0.85	0.48	78,78,78,78	0
56	MG	CA	3086	1/1	0.86	0.16	97,97,97,97	0
56	MG	DA	3165	1/1	0.86	0.45	69,69,69,69	0
56	MG	DA	3148	1/1	0.86	0.24	115,115,115,115	0
62	PEG	DA	3226	7/7	0.86	0.33	58,59,65,67	0
56	MG	CA	3064	1/1	0.86	0.57	267,267,267,267	0
56	MG	BA	1607	1/1	0.86	0.38	162,162,162,162	0
56	MG	CA	3012	1/1	0.86	0.27	130,130,130,130	0
56	MG	CA	3094	1/1	0.86	0.26	159,159,159,159	0
56	MG	CA	3096	1/1	0.86	0.13	116,116,116,116	0
56	MG	AA	1609	1/1	0.86	0.38	107,107,107,107	0
56	MG	DA	3174	1/1	0.86	0.30	78,78,78,78	0
56	MG	CA	3053	1/1	0.87	0.22	108,108,108,108	0
56	MG	CA	3062	1/1	0.87	0.19	237,237,237,237	0
63	EDO	DA	3207	4/4	0.87	0.26	58,60,62,63	0
56	MG	CA	3088	1/1	0.87	0.10	88,88,88,88	0
56	MG	CA	3143	1/1	0.87	0.50	107,107,107,107	0
56	MG	DA	3154	1/1	0.87	0.46	59,59,59,59	0
57	PG4	DS	202	13/13	0.87	0.34	43,51,59,61	0
64	PGE	DD	301	10/10	0.87	0.36	63,67,72,73	0
56	MG	CA	3030	1/1	0.87	0.15	124,124,124,124	0
64	PGE	DU	101	10/10	0.87	0.50	64,72,83,83	0
56	MG	CA	3021	1/1	0.87	1.07	278,278,278,278	0
64	PGE	DA	3216	10/10	0.87	0.39	62,64,65,65	0
62	PEG	DA	3199	7/7	0.87	0.44	60,64,69,70	0
56	MG	DA	3175	1/1	0.87	0.50	75,75,75,75	0
56	MG	CA	3004	1/1	0.87	0.23	223,223,223,223	0
56	MG	AA	1664	1/1	0.87	0.35	186,186,186,186	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	CA	3017	1/1	0.87	0.10	106,106,106,106	0
56	MG	AA	1601	1/1	0.87	1.43	104,104,104,104	0
56	MG	CA	3020	1/1	0.87	0.11	103,103,103,103	0
63	EDO	DA	3001	4/4	0.87	0.37	72,73,75,77	0
56	MG	DA	3095	1/1	0.88	0.17	33,33,33,33	0
56	MG	CA	3052	1/1	0.88	0.13	97,97,97,97	0
56	MG	AA	1649	1/1	0.88	0.12	77,77,77,77	0
58	MPD	DA	3209	8/8	0.88	0.31	68,70,70,71	0
56	MG	BA	1636	1/1	0.88	0.64	172,172,172,172	0
56	MG	CA	3036	1/1	0.88	0.33	203,203,203,203	0
56	MG	AA	1660	1/1	0.88	0.30	286,286,286,286	0
63	EDO	DA	3003	4/4	0.88	0.52	64,64,66,67	0
56	MG	BA	1602	1/1	0.88	0.07	100,100,100,100	0
56	MG	DA	3129	1/1	0.88	1.13	60,60,60,60	0
62	PEG	DL	201	7/7	0.88	0.28	65,69,76,78	0
56	MG	AA	1623	1/1	0.88	0.36	85,85,85,85	0
56	MG	CA	3152	1/1	0.88	0.46	215,215,215,215	0
56	MG	CA	3153	1/1	0.88	0.22	90,90,90,90	0
56	MG	DA	3045	1/1	0.89	0.09	85,85,85,85	0
56	MG	AA	1610	1/1	0.89	0.40	99,99,99,99	0
56	MG	BA	1633	1/1	0.89	0.28	235,235,235,235	0
56	MG	DA	3162	1/1	0.89	0.25	64,64,64,64	0
66	1PE	DA	3185	16/16	0.89	0.31	44,53,71,72	0
56	MG	CA	3019	1/1	0.89	0.10	79,79,79,79	0
56	MG	CA	3035	1/1	0.89	0.26	158,158,158,158	0
56	MG	DA	3156	1/1	0.89	0.34	74,74,74,74	0
59	PUT	DA	3221	6/6	0.89	0.33	44,48,50,50	0
58	MPD	DA	3192	8/8	0.89	0.59	79,79,82,83	0
56	MG	CA	3150	1/1	0.90	0.50	82,82,82,82	0
56	MG	DA	3120	1/1	0.90	0.36	55,55,55,55	0
56	MG	DA	3149	1/1	0.90	0.28	77,77,77,77	0
56	MG	AA	1607	1/1	0.90	0.61	92,92,92,92	0
56	MG	AA	1656	1/1	0.90	0.16	149,149,149,149	0
56	MG	AA	1647	1/1	0.90	0.13	202,202,202,202	0
56	MG	CA	3029	1/1	0.90	0.36	177,177,177,177	0
56	MG	AA	1619	1/1	0.90	0.27	92,92,92,92	0
56	MG	AA	1635	1/1	0.90	0.10	100,100,100,100	0
56	MG	CA	3127	1/1	0.90	0.11	85,85,85,85	0
56	MG	CA	3101	1/1	0.90	0.11	149,149,149,149	0
56	MG	CA	3144	1/1	0.90	0.13	83,83,83,83	0
56	MG	BA	1634	1/1	0.90	0.07	116,116,116,116	0
56	MG	CA	3116	1/1	0.90	0.80	89,89,89,89	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	DA	3166	1/1	0.90	0.86	90,90,90,90	0
65	SPD	DA	3223	10/10	0.90	0.27	40,44,54,55	0
56	MG	CA	3117	1/1	0.90	0.77	109,109,109,109	0
56	MG	DA	3142	1/1	0.90	0.28	79,79,79,79	0
56	MG	CA	3045	1/1	0.90	0.07	93,93,93,93	0
63	EDO	DB	211	4/4	0.90	0.24	73,73,74,75	0
58	MPD	AA	1676	8/8	0.90	0.57	97,100,100,102	0
56	MG	BA	1617	1/1	0.90	0.14	126,126,126,126	0
56	MG	BA	1644	1/1	0.91	0.12	97,97,97,97	0
56	MG	AA	1634	1/1	0.91	0.19	108,108,108,108	0
56	MG	AA	1630	1/1	0.91	0.15	134,134,134,134	0
56	MG	CA	3095	1/1	0.91	0.18	81,81,81,81	0
56	MG	BA	1632	1/1	0.91	0.12	72,72,72,72	0
56	MG	CA	3136	1/1	0.91	0.34	105,105,105,105	0
56	MG	CA	3084	1/1	0.91	0.34	208,208,208,208	0
56	MG	DA	3103	1/1	0.91	0.12	44,44,44,44	0
56	MG	AA	1636	1/1	0.91	0.28	97,97,97,97	0
63	EDO	DA	3197	4/4	0.91	0.26	68,68,69,69	0
56	MG	BA	1640	1/1	0.91	0.82	156,156,156,156	0
56	MG	CA	3100	1/1	0.91	0.31	110,110,110,110	0
56	MG	CA	3089	1/1	0.91	0.22	95,95,95,95	0
56	MG	CA	3103	1/1	0.91	0.15	120,120,120,120	0
56	MG	BA	1609	1/1	0.91	0.16	194,194,194,194	0
60	T1C	AA	1677	42/42	0.92	0.25	89,96,109,110	0
56	MG	DR	201	1/1	0.92	0.60	44,44,44,44	0
61	ZN	AB	301	1/1	0.92	0.30	209,209,209,209	0
64	PGE	DA	3186	10/10	0.92	0.22	39,46,49,50	0
56	MG	DR	203	1/1	0.92	0.42	111,111,111,111	0
59	PUT	DA	3002	6/6	0.92	0.23	45,52,54,55	0
56	MG	BA	1635	1/1	0.92	0.10	111,111,111,111	0
56	MG	CA	3011	1/1	0.92	0.28	117,117,117,117	0
56	MG	DA	3122	1/1	0.92	0.32	80,80,80,80	0
56	MG	BA	1628	1/1	0.92	0.18	111,111,111,111	0
63	EDO	DA	3198	4/4	0.92	0.35	56,57,58,59	0
56	MG	DA	3016	1/1	0.92	0.11	44,44,44,44	0
58	MPD	AA	1671	8/8	0.92	0.53	101,103,104,106	0
56	MG	CA	3118	1/1	0.92	0.45	90,90,90,90	0
56	MG	CA	3043	1/1	0.92	0.14	101,101,101,101	0
56	MG	BA	1645	1/1	0.92	0.05	98,98,98,98	0
56	MG	CA	3042	1/1	0.93	0.12	91,91,91,91	0
56	MG	DA	3094	1/1	0.93	0.21	35,35,35,35	0
56	MG	CA	3102	1/1	0.93	0.27	114,114,114,114	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	AA	1658	1/1	0.93	0.10	100,100,100,100	0
56	MG	CA	3015	1/1	0.93	0.25	83,83,83,83	0
56	MG	DA	3160	1/1	0.93	0.12	72,72,72,72	0
56	MG	DA	3118	1/1	0.93	0.34	76,76,76,76	0
56	MG	CA	3087	1/1	0.93	0.07	97,97,97,97	0
56	MG	AA	1669	1/1	0.93	0.41	118,118,118,118	0
56	MG	CA	3074	1/1	0.93	0.27	206,206,206,206	0
56	MG	DA	3038	1/1	0.93	0.22	29,29,29,29	0
56	MG	DA	3044	1/1	0.93	0.15	36,36,36,36	0
56	MG	CA	3081	1/1	0.93	0.17	134,134,134,134	0
56	MG	DA	3053	1/1	0.93	0.12	78,78,78,78	0
56	MG	AA	1651	1/1	0.93	0.13	70,70,70,70	0
56	MG	CA	3041	1/1	0.94	0.19	71,71,71,71	0
56	MG	DA	3119	1/1	0.94	0.11	63,63,63,63	0
59	PUT	DA	3188	6/6	0.94	0.22	32,35,40,41	0
56	MG	CA	3138	1/1	0.94	0.16	103,103,103,103	0
56	MG	DA	3121	1/1	0.94	0.37	91,91,91,91	0
56	MG	AA	1643	1/1	0.94	0.14	78,78,78,78	0
56	MG	BA	1615	1/1	0.94	0.08	76,76,76,76	0
56	MG	DA	3005	1/1	0.94	0.10	81,81,81,81	0
56	MG	DA	3164	1/1	0.94	0.32	72,72,72,72	0
56	MG	DA	3080	1/1	0.94	0.10	109,109,109,109	0
56	MG	DA	3229	1/1	0.94	0.13	55,55,55,55	0
65	SPD	DA	3187	10/10	0.94	0.24	38,40,48,50	0
59	PUT	DA	3222	6/6	0.94	0.24	50,54,55,55	0
56	MG	DA	3084	1/1	0.94	0.08	57,57,57,57	0
56	MG	CA	3091	1/1	0.94	0.10	96,96,96,96	0
56	MG	AA	1633	1/1	0.94	0.29	101,101,101,101	0
56	MG	DA	3152	1/1	0.94	0.23	47,47,47,47	0
56	MG	DA	3021	1/1	0.94	0.07	48,48,48,48	0
56	MG	CA	3070	1/1	0.94	0.08	112,112,112,112	0
56	MG	DA	3132	1/1	0.94	0.52	77,77,77,77	0
56	MG	DB	208	1/1	0.95	0.26	64,64,64,64	0
56	MG	DA	3081	1/1	0.95	0.17	94,94,94,94	0
56	MG	DA	3082	1/1	0.95	0.08	55,55,55,55	0
56	MG	CA	3114	1/1	0.95	0.47	62,62,62,62	0
56	MG	AA	1653	1/1	0.95	0.04	75,75,75,75	0
56	MG	DA	3009	1/1	0.95	0.12	102,102,102,102	0
56	MG	DA	3097	1/1	0.95	0.14	45,45,45,45	0
56	MG	DA	3135	1/1	0.95	0.27	72,72,72,72	0
56	MG	BA	1613	1/1	0.95	0.18	78,78,78,78	0
56	MG	DA	3108	1/1	0.95	0.18	36,36,36,36	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	DA	3139	1/1	0.95	0.40	64,64,64,64	1
56	MG	DA	3140	1/1	0.95	0.19	57,57,57,57	0
56	MG	BA	1619	1/1	0.95	0.19	107,107,107,107	0
61	ZN	D5	101	1/1	0.95	0.15	60,60,60,60	0
56	MG	BA	1621	1/1	0.95	0.19	42,42,42,42	0
56	MG	DA	3144	1/1	0.95	0.37	65,65,65,65	0
56	MG	AA	1678	1/1	0.95	0.16	74,74,74,74	0
56	MG	DA	3146	1/1	0.95	0.15	72,72,72,72	0
56	MG	DB	201	1/1	0.95	0.14	64,64,64,64	0
56	MG	DB	205	1/1	0.95	0.17	49,49,49,49	0
56	MG	AA	1650	1/1	0.95	0.09	87,87,87,87	0
56	MG	DA	3177	1/1	0.95	0.18	68,68,68,68	0
56	MG	DA	3150	1/1	0.95	0.18	59,59,59,59	0
56	MG	CA	3085	1/1	0.95	0.12	89,89,89,89	0
67	ACY	DA	3191	4/4	0.95	0.27	56,57,58,59	0
56	MG	DA	3069	1/1	0.95	0.17	44,44,44,44	0
56	MG	DA	3070	1/1	0.95	0.15	61,61,61,61	0
56	MG	DA	3076	1/1	0.95	0.20	38,38,38,38	0
56	MG	DA	3127	1/1	0.95	0.43	62,62,62,62	0
56	MG	DA	3098	1/1	0.96	0.09	29,29,29,29	0
56	MG	DA	3099	1/1	0.96	0.13	78,78,78,78	0
56	MG	AA	1641	1/1	0.96	0.08	92,92,92,92	0
56	MG	DA	3137	1/1	0.96	0.26	47,47,47,47	0
56	MG	DA	3105	1/1	0.96	0.19	39,39,39,39	0
56	MG	DA	3049	1/1	0.96	0.17	33,33,33,33	0
56	MG	DA	3050	1/1	0.96	0.12	43,43,43,43	0
56	MG	DA	3115	1/1	0.96	0.15	49,49,49,49	0
56	MG	DA	3117	1/1	0.96	0.11	41,41,41,41	0
56	MG	DA	3006	1/1	0.96	0.11	68,68,68,68	0
56	MG	CA	3037	1/1	0.96	0.43	235,235,235,235	0
56	MG	DA	3008	1/1	0.96	0.05	82,82,82,82	0
56	MG	AA	1629	1/1	0.96	0.14	83,83,83,83	0
56	MG	DA	3013	1/1	0.96	0.13	71,71,71,71	0
56	MG	AA	1666	1/1	0.96	0.05	67,67,67,67	0
56	MG	DA	3020	1/1	0.96	0.32	33,33,33,33	0
56	MG	DM	201	1/1	0.96	0.06	62,62,62,62	0
56	MG	DA	3022	1/1	0.96	0.15	43,43,43,43	0
56	MG	DA	3029	1/1	0.96	0.14	61,61,61,61	0
56	MG	DA	3088	1/1	0.96	0.17	45,45,45,45	0
56	MG	DA	3090	1/1	0.96	0.18	26,26,26,26	0
56	MG	DA	3091	1/1	0.96	0.23	55,55,55,55	0
56	MG	DA	3227	1/1	0.96	0.14	45,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	CA	3073	1/1	0.96	0.28	260,260,260,260	0
56	MG	DA	3158	1/1	0.96	0.17	71,71,71,71	0
56	MG	DA	3043	1/1	0.96	0.08	31,31,31,31	0
56	MG	DB	209	1/1	0.96	0.49	80,80,80,80	0
56	MG	AA	1652	1/1	0.97	0.29	57,57,57,57	0
56	MG	DA	3046	1/1	0.97	0.09	47,47,47,47	0
56	MG	AA	1637	1/1	0.97	0.08	57,57,57,57	0
56	MG	BA	1616	1/1	0.97	0.18	149,149,149,149	0
56	MG	DB	202	1/1	0.97	0.13	29,29,29,29	0
56	MG	DA	3100	1/1	0.97	0.14	30,30,30,30	0
56	MG	DA	3102	1/1	0.97	0.14	56,56,56,56	0
56	MG	DB	203	1/1	0.97	0.05	39,39,39,39	0
56	MG	DA	3017	1/1	0.97	0.13	56,56,56,56	0
56	MG	DA	3018	1/1	0.97	0.25	29,29,29,29	0
56	MG	DA	3109	1/1	0.97	0.10	29,29,29,29	0
56	MG	BA	1605	1/1	0.97	0.09	125,125,125,125	0
56	MG	DA	3114	1/1	0.97	0.11	62,62,62,62	0
56	MG	DA	3073	1/1	0.97	0.15	47,47,47,47	0
56	MG	DA	3075	1/1	0.97	0.07	49,49,49,49	0
56	MG	CA	3046	1/1	0.97	0.14	143,143,143,143	0
56	MG	DA	3077	1/1	0.97	0.18	42,42,42,42	0
56	MG	DA	3078	1/1	0.97	0.10	38,38,38,38	0
56	MG	DA	3079	1/1	0.97	0.07	63,63,63,63	0
56	MG	AA	1667	1/1	0.97	0.12	49,49,49,49	0
56	MG	DA	3028	1/1	0.97	0.14	38,38,38,38	0
56	MG	AA	1638	1/1	0.97	0.09	103,103,103,103	0
56	MG	DA	3083	1/1	0.97	0.09	69,69,69,69	0
56	MG	DA	3031	1/1	0.97	0.21	46,46,46,46	0
56	MG	DD	302	1/1	0.97	0.13	48,48,48,48	0
56	MG	BA	1620	1/1	0.97	0.17	97,97,97,97	0
56	MG	CA	3024	1/1	0.97	0.17	141,141,141,141	0
56	MG	DA	3230	1/1	0.97	0.35	45,45,45,45	0
56	MG	AA	1645	1/1	0.98	0.12	61,61,61,61	0
56	MG	DA	3039	1/1	0.98	0.12	20,20,20,20	0
56	MG	DA	3040	1/1	0.98	0.14	26,26,26,26	0
56	MG	DA	3041	1/1	0.98	0.09	58,58,58,58	0
56	MG	AA	1662	1/1	0.98	0.22	110,110,110,110	0
56	MG	AA	1646	1/1	0.98	0.08	65,65,65,65	0
58	MPD	DS	203	8/8	0.98	0.21	37,40,44,47	0
56	MG	AA	1631	1/1	0.98	0.06	56,56,56,56	0
56	MG	DA	3010	1/1	0.98	0.14	34,34,34,34	0
56	MG	DA	3085	1/1	0.98	0.14	41,41,41,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	DA	3086	1/1	0.98	0.12	39,39,39,39	0
56	MG	DA	3023	1/1	0.98	0.21	34,34,34,34	0
56	MG	DA	3089	1/1	0.98	0.08	36,36,36,36	0
56	MG	DA	3026	1/1	0.98	0.10	40,40,40,40	0
56	MG	DA	3027	1/1	0.98	0.15	71,71,71,71	0
56	MG	DA	3093	1/1	0.98	0.14	36,36,36,36	0
56	MG	DA	3054	1/1	0.98	0.09	57,57,57,57	0
56	MG	DA	3055	1/1	0.98	0.08	49,49,49,49	0
56	MG	DA	3057	1/1	0.98	0.23	57,57,57,57	0
56	MG	DA	3062	1/1	0.98	0.15	37,37,37,37	0
56	MG	CA	3025	1/1	0.98	0.28	105,105,105,105	0
56	MG	DA	3015	1/1	0.98	0.18	18,18,18,18	0
56	MG	DA	3101	1/1	0.98	0.22	30,30,30,30	0
56	MG	DA	3141	1/1	0.98	0.22	66,66,66,66	0
56	MG	DA	3066	1/1	0.98	0.19	29,29,29,29	0
56	MG	DA	3067	1/1	0.98	0.19	55,55,55,55	0
56	MG	DA	3068	1/1	0.98	0.11	62,62,62,62	0
56	MG	DA	3106	1/1	0.98	0.20	31,31,31,31	0
56	MG	DA	3107	1/1	0.98	0.17	47,47,47,47	0
56	MG	DA	3228	1/1	0.98	0.09	53,53,53,53	0
56	MG	BA	1611	1/1	0.98	0.11	66,66,66,66	0
56	MG	DA	3032	1/1	0.98	0.23	42,42,42,42	0
56	MG	DA	3111	1/1	0.98	0.15	32,32,32,32	0
56	MG	DA	3071	1/1	0.98	0.06	91,91,91,91	0
56	MG	DA	3034	1/1	0.98	0.17	28,28,28,28	0
56	MG	DA	3074	1/1	0.98	0.15	33,33,33,33	0
56	MG	DA	3116	1/1	0.98	0.14	28,28,28,28	0
56	MG	DA	3036	1/1	0.98	0.16	34,34,34,34	0
56	MG	DA	3037	1/1	0.98	0.23	31,31,31,31	0
56	MG	DA	3024	1/1	0.99	0.20	32,32,32,32	0
56	MG	DA	3104	1/1	0.99	0.09	42,42,42,42	0
56	MG	DA	3033	1/1	0.99	0.19	26,26,26,26	0
56	MG	DA	3064	1/1	0.99	0.08	59,59,59,59	0
56	MG	DA	3025	1/1	0.99	0.23	25,25,25,25	0
56	MG	DA	3019	1/1	0.99	0.10	43,43,43,43	0
56	MG	DA	3047	1/1	0.99	0.19	27,27,27,27	0
56	MG	DA	3110	1/1	0.99	0.19	19,19,19,19	0
56	MG	DA	3087	1/1	0.99	0.16	48,48,48,48	0
56	MG	DA	3048	1/1	0.99	0.13	42,42,42,42	0
56	MG	AA	1668	1/1	0.99	0.11	54,54,54,54	0
56	MG	AA	1648	1/1	0.99	0.09	76,76,76,76	0
56	MG	DA	3052	1/1	0.99	0.15	36,36,36,36	0

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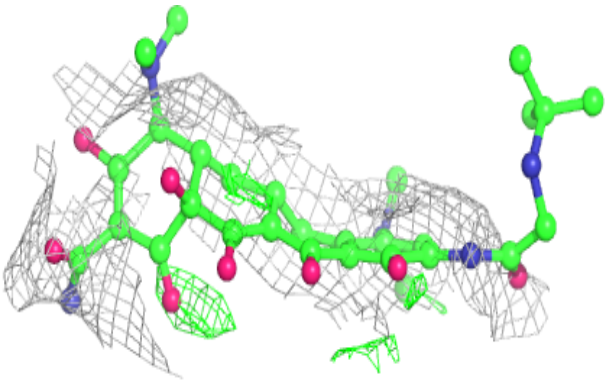
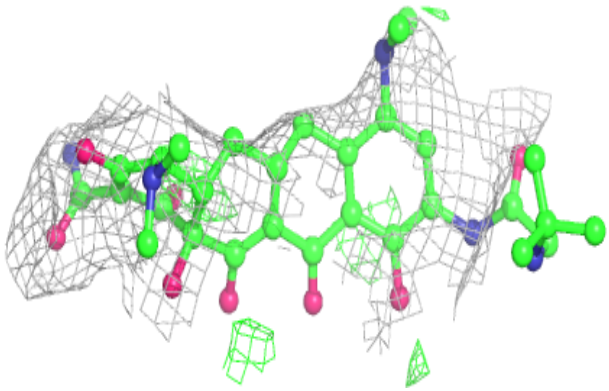
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	DA	3092	1/1	0.99	0.17	31,31,31,31	0
56	MG	DA	3072	1/1	0.99	0.09	47,47,47,47	0
56	MG	DB	204	1/1	0.99	0.15	56,56,56,56	0
56	MG	DA	3030	1/1	0.99	0.14	25,25,25,25	0
56	MG	DA	3096	1/1	0.99	0.11	61,61,61,61	0
56	MG	DA	3014	1/1	0.99	0.25	19,19,19,19	0
56	MG	DA	3056	1/1	0.99	0.17	22,22,22,22	0
56	MG	DA	3042	1/1	0.99	0.16	20,20,20,20	0
56	MG	DA	3058	1/1	0.99	0.08	31,31,31,31	0
56	MG	DA	3060	1/1	0.99	0.11	16,16,16,16	0
56	MG	DA	3061	1/1	0.99	0.15	19,19,19,19	0
56	MG	DA	3051	1/1	1.00	0.14	17,17,17,17	0
56	MG	DA	3011	1/1	1.00	0.17	28,28,28,28	0
56	MG	DA	3012	1/1	1.00	0.09	29,29,29,29	0
56	MG	DA	3113	1/1	1.00	0.22	18,18,18,18	0
56	MG	DA	3035	1/1	1.00	0.18	24,24,24,24	0
56	MG	DA	3059	1/1	1.00	0.15	37,37,37,37	0

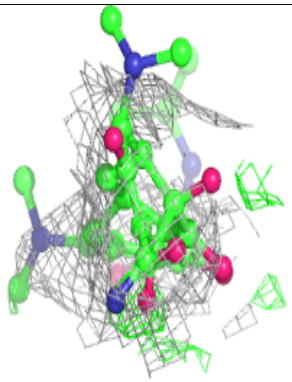
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around T1C BA 1643:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

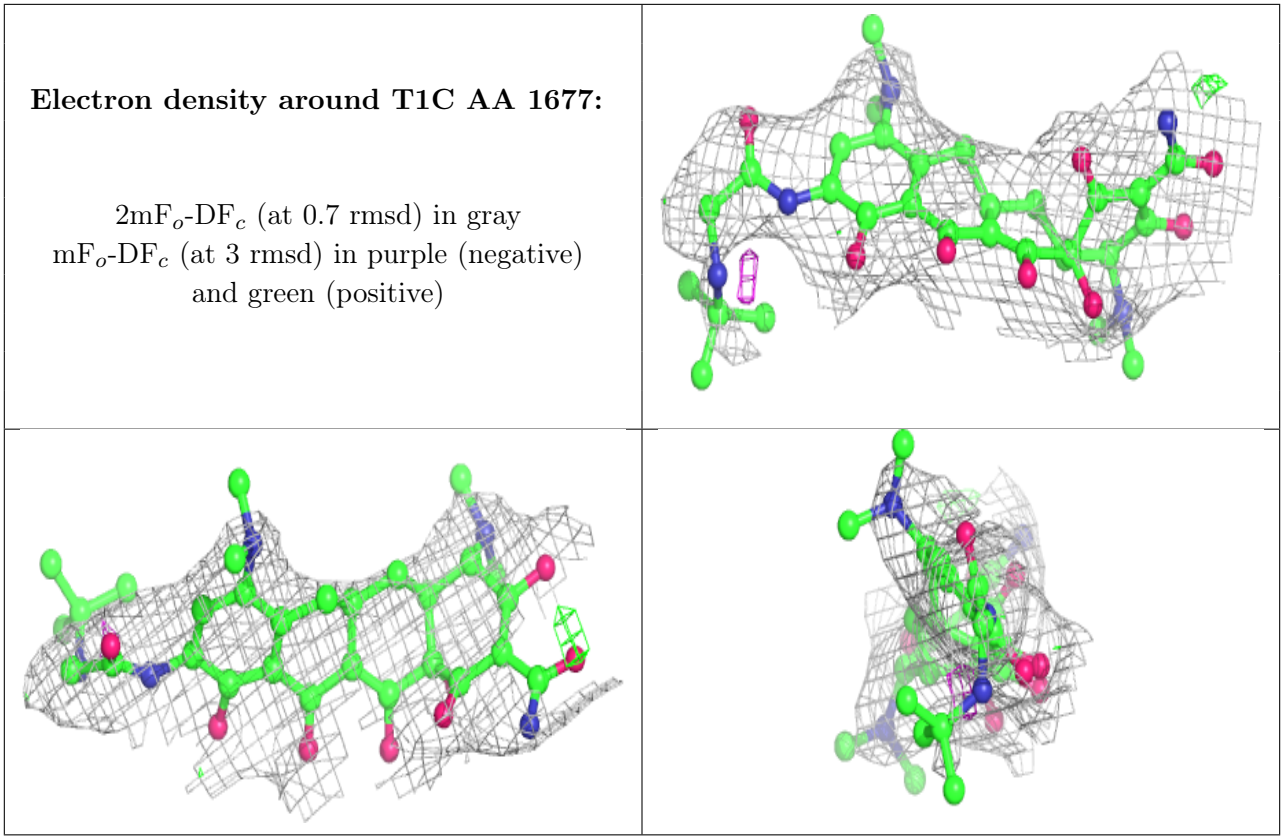






Electron density around T1C AA 1677:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



6.5 Other polymers (i)

There are no such residues in this entry.