



# Full wwPDB X-ray Structure Validation Report ⓘ

Apr 28, 2024 – 02:28 am BST

PDB ID : 5I4L  
Title : Crystal structure of Amicoumacin A bound to the yeast 80S ribosome  
Authors : Prokhorova, I.V.; Yusupova, G.; Yusupov, M.  
Deposited on : 2016-02-12  
Resolution : 3.10 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](mailto: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 ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	<b>FAILED</b>
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

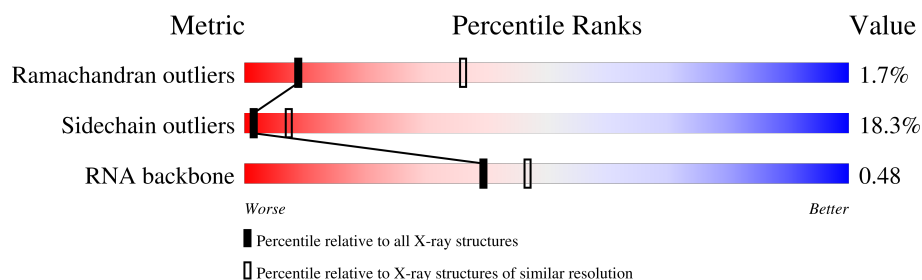
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.10 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))
Ramachandran outliers	138981	1141 (3.10-3.10)
Sidechain outliers	138945	1141 (3.10-3.10)
RNA backbone	3102	1116 (3.40-2.80)











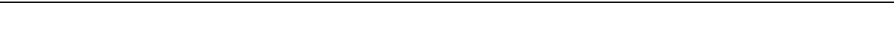

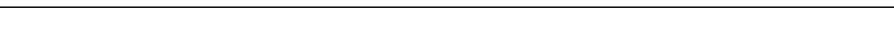
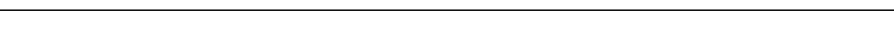











The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria 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  $\leq 5\%$ .

Note EDS failed to run properly.

Mol	Chain	Length	Quality of chain
1	2	1800	70% 27% ..
1	6	1800	72% 26% .
2	S0	206	83% 16%
2	s0	206	80% 18% .
3	S1	216	79% 19% ..
3	s1	216	81% 17% .
4	S2	217	82% 17% .
4	s2	217	81% 18%


























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Mol	Chain	Length	Quality of chain
5	S3	223	 83% 17%
5	s3	223	 84% 16%
6	S4	260	 83% 16% .
6	s4	260	 84% 16%
7	S5	206	 82% 17% .
7	s5	206	 81% 19%
8	S6	226	 88% 12%
8	s6	226	 81% 15% .
9	S7	186	 76% 20% . .
9	s7	186	 78% 21% .
10	S8	200	 81% 12% . 6%
10	s8	200	 79% 14% . 6%
11	S9	185	 82% 17% .
11	s9	185	 82% 17% .
12	C0	98	 80% 17% . .
12	c0	98	 74% 19% . .
13	C1	156	 83% 17% .
13	c1	156	 74% 19% . 6%
14	C2	124	 77% 21% .
14	c2	124	 78% 19% .
15	C3	150	 83% 17% .
15	c3	150	 80% 19% .
16	C4	128	 84% 15% . .
16	c4	128	 81% 18% .
17	C5	142	 73% 14% . 13%












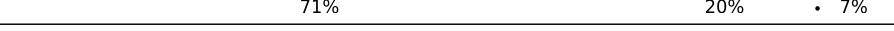







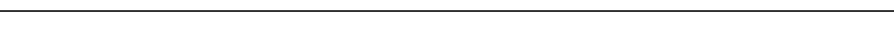

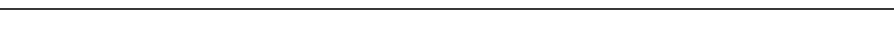
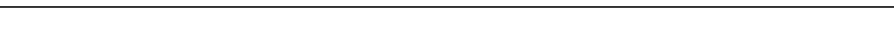


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Mol	Chain	Length	Quality of chain
17	c5	142	 77% 17% 5%
18	C6	142	 77% 20% ..
18	c6	142	 84% 15% .
19	C7	136	 71% 15% .. 12%
19	c7	136	 70% 15% . 14%
20	C8	145	 82% 16% .
20	c8	145	 81% 19% .
21	C9	143	 84% 16%
21	c9	143	 86% 13% .
22	D0	110	 78% 18% ..
22	d0	110	 75% 22% .
23	D1	87	 86% 14%
23	d1	87	 79% 21%
24	D2	129	 81% 16% .
24	d2	129	 88% 10% .
25	D3	144	 81% 18% .
25	d3	144	 85% 15%
26	D4	134	 81% 16% .
26	d4	134	 88% 10% ..
27	D5	70	 74% 24% .
27	d5	70	 83% 16% .
28	D6	97	 76% 19% ..
28	d6	97	 80% 16% .
29	D7	81	 85% 15%
29	d7	81	 84% 16%


























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Mol	Chain	Length	Quality of chain
30	D8	63	 78% 22%
30	d8	63	 81% 19%
31	D9	53	 74% 25% .
31	d9	53	 75% 25%
32	E0	62	 81% 16% .
32	e0	62	 79% 21%
33	E1	76	 68% 17% 8% 7%
33	e1	76	 68% 22% 8% .
34	SR	318	 90% 10%
34	sR	318	 90% 10%
35	SM	176	 75% 15% . 10%
36	1	3396	 71% 20% . 7%
36	5	3396	 71% 20% . 7%
37	3	121	 87% 13%
37	7	121	 84% 15% .
38	4	158	 77% 22% .
38	8	158	 78% 20% .
39	L2	252	 88% 12%
39	l2	252	 83% 17%
40	L3	386	 82% 18%
40	l3	386	 85% 15%
41	L4	361	 85% 14%
41	l4	361	 86% 13% .
42	L5	296	 81% 18% .
42	l5	296	 85% 13% ..


























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Mol	Chain	Length	Quality of chain
43	L6	176	
43	l6	176	
44	L7	223	
44	l7	223	
45	L8	233	
46	L9	191	
46	l9	191	
47	M0	221	
47	m0	221	
48	M1	169	
48	m1	169	
49	M3	194	
49	m3	194	
50	M4	137	
50	m4	137	
51	M5	203	
51	m5	203	
52	M6	197	
52	m6	197	
53	M7	183	
53	m7	183	
54	M8	185	
54	m8	185	
55	M9	188	
55	m9	188	












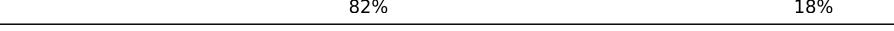







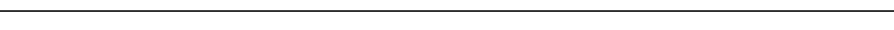

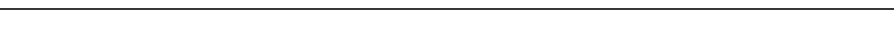
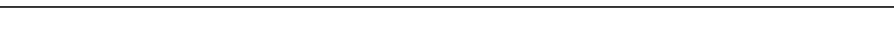


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Mol	Chain	Length	Quality of chain
56	N0	172	 75% 23%
56	n0	172	 79% 21%
57	N1	159	 79% 20%
57	n1	159	 84% 16%
58	N2	100	 82% 18%
58	n2	100	 79% 19%
59	N3	136	 85% 15%
59	n3	136	 88% 12%
60	N4	98	 88% 11%
61	N5	121	 79% 20%
61	n5	121	 83% 16%
62	N6	126	 83% 17%
62	n6	126	 77% 23%
63	N7	135	 84% 16%
63	n7	135	 80% 19%
64	N8	148	 83% 16%
64	n8	148	 80% 19%
65	N9	58	 84% 16%
65	n9	58	 84% 14%
66	O0	100	 81% 16%
66	o0	100	 86% 13%
67	O1	109	 85% 15%
67	o1	109	 81% 19%
68	O2	127	 89% 11%
68	o2	127	 82% 18%

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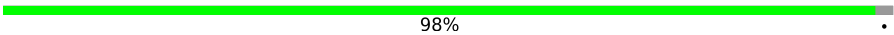
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Mol	Chain	Length	Quality of chain
69	O3	106	 89% 11%
69	o3	106	 91% 9%
70	O4	112	 88% 12% .
70	o4	112	 89% 11%
71	O5	119	 82% 18%
71	o5	119	 85% 15%
72	O6	99	 76% 24%
72	o6	99	 74% 25% .
73	O7	87	 90% 10%
73	o7	87	 84% 16%
74	O8	77	 73% 27%
74	o8	77	 82% 18%
75	O9	50	 90% 10%
75	o9	50	 86% 14%
76	Q0	52	 87% 13%
76	q0	52	 81% 19%
77	Q1	25	 80% 20%
77	q1	25	 72% 28%
78	Q2	105	 83% 16% .
78	q2	105	 81% 19%
79	Q3	91	 85% 15%
79	q3	91	 81% 18% .
80	sM	159	 56% 8% . 35%
81	l8	231	 84% 16%
82	m2	155	 94% . .

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Mol	Chain	Length	Quality of chain
83	n4	135	 86% 13% .
84	p0	312	 38% 8% 54%
85	p1	47	 100%
85	p2	47	 98% .

## 2 Entry composition

There are 89 unique types of molecules in this entry. The entry contains 410475 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 18S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	2	1781	Total	C	N	O	P	0	0	0
			37948	16965	6715	12487	1781			
1	6	1795	Total	C	N	O	P	0	0	0
			38238	17095	6758	12590	1795			

- Molecule 2 is a protein called 40S ribosomal protein S0-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	S0	206	Total	C	N	O	S	0	0	0
			1577	1014	278	283	2			
2	s0	206	Total	C	N	O	S	0	0	0
			1583	1017	281	283	2			

- Molecule 3 is a protein called 40S ribosomal protein S1-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	S1	214	Total	C	N	O	S	0	0	0
			1709	1084	310	311	4			
3	s1	216	Total	C	N	O	S	0	0	0
			1722	1091	312	315	4			

- Molecule 4 is a protein called 40S ribosomal protein S2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	S2	217	Total	C	N	O	S	0	0	0
			1635	1047	289	297	2			
4	s2	217	Total	C	N	O	S	0	0	0
			1635	1047	289	297	2			

- Molecule 5 is a protein called 40S ribosomal protein S3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	S3	223	Total	C	N	O	S	0	0	0
			1734	1101	313	314	6			
5	s3	223	Total	C	N	O	S	0	0	0
			1734	1101	313	314	6			

- Molecule 6 is a protein called 40S ribosomal protein S4-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	S4	260	Total	C	N	O	S	0	0	0
			2068	1316	389	360	3			
6	s4	260	Total	C	N	O	S	0	0	0
			2068	1316	389	360	3			

- Molecule 7 is a protein called 40S ribosomal protein S5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	S5	206	Total	C	N	O	S	0	0	0
			1609	1007	300	299	3			
7	s5	206	Total	C	N	O	S	0	0	0
			1609	1007	300	299	3			

- Molecule 8 is a protein called 40S ribosomal protein S6-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	S6	226	Total	C	N	O	S	0	0	0
			1799	1129	346	321	3			
8	s6	218	Total	C	N	O	S	0	0	0
			1755	1102	337	313	3			

- Molecule 9 is a protein called 40S ribosomal protein S7-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	S7	184	Total	C	N	O		0	0	0
			1481	951	265	265				
9	s7	186	Total	C	N	O		0	0	0
			1491	957	267	267				

- Molecule 10 is a protein called 40S ribosomal protein S8-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	S8	188	Total	C	N	O	S	0	0	0
			1489	925	298	264	2			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	s8	188	Total	C	N	O	S	0	0	0
			1489	925	298	264	2			

- Molecule 11 is a protein called 40S ribosomal protein S9-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	S9	185	Total	C	N	O	S	0	0	0
			1494	943	289	261	1			
11	s9	185	Total	C	N	O	S	0	0	0
			1494	943	289	261	1			

- Molecule 12 is a protein called 40S ribosomal protein S10-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	C0	96	Total	C	N	O	S	0	0	0
			772	499	126	145	2			
12	c0	96	Total	C	N	O	S	0	0	0
			761	490	125	144	2			

- Molecule 13 is a protein called 40S ribosomal protein S11-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	C1	155	Total	C	N	O	S	0	0	0
			1213	774	230	206	3			
13	c1	146	Total	C	N	O	S	0	0	0
			1168	747	221	197	3			

- Molecule 14 is a protein called 40S ribosomal protein S12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	C2	124	Total	C	N	O	S	0	0	0
			890	560	156	172	2			
14	c2	124	Total	C	N	O	S	0	0	0
			890	560	156	172	2			

- Molecule 15 is a protein called 40S ribosomal protein S13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	C3	150	Total	C	N	O	S	0	0	0
			1192	759	224	207	2			
15	c3	150	Total	C	N	O	S	0	0	0
			1192	759	224	207	2			

- Molecule 16 is a protein called 40S ribosomal protein S14-B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	C4	127	Total	C	N	O	S	0	0	0
			891	545	182	163	1			
16	c4	128	Total	C	N	O	S	0	0	0
			949	582	188	176	3			

- Molecule 17 is a protein called 40S ribosomal protein S15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	C5	124	Total	C	N	O	S	0	0	0
			977	622	182	166	7			
17	c5	135	Total	C	N	O	S	0	0	0
			1039	658	196	178	7			

- Molecule 18 is a protein called 40S ribosomal protein S16-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	C6	141	Total	C	N	O		0	0	0
			1105	708	203	194				
18	c6	142	Total	C	N	O		0	0	0
			1111	711	204	196				

- Molecule 19 is a protein called 40S ribosomal protein S17-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	C7	120	Total	C	N	O	S	0	0	0
			926	577	177	170	2			
19	c7	117	Total	C	N	O	S	0	0	0
			906	563	174	167	2			

- Molecule 20 is a protein called 40S ribosomal protein S18-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	C8	145	Total	C	N	O	S	0	0	0
			1192	743	237	210	2			
20	c8	145	Total	C	N	O	S	0	0	0
			1192	743	237	210	2			

- Molecule 21 is a protein called 40S ribosomal protein S19-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
21	C9	143	Total	C	N	O	S	0	0	0
			1112	694	208	208	2			
21	c9	143	Total	C	N	O	S	0	0	0
			1112	694	208	208	2			

- Molecule 22 is a protein called 40S ribosomal protein S20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	D0	107	Total	C	N	O	S	0	0	0
			855	539	156	159	1			
22	d0	110	Total	C	N	O	S	0	0	0
			882	554	161	166	1			

- Molecule 23 is a protein called 40S ribosomal protein S21-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	D1	87	Total	C	N	O	S	0	0	0
			684	420	125	137	2			
23	d1	87	Total	C	N	O	S	0	0	0
			684	420	125	137	2			

- Molecule 24 is a protein called 40S ribosomal protein S22-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	D2	129	Total	C	N	O	S	0	0	0
			1021	650	188	180	3			
24	d2	129	Total	C	N	O	S	0	0	0
			1021	650	188	180	3			

- Molecule 25 is a protein called 40S ribosomal protein S23-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	D3	144	Total	C	N	O	S	0	0	0
			1121	708	220	191	2			
25	d3	144	Total	C	N	O	S	0	0	0
			1121	708	220	191	2			

- Molecule 26 is a protein called 40S ribosomal protein S24-A.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
26	D4	134	Total	C	N	O	0	0	0
			1073	676	208	189			

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
26	d4	134	Total	C	N	O	0	0	0
			1073	676	208	189			

- Molecule 27 is a protein called 40S ribosomal protein S25-A.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
27	D5	70	Total	C	N	O	0	0	0
			563	360	104	99			
27	d5	69	Total	C	N	O	0	0	0
			558	357	103	98			

- Molecule 28 is a protein called 40S ribosomal protein S26-B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	D6	97	Total	C	N	O	S	0	0	0
			769	475	160	129	5			
28	d6	97	Total	C	N	O	S	0	0	0
			769	475	160	129	5			

- Molecule 29 is a protein called 40S ribosomal protein S27-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	D7	81	Total	C	N	O	S	0	0	0
			610	382	110	113	5			
29	d7	81	Total	C	N	O	S	0	0	0
			610	382	110	113	5			

- Molecule 30 is a protein called 40S ribosomal protein S28-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	D8	63	Total	C	N	O	S	0	0	0
			497	306	99	91	1			
30	d8	63	Total	C	N	O	S	0	0	0
			497	306	99	91	1			

- Molecule 31 is a protein called 40S ribosomal protein S29-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	D9	53	Total	C	N	O	S	0	0	0
			442	274	92	72	4			
31	d9	53	Total	C	N	O	S	0	0	0
			442	274	92	72	4			

- Molecule 32 is a protein called 40S ribosomal protein S30-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	E0	60	Total	C	N	O	S	0	0	0
			475	299	98	77	1			
32	e0	62	Total	C	N	O	S	0	0	0
			491	309	101	80	1			

- Molecule 33 is a protein called Ubiquitin-40S ribosomal protein S31.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
33	E1	71	Total	C	N	O	S	0	0	0
			566	362	106	94	4			
33	e1	76	Total	C	N	O	S	0	0	0
			608	388	117	99	4			

- Molecule 34 is a protein called Guanine nucleotide-binding protein subunit beta-like protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
34	SR	318	Total	C	N	O	S	0	0	0
			2437	1541	418	470	8			
34	sR	318	Total	C	N	O	S	0	0	0
			2438	1541	417	472	8			

- Molecule 35 is a protein called Suppressor protein STM1,Suppressor protein STM1,Suppressor protein STM1.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
35	SM	159	Total	C	N	O	0	0	0
			1104	652	221	231			

- Molecule 36 is a RNA chain called 25S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
36	1	3149	Total	C	N	O	P	0	0	0
			67355	30086	12142	21978	3149			
36	5	3150	Total	C	N	O	P	0	0	0
			67376	30095	12145	21987	3149			

- Molecule 37 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
37	3	121	Total	C	N	O	P	0	0	0
			2579	1152	461	845	121			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
37	7	121	Total	C	N	O	P	0	0	0
			2579	1152	461	845	121			

- Molecule 38 is a RNA chain called 5.8S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
38	4	158	Total	C	N	O	P	0	0	0
			3353	1500	586	1109	158			
38	8	158	Total	C	N	O	P	0	0	0
			3353	1500	586	1109	158			

- Molecule 39 is a protein called 60S ribosomal protein L2-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
39	L2	252	Total	C	N	O	S	0	0	0
			1914	1191	388	334	1			
39	l2	252	Total	C	N	O	S	0	0	0
			1912	1190	388	333	1			

- Molecule 40 is a protein called 60S ribosomal protein L3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
40	L3	386	Total	C	N	O	S	0	0	0
			3075	1950	584	533	8			
40	l3	386	Total	C	N	O	S	0	0	0
			3075	1950	584	533	8			

- Molecule 41 is a protein called 60S ribosomal protein L4-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
41	L4	361	Total	C	N	O	S	0	0	0
			2748	1729	522	494	3			
41	l4	361	Total	C	N	O	S	0	0	0
			2748	1729	522	494	3			

- Molecule 42 is a protein called 60S ribosomal protein L5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
42	L5	296	Total	C	N	O	S	0	0	0
			2375	1501	414	458	2			
42	l5	294	Total	C	N	O	S	0	0	0
			2359	1489	412	456	2			

- Molecule 43 is a protein called 60S ribosomal protein L6-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
43	L6	156	Total	C	N	O	S	0	0	0
			1239	800	222	216	1			
43	l6	157	Total	C	N	O	S	0	0	0
			1248	806	224	217	1			

- Molecule 44 is a protein called 60S ribosomal protein L7-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
44	L7	222	Total	C	N	O	S	0	0	0
			1784	1151	324	308	1			
44	l7	223	Total	C	N	O	S	0	0	0
			1791	1155	325	310	1			

- Molecule 45 is a protein called 60S ribosomal protein L8-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
45	L8	233	Total	C	N	O	S	0	0	0
			1804	1151	323	327	3			

- Molecule 46 is a protein called 60S ribosomal protein L9-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
46	L9	191	Total	C	N	O	S	0	0	0
			1518	963	274	277	4			
46	l9	191	Total	C	N	O	S	0	0	0
			1518	963	274	277	4			

- Molecule 47 is a protein called 60S ribosomal protein L10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
47	M0	211	Total	C	N	O	S	0	0	0
			1705	1083	322	294	6			
47	m0	213	Total	C	N	O	S	0	0	0
			1722	1094	325	297	6			

- Molecule 48 is a protein called 60S ribosomal protein L11-B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
48	M1	169	Total	C	N	O	S	0	0	0
			1353	847	253	249	4			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
48	m1	169	Total	C	N	O	S	0	0	0
			1353	847	253	249	4			

- Molecule 49 is a protein called 60S ribosomal protein L13-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
49	M3	193	Total	C	N	O		0	0	0
			1543	962	315	266				
49	m3	194	Total	C	N	O		0	0	0
			1548	965	316	267				

- Molecule 50 is a protein called 60S ribosomal protein L14-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
50	M4	136	Total	C	N	O	S	0	0	0
			1053	675	199	177	2			
50	m4	137	Total	C	N	O	S	0	0	0
			1059	678	200	179	2			

- Molecule 51 is a protein called 60S ribosomal protein L15-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
51	M5	203	Total	C	N	O	S	0	0	0
			1720	1077	361	281	1			
51	m5	203	Total	C	N	O	S	0	0	0
			1720	1077	361	281	1			

- Molecule 52 is a protein called 60S ribosomal protein L16-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
52	M6	197	Total	C	N	O	S	0	0	0
			1555	1003	289	262	1			
52	m6	197	Total	C	N	O	S	0	0	0
			1555	1003	289	262	1			

- Molecule 53 is a protein called 60S ribosomal protein L17-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
53	M7	183	Total	C	N	O		0	0	0
			1420	882	281	257				
53	m7	155	Total	C	N	O		0	0	0
			1227	764	238	225				

- Molecule 54 is a protein called 60S ribosomal protein L18-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
54	M8	185	Total	C	N	O	S	0	0	0
			1441	908	290	241	2			
54	m8	185	Total	C	N	O	S	0	0	0
			1441	908	290	241	2			

- Molecule 55 is a protein called 60S ribosomal protein L19-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
55	M9	188	Total	C	N	O		0	0	0
			1521	935	326	260				
55	m9	188	Total	C	N	O		0	0	0
			1521	935	326	260				

- Molecule 56 is a protein called 60S ribosomal protein L20-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
56	N0	172	Total	C	N	O	S	0	0	0
			1445	930	267	244	4			
56	n0	172	Total	C	N	O	S	0	0	0
			1445	930	267	244	4			

- Molecule 57 is a protein called 60S ribosomal protein L21-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
57	N1	159	Total	C	N	O	S	0	0	0
			1276	805	246	221	4			
57	n1	159	Total	C	N	O	S	0	0	0
			1276	805	246	221	4			

- Molecule 58 is a protein called 60S ribosomal protein L22-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
58	N2	100	Total	C	N	O		0	0	0
			796	516	131	149				
58	n2	98	Total	C	N	O		0	0	0
			778	505	127	146				

- Molecule 59 is a protein called 60S ribosomal protein L23-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
59	N3	136	Total	C	N	O	S	0	0	0
			1003	628	189	179	7			
59	n3	136	Total	C	N	O	S	0	0	0
			1003	628	189	179	7			

- Molecule 60 is a protein called 60S ribosomal protein L24-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
60	N4	98	Total	C	N	O	S	0	0	0
			699	443	137	118	1			

- Molecule 61 is a protein called 60S ribosomal protein L25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
61	N5	121	Total	C	N	O	S	0	0	0
			964	620	169	173	2			
61	n5	120	Total	C	N	O	S	0	0	0
			959	617	168	172	2			

- Molecule 62 is a protein called 60S ribosomal protein L26-A.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
62	N6	126	Total	C	N	O	0	0	0
			993	625	192	176			
62	n6	126	Total	C	N	O	0	0	0
			993	625	192	176			

- Molecule 63 is a protein called 60S ribosomal protein L27-A.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
63	N7	135	Total	C	N	O	0	0	0
			1092	710	202	180			
63	n7	135	Total	C	N	O	0	0	0
			1092	710	202	180			

- Molecule 64 is a protein called 60S ribosomal protein L28.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
64	N8	148	Total	C	N	O	S	0	0	0
			1173	749	231	190	3			
64	n8	148	Total	C	N	O	S	0	0	0
			1173	749	231	190	3			

- Molecule 65 is a protein called 60S ribosomal protein L29.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
65	N9	58	Total	C	N	O	0	0	0
			462	289	100	73			
65	n9	58	Total	C	N	O	0	0	0
			462	289	100	73			

- Molecule 66 is a protein called 60S ribosomal protein L30.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
66	O0	97	Total	C	N	O	S	0	0	0
			743	479	124	139	1			
66	o0	100	Total	C	N	O	S	0	0	0
			767	492	128	146	1			

- Molecule 67 is a protein called 60S ribosomal protein L31-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
67	O1	109	Total	C	N	O	S	0	0	0
			876	556	167	152	1			
67	o1	109	Total	C	N	O	S	0	0	0
			883	559	167	156	1			

- Molecule 68 is a protein called 60S ribosomal protein L32.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
68	O2	127	Total	C	N	O	S	0	0	0
			1020	647	205	167	1			
68	o2	127	Total	C	N	O	S	0	0	0
			1020	647	205	167	1			

- Molecule 69 is a protein called 60S ribosomal protein L33-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
69	O3	106	Total	C	N	O	S	0	0	0
			850	540	165	144	1			
69	o3	106	Total	C	N	O	S	0	0	0
			850	540	165	144	1			

- Molecule 70 is a protein called 60S ribosomal protein L34-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
70	O4	112	Total	C	N	O	S	0	0	0
			880	545	179	152	4			
70	o4	112	Total	C	N	O	S	0	0	0
			880	545	179	152	4			

- Molecule 71 is a protein called 60S ribosomal protein L35-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
71	O5	119	Total	C	N	O	S	0	0	0
			969	615	186	167	1			
71	o5	119	Total	C	N	O	S	0	0	0
			965	612	185	167	1			

- Molecule 72 is a protein called 60S ribosomal protein L36-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
72	O6	99	Total	C	N	O	S	0	0	0
			771	481	156	132	2			
72	o6	99	Total	C	N	O	S	0	0	0
			770	481	156	131	2			

- Molecule 73 is a protein called 60S ribosomal protein L37-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
73	O7	87	Total	C	N	O	S	0	0	0
			681	414	148	114	5			
73	o7	87	Total	C	N	O	S	0	0	0
			681	414	148	114	5			

- Molecule 74 is a protein called 60S ribosomal protein L38.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
74	O8	77	Total	C	N	O	0	0	0
			612	391	115	106			
74	o8	77	Total	C	N	O	0	0	0
			608	388	114	106			

- Molecule 75 is a protein called 60S ribosomal protein L39.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
75	O9	50	Total	C	N	O	S	0	0	0
			436	272	97	65	2			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
75	o9	50	Total	C	N	O	S	0	0	0
			436	272	97	65	2			

- Molecule 76 is a protein called Ubiquitin-60S ribosomal protein L40.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
76	Q0	52	Total	C	N	O	S	0	0	0
			417	259	86	67	5			
76	q0	52	Total	C	N	O	S	0	0	0
			417	259	86	67	5			

- Molecule 77 is a protein called 60S ribosomal protein L41-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
77	Q1	25	Total	C	N	O	S	0	0	0
			233	142	63	27	1			
77	q1	25	Total	C	N	O	S	0	0	0
			233	142	63	27	1			

- Molecule 78 is a protein called 60S ribosomal protein L42-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
78	Q2	105	Total	C	N	O	S	0	0	0
			847	534	170	138	5			
78	q2	105	Total	C	N	O	S	0	0	0
			847	534	170	138	5			

- Molecule 79 is a protein called 60S ribosomal protein L43-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
79	Q3	91	Total	C	N	O	S	0	0	0
			694	429	138	121	6			
79	q3	91	Total	C	N	O	S	0	0	0
			694	429	138	121	6			

- Molecule 80 is a protein called Suppressor protein STM1,Suppressor protein STM1,Suppressor protein STM1.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
80	sM	104	Total	C	N	O	0	0	0
			680	403	140	137			



- Molecule 81 is a protein called 60S ribosomal protein L8-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
81	l8	231	Total	C	N	O	S	0	0	0
			1763	1130	316	314	3			

- Molecule 82 is a protein called 60S ribosomal protein L12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
82	m2	150	Total	C	N	O	S	0	0	0
			750	450	150	150				

- Molecule 83 is a protein called 60S ribosomal protein L24-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
83	n4	135	Total	C	N	O	S	0	0	0
			1038	651	206	180	1			

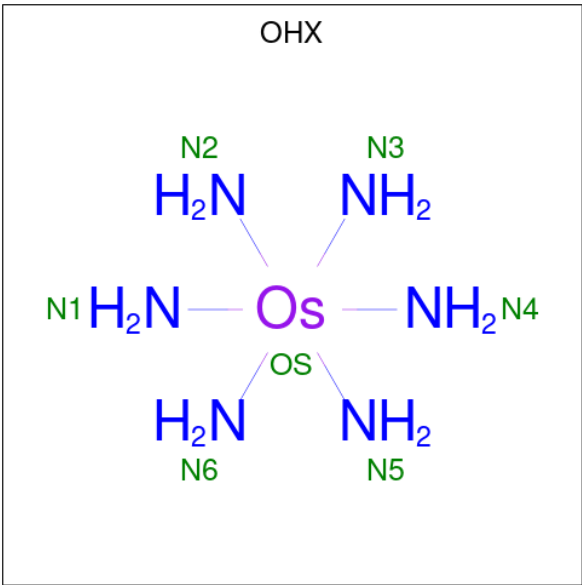
- Molecule 84 is a protein called 60S acidic ribosomal protein P0.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
84	p0	143	Total	C	N	O	S	0	0	0
			1077	687	192	195	3			

- Molecule 85 is a protein called Ribosomal protein P1 alpha, P2 beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
85	p1	47	Total	C	N	O		0	0	0
			235	141	47	47				
85	p2	46	Total	C	N	O		0	0	0
			230	138	46	46				

- Molecule 86 is osmium (III) hexammine (three-letter code: OHX) (formula: H<sub>12</sub>N<sub>6</sub>Os).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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86	2	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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86	1	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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86	1	1	Total	N	Os	0	0
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86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
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86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	1	1	Total	N	Os	0	0
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86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	3	1	Total	N	Os	0	0
			7	6	1		
86	3	1	Total	N	Os	0	0
			7	6	1		
86	3	1	Total	N	Os	0	0
			7	6	1		
86	3	1	Total	N	Os	0	0
			7	6	1		
86	3	1	Total	N	Os	0	0
			7	6	1		
86	3	1	Total	N	Os	0	0
			7	6	1		
86	3	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	4	1	Total	N	Os	0	0
			7	6	1		
86	4	1	Total	N	Os	0	0
			7	6	1		
86	4	1	Total	N	Os	0	0
			7	6	1		
86	4	1	Total	N	Os	0	0
			7	6	1		
86	4	1	Total	N	Os	0	0
			7	6	1		
86	4	1	Total	N	Os	0	0
			7	6	1		
86	4	1	Total	N	Os	0	0
			7	6	1		
86	4	1	Total	N	Os	0	0
			7	6	1		
86	4	1	Total	N	Os	0	0
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86	4	1	Total	N	Os	0	0
			7	6	1		
86	4	1	Total	N	Os	0	0
			7	6	1		
86	4	1	Total	N	Os	0	0
			7	6	1		
86	L3	1	Total	N	Os	0	0
			7	6	1		
86	L3	1	Total	N	Os	0	0
			7	6	1		
86	L4	1	Total	N	Os	0	0
			7	6	1		
86	M0	1	Total	N	Os	0	0
			7	6	1		
86	M5	1	Total	N	Os	0	0
			7	6	1		
86	M7	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	M9	1	Total	N	Os	0	0
			7	6	1		
86	N9	1	Total	N	Os	0	0
			7	6	1		
86	O1	1	Total	N	Os	0	0
			7	6	1		
86	O3	1	Total	N	Os	0	0
			7	6	1		
86	Q2	1	Total	N	Os	0	0
			7	6	1		
86	6	1	Total	N	Os	0	0
			7	6	1		
86	6	1	Total	N	Os	0	0
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86	6	1	Total	N	Os	0	0
			7	6	1		
86	6	1	Total	N	Os	0	0
			7	6	1		
86	6	1	Total	N	Os	0	0
			7	6	1		
86	6	1	Total	N	Os	0	0
			7	6	1		
86	6	1	Total	N	Os	0	0
			7	6	1		
86	6	1	Total	N	Os	0	0
			7	6	1		
86	6	1	Total	N	Os	0	0
			7	6	1		
86	6	1	Total	N	Os	0	0
			7	6	1		
86	6	1	Total	N	Os	0	0
			7	6	1		
86	6	1	Total	N	Os	0	0
			7	6	1		
86	6	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	6	1	Total	N	Os	0	0
			7	6	1		
86	6	1	Total	N	Os	0	0
			7	6	1		
86	6	1	Total	N	Os	0	0
			7	6	1		
86	6	1	Total	N	Os	0	0
			7	6	1		
86	6	1	Total	N	Os	0	0
			7	6	1		
86	6	1	Total	N	Os	0	0
			7	6	1		
86	6	1	Total	N	Os	0	0
			7	6	1		
86	6	1	Total	N	Os	0	0
			7	6	1		
86	6	1	Total	N	Os	0	0
			7	6	1		
86	6	1	Total	N	Os	0	0
			7	6	1		
86	6	1	Total	N	Os	0	0
			7	6	1		
86	6	1	Total	N	Os	0	0
			7	6	1		
86	6	1	Total	N	Os	0	0
			7	6	1		
86	6	1	Total	N	Os	0	0
			7	6	1		
86	6	1	Total	N	Os	0	0
			7	6	1		
86	6	1	Total	N	Os	0	0
			7	6	1		
86	6	1	Total	N	Os	0	0
			7	6	1		
86	6	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	6	1	Total	N	Os	0	0
			7	6	1		
86	6	1	Total	N	Os	0	0
			7	6	1		
86	6	1	Total	N	Os	0	0
			7	6	1		
86	6	1	Total	N	Os	0	0
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86	6	1	Total	N	Os	0	0
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86	6	1	Total	N	Os	0	0
			7	6	1		
86	6	1	Total	N	Os	0	0
			7	6	1		
86	6	1	Total	N	Os	0	0
			7	6	1		
86	6	1	Total	N	Os	0	0
			7	6	1		
86	6	1	Total	N	Os	0	0
			7	6	1		
86	6	1	Total	N	Os	0	0
			7	6	1		
86	6	1	Total	N	Os	0	0
			7	6	1		
86	6	1	Total	N	Os	0	0
			7	6	1		
86	6	1	Total	N	Os	0	0
			7	6	1		
86	6	1	Total	N	Os	0	0
			7	6	1		
86	6	1	Total	N	Os	0	0
			7	6	1		
86	6	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	6	1	Total	N	Os	0	0
			7	6	1		
86	6	1	Total	N	Os	0	0
			7	6	1		
86	6	1	Total	N	Os	0	0
			7	6	1		
86	6	1	Total	N	Os	0	0
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86	6	1	Total	N	Os	0	0
			7	6	1		
86	6	1	Total	N	Os	0	0
			7	6	1		
86	6	1	Total	N	Os	0	0
			7	6	1		
86	6	1	Total	N	Os	0	0
			7	6	1		
86	6	1	Total	N	Os	0	0
			7	6	1		
86	6	1	Total	N	Os	0	0
			7	6	1		
86	6	1	Total	N	Os	0	0
			7	6	1		
86	6	1	Total	N	Os	0	0
			7	6	1		
86	6	1	Total	N	Os	0	0
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86	6	1	Total	N	Os	0	0
			7	6	1		
86	6	1	Total	N	Os	0	0
			7	6	1		
86	6	1	Total	N	Os	0	0
			7	6	1		
86	6	1	Total	N	Os	0	0
			7	6	1		
86	6	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	6	1	Total	N	Os	0	0
			7	6	1		
86	6	1	Total	N	Os	0	0
			7	6	1		
86	6	1	Total	N	Os	0	0
			7	6	1		
86	6	1	Total	N	Os	0	0
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86	6	1	Total	N	Os	0	0
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86	6	1	Total	N	Os	0	0
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86	6	1	Total	N	Os	0	0
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86	6	1	Total	N	Os	0	0
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86	6	1	Total	N	Os	0	0
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86	6	1	Total	N	Os	0	0
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86	6	1	Total	N	Os	0	0
			7	6	1		
86	6	1	Total	N	Os	0	0
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86	6	1	Total	N	Os	0	0
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86	6	1	Total	N	Os	0	0
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86	6	1	Total	N	Os	0	0
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86	6	1	Total	N	Os	0	0
			7	6	1		
86	6	1	Total	N	Os	0	0
			7	6	1		
86	6	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	6	1	Total	N	Os	0	0
			7	6	1		
86	6	1	Total	N	Os	0	0
			7	6	1		
86	6	1	Total	N	Os	0	0
			7	6	1		
86	6	1	Total	N	Os	0	0
			7	6	1		
86	6	1	Total	N	Os	0	0
			7	6	1		
86	6	1	Total	N	Os	0	0
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86	6	1	Total	N	Os	0	0
			7	6	1		
86	6	1	Total	N	Os	0	0
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86	6	1	Total	N	Os	0	0
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86	6	1	Total	N	Os	0	0
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86	6	1	Total	N	Os	0	0
			7	6	1		
86	6	1	Total	N	Os	0	0
			7	6	1		
86	6	1	Total	N	Os	0	0
			7	6	1		
86	6	1	Total	N	Os	0	0
			7	6	1		
86	6	1	Total	N	Os	0	0
			7	6	1		
86	6	1	Total	N	Os	0	0
			7	6	1		
86	6	1	Total	N	Os	0	0
			7	6	1		
86	6	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	6	1	Total 7	N 6	Os 1	0	0
86	6	1	Total 7	N 6	Os 1	0	0
86	6	1	Total 7	N 6	Os 1	0	0
86	6	1	Total 7	N 6	Os 1	0	0
86	6	1	Total 7	N 6	Os 1	0	0
86	6	1	Total 7	N 6	Os 1	0	0
86	6	1	Total 7	N 6	Os 1	0	0
86	6	1	Total 7	N 6	Os 1	0	0
86	6	1	Total 7	N 6	Os 1	0	0
86	6	1	Total 7	N 6	Os 1	0	0
86	6	1	Total 7	N 6	Os 1	0	0
86	6	1	Total 7	N 6	Os 1	0	0
86	6	1	Total 7	N 6	Os 1	0	0
86	6	1	Total 7	N 6	Os 1	0	0
86	6	1	Total 7	N 6	Os 1	0	0
86	6	1	Total 7	N 6	Os 1	0	0
86	s4	1	Total 7	N 6	Os 1	0	0
86	s8	1	Total 7	N 6	Os 1	0	0
86	s9	1	Total 7	N 6	Os 1	0	0
86	c3	1	Total 7	N 6	Os 1	0	0
86	c5	1	Total 7	N 6	Os 1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	c8	1	Total	N	Os	0	0
			7	6	1		
86	sR	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
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86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	5	1	Total	N	Os	0	0
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86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
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86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
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86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
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86	5	1	Total	N	Os	0	0
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86	5	1	Total	N	Os	0	0
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86	5	1	Total	N	Os	0	0
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86	5	1	Total	N	Os	0	0
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86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
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86	5	1	Total	N	Os	0	0
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86	5	1	Total	N	Os	0	0
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86	5	1	Total	N	Os	0	0
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86	5	1	Total	N	Os	0	0
			7	6	1		
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86	5	1	Total	N	Os	0	0
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86	5	1	Total	N	Os	0	0
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86	5	1	Total	N	Os	0	0
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86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	5	1	Total	N	Os	0	0
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86	5	1	Total	N	Os	0	0
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86	5	1	Total	N	Os	0	0
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86	5	1	Total	N	Os	0	0
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86	5	1	Total	N	Os	0	0
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86	5	1	Total	N	Os	0	0
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86	5	1	Total	N	Os	0	0
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86	5	1	Total	N	Os	0	0
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86	5	1	Total	N	Os	0	0
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86	5	1	Total	N	Os	0	0
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86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	5	1	Total	N	Os	0	0
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86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
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			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	7	1	Total	N	Os	0	0
			7	6	1		
86	7	1	Total	N	Os	0	0
			7	6	1		
86	7	1	Total	N	Os	0	0
			7	6	1		
86	7	1	Total	N	Os	0	0
			7	6	1		
86	7	1	Total	N	Os	0	0
			7	6	1		
86	7	1	Total	N	Os	0	0
			7	6	1		
86	7	1	Total	N	Os	0	0
			7	6	1		
86	7	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	7	1	Total	N	Os	0	0
			7	6	1		
86	8	1	Total	N	Os	0	0
			7	6	1		
86	8	1	Total	N	Os	0	0
			7	6	1		
86	8	1	Total	N	Os	0	0
			7	6	1		
86	8	1	Total	N	Os	0	0
			7	6	1		
86	8	1	Total	N	Os	0	0
			7	6	1		
86	8	1	Total	N	Os	0	0
			7	6	1		
86	8	1	Total	N	Os	0	0
			7	6	1		
86	8	1	Total	N	Os	0	0
			7	6	1		
86	8	1	Total	N	Os	0	0
			7	6	1		
86	8	1	Total	N	Os	0	0
			7	6	1		
86	8	1	Total	N	Os	0	0
			7	6	1		
86	13	1	Total	N	Os	0	0
			7	6	1		
86	13	1	Total	N	Os	0	0
			7	6	1		
86	14	1	Total	N	Os	0	0
			7	6	1		
86	15	1	Total	N	Os	0	0
			7	6	1		
86	15	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	l9	1	Total	N	Os	0	0
			7	6	1		
86	m0	1	Total	N	Os	0	0
			7	6	1		
86	m0	1	Total	N	Os	0	0
			7	6	1		
86	m4	1	Total	N	Os	0	0
			7	6	1		
86	m5	1	Total	N	Os	0	0
			7	6	1		
86	m6	1	Total	N	Os	0	0
			7	6	1		
86	n1	1	Total	N	Os	0	0
			7	6	1		
86	n3	1	Total	N	Os	0	0
			7	6	1		
86	n3	1	Total	N	Os	0	0
			7	6	1		
86	n9	1	Total	N	Os	0	0
			7	6	1		
86	o3	1	Total	N	Os	0	0
			7	6	1		
86	o7	1	Total	N	Os	0	0
			7	6	1		
86	q2	1	Total	N	Os	0	0
			7	6	1		

- Molecule 87 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
87	2	91	Total	Mg	0	0
			91	91		
87	S2	1	Total	Mg	0	0
			1	1		
87	D3	1	Total	Mg	0	0
			1	1		
87	1	353	Total	Mg	0	0
			353	353		
87	3	8	Total	Mg	0	0
			8	8		
87	4	17	Total	Mg	0	0
			17	17		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
87	L2	2	Total 2	Mg 2	0	0
87	L3	1	Total 1	Mg 1	0	0
87	L4	1	Total 1	Mg 1	0	0
87	L7	3	Total 3	Mg 3	0	0
87	M0	1	Total 1	Mg 1	0	0
87	M3	2	Total 2	Mg 2	0	0
87	M5	2	Total 2	Mg 2	0	0
87	M7	3	Total 3	Mg 3	0	0
87	M9	1	Total 1	Mg 1	0	0
87	N3	1	Total 1	Mg 1	0	0
87	N8	2	Total 2	Mg 2	0	0
87	O2	1	Total 1	Mg 1	0	0
87	O7	1	Total 1	Mg 1	0	0
87	Q2	1	Total 1	Mg 1	0	0
87	6	98	Total 98	Mg 98	0	0
87	c1	1	Total 1	Mg 1	0	0
87	c6	1	Total 1	Mg 1	0	0
87	d3	1	Total 1	Mg 1	0	0
87	d6	1	Total 1	Mg 1	0	0
87	sM	1	Total 1	Mg 1	0	0
87	5	383	Total 383	Mg 383	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
87	7	11	Total 11	Mg 11	0	0
87	8	9	Total 9	Mg 9	0	0
87	l2	3	Total 3	Mg 3	0	0
87	l3	1	Total 1	Mg 1	0	0
87	m5	3	Total 3	Mg 3	0	0
87	m7	2	Total 2	Mg 2	0	0
87	n3	1	Total 1	Mg 1	0	0
87	n6	2	Total 2	Mg 2	0	0
87	n8	2	Total 2	Mg 2	0	0
87	n9	1	Total 1	Mg 1	0	0
87	o7	2	Total 2	Mg 2	0	0
87	q0	1	Total 1	Mg 1	0	0
87	q1	1	Total 1	Mg 1	0	0
87	q2	1	Total 1	Mg 1	0	0

- Molecule 88 is ZINC ION (three-letter code: ZN) (formula: Zn).

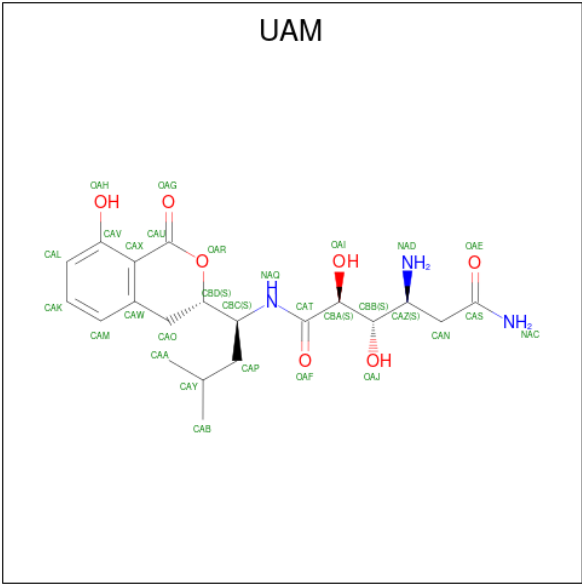
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
88	D6	1	Total 1	Zn 1	0	0
88	D7	1	Total 1	Zn 1	0	0
88	D9	1	Total 1	Zn 1	0	0
88	E1	1	Total 1	Zn 1	0	0
88	O7	1	Total 1	Zn 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
88	Q0	1	Total	Zn	0	0
			1	1		
88	Q2	1	Total	Zn	0	0
			1	1		
88	Q3	1	Total	Zn	0	0
			1	1		
88	d6	1	Total	Zn	0	0
			1	1		
88	d7	1	Total	Zn	0	0
			1	1		
88	d9	1	Total	Zn	0	0
			1	1		
88	e1	1	Total	Zn	0	0
			1	1		
88	o7	1	Total	Zn	0	0
			1	1		
88	q0	1	Total	Zn	0	0
			1	1		
88	q2	1	Total	Zn	0	0
			1	1		
88	q3	1	Total	Zn	0	0
			1	1		

- Molecule 89 is Amicoumacin A (three-letter code: UAM) (formula: C<sub>20</sub>H<sub>29</sub>N<sub>3</sub>O<sub>7</sub>).



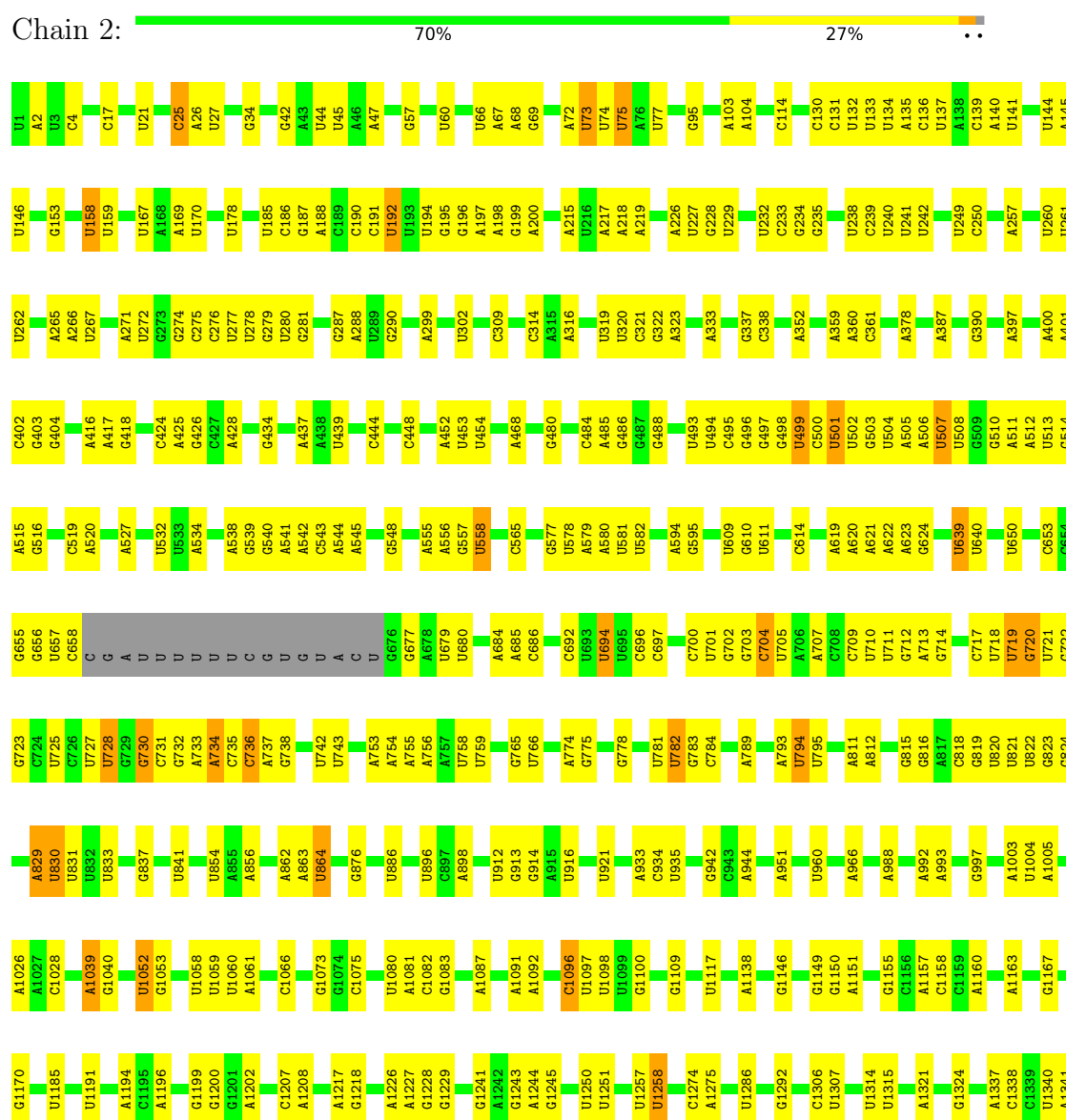
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
89	6	1	Total	C	N	O	0	0
			30	20	3	7		

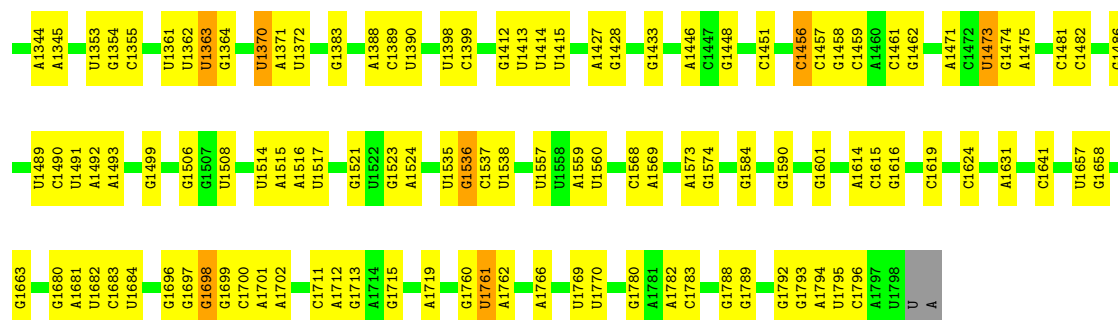
### 3 Residue-property plots

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. 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. 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.

Note EDS failed to run properly.

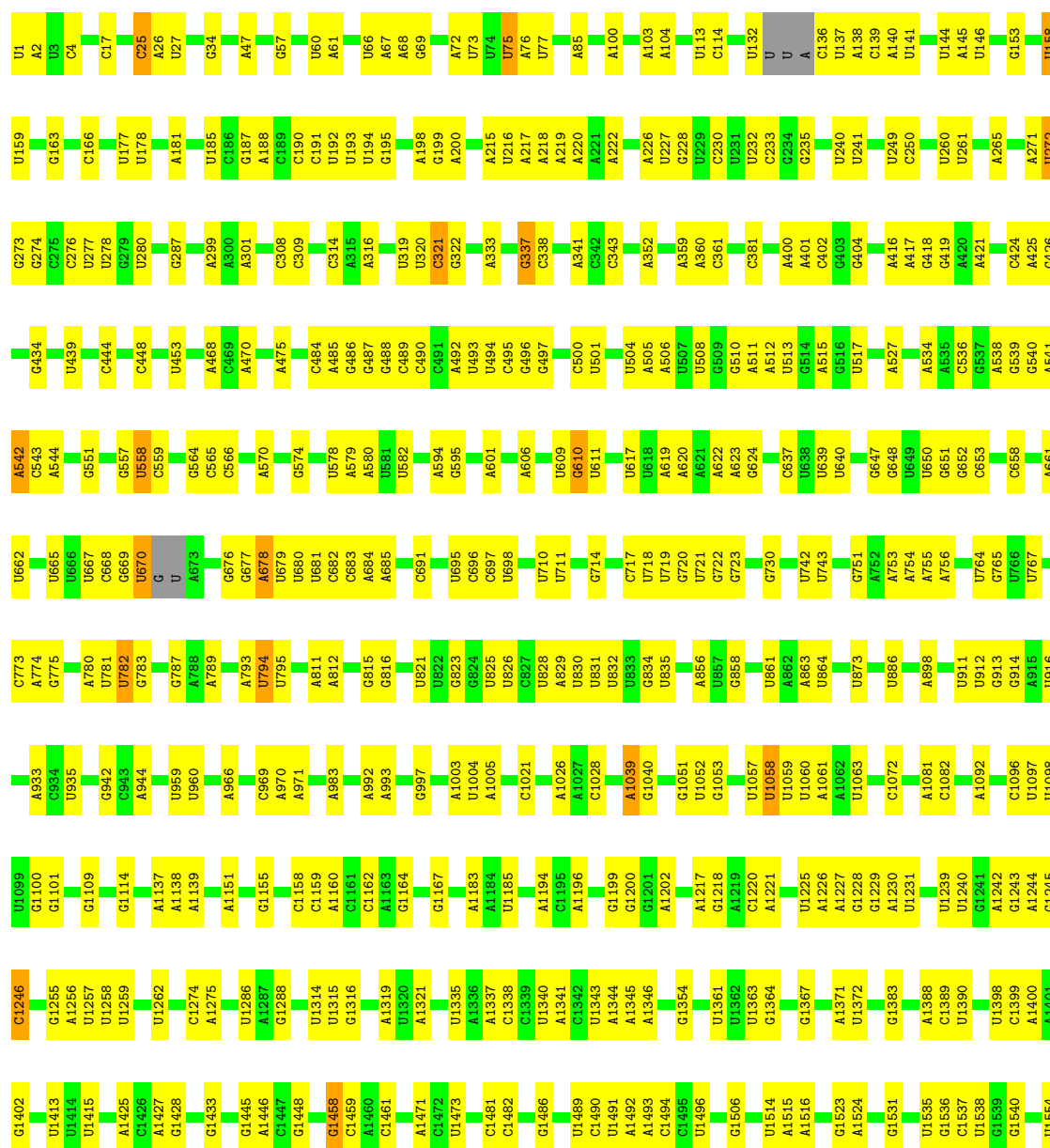
#### • Molecule 1: 18S ribosomal RNA

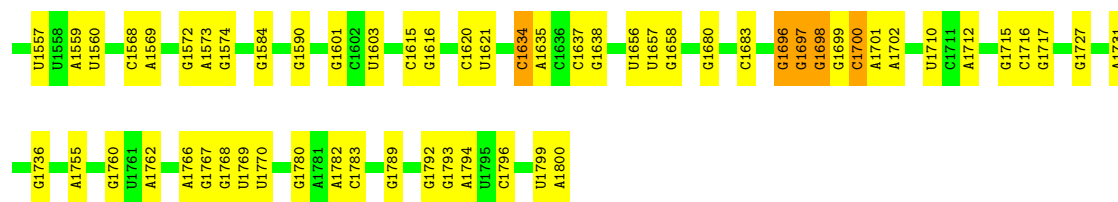




# Molecule 1: 18S ribosomal RNA

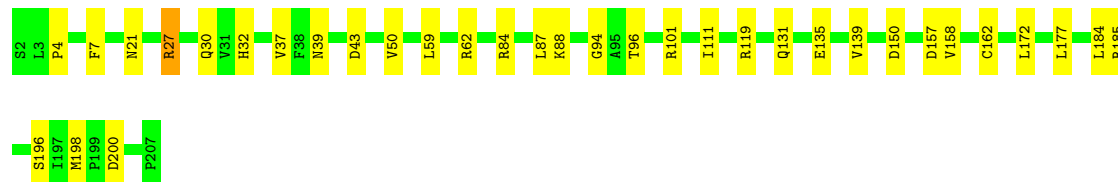
Chain 6: 72% 26%





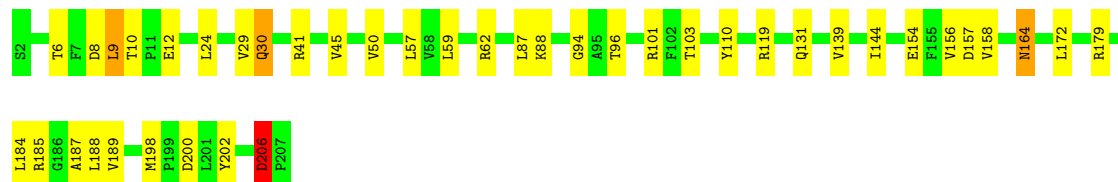
• Molecule 2: 40S ribosomal protein S0-A

Chain S0: 83% 16%



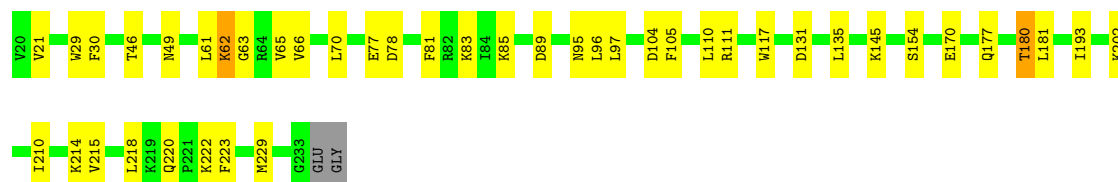
• Molecule 2: 40S ribosomal protein S0-A

Chain s0: 80% 18%



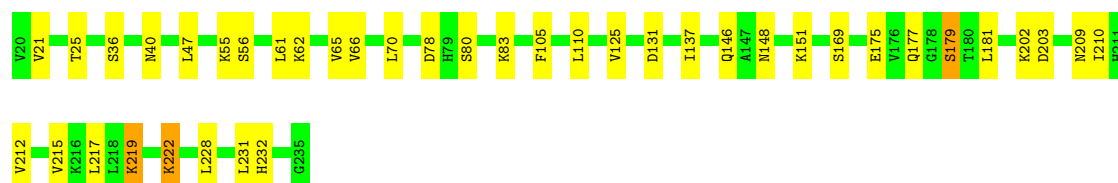
• Molecule 3: 40S ribosomal protein S1-A

Chain S1: 79% 19%




• Molecule 3: 40S ribosomal protein S1-A

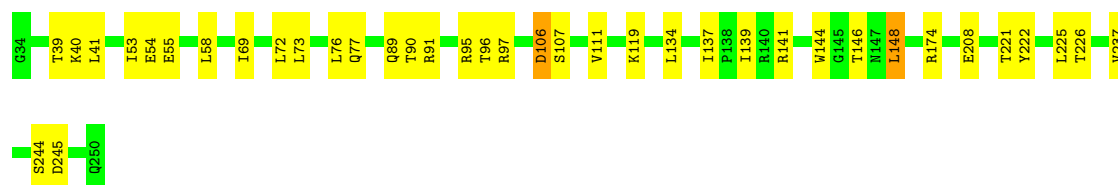
Chain s1: 81% 17%




• Molecule 4: 40S ribosomal protein S2

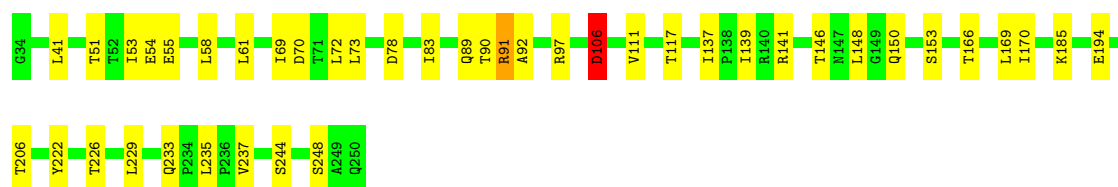


Chain S2:  82% 17%




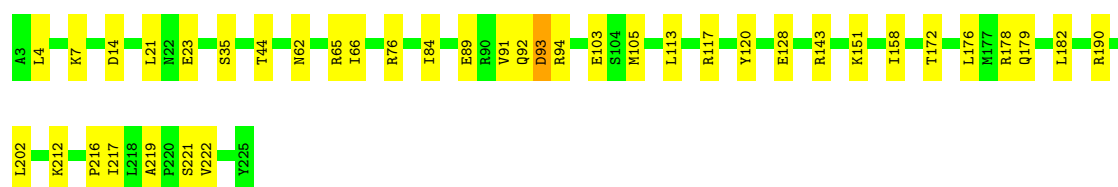
- Molecule 4: 40S ribosomal protein S2

Chain s2:  81% 18%




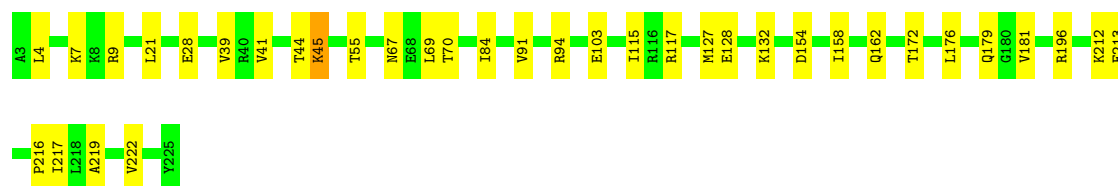
- Molecule 5: 40S ribosomal protein S3

Chain S3:  83% 17%




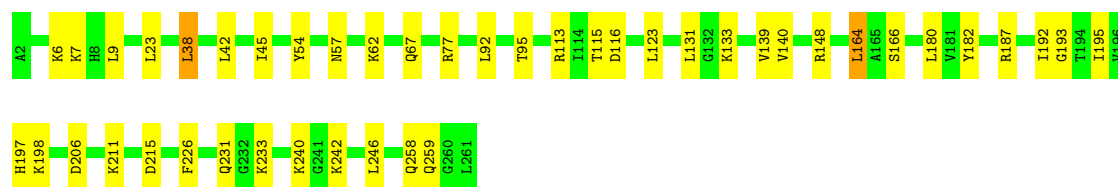
- Molecule 5: 40S ribosomal protein S3

Chain s3:  84% 16%




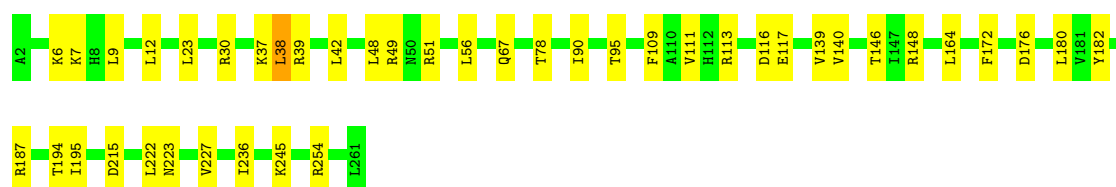
- Molecule 6: 40S ribosomal protein S4-A

Chain S4:  83% 16%




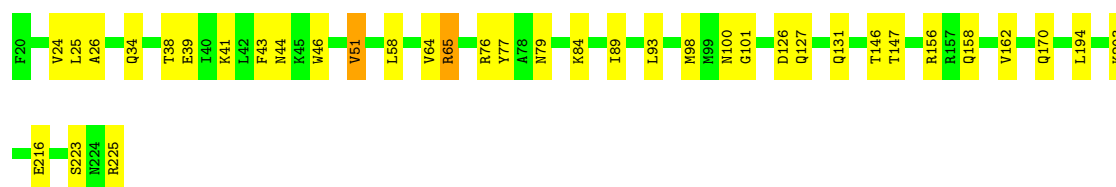
- Molecule 6: 40S ribosomal protein S4-A

Chain s4:  84% 16%




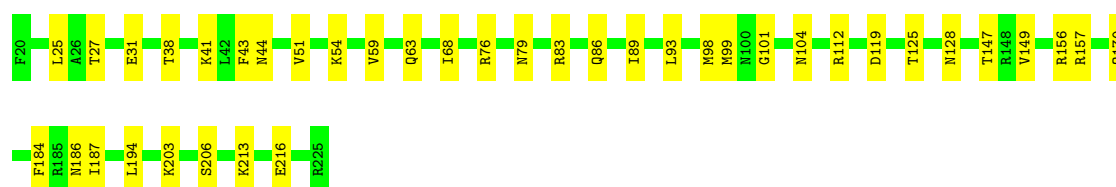
- Molecule 7: 40S ribosomal protein S5

Chain S5:  82% 17% .



- Molecule 7: 40S ribosomal protein S5

Chain s5:  81% 19%




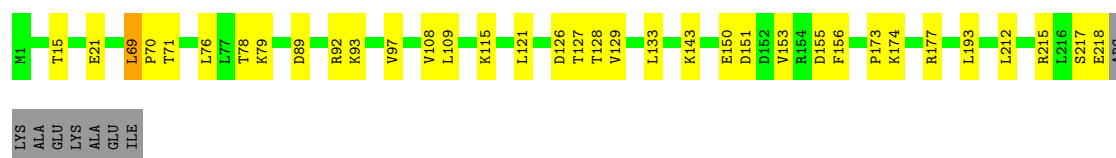
- Molecule 8: 40S ribosomal protein S6-A

Chain S6:  88% 12%




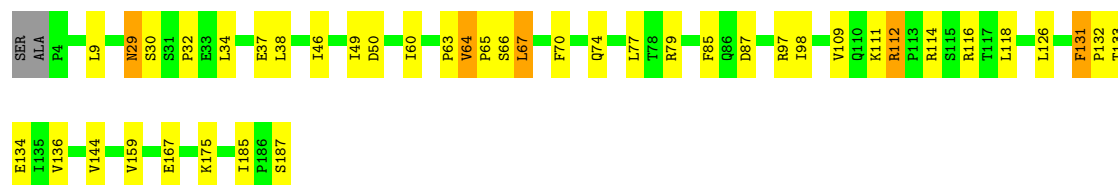
- Molecule 8: 40S ribosomal protein S6-A

Chain s6:  81% 15% .



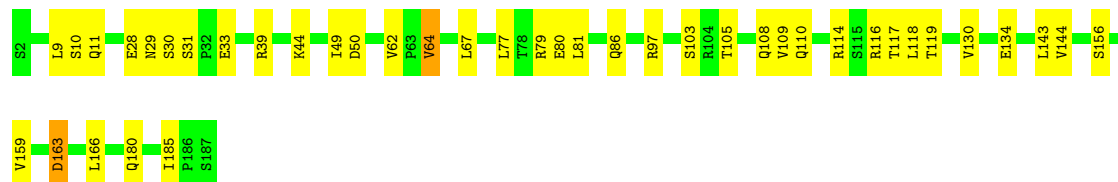
- Molecule 9: 40S ribosomal protein S7-A

Chain S7:  76% 20% ..



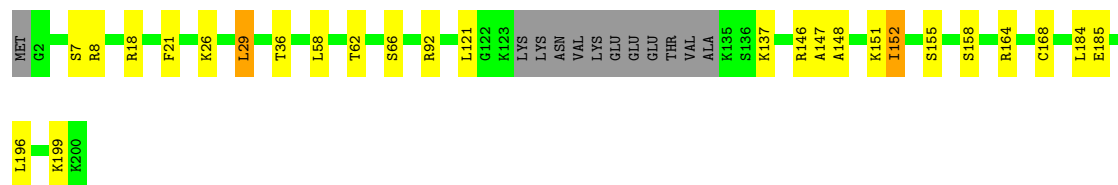
• Molecule 9: 40S ribosomal protein S7-A

Chain s7: 78% 21% .



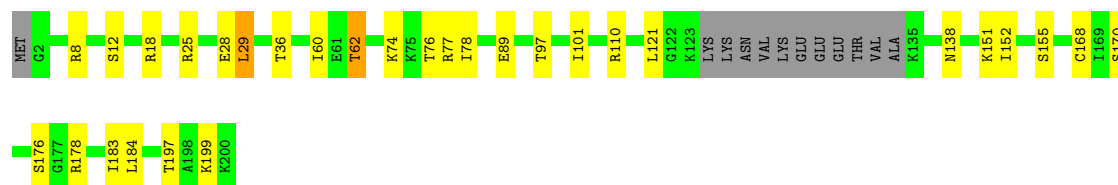
• Molecule 10: 40S ribosomal protein S8-A

Chain S8: 81% 12% 6% .



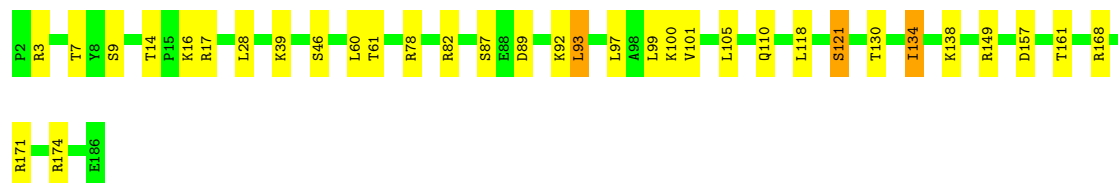
• Molecule 10: 40S ribosomal protein S8-A

Chain s8: 79% 14% 6% .



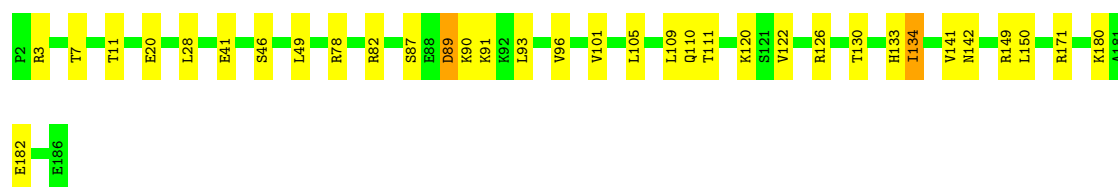
• Molecule 11: 40S ribosomal protein S9-A

Chain S9: 82% 17% .



• Molecule 11: 40S ribosomal protein S9-A

Chain s9: 82% 17% .



- Molecule 12: 40S ribosomal protein S10-A

Chain C0: 80% 17% ..



- Molecule 12: 40S ribosomal protein S10-A

Chain c0: 74% 19% . .



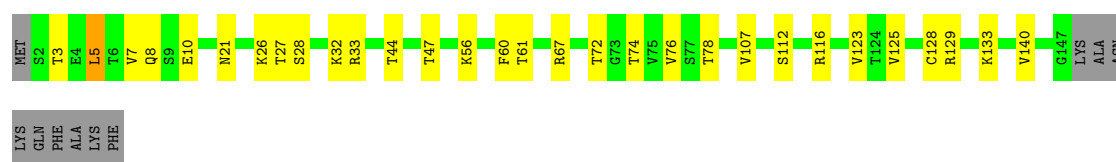
- Molecule 13: 40S ribosomal protein S11-A

Chain C1: 83% 17% .



- Molecule 13: 40S ribosomal protein S11-A

Chain c1: 74% 19% . 6%



- Molecule 14: 40S ribosomal protein S12

Chain C2: 77% 21% .




- Molecule 14: 40S ribosomal protein S12

Chain c2: 78% 19% .



- Molecule 15: 40S ribosomal protein S13

Chain C3:  83% 17% .



- Molecule 15: 40S ribosomal protein S13

Chain c3:  80% 19% .




- Molecule 16: 40S ribosomal protein S14-B

Chain C4:  84% 15% ..



- Molecule 16: 40S ribosomal protein S14-B

Chain c4:  81% 18% .




- Molecule 17: 40S ribosomal protein S15

Chain C5:  73% 14% . 13%




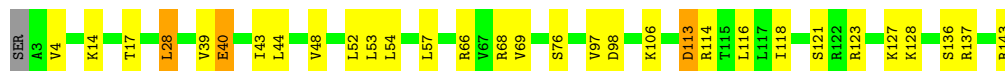
- Molecule 17: 40S ribosomal protein S15

Chain c5:  77% 17% . 5%




- Molecule 18: 40S ribosomal protein S16-A

Chain C6:  77% 20% ..



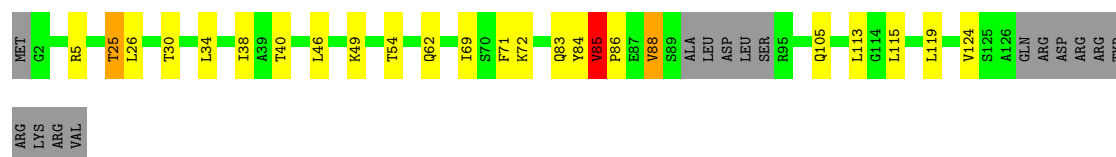
- Molecule 18: 40S ribosomal protein S16-A

Chain c6:  84% 15% .



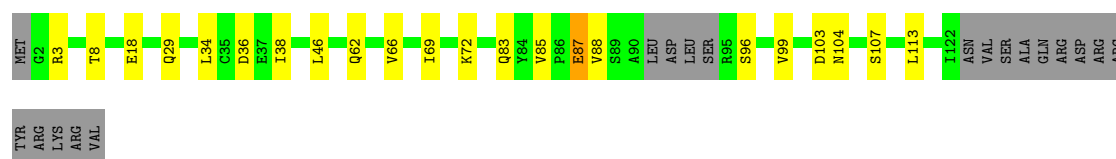
- Molecule 19: 40S ribosomal protein S17-A

Chain C7:  71% 15% .. 12%




- Molecule 19: 40S ribosomal protein S17-A

Chain c7:  70% 15% . 14%




- Molecule 20: 40S ribosomal protein S18-A

Chain C8:  82% 16% .




- Molecule 20: 40S ribosomal protein S18-A

Chain c8:  81% 19% .




- Molecule 21: 40S ribosomal protein S19-A

Chain C9:  84% 16%



- Molecule 21: 40S ribosomal protein S19-A

Chain c9:  86% 13% .



- Molecule 22: 40S ribosomal protein S20

Chain D0: 78% 18% ..



- Molecule 22: 40S ribosomal protein S20

Chain d0: 75% 22% .



- Molecule 23: 40S ribosomal protein S21-A

Chain D1: 86% 14%



- Molecule 23: 40S ribosomal protein S21-A

Chain d1: 79% 21%



- Molecule 24: 40S ribosomal protein S22-A

Chain D2: 81% 16% .



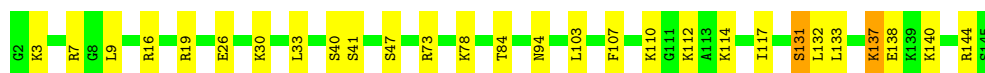
- Molecule 24: 40S ribosomal protein S22-A

Chain d2: 88% 10% .



- Molecule 25: 40S ribosomal protein S23-A

Chain D3: 81% 18% .



- Molecule 25: 40S ribosomal protein S23-A

Chain d3: 85% 15%



- Molecule 26: 40S ribosomal protein S24-A

Chain D4: 81% 16%



- Molecule 26: 40S ribosomal protein S24-A

Chain d4: 88% 10%



- Molecule 27: 40S ribosomal protein S25-A

Chain D5: 74% 24%



- Molecule 27: 40S ribosomal protein S25-A

Chain d5: 83% 16%



- Molecule 28: 40S ribosomal protein S26-B

Chain D6: 76% 19%



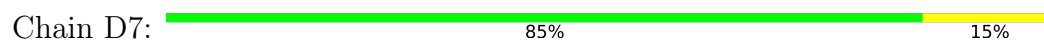
- Molecule 28: 40S ribosomal protein S26-B

Chain d6: 80% 16%

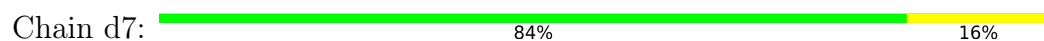




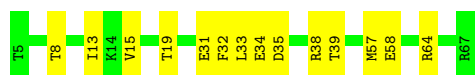
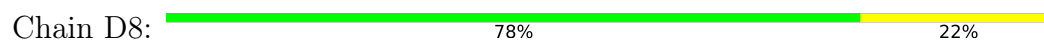
- Molecule 29: 40S ribosomal protein S27-A



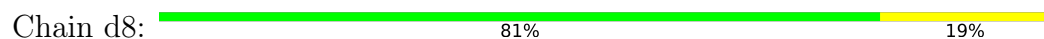
- Molecule 29: 40S ribosomal protein S27-A



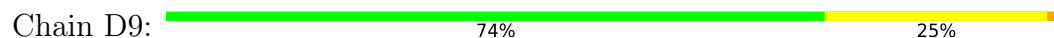
- Molecule 30: 40S ribosomal protein S28-A



- Molecule 30: 40S ribosomal protein S28-A



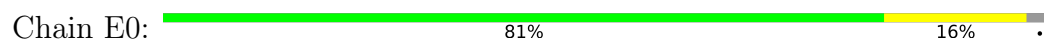
- Molecule 31: 40S ribosomal protein S29-A



- Molecule 31: 40S ribosomal protein S29-A

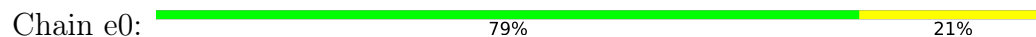


- Molecule 32: 40S ribosomal protein S30-A

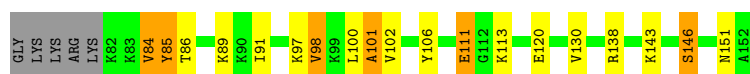




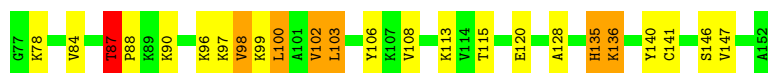
- Molecule 32: 40S ribosomal protein S30-A



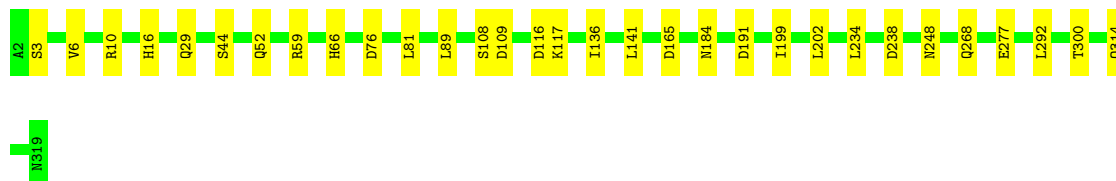
- Molecule 33: Ubiquitin-40S ribosomal protein S31



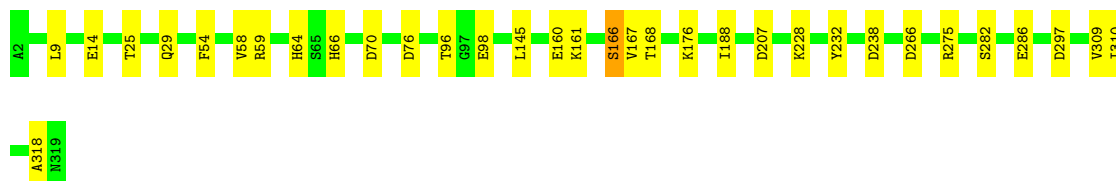
- Molecule 33: Ubiquitin-40S ribosomal protein S31



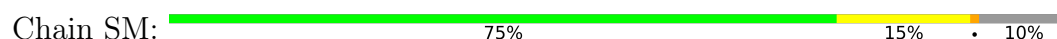
- Molecule 34: Guanine nucleotide-binding protein subunit beta-like protein

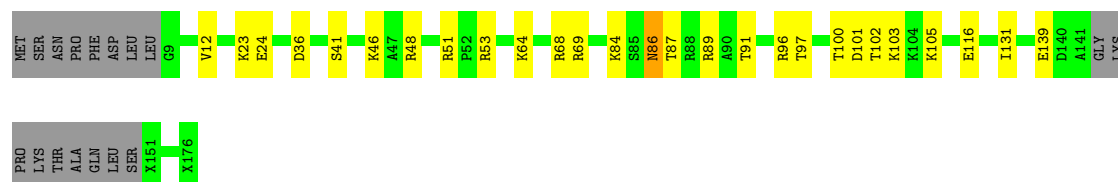


- Molecule 34: Guanine nucleotide-binding protein subunit beta-like protein



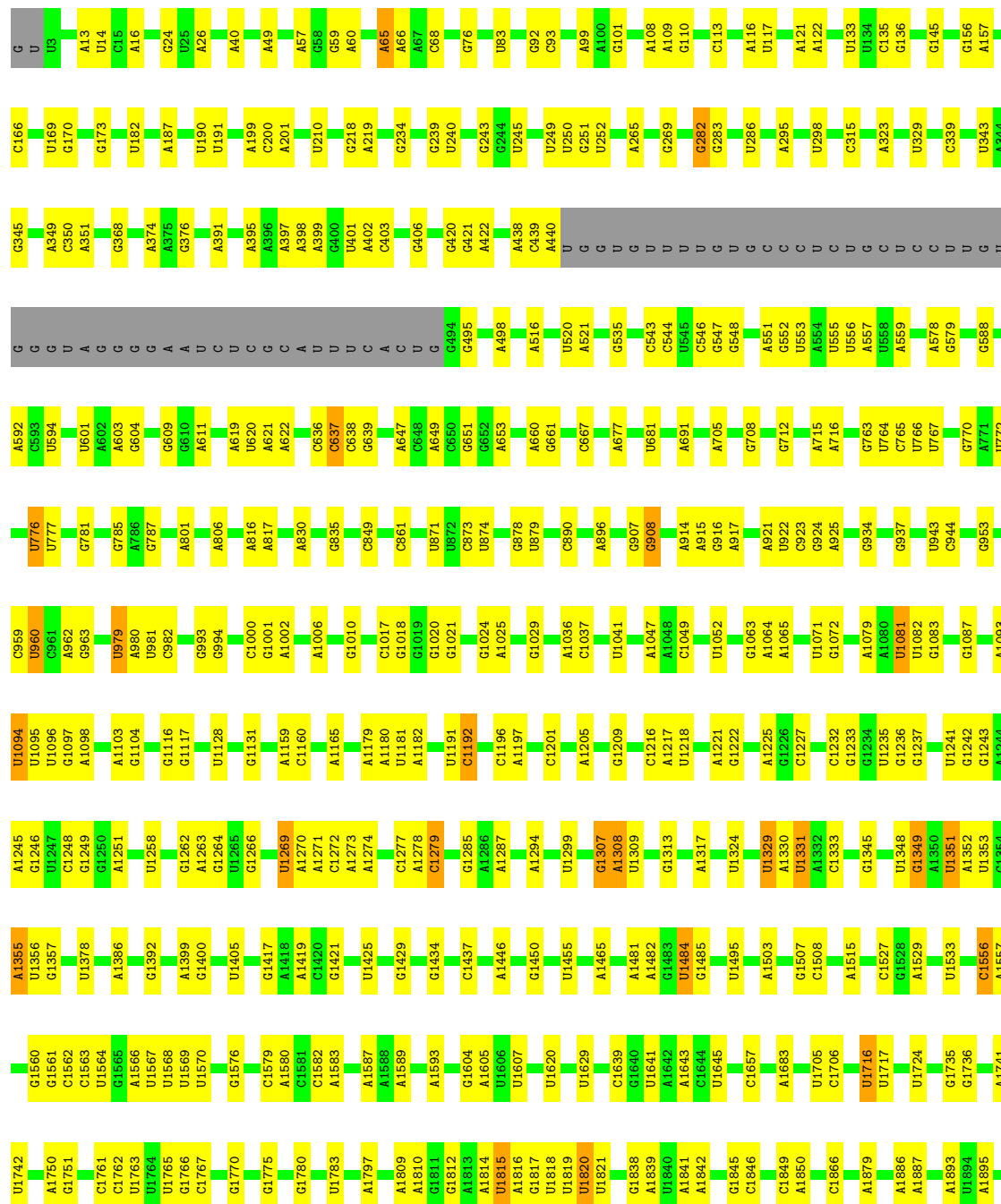
- Molecule 35: Suppressor protein STM1, Suppressor protein STM1, Suppressor protein STM1





• Molecule 36: 25S ribosomal RNA

Chain 1: 71% 20% 7%

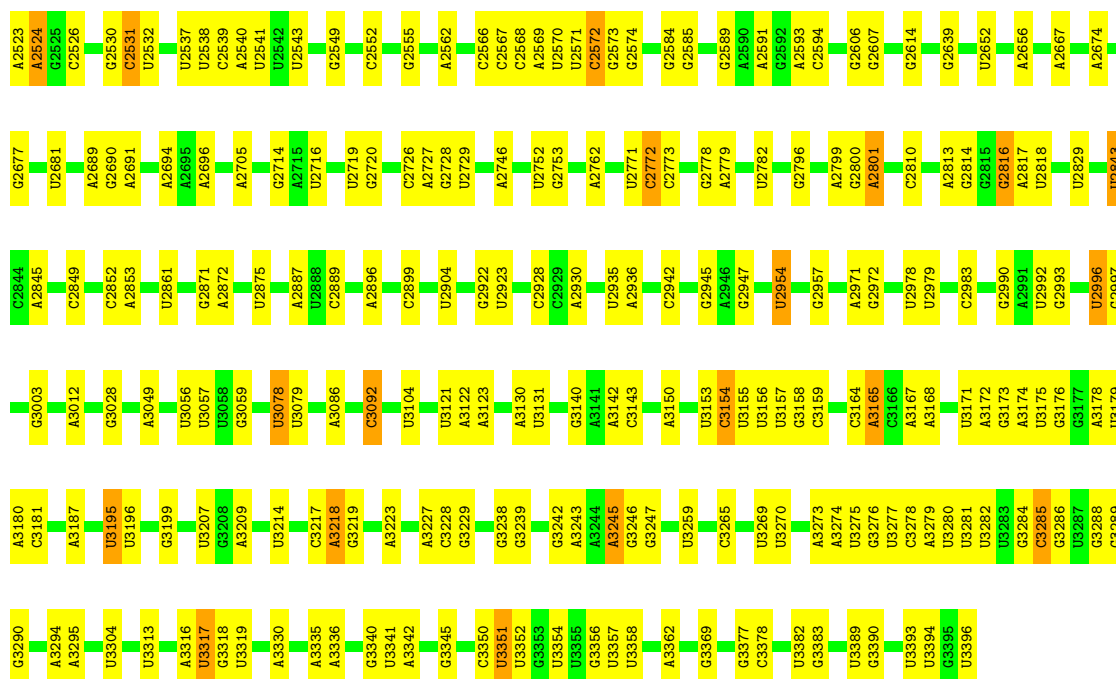




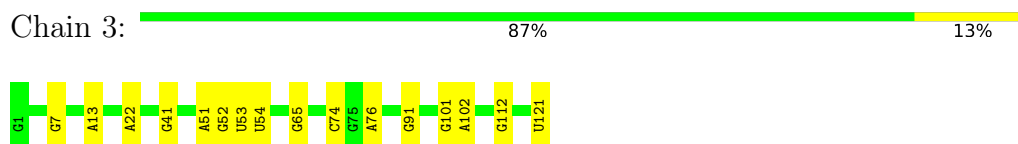
71% 20% 7%



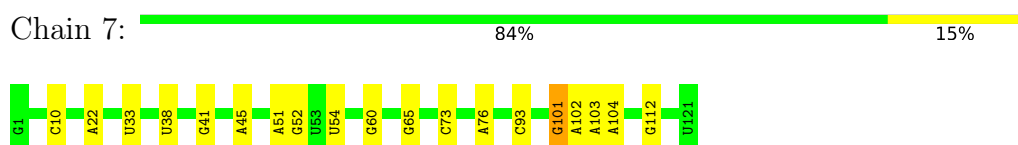




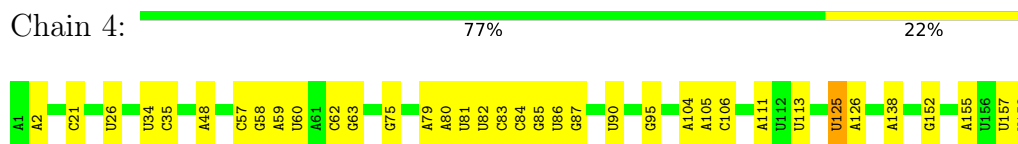
• Molecule 37: 5S ribosomal RNA



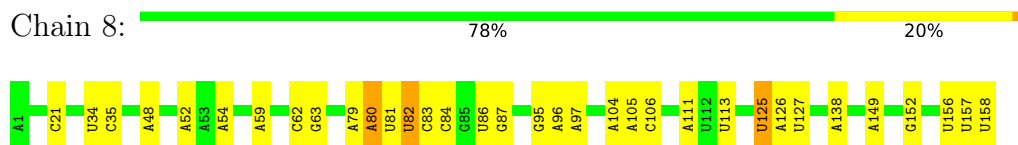
• Molecule 37: 5S ribosomal RNA




• Molecule 38: 5.8S ribosomal RNA



• Molecule 38: 5.8S ribosomal RNA




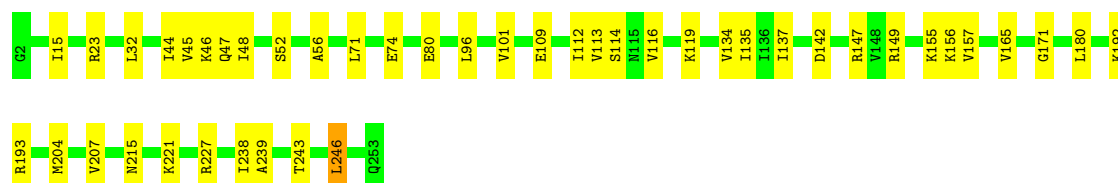
• Molecule 39: 60S ribosomal protein L2-A

Chain L2:  88% 12%




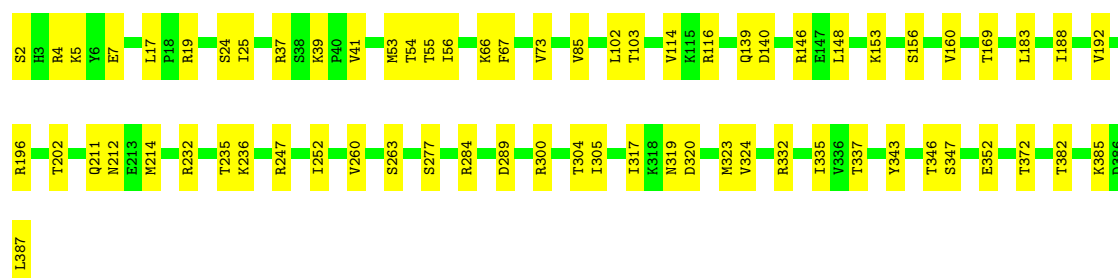
• Molecule 39: 60S ribosomal protein L2-A

Chain l2:  83% 17%




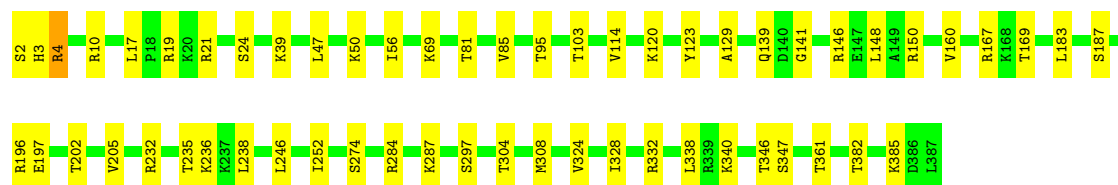
• Molecule 40: 60S ribosomal protein L3

Chain L3:  82% 18%




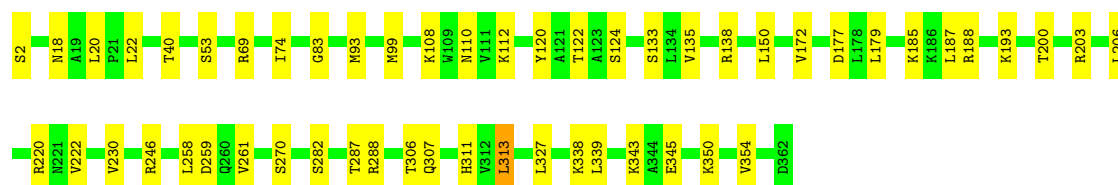
• Molecule 40: 60S ribosomal protein L3

Chain l3:  85% 15%

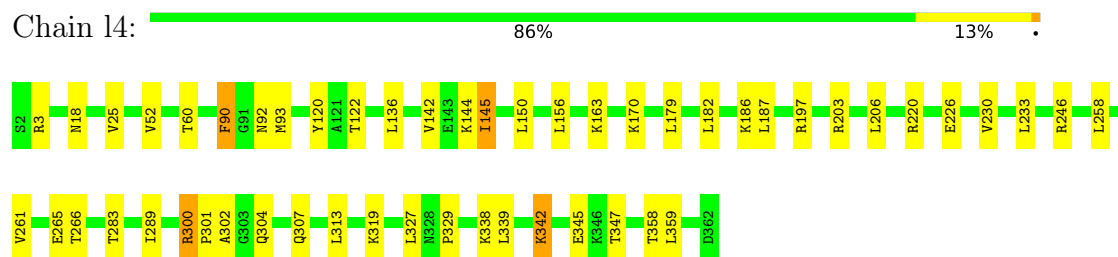


• Molecule 41: 60S ribosomal protein L4-A

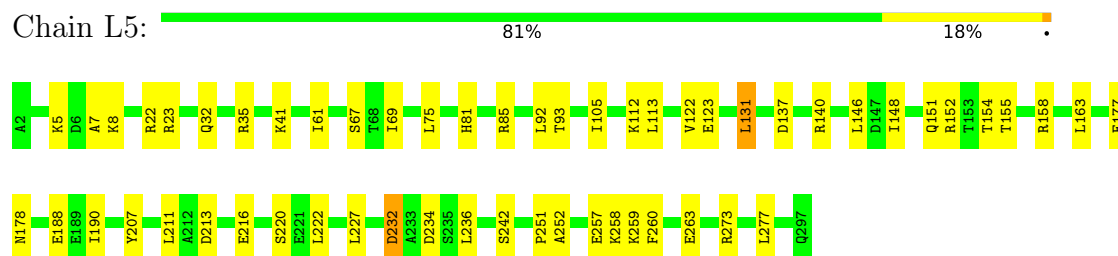
Chain L4:  85% 14%



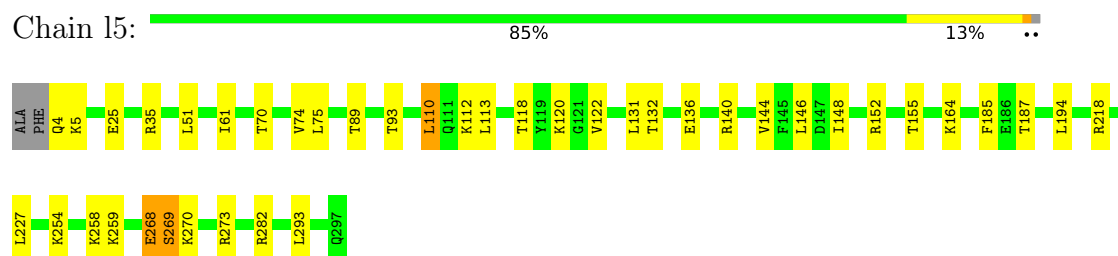
• Molecule 41: 60S ribosomal protein L4-A



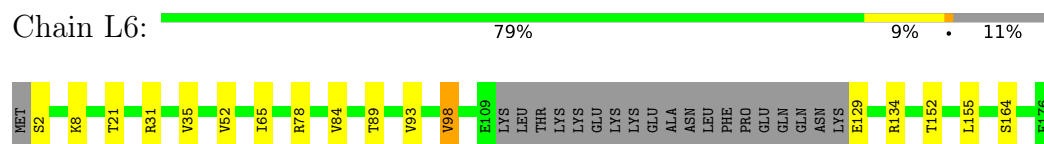
- Molecule 42: 60S ribosomal protein L5



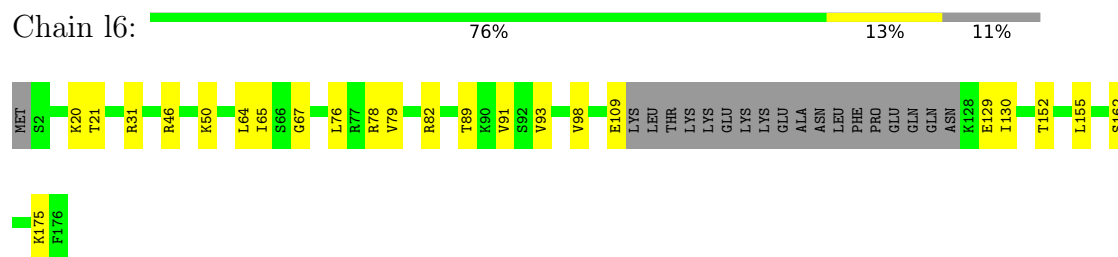
- Molecule 42: 60S ribosomal protein L5



- Molecule 43: 60S ribosomal protein L6-A



- Molecule 43: 60S ribosomal protein L6-A



- Molecule 44: 60S ribosomal protein L7-A







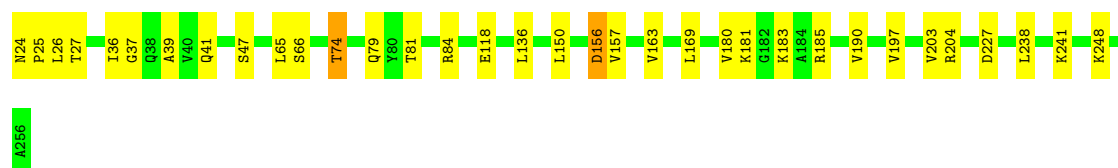
- Molecule 44: 60S ribosomal protein L7-A

Chain 17: 87% 13%



- Molecule 45: 60S ribosomal protein L8-A

Chain L8: 85% 14%



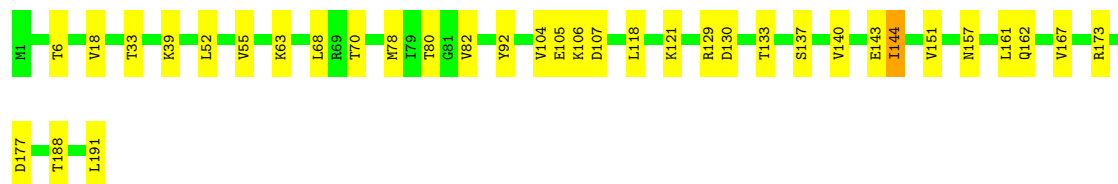
- Molecule 46: 60S ribosomal protein L9-A

Chain L9: 81% 19%



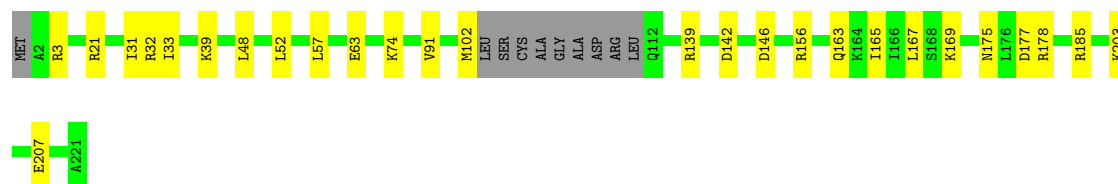
- Molecule 46: 60S ribosomal protein L9-A

Chain 19: 82% 18%

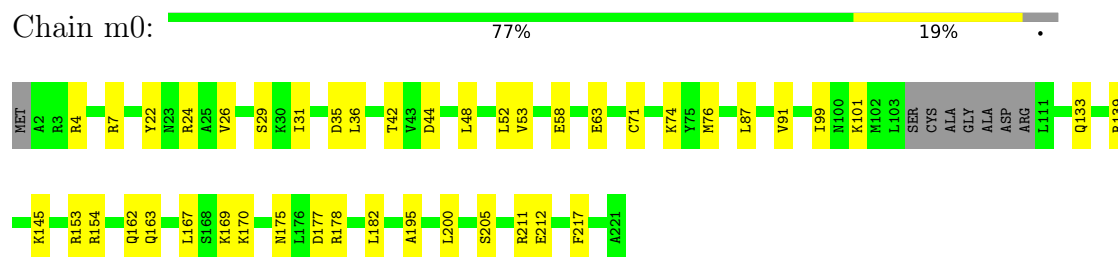


- Molecule 47: 60S ribosomal protein L10

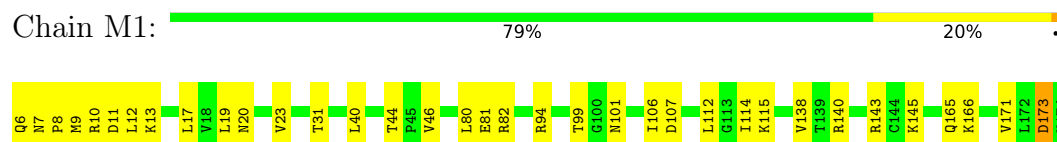
Chain M0: 83% 12% 5%



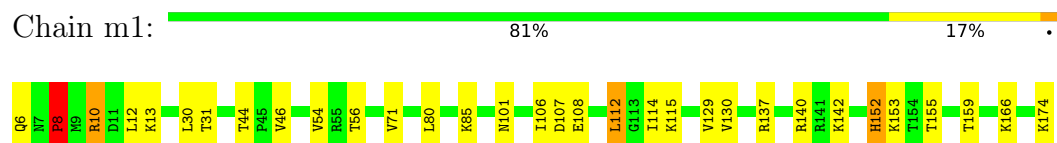
- Molecule 47: 60S ribosomal protein L10



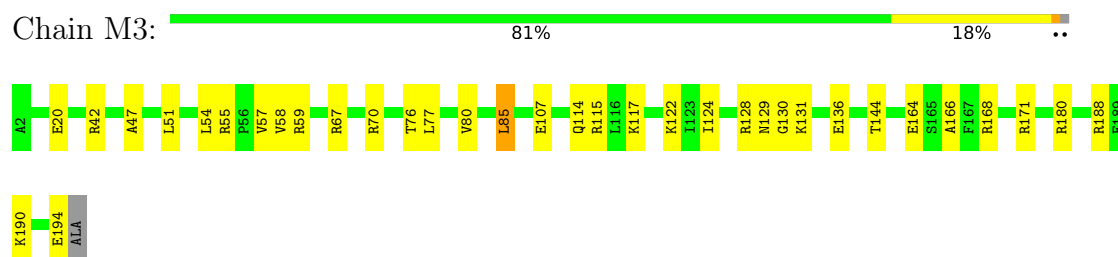
- Molecule 48: 60S ribosomal protein L11-B



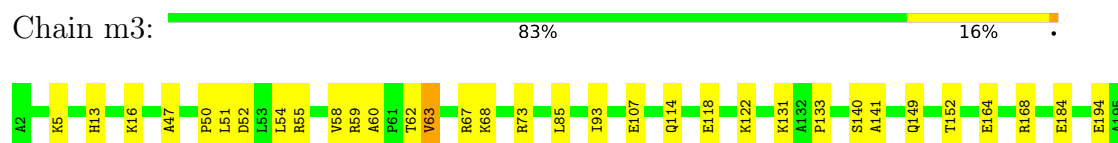
- Molecule 48: 60S ribosomal protein L11-B



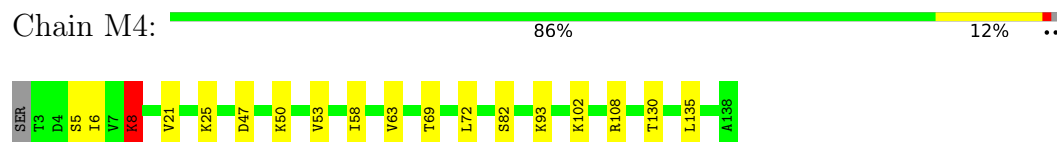
- Molecule 49: 60S ribosomal protein L13-A



- Molecule 49: 60S ribosomal protein L13-A

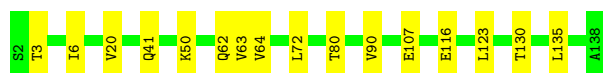


- Molecule 50: 60S ribosomal protein L14-A



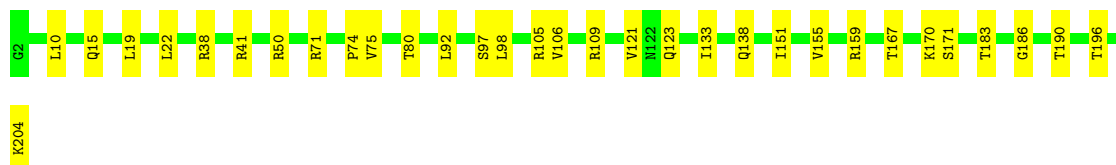
- Molecule 50: 60S ribosomal protein L14-A





- Molecule 51: 60S ribosomal protein L15-A

Chain M5: 84% 16%



- Molecule 51: 60S ribosomal protein L15-A

Chain m5: 84% 15%



- Molecule 52: 60S ribosomal protein L16-A

Chain M6: 85% 15%



- Molecule 52: 60S ribosomal protein L16-A

Chain m6: 85% 15%



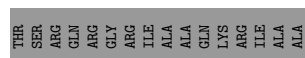
- Molecule 53: 60S ribosomal protein L17-A

Chain M7: 86% 14%



- Molecule 53: 60S ribosomal protein L17-A

Chain m7: 70% 14% 15%




- Molecule 54: 60S ribosomal protein L18-A

Chain M8:  86% 12%



- Molecule 54: 60S ribosomal protein L18-A

Chain m8:  85% 15%



- Molecule 55: 60S ribosomal protein L19-A

Chain M9:  88% 12%




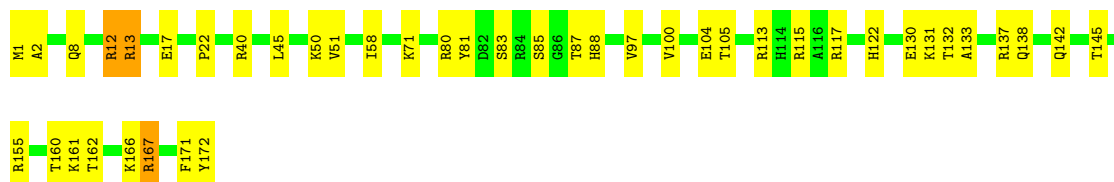
- Molecule 55: 60S ribosomal protein L19-A

Chain m9:  88% 12%




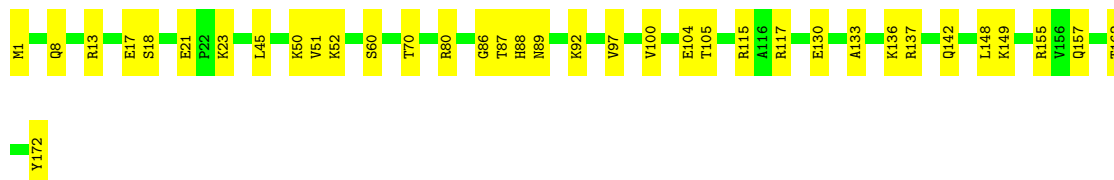
- Molecule 56: 60S ribosomal protein L20-A

Chain N0:  75% 23%

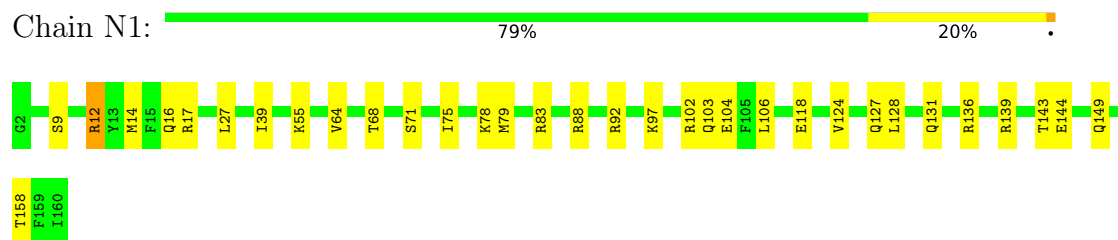


- Molecule 56: 60S ribosomal protein L20-A

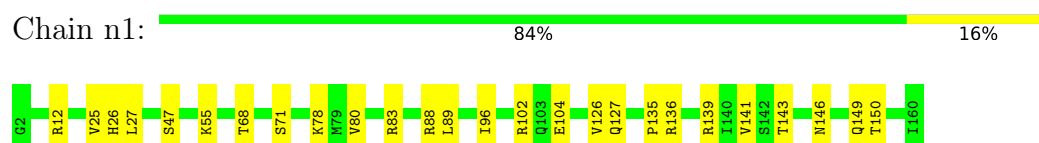
Chain n0:  79% 21%



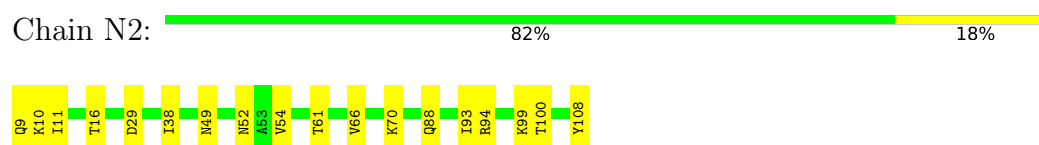
- Molecule 57: 60S ribosomal protein L21-A



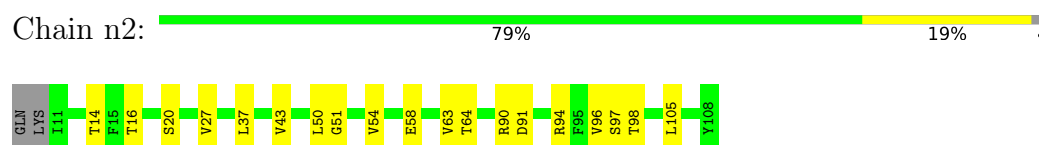
- Molecule 57: 60S ribosomal protein L21-A



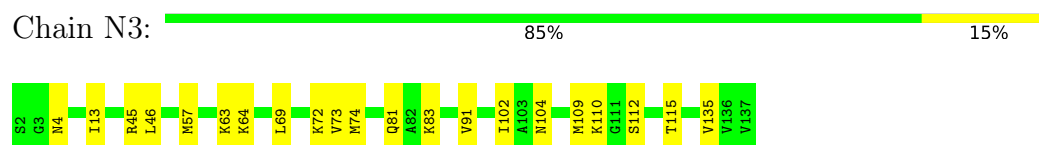
- Molecule 58: 60S ribosomal protein L22-A



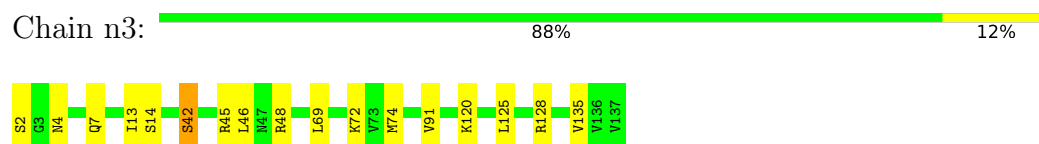
- Molecule 58: 60S ribosomal protein L22-A



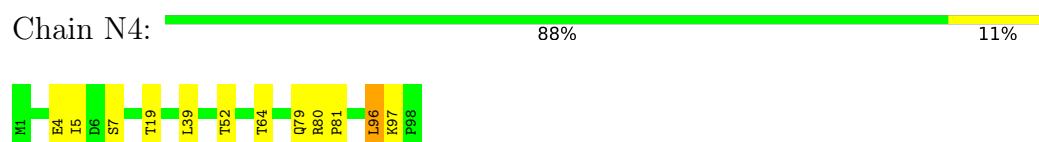
- Molecule 59: 60S ribosomal protein L23-A




- Molecule 59: 60S ribosomal protein L23-A



- Molecule 60: 60S ribosomal protein L24-A




- Molecule 61: 60S ribosomal protein L25

Chain N5:  79% 20%




- Molecule 61: 60S ribosomal protein L25

Chain n5:  83% 16%




- Molecule 62: 60S ribosomal protein L26-A

Chain N6:  83% 17%




- Molecule 62: 60S ribosomal protein L26-A

Chain n6:  77% 23%




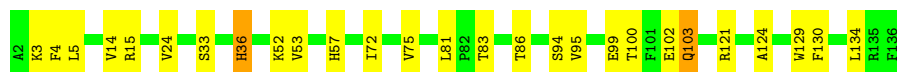
- Molecule 63: 60S ribosomal protein L27-A

Chain N7:  84% 16%




- Molecule 63: 60S ribosomal protein L27-A

Chain n7:  80% 19%




- Molecule 64: 60S ribosomal protein L28

Chain N8:  83% 16%




- Molecule 64: 60S ribosomal protein L28

Chain n8:  80% 19% .




- Molecule 65: 60S ribosomal protein L29

Chain N9:  84% 16%




- Molecule 65: 60S ribosomal protein L29

Chain n9:  84% 14% .




- Molecule 66: 60S ribosomal protein L30

Chain O0:  81% 16% .




- Molecule 66: 60S ribosomal protein L30

Chain o0:  86% 13% .




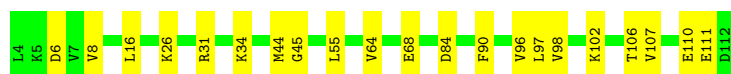
- Molecule 67: 60S ribosomal protein L31-A

Chain O1:  85% 15%



- Molecule 67: 60S ribosomal protein L31-A

Chain o1:  81% 19%




- Molecule 68: 60S ribosomal protein L32

Chain O2:  89% 11%



- Molecule 68: 60S ribosomal protein L32

Chain o2:  82% 18%



- Molecule 69: 60S ribosomal protein L33-A

Chain O3:  89% 11%



- Molecule 69: 60S ribosomal protein L33-A

Chain o3:  91% 9%



- Molecule 70: 60S ribosomal protein L34-A

Chain O4:  88% 12%




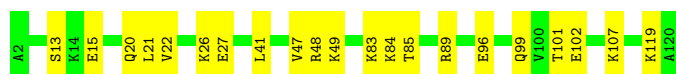
- Molecule 70: 60S ribosomal protein L34-A

Chain o4:  89% 11%




- Molecule 71: 60S ribosomal protein L35-A

Chain O5:  82% 18%




- Molecule 71: 60S ribosomal protein L35-A



Chain o5:  85% 15%




- Molecule 72: 60S ribosomal protein L36-A

Chain O6:  76% 24%



- Molecule 72: 60S ribosomal protein L36-A

Chain o6:  74% 25%




- Molecule 73: 60S ribosomal protein L37-A

Chain O7:  90% 10%




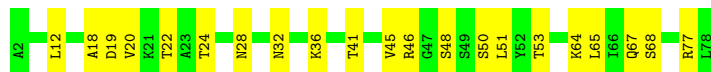
- Molecule 73: 60S ribosomal protein L37-A

Chain o7:  84% 16%




- Molecule 74: 60S ribosomal protein L38

Chain O8:  73% 27%



- Molecule 74: 60S ribosomal protein L38

Chain o8:  82% 18%




- Molecule 75: 60S ribosomal protein L39

Chain O9:  90% 10%




- Molecule 75: 60S ribosomal protein L39

Chain o9:  86% 14%




- Molecule 76: Ubiquitin-60S ribosomal protein L40

Chain Q0:  87% 13%




- Molecule 76: Ubiquitin-60S ribosomal protein L40

Chain q0:  81% 19%



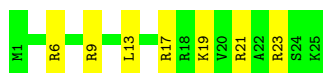
- Molecule 77: 60S ribosomal protein L41-A

Chain Q1:  80% 20%




- Molecule 77: 60S ribosomal protein L41-A

Chain q1:  72% 28%




- Molecule 78: 60S ribosomal protein L42-A

Chain Q2:  83% 16%




- Molecule 78: 60S ribosomal protein L42-A

Chain q2:  81% 19%




- Molecule 79: 60S ribosomal protein L43-A

Chain Q3:  85% 15%



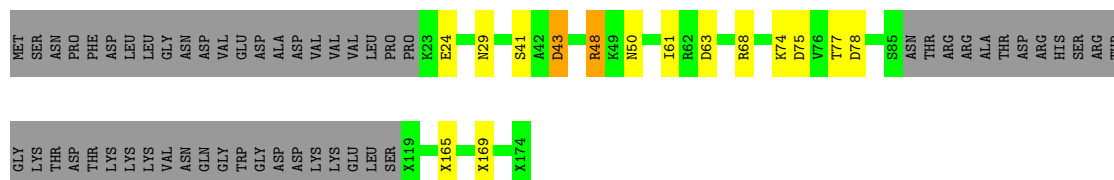
- Molecule 79: 60S ribosomal protein L43-A

Chain q3:  81% 18% .




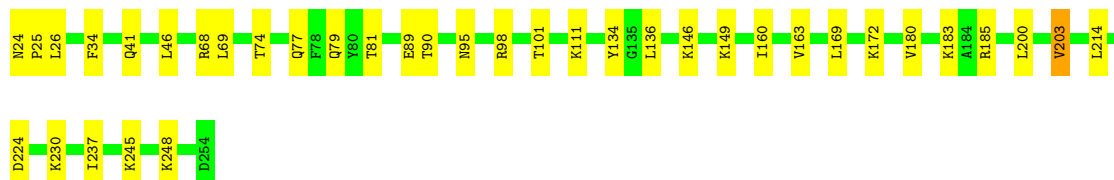
- Molecule 80: Suppressor protein STM1, Suppressor protein STM1, Suppressor protein STM1

Chain sM:  56% 8% . 35%



- Molecule 81: 60S ribosomal protein L8-A

Chain l8:  84% 16%



- Molecule 82: 60S ribosomal protein L12

Chain m2:  94% . .

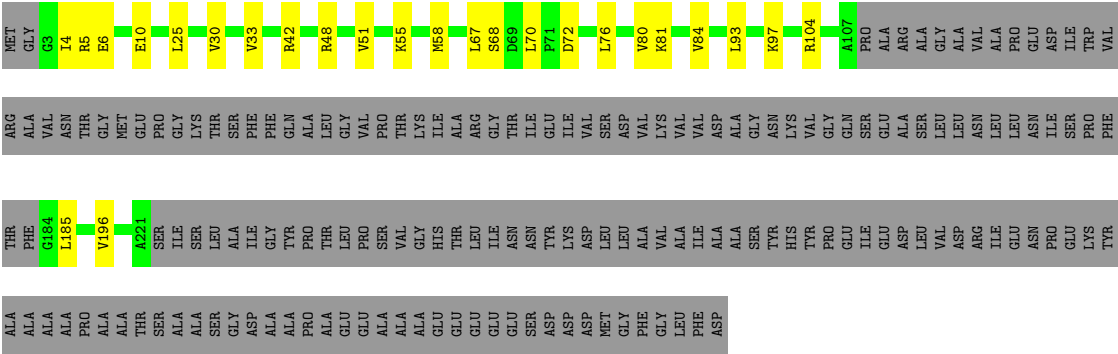
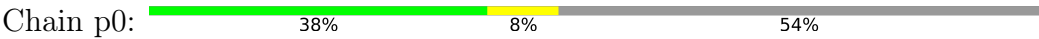


- Molecule 83: 60S ribosomal protein L24-A

Chain n4:  86% 13% .



• Molecule 84: 60S acidic ribosomal protein P0



• Molecule 85: Ribosomal protein P1 alpha, P2 beta



There are no outlier residues recorded for this chain.

• Molecule 85: Ribosomal protein P1 alpha, P2 beta



## 4 Data and refinement statistics

EDS failed to run properly - this section is therefore incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	434.23Å 287.91Å 304.12Å 90.00° 99.11° 90.00°	Depositor
Resolution (Å)	103.62 – 3.10	Depositor
% Data completeness (in resolution range)	100.0 (103.62-3.10)	Depositor
$R_{merge}$	0.23	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	0.94 (at 3.13Å)	Xtriage
Refinement program	PHENIX	Depositor
R, $R_{free}$	0.212 , 0.251	Depositor
Wilson B-factor (Å <sup>2</sup> )	68.5	Xtriage
Anisotropy	0.202	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	410475	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	78.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.57% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  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: ZN, MG, UAM, OHX

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	2	0.37	0/42442	0.93	91/66130 (0.1%)
1	6	0.42	1/42765 (0.0%)	0.93	69/66634 (0.1%)
2	S0	0.33	0/1617	0.59	0/2215
2	s0	0.33	0/1623	0.60	1/2222 (0.0%)
3	S1	0.30	0/1735	0.61	0/2335
3	s1	0.32	1/1748 (0.1%)	0.61	0/2352
4	S2	0.32	0/1665	0.59	0/2263
4	s2	0.33	0/1665	0.62	0/2263
5	S3	0.31	0/1759	0.56	0/2368
5	s3	0.31	0/1759	0.57	0/2368
6	S4	0.32	0/2109	0.63	2/2839 (0.1%)
6	s4	0.34	0/2109	0.66	3/2839 (0.1%)
7	S5	0.28	0/1629	0.56	0/2202
7	s5	0.30	0/1629	0.57	0/2202
8	S6	0.31	0/1823	0.53	0/2439
8	s6	0.34	0/1779	0.58	0/2379
9	S7	0.32	0/1506	0.66	1/2028 (0.0%)
9	s7	0.31	0/1516	0.63	1/2043 (0.0%)
10	S8	0.33	0/1514	0.60	1/2021 (0.0%)
10	s8	0.35	0/1514	0.59	1/2021 (0.0%)
11	S9	0.31	0/1519	0.57	1/2035 (0.0%)
11	s9	0.33	0/1519	0.60	0/2035
12	C0	0.30	0/789	0.67	1/1067 (0.1%)
12	c0	0.30	0/776	0.70	3/1047 (0.3%)
13	C1	0.35	0/1239	0.60	0/1673
13	c1	0.39	1/1194 (0.1%)	0.61	1/1610 (0.1%)
14	C2	0.31	0/898	0.69	1/1220 (0.1%)
14	c2	0.28	0/898	0.67	1/1220 (0.1%)
15	C3	0.33	0/1215	0.55	1/1638 (0.1%)
15	c3	0.31	0/1215	0.60	1/1638 (0.1%)
16	C4	0.30	0/901	0.62	0/1217
16	c4	0.32	0/960	0.57	0/1290

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
17	C5	0.33	0/998	0.60	0/1341
17	c5	0.31	0/1060	0.65	1/1426 (0.1%)
18	C6	0.30	0/1125	0.66	2/1510 (0.1%)
18	c6	0.31	0/1131	0.57	1/1518 (0.1%)
19	C7	0.36	0/935	0.72	2/1254 (0.2%)
19	c7	0.31	0/914	0.60	0/1224
20	C8	0.30	0/1211	0.58	0/1628
20	c8	0.31	0/1211	0.59	1/1628 (0.1%)
21	C9	0.30	0/1130	0.52	0/1517
21	c9	0.35	0/1130	0.55	0/1517
22	D0	0.32	0/865	0.60	0/1169
22	d0	0.32	0/892	0.60	0/1205
23	D1	0.31	0/693	0.58	0/935
23	d1	0.31	0/693	0.58	0/935
24	D2	0.32	0/1038	0.62	3/1395 (0.2%)
24	d2	0.35	0/1038	0.61	1/1395 (0.1%)
25	D3	0.37	0/1139	0.61	0/1518
25	d3	0.38	0/1139	0.60	0/1518
26	D4	0.32	0/1087	0.57	0/1449
26	d4	0.34	0/1087	0.64	1/1449 (0.1%)
27	D5	0.31	0/571	0.62	0/768
27	d5	0.31	0/566	0.51	0/761
28	D6	0.32	0/782	0.67	1/1047 (0.1%)
28	d6	0.34	0/782	0.58	0/1047
29	D7	0.28	0/620	0.61	0/838
29	d7	0.30	0/620	0.63	0/838
30	D8	0.27	0/499	0.54	0/670
30	d8	0.31	0/499	0.59	0/670
31	D9	0.40	0/452	0.68	1/600 (0.2%)
31	d9	0.32	0/452	0.57	0/600
32	E0	0.30	0/483	0.55	0/643
32	e0	0.35	0/499	0.66	0/665
33	E1	0.33	0/577	0.87	1/770 (0.1%)
33	e1	0.35	0/619	0.91	3/822 (0.4%)
34	SR	0.29	0/2490	0.55	0/3389
34	sR	0.28	0/2491	0.56	0/3391
35	SM	0.32	0/984	0.60	0/1323
36	1	0.53	0/75394	0.99	140/117545 (0.1%)
36	5	0.54	1/75414 (0.0%)	0.99	107/117575 (0.1%)
37	3	0.41	0/2883	0.86	1/4491 (0.0%)
37	7	0.52	0/2883	0.96	2/4491 (0.0%)
38	4	0.52	0/3746	0.97	3/5832 (0.1%)
38	8	0.44	0/3746	0.90	5/5832 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
39	L2	0.38	0/1948	0.63	0/2617
39	l2	0.37	0/1946	0.65	1/2614 (0.0%)
40	L3	0.38	0/3146	0.63	0/4228
40	l3	0.43	0/3146	0.65	1/4228 (0.0%)
41	L4	0.41	0/2800	0.66	3/3790 (0.1%)
41	l4	0.38	0/2800	0.65	1/3790 (0.0%)
42	L5	0.34	0/2425	0.60	1/3271 (0.0%)
42	l5	0.39	0/2408	0.59	1/3248 (0.0%)
43	L6	0.37	0/1260	0.58	0/1694
43	l6	0.40	0/1269	0.62	1/1705 (0.1%)
44	L7	0.38	0/1821	0.58	0/2451
44	l7	0.41	0/1828	0.62	2/2461 (0.1%)
45	L8	0.33	0/1836	0.54	0/2481
46	L9	0.33	0/1539	0.56	0/2073
46	l9	0.39	0/1539	0.58	0/2073
47	M0	0.38	0/1741	0.60	1/2335 (0.0%)
47	m0	0.42	0/1758	0.65	0/2358
48	M1	0.32	0/1374	0.56	0/1842
48	m1	0.36	0/1374	0.67	3/1842 (0.2%)
49	M3	0.39	0/1568	0.65	1/2106 (0.0%)
49	m3	0.36	0/1573	0.62	0/2113
50	M4	0.36	0/1068	0.55	0/1438
50	m4	0.40	0/1074	0.56	0/1446
51	M5	0.38	0/1757	0.60	0/2354
51	m5	0.35	0/1757	0.59	0/2354
52	M6	0.42	0/1585	0.57	0/2128
52	m6	0.52	0/1585	0.61	0/2128
53	M7	0.39	0/1443	0.63	0/1944
53	m7	0.43	0/1250	0.61	0/1683
54	M8	0.39	0/1465	0.63	1/1965 (0.1%)
54	m8	0.38	0/1465	0.61	0/1965
55	M9	0.31	0/1538	0.51	1/2050 (0.0%)
55	m9	0.34	0/1538	0.47	0/2050
56	N0	0.37	0/1481	0.62	0/1990
56	n0	0.42	0/1481	0.58	0/1990
57	N1	0.39	0/1300	0.60	0/1743
57	n1	0.43	0/1300	0.59	0/1743
58	N2	0.33	0/812	0.59	0/1099
58	n2	0.32	0/794	0.56	0/1076
59	N3	0.38	0/1018	0.60	0/1369
59	n3	0.43	0/1018	0.65	0/1369
60	N4	0.34	0/712	0.62	2/958 (0.2%)
61	N5	0.35	0/979	0.62	2/1321 (0.2%)



Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
61	n5	0.34	0/974	0.58	0/1314
62	N6	0.38	0/1004	0.65	1/1341 (0.1%)
62	n6	0.36	0/1004	0.63	0/1341
63	N7	0.33	0/1118	0.54	0/1497
63	n7	0.40	1/1118 (0.1%)	0.53	0/1497
64	N8	0.41	0/1204	0.67	1/1612 (0.1%)
64	n8	0.40	0/1204	0.71	1/1612 (0.1%)
65	N9	0.38	0/473	0.57	0/629
65	n9	0.39	0/473	0.64	0/629
66	O0	0.31	0/751	0.52	0/1008
66	o0	0.30	0/775	0.54	1/1040 (0.1%)
67	O1	0.36	0/890	0.55	0/1196
67	o1	0.40	0/897	0.63	0/1205
68	O2	0.46	1/1041 (0.1%)	0.60	0/1394
68	o2	0.42	0/1041	0.65	0/1394
69	O3	0.43	0/868	0.60	0/1168
69	o3	0.46	0/868	0.67	0/1168
70	O4	0.33	0/890	0.59	1/1189 (0.1%)
70	o4	0.33	0/890	0.58	0/1189
71	O5	0.37	0/978	0.60	1/1301 (0.1%)
71	o5	0.33	0/974	0.51	0/1297
72	O6	0.34	0/778	0.57	0/1034
72	o6	0.34	0/777	0.58	0/1033
73	O7	0.41	0/696	0.70	0/923
73	o7	0.38	0/696	0.67	0/923
74	O8	0.33	0/618	0.55	0/826
74	o8	0.31	0/614	0.56	0/822
75	O9	0.41	0/443	0.65	0/588
75	o9	0.38	0/443	0.57	0/588
76	Q0	0.38	0/423	0.62	0/562
76	q0	0.47	0/423	0.66	0/562
77	Q1	0.33	0/234	0.54	0/300
77	q1	0.39	0/234	0.58	0/300
78	Q2	0.39	0/860	0.64	1/1136 (0.1%)
78	q2	0.38	0/860	0.58	0/1136
79	Q3	0.39	0/701	0.62	0/934
79	q3	0.40	0/701	0.63	0/934
80	sM	0.34	0/480	0.64	0/642
81	l8	0.33	0/1795	0.55	0/2429
83	n4	0.37	0/1052	0.63	1/1398 (0.1%)
84	p0	0.33	0/1092	0.55	0/1474
All	All	0.44	6/430471 (0.0%)	0.84	486/632040 (0.1%)

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
2	S0	0	1
2	s0	0	3
3	S1	0	1
3	s1	0	1
4	S2	0	1
4	s2	0	2
5	S3	0	1
5	s3	0	1
6	S4	0	1
7	S5	0	3
7	s5	0	4
9	S7	0	2
9	s7	0	3
10	S8	0	2
10	s8	0	1
11	s9	0	1
14	c2	0	1
15	c3	0	1
16	C4	0	3
16	c4	0	2
17	C5	0	2
17	c5	0	3
18	C6	0	2
18	c6	0	2
19	C7	0	1
19	c7	0	3
20	c8	0	1
22	D0	0	1
22	d0	0	1
23	d1	0	1
24	D2	0	1
24	d2	0	1
25	D3	0	1
25	d3	0	1
26	D4	0	1
26	d4	0	1
27	D5	0	2
27	d5	0	2
28	D6	0	2

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Mol	Chain	#Chirality outliers	#Planarity outliers
32	e0	0	1
33	E1	0	3
33	e1	0	3
34	sR	0	1
39	l2	0	1
40	l3	0	2
41	L4	0	1
41	l4	0	1
42	L5	0	3
42	l5	0	3
43	l6	0	1
44	l7	0	1
45	L8	0	2
46	L9	0	1
48	m1	0	1
49	M3	0	1
49	m3	0	1
50	M4	0	1
50	m4	0	1
51	M5	0	1
51	m5	0	1
52	M6	0	1
52	m6	0	1
53	m7	0	1
56	N0	0	3
56	n0	0	2
57	N1	0	1
58	n2	0	1
60	N4	0	2
63	n7	0	2
64	n8	0	1
65	N9	0	1
65	n9	0	1
66	o0	0	1
67	o1	0	1
70	o4	0	1
71	o5	0	1
79	Q3	0	1
79	q3	0	1
80	sM	0	2
81	l8	0	1
82	m2	0	5

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Mol	Chain	#Chirality outliers	#Planarity outliers
All	All	0	126

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	5	1152	G	N9-C4	-8.63	1.31	1.38
63	n7	36	HIS	C-N	7.01	1.47	1.34
68	O2	51	SER	C-N	-6.35	1.19	1.34
1	6	163	G	N9-C4	-5.93	1.33	1.38
13	c1	128	CYS	CB-SG	-5.29	1.73	1.81
3	s1	219	LYS	C-N	5.21	1.46	1.34

All (486) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	1152	G	N3-C4-N9	-16.34	116.20	126.00
36	5	1152	G	N3-C4-C5	15.93	136.56	128.60
1	6	163	G	N3-C4-N9	-11.53	119.08	126.00
36	1	1308	A	C8-N9-C4	-11.40	101.24	105.80
36	5	2726	C	C6-N1-C2	-10.77	115.99	120.30
36	5	1152	G	C8-N9-C1'	10.49	140.64	127.00
36	5	1152	G	C4-N9-C1'	-10.46	112.90	126.50
36	1	1308	A	N7-C8-N9	10.20	118.90	113.80
1	6	163	G	N3-C4-C5	9.52	133.36	128.60
36	1	406	G	O4'-C1'-N9	9.38	115.70	108.20
1	2	1096	C	N1-C2-O2	9.36	124.52	118.90
36	5	1307	G	P-O3'-C3'	9.30	130.86	119.70
36	1	3217	C	C2-N1-C1'	8.98	128.67	118.80
36	5	2572	C	N1-C2-O2	8.84	124.20	118.90
36	5	2726	C	N3-C2-O2	-8.79	115.75	121.90
1	2	1096	C	C2-N1-C1'	8.68	128.35	118.80
36	5	1152	G	C2-N3-C4	-8.66	107.57	111.90
1	6	453	U	C2-N1-C1'	8.66	128.09	117.70
36	1	3217	C	N1-C2-O2	8.61	124.06	118.90
36	5	3154	C	N1-C2-O2	8.58	124.05	118.90
36	5	3245	A	N7-C8-N9	8.38	117.99	113.80
1	6	163	G	N3-C2-N2	-8.21	114.15	119.90
36	5	2572	C	C2-N1-C1'	8.21	127.83	118.80
48	m1	112	LEU	CA-CB-CG	8.11	133.96	115.30
36	1	1192	C	N1-C2-O2	8.08	123.75	118.90
36	5	3154	C	C2-N1-C1'	8.06	127.67	118.80
1	2	453	U	C2-N1-C1'	8.06	127.37	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	6	194	U	C2-N1-C1'	8.05	127.36	117.70
1	2	1052	U	C2-N1-C1'	8.00	127.30	117.70
36	1	3278	C	N1-C2-O2	8.00	123.70	118.90
36	1	2572	C	C2-N1-C1'	7.92	127.51	118.80
1	2	73	U	O4'-C1'-N1	7.83	114.47	108.20
36	1	979	U	P-O3'-C3'	7.80	129.06	119.70
36	5	2726	C	C5-C4-N4	7.78	125.65	120.20
10	S8	29	LEU	CA-CB-CG	7.74	133.11	115.30
33	e1	87	THR	C-N-CD	-7.74	103.56	120.60
1	6	1634	C	N1-C2-O2	7.66	123.50	118.90
1	6	25	C	C2-N1-C1'	7.66	127.23	118.80
36	1	1495	U	C5-C6-N1	-7.66	118.87	122.70
1	6	1634	C	C2-N1-C1'	7.58	127.14	118.80
36	5	406	G	O4'-C1'-N9	7.58	114.27	108.20
1	6	1	U	C2-N1-C1'	7.55	126.76	117.70
1	6	25	C	N1-C2-O2	7.51	123.41	118.90
14	C2	101	ALA	C-N-CA	-7.50	106.55	122.30
36	1	1192	C	C2-N1-C1'	7.44	126.98	118.80
36	5	2572	C	N3-C2-O2	-7.41	116.71	121.90
36	1	3382	U	N1-C2-O2	7.33	127.93	122.80
36	1	2572	C	N1-C2-O2	7.32	123.29	118.90
1	2	558	U	N1-C2-O2	7.29	127.90	122.80
1	2	830	U	N3-C2-O2	-7.29	117.10	122.20
6	s4	164	LEU	CA-CB-CG	7.27	132.03	115.30
36	1	3217	C	N3-C2-O2	-7.25	116.83	121.90
1	2	558	U	N3-C2-O2	-7.23	117.14	122.20
36	1	3306	U	C5-C4-O4	7.20	130.22	125.90
24	d2	93	LEU	CA-CB-CG	7.19	131.84	115.30
36	1	1351	U	C2-N1-C1'	7.16	126.29	117.70
36	1	2719	U	C2-N1-C1'	-7.15	109.12	117.70
36	1	1351	U	N1-C2-O2	7.15	127.80	122.80
36	1	2617	U	N1-C2-N3	7.14	119.19	114.90
1	2	639	U	N3-C2-O2	-7.14	117.20	122.20
1	6	1473	U	N3-C2-O2	-7.09	117.23	122.20
38	4	125	U	C2-N1-C1'	7.09	126.21	117.70
1	2	507	U	N3-C2-O2	-7.08	117.24	122.20
1	2	192	U	C2-N1-C1'	7.08	126.19	117.70
36	5	981	U	C5-C6-N1	7.04	126.22	122.70
1	2	1363	U	N3-C2-O2	-7.02	117.29	122.20
36	1	960	U	C2-N1-C1'	-7.01	109.29	117.70
1	2	1761	U	P-O3'-C3'	6.99	128.09	119.70
1	6	453	U	N3-C2-O2	-6.98	117.31	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	1363	U	N1-C2-O2	6.97	127.68	122.80
36	5	2816	G	C8-N9-C4	6.97	109.19	106.40
1	2	1096	C	N3-C2-O2	-6.96	117.03	121.90
1	6	453	U	N1-C2-O2	6.95	127.66	122.80
44	17	229	PHE	CB-CG-CD1	6.93	125.65	120.80
38	8	82	U	N3-C2-O2	-6.93	117.35	122.20
40	13	4	ARG	NE-CZ-NH1	6.91	123.75	120.30
1	2	192	U	N1-C2-O2	6.90	127.63	122.80
36	1	770	G	O4'-C1'-N9	6.89	113.71	108.20
36	5	1152	G	N3-C2-N2	-6.88	115.09	119.90
36	1	3382	U	N3-C2-O2	-6.87	117.39	122.20
36	5	767	U	O4'-C1'-N1	6.86	113.69	108.20
36	1	1351	U	N3-C2-O2	-6.84	117.41	122.20
36	1	3278	C	N3-C2-O2	-6.83	117.12	121.90
36	5	2234	G	C5-C6-O6	-6.81	124.51	128.60
36	5	2978	U	O4'-C1'-N1	6.79	113.64	108.20
1	2	507	U	N1-C2-O2	6.79	127.55	122.80
1	6	1473	U	N1-C2-O2	6.78	127.55	122.80
6	S4	193	GLY	N-CA-C	6.78	130.05	113.10
9	s7	9	LEU	CA-CB-CG	6.76	130.85	115.30
36	5	3285	C	C2-N1-C1'	6.75	126.22	118.80
64	n8	98	THR	C-N-CA	6.75	138.56	121.70
36	1	3382	U	C2-N1-C1'	6.74	125.79	117.70
36	5	3245	A	C5-N7-C8	-6.74	100.53	103.90
42	l5	110	LEU	CA-CB-CG	6.74	130.79	115.30
1	2	1363	U	C2-N1-C1'	6.71	125.75	117.70
36	1	2846	U	N3-C2-O2	-6.71	117.50	122.20
2	s0	206	ASP	N-CA-C	6.70	129.10	111.00
36	5	1604	G	C4-N9-C1'	6.69	135.20	126.50
1	2	192	U	N3-C2-O2	-6.68	117.52	122.20
1	2	639	U	N1-C2-O2	6.68	127.48	122.80
36	5	2945	G	O5'-P-OP2	-6.68	99.69	105.70
1	2	1096	C	C6-N1-C1'	-6.67	112.80	120.80
36	1	2617	U	C5-C4-O4	6.67	129.90	125.90
41	14	339	LEU	CA-CB-CG	6.66	130.62	115.30
1	6	25	C	C6-N1-C1'	-6.63	112.84	120.80
1	2	453	U	N1-C2-O2	6.62	127.44	122.80
1	2	453	U	N3-C2-O2	-6.62	117.57	122.20
36	1	1269	U	C2-N1-C1'	6.62	125.64	117.70
1	2	558	U	C2-N1-C1'	6.60	125.62	117.70
1	2	507	U	C2-N1-C1'	6.57	125.58	117.70
1	2	75	U	N3-C2-O2	-6.57	117.60	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	2617	U	C4-C5-C6	6.57	123.64	119.70
36	1	3362	A	O4'-C1'-N9	6.53	113.43	108.20
36	1	3217	C	C6-N1-C1'	-6.53	112.96	120.80
36	5	1856	C	C6-N1-C2	-6.53	117.69	120.30
12	c0	88	PRO	N-CA-CB	6.52	111.12	103.30
1	2	704	C	N1-C2-O2	6.52	122.81	118.90
36	1	979	U	C6-N1-C2	-6.51	117.09	121.00
41	L4	206	LEU	CA-CB-CG	6.51	130.26	115.30
36	5	1495	U	C2-N1-C1'	6.50	125.50	117.70
1	2	75	U	N1-C2-O2	6.48	127.34	122.80
36	1	2996	U	N1-C2-O2	6.48	127.34	122.80
31	D9	36	LEU	CA-CB-CG	6.47	130.18	115.30
19	C7	85	VAL	CA-CB-CG1	6.45	120.58	110.90
36	1	2621	G	O5'-P-OP2	-6.45	99.89	105.70
36	5	1196	C	C6-N1-C2	6.45	122.88	120.30
36	5	2310	U	O5'-P-OP2	-6.45	99.90	105.70
14	c2	58	LEU	CA-CB-CG	6.43	130.10	115.30
36	5	2572	C	C6-N1-C2	-6.43	117.73	120.30
6	s4	12	LEU	CA-CB-CG	6.43	130.08	115.30
1	2	75	U	C2-N1-C1'	6.42	125.41	117.70
12	c0	97	PRO	N-CA-CB	6.42	111.01	103.30
1	2	1456	C	N1-C2-O2	6.42	122.75	118.90
36	1	439	C	N1-C2-O2	6.40	122.74	118.90
1	6	25	C	P-O3'-C3'	6.39	127.37	119.70
1	6	1	U	N1-C2-O2	6.39	127.27	122.80
1	6	1634	C	N3-C2-O2	-6.39	117.43	121.90
36	5	3245	A	C8-N9-C4	-6.39	103.25	105.80
15	c3	58	HIS	C-N-CA	-6.37	108.92	122.30
36	5	3154	C	N3-C2-O2	-6.37	117.44	121.90
1	6	1700	C	C2-N1-C1'	6.36	125.80	118.80
1	2	830	U	N1-C2-O2	6.35	127.25	122.80
1	2	1508	U	N3-C4-C5	-6.35	110.79	114.60
36	5	1115	G	C4-N9-C1'	6.34	134.74	126.50
1	2	728	U	C2-N1-C1'	6.32	125.28	117.70
12	c0	83	PRO	N-CA-CB	6.31	110.87	103.30
1	6	1	U	N3-C2-O2	-6.30	117.79	122.20
36	1	2870	C	C2-N1-C1'	-6.29	111.88	118.80
36	5	2272	G	O4'-C1'-N9	6.29	113.23	108.20
36	1	639	G	N1-C6-O6	6.29	123.67	119.90
41	L4	313	LEU	CA-CB-CG	6.27	129.73	115.30
36	5	38	U	O5'-P-OP2	-6.27	100.05	105.70
36	5	922	U	C5-C6-N1	-6.27	119.56	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	3319	U	P-O3'-C3'	6.27	127.22	119.70
1	2	934	C	C2-N1-C1'	6.25	125.68	118.80
1	6	1634	C	C6-N1-C2	-6.21	117.82	120.30
36	1	1495	U	C2-N1-C1'	-6.21	110.25	117.70
1	6	158	U	P-O3'-C3'	6.20	127.14	119.70
38	8	80	A	N7-C8-N9	6.20	116.90	113.80
48	m1	152	HIS	N-CA-C	-6.20	94.27	111.00
36	5	3195	U	P-O3'-C3'	6.19	127.13	119.70
1	6	163	G	C8-N9-C1'	6.19	135.05	127.00
1	6	1473	U	C2-N1-C1'	6.19	125.13	117.70
39	l2	246	LEU	CA-CB-CG	6.19	129.53	115.30
36	5	3195	U	OP1-P-O3'	6.18	118.80	105.20
1	2	1039	A	O4'-C1'-N9	6.17	113.14	108.20
36	1	1820	U	P-O3'-C3'	6.17	127.10	119.70
1	6	337	G	C4-C5-N7	6.17	113.27	110.80
1	2	1389	C	C2-N1-C1'	6.14	125.56	118.80
1	2	694	U	N1-C2-O2	6.12	127.08	122.80
1	6	794	U	C2-N1-C1'	6.12	125.04	117.70
1	2	1698	G	P-O3'-C3'	6.11	127.03	119.70
36	1	3275	U	OP1-P-O3'	6.10	118.62	105.20
9	S7	64	VAL	N-CA-C	-6.09	94.55	111.00
36	1	2550	U	C5-C6-N1	6.09	125.74	122.70
1	2	1324	G	N3-C4-N9	-6.08	122.35	126.00
18	C6	28	LEU	CA-CB-CG	6.08	129.28	115.30
36	1	776	U	C4-C5-C6	6.07	123.34	119.70
36	1	3306	U	N3-C2-O2	-6.06	117.96	122.20
36	5	873	C	P-O3'-C3'	6.06	126.97	119.70
36	1	922	U	C2-N1-C1'	6.05	124.96	117.70
36	1	1269	U	N1-C2-O2	6.04	127.03	122.80
36	1	2978	U	O4'-C1'-N1	6.04	113.03	108.20
36	1	2772	C	O4'-C1'-N1	6.03	113.03	108.20
36	5	2524	A	O4'-C1'-N9	6.03	113.02	108.20
10	s8	29	LEU	CA-CB-CG	6.03	129.16	115.30
36	1	1299	U	O5'-P-OP2	-6.01	100.29	105.70
1	2	287	G	O4'-C1'-N9	6.01	113.01	108.20
36	5	2531	C	C2-N1-C1'	6.00	125.41	118.80
36	1	1192	C	C6-N1-C1'	-6.00	113.60	120.80
36	1	2726	C	N3-C2-O2	-5.99	117.71	121.90
36	1	282	G	C8-N9-C4	-5.98	104.01	106.40
1	2	694	U	C2-N1-C1'	5.98	124.88	117.70
1	2	1052	U	N1-C2-O2	5.98	126.98	122.80
12	C0	88	PRO	N-CA-CB	5.97	110.46	103.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	c5	36	LEU	CA-CB-CG	5.97	129.03	115.30
1	2	323	A	O5'-P-OP2	-5.96	100.33	105.70
36	5	1239	C	C5-C6-N1	5.96	123.98	121.00
70	O4	51	LEU	CA-CB-CG	5.96	129.01	115.30
36	5	3362	A	O4'-C1'-N9	5.96	112.97	108.20
36	1	1604	G	C4-N9-C1'	5.95	134.23	126.50
36	5	2726	C	N3-C4-C5	-5.95	119.52	121.90
36	1	1495	U	C4-C5-C6	5.93	123.26	119.70
36	1	2836	C	N3-C2-O2	-5.93	117.75	121.90
36	5	1481	A	P-O3'-C3'	5.93	126.82	119.70
36	5	1308	A	O5'-P-OP1	-5.92	100.38	105.70
36	5	1152	G	C4-C5-C6	-5.91	115.25	118.80
36	1	922	U	N1-C2-O2	5.91	126.94	122.80
1	6	321	C	N3-C2-O2	-5.91	117.76	121.90
36	1	345	G	N3-C4-C5	-5.89	125.65	128.60
1	2	734	A	P-O3'-C3'	5.89	126.76	119.70
1	6	25	C	OP2-P-O3'	5.89	118.15	105.20
1	2	1370	U	P-O3'-C3'	5.88	126.76	119.70
36	1	2572	C	N3-C2-O2	-5.88	117.78	121.90
36	1	2714	G	N3-C4-C5	5.88	131.54	128.60
1	6	75	U	O4'-C1'-N1	5.88	112.90	108.20
1	6	678	A	P-O3'-C3'	5.88	126.75	119.70
1	2	829	A	P-O3'-C3'	5.88	126.75	119.70
1	6	272	U	P-O3'-C3'	5.85	126.72	119.70
1	6	1768	G	N3-C4-N9	-5.85	122.49	126.00
1	6	542	A	P-O3'-C3'	5.85	126.72	119.70
36	1	2617	U	N3-C2-O2	-5.83	118.11	122.20
36	1	2996	U	C2-N1-C1'	5.83	124.69	117.70
71	O5	21	LEU	CA-CB-CG	5.82	128.68	115.30
1	2	734	A	OP1-P-O3'	5.81	117.98	105.20
1	2	581	U	C2-N1-C1'	5.80	124.66	117.70
36	5	1582	C	C6-N1-C2	-5.80	117.98	120.30
1	6	1039	A	O4'-C1'-N9	5.80	112.84	108.20
36	5	1604	G	C8-N9-C1'	-5.80	119.47	127.00
41	L4	339	LEU	CA-CB-CG	5.79	128.62	115.30
18	C6	40	GLU	C-N-CD	-5.78	107.88	120.60
1	6	558	U	C2-N1-C1'	5.78	124.64	117.70
1	2	1258	U	N3-C2-O2	-5.77	118.16	122.20
1	2	1324	G	N3-C2-N2	-5.77	115.86	119.90
36	1	1349	G	N3-C4-C5	-5.77	125.71	128.60
36	1	2942	C	C2-N1-C1'	-5.77	112.45	118.80
36	1	439	C	C2-N1-C1'	5.76	125.14	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	D2	104	LEU	CA-CB-CG	5.76	128.55	115.30
36	1	1484	U	P-O3'-C3'	5.76	126.61	119.70
36	1	1269	U	N3-C2-O2	-5.75	118.17	122.20
36	1	1307	G	P-O3'-C3'	5.75	126.60	119.70
1	6	163	G	C4-N9-C1'	-5.75	119.03	126.50
36	5	3154	C	C6-N1-C1'	-5.75	113.90	120.80
1	6	610	G	C4-N9-C1'	5.75	133.97	126.50
1	2	720	G	P-O3'-C3'	5.74	126.58	119.70
1	6	542	A	O4'-C1'-N9	5.74	112.79	108.20
36	1	2719	U	N1-C2-O2	-5.73	118.79	122.80
36	5	2843	U	N3-C2-O2	-5.72	118.19	122.20
1	6	1058	U	OP1-P-O3'	5.71	117.77	105.20
36	5	1152	G	C5-N7-C8	-5.69	101.45	104.30
1	6	782	U	N3-C2-O2	-5.69	118.22	122.20
36	1	2522	G	C4-N9-C1'	5.68	133.88	126.50
1	6	194	U	N1-C2-O2	5.68	126.77	122.80
83	n4	75	THR	C-N-CA	5.68	135.89	121.70
1	2	1389	C	N1-C2-O2	5.67	122.30	118.90
36	5	3285	C	N1-C2-O2	5.67	122.30	118.90
36	5	3209	A	C4-N9-C1'	5.67	136.50	126.30
36	1	2541	U	C2-N1-C1'	5.66	124.50	117.70
18	c6	117	LEU	CA-CB-CG	5.66	128.31	115.30
1	2	720	G	OP1-P-O3'	5.65	117.64	105.20
36	1	1308	A	C4-C5-C6	5.65	119.83	117.00
1	6	1700	C	N1-C2-O2	5.65	122.29	118.90
1	6	1274	C	N1-C2-O2	5.64	122.29	118.90
44	l7	229	PHE	CB-CG-CD2	-5.64	116.85	120.80
36	5	3351	U	N3-C2-O2	-5.63	118.26	122.20
24	D2	93	LEU	CA-CB-CG	5.63	128.25	115.30
36	1	1815	U	P-O3'-C3'	5.63	126.45	119.70
1	6	858	G	O4'-C1'-N9	5.62	112.70	108.20
36	1	1331	U	O4'-C1'-N1	-5.62	103.70	108.20
1	6	1698	G	P-O3'-C3'	5.62	126.45	119.70
1	2	1761	U	C6-N1-C2	-5.62	117.63	121.00
36	5	1314	C	C2-N1-C1'	5.62	124.98	118.80
36	5	1115	G	C8-N9-C1'	-5.61	119.71	127.00
36	1	3344	A	N7-C8-N9	5.61	116.60	113.80
36	1	2355	G	N1-C6-O6	5.61	123.26	119.90
36	5	1483	G	O4'-C1'-N9	5.61	112.68	108.20
36	5	1481	A	C8-N9-C4	-5.60	103.56	105.80
37	7	101	G	N1-C6-O6	5.59	123.26	119.90
1	6	163	G	C2-N3-C4	-5.59	109.11	111.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	C7	85	VAL	CB-CA-C	5.58	121.99	111.40
36	1	2572	C	C6-N1-C1'	-5.57	114.12	120.80
36	1	776	U	C5-C6-N1	-5.56	119.92	122.70
61	N5	38	LEU	CA-CB-CG	5.56	128.09	115.30
36	1	3316	A	OP2-P-O3'	5.56	117.43	105.20
1	6	321	C	N1-C2-O2	5.55	122.23	118.90
36	1	65	A	P-O3'-C3'	5.54	126.34	119.70
1	2	1536	G	C4-N9-C1'	5.54	133.70	126.50
36	5	981	U	C6-N1-C2	-5.54	117.68	121.00
1	6	453	U	C6-N1-C1'	-5.53	113.45	121.20
1	2	73	U	OP1-P-O3'	5.53	117.37	105.20
38	8	80	A	C8-N9-C4	-5.53	103.59	105.80
1	2	1560	U	N3-C2-O2	-5.52	118.33	122.20
36	1	2550	U	C6-N1-C2	-5.52	117.69	121.00
43	l6	67	GLY	C-N-CD	-5.52	108.45	120.60
1	2	25	C	P-O3'-C3'	5.52	126.32	119.70
1	2	736	C	C2-N1-C1'	5.51	124.87	118.80
1	2	794	U	P-O3'-C3'	5.51	126.31	119.70
36	1	2679	A	O4'-C1'-N9	5.50	112.60	108.20
36	1	2714	G	N3-C4-N9	-5.50	122.70	126.00
36	1	2541	U	P-O3'-C3'	5.50	126.30	119.70
36	1	1838	G	C5-C6-O6	-5.49	125.30	128.60
1	2	1456	C	N3-C2-O2	-5.49	118.06	121.90
36	1	2571	U	C2-N1-C1'	5.49	124.28	117.70
36	5	3214	U	N3-C2-O2	-5.49	118.36	122.20
36	1	2870	C	C6-N1-C1'	5.48	127.37	120.80
36	1	1838	G	C6-C5-N7	-5.48	127.11	130.40
1	2	25	C	OP2-P-O3'	5.47	117.24	105.20
36	5	2283	G	C5-C6-O6	-5.47	125.31	128.60
36	5	2801	A	C8-N9-C4	5.47	107.99	105.80
36	5	1115	G	N3-C4-N9	5.47	129.28	126.00
36	5	2996	U	N1-C2-O2	5.47	126.63	122.80
36	5	2234	G	N1-C6-O6	5.47	123.18	119.90
1	2	1473	U	N1-C2-O2	5.46	126.63	122.80
36	1	2513	U	O4'-C1'-N1	5.46	112.57	108.20
1	2	1456	C	C2-N1-C1'	5.46	124.81	118.80
36	1	1329	U	P-O3'-C3'	5.46	126.25	119.70
36	5	2257	C	C6-N1-C2	-5.46	118.12	120.30
64	N8	29	PRO	C-N-CA	-5.46	110.84	122.30
1	2	782	U	P-O3'-C3'	5.45	126.24	119.70
36	5	2273	G	C4-N9-C1'	-5.44	119.42	126.50
36	1	3344	A	O4'-C1'-N9	5.44	112.55	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	637	C	P-O3'-C3'	5.44	126.22	119.70
1	6	610	G	C8-N9-C1'	-5.43	119.94	127.00
33	e1	103	LEU	CA-CB-CG	-5.43	102.82	115.30
36	1	3218	A	P-O3'-C3'	5.41	126.20	119.70
36	5	1152	G	N1-C2-N2	5.41	121.07	116.20
66	o0	41	LEU	CA-CB-CG	5.41	127.74	115.30
36	1	3154	C	C2-N1-C1'	5.39	124.73	118.80
36	5	2372	A	C8-N9-C4	-5.39	103.64	105.80
36	1	1279	C	C6-N1-C2	-5.39	118.14	120.30
24	D2	65	LEU	CA-CB-CG	5.39	127.69	115.30
36	1	934	G	C4-N9-C1'	5.39	133.50	126.50
1	6	1274	C	C2-N1-C1'	5.39	124.72	118.80
6	s4	38	LEU	CA-CB-CG	5.38	127.69	115.30
1	6	163	G	N9-C4-C5	5.38	107.55	105.40
15	C3	22	ALA	C-N-CD	-5.38	108.76	120.60
36	1	1838	G	N3-C4-N9	5.38	129.22	126.00
1	2	158	U	P-O3'-C3'	5.37	126.15	119.70
36	5	3351	U	N1-C2-O2	5.37	126.56	122.80
36	1	908	G	C4-N9-C1'	5.37	133.48	126.50
1	2	577	G	N1-C6-O6	5.37	123.12	119.90
36	1	1887	A	O5'-P-OP2	5.37	117.14	110.70
1	2	864	U	N3-C2-O2	-5.36	118.45	122.20
36	1	908	G	O4'-C1'-N9	-5.36	103.91	108.20
36	1	3057	U	N3-C2-O2	-5.36	118.45	122.20
33	e1	100	LEU	CA-CB-CG	5.36	127.62	115.30
36	5	3078	U	N1-C2-O2	5.36	126.55	122.80
36	1	2571	U	N1-C2-O2	5.35	126.55	122.80
1	2	1473	U	N3-C2-O2	-5.35	118.45	122.20
36	5	3092	C	C2-N1-C1'	-5.35	112.92	118.80
36	1	2513	U	P-O3'-C3'	5.35	126.12	119.70
1	2	1761	U	N3-C2-O2	-5.34	118.46	122.20
36	5	1931	U	C2-N1-C1'	-5.34	111.29	117.70
60	N4	81	PRO	N-CA-C	5.34	125.97	112.10
36	5	2572	C	C6-N1-C1'	-5.33	114.40	120.80
1	2	1052	U	C6-N1-C1'	-5.32	113.75	121.20
36	5	1355	A	P-O3'-C3'	5.32	126.08	119.70
36	1	199	A	O4'-C1'-N9	5.32	112.45	108.20
36	1	922	U	N3-C2-O2	-5.32	118.48	122.20
1	6	1458	G	C4-N9-C1'	5.31	133.41	126.50
36	1	2373	A	O5'-P-OP1	-5.31	100.92	105.70
36	5	1561	G	O4'-C1'-N9	5.31	112.45	108.20
36	5	1716	U	P-O3'-C3'	5.30	126.06	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	3209	A	O4'-C1'-N9	5.30	112.44	108.20
1	6	677	G	C4-N9-C1'	-5.30	119.61	126.50
36	5	3218	A	P-O3'-C3'	5.30	126.06	119.70
55	M9	129	GLY	C-N-CA	-5.30	108.45	121.70
36	1	1349	G	N3-C4-N9	5.29	129.17	126.00
36	1	2572	C	C6-N1-C2	-5.29	118.19	120.30
36	5	1169	A	OP2-P-O3'	5.29	116.83	105.20
13	c1	5	LEU	CA-CB-CG	5.28	127.45	115.30
1	6	194	U	N3-C2-O2	-5.28	118.50	122.20
36	1	101	G	O4'-C1'-N9	5.28	112.42	108.20
36	1	1308	A	C6-C5-N7	-5.28	128.61	132.30
36	5	2843	U	N1-C2-O2	5.28	126.49	122.80
1	6	1389	C	C2-N1-C1'	5.27	124.60	118.80
36	1	979	U	N1-C2-N3	5.26	118.06	114.90
36	5	2541	U	C2-N1-C1'	5.26	124.02	117.70
36	5	1238	C	P-O3'-C3'	5.26	126.01	119.70
36	5	2930	A	O4'-C1'-N9	5.26	112.41	108.20
36	1	2827	U	C2-N1-C1'	-5.26	111.39	117.70
36	1	1192	C	N3-C2-O2	-5.26	118.22	121.90
49	M3	85	LEU	CA-CB-CG	5.25	127.38	115.30
1	2	794	U	N1-C2-O2	5.25	126.47	122.80
36	1	1556	C	P-O3'-C3'	5.24	125.99	119.70
1	6	795	U	C2-N1-C1'	5.24	123.99	117.70
1	2	730	G	C4-N9-C1'	5.23	133.30	126.50
36	1	835	G	O4'-C1'-N9	5.23	112.38	108.20
36	1	1355	A	P-O3'-C3'	5.23	125.98	119.70
36	5	1314	C	C6-N1-C1'	-5.23	114.52	120.80
1	2	73	U	P-O3'-C3'	5.23	125.97	119.70
36	1	2846	U	N1-C2-O2	5.22	126.46	122.80
36	5	2772	C	P-O3'-C3'	5.22	125.97	119.70
1	2	704	C	C2-N1-C1'	5.22	124.54	118.80
47	M0	57	LEU	CA-CB-CG	5.22	127.30	115.30
38	4	125	U	N1-C2-O2	5.20	126.44	122.80
42	L5	131	LEU	CA-CB-CG	5.20	127.27	115.30
36	5	183	G	P-O3'-C3'	5.20	125.94	119.70
36	1	282	G	C2'-C3'-O3'	5.20	122.02	113.70
36	5	2954	U	N1-C2-O2	5.20	126.44	122.80
36	1	3278	C	C2-N1-C1'	5.20	124.52	118.80
38	8	125	U	C2-N1-C1'	5.20	123.94	117.70
1	2	830	U	C2-N1-C1'	5.20	123.94	117.70
36	1	915	A	C8-N9-C4	-5.20	103.72	105.80
1	6	1114	G	O4'-C1'-N9	5.20	112.36	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	2719	U	C6-N1-C1'	5.19	128.47	121.20
36	1	1294	A	O4'-C1'-N9	5.19	112.35	108.20
36	1	2101	C	P-O3'-C3'	5.19	125.92	119.70
33	E1	85	TYR	CA-CB-CG	5.18	123.25	113.40
1	2	1170	G	C4-N9-C1'	5.18	133.24	126.50
36	1	1820	U	OP2-P-O3'	5.18	116.60	105.20
1	2	694	U	N3-C2-O2	-5.17	118.58	122.20
60	N4	79	GLN	C-N-CA	5.17	134.64	121.70
36	5	2392	C	C2-N1-C1'	-5.17	113.11	118.80
78	Q2	93	LEU	CA-CB-CG	5.17	127.18	115.30
1	2	1324	G	C8-N9-C1'	5.16	133.71	127.00
1	2	499	U	P-O3'-C3'	5.15	125.89	119.70
36	1	1081	U	C2-N1-C1'	5.15	123.88	117.70
1	6	163	G	N1-C2-N2	5.14	120.83	116.20
36	5	3078	U	N3-C2-O2	-5.14	118.60	122.20
1	2	704	C	N3-C2-O2	-5.14	118.30	121.90
1	2	1052	U	N3-C2-O2	-5.14	118.60	122.20
36	5	3245	A	C6-C5-N7	-5.14	128.70	132.30
36	1	406	G	C4-N9-C1'	-5.14	119.82	126.50
20	c8	15	LEU	CA-CB-CG	5.14	127.12	115.30
1	2	1274	C	N1-C2-O2	5.13	121.98	118.90
36	5	776	U	C5-C6-N1	-5.13	120.14	122.70
36	1	3277	U	N3-C2-O2	-5.13	118.61	122.20
36	5	2385	G	C8-N9-C4	5.12	108.45	106.40
36	1	2572	C	O4'-C1'-N1	5.12	112.30	108.20
1	6	1697	G	N3-C4-C5	-5.12	126.04	128.60
36	5	1014	U	C2-N1-C1'	5.12	123.84	117.70
1	6	1246	C	C2-N1-C1'	5.12	124.43	118.80
6	S4	38	LEU	CA-CB-CG	5.12	127.07	115.30
36	5	374	A	P-O3'-C3'	5.12	125.84	119.70
36	5	1284	C	P-O3'-C3'	5.12	125.84	119.70
1	2	1208	A	O4'-C1'-N9	5.11	112.29	108.20
1	6	194	U	C6-N1-C1'	-5.11	114.05	121.20
1	6	558	U	P-O3'-C3'	5.11	125.83	119.70
36	5	3092	C	O4'-C1'-N1	5.11	112.29	108.20
38	8	82	U	C5-C4-O4	5.11	128.96	125.90
1	2	782	U	OP2-P-O3'	5.10	116.43	105.20
28	D6	86	VAL	N-CA-C	-5.10	97.23	111.00
36	1	1716	U	P-O3'-C3'	5.10	125.82	119.70
38	4	125	U	C6-N1-C1'	-5.09	114.07	121.20
36	1	1308	A	C5-N7-C8	-5.09	101.35	103.90
1	6	1560	U	C2-N1-C1'	5.09	123.81	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	719	U	C2-N1-C1'	5.09	123.81	117.70
61	N5	113	LEU	CA-CB-CG	5.08	126.99	115.30
36	1	1094	U	OP1-P-O3'	5.08	116.38	105.20
1	6	1696	G	C3'-C2'-C1'	5.08	105.56	101.50
1	2	501	U	OP1-P-O3'	5.07	116.36	105.20
36	1	2606	G	N3-C4-N9	5.07	129.04	126.00
1	6	1768	G	N3-C4-C5	5.07	131.14	128.60
48	m1	8	PRO	C-N-CA	5.07	134.38	121.70
1	2	1389	C	C6-N1-C2	-5.07	118.27	120.30
1	6	1058	U	P-O3'-C3'	5.07	125.78	119.70
36	5	404	G	O5'-P-OP2	-5.07	101.14	105.70
36	1	2719	U	C5-C6-N1	-5.06	120.17	122.70
36	5	1495	U	C5-C6-N1	5.06	125.23	122.70
36	5	3285	C	C6-N1-C1'	-5.06	114.73	120.80
36	1	2112	U	P-O3'-C3'	5.06	125.77	119.70
36	1	2314	U	C2-N1-C1'	5.06	123.77	117.70
36	1	3217	C	C6-N1-C2	-5.05	118.28	120.30
36	5	3140	G	C5-C6-O6	-5.05	125.57	128.60
36	5	3317	U	P-O3'-C3'	5.05	125.76	119.70
36	1	3110	C	C6-N1-C2	-5.05	118.28	120.30
1	2	1389	C	N3-C2-O2	-5.04	118.37	121.90
36	1	1556	C	N1-C2-O2	5.04	121.92	118.90
1	6	670	U	C2-N1-C1'	5.04	123.75	117.70
54	M8	41	ASP	CB-CG-OD1	5.03	122.83	118.30
36	5	3214	U	N1-C2-O2	5.03	126.32	122.80
36	5	3377	G	C5-C6-O6	-5.03	125.58	128.60
26	d4	121	THR	C-N-CA	-5.02	111.75	122.30
36	1	2996	U	N3-C2-O2	-5.02	118.69	122.20
36	1	3306	U	N3-C4-O4	-5.02	115.89	119.40
36	1	1116	G	OP2-P-O3'	5.01	116.23	105.20
62	N6	126	LEU	CA-CB-CG	5.01	126.83	115.30
36	5	2439	A	O5'-P-OP1	5.01	116.72	110.70
37	3	52	G	P-O3'-C3'	5.01	125.71	119.70
1	2	1508	U	C6-N1-C2	-5.01	117.99	121.00
1	6	75	U	P-O3'-C3'	5.01	125.71	119.70
1	6	1340	U	N3-C2-O2	-5.01	118.69	122.20
37	7	101	G	C5-C6-O6	-5.01	125.60	128.60
1	2	704	C	O4'-C1'-N1	5.00	112.20	108.20
11	S9	93	LEU	CA-CB-CG	5.00	126.80	115.30

There are no chirality outliers.

All (126) planarity outliers are listed below:



Mol	Chain	Res	Type	Group
16	C4	123	SER	Peptide
16	C4	38	THR	Peptide
16	C4	49	LYS	Peptide
17	C5	124	THR	Peptide
17	C5	27	GLU	Peptide
18	C6	113	ASP	Peptide
18	C6	40	GLU	Peptide
19	C7	85	VAL	Peptide
22	D0	73	GLY	Peptide
24	D2	54	ASP	Peptide
25	D3	137	LYS	Peptide
26	D4	46	GLU	Peptide
27	D5	54	VAL	Peptide
27	D5	94	LYS	Peptide
28	D6	10	ARG	Peptide
28	D6	84	VAL	Peptide
33	E1	101	ALA	Peptide
33	E1	143	LYS	Peptide
33	E1	146	SER	Peptide
41	L4	83	GLY	Peptide
42	L5	232	ASP	Peptide
42	L5	251	PRO	Peptide
42	L5	7	ALA	Peptide
45	L8	24	ASN	Peptide
45	L8	74	THR	Peptide
46	L9	108	GLY	Peptide
49	M3	130	GLY	Peptide
50	M4	8	LYS	Peptide
51	M5	186	GLY	Peptide
52	M6	110	PRO	Peptide
56	N0	12	ARG	Peptide
56	N0	133	ALA	Peptide
56	N0	22	PRO	Peptide
57	N1	16	GLN	Peptide
60	N4	80	ARG	Peptide
60	N4	96	LEU	Peptide
65	N9	20	GLY	Peptide
79	Q3	49	ARG	Peptide
2	S0	94	GLY	Peptide
3	S1	131	ASP	Peptide
4	S2	106	ASP	Peptide
5	S3	219	ALA	Peptide
6	S4	57	ASN	Peptide

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Mol	Chain	Res	Type	Group
7	S5	100	ASN	Peptide
7	S5	44	ASN	Peptide
7	S5	65	ARG	Peptide
9	S7	131	PHE	Peptide
9	S7	29	ASN	Peptide
10	S8	146	ARG	Peptide
10	S8	147	ALA	Peptide
14	c2	101	ALA	Peptide
15	c3	59	GLY	Peptide
16	c4	125	SER	Peptide
16	c4	90	ARG	Peptide
17	c5	124	THR	Peptide
17	c5	50	THR	Peptide
17	c5	52	LYS	Peptide
18	c6	115	THR	Peptide
18	c6	40	GLU	Peptide
19	c7	66	VAL	Peptide
19	c7	87	GLU	Peptide
19	c7	96	SER	Peptide
20	c8	90	ASN	Peptide
22	d0	70	THR	Peptide
23	d1	43	GLY	Peptide
24	d2	54	ASP	Peptide
25	d3	44	GLY	Peptide
26	d4	35	VAL	Peptide
27	d5	69	LEU	Peptide
27	d5	86	GLU	Peptide
32	e0	51	ASN	Peptide
33	e1	128	ALA	Peptide
33	e1	135	HIS	Peptide
33	e1	87	THR	Peptide
39	l2	171	GLY	Peptide
40	l3	141	GLY	Peptide
40	l3	2	SER	Peptide
41	l4	300	ARG	Peptide
42	l5	268	GLU	Peptide
42	l5	269	SER	Peptide
42	l5	270	LYS	Peptide
43	l6	129	GLU	Peptide
44	l7	192	GLY	Peptide
81	l8	24	ASN	Peptide
48	m1	8	PRO	Peptide

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Mol	Chain	Res	Type	Group
82	m2	103	UNK	Peptide
82	m2	117	UNK	Peptide
82	m2	55	UNK	Peptide
82	m2	56	UNK	Peptide
82	m2	59	UNK	Peptide
49	m3	133	PRO	Peptide
50	m4	20	VAL	Peptide
51	m5	181	ASN	Peptide
52	m6	109	PRO	Peptide
53	m7	119	VAL	Peptide
56	n0	133	ALA	Peptide
56	n0	86	GLY	Peptide
58	n2	51	GLY	Peptide
63	n7	124	ALA	Peptide
63	n7	4	PHE	Peptide
64	n8	66	ALA	Peptide
65	n9	19	ASN	Peptide
66	o0	99	ASP	Peptide
67	o1	90	PHE	Peptide
70	o4	80	ARG	Peptide
71	o5	118	ILE	Peptide
79	q3	49	ARG	Peptide
2	s0	187	ALA	Peptide
2	s0	206	ASP	Peptide
2	s0	94	GLY	Peptide
3	s1	222	LYS	Peptide
4	s2	106	ASP	Peptide
4	s2	91	ARG	Peptide
5	s3	219	ALA	Peptide
7	s5	206	SER	Peptide
7	s5	44	ASN	Peptide
7	s5	54	LYS	Peptide
7	s5	99	MET	Peptide
9	s7	130	VAL	Peptide
9	s7	29	ASN	Peptide
9	s7	64	VAL	Peptide
10	s8	60	ILE	Peptide
11	s9	89	ASP	Peptide
80	sM	165	UNK	Peptide
80	sM	169	UNK	Peptide
34	sR	161	LYS	Peptide

## 5.2 Too-close contacts [i](#)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

## 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	S0	204/206 (99%)	173 (85%)	27 (13%)	4 (2%)	7	31
2	s0	204/206 (99%)	175 (86%)	21 (10%)	8 (4%)	3	18
3	S1	212/216 (98%)	167 (79%)	40 (19%)	5 (2%)	6	27
3	s1	214/216 (99%)	182 (85%)	29 (14%)	3 (1%)	11	40
4	S2	215/217 (99%)	200 (93%)	11 (5%)	4 (2%)	8	33
4	s2	215/217 (99%)	195 (91%)	17 (8%)	3 (1%)	11	40
5	S3	221/223 (99%)	194 (88%)	23 (10%)	4 (2%)	8	34
5	s3	221/223 (99%)	185 (84%)	31 (14%)	5 (2%)	6	28
6	S4	258/260 (99%)	232 (90%)	24 (9%)	2 (1%)	19	54
6	s4	258/260 (99%)	230 (89%)	25 (10%)	3 (1%)	13	44
7	S5	204/206 (99%)	181 (89%)	15 (7%)	8 (4%)	3	18
7	s5	204/206 (99%)	182 (89%)	19 (9%)	3 (2%)	10	39
8	S6	224/226 (99%)	207 (92%)	14 (6%)	3 (1%)	12	42
8	s6	216/226 (96%)	198 (92%)	14 (6%)	4 (2%)	8	33
9	S7	182/186 (98%)	148 (81%)	20 (11%)	14 (8%)	1	5
9	s7	184/186 (99%)	154 (84%)	27 (15%)	3 (2%)	9	37
10	S8	184/200 (92%)	161 (88%)	21 (11%)	2 (1%)	14	46
10	s8	184/200 (92%)	170 (92%)	11 (6%)	3 (2%)	9	37
11	S9	183/185 (99%)	163 (89%)	16 (9%)	4 (2%)	6	29
11	s9	183/185 (99%)	164 (90%)	18 (10%)	1 (0%)	29	64
12	C0	94/98 (96%)	75 (80%)	17 (18%)	2 (2%)	7	30

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
12	c0	92/98 (94%)	67 (73%)	14 (15%)	11 (12%)	0	1
13	C1	153/156 (98%)	131 (86%)	20 (13%)	2 (1%)	12	42
13	c1	144/156 (92%)	124 (86%)	15 (10%)	5 (4%)	3	20
14	C2	122/124 (98%)	89 (73%)	27 (22%)	6 (5%)	2	14
14	c2	122/124 (98%)	85 (70%)	33 (27%)	4 (3%)	4	21
15	C3	148/150 (99%)	138 (93%)	9 (6%)	1 (1%)	22	57
15	c3	148/150 (99%)	130 (88%)	15 (10%)	3 (2%)	7	31
16	C4	125/128 (98%)	111 (89%)	12 (10%)	2 (2%)	9	37
16	c4	126/128 (98%)	111 (88%)	14 (11%)	1 (1%)	19	54
17	C5	122/142 (86%)	102 (84%)	14 (12%)	6 (5%)	2	14
17	c5	133/142 (94%)	109 (82%)	17 (13%)	7 (5%)	2	12
18	C6	139/142 (98%)	124 (89%)	13 (9%)	2 (1%)	11	40
18	c6	140/142 (99%)	131 (94%)	9 (6%)	0	100	100
19	C7	116/136 (85%)	100 (86%)	11 (10%)	5 (4%)	2	16
19	c7	113/136 (83%)	99 (88%)	11 (10%)	3 (3%)	5	25
20	C8	143/145 (99%)	120 (84%)	18 (13%)	5 (4%)	3	20
20	c8	143/145 (99%)	121 (85%)	17 (12%)	5 (4%)	3	20
21	C9	141/143 (99%)	127 (90%)	14 (10%)	0	100	100
21	c9	141/143 (99%)	125 (89%)	14 (10%)	2 (1%)	11	40
22	D0	105/110 (96%)	91 (87%)	13 (12%)	1 (1%)	15	49
22	d0	108/110 (98%)	89 (82%)	14 (13%)	5 (5%)	2	15
23	D1	85/87 (98%)	71 (84%)	13 (15%)	1 (1%)	13	44
23	d1	85/87 (98%)	75 (88%)	9 (11%)	1 (1%)	13	44
24	D2	127/129 (98%)	118 (93%)	6 (5%)	3 (2%)	6	27
24	d2	127/129 (98%)	119 (94%)	7 (6%)	1 (1%)	19	54
25	D3	142/144 (99%)	118 (83%)	19 (13%)	5 (4%)	3	20
25	d3	142/144 (99%)	131 (92%)	11 (8%)	0	100	100
26	D4	132/134 (98%)	117 (89%)	9 (7%)	6 (4%)	2	15
26	d4	132/134 (98%)	111 (84%)	18 (14%)	3 (2%)	6	28
27	D5	68/70 (97%)	51 (75%)	14 (21%)	3 (4%)	2	15
27	d5	67/70 (96%)	58 (87%)	8 (12%)	1 (2%)	10	39

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
28	D6	95/97 (98%)	70 (74%)	19 (20%)	6 (6%)	1	8
28	d6	95/97 (98%)	76 (80%)	12 (13%)	7 (7%)	1	6
29	D7	79/81 (98%)	69 (87%)	8 (10%)	2 (2%)	5	27
29	d7	79/81 (98%)	72 (91%)	6 (8%)	1 (1%)	12	42
30	D8	61/63 (97%)	54 (88%)	7 (12%)	0	100	100
30	d8	61/63 (97%)	49 (80%)	12 (20%)	0	100	100
31	D9	51/53 (96%)	47 (92%)	4 (8%)	0	100	100
31	d9	51/53 (96%)	48 (94%)	2 (4%)	1 (2%)	7	31
32	E0	58/62 (94%)	49 (84%)	7 (12%)	2 (3%)	3	21
32	e0	60/62 (97%)	51 (85%)	7 (12%)	2 (3%)	4	21
33	E1	69/76 (91%)	45 (65%)	18 (26%)	6 (9%)	1	4
33	e1	74/76 (97%)	49 (66%)	18 (24%)	7 (10%)	0	3
34	SR	316/318 (99%)	288 (91%)	28 (9%)	0	100	100
34	sR	316/318 (99%)	286 (90%)	26 (8%)	4 (1%)	12	42
35	SM	131/176 (74%)	108 (82%)	17 (13%)	6 (5%)	2	15
39	L2	250/252 (99%)	234 (94%)	15 (6%)	1 (0%)	34	69
39	l2	250/252 (99%)	225 (90%)	22 (9%)	3 (1%)	13	44
40	L3	384/386 (100%)	356 (93%)	24 (6%)	4 (1%)	15	49
40	l3	384/386 (100%)	362 (94%)	20 (5%)	2 (0%)	29	64
41	L4	359/361 (99%)	327 (91%)	32 (9%)	0	100	100
41	l4	359/361 (99%)	327 (91%)	25 (7%)	7 (2%)	8	33
42	L5	294/296 (99%)	257 (87%)	33 (11%)	4 (1%)	11	40
42	l5	292/296 (99%)	275 (94%)	17 (6%)	0	100	100
43	L6	152/176 (86%)	145 (95%)	6 (4%)	1 (1%)	22	57
43	l6	153/176 (87%)	139 (91%)	12 (8%)	2 (1%)	12	42
44	L7	220/223 (99%)	208 (94%)	11 (5%)	1 (0%)	29	64
44	l7	221/223 (99%)	208 (94%)	11 (5%)	2 (1%)	17	52
45	L8	231/233 (99%)	203 (88%)	22 (10%)	6 (3%)	5	26
46	L9	189/191 (99%)	171 (90%)	17 (9%)	1 (0%)	29	64
46	l9	189/191 (99%)	175 (93%)	12 (6%)	2 (1%)	14	46
47	M0	207/221 (94%)	188 (91%)	19 (9%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
47	m0	209/221 (95%)	188 (90%)	18 (9%)	3 (1%)	11	40
48	M1	167/169 (99%)	141 (84%)	20 (12%)	6 (4%)	3	20
48	m1	167/169 (99%)	143 (86%)	18 (11%)	6 (4%)	3	20
49	M3	191/194 (98%)	171 (90%)	14 (7%)	6 (3%)	4	23
49	m3	192/194 (99%)	166 (86%)	17 (9%)	9 (5%)	2	14
50	M4	134/137 (98%)	125 (93%)	7 (5%)	2 (2%)	10	39
50	m4	135/137 (98%)	132 (98%)	3 (2%)	0	100	100
51	M5	201/203 (99%)	191 (95%)	8 (4%)	2 (1%)	15	49
51	m5	201/203 (99%)	186 (92%)	12 (6%)	3 (2%)	10	39
52	M6	195/197 (99%)	189 (97%)	4 (2%)	2 (1%)	15	49
52	m6	195/197 (99%)	184 (94%)	11 (6%)	0	100	100
53	M7	181/183 (99%)	169 (93%)	12 (7%)	0	100	100
53	m7	153/183 (84%)	146 (95%)	7 (5%)	0	100	100
54	M8	183/185 (99%)	169 (92%)	12 (7%)	2 (1%)	14	46
54	m8	183/185 (99%)	169 (92%)	13 (7%)	1 (0%)	29	64
55	M9	186/188 (99%)	175 (94%)	9 (5%)	2 (1%)	14	46
55	m9	186/188 (99%)	173 (93%)	13 (7%)	0	100	100
56	N0	170/172 (99%)	158 (93%)	9 (5%)	3 (2%)	8	34
56	n0	170/172 (99%)	163 (96%)	7 (4%)	0	100	100
57	N1	157/159 (99%)	142 (90%)	13 (8%)	2 (1%)	12	42
57	n1	157/159 (99%)	149 (95%)	6 (4%)	2 (1%)	12	42
58	N2	98/100 (98%)	85 (87%)	12 (12%)	1 (1%)	15	49
58	n2	96/100 (96%)	91 (95%)	4 (4%)	1 (1%)	15	49
59	N3	134/136 (98%)	128 (96%)	6 (4%)	0	100	100
59	n3	134/136 (98%)	130 (97%)	3 (2%)	1 (1%)	22	57
60	N4	96/98 (98%)	84 (88%)	10 (10%)	2 (2%)	7	30
61	N5	119/121 (98%)	113 (95%)	6 (5%)	0	100	100
61	n5	118/121 (98%)	104 (88%)	14 (12%)	0	100	100
62	N6	124/126 (98%)	115 (93%)	9 (7%)	0	100	100
62	n6	124/126 (98%)	119 (96%)	3 (2%)	2 (2%)	9	37
63	N7	133/135 (98%)	124 (93%)	6 (4%)	3 (2%)	6	28

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
63	n7	133/135 (98%)	115 (86%)	15 (11%)	3 (2%)	6	28
64	N8	146/148 (99%)	131 (90%)	12 (8%)	3 (2%)	7	30
64	n8	146/148 (99%)	131 (90%)	13 (9%)	2 (1%)	11	40
65	N9	56/58 (97%)	49 (88%)	7 (12%)	0	100	100
65	n9	56/58 (97%)	46 (82%)	9 (16%)	1 (2%)	8	34
66	O0	95/100 (95%)	93 (98%)	2 (2%)	0	100	100
66	o0	98/100 (98%)	89 (91%)	9 (9%)	0	100	100
67	O1	107/109 (98%)	100 (94%)	6 (6%)	1 (1%)	17	52
67	o1	107/109 (98%)	100 (94%)	6 (6%)	1 (1%)	17	52
68	O2	125/127 (98%)	121 (97%)	4 (3%)	0	100	100
68	o2	125/127 (98%)	116 (93%)	6 (5%)	3 (2%)	6	27
69	O3	104/106 (98%)	99 (95%)	5 (5%)	0	100	100
69	o3	104/106 (98%)	97 (93%)	7 (7%)	0	100	100
70	O4	110/112 (98%)	104 (94%)	6 (6%)	0	100	100
70	o4	110/112 (98%)	102 (93%)	7 (6%)	1 (1%)	17	52
71	O5	117/119 (98%)	108 (92%)	9 (8%)	0	100	100
71	o5	117/119 (98%)	106 (91%)	11 (9%)	0	100	100
72	O6	97/99 (98%)	79 (81%)	15 (16%)	3 (3%)	4	23
72	o6	97/99 (98%)	87 (90%)	8 (8%)	2 (2%)	7	30
73	O7	85/87 (98%)	78 (92%)	7 (8%)	0	100	100
73	o7	85/87 (98%)	78 (92%)	6 (7%)	1 (1%)	13	44
74	O8	75/77 (97%)	66 (88%)	6 (8%)	3 (4%)	3	17
74	o8	75/77 (97%)	67 (89%)	7 (9%)	1 (1%)	12	42
75	O9	48/50 (96%)	46 (96%)	2 (4%)	0	100	100
75	o9	48/50 (96%)	44 (92%)	4 (8%)	0	100	100
76	Q0	50/52 (96%)	47 (94%)	3 (6%)	0	100	100
76	q0	50/52 (96%)	46 (92%)	3 (6%)	1 (2%)	7	31
77	Q1	23/25 (92%)	22 (96%)	1 (4%)	0	100	100
77	q1	23/25 (92%)	23 (100%)	0	0	100	100
78	Q2	103/105 (98%)	89 (86%)	14 (14%)	0	100	100
78	q2	103/105 (98%)	96 (93%)	6 (6%)	1 (1%)	15	49

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
79	Q3	89/91 (98%)	81 (91%)	7 (8%)	1 (1%)	14	46
79	q3	89/91 (98%)	85 (96%)	3 (3%)	1 (1%)	14	46
80	sM	61/159 (38%)	50 (82%)	8 (13%)	3 (5%)	2	14
81	l8	229/231 (99%)	197 (86%)	28 (12%)	4 (2%)	9	36
83	n4	133/135 (98%)	111 (84%)	16 (12%)	6 (4%)	2	15
84	p0	139/312 (45%)	126 (91%)	12 (9%)	1 (1%)	22	57
All	All	22272/23122 (96%)	19937 (90%)	1963 (9%)	372 (2%)	9	36

All (372) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
9	S7	64	VAL
9	S7	111	LYS
9	S7	131	PHE
9	S7	133	THR
12	C0	87	VAL
12	C0	88	PRO
14	C2	126	TRP
18	C6	39	VAL
19	C7	85	VAL
19	C7	86	PRO
20	C8	28	ILE
24	D2	83	ILE
26	D4	35	VAL
27	D5	39	ALA
32	E0	47	VAL
40	L3	140	ASP
43	L6	98	VAL
45	L8	36	ILE
46	L9	50	ASN
48	M1	11	ASP
49	M3	129	ASN
52	M6	111	PRO
72	O6	33	ALA
72	O6	34	SER
2	s0	189	VAL
3	s1	210	ILE
4	s2	92	ALA
9	s7	64	VAL
12	c0	83	PRO

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Mol	Chain	Res	Type
12	c0	88	PRO
12	c0	97	PRO
14	c2	91	VAL
17	c5	126	VAL
20	c8	91	ASP
24	d2	6	VAL
33	e1	87	THR
33	e1	102	VAL
39	l2	239	ALA
43	l6	98	VAL
43	l6	130	ILE
48	m1	152	HIS
49	m3	63	VAL
51	m5	184	LYS
83	n4	76	VAL
63	n7	130	PHE
65	n9	21	ILE
3	S1	63	GLY
5	S3	217	ILE
9	S7	66	SER
9	S7	112	ARG
10	S8	148	ALA
13	C1	7	VAL
14	C2	89	ILE
14	C2	91	VAL
16	C4	40	ALA
17	C5	69	GLU
17	C5	70	ASN
17	C5	126	VAL
18	C6	113	ASP
19	C7	88	VAL
19	C7	124	VAL
22	D0	18	GLN
23	D1	82	VAL
24	D2	30	SER
26	D4	5	VAL
28	D6	46	GLU
28	D6	75	VAL
29	D7	62	ILE
33	E1	98	VAL
35	SM	87	THR
40	L3	4	ARG

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Mol	Chain	Res	Type
40	L3	5	LYS
42	L5	252	ALA
42	L5	259	LYS
45	L8	37	GLY
48	M1	115	LYS
50	M4	8	LYS
51	M5	75	VAL
54	M8	99	THR
55	M9	131	ALA
56	N0	13	ARG
57	N1	124	VAL
60	N4	96	LEU
63	N7	30	ASP
74	O8	19	ASP
5	s3	216	PRO
5	s3	217	ILE
5	s3	222	VAL
8	s6	173	PRO
8	s6	174	LYS
9	s7	10	SER
12	c0	82	LEU
13	c1	7	VAL
13	c1	133	LYS
14	c2	84	ASN
15	c3	66	ILE
17	c5	51	SER
19	c7	88	VAL
20	c8	92	ILE
22	d0	15	GLN
22	d0	118	VAL
23	d1	6	GLY
26	d4	52	LYS
26	d4	123	LYS
29	d7	62	ILE
33	e1	98	VAL
33	e1	103	LEU
33	e1	136	LYS
39	l2	238	ILE
41	l4	302	ALA
47	m0	175	ASN
54	m8	99	THR
62	n6	125	LYS

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Mol	Chain	Res	Type
72	o6	63	ASN
74	o8	19	ASP
2	S0	4	PRO
3	S1	62	LYS
5	S3	221	SER
7	S5	58	LEU
7	S5	64	VAL
9	S7	65	PRO
9	S7	67	LEU
9	S7	132	PRO
9	S7	134	GLU
13	C1	6	THR
24	D2	31	SER
25	D3	3	LYS
26	D4	4	ALA
27	D5	71	ILE
33	E1	101	ALA
35	SM	46	LYS
35	SM	86	ASN
35	SM	102	THR
39	L2	251	LYS
48	M1	8	PRO
48	M1	165	GLN
49	M3	51	LEU
49	M3	77	LEU
49	M3	166	ALA
51	M5	74	PRO
56	N0	2	ALA
56	N0	167	ARG
64	N8	79	TRP
2	s0	164	ASN
3	s1	179	SER
7	s5	43	PHE
7	s5	184	PHE
8	s6	70	PRO
13	c1	61	THR
16	c4	126	THR
17	c5	7	ALA
17	c5	125	PRO
20	c8	8	GLN
22	d0	51	VAL
26	d4	35	VAL

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Mol	Chain	Res	Type
28	d6	61	GLU
28	d6	62	TYR
33	e1	84	VAL
34	sR	54	PHE
34	sR	166	SER
41	l4	90	PHE
41	l4	329	PRO
44	l7	229	PHE
48	m1	115	LYS
49	m3	47	ALA
49	m3	140	SER
49	m3	141	ALA
57	n1	136	ARG
59	n3	42	SER
83	n4	63	ILE
83	n4	73	ARG
83	n4	77	LYS
64	n8	78	LEU
3	S1	180	THR
4	S2	40	LYS
4	S2	144	TRP
4	S2	148	LEU
6	S4	164	LEU
8	S6	70	PRO
9	S7	32	PRO
10	S8	152	ILE
14	C2	106	ILE
17	C5	54	ALA
20	C8	61	LEU
20	C8	91	ASP
20	C8	144	ARG
26	D4	36	SER
27	D5	88	ILE
28	D6	45	VAL
28	D6	61	GLU
33	E1	100	LEU
33	E1	111	GLU
48	M1	173	ASP
49	M3	47	ALA
52	M6	110	PRO
55	M9	53	LYS
3	s1	209	ASN

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Mol	Chain	Res	Type
5	s3	45	LYS
7	s5	101	GLY
10	s8	62	THR
11	s9	134	ILE
12	c0	32	HIS
12	c0	94	GLU
13	c1	8	GLN
14	c2	106	ILE
17	c5	128	HIS
17	c5	129	GLY
27	d5	104	ALA
28	d6	15	ARG
33	e1	88	PRO
34	sR	318	ALA
80	sM	48	ARG
80	sM	50	ASN
40	l3	129	ALA
41	l4	342	LYS
44	l7	191	VAL
48	m1	8	PRO
49	m3	51	LEU
83	n4	72	SER
83	n4	133	THR
63	n7	129	TRP
68	o2	12	LYS
70	o4	82	ALA
72	o6	98	ARG
4	S2	39	THR
5	S3	93	ASP
5	S3	216	PRO
7	S5	26	ALA
7	S5	39	GLU
7	S5	51	VAL
7	S5	77	TYR
7	S5	127	GLN
11	S9	100	LYS
11	S9	121	SER
11	S9	134	ILE
14	C2	125	ASN
14	C2	128	ALA
15	C3	22	ALA
17	C5	125	PRO

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Mol	Chain	Res	Type
19	C7	25	THR
20	C8	14	ILE
25	D3	131	SER
25	D3	137	LYS
26	D4	6	THR
29	D7	38	PRO
33	E1	106	TYR
40	L3	317	ILE
42	L5	258	LYS
45	L8	25	PRO
45	L8	39	ALA
45	L8	157	VAL
48	M1	114	ILE
49	M3	76	THR
63	N7	102	GLU
64	N8	48	TYR
64	N8	78	LEU
74	O8	18	ALA
79	Q3	51	ALA
2	s0	9	LEU
2	s0	103	THR
2	s0	206	ASP
4	s2	106	ASP
5	s3	179	GLN
6	s4	172	PHE
9	s7	163	ASP
12	c0	30	ALA
14	c2	66	VAL
17	c5	68	PRO
19	c7	103	ASP
21	c9	142	GLU
28	d6	13	LYS
81	l8	25	PRO
81	l8	34	PHE
81	l8	203	VAL
46	l9	144	ILE
48	m1	10	ARG
48	m1	108	GLU
48	m1	114	ILE
49	m3	50	PRO
49	m3	62	THR
51	m5	183	THR

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Mol	Chain	Res	Type
58	n2	91	ASP
62	n6	126	LEU
63	n7	103	GLN
68	o2	5	PRO
73	o7	86	ALA
78	q2	76	LYS
79	q3	51	ALA
2	S0	27	ARG
2	S0	39	ASN
3	S1	49	ASN
6	S4	195	ILE
8	S6	69	LEU
9	S7	74	GLN
25	D3	112	LYS
28	D6	82	ARG
28	D6	84	VAL
33	E1	84	VAL
42	L5	260	PHE
45	L8	156	ASP
57	N1	12	ARG
58	N2	11	ILE
60	N4	97	LYS
63	N7	103	GLN
67	O1	7	VAL
2	s0	30	GLN
4	s2	235	LEU
12	c0	31	LYS
15	c3	60	VAL
21	c9	34	VAL
22	d0	96	PRO
28	d6	34	LYS
34	sR	160	GLU
39	l2	56	ALA
40	l3	187	SER
47	m0	170	LYS
47	m0	195	ALA
68	o2	6	HIS
76	q0	78	ILE
84	p0	33	VAL
2	S0	158	VAL
3	S1	210	ILE
7	S5	101	GLY

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Mol	Chain	Res	Type
9	S7	98	ILE
16	C4	42	VAL
17	C5	53	PRO
26	D4	47	VAL
35	SM	12	VAL
50	M4	6	ILE
72	O6	3	VAL
10	s8	78	ILE
12	c0	35	ILE
12	c0	92	ILE
19	c7	99	VAL
22	d0	97	VAL
81	l8	237	ILE
64	n8	28	HIS
9	S7	63	PRO
8	s6	69	LEU
10	s8	101	ILE
20	c8	14	ILE
32	e0	47	VAL
51	m5	76	PRO
57	n1	135	PRO
8	S6	173	PRO
35	SM	53	ARG
54	M8	162	ALA
74	O8	36	LYS
2	s0	10	THR
2	s0	158	VAL
6	s4	30	ARG
6	s4	90	ILE
15	c3	22	ALA
20	c8	135	GLY
31	d9	6	VAL
41	l4	301	PRO
46	l9	167	VAL
49	m3	93	ILE
11	S9	168	ARG
32	E0	45	VAL
44	L7	178	ILE
13	c1	129	ARG
28	d6	58	VAL
32	e0	60	PRO
80	sM	43	ASP

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Mol	Chain	Res	Type
41	l4	142	VAL
49	m3	60	ALA
67	o1	45	GLY
25	D3	41	SER
12	c0	3	MET
28	d6	59	TYR
41	l4	145	ILE

### 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	S0	164/173 (95%)	134 (82%)	30 (18%)	1	7
2	s0	165/173 (95%)	131 (79%)	34 (21%)	1	5
3	S1	191/192 (100%)	152 (80%)	39 (20%)	1	5
3	s1	192/192 (100%)	154 (80%)	38 (20%)	1	5
4	S2	176/176 (100%)	141 (80%)	35 (20%)	1	5
4	s2	176/176 (100%)	136 (77%)	40 (23%)	1	3
5	S3	182/182 (100%)	147 (81%)	35 (19%)	1	6
5	s3	182/182 (100%)	151 (83%)	31 (17%)	2	9
6	S4	221/221 (100%)	180 (81%)	41 (19%)	1	7
6	s4	221/221 (100%)	184 (83%)	37 (17%)	2	9
7	S5	173/173 (100%)	145 (84%)	28 (16%)	2	10
7	s5	173/173 (100%)	141 (82%)	32 (18%)	1	7
8	S6	188/193 (97%)	162 (86%)	26 (14%)	3	16
8	s6	187/193 (97%)	155 (83%)	32 (17%)	2	9
9	S7	165/166 (99%)	135 (82%)	30 (18%)	1	7
9	s7	165/166 (99%)	129 (78%)	36 (22%)	1	4
10	S8	150/161 (93%)	127 (85%)	23 (15%)	2	12
10	s8	150/161 (93%)	123 (82%)	27 (18%)	1	7

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
11	S9	158/158 (100%)	126 (80%)	32 (20%)	1	5
11	s9	158/158 (100%)	124 (78%)	34 (22%)	1	4
12	C0	77/91 (85%)	61 (79%)	16 (21%)	1	5
12	c0	73/91 (80%)	60 (82%)	13 (18%)	2	8
13	C1	129/137 (94%)	105 (81%)	24 (19%)	1	7
13	c1	129/137 (94%)	105 (81%)	24 (19%)	1	7
14	C2	88/100 (88%)	65 (74%)	23 (26%)	0	1
14	c2	88/100 (88%)	64 (73%)	24 (27%)	0	1
15	C3	127/127 (100%)	102 (80%)	25 (20%)	1	6
15	c3	127/127 (100%)	101 (80%)	26 (20%)	1	5
16	C4	81/97 (84%)	65 (80%)	16 (20%)	1	5
16	c4	97/97 (100%)	75 (77%)	22 (23%)	1	3
17	C5	101/118 (86%)	87 (86%)	14 (14%)	3	15
17	c5	103/118 (87%)	86 (84%)	17 (16%)	2	10
18	C6	117/118 (99%)	89 (76%)	28 (24%)	0	2
18	c6	118/118 (100%)	97 (82%)	21 (18%)	2	8
19	C7	94/124 (76%)	72 (77%)	22 (23%)	1	3
19	c7	92/124 (74%)	75 (82%)	17 (18%)	1	7
20	C8	128/128 (100%)	104 (81%)	24 (19%)	1	6
20	c8	128/128 (100%)	106 (83%)	22 (17%)	2	9
21	C9	115/115 (100%)	92 (80%)	23 (20%)	1	5
21	c9	115/115 (100%)	96 (84%)	19 (16%)	2	10
22	D0	100/103 (97%)	80 (80%)	20 (20%)	1	5
22	d0	103/103 (100%)	77 (75%)	26 (25%)	0	1
23	D1	74/74 (100%)	63 (85%)	11 (15%)	3	13
23	d1	74/74 (100%)	58 (78%)	16 (22%)	1	4
24	D2	110/110 (100%)	89 (81%)	21 (19%)	1	6
24	d2	110/110 (100%)	96 (87%)	14 (13%)	4	18
25	D3	119/119 (100%)	95 (80%)	24 (20%)	1	5
25	d3	119/119 (100%)	99 (83%)	20 (17%)	2	9
26	D4	112/112 (100%)	91 (81%)	21 (19%)	1	6

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
26	d4	112/112 (100%)	98 (88%)	14 (12%)	4	18
27	D5	61/61 (100%)	47 (77%)	14 (23%)	1	3
27	d5	61/61 (100%)	53 (87%)	8 (13%)	4	17
28	D6	83/83 (100%)	63 (76%)	20 (24%)	0	2
28	d6	83/83 (100%)	68 (82%)	15 (18%)	1	7
29	D7	70/70 (100%)	60 (86%)	10 (14%)	3	14
29	d7	70/70 (100%)	58 (83%)	12 (17%)	2	9
30	D8	56/56 (100%)	42 (75%)	14 (25%)	0	2
30	d8	56/56 (100%)	44 (79%)	12 (21%)	1	4
31	D9	47/47 (100%)	33 (70%)	14 (30%)	0	1
31	d9	47/47 (100%)	35 (74%)	12 (26%)	0	1
32	E0	51/53 (96%)	43 (84%)	8 (16%)	2	11
32	e0	53/53 (100%)	43 (81%)	10 (19%)	1	6
33	E1	62/66 (94%)	47 (76%)	15 (24%)	0	2
33	e1	66/66 (100%)	47 (71%)	19 (29%)	0	1
34	SR	259/261 (99%)	228 (88%)	31 (12%)	5	20
34	sR	259/261 (99%)	230 (89%)	29 (11%)	6	24
35	SM	97/122 (80%)	75 (77%)	22 (23%)	1	3
39	L2	193/194 (100%)	163 (84%)	30 (16%)	2	11
39	l2	192/194 (99%)	152 (79%)	40 (21%)	1	5
40	L3	320/322 (99%)	256 (80%)	64 (20%)	1	5
40	l3	319/322 (99%)	266 (83%)	53 (17%)	2	9
41	L4	288/288 (100%)	238 (83%)	50 (17%)	2	9
41	l4	288/288 (100%)	241 (84%)	47 (16%)	2	10
42	L5	244/244 (100%)	194 (80%)	50 (20%)	1	5
42	l5	243/244 (100%)	203 (84%)	40 (16%)	2	10
43	L6	134/153 (88%)	117 (87%)	17 (13%)	4	18
43	l6	135/153 (88%)	116 (86%)	19 (14%)	3	15
44	L7	186/187 (100%)	160 (86%)	26 (14%)	3	15
44	l7	187/187 (100%)	159 (85%)	28 (15%)	3	12
45	L8	187/191 (98%)	159 (85%)	28 (15%)	3	12

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
46	L9	171/171 (100%)	136 (80%)	35 (20%)	1	5
46	l9	171/171 (100%)	137 (80%)	34 (20%)	1	5
47	M0	177/187 (95%)	151 (85%)	26 (15%)	3	13
47	m0	179/187 (96%)	139 (78%)	40 (22%)	1	3
48	M1	147/147 (100%)	117 (80%)	30 (20%)	1	5
48	m1	147/147 (100%)	120 (82%)	27 (18%)	1	7
49	M3	154/154 (100%)	126 (82%)	28 (18%)	1	7
49	m3	154/154 (100%)	130 (84%)	24 (16%)	2	11
50	M4	107/108 (99%)	90 (84%)	17 (16%)	2	11
50	m4	108/108 (100%)	93 (86%)	15 (14%)	3	15
51	M5	175/175 (100%)	146 (83%)	29 (17%)	2	9
51	m5	175/175 (100%)	146 (83%)	29 (17%)	2	9
52	M6	160/160 (100%)	132 (82%)	28 (18%)	2	8
52	m6	160/160 (100%)	132 (82%)	28 (18%)	2	8
53	M7	140/145 (97%)	115 (82%)	25 (18%)	2	8
53	m7	125/145 (86%)	100 (80%)	25 (20%)	1	5
54	M8	150/150 (100%)	126 (84%)	24 (16%)	2	11
54	m8	150/150 (100%)	124 (83%)	26 (17%)	2	9
55	M9	153/153 (100%)	134 (88%)	19 (12%)	4	19
55	m9	153/153 (100%)	130 (85%)	23 (15%)	3	12
56	N0	156/156 (100%)	116 (74%)	40 (26%)	0	1
56	n0	156/156 (100%)	122 (78%)	34 (22%)	1	4
57	N1	136/136 (100%)	105 (77%)	31 (23%)	1	3
57	n1	136/136 (100%)	112 (82%)	24 (18%)	2	8
58	N2	87/87 (100%)	70 (80%)	17 (20%)	1	6
58	n2	85/87 (98%)	68 (80%)	17 (20%)	1	5
59	N3	104/104 (100%)	83 (80%)	21 (20%)	1	5
59	n3	104/104 (100%)	87 (84%)	17 (16%)	2	10
60	N4	57/86 (66%)	50 (88%)	7 (12%)	4	19
61	N5	104/105 (99%)	78 (75%)	26 (25%)	0	2
61	n5	104/105 (99%)	85 (82%)	19 (18%)	1	7

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
62	N6	109/109 (100%)	87 (80%)	22 (20%)	1	5
62	n6	109/109 (100%)	82 (75%)	27 (25%)	0	2
63	N7	115/115 (100%)	95 (83%)	20 (17%)	2	9
63	n7	115/115 (100%)	92 (80%)	23 (20%)	1	5
64	N8	118/118 (100%)	96 (81%)	22 (19%)	1	7
64	n8	118/118 (100%)	90 (76%)	28 (24%)	1	2
65	N9	46/46 (100%)	38 (83%)	8 (17%)	2	9
65	n9	46/46 (100%)	38 (83%)	8 (17%)	2	9
66	O0	81/84 (96%)	65 (80%)	16 (20%)	1	5
66	o0	84/84 (100%)	71 (84%)	13 (16%)	2	11
67	O1	92/96 (96%)	77 (84%)	15 (16%)	2	10
67	o1	94/96 (98%)	75 (80%)	19 (20%)	1	5
68	O2	109/109 (100%)	96 (88%)	13 (12%)	5	20
68	o2	109/109 (100%)	89 (82%)	20 (18%)	1	7
69	O3	90/90 (100%)	78 (87%)	12 (13%)	4	16
69	o3	90/90 (100%)	80 (89%)	10 (11%)	6	24
70	O4	95/95 (100%)	81 (85%)	14 (15%)	3	13
70	o4	95/95 (100%)	85 (90%)	10 (10%)	7	26
71	O5	104/104 (100%)	84 (81%)	20 (19%)	1	6
71	o5	103/104 (99%)	86 (84%)	17 (16%)	2	10
72	O6	81/81 (100%)	60 (74%)	21 (26%)	0	1
72	o6	80/81 (99%)	55 (69%)	25 (31%)	0	0
73	O7	70/70 (100%)	61 (87%)	9 (13%)	4	18
73	o7	70/70 (100%)	57 (81%)	13 (19%)	1	7
74	O8	68/68 (100%)	50 (74%)	18 (26%)	0	1
74	o8	67/68 (98%)	54 (81%)	13 (19%)	1	6
75	O9	45/45 (100%)	40 (89%)	5 (11%)	6	24
75	o9	45/45 (100%)	38 (84%)	7 (16%)	2	11
76	Q0	47/47 (100%)	40 (85%)	7 (15%)	3	13
76	q0	47/47 (100%)	38 (81%)	9 (19%)	1	6
77	Q1	23/23 (100%)	18 (78%)	5 (22%)	1	4

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
77	q1	23/23 (100%)	16 (70%)	7 (30%)	0	0
78	Q2	90/90 (100%)	72 (80%)	18 (20%)	1	5
78	q2	90/90 (100%)	71 (79%)	19 (21%)	1	5
79	Q3	71/71 (100%)	59 (83%)	12 (17%)	2	9
79	q3	71/71 (100%)	55 (78%)	16 (22%)	1	3
80	sM	54/103 (52%)	42 (78%)	12 (22%)	1	4
81	l8	177/190 (93%)	144 (81%)	33 (19%)	1	7
83	n4	100/114 (88%)	87 (87%)	13 (13%)	4	18
84	p0	105/254 (41%)	81 (77%)	24 (23%)	1	3
All	All	18725/19364 (97%)	15293 (82%)	3432 (18%)	1	7

All (3432) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	S0	7	PHE
2	S0	21	ASN
2	S0	27	ARG
2	S0	30	GLN
2	S0	32	HIS
2	S0	37	VAL
2	S0	43	ASP
2	S0	50	VAL
2	S0	59	LEU
2	S0	62	ARG
2	S0	84	ARG
2	S0	87	LEU
2	S0	88	LYS
2	S0	96	THR
2	S0	101	ARG
2	S0	111	ILE
2	S0	119	ARG
2	S0	131	GLN
2	S0	135	GLU
2	S0	139	VAL
2	S0	150	ASP
2	S0	157	ASP
2	S0	162	CYS
2	S0	172	LEU
2	S0	177	LEU

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Mol	Chain	Res	Type
2	S0	184	LEU
2	S0	185	ARG
2	S0	196	SER
2	S0	198	MET
2	S0	200	ASP
3	S1	21	VAL
3	S1	29	TRP
3	S1	30	PHE
3	S1	46	THR
3	S1	61	LEU
3	S1	62	LYS
3	S1	65	VAL
3	S1	66	VAL
3	S1	70	LEU
3	S1	77	GLU
3	S1	78	ASP
3	S1	81	PHE
3	S1	83	LYS
3	S1	85	LYS
3	S1	89	ASP
3	S1	95	ASN
3	S1	96	LEU
3	S1	97	LEU
3	S1	104	ASP
3	S1	105	PHE
3	S1	110	LEU
3	S1	111	ARG
3	S1	117	TRP
3	S1	135	LEU
3	S1	145	LYS
3	S1	154	SER
3	S1	170	GLU
3	S1	177	GLN
3	S1	180	THR
3	S1	181	LEU
3	S1	193	ILE
3	S1	202	LYS
3	S1	214	LYS
3	S1	215	VAL
3	S1	218	LEU
3	S1	220	GLN
3	S1	222	LYS

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Mol	Chain	Res	Type
3	S1	223	PHE
3	S1	229	MET
4	S2	41	LEU
4	S2	53	ILE
4	S2	54	GLU
4	S2	55	GLU
4	S2	58	LEU
4	S2	69	ILE
4	S2	72	LEU
4	S2	73	LEU
4	S2	76	LEU
4	S2	77	GLN
4	S2	89	GLN
4	S2	90	THR
4	S2	91	ARG
4	S2	95	ARG
4	S2	96	THR
4	S2	97	ARG
4	S2	106	ASP
4	S2	107	SER
4	S2	111	VAL
4	S2	119	LYS
4	S2	134	LEU
4	S2	137	ILE
4	S2	139	ILE
4	S2	141	ARG
4	S2	146	THR
4	S2	148	LEU
4	S2	174	ARG
4	S2	208	GLU
4	S2	221	THR
4	S2	222	TYR
4	S2	225	LEU
4	S2	226	THR
4	S2	237	VAL
4	S2	244	SER
4	S2	245	ASP
5	S3	4	LEU
5	S3	7	LYS
5	S3	14	ASP
5	S3	21	LEU
5	S3	23	GLU

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Mol	Chain	Res	Type
5	S3	35	SER
5	S3	44	THR
5	S3	62	ASN
5	S3	65	ARG
5	S3	66	ILE
5	S3	76	ARG
5	S3	84	ILE
5	S3	89	GLU
5	S3	91	VAL
5	S3	92	GLN
5	S3	93	ASP
5	S3	94	ARG
5	S3	103	GLU
5	S3	105	MET
5	S3	113	LEU
5	S3	117	ARG
5	S3	120	TYR
5	S3	128	GLU
5	S3	143	ARG
5	S3	151	LYS
5	S3	158	ILE
5	S3	172	THR
5	S3	176	LEU
5	S3	178	ARG
5	S3	179	GLN
5	S3	182	LEU
5	S3	190	ARG
5	S3	202	LEU
5	S3	212	LYS
5	S3	222	VAL
6	S4	6	LYS
6	S4	7	LYS
6	S4	9	LEU
6	S4	23	LEU
6	S4	38	LEU
6	S4	42	LEU
6	S4	45	ILE
6	S4	54	TYR
6	S4	62	LYS
6	S4	67	GLN
6	S4	77	ARG
6	S4	92	LEU

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Mol	Chain	Res	Type
6	S4	95	THR
6	S4	113	ARG
6	S4	115	THR
6	S4	116	ASP
6	S4	123	LEU
6	S4	131	LEU
6	S4	133	LYS
6	S4	139	VAL
6	S4	140	VAL
6	S4	148	ARG
6	S4	164	LEU
6	S4	166	SER
6	S4	180	LEU
6	S4	182	TYR
6	S4	187	ARG
6	S4	192	ILE
6	S4	197	HIS
6	S4	198	LYS
6	S4	206	ASP
6	S4	211	LYS
6	S4	215	ASP
6	S4	226	PHE
6	S4	231	GLN
6	S4	233	LYS
6	S4	240	LYS
6	S4	242	LYS
6	S4	246	LEU
6	S4	258	GLN
6	S4	259	GLN
7	S5	24	VAL
7	S5	25	LEU
7	S5	34	GLN
7	S5	38	THR
7	S5	41	LYS
7	S5	43	PHE
7	S5	46	TRP
7	S5	51	VAL
7	S5	65	ARG
7	S5	76	ARG
7	S5	79	ASN
7	S5	84	LYS
7	S5	89	ILE

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Mol	Chain	Res	Type
7	S5	93	LEU
7	S5	98	MET
7	S5	126	ASP
7	S5	131	GLN
7	S5	146	THR
7	S5	147	THR
7	S5	156	ARG
7	S5	158	GLN
7	S5	162	VAL
7	S5	170	GLN
7	S5	194	LEU
7	S5	203	LYS
7	S5	216	GLU
7	S5	223	SER
7	S5	225	ARG
8	S6	7	TYR
8	S6	10	ASN
8	S6	19	ASP
8	S6	58	LYS
8	S6	69	LEU
8	S6	76	LEU
8	S6	78	THR
8	S6	79	LYS
8	S6	81	VAL
8	S6	82	SER
8	S6	98	ARG
8	S6	109	LEU
8	S6	126	ASP
8	S6	127	THR
8	S6	128	THR
8	S6	129	VAL
8	S6	133	LEU
8	S6	144	PHE
8	S6	151	ASP
8	S6	154	ARG
8	S6	155	ASP
8	S6	169	TYR
8	S6	174	LYS
8	S6	193	LEU
8	S6	211	LEU
8	S6	223	LYS
9	S7	9	LEU

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Mol	Chain	Res	Type
9	S7	29	ASN
9	S7	30	SER
9	S7	34	LEU
9	S7	37	GLU
9	S7	38	LEU
9	S7	46	ILE
9	S7	49	ILE
9	S7	50	ASP
9	S7	60	ILE
9	S7	67	LEU
9	S7	70	PHE
9	S7	77	LEU
9	S7	79	ARG
9	S7	85	PHE
9	S7	87	ASP
9	S7	97	ARG
9	S7	109	VAL
9	S7	112	ARG
9	S7	114	ARG
9	S7	116	ARG
9	S7	118	LEU
9	S7	126	LEU
9	S7	136	VAL
9	S7	144	VAL
9	S7	159	VAL
9	S7	167	GLU
9	S7	175	LYS
9	S7	185	ILE
9	S7	187	SER
10	S8	7	SER
10	S8	8	ARG
10	S8	18	ARG
10	S8	21	PHE
10	S8	26	LYS
10	S8	29	LEU
10	S8	36	THR
10	S8	58	LEU
10	S8	62	THR
10	S8	66	SER
10	S8	92	ARG
10	S8	121	LEU
10	S8	137	LYS

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Mol	Chain	Res	Type
10	S8	151	LYS
10	S8	152	ILE
10	S8	155	SER
10	S8	158	SER
10	S8	164	ARG
10	S8	168	CYS
10	S8	184	LEU
10	S8	185	GLU
10	S8	196	LEU
10	S8	199	LYS
11	S9	3	ARG
11	S9	7	THR
11	S9	9	SER
11	S9	14	THR
11	S9	16	LYS
11	S9	17	ARG
11	S9	28	LEU
11	S9	39	LYS
11	S9	46	SER
11	S9	60	LEU
11	S9	61	THR
11	S9	78	ARG
11	S9	82	ARG
11	S9	87	SER
11	S9	89	ASP
11	S9	92	LYS
11	S9	93	LEU
11	S9	97	LEU
11	S9	99	LEU
11	S9	101	VAL
11	S9	105	LEU
11	S9	110	GLN
11	S9	118	LEU
11	S9	121	SER
11	S9	130	THR
11	S9	134	ILE
11	S9	138	LYS
11	S9	149	ARG
11	S9	157	ASP
11	S9	161	THR
11	S9	171	ARG
11	S9	174	ARG

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Mol	Chain	Res	Type
12	C0	1	MET
12	C0	7	ASP
12	C0	8	ARG
12	C0	18	GLU
12	C0	20	VAL
12	C0	27	PHE
12	C0	32	HIS
12	C0	46	LEU
12	C0	49	LEU
12	C0	52	LYS
12	C0	55	VAL
12	C0	56	LYS
12	C0	71	GLU
12	C0	76	LEU
12	C0	81	ASN
12	C0	82	LEU
13	C1	2	SER
13	C1	5	LEU
13	C1	21	ASN
13	C1	27	THR
13	C1	29	LYS
13	C1	40	LEU
13	C1	44	THR
13	C1	56	LYS
13	C1	67	ARG
13	C1	69	LYS
13	C1	74	THR
13	C1	80	MET
13	C1	109	VAL
13	C1	112	SER
13	C1	118	GLN
13	C1	119	VAL
13	C1	123	VAL
13	C1	125	VAL
13	C1	127	GLN
13	C1	128	CYS
13	C1	136	ARG
13	C1	140	VAL
13	C1	141	LYS
13	C1	143	SER
14	C2	28	LEU
14	C2	36	LEU

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Mol	Chain	Res	Type
14	C2	37	VAL
14	C2	43	ARG
14	C2	45	LEU
14	C2	46	ARG
14	C2	50	LYS
14	C2	52	LEU
14	C2	61	VAL
14	C2	62	LEU
14	C2	65	SER
14	C2	66	VAL
14	C2	71	ILE
14	C2	74	LEU
14	C2	83	GLU
14	C2	89	ILE
14	C2	103	LEU
14	C2	119	SER
14	C2	126	TRP
14	C2	129	GLU
14	C2	132	GLU
14	C2	139	HIS
14	C2	140	PHE
15	C3	3	ARG
15	C3	9	LYS
15	C3	16	ILE
15	C3	27	LYS
15	C3	31	GLU
15	C3	39	LYS
15	C3	45	LEU
15	C3	64	ARG
15	C3	65	VAL
15	C3	66	ILE
15	C3	73	ARG
15	C3	76	LYS
15	C3	83	GLU
15	C3	88	LEU
15	C3	94	LYS
15	C3	102	LEU
15	C3	103	GLU
15	C3	105	ASN
15	C3	115	LEU
15	C3	120	SER
15	C3	125	LEU

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Mol	Chain	Res	Type
15	C3	134	VAL
15	C3	142	GLU
15	C3	145	THR
15	C3	151	ASN
16	C4	13	VAL
16	C4	14	PHE
16	C4	24	ASN
16	C4	29	HIS
16	C4	39	ILE
16	C4	43	THR
16	C4	48	VAL
16	C4	51	ASP
16	C4	92	LYS
16	C4	96	PRO
16	C4	103	ARG
16	C4	108	SER
16	C4	123	SER
16	C4	132	ARG
16	C4	136	ARG
16	C4	137	LEU
17	C5	11	VAL
17	C5	22	LEU
17	C5	27	GLU
17	C5	28	MET
17	C5	34	VAL
17	C5	35	LYS
17	C5	44	ARG
17	C5	47	ARG
17	C5	52	LYS
17	C5	86	VAL
17	C5	89	MET
17	C5	110	GLU
17	C5	121	ILE
17	C5	128	HIS
18	C6	4	VAL
18	C6	14	LYS
18	C6	17	THR
18	C6	28	LEU
18	C6	43	ILE
18	C6	44	LEU
18	C6	48	VAL
18	C6	52	LEU

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Mol	Chain	Res	Type
18	C6	53	LEU
18	C6	54	LEU
18	C6	57	LEU
18	C6	66	ARG
18	C6	68	ARG
18	C6	69	VAL
18	C6	76	SER
18	C6	97	VAL
18	C6	98	ASP
18	C6	106	LYS
18	C6	114	ARG
18	C6	116	LEU
18	C6	118	ILE
18	C6	121	SER
18	C6	123	ARG
18	C6	127	LYS
18	C6	128	LYS
18	C6	136	SER
18	C6	137	ARG
18	C6	143	ARG
19	C7	5	ARG
19	C7	25	THR
19	C7	26	LEU
19	C7	30	THR
19	C7	34	LEU
19	C7	38	ILE
19	C7	40	THR
19	C7	46	LEU
19	C7	49	LYS
19	C7	54	THR
19	C7	62	GLN
19	C7	69	ILE
19	C7	71	PHE
19	C7	72	LYS
19	C7	83	GLN
19	C7	84	TYR
19	C7	85	VAL
19	C7	88	VAL
19	C7	105	GLN
19	C7	113	LEU
19	C7	115	LEU
19	C7	119	LEU

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Mol	Chain	Res	Type
20	C8	3	LEU
20	C8	5	VAL
20	C8	8	GLN
20	C8	11	PHE
20	C8	13	HIS
20	C8	14	ILE
20	C8	15	LEU
20	C8	17	LEU
20	C8	26	ILE
20	C8	28	ILE
20	C8	53	ASP
20	C8	54	LEU
20	C8	60	GLU
20	C8	61	LEU
20	C8	71	GLN
20	C8	74	GLN
20	C8	80	LYS
20	C8	86	LEU
20	C8	92	ILE
20	C8	93	THR
20	C8	97	ASP
20	C8	132	ARG
20	C8	133	VAL
20	C8	143	ARG
21	C9	6	VAL
21	C9	13	ASP
21	C9	22	LEU
21	C9	25	GLN
21	C9	28	LEU
21	C9	33	TYR
21	C9	35	ASP
21	C9	36	ILE
21	C9	41	SER
21	C9	63	ARG
21	C9	67	MET
21	C9	70	GLN
21	C9	79	LEU
21	C9	86	ARG
21	C9	94	ILE
21	C9	117	SER
21	C9	122	ARG
21	C9	125	SER

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Mol	Chain	Res	Type
21	C9	126	GLU
21	C9	130	ARG
21	C9	131	ASP
21	C9	134	ARG
21	C9	144	GLU
22	D0	15	GLN
22	D0	18	GLN
22	D0	23	ARG
22	D0	27	THR
22	D0	31	VAL
22	D0	34	LEU
22	D0	35	GLU
22	D0	41	ILE
22	D0	47	GLN
22	D0	48	HIS
22	D0	51	VAL
22	D0	61	LYS
22	D0	70	THR
22	D0	72	ASN
22	D0	74	GLU
22	D0	81	THR
22	D0	89	ARG
22	D0	103	ILE
22	D0	108	ILE
22	D0	121	ASN
23	D1	1	MET
23	D1	3	ASN
23	D1	5	LYS
23	D1	7	GLN
23	D1	60	ARG
23	D1	62	ARG
23	D1	68	SER
23	D1	69	LEU
23	D1	75	ASN
23	D1	80	LYS
23	D1	84	SER
24	D2	4	SER
24	D2	7	LEU
24	D2	12	ASN
24	D2	24	GLN
24	D2	30	SER
24	D2	42	GLN

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Mol	Chain	Res	Type
24	D2	43	LYS
24	D2	53	ILE
24	D2	56	HIS
24	D2	65	LEU
24	D2	66	ASN
24	D2	81	VAL
24	D2	93	LEU
24	D2	97	ARG
24	D2	98	GLN
24	D2	103	ILE
24	D2	104	LEU
24	D2	105	THR
24	D2	121	VAL
24	D2	122	SER
24	D2	125	ILE
25	D3	7	ARG
25	D3	9	LEU
25	D3	16	ARG
25	D3	19	ARG
25	D3	26	GLU
25	D3	30	LYS
25	D3	33	LEU
25	D3	40	SER
25	D3	47	SER
25	D3	73	ARG
25	D3	78	LYS
25	D3	84	THR
25	D3	94	ASN
25	D3	103	LEU
25	D3	107	PHE
25	D3	110	LYS
25	D3	114	LYS
25	D3	117	ILE
25	D3	131	SER
25	D3	132	LEU
25	D3	133	LEU
25	D3	138	GLU
25	D3	140	LYS
25	D3	144	ARG
26	D4	2	SER
26	D4	14	SER
26	D4	32	ARG

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Mol	Chain	Res	Type
26	D4	35	VAL
26	D4	46	GLU
26	D4	47	VAL
26	D4	51	GLU
26	D4	57	VAL
26	D4	61	ARG
26	D4	62	THR
26	D4	81	GLU
26	D4	84	LYS
26	D4	96	LEU
26	D4	100	VAL
26	D4	102	LYS
26	D4	104	SER
26	D4	105	ARG
26	D4	121	THR
26	D4	123	LYS
26	D4	127	LYS
26	D4	128	LYS
27	D5	40	VAL
27	D5	42	LEU
27	D5	59	TYR
27	D5	63	SER
27	D5	67	ASP
27	D5	69	LEU
27	D5	71	ILE
27	D5	75	LEU
27	D5	77	ARG
27	D5	85	LYS
27	D5	93	SER
27	D5	95	HIS
27	D5	96	SER
27	D5	100	ILE
28	D6	12	LYS
28	D6	15	ARG
28	D6	36	ILE
28	D6	41	ILE
28	D6	44	ILE
28	D6	45	VAL
28	D6	61	GLU
28	D6	64	LEU
28	D6	66	LYS
28	D6	69	ASN

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Mol	Chain	Res	Type
28	D6	70	LYS
28	D6	74	CYS
28	D6	82	ARG
28	D6	83	ILE
28	D6	84	VAL
28	D6	85	ARG
28	D6	86	VAL
28	D6	87	ARG
28	D6	89	ARG
28	D6	90	GLU
29	D7	3	LEU
29	D7	4	VAL
29	D7	20	LYS
29	D7	33	LEU
29	D7	34	ASP
29	D7	36	LYS
29	D7	56	CYS
29	D7	60	SER
29	D7	61	THR
29	D7	72	LYS
30	D8	8	THR
30	D8	13	ILE
30	D8	15	VAL
30	D8	19	THR
30	D8	31	GLU
30	D8	32	PHE
30	D8	33	LEU
30	D8	34	GLU
30	D8	35	ASP
30	D8	38	ARG
30	D8	39	THR
30	D8	57	MET
30	D8	58	GLU
30	D8	64	ARG
31	D9	6	VAL
31	D9	8	PHE
31	D9	9	SER
31	D9	12	ARG
31	D9	19	ARG
31	D9	21	CYS
31	D9	22	ARG
31	D9	23	VAL

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Mol	Chain	Res	Type
31	D9	25	SER
31	D9	30	LEU
31	D9	32	ARG
31	D9	36	LEU
31	D9	40	ARG
31	D9	49	ASP
32	E0	20	LYS
32	E0	28	LYS
32	E0	39	LEU
32	E0	42	ARG
32	E0	48	THR
32	E0	49	LEU
32	E0	50	VAL
32	E0	56	MET
33	E1	84	VAL
33	E1	85	TYR
33	E1	86	THR
33	E1	89	LYS
33	E1	91	ILE
33	E1	97	LYS
33	E1	98	VAL
33	E1	102	VAL
33	E1	111	GLU
33	E1	113	LYS
33	E1	120	GLU
33	E1	130	VAL
33	E1	138	ARG
33	E1	146	SER
33	E1	151	ASN
34	SR	3	SER
34	SR	6	VAL
34	SR	10	ARG
34	SR	16	HIS
34	SR	29	GLN
34	SR	44	SER
34	SR	52	GLN
34	SR	59	ARG
34	SR	66	HIS
34	SR	76	ASP
34	SR	81	LEU
34	SR	89	LEU
34	SR	108	SER

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Mol	Chain	Res	Type
34	SR	109	ASP
34	SR	116	ASP
34	SR	117	LYS
34	SR	136	ILE
34	SR	141	LEU
34	SR	165	ASP
34	SR	184	ASN
34	SR	191	ASP
34	SR	199	ILE
34	SR	202	LEU
34	SR	234	LEU
34	SR	238	ASP
34	SR	248	ASN
34	SR	268	GLN
34	SR	277	GLU
34	SR	292	LEU
34	SR	300	THR
34	SR	314	GLN
35	SM	23	LYS
35	SM	24	GLU
35	SM	36	ASP
35	SM	41	SER
35	SM	48	ARG
35	SM	51	ARG
35	SM	64	LYS
35	SM	68	ARG
35	SM	69	ARG
35	SM	84	LYS
35	SM	86	ASN
35	SM	89	ARG
35	SM	91	THR
35	SM	96	ARG
35	SM	97	THR
35	SM	100	THR
35	SM	101	ASP
35	SM	103	LYS
35	SM	105	LYS
35	SM	116	GLU
35	SM	131	ILE
35	SM	139	GLU
39	L2	10	LYS
39	L2	23	ARG

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Mol	Chain	Res	Type
39	L2	44	ILE
39	L2	45	VAL
39	L2	48	ILE
39	L2	70	ARG
39	L2	71	LEU
39	L2	74	GLU
39	L2	84	THR
39	L2	88	ILE
39	L2	101	VAL
39	L2	104	LEU
39	L2	109	GLU
39	L2	113	VAL
39	L2	143	GLU
39	L2	157	VAL
39	L2	165	VAL
39	L2	177	LYS
39	L2	179	LEU
39	L2	180	LEU
39	L2	181	LYS
39	L2	191	LEU
39	L2	202	VAL
39	L2	204	MET
39	L2	227	ARG
39	L2	230	VAL
39	L2	231	SER
39	L2	241	ARG
39	L2	247	ARG
39	L2	250	GLN
40	L3	2	SER
40	L3	7	GLU
40	L3	17	LEU
40	L3	19	ARG
40	L3	24	SER
40	L3	25	ILE
40	L3	37	ARG
40	L3	39	LYS
40	L3	41	VAL
40	L3	53	MET
40	L3	54	THR
40	L3	55	THR
40	L3	56	ILE
40	L3	66	LYS

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Mol	Chain	Res	Type
40	L3	67	PHE
40	L3	73	VAL
40	L3	85	VAL
40	L3	102	LEU
40	L3	103	THR
40	L3	114	VAL
40	L3	116	ARG
40	L3	139	GLN
40	L3	146	ARG
40	L3	148	LEU
40	L3	153	LYS
40	L3	156	SER
40	L3	160	VAL
40	L3	169	THR
40	L3	183	LEU
40	L3	188	ILE
40	L3	192	VAL
40	L3	196	ARG
40	L3	202	THR
40	L3	211	GLN
40	L3	212	ASN
40	L3	214	MET
40	L3	232	ARG
40	L3	235	THR
40	L3	236	LYS
40	L3	247	ARG
40	L3	252	ILE
40	L3	260	VAL
40	L3	263	SER
40	L3	277	SER
40	L3	284	ARG
40	L3	289	ASP
40	L3	300	ARG
40	L3	304	THR
40	L3	305	ILE
40	L3	319	ASN
40	L3	320	ASP
40	L3	323	MET
40	L3	324	VAL
40	L3	332	ARG
40	L3	335	ILE
40	L3	337	THR

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Mol	Chain	Res	Type
40	L3	343	TYR
40	L3	346	THR
40	L3	347	SER
40	L3	352	GLU
40	L3	372	THR
40	L3	382	THR
40	L3	385	LYS
40	L3	387	LEU
41	L4	2	SER
41	L4	18	ASN
41	L4	20	LEU
41	L4	22	LEU
41	L4	40	THR
41	L4	53	SER
41	L4	69	ARG
41	L4	74	ILE
41	L4	93	MET
41	L4	99	MET
41	L4	108	LYS
41	L4	110	ASN
41	L4	112	LYS
41	L4	120	TYR
41	L4	122	THR
41	L4	124	SER
41	L4	133	SER
41	L4	135	VAL
41	L4	138	ARG
41	L4	150	LEU
41	L4	172	VAL
41	L4	177	ASP
41	L4	179	LEU
41	L4	185	LYS
41	L4	187	LEU
41	L4	188	ARG
41	L4	193	LYS
41	L4	200	THR
41	L4	203	ARG
41	L4	220	ARG
41	L4	222	VAL
41	L4	230	VAL
41	L4	246	ARG
41	L4	258	LEU

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Mol	Chain	Res	Type
41	L4	259	ASP
41	L4	261	VAL
41	L4	270	SER
41	L4	282	SER
41	L4	287	THR
41	L4	288	ARG
41	L4	306	THR
41	L4	307	GLN
41	L4	311	HIS
41	L4	313	LEU
41	L4	327	LEU
41	L4	338	LYS
41	L4	343	LYS
41	L4	345	GLU
41	L4	350	LYS
41	L4	354	VAL
42	L5	5	LYS
42	L5	8	LYS
42	L5	22	ARG
42	L5	23	ARG
42	L5	32	GLN
42	L5	35	ARG
42	L5	41	LYS
42	L5	61	ILE
42	L5	67	SER
42	L5	69	ILE
42	L5	75	LEU
42	L5	81	HIS
42	L5	85	ARG
42	L5	92	LEU
42	L5	93	THR
42	L5	105	ILE
42	L5	112	LYS
42	L5	113	LEU
42	L5	122	VAL
42	L5	123	GLU
42	L5	131	LEU
42	L5	137	ASP
42	L5	140	ARG
42	L5	146	LEU
42	L5	148	ILE
42	L5	151	GLN

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Mol	Chain	Res	Type
42	L5	152	ARG
42	L5	154	THR
42	L5	155	THR
42	L5	158	ARG
42	L5	163	LEU
42	L5	177	GLU
42	L5	178	ASN
42	L5	188	GLU
42	L5	190	ILE
42	L5	207	TYR
42	L5	211	LEU
42	L5	213	ASP
42	L5	216	GLU
42	L5	220	SER
42	L5	222	LEU
42	L5	227	LEU
42	L5	232	ASP
42	L5	234	ASP
42	L5	236	LEU
42	L5	242	SER
42	L5	257	GLU
42	L5	263	GLU
42	L5	273	ARG
42	L5	277	LEU
43	L6	2	SER
43	L6	8	LYS
43	L6	21	THR
43	L6	31	ARG
43	L6	35	VAL
43	L6	52	VAL
43	L6	65	ILE
43	L6	78	ARG
43	L6	84	VAL
43	L6	89	THR
43	L6	93	VAL
43	L6	98	VAL
43	L6	129	GLU
43	L6	134	ARG
43	L6	152	THR
43	L6	155	LEU
43	L6	164	SER
44	L7	24	GLU

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Mol	Chain	Res	Type
44	L7	25	GLN
44	L7	39	GLU
44	L7	40	LYS
44	L7	45	LEU
44	L7	46	GLU
44	L7	80	GLN
44	L7	84	VAL
44	L7	87	VAL
44	L7	92	ILE
44	L7	93	ASN
44	L7	108	LEU
44	L7	118	LYS
44	L7	124	LEU
44	L7	145	ARG
44	L7	158	LYS
44	L7	173	LEU
44	L7	175	LYS
44	L7	179	LEU
44	L7	182	ASP
44	L7	184	LEU
44	L7	211	SER
44	L7	225	GLN
44	L7	229	PHE
44	L7	239	LEU
44	L7	244	ASN
45	L8	26	LEU
45	L8	27	THR
45	L8	41	GLN
45	L8	47	SER
45	L8	65	LEU
45	L8	66	SER
45	L8	74	THR
45	L8	79	GLN
45	L8	81	THR
45	L8	84	ARG
45	L8	118	GLU
45	L8	136	LEU
45	L8	150	LEU
45	L8	156	ASP
45	L8	163	VAL
45	L8	169	LEU
45	L8	180	VAL

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Mol	Chain	Res	Type
45	L8	181	LYS
45	L8	183	LYS
45	L8	185	ARG
45	L8	190	VAL
45	L8	197	VAL
45	L8	203	VAL
45	L8	204	ARG
45	L8	227	ASP
45	L8	238	LEU
45	L8	241	LYS
45	L8	248	LYS
46	L9	1	MET
46	L9	2	LYS
46	L9	4	ILE
46	L9	5	GLN
46	L9	9	GLN
46	L9	22	SER
46	L9	41	ILE
46	L9	44	THR
46	L9	49	ASN
46	L9	52	LEU
46	L9	62	ARG
46	L9	65	VAL
46	L9	68	LEU
46	L9	69	ARG
46	L9	70	THR
46	L9	82	VAL
46	L9	92	TYR
46	L9	93	VAL
46	L9	107	ASP
46	L9	132	VAL
46	L9	139	ASN
46	L9	140	VAL
46	L9	151	VAL
46	L9	152	GLU
46	L9	157	ASN
46	L9	161	LEU
46	L9	162	GLN
46	L9	164	ILE
46	L9	170	LYS
46	L9	172	ILE
46	L9	173	ARG

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Mol	Chain	Res	Type
46	L9	177	ASP
46	L9	189	GLU
46	L9	190	ASP
46	L9	191	LEU
47	M0	3	ARG
47	M0	21	ARG
47	M0	31	ILE
47	M0	32	ARG
47	M0	33	ILE
47	M0	39	LYS
47	M0	48	LEU
47	M0	52	LEU
47	M0	63	GLU
47	M0	74	LYS
47	M0	91	VAL
47	M0	102	MET
47	M0	139	ARG
47	M0	142	ASP
47	M0	146	ASP
47	M0	156	ARG
47	M0	163	GLN
47	M0	165	ILE
47	M0	167	LEU
47	M0	169	LYS
47	M0	175	ASN
47	M0	177	ASP
47	M0	178	ARG
47	M0	185	ARG
47	M0	203	LYS
47	M0	207	GLU
48	M1	6	GLN
48	M1	7	ASN
48	M1	9	MET
48	M1	10	ARG
48	M1	12	LEU
48	M1	13	LYS
48	M1	17	LEU
48	M1	19	LEU
48	M1	20	ASN
48	M1	23	VAL
48	M1	31	THR
48	M1	40	LEU

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Mol	Chain	Res	Type
48	M1	44	THR
48	M1	46	VAL
48	M1	80	LEU
48	M1	81	GLU
48	M1	82	ARG
48	M1	94	ARG
48	M1	99	THR
48	M1	101	ASN
48	M1	106	ILE
48	M1	107	ASP
48	M1	112	LEU
48	M1	138	VAL
48	M1	140	ARG
48	M1	143	ARG
48	M1	145	LYS
48	M1	166	LYS
48	M1	171	VAL
48	M1	173	ASP
49	M3	20	GLU
49	M3	42	ARG
49	M3	54	LEU
49	M3	55	ARG
49	M3	57	VAL
49	M3	58	VAL
49	M3	59	ARG
49	M3	67	ARG
49	M3	70	ARG
49	M3	80	VAL
49	M3	85	LEU
49	M3	107	GLU
49	M3	114	GLN
49	M3	115	ARG
49	M3	117	LYS
49	M3	122	LYS
49	M3	124	ILE
49	M3	128	ARG
49	M3	131	LYS
49	M3	136	GLU
49	M3	144	THR
49	M3	164	GLU
49	M3	168	ARG
49	M3	171	ARG

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Mol	Chain	Res	Type
49	M3	180	ARG
49	M3	188	ARG
49	M3	190	LYS
49	M3	194	GLU
50	M4	5	SER
50	M4	8	LYS
50	M4	21	VAL
50	M4	25	LYS
50	M4	47	ASP
50	M4	50	LYS
50	M4	53	VAL
50	M4	58	ILE
50	M4	63	VAL
50	M4	69	THR
50	M4	72	LEU
50	M4	82	SER
50	M4	93	LYS
50	M4	102	LYS
50	M4	108	ARG
50	M4	130	THR
50	M4	135	LEU
51	M5	10	LEU
51	M5	15	GLN
51	M5	19	LEU
51	M5	22	LEU
51	M5	38	ARG
51	M5	41	ARG
51	M5	50	ARG
51	M5	71	ARG
51	M5	80	THR
51	M5	92	LEU
51	M5	97	SER
51	M5	98	LEU
51	M5	105	ARG
51	M5	106	VAL
51	M5	109	ARG
51	M5	121	VAL
51	M5	123	GLN
51	M5	133	ILE
51	M5	138	GLN
51	M5	151	ILE
51	M5	155	VAL

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Mol	Chain	Res	Type
51	M5	159	ARG
51	M5	167	THR
51	M5	170	LYS
51	M5	171	SER
51	M5	183	THR
51	M5	190	THR
51	M5	196	THR
51	M5	204	LYS
52	M6	22	VAL
52	M6	27	LEU
52	M6	33	ILE
52	M6	58	LEU
52	M6	68	ARG
52	M6	78	ARG
52	M6	84	LEU
52	M6	85	ARG
52	M6	94	ARG
52	M6	100	GLU
52	M6	106	GLU
52	M6	114	LYS
52	M6	117	ARG
52	M6	119	VAL
52	M6	124	LEU
52	M6	126	VAL
52	M6	128	ARG
52	M6	129	LEU
52	M6	134	LYS
52	M6	143	THR
52	M6	160	ARG
52	M6	161	LYS
52	M6	162	VAL
52	M6	166	GLU
52	M6	180	SER
52	M6	182	ASN
52	M6	184	THR
52	M6	187	GLU
53	M7	3	ARG
53	M7	9	THR
53	M7	18	ARG
53	M7	24	VAL
53	M7	25	SER
53	M7	29	THR

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Mol	Chain	Res	Type
53	M7	32	THR
53	M7	36	ILE
53	M7	40	GLU
53	M7	52	LEU
53	M7	55	GLN
53	M7	78	VAL
53	M7	111	LYS
53	M7	112	LEU
53	M7	127	ARG
53	M7	128	ARG
53	M7	136	ILE
53	M7	142	SER
53	M7	144	SER
53	M7	165	VAL
53	M7	168	LEU
53	M7	171	ARG
53	M7	173	ARG
53	M7	180	LYS
53	M7	181	ARG
54	M8	3	ILE
54	M8	11	LYS
54	M8	17	THR
54	M8	24	VAL
54	M8	26	LEU
54	M8	32	LEU
54	M8	34	THR
54	M8	39	ARG
54	M8	41	ASP
54	M8	49	LEU
54	M8	57	ILE
54	M8	64	VAL
54	M8	69	ARG
54	M8	81	VAL
54	M8	99	THR
54	M8	111	ARG
54	M8	113	LYS
54	M8	122	ILE
54	M8	135	GLN
54	M8	138	LEU
54	M8	144	ARG
54	M8	150	VAL
54	M8	165	ILE

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Mol	Chain	Res	Type
54	M8	168	THR
55	M9	10	LEU
55	M9	20	ARG
55	M9	24	LEU
55	M9	29	THR
55	M9	41	ILE
55	M9	44	LEU
55	M9	55	VAL
55	M9	63	THR
55	M9	71	ARG
55	M9	74	ARG
55	M9	98	ARG
55	M9	99	LEU
55	M9	103	ARG
55	M9	104	ARG
55	M9	106	LEU
55	M9	115	ILE
55	M9	116	ASP
55	M9	138	LEU
55	M9	175	GLN
56	N0	1	MET
56	N0	8	GLN
56	N0	12	ARG
56	N0	13	ARG
56	N0	17	GLU
56	N0	40	ARG
56	N0	45	LEU
56	N0	50	LYS
56	N0	51	VAL
56	N0	58	ILE
56	N0	71	LYS
56	N0	80	ARG
56	N0	81	TYR
56	N0	83	SER
56	N0	85	SER
56	N0	87	THR
56	N0	88	HIS
56	N0	97	VAL
56	N0	100	VAL
56	N0	104	GLU
56	N0	105	THR
56	N0	113	ARG

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Mol	Chain	Res	Type
56	N0	115	ARG
56	N0	117	ARG
56	N0	122	HIS
56	N0	130	GLU
56	N0	131	LYS
56	N0	132	THR
56	N0	137	ARG
56	N0	138	GLN
56	N0	142	GLN
56	N0	145	THR
56	N0	155	ARG
56	N0	160	THR
56	N0	161	LYS
56	N0	162	THR
56	N0	166	LYS
56	N0	167	ARG
56	N0	171	PHE
56	N0	172	TYR
57	N1	9	SER
57	N1	12	ARG
57	N1	14	MET
57	N1	17	ARG
57	N1	27	LEU
57	N1	39	ILE
57	N1	55	LYS
57	N1	64	VAL
57	N1	68	THR
57	N1	71	SER
57	N1	75	ILE
57	N1	78	LYS
57	N1	79	MET
57	N1	83	ARG
57	N1	88	ARG
57	N1	92	ARG
57	N1	97	LYS
57	N1	102	ARG
57	N1	103	GLN
57	N1	104	GLU
57	N1	106	LEU
57	N1	118	GLU
57	N1	127	GLN
57	N1	128	LEU

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Mol	Chain	Res	Type
57	N1	131	GLN
57	N1	136	ARG
57	N1	139	ARG
57	N1	143	THR
57	N1	144	GLU
57	N1	149	GLN
57	N1	158	THR
58	N2	9	GLN
58	N2	10	LYS
58	N2	16	THR
58	N2	29	ASP
58	N2	38	ILE
58	N2	49	ASN
58	N2	52	ASN
58	N2	54	VAL
58	N2	61	THR
58	N2	66	VAL
58	N2	70	LYS
58	N2	88	GLN
58	N2	93	ILE
58	N2	94	ARG
58	N2	99	LYS
58	N2	100	THR
58	N2	108	TYR
59	N3	4	ASN
59	N3	13	ILE
59	N3	45	ARG
59	N3	46	LEU
59	N3	57	MET
59	N3	63	LYS
59	N3	64	LYS
59	N3	69	LEU
59	N3	72	LYS
59	N3	73	VAL
59	N3	74	MET
59	N3	81	GLN
59	N3	83	LYS
59	N3	91	VAL
59	N3	102	ILE
59	N3	104	ASN
59	N3	109	MET
59	N3	110	LYS

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Mol	Chain	Res	Type
59	N3	112	SER
59	N3	115	THR
59	N3	135	VAL
60	N4	4	GLU
60	N4	5	ILE
60	N4	7	SER
60	N4	19	THR
60	N4	39	LEU
60	N4	52	THR
60	N4	64	THR
61	N5	26	VAL
61	N5	27	ARG
61	N5	28	THR
61	N5	34	LEU
61	N5	37	THR
61	N5	38	LEU
61	N5	39	LYS
61	N5	40	LEU
61	N5	45	LYS
61	N5	48	SER
61	N5	51	VAL
61	N5	63	ILE
61	N5	71	THR
61	N5	73	MET
61	N5	81	ILE
61	N5	89	LYS
61	N5	96	LYS
61	N5	108	LEU
61	N5	113	LEU
61	N5	115	ARG
61	N5	125	ARG
61	N5	127	THR
61	N5	133	LEU
61	N5	135	ILE
61	N5	139	ILE
61	N5	142	ILE
62	N6	3	LYS
62	N6	4	GLN
62	N6	13	ARG
62	N6	17	LYS
62	N6	37	LYS
62	N6	42	GLN

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Mol	Chain	Res	Type
62	N6	45	ILE
62	N6	50	ILE
62	N6	51	ARG
62	N6	56	VAL
62	N6	57	LEU
62	N6	60	ARG
62	N6	70	ILE
62	N6	74	TYR
62	N6	76	LEU
62	N6	97	ILE
62	N6	105	VAL
62	N6	114	ASP
62	N6	115	ARG
62	N6	125	LYS
62	N6	126	LEU
62	N6	127	GLU
63	N7	14	VAL
63	N7	24	VAL
63	N7	46	ILE
63	N7	53	VAL
63	N7	54	THR
63	N7	55	LYS
63	N7	64	LYS
63	N7	72	ILE
63	N7	75	VAL
63	N7	81	LEU
63	N7	83	THR
63	N7	86	THR
63	N7	90	GLU
63	N7	92	PHE
63	N7	99	GLU
63	N7	102	GLU
63	N7	109	GLU
63	N7	127	ASN
63	N7	134	LEU
63	N7	135	ARG
64	N8	4	ARG
64	N8	6	THR
64	N8	8	THR
64	N8	10	LYS
64	N8	12	ARG
64	N8	14	HIS

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Mol	Chain	Res	Type
64	N8	16	SER
64	N8	32	ARG
64	N8	34	MET
64	N8	42	ARG
64	N8	46	ASP
64	N8	47	LYS
64	N8	60	TYR
64	N8	72	VAL
64	N8	76	ASP
64	N8	78	LEU
64	N8	88	ASP
64	N8	115	LYS
64	N8	120	ASN
64	N8	130	VAL
64	N8	133	LEU
64	N8	139	ARG
65	N9	4	SER
65	N9	13	THR
65	N9	22	LYS
65	N9	25	LYS
65	N9	28	LYS
65	N9	29	TYR
65	N9	50	THR
65	N9	59	LYS
66	O0	14	LEU
66	O0	16	LEU
66	O0	24	THR
66	O0	32	LYS
66	O0	50	VAL
66	O0	53	LYS
66	O0	54	SER
66	O0	61	MET
66	O0	66	LYS
66	O0	83	LYS
66	O0	87	VAL
66	O0	97	ASP
66	O0	99	ASP
66	O0	100	ILE
66	O0	101	LEU
66	O0	104	LEU
67	O1	16	LEU
67	O1	26	LYS

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Mol	Chain	Res	Type
67	O1	31	ARG
67	O1	41	LYS
67	O1	47	ASP
67	O1	55	LEU
67	O1	64	VAL
67	O1	68	GLU
67	O1	76	SER
67	O1	79	ARG
67	O1	82	GLU
67	O1	84	ASP
67	O1	96	VAL
67	O1	105	GLN
67	O1	106	THR
68	O2	19	ARG
68	O2	27	ARG
68	O2	33	ARG
68	O2	34	LYS
68	O2	41	VAL
68	O2	44	ARG
68	O2	62	LYS
68	O2	73	THR
68	O2	75	LEU
68	O2	76	VAL
68	O2	106	VAL
68	O2	125	ARG
68	O2	128	LEU
69	O3	4	SER
69	O3	10	LYS
69	O3	15	SER
69	O3	28	SER
69	O3	31	LYS
69	O3	33	GLU
69	O3	59	VAL
69	O3	70	LYS
69	O3	86	ARG
69	O3	98	VAL
69	O3	99	ARG
69	O3	106	ASN
70	O4	5	VAL
70	O4	20	ILE
70	O4	24	LYS
70	O4	29	ILE

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Mol	Chain	Res	Type
70	O4	51	LEU
70	O4	58	ARG
70	O4	60	ARG
70	O4	65	VAL
70	O4	71	THR
70	O4	74	ARG
70	O4	86	LYS
70	O4	87	GLU
70	O4	102	LYS
70	O4	104	VAL
71	O5	13	SER
71	O5	15	GLU
71	O5	20	GLN
71	O5	22	VAL
71	O5	26	LYS
71	O5	27	GLU
71	O5	41	LEU
71	O5	47	VAL
71	O5	48	ARG
71	O5	49	LYS
71	O5	83	LYS
71	O5	84	LYS
71	O5	85	THR
71	O5	89	ARG
71	O5	96	GLU
71	O5	99	GLN
71	O5	101	THR
71	O5	102	GLU
71	O5	107	LYS
71	O5	119	LYS
72	O6	11	LEU
72	O6	13	LYS
72	O6	17	VAL
72	O6	18	THR
72	O6	25	LYS
72	O6	26	ILE
72	O6	36	ARG
72	O6	42	SER
72	O6	45	ARG
72	O6	57	LEU
72	O6	58	ILE
72	O6	60	LEU

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Mol	Chain	Res	Type
72	O6	64	SER
72	O6	66	GLU
72	O6	68	ARG
72	O6	76	ARG
72	O6	81	THR
72	O6	89	GLU
72	O6	90	MET
72	O6	98	ARG
72	O6	99	ARG
73	O7	24	ARG
73	O7	25	ARG
73	O7	33	THR
73	O7	45	ARG
73	O7	55	ARG
73	O7	58	THR
73	O7	59	THR
73	O7	67	LEU
73	O7	82	SER
74	O8	12	LEU
74	O8	20	VAL
74	O8	22	THR
74	O8	24	THR
74	O8	28	ASN
74	O8	32	ASN
74	O8	41	THR
74	O8	45	VAL
74	O8	46	ARG
74	O8	48	SER
74	O8	50	SER
74	O8	51	LEU
74	O8	53	THR
74	O8	64	LYS
74	O8	65	LEU
74	O8	67	GLN
74	O8	68	SER
74	O8	77	ARG
75	O9	4	GLN
75	O9	5	LYS
75	O9	21	ARG
75	O9	27	ILE
75	O9	29	LEU
76	Q0	77	ILE

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Mol	Chain	Res	Type
76	Q0	78	ILE
76	Q0	83	LYS
76	Q0	85	LEU
76	Q0	113	ARG
76	Q0	114	LYS
76	Q0	127	LEU
77	Q1	4	LYS
77	Q1	9	ARG
77	Q1	10	THR
77	Q1	11	ARG
77	Q1	23	ARG
78	Q2	4	VAL
78	Q2	8	ARG
78	Q2	17	CYS
78	Q2	21	THR
78	Q2	22	GLN
78	Q2	35	LEU
78	Q2	47	GLN
78	Q2	60	LYS
78	Q2	61	LYS
78	Q2	78	LYS
78	Q2	83	LEU
78	Q2	84	THR
78	Q2	85	LEU
78	Q2	87	ARG
78	Q2	92	GLU
78	Q2	93	LEU
78	Q2	100	LYS
78	Q2	104	LEU
79	Q3	11	THR
79	Q3	16	VAL
79	Q3	24	ARG
79	Q3	25	GLN
79	Q3	32	GLN
79	Q3	40	SER
79	Q3	45	LYS
79	Q3	46	THR
79	Q3	56	THR
79	Q3	60	CYS
79	Q3	73	THR
79	Q3	88	GLU
2	s0	6	THR

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Mol	Chain	Res	Type
2	s0	8	ASP
2	s0	9	LEU
2	s0	12	GLU
2	s0	24	LEU
2	s0	29	VAL
2	s0	30	GLN
2	s0	41	ARG
2	s0	45	VAL
2	s0	50	VAL
2	s0	57	LEU
2	s0	59	LEU
2	s0	62	ARG
2	s0	87	LEU
2	s0	88	LYS
2	s0	96	THR
2	s0	101	ARG
2	s0	110	TYR
2	s0	119	ARG
2	s0	131	GLN
2	s0	139	VAL
2	s0	144	ILE
2	s0	154	GLU
2	s0	156	VAL
2	s0	157	ASP
2	s0	164	ASN
2	s0	172	LEU
2	s0	179	ARG
2	s0	184	LEU
2	s0	185	ARG
2	s0	188	LEU
2	s0	198	MET
2	s0	200	ASP
2	s0	202	TYR
3	s1	21	VAL
3	s1	25	THR
3	s1	36	SER
3	s1	40	ASN
3	s1	47	LEU
3	s1	55	LYS
3	s1	56	SER
3	s1	61	LEU
3	s1	62	LYS

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Mol	Chain	Res	Type
3	s1	65	VAL
3	s1	66	VAL
3	s1	70	LEU
3	s1	78	ASP
3	s1	80	SER
3	s1	83	LYS
3	s1	105	PHE
3	s1	110	LEU
3	s1	125	VAL
3	s1	131	ASP
3	s1	137	ILE
3	s1	146	GLN
3	s1	148	ASN
3	s1	151	LYS
3	s1	169	SER
3	s1	175	GLU
3	s1	177	GLN
3	s1	179	SER
3	s1	181	LEU
3	s1	202	LYS
3	s1	203	ASP
3	s1	212	VAL
3	s1	215	VAL
3	s1	217	LEU
3	s1	219	LYS
3	s1	222	LYS
3	s1	228	LEU
3	s1	231	LEU
3	s1	232	HIS
4	s2	41	LEU
4	s2	51	THR
4	s2	53	ILE
4	s2	54	GLU
4	s2	55	GLU
4	s2	58	LEU
4	s2	61	LEU
4	s2	69	ILE
4	s2	70	ASP
4	s2	72	LEU
4	s2	73	LEU
4	s2	78	ASP
4	s2	83	ILE

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Mol	Chain	Res	Type
4	s2	89	GLN
4	s2	90	THR
4	s2	91	ARG
4	s2	97	ARG
4	s2	106	ASP
4	s2	111	VAL
4	s2	117	THR
4	s2	137	ILE
4	s2	139	ILE
4	s2	141	ARG
4	s2	146	THR
4	s2	148	LEU
4	s2	150	GLN
4	s2	153	SER
4	s2	166	THR
4	s2	169	LEU
4	s2	170	ILE
4	s2	185	LYS
4	s2	194	GLU
4	s2	206	THR
4	s2	222	TYR
4	s2	226	THR
4	s2	229	LEU
4	s2	233	GLN
4	s2	237	VAL
4	s2	244	SER
4	s2	248	SER
5	s3	4	LEU
5	s3	7	LYS
5	s3	9	ARG
5	s3	21	LEU
5	s3	28	GLU
5	s3	39	VAL
5	s3	41	VAL
5	s3	44	THR
5	s3	45	LYS
5	s3	55	THR
5	s3	67	ASN
5	s3	69	LEU
5	s3	70	THR
5	s3	84	ILE
5	s3	91	VAL

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Mol	Chain	Res	Type
5	s3	94	ARG
5	s3	103	GLU
5	s3	115	ILE
5	s3	117	ARG
5	s3	127	MET
5	s3	128	GLU
5	s3	132	LYS
5	s3	154	ASP
5	s3	158	ILE
5	s3	162	GLN
5	s3	172	THR
5	s3	176	LEU
5	s3	181	VAL
5	s3	196	ARG
5	s3	212	LYS
5	s3	213	GLU
6	s4	6	LYS
6	s4	7	LYS
6	s4	9	LEU
6	s4	23	LEU
6	s4	37	LYS
6	s4	38	LEU
6	s4	39	ARG
6	s4	42	LEU
6	s4	48	LEU
6	s4	49	ARG
6	s4	51	ARG
6	s4	56	LEU
6	s4	67	GLN
6	s4	78	THR
6	s4	95	THR
6	s4	109	PHE
6	s4	111	VAL
6	s4	113	ARG
6	s4	116	ASP
6	s4	117	GLU
6	s4	139	VAL
6	s4	140	VAL
6	s4	146	THR
6	s4	148	ARG
6	s4	176	ASP
6	s4	180	LEU

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Mol	Chain	Res	Type
6	s4	182	TYR
6	s4	187	ARG
6	s4	194	THR
6	s4	195	ILE
6	s4	215	ASP
6	s4	222	LEU
6	s4	223	ASN
6	s4	227	VAL
6	s4	236	ILE
6	s4	245	LYS
6	s4	254	ARG
7	s5	25	LEU
7	s5	27	THR
7	s5	31	GLU
7	s5	38	THR
7	s5	41	LYS
7	s5	51	VAL
7	s5	59	VAL
7	s5	63	GLN
7	s5	68	ILE
7	s5	76	ARG
7	s5	79	ASN
7	s5	83	ARG
7	s5	86	GLN
7	s5	89	ILE
7	s5	93	LEU
7	s5	98	MET
7	s5	104	ASN
7	s5	112	ARG
7	s5	119	ASP
7	s5	125	THR
7	s5	128	ASN
7	s5	147	THR
7	s5	149	VAL
7	s5	156	ARG
7	s5	157	ARG
7	s5	170	GLN
7	s5	186	ASN
7	s5	187	ILE
7	s5	194	LEU
7	s5	203	LYS
7	s5	213	LYS

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Mol	Chain	Res	Type
7	s5	216	GLU
8	s6	15	THR
8	s6	21	GLU
8	s6	69	LEU
8	s6	71	THR
8	s6	76	LEU
8	s6	78	THR
8	s6	79	LYS
8	s6	89	ASP
8	s6	92	ARG
8	s6	93	LYS
8	s6	97	VAL
8	s6	108	VAL
8	s6	109	LEU
8	s6	115	LYS
8	s6	121	LEU
8	s6	126	ASP
8	s6	127	THR
8	s6	128	THR
8	s6	129	VAL
8	s6	133	LEU
8	s6	143	LYS
8	s6	150	GLU
8	s6	151	ASP
8	s6	153	VAL
8	s6	155	ASP
8	s6	156	PHE
8	s6	177	ARG
8	s6	193	LEU
8	s6	212	LEU
8	s6	215	ARG
8	s6	217	SER
8	s6	218	GLU
9	s7	11	GLN
9	s7	28	GLU
9	s7	30	SER
9	s7	31	SER
9	s7	33	GLU
9	s7	39	ARG
9	s7	44	LYS
9	s7	49	ILE
9	s7	50	ASP

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Mol	Chain	Res	Type
9	s7	62	VAL
9	s7	67	LEU
9	s7	77	LEU
9	s7	79	ARG
9	s7	80	GLU
9	s7	81	LEU
9	s7	86	GLN
9	s7	97	ARG
9	s7	103	SER
9	s7	105	THR
9	s7	108	GLN
9	s7	109	VAL
9	s7	110	GLN
9	s7	114	ARG
9	s7	116	ARG
9	s7	117	THR
9	s7	118	LEU
9	s7	119	THR
9	s7	134	GLU
9	s7	143	LEU
9	s7	144	VAL
9	s7	156	SER
9	s7	159	VAL
9	s7	163	ASP
9	s7	166	LEU
9	s7	180	GLN
9	s7	185	ILE
10	s8	8	ARG
10	s8	12	SER
10	s8	18	ARG
10	s8	25	ARG
10	s8	28	GLU
10	s8	29	LEU
10	s8	36	THR
10	s8	62	THR
10	s8	74	LYS
10	s8	76	THR
10	s8	77	ARG
10	s8	89	GLU
10	s8	97	THR
10	s8	110	ARG
10	s8	121	LEU

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Mol	Chain	Res	Type
10	s8	138	ASN
10	s8	151	LYS
10	s8	152	ILE
10	s8	155	SER
10	s8	168	CYS
10	s8	170	SER
10	s8	176	SER
10	s8	178	ARG
10	s8	183	ILE
10	s8	184	LEU
10	s8	197	THR
10	s8	199	LYS
11	s9	3	ARG
11	s9	7	THR
11	s9	11	THR
11	s9	20	GLU
11	s9	28	LEU
11	s9	41	GLU
11	s9	46	SER
11	s9	49	LEU
11	s9	78	ARG
11	s9	82	ARG
11	s9	87	SER
11	s9	89	ASP
11	s9	90	LYS
11	s9	91	LYS
11	s9	93	LEU
11	s9	96	VAL
11	s9	101	VAL
11	s9	105	LEU
11	s9	109	LEU
11	s9	110	GLN
11	s9	111	THR
11	s9	120	LYS
11	s9	122	VAL
11	s9	126	ARG
11	s9	130	THR
11	s9	133	HIS
11	s9	134	ILE
11	s9	141	VAL
11	s9	142	ASN
11	s9	149	ARG

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Mol	Chain	Res	Type
11	s9	150	LEU
11	s9	171	ARG
11	s9	180	LYS
11	s9	182	GLU
12	c0	2	LEU
12	c0	3	MET
12	c0	15	LEU
12	c0	22	VAL
12	c0	28	ASN
12	c0	36	ASP
12	c0	47	GLN
12	c0	50	THR
12	c0	55	VAL
12	c0	57	THR
12	c0	67	THR
12	c0	71	GLU
12	c0	77	ARG
13	c1	3	THR
13	c1	5	LEU
13	c1	10	GLU
13	c1	21	ASN
13	c1	26	LYS
13	c1	27	THR
13	c1	28	SER
13	c1	32	LYS
13	c1	33	ARG
13	c1	44	THR
13	c1	47	THR
13	c1	56	LYS
13	c1	60	PHE
13	c1	67	ARG
13	c1	72	THR
13	c1	74	THR
13	c1	76	VAL
13	c1	78	THR
13	c1	107	VAL
13	c1	112	SER
13	c1	116	ARG
13	c1	123	VAL
13	c1	125	VAL
13	c1	140	VAL
14	c2	28	LEU

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Mol	Chain	Res	Type
14	c2	36	LEU
14	c2	39	ASP
14	c2	43	ARG
14	c2	45	LEU
14	c2	54	ARG
14	c2	58	LEU
14	c2	59	LEU
14	c2	61	VAL
14	c2	62	LEU
14	c2	63	VAL
14	c2	66	VAL
14	c2	71	ILE
14	c2	74	LEU
14	c2	85	LYS
14	c2	89	ILE
14	c2	91	VAL
14	c2	97	LEU
14	c2	103	LEU
14	c2	121	VAL
14	c2	129	GLU
14	c2	132	GLU
14	c2	136	ILE
14	c2	140	PHE
15	c3	4	MET
15	c3	6	SER
15	c3	12	SER
15	c3	14	SER
15	c3	16	ILE
15	c3	27	LYS
15	c3	28	LEU
15	c3	33	VAL
15	c3	35	GLU
15	c3	62	GLN
15	c3	64	ARG
15	c3	66	ILE
15	c3	67	THR
15	c3	75	LEU
15	c3	76	LYS
15	c3	80	LEU
15	c3	84	ILE
15	c3	88	LEU
15	c3	102	LEU

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Mol	Chain	Res	Type
15	c3	104	ARG
15	c3	115	LEU
15	c3	125	LEU
15	c3	127	ARG
15	c3	131	THR
15	c3	134	VAL
15	c3	138	ASN
16	c4	13	VAL
16	c4	20	TYR
16	c4	26	THR
16	c4	31	THR
16	c4	43	THR
16	c4	55	SER
16	c4	65	GLN
16	c4	66	ASP
16	c4	79	VAL
16	c4	81	VAL
16	c4	84	ARG
16	c4	92	LYS
16	c4	102	LEU
16	c4	107	ARG
16	c4	114	ARG
16	c4	119	THR
16	c4	124	ASP
16	c4	126	THR
16	c4	132	ARG
16	c4	133	ARG
16	c4	136	ARG
16	c4	137	LEU
17	c5	12	PHE
17	c5	20	VAL
17	c5	21	ASP
17	c5	28	MET
17	c5	36	LEU
17	c5	43	ARG
17	c5	44	ARG
17	c5	49	MET
17	c5	69	GLU
17	c5	92	SER
17	c5	97	TYR
17	c5	107	ILE
17	c5	110	GLU

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Mol	Chain	Res	Type
17	c5	121	ILE
17	c5	122	THR
17	c5	124	THR
17	c5	127	ARG
18	c6	7	VAL
18	c6	17	THR
18	c6	23	LYS
18	c6	28	LEU
18	c6	32	ASN
18	c6	36	ILE
18	c6	37	THR
18	c6	43	ILE
18	c6	53	LEU
18	c6	57	LEU
18	c6	66	ARG
18	c6	68	ARG
18	c6	69	VAL
18	c6	70	THR
18	c6	83	GLN
18	c6	98	ASP
18	c6	110	THR
18	c6	113	ASP
18	c6	114	ARG
18	c6	117	LEU
18	c6	137	ARG
19	c7	3	ARG
19	c7	8	THR
19	c7	18	GLU
19	c7	29	GLN
19	c7	34	LEU
19	c7	36	ASP
19	c7	38	ILE
19	c7	46	LEU
19	c7	62	GLN
19	c7	69	ILE
19	c7	72	LYS
19	c7	83	GLN
19	c7	85	VAL
19	c7	87	GLU
19	c7	104	ASN
19	c7	107	SER
19	c7	113	LEU

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Mol	Chain	Res	Type
20	c8	3	LEU
20	c8	4	VAL
20	c8	5	VAL
20	c8	10	SER
20	c8	13	HIS
20	c8	15	LEU
20	c8	18	LEU
20	c8	25	ASN
20	c8	28	ILE
20	c8	36	LYS
20	c8	40	ARG
20	c8	61	LEU
20	c8	63	GLN
20	c8	66	LEU
20	c8	94	ASP
20	c8	110	ARG
20	c8	116	LEU
20	c8	119	ILE
20	c8	134	ARG
20	c8	136	GLN
20	c8	141	THR
20	c8	143	ARG
21	c9	6	VAL
21	c9	20	SER
21	c9	27	LYS
21	c9	28	LEU
21	c9	37	VAL
21	c9	41	SER
21	c9	57	ARG
21	c9	68	ARG
21	c9	70	GLN
21	c9	84	LYS
21	c9	89	ARG
21	c9	123	ARG
21	c9	131	ASP
21	c9	132	LEU
21	c9	134	ARG
21	c9	135	ILE
21	c9	140	LEU
21	c9	142	GLU
21	c9	144	GLU
22	d0	12	GLN

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Mol	Chain	Res	Type
22	d0	13	GLU
22	d0	16	GLN
22	d0	21	LYS
22	d0	23	ARG
22	d0	27	THR
22	d0	31	VAL
22	d0	34	LEU
22	d0	39	SER
22	d0	44	ASN
22	d0	47	GLN
22	d0	51	VAL
22	d0	57	ARG
22	d0	60	THR
22	d0	63	LEU
22	d0	70	THR
22	d0	74	GLU
22	d0	77	LYS
22	d0	97	VAL
22	d0	98	GLN
22	d0	99	ILE
22	d0	103	ILE
22	d0	107	THR
22	d0	108	ILE
22	d0	115	GLU
22	d0	118	VAL
23	d1	2	GLU
23	d1	5	LYS
23	d1	10	GLU
23	d1	11	LEU
23	d1	12	TYR
23	d1	15	ARG
23	d1	18	SER
23	d1	32	VAL
23	d1	44	ARG
23	d1	52	THR
23	d1	65	SER
23	d1	67	ASP
23	d1	68	SER
23	d1	75	ASN
23	d1	78	LEU
23	d1	87	ARG
24	d2	6	VAL

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Mol	Chain	Res	Type
24	d2	7	LEU
24	d2	15	ASN
24	d2	22	LYS
24	d2	23	ARG
24	d2	26	LEU
24	d2	47	ILE
24	d2	65	LEU
24	d2	83	ILE
24	d2	93	LEU
24	d2	98	GLN
24	d2	103	ILE
24	d2	105	THR
24	d2	111	MET
25	d3	9	LEU
25	d3	14	LYS
25	d3	16	ARG
25	d3	19	ARG
25	d3	36	THR
25	d3	40	SER
25	d3	55	GLU
25	d3	66	SER
25	d3	73	ARG
25	d3	79	ASN
25	d3	83	VAL
25	d3	84	THR
25	d3	100	ASP
25	d3	103	LEU
25	d3	107	PHE
25	d3	109	ARG
25	d3	114	LYS
25	d3	126	LYS
25	d3	127	VAL
25	d3	128	SER
26	d4	10	ARG
26	d4	26	ASP
26	d4	34	ASN
26	d4	35	VAL
26	d4	43	LYS
26	d4	47	VAL
26	d4	49	LYS
26	d4	51	GLU
26	d4	58	PHE

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Mol	Chain	Res	Type
26	d4	62	THR
26	d4	83	LYS
26	d4	88	THR
26	d4	121	THR
26	d4	128	LYS
27	d5	43	ASP
27	d5	51	LEU
27	d5	53	GLU
27	d5	57	TYR
27	d5	60	VAL
27	d5	68	ARG
27	d5	71	ILE
27	d5	81	ARG
28	d6	5	ARG
28	d6	10	ARG
28	d6	12	LYS
28	d6	18	VAL
28	d6	28	LYS
28	d6	34	LYS
28	d6	39	MET
28	d6	53	LEU
28	d6	58	VAL
28	d6	61	GLU
28	d6	67	THR
28	d6	82	ARG
28	d6	84	VAL
28	d6	89	ARG
28	d6	90	GLU
29	d7	8	LEU
29	d7	15	GLU
29	d7	40	CYS
29	d7	41	LEU
29	d7	43	ILE
29	d7	44	THR
29	d7	52	THR
29	d7	60	SER
29	d7	61	THR
29	d7	72	LYS
29	d7	77	THR
29	d7	81	ARG
30	d8	15	VAL
30	d8	22	ARG

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Mol	Chain	Res	Type
30	d8	28	VAL
30	d8	30	VAL
30	d8	32	PHE
30	d8	33	LEU
30	d8	36	THR
30	d8	39	THR
30	d8	62	GLU
30	d8	64	ARG
30	d8	65	ARG
30	d8	67	ARG
31	d9	10	HIS
31	d9	12	ARG
31	d9	24	CYS
31	d9	25	SER
31	d9	30	LEU
31	d9	32	ARG
31	d9	36	LEU
31	d9	38	ILE
31	d9	39	CYS
31	d9	42	CYS
31	d9	49	ASP
31	d9	54	LYS
32	e0	24	THR
32	e0	28	LYS
32	e0	29	LYS
32	e0	38	LEU
32	e0	39	LEU
32	e0	44	PHE
32	e0	46	ASN
32	e0	49	LEU
32	e0	55	ARG
32	e0	56	MET
33	e1	78	LYS
33	e1	90	LYS
33	e1	96	LYS
33	e1	97	LYS
33	e1	98	VAL
33	e1	99	LYS
33	e1	100	LEU
33	e1	102	VAL
33	e1	106	TYR
33	e1	108	VAL

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Mol	Chain	Res	Type
33	e1	113	LYS
33	e1	115	THR
33	e1	120	GLU
33	e1	135	HIS
33	e1	136	LYS
33	e1	140	TYR
33	e1	141	CYS
33	e1	146	SER
33	e1	147	VAL
34	sR	9	LEU
34	sR	14	GLU
34	sR	25	THR
34	sR	29	GLN
34	sR	58	VAL
34	sR	59	ARG
34	sR	64	HIS
34	sR	66	HIS
34	sR	70	ASP
34	sR	76	ASP
34	sR	96	THR
34	sR	98	GLU
34	sR	145	LEU
34	sR	166	SER
34	sR	167	VAL
34	sR	168	THR
34	sR	176	LYS
34	sR	188	ILE
34	sR	207	ASP
34	sR	228	LYS
34	sR	232	TYR
34	sR	238	ASP
34	sR	266	ASP
34	sR	275	ARG
34	sR	282	SER
34	sR	286	GLU
34	sR	297	ASP
34	sR	309	VAL
34	sR	310	ILE
80	sM	24	GLU
80	sM	29	ASN
80	sM	41	SER
80	sM	43	ASP

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Mol	Chain	Res	Type
80	sM	48	ARG
80	sM	61	ILE
80	sM	63	ASP
80	sM	68	ARG
80	sM	74	LYS
80	sM	75	ASP
80	sM	77	THR
80	sM	78	ASP
39	l2	15	ILE
39	l2	23	ARG
39	l2	32	LEU
39	l2	44	ILE
39	l2	45	VAL
39	l2	46	LYS
39	l2	47	GLN
39	l2	48	ILE
39	l2	52	SER
39	l2	71	LEU
39	l2	74	GLU
39	l2	80	GLU
39	l2	96	LEU
39	l2	101	VAL
39	l2	109	GLU
39	l2	112	ILE
39	l2	113	VAL
39	l2	114	SER
39	l2	116	VAL
39	l2	119	LYS
39	l2	134	VAL
39	l2	135	ILE
39	l2	137	ILE
39	l2	142	ASP
39	l2	147	ARG
39	l2	149	ARG
39	l2	155	LYS
39	l2	156	LYS
39	l2	157	VAL
39	l2	165	VAL
39	l2	180	LEU
39	l2	192	LYS
39	l2	193	ARG
39	l2	204	MET

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Mol	Chain	Res	Type
39	l2	207	VAL
39	l2	215	ASN
39	l2	221	LYS
39	l2	227	ARG
39	l2	243	THR
39	l2	246	LEU
40	l3	3	HIS
40	l3	4	ARG
40	l3	10	ARG
40	l3	17	LEU
40	l3	19	ARG
40	l3	21	ARG
40	l3	24	SER
40	l3	39	LYS
40	l3	47	LEU
40	l3	50	LYS
40	l3	56	ILE
40	l3	69	LYS
40	l3	81	THR
40	l3	85	VAL
40	l3	95	THR
40	l3	103	THR
40	l3	114	VAL
40	l3	120	LYS
40	l3	123	TYR
40	l3	139	GLN
40	l3	146	ARG
40	l3	148	LEU
40	l3	150	ARG
40	l3	160	VAL
40	l3	167	ARG
40	l3	169	THR
40	l3	183	LEU
40	l3	196	ARG
40	l3	197	GLU
40	l3	202	THR
40	l3	205	VAL
40	l3	232	ARG
40	l3	235	THR
40	l3	236	LYS
40	l3	238	LEU
40	l3	246	LEU

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Mol	Chain	Res	Type
40	l3	252	ILE
40	l3	274	SER
40	l3	284	ARG
40	l3	287	LYS
40	l3	297	SER
40	l3	304	THR
40	l3	308	MET
40	l3	324	VAL
40	l3	328	ILE
40	l3	332	ARG
40	l3	338	LEU
40	l3	340	LYS
40	l3	346	THR
40	l3	347	SER
40	l3	361	THR
40	l3	382	THR
40	l3	385	LYS
41	l4	3	ARG
41	l4	18	ASN
41	l4	25	VAL
41	l4	52	VAL
41	l4	60	THR
41	l4	90	PHE
41	l4	92	ASN
41	l4	93	MET
41	l4	120	TYR
41	l4	122	THR
41	l4	136	LEU
41	l4	144	LYS
41	l4	145	ILE
41	l4	150	LEU
41	l4	156	LEU
41	l4	163	LYS
41	l4	170	LYS
41	l4	179	LEU
41	l4	182	LEU
41	l4	186	LYS
41	l4	187	LEU
41	l4	197	ARG
41	l4	203	ARG
41	l4	206	LEU
41	l4	220	ARG

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Mol	Chain	Res	Type
41	14	226	GLU
41	14	230	VAL
41	14	233	LEU
41	14	246	ARG
41	14	258	LEU
41	14	261	VAL
41	14	265	GLU
41	14	266	THR
41	14	283	THR
41	14	289	ILE
41	14	300	ARG
41	14	304	GLN
41	14	307	GLN
41	14	313	LEU
41	14	319	LYS
41	14	327	LEU
41	14	338	LYS
41	14	342	LYS
41	14	345	GLU
41	14	347	THR
41	14	358	THR
41	14	359	LEU
42	15	4	GLN
42	15	5	LYS
42	15	25	GLU
42	15	35	ARG
42	15	51	LEU
42	15	61	ILE
42	15	70	THR
42	15	74	VAL
42	15	75	LEU
42	15	89	THR
42	15	93	THR
42	15	110	LEU
42	15	112	LYS
42	15	113	LEU
42	15	118	THR
42	15	120	LYS
42	15	122	VAL
42	15	131	LEU
42	15	132	THR
42	15	136	GLU

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Mol	Chain	Res	Type
42	15	140	ARG
42	15	144	VAL
42	15	146	LEU
42	15	148	ILE
42	15	152	ARG
42	15	155	THR
42	15	164	LYS
42	15	185	PHE
42	15	187	THR
42	15	194	LEU
42	15	218	ARG
42	15	227	LEU
42	15	254	LYS
42	15	258	LYS
42	15	259	LYS
42	15	268	GLU
42	15	269	SER
42	15	273	ARG
42	15	282	ARG
42	15	293	LEU
43	16	20	LYS
43	16	21	THR
43	16	31	ARG
43	16	46	ARG
43	16	50	LYS
43	16	64	LEU
43	16	65	ILE
43	16	76	LEU
43	16	78	ARG
43	16	79	VAL
43	16	82	ARG
43	16	89	THR
43	16	91	VAL
43	16	93	VAL
43	16	109	GLU
43	16	152	THR
43	16	155	LEU
43	16	162	SER
43	16	175	LYS
44	17	22	THR
44	17	29	GLU
44	17	30	ARG

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Mol	Chain	Res	Type
44	17	39	GLU
44	17	41	ARG
44	17	45	LEU
44	17	56	GLU
44	17	60	ARG
44	17	77	VAL
44	17	83	LEU
44	17	84	VAL
44	17	87	VAL
44	17	88	ARG
44	17	98	LYS
44	17	100	ARG
44	17	111	ILE
44	17	147	LEU
44	17	156	ILE
44	17	157	ASN
44	17	158	LYS
44	17	164	SER
44	17	173	LEU
44	17	179	LEU
44	17	184	LEU
44	17	219	LYS
44	17	229	PHE
44	17	239	LEU
44	17	244	ASN
81	18	26	LEU
81	18	41	GLN
81	18	46	LEU
81	18	68	ARG
81	18	69	LEU
81	18	74	THR
81	18	77	GLN
81	18	79	GLN
81	18	81	THR
81	18	89	GLU
81	18	90	THR
81	18	95	ASN
81	18	98	ARG
81	18	101	THR
81	18	111	LYS
81	18	134	TYR
81	18	136	LEU

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Mol	Chain	Res	Type
81	18	146	LYS
81	18	149	LYS
81	18	160	ILE
81	18	163	VAL
81	18	169	LEU
81	18	172	LYS
81	18	180	VAL
81	18	183	LYS
81	18	185	ARG
81	18	200	LEU
81	18	203	VAL
81	18	214	LEU
81	18	224	ASP
81	18	230	LYS
81	18	245	LYS
81	18	248	LYS
46	19	6	THR
46	19	18	VAL
46	19	33	THR
46	19	39	LYS
46	19	52	LEU
46	19	55	VAL
46	19	63	LYS
46	19	68	LEU
46	19	70	THR
46	19	78	MET
46	19	80	THR
46	19	82	VAL
46	19	92	TYR
46	19	104	VAL
46	19	105	GLU
46	19	106	LYS
46	19	107	ASP
46	19	118	LEU
46	19	121	LYS
46	19	129	ARG
46	19	130	ASP
46	19	133	THR
46	19	137	SER
46	19	140	VAL
46	19	143	GLU
46	19	144	ILE

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Mol	Chain	Res	Type
46	l9	151	VAL
46	l9	157	ASN
46	l9	161	LEU
46	l9	162	GLN
46	l9	173	ARG
46	l9	177	ASP
46	l9	188	THR
46	l9	191	LEU
47	m0	4	ARG
47	m0	7	ARG
47	m0	22	TYR
47	m0	24	ARG
47	m0	26	VAL
47	m0	29	SER
47	m0	31	ILE
47	m0	35	ASP
47	m0	36	LEU
47	m0	42	THR
47	m0	44	ASP
47	m0	48	LEU
47	m0	52	LEU
47	m0	53	VAL
47	m0	58	GLU
47	m0	63	GLU
47	m0	71	CYS
47	m0	74	LYS
47	m0	76	MET
47	m0	87	LEU
47	m0	91	VAL
47	m0	99	ILE
47	m0	101	LYS
47	m0	133	GLN
47	m0	139	ARG
47	m0	145	LYS
47	m0	153	ARG
47	m0	154	ARG
47	m0	162	GLN
47	m0	163	GLN
47	m0	167	LEU
47	m0	169	LYS
47	m0	177	ASP
47	m0	178	ARG

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Mol	Chain	Res	Type
47	m0	182	LEU
47	m0	200	LEU
47	m0	205	SER
47	m0	211	ARG
47	m0	212	GLU
47	m0	217	PHE
48	m1	6	GLN
48	m1	10	ARG
48	m1	12	LEU
48	m1	13	LYS
48	m1	30	LEU
48	m1	31	THR
48	m1	44	THR
48	m1	46	VAL
48	m1	54	VAL
48	m1	56	THR
48	m1	71	VAL
48	m1	80	LEU
48	m1	85	LYS
48	m1	101	ASN
48	m1	106	ILE
48	m1	107	ASP
48	m1	112	LEU
48	m1	129	VAL
48	m1	130	VAL
48	m1	137	ARG
48	m1	140	ARG
48	m1	142	LYS
48	m1	153	LYS
48	m1	155	THR
48	m1	159	THR
48	m1	166	LYS
48	m1	174	LYS
49	m3	5	LYS
49	m3	13	HIS
49	m3	16	LYS
49	m3	52	ASP
49	m3	54	LEU
49	m3	55	ARG
49	m3	58	VAL
49	m3	59	ARG
49	m3	63	VAL

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Mol	Chain	Res	Type
49	m3	67	ARG
49	m3	68	LYS
49	m3	73	ARG
49	m3	85	LEU
49	m3	107	GLU
49	m3	114	GLN
49	m3	118	GLU
49	m3	122	LYS
49	m3	131	LYS
49	m3	149	GLN
49	m3	152	THR
49	m3	164	GLU
49	m3	168	ARG
49	m3	184	GLU
49	m3	194	GLU
50	m4	3	THR
50	m4	6	ILE
50	m4	41	GLN
50	m4	50	LYS
50	m4	62	GLN
50	m4	63	VAL
50	m4	64	VAL
50	m4	72	LEU
50	m4	80	THR
50	m4	90	VAL
50	m4	107	GLU
50	m4	116	GLU
50	m4	123	LEU
50	m4	130	THR
50	m4	135	LEU
51	m5	5	LYS
51	m5	8	GLU
51	m5	10	LEU
51	m5	12	ARG
51	m5	15	GLN
51	m5	22	LEU
51	m5	24	ARG
51	m5	27	VAL
51	m5	49	ARG
51	m5	67	ARG
51	m5	68	ARG
51	m5	75	VAL

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Mol	Chain	Res	Type
51	m5	80	THR
51	m5	85	THR
51	m5	92	LEU
51	m5	97	SER
51	m5	98	LEU
51	m5	104	GLU
51	m5	138	GLN
51	m5	153	ASP
51	m5	155	VAL
51	m5	159	ARG
51	m5	175	ASN
51	m5	176	LYS
51	m5	183	THR
51	m5	187	ARG
51	m5	190	THR
51	m5	198	SER
51	m5	204	LYS
52	m6	3	VAL
52	m6	22	VAL
52	m6	25	LYS
52	m6	34	VAL
52	m6	41	LEU
52	m6	58	LEU
52	m6	67	THR
52	m6	74	ARG
52	m6	78	ARG
52	m6	79	ILE
52	m6	84	LEU
52	m6	85	ARG
52	m6	100	GLU
52	m6	106	GLU
52	m6	117	ARG
52	m6	119	VAL
52	m6	124	LEU
52	m6	126	VAL
52	m6	128	ARG
52	m6	129	LEU
52	m6	152	VAL
52	m6	170	LYS
52	m6	171	LYS
52	m6	175	THR
52	m6	180	SER

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Mol	Chain	Res	Type
52	m6	182	ASN
52	m6	184	THR
52	m6	197	LEU
53	m7	7	THR
53	m7	9	THR
53	m7	24	VAL
53	m7	29	THR
53	m7	31	GLU
53	m7	32	THR
53	m7	42	THR
53	m7	43	LYS
53	m7	52	LEU
53	m7	56	ARG
53	m7	78	VAL
53	m7	79	THR
53	m7	80	LYS
53	m7	89	LYS
53	m7	96	GLN
53	m7	107	LEU
53	m7	112	LEU
53	m7	114	VAL
53	m7	118	GLN
53	m7	121	GLN
53	m7	126	ARG
53	m7	127	ARG
53	m7	144	SER
53	m7	153	LYS
53	m7	155	GLU
54	m8	3	ILE
54	m8	7	SER
54	m8	12	ARG
54	m8	23	ASN
54	m8	24	VAL
54	m8	26	LEU
54	m8	32	LEU
54	m8	34	THR
54	m8	49	LEU
54	m8	57	ILE
54	m8	63	SER
54	m8	64	VAL
54	m8	74	GLU
54	m8	80	THR

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Mol	Chain	Res	Type
54	m8	93	ILE
54	m8	111	ARG
54	m8	113	LYS
54	m8	127	LEU
54	m8	135	GLN
54	m8	137	THR
54	m8	138	LEU
54	m8	161	LYS
54	m8	165	ILE
54	m8	170	ARG
54	m8	174	ARG
54	m8	180	ARG
55	m9	10	LEU
55	m9	29	THR
55	m9	36	ASN
55	m9	43	LYS
55	m9	49	THR
55	m9	52	LYS
55	m9	63	THR
55	m9	70	LYS
55	m9	71	ARG
55	m9	74	ARG
55	m9	76	SER
55	m9	88	ARG
55	m9	99	LEU
55	m9	116	ASP
55	m9	128	LYS
55	m9	138	LEU
55	m9	152	GLU
55	m9	153	LYS
55	m9	164	LEU
55	m9	167	ARG
55	m9	171	ASP
55	m9	173	ARG
55	m9	177	VAL
56	n0	1	MET
56	n0	8	GLN
56	n0	13	ARG
56	n0	17	GLU
56	n0	18	SER
56	n0	21	GLU
56	n0	23	LYS

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Mol	Chain	Res	Type
56	n0	45	LEU
56	n0	50	LYS
56	n0	51	VAL
56	n0	52	LYS
56	n0	60	SER
56	n0	70	THR
56	n0	80	ARG
56	n0	87	THR
56	n0	88	HIS
56	n0	89	ASN
56	n0	92	LYS
56	n0	97	VAL
56	n0	100	VAL
56	n0	104	GLU
56	n0	105	THR
56	n0	115	ARG
56	n0	117	ARG
56	n0	130	GLU
56	n0	136	LYS
56	n0	137	ARG
56	n0	142	GLN
56	n0	148	LEU
56	n0	149	LYS
56	n0	155	ARG
56	n0	157	GLN
56	n0	162	THR
56	n0	172	TYR
57	n1	12	ARG
57	n1	25	VAL
57	n1	26	HIS
57	n1	27	LEU
57	n1	47	SER
57	n1	55	LYS
57	n1	68	THR
57	n1	71	SER
57	n1	78	LYS
57	n1	80	VAL
57	n1	83	ARG
57	n1	88	ARG
57	n1	89	LEU
57	n1	96	ILE
57	n1	102	ARG

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Mol	Chain	Res	Type
57	n1	104	GLU
57	n1	126	VAL
57	n1	127	GLN
57	n1	139	ARG
57	n1	141	VAL
57	n1	143	THR
57	n1	146	ASN
57	n1	149	GLN
57	n1	150	THR
58	n2	14	THR
58	n2	16	THR
58	n2	20	SER
58	n2	27	VAL
58	n2	37	LEU
58	n2	43	VAL
58	n2	50	LEU
58	n2	54	VAL
58	n2	58	GLU
58	n2	63	VAL
58	n2	64	THR
58	n2	90	ARG
58	n2	94	ARG
58	n2	96	VAL
58	n2	97	SER
58	n2	98	THR
58	n2	105	LEU
59	n3	2	SER
59	n3	4	ASN
59	n3	7	GLN
59	n3	13	ILE
59	n3	14	SER
59	n3	42	SER
59	n3	45	ARG
59	n3	46	LEU
59	n3	48	ARG
59	n3	69	LEU
59	n3	72	LYS
59	n3	74	MET
59	n3	91	VAL
59	n3	120	LYS
59	n3	125	LEU
59	n3	128	ARG

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Mol	Chain	Res	Type
59	n3	135	VAL
83	n4	1	MET
83	n4	5	ILE
83	n4	39	LEU
83	n4	54	LEU
83	n4	63	ILE
83	n4	96	LEU
83	n4	97	LYS
83	n4	99	GLU
83	n4	100	VAL
83	n4	105	ARG
83	n4	107	GLU
83	n4	127	LYS
83	n4	130	SER
61	n5	24	LEU
61	n5	27	ARG
61	n5	34	LEU
61	n5	37	THR
61	n5	39	LYS
61	n5	45	LYS
61	n5	49	LYS
61	n5	56	ARG
61	n5	63	ILE
61	n5	71	THR
61	n5	86	VAL
61	n5	108	LEU
61	n5	109	LYS
61	n5	112	THR
61	n5	115	ARG
61	n5	125	ARG
61	n5	127	THR
61	n5	135	ILE
61	n5	142	ILE
62	n6	8	VAL
62	n6	12	ARG
62	n6	13	ARG
62	n6	14	LYS
62	n6	17	LYS
62	n6	37	LYS
62	n6	39	LEU
62	n6	40	ARG
62	n6	45	ILE

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Mol	Chain	Res	Type
62	n6	50	ILE
62	n6	52	ARG
62	n6	56	VAL
62	n6	57	LEU
62	n6	62	SER
62	n6	64	LYS
62	n6	66	GLN
62	n6	70	ILE
62	n6	74	TYR
62	n6	76	LEU
62	n6	80	VAL
62	n6	89	LYS
62	n6	94	SER
62	n6	95	VAL
62	n6	106	ILE
62	n6	112	ASP
62	n6	115	ARG
62	n6	120	GLN
63	n7	3	LYS
63	n7	5	LEU
63	n7	14	VAL
63	n7	15	ARG
63	n7	24	VAL
63	n7	33	SER
63	n7	36	HIS
63	n7	52	LYS
63	n7	53	VAL
63	n7	57	HIS
63	n7	72	ILE
63	n7	75	VAL
63	n7	81	LEU
63	n7	83	THR
63	n7	86	THR
63	n7	94	SER
63	n7	95	VAL
63	n7	99	GLU
63	n7	100	THR
63	n7	102	GLU
63	n7	103	GLN
63	n7	121	ARG
63	n7	134	LEU
64	n8	4	ARG

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Mol	Chain	Res	Type
64	n8	6	THR
64	n8	7	LYS
64	n8	8	THR
64	n8	10	LYS
64	n8	12	ARG
64	n8	14	HIS
64	n8	25	HIS
64	n8	27	LYS
64	n8	34	MET
64	n8	42	ARG
64	n8	46	ASP
64	n8	47	LYS
64	n8	56	VAL
64	n8	60	TYR
64	n8	65	GLN
64	n8	78	LEU
64	n8	84	GLU
64	n8	85	ASP
64	n8	89	GLN
64	n8	91	LEU
64	n8	97	GLU
64	n8	98	THR
64	n8	115	LYS
64	n8	117	ARG
64	n8	124	ILE
64	n8	132	LYS
64	n8	133	LEU
65	n9	3	LYS
65	n9	14	ARG
65	n9	21	ILE
65	n9	26	THR
65	n9	31	SER
65	n9	38	LYS
65	n9	58	LYS
65	n9	59	LYS
66	o0	8	GLU
66	o0	10	ILE
66	o0	16	LEU
66	o0	19	LYS
66	o0	40	LYS
66	o0	41	LEU
66	o0	55	GLU

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Mol	Chain	Res	Type
66	o0	61	MET
66	o0	68	TYR
66	o0	74	ASN
66	o0	86	ARG
66	o0	101	LEU
66	o0	103	THR
67	o1	6	ASP
67	o1	8	VAL
67	o1	16	LEU
67	o1	26	LYS
67	o1	31	ARG
67	o1	34	LYS
67	o1	44	MET
67	o1	55	LEU
67	o1	64	VAL
67	o1	68	GLU
67	o1	84	ASP
67	o1	96	VAL
67	o1	97	LEU
67	o1	98	VAL
67	o1	102	LYS
67	o1	106	THR
67	o1	107	VAL
67	o1	110	GLU
67	o1	111	GLU
68	o2	3	SER
68	o2	4	LEU
68	o2	14	THR
68	o2	16	LYS
68	o2	19	ARG
68	o2	24	ARG
68	o2	31	ASN
68	o2	33	ARG
68	o2	35	GLN
68	o2	41	VAL
68	o2	51	SER
68	o2	54	LYS
68	o2	73	THR
68	o2	75	LEU
68	o2	82	LEU
68	o2	89	THR
68	o2	95	GLU

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Mol	Chain	Res	Type
68	o2	106	VAL
68	o2	125	ARG
68	o2	126	LEU
69	o3	4	SER
69	o3	31	LYS
69	o3	49	ILE
69	o3	70	LYS
69	o3	73	ARG
69	o3	74	THR
69	o3	81	VAL
69	o3	84	THR
69	o3	86	ARG
69	o3	98	VAL
70	o4	5	VAL
70	o4	24	LYS
70	o4	44	CYS
70	o4	46	ASP
70	o4	58	ARG
70	o4	65	VAL
70	o4	81	CYS
70	o4	83	ASN
70	o4	88	ARG
70	o4	102	LYS
71	o5	4	VAL
71	o5	20	GLN
71	o5	21	LEU
71	o5	27	GLU
71	o5	36	LEU
71	o5	37	SER
71	o5	45	LYS
71	o5	47	VAL
71	o5	62	GLN
71	o5	69	LEU
71	o5	81	ARG
71	o5	85	THR
71	o5	86	ARG
71	o5	89	ARG
71	o5	90	ARG
71	o5	101	THR
71	o5	107	LYS
72	o6	2	THR
72	o6	5	THR

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Mol	Chain	Res	Type
72	o6	7	ILE
72	o6	9	ILE
72	o6	11	LEU
72	o6	17	VAL
72	o6	21	THR
72	o6	26	ILE
72	o6	29	LYS
72	o6	35	ASN
72	o6	36	ARG
72	o6	37	THR
72	o6	40	VAL
72	o6	42	SER
72	o6	43	LEU
72	o6	45	ARG
72	o6	57	LEU
72	o6	58	ILE
72	o6	59	ASP
72	o6	60	LEU
72	o6	62	ARG
72	o6	71	LYS
72	o6	88	GLU
72	o6	94	ILE
72	o6	98	ARG
73	o7	3	LYS
73	o7	17	THR
73	o7	24	ARG
73	o7	25	ARG
73	o7	30	GLN
73	o7	33	THR
73	o7	44	THR
73	o7	46	SER
73	o7	55	ARG
73	o7	65	ARG
73	o7	68	LYS
73	o7	75	LYS
73	o7	80	THR
74	o8	5	ILE
74	o8	12	LEU
74	o8	17	ARG
74	o8	24	THR
74	o8	31	LEU
74	o8	41	THR

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Mol	Chain	Res	Type
74	o8	46	ARG
74	o8	50	SER
74	o8	53	THR
74	o8	61	LYS
74	o8	64	LYS
74	o8	65	LEU
74	o8	78	LEU
75	o9	4	GLN
75	o9	15	LYS
75	o9	17	LYS
75	o9	21	ARG
75	o9	23	LEU
75	o9	28	ARG
75	o9	29	LEU
76	q0	85	LEU
76	q0	88	LYS
76	q0	106	ARG
76	q0	112	LYS
76	q0	113	ARG
76	q0	114	LYS
76	q0	119	ASN
76	q0	127	LEU
76	q0	128	LYS
77	q1	6	ARG
77	q1	9	ARG
77	q1	13	LEU
77	q1	17	ARG
77	q1	19	LYS
77	q1	21	ARG
77	q1	23	ARG
78	q2	6	LYS
78	q2	7	THR
78	q2	8	ARG
78	q2	18	ARG
78	q2	20	HIS
78	q2	22	GLN
78	q2	26	THR
78	q2	45	ARG
78	q2	61	LYS
78	q2	64	THR
78	q2	78	LYS
78	q2	83	LEU

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Mol	Chain	Res	Type
78	q2	84	THR
78	q2	85	LEU
78	q2	93	LEU
78	q2	98	LYS
78	q2	100	LYS
78	q2	104	LEU
78	q2	105	GLN
79	q3	5	THR
79	q3	20	SER
79	q3	21	SER
79	q3	24	ARG
79	q3	26	VAL
79	q3	30	GLU
79	q3	36	ARG
79	q3	42	CYS
79	q3	45	LYS
79	q3	48	LYS
79	q3	49	ARG
79	q3	54	ILE
79	q3	56	THR
79	q3	59	CYS
79	q3	70	THR
79	q3	81	SER
84	p0	4	ILE
84	p0	5	ARG
84	p0	6	GLU
84	p0	10	GLU
84	p0	25	LEU
84	p0	30	VAL
84	p0	42	ARG
84	p0	48	ARG
84	p0	51	VAL
84	p0	55	LYS
84	p0	58	MET
84	p0	67	LEU
84	p0	68	SER
84	p0	70	LEU
84	p0	72	ASP
84	p0	76	LEU
84	p0	80	VAL
84	p0	81	LYS
84	p0	84	VAL

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Mol	Chain	Res	Type
84	p0	93	LEU
84	p0	97	LYS
84	p0	104	ARG
84	p0	185	LEU
84	p0	196	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (38) such sidechains are listed below:

Mol	Chain	Res	Type
8	S6	22	HIS
9	S7	74	GLN
11	S9	110	GLN
15	C3	62	GLN
18	C6	32	ASN
19	C7	48	ASN
23	D1	74	GLN
24	D2	56	HIS
27	D5	95	HIS
32	E0	17	GLN
41	L4	311	HIS
42	L5	40	HIS
44	L7	244	ASN
51	M5	194	GLN
53	M7	10	ASN
53	M7	34	GLN
59	N3	98	ASN
78	Q2	47	GLN
2	s0	140	ASN
3	s1	149	GLN
11	s9	110	GLN
11	s9	123	HIS
11	s9	124	HIS
11	s9	142	ASN
15	c3	49	GLN
22	d0	48	HIS
22	d0	72	ASN
26	d4	22	GLN
33	e1	93	HIS
34	sR	314	GLN
39	l2	47	GLN
39	l2	100	ASN
46	l9	8	GLN

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Mol	Chain	Res	Type
64	n8	28	HIS
64	n8	44	ASN
70	o4	3	GLN
71	o5	68	GLN
76	q0	119	ASN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	2	1777/1800 (98%)	480 (27%)	60 (3%)
1	6	1793/1800 (99%)	466 (25%)	52 (2%)
36	1	3145/3396 (92%)	667 (21%)	76 (2%)
36	5	3145/3396 (92%)	677 (21%)	67 (2%)
37	3	120/121 (99%)	15 (12%)	0
37	7	120/121 (99%)	19 (15%)	0
38	4	157/158 (99%)	35 (22%)	2 (1%)
38	8	157/158 (99%)	34 (21%)	3 (1%)
All	All	10414/10950 (95%)	2393 (22%)	260 (2%)

All (2393) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	2	2	A
1	2	4	C
1	2	17	C
1	2	21	U
1	2	25	C
1	2	26	A
1	2	27	U
1	2	34	G
1	2	42	G
1	2	44	U
1	2	45	U
1	2	47	A
1	2	57	G
1	2	60	U
1	2	66	U
1	2	67	A
1	2	68	A
1	2	69	G
1	2	72	A

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Mol	Chain	Res	Type
1	2	73	U
1	2	74	U
1	2	75	U
1	2	77	U
1	2	95	G
1	2	103	A
1	2	104	A
1	2	114	C
1	2	131	C
1	2	132	U
1	2	133	U
1	2	134	U
1	2	135	A
1	2	136	C
1	2	137	U
1	2	140	A
1	2	141	U
1	2	145	A
1	2	146	U
1	2	153	G
1	2	158	U
1	2	159	U
1	2	167	U
1	2	169	A
1	2	170	U
1	2	178	U
1	2	185	U
1	2	186	C
1	2	188	A
1	2	190	C
1	2	191	C
1	2	192	U
1	2	194	U
1	2	195	G
1	2	196	G
1	2	197	A
1	2	198	A
1	2	199	G
1	2	200	A
1	2	215	A
1	2	217	A
1	2	218	A

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Mol	Chain	Res	Type
1	2	219	A
1	2	226	A
1	2	227	U
1	2	228	G
1	2	229	U
1	2	233	C
1	2	234	G
1	2	235	G
1	2	238	U
1	2	239	C
1	2	240	U
1	2	241	U
1	2	242	U
1	2	249	U
1	2	250	C
1	2	257	A
1	2	260	U
1	2	261	U
1	2	262	U
1	2	265	A
1	2	266	A
1	2	267	U
1	2	271	A
1	2	272	U
1	2	274	G
1	2	275	C
1	2	276	C
1	2	277	U
1	2	278	U
1	2	279	G
1	2	280	U
1	2	281	G
1	2	288	A
1	2	290	G
1	2	299	A
1	2	302	U
1	2	309	C
1	2	314	C
1	2	316	A
1	2	320	U
1	2	321	C
1	2	322	G

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Mol	Chain	Res	Type
1	2	333	A
1	2	337	G
1	2	338	C
1	2	352	A
1	2	359	A
1	2	360	A
1	2	361	C
1	2	378	A
1	2	387	A
1	2	390	G
1	2	397	A
1	2	400	A
1	2	401	A
1	2	402	C
1	2	403	G
1	2	404	G
1	2	416	A
1	2	418	G
1	2	424	C
1	2	425	A
1	2	426	G
1	2	428	A
1	2	434	G
1	2	437	A
1	2	439	U
1	2	444	C
1	2	448	C
1	2	452	A
1	2	454	U
1	2	468	A
1	2	480	G
1	2	484	C
1	2	485	A
1	2	486	G
1	2	488	G
1	2	493	U
1	2	494	U
1	2	495	C
1	2	496	G
1	2	497	G
1	2	498	G
1	2	499	U

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Mol	Chain	Res	Type
1	2	500	C
1	2	502	U
1	2	503	G
1	2	504	U
1	2	505	A
1	2	506	A
1	2	507	U
1	2	508	U
1	2	510	G
1	2	511	A
1	2	512	A
1	2	513	U
1	2	514	G
1	2	515	A
1	2	516	G
1	2	519	C
1	2	520	A
1	2	527	A
1	2	532	U
1	2	534	A
1	2	538	A
1	2	539	G
1	2	540	G
1	2	541	A
1	2	542	A
1	2	543	C
1	2	544	A
1	2	545	A
1	2	548	G
1	2	555	A
1	2	556	A
1	2	557	G
1	2	558	U
1	2	565	C
1	2	578	U
1	2	579	A
1	2	580	A
1	2	582	U
1	2	594	A
1	2	595	G
1	2	609	U
1	2	610	G

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Mol	Chain	Res	Type
1	2	611	U
1	2	614	C
1	2	619	A
1	2	620	A
1	2	621	A
1	2	622	A
1	2	623	A
1	2	624	G
1	2	639	U
1	2	640	U
1	2	650	U
1	2	653	C
1	2	655	G
1	2	656	G
1	2	657	U
1	2	658	C
1	2	677	G
1	2	679	U
1	2	680	U
1	2	684	A
1	2	685	A
1	2	686	C
1	2	692	C
1	2	694	U
1	2	696	C
1	2	697	C
1	2	700	C
1	2	701	U
1	2	702	G
1	2	703	G
1	2	704	C
1	2	705	U
1	2	707	A
1	2	709	C
1	2	710	U
1	2	711	U
1	2	712	G
1	2	713	A
1	2	714	G
1	2	717	C
1	2	718	U
1	2	719	U

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Mol	Chain	Res	Type
1	2	720	G
1	2	721	U
1	2	722	G
1	2	723	G
1	2	725	U
1	2	727	U
1	2	728	U
1	2	730	G
1	2	731	C
1	2	732	G
1	2	733	A
1	2	734	A
1	2	735	C
1	2	736	C
1	2	737	A
1	2	738	G
1	2	742	U
1	2	743	U
1	2	753	A
1	2	754	A
1	2	755	A
1	2	756	A
1	2	758	U
1	2	759	U
1	2	765	G
1	2	766	U
1	2	774	A
1	2	775	G
1	2	778	G
1	2	781	U
1	2	782	U
1	2	783	G
1	2	784	C
1	2	789	A
1	2	793	A
1	2	794	U
1	2	795	U
1	2	812	A
1	2	815	G
1	2	816	G
1	2	818	C
1	2	819	G

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Mol	Chain	Res	Type
1	2	820	U
1	2	821	U
1	2	822	U
1	2	823	G
1	2	824	G
1	2	829	A
1	2	830	U
1	2	831	U
1	2	833	U
1	2	837	G
1	2	841	U
1	2	854	U
1	2	856	A
1	2	862	A
1	2	863	A
1	2	864	U
1	2	876	G
1	2	886	U
1	2	896	U
1	2	898	A
1	2	912	U
1	2	913	G
1	2	914	G
1	2	916	U
1	2	921	U
1	2	933	A
1	2	935	U
1	2	942	G
1	2	944	A
1	2	951	A
1	2	960	U
1	2	966	A
1	2	988	A
1	2	992	A
1	2	993	A
1	2	997	G
1	2	1003	A
1	2	1004	U
1	2	1005	A
1	2	1026	A
1	2	1028	C
1	2	1039	A

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Mol	Chain	Res	Type
1	2	1040	G
1	2	1052	U
1	2	1053	G
1	2	1058	U
1	2	1059	U
1	2	1060	U
1	2	1061	A
1	2	1066	C
1	2	1073	G
1	2	1075	C
1	2	1080	U
1	2	1082	C
1	2	1083	G
1	2	1087	A
1	2	1091	A
1	2	1092	A
1	2	1096	C
1	2	1097	U
1	2	1098	U
1	2	1100	G
1	2	1109	G
1	2	1117	U
1	2	1138	A
1	2	1146	G
1	2	1149	G
1	2	1150	G
1	2	1151	A
1	2	1155	G
1	2	1157	A
1	2	1158	C
1	2	1160	A
1	2	1163	A
1	2	1167	G
1	2	1185	U
1	2	1191	U
1	2	1194	A
1	2	1196	A
1	2	1199	G
1	2	1200	G
1	2	1202	A
1	2	1207	C
1	2	1217	A

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Mol	Chain	Res	Type
1	2	1218	G
1	2	1227	A
1	2	1228	G
1	2	1229	G
1	2	1241	G
1	2	1243	G
1	2	1244	A
1	2	1245	G
1	2	1251	U
1	2	1257	U
1	2	1258	U
1	2	1275	A
1	2	1286	U
1	2	1292	G
1	2	1306	C
1	2	1307	U
1	2	1314	U
1	2	1315	U
1	2	1321	A
1	2	1337	A
1	2	1338	C
1	2	1340	U
1	2	1341	A
1	2	1344	A
1	2	1345	A
1	2	1354	G
1	2	1355	C
1	2	1361	U
1	2	1362	U
1	2	1363	U
1	2	1364	G
1	2	1370	U
1	2	1371	A
1	2	1372	U
1	2	1383	G
1	2	1388	A
1	2	1390	U
1	2	1398	U
1	2	1399	C
1	2	1412	G
1	2	1413	U
1	2	1414	U

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Mol	Chain	Res	Type
1	2	1415	U
1	2	1427	A
1	2	1428	G
1	2	1433	G
1	2	1446	A
1	2	1448	G
1	2	1451	C
1	2	1456	C
1	2	1457	C
1	2	1458	G
1	2	1459	C
1	2	1461	C
1	2	1462	G
1	2	1471	A
1	2	1473	U
1	2	1474	G
1	2	1475	A
1	2	1482	C
1	2	1486	G
1	2	1489	U
1	2	1490	C
1	2	1491	U
1	2	1492	A
1	2	1493	A
1	2	1499	G
1	2	1506	G
1	2	1514	U
1	2	1515	A
1	2	1516	A
1	2	1517	U
1	2	1521	G
1	2	1523	G
1	2	1524	A
1	2	1535	U
1	2	1536	G
1	2	1537	C
1	2	1538	U
1	2	1557	U
1	2	1559	A
1	2	1569	A
1	2	1574	G
1	2	1584	G

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Mol	Chain	Res	Type
1	2	1590	G
1	2	1601	G
1	2	1614	A
1	2	1616	G
1	2	1619	C
1	2	1624	C
1	2	1631	A
1	2	1641	C
1	2	1657	U
1	2	1658	G
1	2	1663	G
1	2	1680	G
1	2	1681	A
1	2	1682	U
1	2	1683	C
1	2	1684	U
1	2	1697	G
1	2	1698	G
1	2	1699	G
1	2	1700	C
1	2	1701	A
1	2	1702	A
1	2	1712	A
1	2	1713	G
1	2	1715	G
1	2	1719	A
1	2	1760	G
1	2	1762	A
1	2	1766	A
1	2	1769	U
1	2	1770	U
1	2	1780	G
1	2	1782	A
1	2	1783	C
1	2	1788	G
1	2	1789	G
1	2	1792	G
1	2	1793	G
1	2	1794	A
1	2	1795	U
1	2	1796	C
36	1	13	A

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Mol	Chain	Res	Type
36	1	14	U
36	1	16	A
36	1	24	G
36	1	26	A
36	1	40	A
36	1	49	A
36	1	57	A
36	1	59	G
36	1	60	A
36	1	65	A
36	1	66	A
36	1	68	C
36	1	76	G
36	1	83	U
36	1	92	G
36	1	93	C
36	1	99	A
36	1	108	A
36	1	109	A
36	1	110	G
36	1	113	C
36	1	116	A
36	1	117	U
36	1	121	A
36	1	122	A
36	1	133	U
36	1	135	C
36	1	136	G
36	1	145	G
36	1	156	G
36	1	157	A
36	1	166	C
36	1	170	G
36	1	173	G
36	1	182	U
36	1	187	A
36	1	190	U
36	1	191	U
36	1	200	C
36	1	201	A
36	1	210	U
36	1	218	G

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Mol	Chain	Res	Type
36	1	219	A
36	1	234	G
36	1	240	U
36	1	243	G
36	1	245	U
36	1	249	U
36	1	250	U
36	1	251	G
36	1	252	U
36	1	265	A
36	1	269	G
36	1	282	G
36	1	283	G
36	1	286	U
36	1	295	A
36	1	298	U
36	1	315	C
36	1	323	A
36	1	329	U
36	1	339	C
36	1	343	U
36	1	349	A
36	1	350	C
36	1	351	A
36	1	368	G
36	1	374	A
36	1	376	G
36	1	391	A
36	1	395	A
36	1	398	A
36	1	399	A
36	1	401	U
36	1	402	A
36	1	403	C
36	1	420	G
36	1	421	G
36	1	422	A
36	1	438	A
36	1	440	A
36	1	495	G
36	1	498	A
36	1	516	A

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Mol	Chain	Res	Type
36	1	520	U
36	1	521	A
36	1	535	G
36	1	543	C
36	1	544	C
36	1	546	C
36	1	547	G
36	1	548	G
36	1	551	A
36	1	552	G
36	1	553	U
36	1	555	U
36	1	556	U
36	1	557	A
36	1	559	A
36	1	578	A
36	1	579	G
36	1	592	A
36	1	601	U
36	1	603	A
36	1	604	G
36	1	609	G
36	1	611	A
36	1	619	A
36	1	620	U
36	1	621	A
36	1	622	A
36	1	636	C
36	1	638	C
36	1	647	A
36	1	649	A
36	1	651	G
36	1	653	A
36	1	660	A
36	1	661	G
36	1	667	C
36	1	677	A
36	1	681	U
36	1	691	A
36	1	705	A
36	1	708	G
36	1	712	G

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Mol	Chain	Res	Type
36	1	715	A
36	1	716	A
36	1	764	U
36	1	765	C
36	1	766	U
36	1	767	U
36	1	772	U
36	1	776	U
36	1	777	U
36	1	781	G
36	1	785	G
36	1	787	G
36	1	801	A
36	1	806	A
36	1	816	A
36	1	817	A
36	1	830	A
36	1	849	C
36	1	861	C
36	1	871	U
36	1	874	U
36	1	878	G
36	1	879	U
36	1	890	C
36	1	896	A
36	1	907	G
36	1	908	G
36	1	914	A
36	1	916	G
36	1	917	A
36	1	921	A
36	1	923	C
36	1	924	G
36	1	925	A
36	1	937	G
36	1	943	U
36	1	944	C
36	1	953	G
36	1	959	C
36	1	960	U
36	1	962	A
36	1	963	G

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Mol	Chain	Res	Type
36	1	979	U
36	1	980	A
36	1	981	U
36	1	982	C
36	1	994	G
36	1	1000	C
36	1	1001	G
36	1	1002	A
36	1	1006	A
36	1	1010	G
36	1	1017	C
36	1	1018	G
36	1	1020	G
36	1	1021	G
36	1	1024	G
36	1	1025	A
36	1	1029	G
36	1	1036	A
36	1	1037	C
36	1	1041	U
36	1	1047	A
36	1	1049	C
36	1	1052	U
36	1	1063	G
36	1	1064	A
36	1	1065	A
36	1	1071	U
36	1	1072	G
36	1	1079	A
36	1	1081	U
36	1	1082	U
36	1	1083	G
36	1	1087	G
36	1	1093	A
36	1	1094	U
36	1	1095	U
36	1	1096	U
36	1	1097	G
36	1	1098	A
36	1	1103	A
36	1	1104	G
36	1	1117	G

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Mol	Chain	Res	Type
36	1	1128	U
36	1	1131	G
36	1	1159	A
36	1	1160	C
36	1	1165	A
36	1	1179	A
36	1	1180	A
36	1	1181	U
36	1	1182	A
36	1	1191	U
36	1	1192	C
36	1	1197	A
36	1	1201	C
36	1	1205	A
36	1	1209	G
36	1	1216	C
36	1	1217	A
36	1	1218	U
36	1	1221	A
36	1	1222	G
36	1	1225	A
36	1	1227	C
36	1	1232	C
36	1	1233	G
36	1	1235	U
36	1	1236	G
36	1	1237	G
36	1	1241	U
36	1	1242	G
36	1	1243	G
36	1	1245	A
36	1	1246	G
36	1	1248	C
36	1	1249	G
36	1	1251	A
36	1	1258	U
36	1	1262	G
36	1	1263	A
36	1	1264	G
36	1	1266	G
36	1	1269	U
36	1	1270	A

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Mol	Chain	Res	Type
36	1	1271	A
36	1	1272	C
36	1	1274	A
36	1	1277	C
36	1	1278	A
36	1	1279	C
36	1	1285	G
36	1	1287	A
36	1	1307	G
36	1	1308	A
36	1	1309	U
36	1	1313	G
36	1	1324	U
36	1	1330	A
36	1	1331	U
36	1	1333	C
36	1	1345	G
36	1	1348	U
36	1	1349	G
36	1	1351	U
36	1	1352	A
36	1	1353	U
36	1	1355	A
36	1	1356	U
36	1	1357	G
36	1	1378	U
36	1	1386	A
36	1	1392	G
36	1	1399	A
36	1	1400	G
36	1	1405	U
36	1	1417	G
36	1	1419	A
36	1	1421	G
36	1	1425	U
36	1	1429	G
36	1	1434	G
36	1	1437	C
36	1	1446	A
36	1	1450	G
36	1	1455	U
36	1	1465	A

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Mol	Chain	Res	Type
36	1	1481	A
36	1	1482	A
36	1	1485	G
36	1	1503	A
36	1	1508	C
36	1	1515	A
36	1	1527	C
36	1	1529	A
36	1	1533	U
36	1	1556	C
36	1	1557	A
36	1	1560	G
36	1	1561	G
36	1	1562	C
36	1	1563	C
36	1	1564	U
36	1	1566	A
36	1	1567	U
36	1	1568	U
36	1	1569	U
36	1	1570	U
36	1	1576	G
36	1	1579	C
36	1	1580	A
36	1	1582	C
36	1	1583	A
36	1	1587	A
36	1	1589	A
36	1	1593	A
36	1	1605	A
36	1	1607	U
36	1	1620	U
36	1	1629	U
36	1	1639	C
36	1	1641	U
36	1	1643	A
36	1	1645	U
36	1	1657	C
36	1	1683	A
36	1	1705	U
36	1	1706	C
36	1	1716	U

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Mol	Chain	Res	Type
36	1	1717	U
36	1	1724	U
36	1	1735	G
36	1	1736	G
36	1	1741	A
36	1	1742	U
36	1	1750	A
36	1	1751	G
36	1	1761	C
36	1	1762	C
36	1	1763	U
36	1	1765	U
36	1	1766	G
36	1	1767	C
36	1	1770	G
36	1	1775	G
36	1	1780	G
36	1	1783	U
36	1	1797	A
36	1	1809	A
36	1	1810	A
36	1	1812	G
36	1	1814	A
36	1	1816	A
36	1	1817	G
36	1	1818	U
36	1	1819	U
36	1	1820	U
36	1	1821	U
36	1	1839	A
36	1	1841	A
36	1	1842	A
36	1	1845	G
36	1	1846	C
36	1	1849	C
36	1	1850	A
36	1	1866	C
36	1	1879	A
36	1	1886	A
36	1	1893	A
36	1	1895	A
36	1	1903	U

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Mol	Chain	Res	Type
36	1	1906	G
36	1	1927	G
36	1	1935	G
36	1	1951	C
36	1	1952	G
36	1	1953	G
36	1	1954	G
36	1	2094	C
36	1	2101	C
36	1	2102	U
36	1	2111	G
36	1	2112	U
36	1	2113	A
36	1	2114	C
36	1	2115	G
36	1	2116	G
36	1	2121	G
36	1	2122	G
36	1	2131	A
36	1	2134	G
36	1	2140	U
36	1	2144	A
36	1	2158	A
36	1	2168	A
36	1	2169	G
36	1	2188	A
36	1	2198	A
36	1	2205	U
36	1	2206	G
36	1	2208	A
36	1	2209	U
36	1	2210	G
36	1	2228	A
36	1	2244	A
36	1	2249	G
36	1	2250	G
36	1	2254	U
36	1	2255	A
36	1	2256	A
36	1	2262	A
36	1	2272	G
36	1	2273	G

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Mol	Chain	Res	Type
36	1	2279	A
36	1	2281	A
36	1	2282	U
36	1	2284	C
36	1	2307	G
36	1	2310	U
36	1	2313	A
36	1	2314	U
36	1	2315	G
36	1	2334	U
36	1	2336	U
36	1	2361	A
36	1	2367	A
36	1	2373	A
36	1	2374	C
36	1	2375	G
36	1	2385	G
36	1	2388	U
36	1	2393	G
36	1	2394	G
36	1	2397	A
36	1	2401	A
36	1	2402	A
36	1	2403	G
36	1	2406	C
36	1	2411	U
36	1	2418	G
36	1	2419	A
36	1	2437	G
36	1	2444	C
36	1	2445	A
36	1	2502	A
36	1	2503	G
36	1	2507	C
36	1	2514	U
36	1	2515	A
36	1	2522	G
36	1	2523	A
36	1	2532	U
36	1	2533	G
36	1	2534	G
36	1	2537	U

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Mol	Chain	Res	Type
36	1	2538	U
36	1	2539	C
36	1	2540	A
36	1	2541	U
36	1	2542	U
36	1	2543	U
36	1	2547	A
36	1	2548	C
36	1	2549	G
36	1	2551	U
36	1	2552	C
36	1	2554	A
36	1	2555	G
36	1	2560	C
36	1	2561	A
36	1	2567	C
36	1	2568	C
36	1	2569	A
36	1	2570	U
36	1	2571	U
36	1	2572	C
36	1	2573	G
36	1	2576	G
36	1	2582	C
36	1	2585	G
36	1	2589	G
36	1	2593	A
36	1	2594	C
36	1	2606	G
36	1	2607	G
36	1	2614	G
36	1	2637	A
36	1	2638	C
36	1	2652	U
36	1	2656	A
36	1	2672	G
36	1	2674	A
36	1	2677	G
36	1	2681	U
36	1	2689	A
36	1	2690	G
36	1	2691	A

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Mol	Chain	Res	Type
36	1	2694	A
36	1	2695	A
36	1	2696	A
36	1	2704	A
36	1	2714	G
36	1	2728	G
36	1	2729	U
36	1	2737	C
36	1	2744	U
36	1	2752	U
36	1	2753	G
36	1	2755	C
36	1	2772	C
36	1	2777	G
36	1	2778	G
36	1	2780	A
36	1	2796	G
36	1	2799	A
36	1	2800	G
36	1	2801	A
36	1	2803	A
36	1	2810	C
36	1	2816	G
36	1	2817	A
36	1	2818	U
36	1	2829	U
36	1	2834	G
36	1	2837	A
36	1	2842	U
36	1	2843	U
36	1	2845	A
36	1	2847	A
36	1	2849	C
36	1	2853	A
36	1	2856	G
36	1	2860	U
36	1	2867	C
36	1	2871	G
36	1	2872	A
36	1	2875	U
36	1	2887	A
36	1	2889	C

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Mol	Chain	Res	Type
36	1	2896	A
36	1	2898	G
36	1	2899	C
36	1	2923	U
36	1	2935	U
36	1	2936	A
36	1	2937	G
36	1	2938	G
36	1	2939	G
36	1	2942	C
36	1	2943	G
36	1	2946	A
36	1	2947	G
36	1	2954	U
36	1	2971	A
36	1	2974	U
36	1	2977	G
36	1	2983	C
36	1	2990	G
36	1	2992	U
36	1	2996	U
36	1	2997	G
36	1	3012	A
36	1	3034	C
36	1	3054	U
36	1	3059	G
36	1	3078	U
36	1	3079	U
36	1	3080	G
36	1	3086	A
36	1	3087	A
36	1	3092	C
36	1	3113	A
36	1	3119	U
36	1	3122	A
36	1	3130	A
36	1	3131	U
36	1	3134	A
36	1	3139	A
36	1	3142	A
36	1	3143	C
36	1	3151	U

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Mol	Chain	Res	Type
36	1	3153	U
36	1	3154	C
36	1	3155	U
36	1	3156	U
36	1	3157	U
36	1	3164	C
36	1	3165	A
36	1	3168	A
36	1	3169	U
36	1	3170	A
36	1	3171	U
36	1	3173	G
36	1	3174	A
36	1	3176	G
36	1	3179	U
36	1	3181	C
36	1	3187	A
36	1	3195	U
36	1	3196	U
36	1	3197	G
36	1	3198	U
36	1	3207	U
36	1	3210	A
36	1	3217	C
36	1	3218	A
36	1	3219	G
36	1	3220	G
36	1	3228	C
36	1	3229	G
36	1	3235	C
36	1	3243	A
36	1	3245	A
36	1	3246	G
36	1	3247	G
36	1	3253	G
36	1	3259	U
36	1	3263	G
36	1	3269	U
36	1	3270	U
36	1	3272	C
36	1	3276	G
36	1	3279	A

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Mol	Chain	Res	Type
36	1	3281	U
36	1	3286	G
36	1	3287	U
36	1	3288	G
36	1	3289	G
36	1	3293	U
36	1	3294	A
36	1	3295	A
36	1	3304	U
36	1	3307	A
36	1	3313	U
36	1	3316	A
36	1	3317	U
36	1	3318	G
36	1	3319	U
36	1	3320	A
36	1	3341	U
36	1	3342	A
36	1	3344	A
36	1	3345	G
36	1	3349	C
36	1	3351	U
36	1	3352	U
36	1	3353	G
36	1	3354	U
36	1	3355	U
36	1	3356	G
36	1	3360	C
36	1	3369	G
36	1	3375	A
36	1	3376	A
36	1	3378	C
36	1	3382	U
36	1	3383	G
36	1	3389	U
36	1	3396	U
37	3	7	G
37	3	13	A
37	3	22	A
37	3	41	G
37	3	51	A
37	3	53	U

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Mol	Chain	Res	Type
37	3	54	U
37	3	65	G
37	3	74	C
37	3	76	A
37	3	91	G
37	3	101	G
37	3	102	A
37	3	112	G
37	3	121	U
38	4	2	A
38	4	21	C
38	4	26	U
38	4	34	U
38	4	35	C
38	4	48	A
38	4	57	C
38	4	58	G
38	4	59	A
38	4	60	U
38	4	62	C
38	4	63	G
38	4	75	G
38	4	79	A
38	4	80	A
38	4	81	U
38	4	82	U
38	4	83	C
38	4	84	C
38	4	86	U
38	4	87	G
38	4	90	U
38	4	95	G
38	4	104	A
38	4	105	A
38	4	106	C
38	4	111	A
38	4	113	U
38	4	125	U
38	4	126	A
38	4	138	A
38	4	152	G
38	4	155	A

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Mol	Chain	Res	Type
38	4	157	U
38	4	158	U
1	6	2	A
1	6	4	C
1	6	17	C
1	6	25	C
1	6	26	A
1	6	27	U
1	6	34	G
1	6	47	A
1	6	57	G
1	6	60	U
1	6	61	A
1	6	66	U
1	6	67	A
1	6	68	A
1	6	69	G
1	6	72	A
1	6	73	U
1	6	75	U
1	6	76	A
1	6	77	U
1	6	85	A
1	6	100	A
1	6	104	A
1	6	113	U
1	6	114	C
1	6	132	U
1	6	137	U
1	6	138	A
1	6	140	A
1	6	141	U
1	6	144	U
1	6	145	A
1	6	146	U
1	6	153	G
1	6	158	U
1	6	159	U
1	6	166	C
1	6	177	U
1	6	178	U
1	6	181	A

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Mol	Chain	Res	Type
1	6	185	U
1	6	188	A
1	6	190	C
1	6	191	C
1	6	192	U
1	6	193	U
1	6	195	G
1	6	198	A
1	6	199	G
1	6	200	A
1	6	215	A
1	6	216	U
1	6	217	A
1	6	218	A
1	6	219	A
1	6	220	A
1	6	222	A
1	6	226	A
1	6	227	U
1	6	228	G
1	6	230	C
1	6	232	U
1	6	233	C
1	6	235	G
1	6	240	U
1	6	241	U
1	6	249	U
1	6	250	C
1	6	260	U
1	6	261	U
1	6	265	A
1	6	271	A
1	6	272	U
1	6	273	G
1	6	274	G
1	6	276	C
1	6	277	U
1	6	278	U
1	6	280	U
1	6	287	G
1	6	299	A
1	6	301	A

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Mol	Chain	Res	Type
1	6	308	C
1	6	309	C
1	6	314	C
1	6	316	A
1	6	319	U
1	6	320	U
1	6	321	C
1	6	322	G
1	6	333	A
1	6	337	G
1	6	338	C
1	6	341	A
1	6	343	C
1	6	352	A
1	6	359	A
1	6	360	A
1	6	361	C
1	6	381	C
1	6	400	A
1	6	401	A
1	6	402	C
1	6	404	G
1	6	416	A
1	6	417	A
1	6	418	G
1	6	419	G
1	6	421	A
1	6	424	C
1	6	425	A
1	6	426	G
1	6	434	G
1	6	439	U
1	6	444	C
1	6	448	C
1	6	468	A
1	6	470	A
1	6	475	A
1	6	484	C
1	6	485	A
1	6	486	G
1	6	487	G
1	6	488	G

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Mol	Chain	Res	Type
1	6	489	C
1	6	490	C
1	6	492	A
1	6	493	U
1	6	494	U
1	6	495	C
1	6	496	G
1	6	497	G
1	6	500	C
1	6	501	U
1	6	504	U
1	6	505	A
1	6	506	A
1	6	508	U
1	6	510	G
1	6	511	A
1	6	512	A
1	6	513	U
1	6	515	A
1	6	517	U
1	6	527	A
1	6	534	A
1	6	536	C
1	6	538	A
1	6	539	G
1	6	540	G
1	6	541	A
1	6	542	A
1	6	543	C
1	6	544	A
1	6	551	G
1	6	557	G
1	6	558	U
1	6	559	C
1	6	564	G
1	6	565	C
1	6	566	C
1	6	570	A
1	6	574	G
1	6	578	U
1	6	579	A
1	6	580	A

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Mol	Chain	Res	Type
1	6	582	U
1	6	594	A
1	6	595	G
1	6	601	A
1	6	606	A
1	6	609	U
1	6	610	G
1	6	611	U
1	6	617	U
1	6	619	A
1	6	620	A
1	6	622	A
1	6	623	A
1	6	624	G
1	6	637	C
1	6	639	U
1	6	640	U
1	6	648	G
1	6	650	U
1	6	652	G
1	6	653	C
1	6	658	C
1	6	661	A
1	6	662	U
1	6	665	U
1	6	667	U
1	6	668	C
1	6	669	G
1	6	670	U
1	6	676	G
1	6	678	A
1	6	679	U
1	6	680	U
1	6	681	U
1	6	682	C
1	6	683	C
1	6	684	A
1	6	685	A
1	6	691	C
1	6	695	U
1	6	696	C
1	6	697	C

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Mol	Chain	Res	Type
1	6	698	U
1	6	710	U
1	6	711	U
1	6	714	G
1	6	718	U
1	6	719	U
1	6	720	G
1	6	721	U
1	6	722	G
1	6	723	G
1	6	730	G
1	6	742	U
1	6	743	U
1	6	751	G
1	6	753	A
1	6	754	A
1	6	755	A
1	6	756	A
1	6	764	U
1	6	765	G
1	6	767	U
1	6	773	C
1	6	774	A
1	6	775	G
1	6	780	A
1	6	781	U
1	6	782	U
1	6	783	G
1	6	787	G
1	6	789	A
1	6	793	A
1	6	794	U
1	6	811	A
1	6	812	A
1	6	815	G
1	6	816	G
1	6	821	U
1	6	823	G
1	6	825	U
1	6	826	U
1	6	828	U
1	6	829	A

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Mol	Chain	Res	Type
1	6	830	U
1	6	831	U
1	6	832	U
1	6	834	G
1	6	835	U
1	6	856	A
1	6	861	U
1	6	863	A
1	6	864	U
1	6	873	U
1	6	886	U
1	6	898	A
1	6	911	U
1	6	912	U
1	6	913	G
1	6	914	G
1	6	916	U
1	6	933	A
1	6	935	U
1	6	942	G
1	6	944	A
1	6	959	U
1	6	960	U
1	6	966	A
1	6	969	C
1	6	970	A
1	6	971	A
1	6	983	A
1	6	992	A
1	6	993	A
1	6	997	G
1	6	1003	A
1	6	1004	U
1	6	1005	A
1	6	1021	C
1	6	1026	A
1	6	1028	C
1	6	1039	A
1	6	1040	G
1	6	1052	U
1	6	1053	G
1	6	1057	U

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Mol	Chain	Res	Type
1	6	1058	U
1	6	1059	U
1	6	1060	U
1	6	1061	A
1	6	1063	U
1	6	1072	C
1	6	1081	A
1	6	1082	C
1	6	1092	A
1	6	1096	C
1	6	1097	U
1	6	1098	U
1	6	1100	G
1	6	1101	G
1	6	1109	G
1	6	1137	A
1	6	1138	A
1	6	1139	A
1	6	1151	A
1	6	1155	G
1	6	1158	C
1	6	1159	C
1	6	1160	A
1	6	1162	C
1	6	1164	G
1	6	1167	G
1	6	1183	A
1	6	1185	U
1	6	1194	A
1	6	1196	A
1	6	1199	G
1	6	1200	G
1	6	1202	A
1	6	1217	A
1	6	1218	G
1	6	1220	C
1	6	1221	A
1	6	1225	U
1	6	1226	A
1	6	1228	G
1	6	1229	G
1	6	1230	A

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Mol	Chain	Res	Type
1	6	1231	U
1	6	1239	U
1	6	1240	U
1	6	1242	A
1	6	1243	G
1	6	1244	A
1	6	1245	G
1	6	1246	C
1	6	1255	G
1	6	1256	A
1	6	1257	U
1	6	1258	U
1	6	1259	U
1	6	1262	U
1	6	1275	A
1	6	1286	U
1	6	1288	G
1	6	1314	U
1	6	1315	U
1	6	1316	G
1	6	1319	A
1	6	1321	A
1	6	1335	U
1	6	1337	A
1	6	1338	C
1	6	1341	A
1	6	1343	U
1	6	1344	A
1	6	1345	A
1	6	1346	A
1	6	1354	G
1	6	1361	U
1	6	1363	U
1	6	1364	G
1	6	1367	G
1	6	1371	A
1	6	1372	U
1	6	1383	G
1	6	1388	A
1	6	1390	U
1	6	1398	U
1	6	1399	C

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Mol	Chain	Res	Type
1	6	1400	A
1	6	1402	G
1	6	1413	U
1	6	1415	U
1	6	1425	A
1	6	1427	A
1	6	1428	G
1	6	1433	G
1	6	1445	G
1	6	1446	A
1	6	1448	G
1	6	1458	G
1	6	1459	C
1	6	1461	C
1	6	1471	A
1	6	1482	C
1	6	1486	G
1	6	1489	U
1	6	1490	C
1	6	1491	U
1	6	1492	A
1	6	1493	A
1	6	1494	C
1	6	1496	U
1	6	1506	G
1	6	1514	U
1	6	1515	A
1	6	1516	A
1	6	1523	G
1	6	1524	A
1	6	1531	G
1	6	1535	U
1	6	1536	G
1	6	1537	C
1	6	1538	U
1	6	1540	G
1	6	1554	U
1	6	1557	U
1	6	1559	A
1	6	1569	A
1	6	1573	A
1	6	1574	G

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Mol	Chain	Res	Type
1	6	1584	G
1	6	1590	G
1	6	1601	G
1	6	1603	U
1	6	1616	G
1	6	1620	C
1	6	1621	U
1	6	1634	C
1	6	1635	A
1	6	1637	C
1	6	1638	G
1	6	1656	U
1	6	1657	U
1	6	1658	G
1	6	1680	G
1	6	1683	C
1	6	1696	G
1	6	1697	G
1	6	1698	G
1	6	1699	G
1	6	1700	C
1	6	1701	A
1	6	1702	A
1	6	1710	U
1	6	1712	A
1	6	1715	G
1	6	1716	C
1	6	1717	G
1	6	1727	G
1	6	1731	A
1	6	1736	G
1	6	1755	A
1	6	1760	G
1	6	1762	A
1	6	1766	A
1	6	1767	G
1	6	1769	U
1	6	1770	U
1	6	1780	G
1	6	1782	A
1	6	1783	C
1	6	1789	G

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Mol	Chain	Res	Type
1	6	1792	G
1	6	1793	G
1	6	1794	A
1	6	1796	C
1	6	1799	U
1	6	1800	A
36	5	15	C
36	5	16	A
36	5	21	G
36	5	24	G
36	5	26	A
36	5	40	A
36	5	44	U
36	5	45	A
36	5	49	A
36	5	57	A
36	5	59	G
36	5	60	A
36	5	65	A
36	5	66	A
36	5	73	C
36	5	76	G
36	5	83	U
36	5	93	C
36	5	96	G
36	5	99	A
36	5	109	A
36	5	110	G
36	5	111	C
36	5	113	C
36	5	116	A
36	5	120	G
36	5	121	A
36	5	122	A
36	5	133	U
36	5	134	U
36	5	135	C
36	5	136	G
36	5	150	A
36	5	152	U
36	5	156	G
36	5	157	A

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Mol	Chain	Res	Type
36	5	165	A
36	5	166	C
36	5	170	G
36	5	171	G
36	5	172	G
36	5	173	G
36	5	174	C
36	5	178	U
36	5	182	U
36	5	183	G
36	5	184	U
36	5	187	A
36	5	190	U
36	5	191	U
36	5	200	C
36	5	210	U
36	5	218	G
36	5	219	A
36	5	220	G
36	5	221	A
36	5	227	G
36	5	239	G
36	5	240	U
36	5	243	G
36	5	244	G
36	5	246	U
36	5	248	U
36	5	249	U
36	5	250	U
36	5	251	G
36	5	252	U
36	5	253	A
36	5	254	A
36	5	259	C
36	5	269	G
36	5	270	U
36	5	284	A
36	5	286	U
36	5	295	A
36	5	298	U
36	5	310	U
36	5	315	C

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Mol	Chain	Res	Type
36	5	316	U
36	5	323	A
36	5	329	U
36	5	339	C
36	5	349	A
36	5	350	C
36	5	351	A
36	5	370	U
36	5	375	A
36	5	376	G
36	5	398	A
36	5	399	A
36	5	401	U
36	5	402	A
36	5	403	C
36	5	404	G
36	5	421	G
36	5	422	A
36	5	436	A
36	5	437	G
36	5	438	A
36	5	439	C
36	5	440	A
36	5	441	U
36	5	442	G
36	5	492	U
36	5	521	A
36	5	532	A
36	5	535	G
36	5	542	G
36	5	546	C
36	5	547	G
36	5	548	G
36	5	555	U
36	5	557	A
36	5	559	A
36	5	578	A
36	5	579	G
36	5	592	A
36	5	594	U
36	5	595	G
36	5	600	G

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Mol	Chain	Res	Type
36	5	604	G
36	5	608	A
36	5	609	G
36	5	611	A
36	5	612	U
36	5	619	A
36	5	620	U
36	5	621	A
36	5	636	C
36	5	640	U
36	5	647	A
36	5	649	A
36	5	651	G
36	5	653	A
36	5	660	A
36	5	661	G
36	5	675	C
36	5	677	A
36	5	680	G
36	5	681	U
36	5	683	U
36	5	691	A
36	5	705	A
36	5	708	G
36	5	712	G
36	5	715	A
36	5	716	A
36	5	725	G
36	5	727	G
36	5	758	C
36	5	766	U
36	5	767	U
36	5	776	U
36	5	777	U
36	5	778	U
36	5	780	A
36	5	781	G
36	5	785	G
36	5	786	A
36	5	806	A
36	5	817	A
36	5	830	A

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Mol	Chain	Res	Type
36	5	851	C
36	5	861	C
36	5	874	U
36	5	879	U
36	5	885	U
36	5	896	A
36	5	907	G
36	5	908	G
36	5	909	G
36	5	914	A
36	5	916	G
36	5	917	A
36	5	921	A
36	5	924	G
36	5	937	G
36	5	944	C
36	5	953	G
36	5	959	C
36	5	960	U
36	5	961	C
36	5	963	G
36	5	973	A
36	5	979	U
36	5	983	A
36	5	994	G
36	5	1000	C
36	5	1001	G
36	5	1002	A
36	5	1006	A
36	5	1010	G
36	5	1015	U
36	5	1016	C
36	5	1017	C
36	5	1018	G
36	5	1019	G
36	5	1021	G
36	5	1024	G
36	5	1025	A
36	5	1026	A
36	5	1027	A
36	5	1028	U
36	5	1029	G

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Mol	Chain	Res	Type
36	5	1032	C
36	5	1033	U
36	5	1035	G
36	5	1047	A
36	5	1049	C
36	5	1064	A
36	5	1065	A
36	5	1072	G
36	5	1081	U
36	5	1082	U
36	5	1085	A
36	5	1093	A
36	5	1094	U
36	5	1095	U
36	5	1096	U
36	5	1097	G
36	5	1098	A
36	5	1103	A
36	5	1104	G
36	5	1117	G
36	5	1131	G
36	5	1152	G
36	5	1153	A
36	5	1159	A
36	5	1174	G
36	5	1180	A
36	5	1181	U
36	5	1182	A
36	5	1190	A
36	5	1191	U
36	5	1192	C
36	5	1193	A
36	5	1196	C
36	5	1197	A
36	5	1201	C
36	5	1202	A
36	5	1209	G
36	5	1222	G
36	5	1232	C
36	5	1236	G
36	5	1237	G
36	5	1239	C

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Mol	Chain	Res	Type
36	5	1241	U
36	5	1242	G
36	5	1243	G
36	5	1245	A
36	5	1246	G
36	5	1252	A
36	5	1258	U
36	5	1259	A
36	5	1262	G
36	5	1263	A
36	5	1264	G
36	5	1265	U
36	5	1266	G
36	5	1285	G
36	5	1307	G
36	5	1308	A
36	5	1309	U
36	5	1329	U
36	5	1330	A
36	5	1331	U
36	5	1349	G
36	5	1351	U
36	5	1352	A
36	5	1353	U
36	5	1355	A
36	5	1356	U
36	5	1357	G
36	5	1385	C
36	5	1386	A
36	5	1387	G
36	5	1391	C
36	5	1392	G
36	5	1398	U
36	5	1399	A
36	5	1400	G
36	5	1418	A
36	5	1419	A
36	5	1420	C
36	5	1421	G
36	5	1429	G
36	5	1431	G
36	5	1433	A

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Mol	Chain	Res	Type
36	5	1434	G
36	5	1437	C
36	5	1446	A
36	5	1450	G
36	5	1455	U
36	5	1465	A
36	5	1481	A
36	5	1482	A
36	5	1490	A
36	5	1503	A
36	5	1508	C
36	5	1514	G
36	5	1533	U
36	5	1536	G
36	5	1553	U
36	5	1554	U
36	5	1555	U
36	5	1556	C
36	5	1558	A
36	5	1560	G
36	5	1561	G
36	5	1562	C
36	5	1563	C
36	5	1565	G
36	5	1566	A
36	5	1567	U
36	5	1568	U
36	5	1569	U
36	5	1570	U
36	5	1571	A
36	5	1572	U
36	5	1574	C
36	5	1575	A
36	5	1576	G
36	5	1577	G
36	5	1578	C
36	5	1579	C
36	5	1581	C
36	5	1583	A
36	5	1587	A
36	5	1589	A
36	5	1605	A

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Mol	Chain	Res	Type
36	5	1620	U
36	5	1629	U
36	5	1639	C
36	5	1643	A
36	5	1644	C
36	5	1645	U
36	5	1655	G
36	5	1657	C
36	5	1658	G
36	5	1683	A
36	5	1716	U
36	5	1717	U
36	5	1718	G
36	5	1724	U
36	5	1725	C
36	5	1736	G
36	5	1750	A
36	5	1751	G
36	5	1756	C
36	5	1762	C
36	5	1764	U
36	5	1765	U
36	5	1766	G
36	5	1770	G
36	5	1775	G
36	5	1778	G
36	5	1780	G
36	5	1793	C
36	5	1797	A
36	5	1808	G
36	5	1810	A
36	5	1812	G
36	5	1814	A
36	5	1815	U
36	5	1816	A
36	5	1817	G
36	5	1818	U
36	5	1820	U
36	5	1821	U
36	5	1839	A
36	5	1841	A
36	5	1842	A

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Mol	Chain	Res	Type
36	5	1846	C
36	5	1849	C
36	5	1850	A
36	5	1878	G
36	5	1879	A
36	5	1880	U
36	5	1893	A
36	5	1906	G
36	5	1907	C
36	5	1909	A
36	5	1952	G
36	5	1953	G
36	5	2100	A
36	5	2101	C
36	5	2102	U
36	5	2112	U
36	5	2113	A
36	5	2121	G
36	5	2122	G
36	5	2131	A
36	5	2134	G
36	5	2140	U
36	5	2144	A
36	5	2158	A
36	5	2169	G
36	5	2170	U
36	5	2187	G
36	5	2188	A
36	5	2192	C
36	5	2201	G
36	5	2205	U
36	5	2206	G
36	5	2208	A
36	5	2210	G
36	5	2228	A
36	5	2244	A
36	5	2245	C
36	5	2252	A
36	5	2253	G
36	5	2255	A
36	5	2256	A
36	5	2257	C

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Mol	Chain	Res	Type
36	5	2258	U
36	5	2264	U
36	5	2270	A
36	5	2273	G
36	5	2279	A
36	5	2281	A
36	5	2282	U
36	5	2288	G
36	5	2303	A
36	5	2307	G
36	5	2310	U
36	5	2313	A
36	5	2315	G
36	5	2330	C
36	5	2331	C
36	5	2334	U
36	5	2336	U
36	5	2372	A
36	5	2373	A
36	5	2374	C
36	5	2375	G
36	5	2385	G
36	5	2393	G
36	5	2397	A
36	5	2400	G
36	5	2401	A
36	5	2402	A
36	5	2403	G
36	5	2404	A
36	5	2405	C
36	5	2411	U
36	5	2418	G
36	5	2419	A
36	5	2435	G
36	5	2438	A
36	5	2439	A
36	5	2440	G
36	5	2441	A
36	5	2443	A
36	5	2504	U
36	5	2505	U
36	5	2506	U

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Mol	Chain	Res	Type
36	5	2507	C
36	5	2508	U
36	5	2510	U
36	5	2511	A
36	5	2512	C
36	5	2514	U
36	5	2515	A
36	5	2522	G
36	5	2523	A
36	5	2524	A
36	5	2526	C
36	5	2530	G
36	5	2531	C
36	5	2532	U
36	5	2537	U
36	5	2538	U
36	5	2539	C
36	5	2540	A
36	5	2543	U
36	5	2549	G
36	5	2552	C
36	5	2555	G
36	5	2562	A
36	5	2566	C
36	5	2567	C
36	5	2568	C
36	5	2569	A
36	5	2570	U
36	5	2571	U
36	5	2572	C
36	5	2573	G
36	5	2574	G
36	5	2584	G
36	5	2585	G
36	5	2589	G
36	5	2591	A
36	5	2593	A
36	5	2594	C
36	5	2606	G
36	5	2607	G
36	5	2614	G
36	5	2639	G

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Mol	Chain	Res	Type
36	5	2652	U
36	5	2656	A
36	5	2667	A
36	5	2674	A
36	5	2677	G
36	5	2681	U
36	5	2689	A
36	5	2690	G
36	5	2691	A
36	5	2694	A
36	5	2696	A
36	5	2705	A
36	5	2714	G
36	5	2716	U
36	5	2719	U
36	5	2720	G
36	5	2727	A
36	5	2728	G
36	5	2729	U
36	5	2746	A
36	5	2752	U
36	5	2753	G
36	5	2762	A
36	5	2771	U
36	5	2772	C
36	5	2773	C
36	5	2778	G
36	5	2779	A
36	5	2782	U
36	5	2796	G
36	5	2799	A
36	5	2800	G
36	5	2801	A
36	5	2810	C
36	5	2813	A
36	5	2814	G
36	5	2816	G
36	5	2817	A
36	5	2818	U
36	5	2829	U
36	5	2843	U
36	5	2845	A

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Mol	Chain	Res	Type
36	5	2849	C
36	5	2852	C
36	5	2853	A
36	5	2861	U
36	5	2871	G
36	5	2872	A
36	5	2875	U
36	5	2887	A
36	5	2889	C
36	5	2896	A
36	5	2899	C
36	5	2904	U
36	5	2922	G
36	5	2923	U
36	5	2928	C
36	5	2935	U
36	5	2936	A
36	5	2942	C
36	5	2947	G
36	5	2954	U
36	5	2957	G
36	5	2971	A
36	5	2972	G
36	5	2979	U
36	5	2983	C
36	5	2990	G
36	5	2992	U
36	5	2993	G
36	5	2996	U
36	5	2997	G
36	5	3003	G
36	5	3012	A
36	5	3028	G
36	5	3049	A
36	5	3056	U
36	5	3057	U
36	5	3059	G
36	5	3078	U
36	5	3079	U
36	5	3086	A
36	5	3092	C
36	5	3104	U

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Mol	Chain	Res	Type
36	5	3122	A
36	5	3123	A
36	5	3130	A
36	5	3131	U
36	5	3142	A
36	5	3143	C
36	5	3150	A
36	5	3153	U
36	5	3155	U
36	5	3156	U
36	5	3157	U
36	5	3158	G
36	5	3159	C
36	5	3164	C
36	5	3165	A
36	5	3167	A
36	5	3168	A
36	5	3171	U
36	5	3172	A
36	5	3173	G
36	5	3174	A
36	5	3175	U
36	5	3176	G
36	5	3178	A
36	5	3179	U
36	5	3180	A
36	5	3181	C
36	5	3187	A
36	5	3195	U
36	5	3196	U
36	5	3199	G
36	5	3207	U
36	5	3217	C
36	5	3218	A
36	5	3219	G
36	5	3223	A
36	5	3227	A
36	5	3228	C
36	5	3229	G
36	5	3238	G
36	5	3239	G
36	5	3242	G

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Mol	Chain	Res	Type
36	5	3243	A
36	5	3245	A
36	5	3246	G
36	5	3247	G
36	5	3259	U
36	5	3265	C
36	5	3269	U
36	5	3270	U
36	5	3273	A
36	5	3274	A
36	5	3275	U
36	5	3276	G
36	5	3277	U
36	5	3278	C
36	5	3279	A
36	5	3280	U
36	5	3281	U
36	5	3282	U
36	5	3284	G
36	5	3285	C
36	5	3286	G
36	5	3288	G
36	5	3289	G
36	5	3290	G
36	5	3294	A
36	5	3295	A
36	5	3304	U
36	5	3313	U
36	5	3316	A
36	5	3317	U
36	5	3318	G
36	5	3319	U
36	5	3330	A
36	5	3335	A
36	5	3336	A
36	5	3341	U
36	5	3342	A
36	5	3345	G
36	5	3350	C
36	5	3351	U
36	5	3352	U
36	5	3354	U

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Mol	Chain	Res	Type
36	5	3356	G
36	5	3358	U
36	5	3369	G
36	5	3378	C
36	5	3382	U
36	5	3383	G
36	5	3389	U
36	5	3390	G
36	5	3393	U
36	5	3394	U
36	5	3396	U
37	7	10	C
37	7	22	A
37	7	33	U
37	7	38	U
37	7	41	G
37	7	45	A
37	7	51	A
37	7	52	G
37	7	54	U
37	7	60	G
37	7	65	G
37	7	73	C
37	7	76	A
37	7	93	C
37	7	101	G
37	7	102	A
37	7	103	A
37	7	104	A
37	7	112	G
38	8	21	C
38	8	34	U
38	8	35	C
38	8	48	A
38	8	52	A
38	8	54	A
38	8	59	A
38	8	62	C
38	8	63	G
38	8	79	A
38	8	80	A
38	8	81	U

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Mol	Chain	Res	Type
38	8	82	U
38	8	83	C
38	8	84	C
38	8	86	U
38	8	87	G
38	8	95	G
38	8	96	A
38	8	97	A
38	8	104	A
38	8	105	A
38	8	106	C
38	8	111	A
38	8	113	U
38	8	125	U
38	8	126	A
38	8	127	U
38	8	138	A
38	8	149	A
38	8	152	G
38	8	156	U
38	8	157	U
38	8	158	U

All (260) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	2	25	C
1	2	45	U
1	2	68	A
1	2	73	U
1	2	74	U
1	2	103	A
1	2	114	C
1	2	130	C
1	2	131	C
1	2	132	U
1	2	136	C
1	2	139	C
1	2	144	U
1	2	158	U
1	2	187	G
1	2	217	A

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Mol	Chain	Res	Type
1	2	218	A
1	2	232	U
1	2	240	U
1	2	278	U
1	2	280	U
1	2	319	U
1	2	417	A
1	2	497	G
1	2	499	U
1	2	501	U
1	2	503	G
1	2	512	A
1	2	555	A
1	2	582	U
1	2	622	A
1	2	685	A
1	2	704	C
1	2	720	G
1	2	721	U
1	2	755	A
1	2	782	U
1	2	794	U
1	2	811	A
1	2	829	A
1	2	913	G
1	2	1058	U
1	2	1081	A
1	2	1157	A
1	2	1226	A
1	2	1244	A
1	2	1250	U
1	2	1344	A
1	2	1370	U
1	2	1457	C
1	2	1481	C
1	2	1489	U
1	2	1568	C
1	2	1573	A
1	2	1615	C
1	2	1657	U
1	2	1696	G
1	2	1698	G

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Mol	Chain	Res	Type
1	2	1711	C
1	2	1761	U
36	1	13	A
36	1	65	A
36	1	93	C
36	1	169	U
36	1	210	U
36	1	239	G
36	1	282	G
36	1	397	A
36	1	547	G
36	1	588	G
36	1	594	U
36	1	637	C
36	1	715	A
36	1	763	G
36	1	873	C
36	1	916	G
36	1	979	U
36	1	981	U
36	1	993	G
36	1	1064	A
36	1	1094	U
36	1	1097	G
36	1	1103	A
36	1	1196	C
36	1	1273	A
36	1	1307	G
36	1	1317	A
36	1	1329	U
36	1	1331	U
36	1	1352	A
36	1	1355	A
36	1	1484	U
36	1	1507	G
36	1	1556	C
36	1	1562	C
36	1	1582	C
36	1	1589	A
36	1	1716	U
36	1	1815	U
36	1	1816	A

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Mol	Chain	Res	Type
36	1	1820	U
36	1	1842	A
36	1	2101	C
36	1	2112	U
36	1	2209	U
36	1	2227	C
36	1	2249	G
36	1	2360	C
36	1	2418	G
36	1	2513	U
36	1	2522	G
36	1	2537	U
36	1	2538	U
36	1	2541	U
36	1	2554	A
36	1	2585	G
36	1	2593	A
36	1	2817	A
36	1	2818	U
36	1	3078	U
36	1	3121	U
36	1	3139	A
36	1	3169	U
36	1	3195	U
36	1	3207	U
36	1	3218	A
36	1	3228	C
36	1	3269	U
36	1	3275	U
36	1	3276	G
36	1	3316	A
36	1	3319	U
36	1	3350	C
36	1	3351	U
36	1	3353	G
36	1	3375	A
38	4	85	G
38	4	125	U
1	6	25	C
1	6	66	U
1	6	76	A
1	6	103	A

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Mol	Chain	Res	Type
1	6	114	C
1	6	136	C
1	6	139	C
1	6	145	A
1	6	158	U
1	6	187	G
1	6	192	U
1	6	217	A
1	6	240	U
1	6	272	U
1	6	277	U
1	6	417	A
1	6	512	A
1	6	542	A
1	6	543	C
1	6	557	G
1	6	558	U
1	6	622	A
1	6	647	G
1	6	651	G
1	6	667	U
1	6	697	C
1	6	717	C
1	6	755	A
1	6	829	A
1	6	834	G
1	6	1051	G
1	6	1058	U
1	6	1081	A
1	6	1097	U
1	6	1098	U
1	6	1227	A
1	6	1244	A
1	6	1255	G
1	6	1344	A
1	6	1481	C
1	6	1489	U
1	6	1491	U
1	6	1535	U
1	6	1568	C
1	6	1572	G
1	6	1573	A

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Mol	Chain	Res	Type
1	6	1615	C
1	6	1620	C
1	6	1657	U
1	6	1696	G
1	6	1698	G
1	6	1700	C
36	5	151	A
36	5	183	G
36	5	238	A
36	5	374	A
36	5	438	A
36	5	588	G
36	5	765	C
36	5	873	C
36	5	916	G
36	5	960	U
36	5	993	G
36	5	1027	A
36	5	1064	A
36	5	1081	U
36	5	1152	G
36	5	1181	U
36	5	1238	C
36	5	1241	U
36	5	1284	C
36	5	1307	G
36	5	1329	U
36	5	1331	U
36	5	1352	A
36	5	1355	A
36	5	1481	A
36	5	1554	U
36	5	1560	G
36	5	1574	C
36	5	1580	A
36	5	1589	A
36	5	1716	U
36	5	1815	U
36	5	1816	A
36	5	1846	C
36	5	1879	A
36	5	2101	C

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Mol	Chain	Res	Type
36	5	2112	U
36	5	2204	C
36	5	2209	U
36	5	2257	C
36	5	2372	A
36	5	2373	A
36	5	2374	C
36	5	2440	G
36	5	2507	C
36	5	2513	U
36	5	2531	C
36	5	2728	G
36	5	2772	C
36	5	2818	U
36	5	2887	A
36	5	2896	A
36	5	2971	A
36	5	3078	U
36	5	3121	U
36	5	3154	C
36	5	3155	U
36	5	3195	U
36	5	3218	A
36	5	3228	C
36	5	3269	U
36	5	3275	U
36	5	3289	G
36	5	3317	U
36	5	3340	G
36	5	3341	U
36	5	3357	U
38	8	111	A
38	8	126	A
38	8	156	U

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

There are no non-standard protein/DNA/RNA residues in this entry.



## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 2029 ligands modelled in this entry, 1035 are monoatomic - leaving 994 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	$\# Z  > 2$
86	OHX	5	3589	-	0,6,6	-	-	-		
86	OHX	1	3487	-	0,6,6	-	-	-		
86	OHX	5	3492	-	0,6,6	-	-	-		
86	OHX	5	3721	-	0,6,6	-	-	-		
86	OHX	2	1981	-	0,6,6	-	-	-		
86	OHX	2	2004	-	0,6,6	-	-	-		
86	OHX	1	3535	-	0,6,6	-	-	-		
86	OHX	8	214	-	0,6,6	-	-	-		
86	OHX	1	3484	-	0,6,6	-	-	-		
86	OHX	1	3504	-	0,6,6	-	-	-		
86	OHX	1	3670	-	0,6,6	-	-	-		
86	OHX	5	3504	36	0,6,6	-	-	-		
86	OHX	4	205	-	0,6,6	-	-	-		
86	OHX	6	1992	-	0,6,6	-	-	-		
86	OHX	2	2026	-	0,6,6	-	-	-		
86	OHX	5	3555	-	0,6,6	-	-	-		
86	OHX	5	3602	-	0,6,6	-	-	-		
86	OHX	C5	201	-	0,6,6	-	-	-		
86	OHX	5	3498	-	0,6,6	-	-	-		
86	OHX	6	1948	-	0,6,6	-	-	-		
86	OHX	1	3436	-	0,6,6	-	-	-		
86	OHX	5	3587	-	0,6,6	-	-	-		
86	OHX	5	3706	-	0,6,6	-	-	-		
86	OHX	1	3420	-	0,6,6	-	-	-		
86	OHX	1	3463	-	0,6,6	-	-	-		
86	OHX	6	1917	-	0,6,6	-	-	-		
86	OHX	5	3717	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
86	OHX	m0	302	-	0,6,6	-	-	-		
86	OHX	1	3404	-	0,6,6	-	-	-		
86	OHX	1	3685	-	0,6,6	-	-	-		
86	OHX	5	3408	-	0,6,6	-	-	-		
86	OHX	2	1941	-	0,6,6	-	-	-		
86	OHX	2	1949	-	0,6,6	-	-	-		
86	OHX	1	3454	-	0,6,6	-	-	-		
86	OHX	5	3650	-	0,6,6	-	-	-		
86	OHX	3	204	-	0,6,6	-	-	-		
86	OHX	5	3515	-	0,6,6	-	-	-		
86	OHX	5	3654	-	0,6,6	-	-	-		
86	OHX	1	3597	-	0,6,6	-	-	-		
86	OHX	5	3418	-	0,6,6	-	-	-		
86	OHX	1	3427	-	0,6,6	-	-	-		
86	OHX	5	3712	-	0,6,6	-	-	-		
86	OHX	1	3534	-	0,6,6	-	-	-		
86	OHX	2	1999	-	0,6,6	-	-	-		
86	OHX	2	1964	-	0,6,6	-	-	-		
86	OHX	1	3702	-	0,6,6	-	-	-		
86	OHX	5	3628	-	0,6,6	-	-	-		
86	OHX	2	2018	-	0,6,6	-	-	-		
86	OHX	6	1970	-	0,6,6	-	-	-		
86	OHX	1	3707	-	0,6,6	-	-	-		
86	OHX	5	3609	-	0,6,6	-	-	-		
86	OHX	1	3653	-	0,6,6	-	-	-		
86	OHX	6	1943	-	0,6,6	-	-	-		
86	OHX	1	3525	-	0,6,6	-	-	-		
86	OHX	1	3659	-	0,6,6	-	-	-		
86	OHX	2	1925	-	0,6,6	-	-	-		
86	OHX	5	3577	-	0,6,6	-	-	-		
86	OHX	1	3486	-	0,6,6	-	-	-		
86	OHX	1	3664	-	0,6,6	-	-	-		
86	OHX	2	1960	-	0,6,6	-	-	-		
86	OHX	2	1923	-	0,6,6	-	-	-		
86	OHX	5	3449	-	0,6,6	-	-	-		
86	OHX	6	1902	-	0,6,6	-	-	-		
86	OHX	1	3413	-	0,6,6	-	-	-		
86	OHX	1	3551	-	0,6,6	-	-	-		
86	OHX	1	3610	-	0,6,6	-	-	-		
86	OHX	5	3698	-	0,6,6	-	-	-		
86	OHX	5	3468	-	0,6,6	-	-	-		
86	OHX	5	3571	-	0,6,6	-	-	-		
86	OHX	2	1994	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
86	OHX	6	2031	-	0,6,6	-	-	-		
86	OHX	2	2001	-	0,6,6	-	-	-		
86	OHX	1	3679	-	0,6,6	-	-	-		
86	OHX	c8	201	-	0,6,6	-	-	-		
86	OHX	5	3578	-	0,6,6	-	-	-		
86	OHX	2	1913	-	0,6,6	-	-	-		
86	OHX	1	3700	-	0,6,6	-	-	-		
86	OHX	6	1939	-	0,6,6	-	-	-		
86	OHX	n3	201	-	0,6,6	-	-	-		
86	OHX	5	3444	-	0,6,6	-	-	-		
86	OHX	2	1906	-	0,6,6	-	-	-		
86	OHX	6	1967	-	0,6,6	-	-	-		
86	OHX	5	3465	-	0,6,6	-	-	-		
86	OHX	5	3637	-	0,6,6	-	-	-		
86	OHX	5	3620	-	0,6,6	-	-	-		
86	OHX	2	1958	-	0,6,6	-	-	-		
86	OHX	1	3432	-	0,6,6	-	-	-		
86	OHX	1	3589	-	0,6,6	-	-	-		
86	OHX	5	3422	-	0,6,6	-	-	-		
86	OHX	6	1968	-	0,6,6	-	-	-		
86	OHX	5	3476	-	0,6,6	-	-	-		
86	OHX	1	3506	-	0,6,6	-	-	-		
86	OHX	2	1991	-	0,6,6	-	-	-		
86	OHX	5	3440	-	0,6,6	-	-	-		
86	OHX	5	3410	-	0,6,6	-	-	-		
86	OHX	2	1924	-	0,6,6	-	-	-		
86	OHX	1	3644	-	0,6,6	-	-	-		
86	OHX	1	3468	-	0,6,6	-	-	-		
86	OHX	8	212	-	0,6,6	-	-	-		
86	OHX	4	209	-	0,6,6	-	-	-		
86	OHX	2	1914	-	0,6,6	-	-	-		
86	OHX	2	2027	-	0,6,6	-	-	-		
86	OHX	6	1954	-	0,6,6	-	-	-		
86	OHX	5	3618	-	0,6,6	-	-	-		
86	OHX	7	205	-	0,6,6	-	-	-		
86	OHX	2	1997	-	0,6,6	-	-	-		
86	OHX	4	212	-	0,6,6	-	-	-		
86	OHX	6	1966	-	0,6,6	-	-	-		
86	OHX	2	1912	-	0,6,6	-	-	-		
86	OHX	6	2000	-	0,6,6	-	-	-		
86	OHX	6	2011	-	0,6,6	-	-	-		
86	OHX	1	3528	-	0,6,6	-	-	-		
86	OHX	5	3576	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
86	OHX	5	3687	-	0,6,6	-	-	-		
86	OHX	2	1967	-	0,6,6	-	-	-		
86	OHX	5	3699	-	0,6,6	-	-	-		
86	OHX	6	2026	-	0,6,6	-	-	-		
86	OHX	5	3563	-	0,6,6	-	-	-		
86	OHX	5	3570	-	0,6,6	-	-	-		
86	OHX	5	3436	-	0,6,6	-	-	-		
86	OHX	2	1930	-	0,6,6	-	-	-		
86	OHX	5	3646	-	0,6,6	-	-	-		
86	OHX	2	2017	-	0,6,6	-	-	-		
86	OHX	5	3607	-	0,6,6	-	-	-		
86	OHX	6	1932	-	0,6,6	-	-	-		
86	OHX	2	1963	-	0,6,6	-	-	-		
86	OHX	5	3495	-	0,6,6	-	-	-		
86	OHX	5	3524	-	0,6,6	-	-	-		
86	OHX	1	3479	-	0,6,6	-	-	-		
86	OHX	5	3692	-	0,6,6	-	-	-		
86	OHX	5	3615	-	0,6,6	-	-	-		
86	OHX	1	3643	-	0,6,6	-	-	-		
86	OHX	6	1976	-	0,6,6	-	-	-		
86	OHX	5	3426	-	0,6,6	-	-	-		
86	OHX	5	3635	-	0,6,6	-	-	-		
86	OHX	2	1920	-	0,6,6	-	-	-		
86	OHX	2	1910	-	0,6,6	-	-	-		
86	OHX	1	3417	-	0,6,6	-	-	-		
86	OHX	5	3591	-	0,6,6	-	-	-		
86	OHX	1	3582	-	0,6,6	-	-	-		
86	OHX	1	3517	-	0,6,6	-	-	-		
86	OHX	7	206	-	0,6,6	-	-	-		
86	OHX	1	3613	-	0,6,6	-	-	-		
86	OHX	6	2024	-	0,6,6	-	-	-		
86	OHX	5	3536	-	0,6,6	-	-	-		
86	OHX	5	3702	-	0,6,6	-	-	-		
86	OHX	5	3662	-	0,6,6	-	-	-		
86	OHX	1	3619	-	0,6,6	-	-	-		
86	OHX	2	2014	-	0,6,6	-	-	-		
86	OHX	3	203	-	0,6,6	-	-	-		
86	OHX	5	3693	-	0,6,6	-	-	-		
86	OHX	1	3522	-	0,6,6	-	-	-		
86	OHX	6	2028	-	0,6,6	-	-	-		
86	OHX	1	3669	-	0,6,6	-	-	-		
86	OHX	6	2007	-	0,6,6	-	-	-		
86	OHX	2	2008	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
86	OHX	6	2034	-	0,6,6	-	-	-		
86	OHX	5	3554	-	0,6,6	-	-	-		
86	OHX	5	3641	-	0,6,6	-	-	-		
86	OHX	5	3653	-	0,6,6	-	-	-		
86	OHX	5	3656	-	0,6,6	-	-	-		
86	OHX	o3	201	-	0,6,6	-	-	-		
86	OHX	1	3596	-	0,6,6	-	-	-		
86	OHX	1	3565	-	0,6,6	-	-	-		
86	OHX	1	3647	-	0,6,6	-	-	-		
86	OHX	5	3719	-	0,6,6	-	-	-		
86	OHX	1	3667	-	0,6,6	-	-	-		
86	OHX	1	3411	-	0,6,6	-	-	-		
86	OHX	1	3429	36	0,6,6	-	-	-		
86	OHX	1	3686	-	0,6,6	-	-	-		
86	OHX	1	3633	-	0,6,6	-	-	-		
86	OHX	6	1972	-	0,6,6	-	-	-		
86	OHX	5	3494	-	0,6,6	-	-	-		
86	OHX	5	3584	-	0,6,6	-	-	-		
86	OHX	1	3546	-	0,6,6	-	-	-		
86	OHX	7	204	-	0,6,6	-	-	-		
86	OHX	1	3586	-	0,6,6	-	-	-		
86	OHX	4	215	-	0,6,6	-	-	-		
86	OHX	1	3455	-	0,6,6	-	-	-		
86	OHX	1	3539	-	0,6,6	-	-	-		
86	OHX	5	3453	-	0,6,6	-	-	-		
86	OHX	1	3460	-	0,6,6	-	-	-		
86	OHX	1	3656	-	0,6,6	-	-	-		
86	OHX	6	2004	-	0,6,6	-	-	-		
86	OHX	s4	301	-	0,6,6	-	-	-		
86	OHX	5	3479	-	0,6,6	-	-	-		
86	OHX	5	3689	-	0,6,6	-	-	-		
86	OHX	5	3474	-	0,6,6	-	-	-		
86	OHX	5	3690	-	0,6,6	-	-	-		
86	OHX	2	1978	-	0,6,6	-	-	-		
86	OHX	1	3521	-	0,6,6	-	-	-		
86	OHX	M5	301	-	0,6,6	-	-	-		
86	OHX	5	3655	-	0,6,6	-	-	-		
86	OHX	1	3564	-	0,6,6	-	-	-		
86	OHX	5	3484	-	0,6,6	-	-	-		
86	OHX	1	3418	-	0,6,6	-	-	-		
86	OHX	6	1916	-	0,6,6	-	-	-		
86	OHX	4	211	-	0,6,6	-	-	-		
86	OHX	1	3590	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
86	OHX	4	214	-	0,6,6	-	-	-		
86	OHX	5	3639	-	0,6,6	-	-	-		
86	OHX	5	3565	-	0,6,6	-	-	-		
86	OHX	7	207	-	0,6,6	-	-	-		
86	OHX	5	3412	-	0,6,6	-	-	-		
86	OHX	5	3529	-	0,6,6	-	-	-		
86	OHX	5	3642	-	0,6,6	-	-	-		
86	OHX	5	3660	-	0,6,6	-	-	-		
86	OHX	2	1972	-	0,6,6	-	-	-		
86	OHX	5	3697	-	0,6,6	-	-	-		
86	OHX	1	3705	-	0,6,6	-	-	-		
86	OHX	5	3601	-	0,6,6	-	-	-		
86	OHX	5	3705	-	0,6,6	-	-	-		
86	OHX	5	3456	-	0,6,6	-	-	-		
86	OHX	1	3645	-	0,6,6	-	-	-		
86	OHX	M7	202	-	0,6,6	-	-	-		
86	OHX	5	3553	-	0,6,6	-	-	-		
86	OHX	6	1904	-	0,6,6	-	-	-		
86	OHX	2	1918	-	0,6,6	-	-	-		
86	OHX	5	3454	-	0,6,6	-	-	-		
86	OHX	5	3543	-	0,6,6	-	-	-		
86	OHX	5	3683	-	0,6,6	-	-	-		
86	OHX	1	3461	-	0,6,6	-	-	-		
86	OHX	6	2019	-	0,6,6	-	-	-		
86	OHX	1	3566	-	0,6,6	-	-	-		
86	OHX	6	1919	-	0,6,6	-	-	-		
86	OHX	5	3472	-	0,6,6	-	-	-		
86	OHX	6	1951	-	0,6,6	-	-	-		
86	OHX	6	1961	-	0,6,6	-	-	-		
86	OHX	1	3495	-	0,6,6	-	-	-		
86	OHX	5	3466	-	0,6,6	-	-	-		
86	OHX	6	2002	-	0,6,6	-	-	-		
86	OHX	m4	201	-	0,6,6	-	-	-		
86	OHX	2	2016	-	0,6,6	-	-	-		
86	OHX	2	1951	-	0,6,6	-	-	-		
86	OHX	5	3675	-	0,6,6	-	-	-		
86	OHX	1	3583	36	0,6,6	-	-	-		
86	OHX	2	1904	-	0,6,6	-	-	-		
86	OHX	2	1942	-	0,6,6	-	-	-		
86	OHX	1	3638	-	0,6,6	-	-	-		
86	OHX	5	3643	-	0,6,6	-	-	-		
86	OHX	1	3637	-	0,6,6	-	-	-		
86	OHX	1	3661	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
86	OHX	1	3620	-	0,6,6	-	-	-		
86	OHX	1	3587	-	0,6,6	-	-	-		
86	OHX	5	3604	-	0,6,6	-	-	-		
86	OHX	1	3433	-	0,6,6	-	-	-		
86	OHX	2	1944	-	0,6,6	-	-	-		
86	OHX	1	3403	-	0,6,6	-	-	-		
86	OHX	6	2022	-	0,6,6	-	-	-		
86	OHX	5	3413	-	0,6,6	-	-	-		
86	OHX	5	3517	-	0,6,6	-	-	-		
86	OHX	5	3600	-	0,6,6	-	-	-		
86	OHX	2	2019	-	0,6,6	-	-	-		
86	OHX	1	3530	-	0,6,6	-	-	-		
89	UAM	6	2134	-	31,31,31	0.18	0	38,44,44	0.55	1 (2%)
86	OHX	6	1969	-	0,6,6	-	-	-		
86	OHX	1	3440	-	0,6,6	-	-	-		
86	OHX	1	3567	-	0,6,6	-	-	-		
86	OHX	5	3622	-	0,6,6	-	-	-		
86	OHX	5	3708	-	0,6,6	-	-	-		
86	OHX	1	3405	-	0,6,6	-	-	-		
86	OHX	5	3700	-	0,6,6	-	-	-		
86	OHX	5	3608	-	0,6,6	-	-	-		
86	OHX	5	3558	-	0,6,6	-	-	-		
86	OHX	5	3682	-	0,6,6	-	-	-		
86	OHX	5	3585	-	0,6,6	-	-	-		
86	OHX	6	1924	-	0,6,6	-	-	-		
86	OHX	5	3527	-	0,6,6	-	-	-		
86	OHX	5	3633	-	0,6,6	-	-	-		
86	OHX	c5	201	-	0,6,6	-	-	-		
86	OHX	5	3523	-	0,6,6	-	-	-		
86	OHX	6	1979	-	0,6,6	-	-	-		
86	OHX	5	3676	-	0,6,6	-	-	-		
86	OHX	5	3623	-	0,6,6	-	-	-		
86	OHX	2	1908	-	0,6,6	-	-	-		
86	OHX	1	3577	-	0,6,6	-	-	-		
86	OHX	1	3622	-	0,6,6	-	-	-		
86	OHX	8	216	-	0,6,6	-	-	-		
86	OHX	2	1969	-	0,6,6	-	-	-		
86	OHX	1	3550	-	0,6,6	-	-	-		
86	OHX	5	3701	-	0,6,6	-	-	-		
86	OHX	6	1928	-	0,6,6	-	-	-		
86	OHX	1	3501	-	0,6,6	-	-	-		
86	OHX	1	3709	-	0,6,6	-	-	-		
86	OHX	1	3426	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
86	OHX	1	3449	-	0,6,6	-	-	-		
86	OHX	5	3458	-	0,6,6	-	-	-		
86	OHX	5	3486	-	0,6,6	-	-	-		
86	OHX	5	3674	-	0,6,6	-	-	-		
86	OHX	8	206	-	0,6,6	-	-	-		
86	OHX	1	3547	-	0,6,6	-	-	-		
86	OHX	5	3720	-	0,6,6	-	-	-		
86	OHX	2	1954	-	0,6,6	-	-	-		
86	OHX	1	3698	-	0,6,6	-	-	-		
86	OHX	1	3571	-	0,6,6	-	-	-		
86	OHX	2	1965	-	0,6,6	-	-	-		
86	OHX	1	3536	-	0,6,6	-	-	-		
86	OHX	1	3588	-	0,6,6	-	-	-		
86	OHX	5	3636	-	0,6,6	-	-	-		
86	OHX	1	3523	-	0,6,6	-	-	-		
86	OHX	1	3452	-	0,6,6	-	-	-		
86	OHX	1	3537	-	0,6,6	-	-	-		
86	OHX	1	3618	-	0,6,6	-	-	-		
86	OHX	L3	402	-	0,6,6	-	-	-		
86	OHX	2	1932	-	0,6,6	-	-	-		
86	OHX	5	3551	-	0,6,6	-	-	-		
86	OHX	5	3663	-	0,6,6	-	-	-		
86	OHX	4	213	-	0,6,6	-	-	-		
86	OHX	2	1952	-	0,6,6	-	-	-		
86	OHX	5	3581	-	0,6,6	-	-	-		
86	OHX	1	3710	-	0,6,6	-	-	-		
86	OHX	5	3617	-	0,6,6	-	-	-		
86	OHX	2	1915	-	0,6,6	-	-	-		
86	OHX	6	1987	-	0,6,6	-	-	-		
86	OHX	6	1944	-	0,6,6	-	-	-		
86	OHX	7	209	-	0,6,6	-	-	-		
86	OHX	5	3559	-	0,6,6	-	-	-		
86	OHX	5	3595	-	0,6,6	-	-	-		
86	OHX	1	3511	-	0,6,6	-	-	-		
86	OHX	5	3715	-	0,6,6	-	-	-		
86	OHX	5	3416	-	0,6,6	-	-	-		
86	OHX	8	204	-	0,6,6	-	-	-		
86	OHX	1	3480	-	0,6,6	-	-	-		
86	OHX	1	3706	-	0,6,6	-	-	-		
86	OHX	2	1928	-	0,6,6	-	-	-		
86	OHX	1	3414	-	0,6,6	-	-	-		
86	OHX	O1	201	-	0,6,6	-	-	-		
86	OHX	6	2035	-	0,6,6	-	-	-		



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
86	OHX	5	3480	-	0,6,6	-	-	-		
86	OHX	1	3692	-	0,6,6	-	-	-		
86	OHX	N9	101	-	0,6,6	-	-	-		
86	OHX	1	3476	-	0,6,6	-	-	-		
86	OHX	6	1908	-	0,6,6	-	-	-		
86	OHX	5	3505	-	0,6,6	-	-	-		
86	OHX	1	3690	-	0,6,6	-	-	-		
86	OHX	2	1985	-	0,6,6	-	-	-		
86	OHX	5	3420	-	0,6,6	-	-	-		
86	OHX	1	3594	-	0,6,6	-	-	-		
86	OHX	5	3548	-	0,6,6	-	-	-		
86	OHX	2	1953	-	0,6,6	-	-	-		
86	OHX	1	3542	-	0,6,6	-	-	-		
86	OHX	5	3478	-	0,6,6	-	-	-		
86	OHX	1	3612	-	0,6,6	-	-	-		
86	OHX	2	1975	-	0,6,6	-	-	-		
86	OHX	2	1987	-	0,6,6	-	-	-		
86	OHX	5	3411	-	0,6,6	-	-	-		
86	OHX	2	1973	-	0,6,6	-	-	-		
86	OHX	1	3422	-	0,6,6	-	-	-		
86	OHX	1	3576	-	0,6,6	-	-	-		
86	OHX	1	3684	-	0,6,6	-	-	-		
86	OHX	5	3429	-	0,6,6	-	-	-		
86	OHX	1	3699	-	0,6,6	-	-	-		
86	OHX	5	3545	-	0,6,6	-	-	-		
86	OHX	5	3686	-	0,6,6	-	-	-		
86	OHX	1	3410	-	0,6,6	-	-	-		
86	OHX	1	3556	-	0,6,6	-	-	-		
86	OHX	5	3460	-	0,6,6	-	-	-		
86	OHX	5	3403	-	0,6,6	-	-	-		
86	OHX	5	3668	-	0,6,6	-	-	-		
86	OHX	6	1949	-	0,6,6	-	-	-		
86	OHX	5	3672	-	0,6,6	-	-	-		
86	OHX	2	1977	-	0,6,6	-	-	-		
86	OHX	2	2006	-	0,6,6	-	-	-		
86	OHX	5	3407	-	0,6,6	-	-	-		
86	OHX	5	3534	-	0,6,6	-	-	-		
86	OHX	5	3594	-	0,6,6	-	-	-		
86	OHX	6	1999	-	0,6,6	-	-	-		
86	OHX	1	3639	-	0,6,6	-	-	-		
86	OHX	7	211	-	0,6,6	-	-	-		
86	OHX	1	3561	-	0,6,6	-	-	-		
86	OHX	5	3462	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
86	OHX	1	3474	-	0,6,6	-	-	-		
86	OHX	1	3642	-	0,6,6	-	-	-		
86	OHX	2	1905	-	0,6,6	-	-	-		
86	OHX	6	1935	-	0,6,6	-	-	-		
86	OHX	L4	401	-	0,6,6	-	-	-		
86	OHX	2	1902	-	0,6,6	-	-	-		
86	OHX	1	3695	-	0,6,6	-	-	-		
86	OHX	6	1915	-	0,6,6	-	-	-		
86	OHX	6	1953	-	0,6,6	-	-	-		
86	OHX	8	213	-	0,6,6	-	-	-		
86	OHX	6	1903	-	0,6,6	-	-	-		
86	OHX	6	2033	-	0,6,6	-	-	-		
86	OHX	5	3435	-	0,6,6	-	-	-		
86	OHX	2	2013	-	0,6,6	-	-	-		
86	OHX	6	2036	-	0,6,6	-	-	-		
86	OHX	5	3464	-	0,6,6	-	-	-		
86	OHX	5	3572	-	0,6,6	-	-	-		
86	OHX	5	3649	-	0,6,6	-	-	-		
86	OHX	5	3677	-	0,6,6	-	-	-		
86	OHX	6	1906	-	0,6,6	-	-	-		
86	OHX	1	3498	-	0,6,6	-	-	-		
86	OHX	1	3640	-	0,6,6	-	-	-		
86	OHX	15	301	-	0,6,6	-	-	-		
86	OHX	5	3493	-	0,6,6	-	-	-		
86	OHX	5	3648	-	0,6,6	-	-	-		
86	OHX	8	203	-	0,6,6	-	-	-		
86	OHX	5	3665	-	0,6,6	-	-	-		
86	OHX	5	3424	-	0,6,6	-	-	-		
86	OHX	1	3514	-	0,6,6	-	-	-		
86	OHX	6	1974	-	0,6,6	-	-	-		
86	OHX	6	2014	-	0,6,6	-	-	-		
86	OHX	8	215	-	0,6,6	-	-	-		
86	OHX	4	203	-	0,6,6	-	-	-		
86	OHX	5	3490	-	0,6,6	-	-	-		
86	OHX	1	3579	-	0,6,6	-	-	-		
86	OHX	1	3520	-	0,6,6	-	-	-		
86	OHX	2	1971	-	0,6,6	-	-	-		
86	OHX	2	1974	-	0,6,6	-	-	-		
86	OHX	5	3590	-	0,6,6	-	-	-		
86	OHX	n3	202	-	0,6,6	-	-	-		
86	OHX	1	3401	-	0,6,6	-	-	-		
86	OHX	1	3437	-	0,6,6	-	-	-		
86	OHX	4	207	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
86	OHX	6	1907	-	0,6,6	-	-	-		
86	OHX	5	3428	-	0,6,6	-	-	-		
86	OHX	1	3655	-	0,6,6	-	-	-		
86	OHX	1	3675	-	0,6,6	-	-	-		
86	OHX	1	3712	-	0,6,6	-	-	-		
86	OHX	S9	201	-	0,6,6	-	-	-		
86	OHX	5	3537	-	0,6,6	-	-	-		
86	OHX	1	3708	-	0,6,6	-	-	-		
86	OHX	5	3526	-	0,6,6	-	-	-		
86	OHX	2	1936	-	0,6,6	-	-	-		
86	OHX	2	1922	-	0,6,6	-	-	-		
86	OHX	5	3443	-	0,6,6	-	-	-		
86	OHX	5	3583	-	0,6,6	-	-	-		
86	OHX	2	1995	-	0,6,6	-	-	-		
86	OHX	6	1977	-	0,6,6	-	-	-		
86	OHX	5	3511	-	0,6,6	-	-	-		
86	OHX	6	2006	-	0,6,6	-	-	-		
86	OHX	5	3713	-	0,6,6	-	-	-		
86	OHX	1	3607	-	0,6,6	-	-	-		
86	OHX	1	3660	-	0,6,6	-	-	-		
86	OHX	6	2013	-	0,6,6	-	-	-		
86	OHX	1	3562	-	0,6,6	-	-	-		
86	OHX	5	3433	-	0,6,6	-	-	-		
86	OHX	5	3626	-	0,6,6	-	-	-		
86	OHX	2	1934	-	0,6,6	-	-	-		
86	OHX	1	3496	-	0,6,6	-	-	-		
86	OHX	2	1940	-	0,6,6	-	-	-		
86	OHX	1	3553	-	0,6,6	-	-	-		
86	OHX	6	1989	-	0,6,6	-	-	-		
86	OHX	1	3402	-	0,6,6	-	-	-		
86	OHX	2	1907	-	0,6,6	-	-	-		
86	OHX	1	3671	-	0,6,6	-	-	-		
86	OHX	6	1959	-	0,6,6	-	-	-		
86	OHX	2	1970	-	0,6,6	-	-	-		
86	OHX	5	3405	-	0,6,6	-	-	-		
86	OHX	1	3697	-	0,6,6	-	-	-		
86	OHX	1	3499	-	0,6,6	-	-	-		
86	OHX	1	3472	-	0,6,6	-	-	-		
86	OHX	2	1982	-	0,6,6	-	-	-		
86	OHX	6	1986	-	0,6,6	-	-	-		
86	OHX	1	3606	-	0,6,6	-	-	-		
86	OHX	2	1947	-	0,6,6	-	-	-		
86	OHX	6	1922	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
86	OHX	4	217	-	0,6,6	-	-	-		
86	OHX	5	3500	-	0,6,6	-	-	-		
86	OHX	5	3724	-	0,6,6	-	-	-		
86	OHX	2	1968	-	0,6,6	-	-	-		
86	OHX	1	3573	-	0,6,6	-	-	-		
86	OHX	7	210	-	0,6,6	-	-	-		
86	OHX	6	1965	-	0,6,6	-	-	-		
86	OHX	1	3657	-	0,6,6	-	-	-		
86	OHX	5	3561	-	0,6,6	-	-	-		
86	OHX	5	3678	-	0,6,6	-	-	-		
86	OHX	2	1943	-	0,6,6	-	-	-		
86	OHX	2	1911	-	0,6,6	-	-	-		
86	OHX	1	3419	-	0,6,6	-	-	-		
86	OHX	1	3572	-	0,6,6	-	-	-		
86	OHX	5	3425	-	0,6,6	-	-	-		
86	OHX	5	3470	-	0,6,6	-	-	-		
86	OHX	1	3701	-	0,6,6	-	-	-		
86	OHX	2	2011	-	0,6,6	-	-	-		
86	OHX	1	3636	-	0,6,6	-	-	-		
86	OHX	7	201	-	0,6,6	-	-	-		
86	OHX	n1	201	-	0,6,6	-	-	-		
86	OHX	6	1995	-	0,6,6	-	-	-		
86	OHX	1	3478	-	0,6,6	-	-	-		
86	OHX	1	3416	-	0,6,6	-	-	-		
86	OHX	1	3569	-	0,6,6	-	-	-		
86	OHX	5	3704	-	0,6,6	-	-	-		
86	OHX	1	3508	-	0,6,6	-	-	-		
86	OHX	5	3621	-	0,6,6	-	-	-		
86	OHX	5	3521	-	0,6,6	-	-	-		
86	OHX	6	1983	-	0,6,6	-	-	-		
86	OHX	6	1991	-	0,6,6	-	-	-		
86	OHX	2	1937	-	0,6,6	-	-	-		
86	OHX	5	3546	-	0,6,6	-	-	-		
86	OHX	o7	502	-	0,6,6	-	-	-		
86	OHX	1	3524	-	0,6,6	-	-	-		
86	OHX	5	3580	-	0,6,6	-	-	-		
86	OHX	1	3676	-	0,6,6	-	-	-		
86	OHX	5	3519	-	0,6,6	-	-	-		
86	OHX	2	2003	-	0,6,6	-	-	-		
86	OHX	1	3483	-	0,6,6	-	-	-		
86	OHX	5	3401	-	0,6,6	-	-	-		
86	OHX	5	3645	-	0,6,6	-	-	-		
86	OHX	2	1916	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
86	OHX	4	208	-	0,6,6	-	-	-		
86	OHX	5	3510	-	0,6,6	-	-	-		
86	OHX	1	3471	-	0,6,6	-	-	-		
86	OHX	s9	201	-	0,6,6	-	-	-		
86	OHX	1	3674	-	0,6,6	-	-	-		
86	OHX	3	207	-	0,6,6	-	-	-		
86	OHX	5	3441	-	0,6,6	-	-	-		
86	OHX	6	1937	-	0,6,6	-	-	-		
86	OHX	1	3668	-	0,6,6	-	-	-		
86	OHX	1	3541	-	0,6,6	-	-	-		
86	OHX	6	2008	-	0,6,6	-	-	-		
86	OHX	5	3541	-	0,6,6	-	-	-		
86	OHX	5	3659	-	0,6,6	-	-	-		
86	OHX	1	3635	-	0,6,6	-	-	-		
86	OHX	5	3431	-	0,6,6	-	-	-		
86	OHX	5	3566	-	0,6,6	-	-	-		
86	OHX	1	3435	-	0,6,6	-	-	-		
86	OHX	5	3451	-	0,6,6	-	-	-		
86	OHX	1	3555	-	0,6,6	-	-	-		
86	OHX	1	3663	-	0,6,6	-	-	-		
86	OHX	1	3649	-	0,6,6	-	-	-		
86	OHX	5	3670	-	0,6,6	-	-	-		
86	OHX	6	1942	-	0,6,6	-	-	-		
86	OHX	5	3685	-	0,6,6	-	-	-		
86	OHX	1	3448	-	0,6,6	-	-	-		
86	OHX	1	3493	-	0,6,6	-	-	-		
86	OHX	1	3485	-	0,6,6	-	-	-		
86	OHX	1	3518	-	0,6,6	-	-	-		
86	OHX	1	3559	-	0,6,6	-	-	-		
86	OHX	6	1914	-	0,6,6	-	-	-		
86	OHX	5	3438	-	0,6,6	-	-	-		
86	OHX	5	3489	-	0,6,6	-	-	-		
86	OHX	1	3688	-	0,6,6	-	-	-		
86	OHX	5	3512	-	0,6,6	-	-	-		
86	OHX	5	3560	-	0,6,6	-	-	-		
86	OHX	2	1948	-	0,6,6	-	-	-		
86	OHX	1	3641	-	0,6,6	-	-	-		
86	OHX	5	3507	-	0,6,6	-	-	-		
86	OHX	1	3446	-	0,6,6	-	-	-		
86	OHX	5	3439	-	0,6,6	-	-	-		
86	OHX	5	3640	-	0,6,6	-	-	-		
86	OHX	6	1945	-	0,6,6	-	-	-		
86	OHX	1	3628	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
86	OHX	5	3499	-	0,6,6	-	-	-		
86	OHX	5	3695	-	0,6,6	-	-	-		
86	OHX	1	3505	-	0,6,6	-	-	-		
86	OHX	5	3681	-	0,6,6	-	-	-		
86	OHX	1	3457	-	0,6,6	-	-	-		
86	OHX	1	3488	-	0,6,6	-	-	-		
86	OHX	3	208	-	0,6,6	-	-	-		
86	OHX	1	3464	-	0,6,6	-	-	-		
86	OHX	6	1997	-	0,6,6	-	-	-		
86	OHX	5	3532	-	0,6,6	-	-	-		
86	OHX	5	3625	-	0,6,6	-	-	-		
86	OHX	5	3631	-	0,6,6	-	-	-		
86	OHX	1	3605	-	0,6,6	-	-	-		
86	OHX	5	3471	-	0,6,6	-	-	-		
86	OHX	5	3544	-	0,6,6	-	-	-		
86	OHX	5	3592	-	0,6,6	-	-	-		
86	OHX	1	3545	-	0,6,6	-	-	-		
86	OHX	5	3657	-	0,6,6	-	-	-		
86	OHX	2	2022	-	0,6,6	-	-	-		
86	OHX	5	3710	-	0,6,6	-	-	-		
86	OHX	5	3485	-	0,6,6	-	-	-		
86	OHX	m0	301	-	0,6,6	-	-	-		
86	OHX	5	3680	-	0,6,6	-	-	-		
86	OHX	5	3716	-	0,6,6	-	-	-		
86	OHX	2	1996	-	0,6,6	-	-	-		
86	OHX	1	3438	-	0,6,6	-	-	-		
86	OHX	1	3412	-	0,6,6	-	-	-		
86	OHX	1	3558	-	0,6,6	-	-	-		
86	OHX	1	3694	-	0,6,6	-	-	-		
86	OHX	1	3458	-	0,6,6	-	-	-		
86	OHX	6	1960	-	0,6,6	-	-	-		
86	OHX	1	3407	-	0,6,6	-	-	-		
86	OHX	1	3415	-	0,6,6	-	-	-		
86	OHX	1	3527	-	0,6,6	-	-	-		
86	OHX	6	1973	-	0,6,6	-	-	-		
86	OHX	5	3491	-	0,6,6	-	-	-		
86	OHX	5	3457	-	0,6,6	-	-	-		
86	OHX	5	3614	-	0,6,6	-	-	-		
86	OHX	5	3619	-	0,6,6	-	-	-		
86	OHX	2	1961	-	0,6,6	-	-	-		
86	OHX	1	3494	-	0,6,6	-	-	-		
86	OHX	6	1918	-	0,6,6	-	-	-		
86	OHX	2	2012	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
86	OHX	5	3552	-	0,6,6	-	-	-		
86	OHX	1	3462	-	0,6,6	-	-	-		
86	OHX	5	3596	-	0,6,6	-	-	-		
86	OHX	1	3626	-	0,6,6	-	-	-		
86	OHX	2	1990	-	0,6,6	-	-	-		
86	OHX	6	1980	-	0,6,6	-	-	-		
86	OHX	5	3630	-	0,6,6	-	-	-		
86	OHX	5	3487	-	0,6,6	-	-	-		
86	OHX	8	211	-	0,6,6	-	-	-		
86	OHX	1	3538	-	0,6,6	-	-	-		
86	OHX	1	3683	-	0,6,6	-	-	-		
86	OHX	6	1978	-	0,6,6	-	-	-		
86	OHX	5	3588	-	0,6,6	-	-	-		
86	OHX	6	1993	-	0,6,6	-	-	-		
86	OHX	7	202	-	0,6,6	-	-	-		
86	OHX	5	3496	-	0,6,6	-	-	-		
86	OHX	3	202	-	0,6,6	-	-	-		
86	OHX	2	1933	-	0,6,6	-	-	-		
86	OHX	6	2037	-	0,6,6	-	-	-		
86	OHX	5	3402	-	0,6,6	-	-	-		
86	OHX	1	3648	-	0,6,6	-	-	-		
86	OHX	5	3434	-	0,6,6	-	-	-		
86	OHX	5	3711	-	0,6,6	-	-	-		
86	OHX	6	2009	-	0,6,6	-	-	-		
86	OHX	5	3671	-	0,6,6	-	-	-		
86	OHX	1	3466	-	0,6,6	-	-	-		
86	OHX	6	1982	-	0,6,6	-	-	-		
86	OHX	1	3490	-	0,6,6	-	-	-		
86	OHX	2	1931	-	0,6,6	-	-	-		
86	OHX	1	3651	-	0,6,6	-	-	-		
86	OHX	1	3689	-	0,6,6	-	-	-		
86	OHX	4	210	-	0,6,6	-	-	-		
86	OHX	3	201	-	0,6,6	-	-	-		
86	OHX	2	2002	-	0,6,6	-	-	-		
86	OHX	6	2003	-	0,6,6	-	-	-		
86	OHX	5	3568	-	0,6,6	-	-	-		
86	OHX	q2	502	-	0,6,6	-	-	-		
86	OHX	5	3718	-	0,6,6	-	-	-		
86	OHX	2	1986	-	0,6,6	-	-	-		
86	OHX	1	3604	-	0,6,6	-	-	-		
86	OHX	5	3714	-	0,6,6	-	-	-		
86	OHX	6	2021	-	0,6,6	-	-	-		
86	OHX	2	1979	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
86	OHX	6	1958	-	0,6,6	-	-	-		
86	OHX	6	1923	-	0,6,6	-	-	-		
86	OHX	1	3557	-	0,6,6	-	-	-		
86	OHX	5	3448	-	0,6,6	-	-	-		
86	OHX	1	3470	-	0,6,6	-	-	-		
86	OHX	1	3533	-	0,6,6	-	-	-		
86	OHX	m5	302	-	0,6,6	-	-	-		
86	OHX	1	3516	-	0,6,6	-	-	-		
86	OHX	5	3473	-	0,6,6	-	-	-		
86	OHX	5	3447	-	0,6,6	-	-	-		
86	OHX	C1	201	-	0,6,6	-	-	-		
86	OHX	5	3612	-	0,6,6	-	-	-		
86	OHX	1	3580	-	0,6,6	-	-	-		
86	OHX	1	3598	-	0,6,6	-	-	-		
86	OHX	8	209	-	0,6,6	-	-	-		
86	OHX	1	3666	-	0,6,6	-	-	-		
86	OHX	6	1957	-	0,6,6	-	-	-		
86	OHX	5	3442	-	0,6,6	-	-	-		
86	OHX	1	3608	-	0,6,6	-	-	-		
86	OHX	1	3593	-	0,6,6	-	-	-		
86	OHX	5	3508	-	0,6,6	-	-	-		
86	OHX	5	3616	-	0,6,6	-	-	-		
86	OHX	2	1955	-	0,6,6	-	-	-		
86	OHX	1	3634	-	0,6,6	-	-	-		
86	OHX	1	3441	-	0,6,6	-	-	-		
86	OHX	1	3467	-	0,6,6	-	-	-		
86	OHX	C8	201	-	0,6,6	-	-	-		
86	OHX	5	3723	-	0,6,6	-	-	-		
86	OHX	5	3709	-	0,6,6	-	-	-		
86	OHX	m6	201	-	0,6,6	-	-	-		
86	OHX	1	3451	-	0,6,6	-	-	-		
86	OHX	1	3500	-	0,6,6	-	-	-		
86	OHX	2	2005	-	0,6,6	-	-	-		
86	OHX	1	3672	-	0,6,6	-	-	-		
86	OHX	5	3579	-	0,6,6	-	-	-		
86	OHX	5	3647	-	0,6,6	-	-	-		
86	OHX	7	208	-	0,6,6	-	-	-		
86	OHX	5	3509	-	0,6,6	-	-	-		
86	OHX	2	1919	-	0,6,6	-	-	-		
86	OHX	5	3415	-	0,6,6	-	-	-		
86	OHX	6	2012	-	0,6,6	-	-	-		
86	OHX	2	1909	1	0,6,6	-	-	-		
86	OHX	1	3602	-	0,6,6	-	-	-		



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
86	OHX	1	3678	-	0,6,6	-	-	-		
86	OHX	6	1941	-	0,6,6	-	-	-		
86	OHX	5	3574	-	0,6,6	-	-	-		
86	OHX	1	3548	-	0,6,6	-	-	-		
86	OHX	3	206	-	0,6,6	-	-	-		
86	OHX	1	3563	-	0,6,6	-	-	-		
86	OHX	2	1903	-	0,6,6	-	-	-		
86	OHX	5	3667	-	0,6,6	-	-	-		
86	OHX	1	3599	-	0,6,6	-	-	-		
86	OHX	1	3681	-	0,6,6	-	-	-		
86	OHX	S8	301	-	0,6,6	-	-	-		
86	OHX	1	3623	-	0,6,6	-	-	-		
86	OHX	1	3711	-	0,6,6	-	-	-		
86	OHX	14	401	-	0,6,6	-	-	-		
86	OHX	1	3503	-	0,6,6	-	-	-		
86	OHX	5	3638	-	0,6,6	-	-	-		
86	OHX	1	3406	-	0,6,6	-	-	-		
86	OHX	1	3652	-	0,6,6	-	-	-		
86	OHX	1	3544	-	0,6,6	-	-	-		
86	OHX	2	1988	-	0,6,6	-	-	-		
86	OHX	6	1926	-	0,6,6	-	-	-		
86	OHX	1	3428	-	0,6,6	-	-	-		
86	OHX	7	203	-	0,6,6	-	-	-		
86	OHX	1	3456	-	0,6,6	-	-	-		
86	OHX	1	3662	36	0,6,6	-	-	-		
86	OHX	5	3624	-	0,6,6	-	-	-		
86	OHX	5	3567	-	0,6,6	-	-	-		
86	OHX	6	2005	-	0,6,6	-	-	-		
86	OHX	6	2001	-	0,6,6	-	-	-		
86	OHX	5	3722	-	0,6,6	-	-	-		
86	OHX	1	3704	-	0,6,6	-	-	-		
86	OHX	5	3421	-	0,6,6	-	-	-		
86	OHX	1	3439	-	0,6,6	-	-	-		
86	OHX	1	3502	-	0,6,6	-	-	-		
86	OHX	5	3488	-	0,6,6	-	-	-		
86	OHX	1	3497	-	0,6,6	-	-	-		
86	OHX	5	3502	-	0,6,6	-	-	-		
86	OHX	1	3510	-	0,6,6	-	-	-		
86	OHX	2	1959	-	0,6,6	-	-	-		
86	OHX	5	3605	-	0,6,6	-	-	-		
86	OHX	L3	401	-	0,6,6	-	-	-		
86	OHX	2	1921	-	0,6,6	-	-	-		
86	OHX	1	3578	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
86	OHX	1	3473	-	0,6,6	-	-	-		
86	OHX	1	3615	-	0,6,6	-	-	-		
86	OHX	1	3680	-	0,6,6	-	-	-		
86	OHX	6	1962	-	0,6,6	-	-	-		
86	OHX	5	3611	-	0,6,6	-	-	-		
86	OHX	2	1926	-	0,6,6	-	-	-		
86	OHX	1	3409	-	0,6,6	-	-	-		
86	OHX	1	3601	-	0,6,6	-	-	-		
86	OHX	5	3450	-	0,6,6	-	-	-		
86	OHX	1	3431	-	0,6,6	-	-	-		
86	OHX	1	3693	-	0,6,6	-	-	-		
86	OHX	5	3446	-	0,6,6	-	-	-		
86	OHX	5	3550	-	0,6,6	-	-	-		
86	OHX	5	3530	-	0,6,6	-	-	-		
86	OHX	8	207	-	0,6,6	-	-	-		
86	OHX	2	1935	-	0,6,6	-	-	-		
86	OHX	1	3554	-	0,6,6	-	-	-		
86	OHX	5	3430	-	0,6,6	-	-	-		
86	OHX	5	3482	-	0,6,6	-	-	-		
86	OHX	2	1966	-	0,6,6	-	-	-		
86	OHX	1	3677	-	0,6,6	-	-	-		
86	OHX	5	3606	-	0,6,6	-	-	-		
86	OHX	1	3423	-	0,6,6	-	-	-		
86	OHX	5	3694	-	0,6,6	-	-	-		
86	OHX	5	3691	-	0,6,6	-	-	-		
86	OHX	5	3696	-	0,6,6	-	-	-		
86	OHX	SR	401	-	0,6,6	-	-	-		
86	OHX	1	3515	-	0,6,6	-	-	-		
86	OHX	6	1950	-	0,6,6	-	-	-		
86	OHX	5	3497	-	0,6,6	-	-	-		
86	OHX	6	1930	-	0,6,6	-	-	-		
86	OHX	1	3603	-	0,6,6	-	-	-		
86	OHX	6	2032	-	0,6,6	-	-	-		
86	OHX	2	1901	-	0,6,6	-	-	-		
86	OHX	5	3538	-	0,6,6	-	-	-		
86	OHX	1	3631	-	0,6,6	-	-	-		
86	OHX	1	3625	-	0,6,6	-	-	-		
86	OHX	6	1964	-	0,6,6	-	-	-		
86	OHX	2	1950	-	0,6,6	-	-	-		
86	OHX	6	2018	-	0,6,6	-	-	-		
86	OHX	6	1963	-	0,6,6	-	-	-		
86	OHX	2	2009	-	0,6,6	-	-	-		
86	OHX	1	3512	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
86	OHX	2	1976	-	0,6,6	-	-	-		
86	OHX	5	3459	-	0,6,6	-	-	-		
86	OHX	6	1971	-	0,6,6	-	-	-		
86	OHX	5	3651	-	0,6,6	-	-	-		
86	OHX	2	1984	-	0,6,6	-	-	-		
86	OHX	2	1938	-	0,6,6	-	-	-		
86	OHX	6	1912	-	0,6,6	-	-	-		
86	OHX	O3	201	-	0,6,6	-	-	-		
86	OHX	6	1901	-	0,6,6	-	-	-		
86	OHX	6	1913	-	0,6,6	-	-	-		
86	OHX	1	3646	-	0,6,6	-	-	-		
86	OHX	6	1921	-	0,6,6	-	-	-		
86	OHX	5	3469	-	0,6,6	-	-	-		
86	OHX	5	3535	-	0,6,6	-	-	-		
86	OHX	2	1939	-	0,6,6	-	-	-		
86	OHX	5	3409	-	0,6,6	-	-	-		
86	OHX	5	3549	-	0,6,6	-	-	-		
86	OHX	1	3682	-	0,6,6	-	-	-		
86	OHX	1	3614	-	0,6,6	-	-	-		
86	OHX	6	2017	-	0,6,6	-	-	-		
86	OHX	1	3424	-	0,6,6	-	-	-		
86	OHX	3	205	-	0,6,6	-	-	-		
86	OHX	5	3629	-	0,6,6	-	-	-		
86	OHX	1	3552	-	0,6,6	-	-	-		
86	OHX	1	3568	-	0,6,6	-	-	-		
86	OHX	1	3595	-	0,6,6	-	-	-		
86	OHX	5	3658	-	0,6,6	-	-	-		
86	OHX	5	3406	-	0,6,6	-	-	-		
86	OHX	5	3556	-	0,6,6	-	-	-		
86	OHX	5	3632	-	0,6,6	-	-	-		
86	OHX	2	1927	-	0,6,6	-	-	-		
86	OHX	2	1946	-	0,6,6	-	-	-		
86	OHX	6	2027	1	0,6,6	-	-	-		
86	OHX	5	3481	-	0,6,6	-	-	-		
86	OHX	6	1934	-	0,6,6	-	-	-		
86	OHX	2	1989	-	0,6,6	-	-	-		
86	OHX	1	3703	-	0,6,6	-	-	-		
86	OHX	6	1998	-	0,6,6	-	-	-		
86	OHX	5	3513	-	0,6,6	-	-	-		
86	OHX	1	3540	-	0,6,6	-	-	-		
86	OHX	2	2028	-	0,6,6	-	-	-		
86	OHX	1	3630	-	0,6,6	-	-	-		
86	OHX	5	3452	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
86	OHX	1	3477	-	0,6,6	-	-	-		
86	OHX	6	1996	-	0,6,6	-	-	-		
86	OHX	5	3533	-	0,6,6	-	-	-		
86	OHX	6	1956	-	0,6,6	-	-	-		
86	OHX	1	3560	-	0,6,6	-	-	-		
86	OHX	5	3586	-	0,6,6	-	-	-		
86	OHX	5	3542	-	0,6,6	-	-	-		
86	OHX	6	1955	-	0,6,6	-	-	-		
86	OHX	1	3447	-	0,6,6	-	-	-		
86	OHX	2	2025	-	0,6,6	-	-	-		
86	OHX	6	1910	-	0,6,6	-	-	-		
86	OHX	5	3437	-	0,6,6	-	-	-		
86	OHX	5	3463	36	0,6,6	-	-	-		
86	OHX	5	3666	-	0,6,6	-	-	-		
86	OHX	2	1962	-	0,6,6	-	-	-		
86	OHX	1	3581	-	0,6,6	-	-	-		
86	OHX	6	1946	-	0,6,6	-	-	-		
86	OHX	1	3585	-	0,6,6	-	-	-		
86	OHX	2	2023	-	0,6,6	-	-	-		
86	OHX	5	3404	-	0,6,6	-	-	-		
86	OHX	5	3598	-	0,6,6	-	-	-		
86	OHX	1	3475	-	0,6,6	-	-	-		
86	OHX	1	3509	-	0,6,6	-	-	-		
86	OHX	8	205	-	0,6,6	-	-	-		
86	OHX	2	1945	-	0,6,6	-	-	-		
86	OHX	5	3467	-	0,6,6	-	-	-		
86	OHX	5	3445	-	0,6,6	-	-	-		
86	OHX	5	3627	-	0,6,6	-	-	-		
86	OHX	1	3575	-	0,6,6	-	-	-		
86	OHX	2	1998	-	0,6,6	-	-	-		
86	OHX	5	3427	-	0,6,6	-	-	-		
86	OHX	1	3687	-	0,6,6	-	-	-		
86	OHX	5	3688	-	0,6,6	-	-	-		
86	OHX	n9	102	-	0,6,6	-	-	-		
86	OHX	2	1956	-	0,6,6	-	-	-		
86	OHX	5	3562	-	0,6,6	-	-	-		
86	OHX	1	3691	-	0,6,6	-	-	-		
86	OHX	2	2024	-	0,6,6	-	-	-		
86	OHX	5	3679	-	0,6,6	-	-	-		
86	OHX	5	3525	-	0,6,6	-	-	-		
86	OHX	6	2023	-	0,6,6	-	-	-		
86	OHX	5	3483	-	0,6,6	-	-	-		
86	OHX	15	302	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
86	OHX	1	3624	-	0,6,6	-	-	-		
86	OHX	5	3557	-	0,6,6	-	-	-		
86	OHX	6	1947	-	0,6,6	-	-	-		
86	OHX	C3	201	-	0,6,6	-	-	-		
86	OHX	1	3621	-	0,6,6	-	-	-		
86	OHX	5	3531	-	0,6,6	-	-	-		
86	OHX	5	3599	-	0,6,6	-	-	-		
86	OHX	1	3584	-	0,6,6	-	-	-		
86	OHX	6	1927	1	0,6,6	-	-	-		
86	OHX	5	3516	-	0,6,6	-	-	-		
86	OHX	5	3575	-	0,6,6	-	-	-		
86	OHX	5	3503	-	0,6,6	-	-	-		
86	OHX	2	1983	-	0,6,6	-	-	-		
86	OHX	1	3543	-	0,6,6	-	-	-		
86	OHX	6	2010	-	0,6,6	-	-	-		
86	OHX	1	3592	-	0,6,6	-	-	-		
86	OHX	1	3616	-	0,6,6	-	-	-		
86	OHX	5	3432	-	0,6,6	-	-	-		
86	OHX	5	3673	-	0,6,6	-	-	-		
86	OHX	1	3408	-	0,6,6	-	-	-		
86	OHX	1	3570	-	0,6,6	-	-	-		
86	OHX	5	3661	-	0,6,6	-	-	-		
86	OHX	2	2007	-	0,6,6	-	-	-		
86	OHX	6	2025	-	0,6,6	-	-	-		
86	OHX	1	3489	-	0,6,6	-	-	-		
86	OHX	1	3665	-	0,6,6	-	-	-		
86	OHX	1	3632	-	0,6,6	-	-	-		
86	OHX	1	3609	-	0,6,6	-	-	-		
86	OHX	1	3526	-	0,6,6	-	-	-		
86	OHX	5	3540	-	0,6,6	-	-	-		
86	OHX	5	3528	-	0,6,6	-	-	-		
86	OHX	6	2016	-	0,6,6	-	-	-		
86	OHX	2	2000	-	0,6,6	-	-	-		
86	OHX	sR	401	-	0,6,6	-	-	-		
86	OHX	2	1980	-	0,6,6	-	-	-		
86	OHX	s8	301	-	0,6,6	-	-	-		
86	OHX	5	3520	-	0,6,6	-	-	-		
86	OHX	2	2010	-	0,6,6	-	-	-		
86	OHX	1	3421	-	0,6,6	-	-	-		
86	OHX	M0	301	-	0,6,6	-	-	-		
86	OHX	5	3539	-	0,6,6	-	-	-		
86	OHX	5	3707	-	0,6,6	-	-	-		
86	OHX	5	3514	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
86	OHX	6	2015	-	0,6,6	-	-	-		
86	OHX	5	3597	-	0,6,6	-	-	-		
86	OHX	1	3425	-	0,6,6	-	-	-		
86	OHX	1	3430	-	0,6,6	-	-	-		
86	OHX	5	3477	-	0,6,6	-	-	-		
86	OHX	1	3442	-	0,6,6	-	-	-		
86	OHX	6	1936	-	0,6,6	-	-	-		
86	OHX	6	1925	-	0,6,6	-	-	-		
86	OHX	6	1931	-	0,6,6	-	-	-		
86	OHX	1	3532	-	0,6,6	-	-	-		
86	OHX	2	1929	-	0,6,6	-	-	-		
86	OHX	6	1984	-	0,6,6	-	-	-		
86	OHX	1	3492	-	0,6,6	-	-	-		
86	OHX	5	3423	-	0,6,6	-	-	-		
86	OHX	1	3445	-	0,6,6	-	-	-		
86	OHX	5	3547	-	0,6,6	-	-	-		
86	OHX	5	3664	-	0,6,6	-	-	-		
86	OHX	5	3501	36	0,6,6	-	-	-		
86	OHX	5	3569	-	0,6,6	-	-	-		
86	OHX	6	1920	-	0,6,6	-	-	-		
86	OHX	5	3475	-	0,6,6	-	-	-		
86	OHX	5	3417	-	0,6,6	-	-	-		
86	OHX	2	2015	-	0,6,6	-	-	-		
86	OHX	1	3549	-	0,6,6	-	-	-		
86	OHX	4	204	-	0,6,6	-	-	-		
86	OHX	2	2021	-	0,6,6	-	-	-		
86	OHX	5	3582	-	0,6,6	-	-	-		
86	OHX	5	3610	-	0,6,6	-	-	-		
86	OHX	6	1938	-	0,6,6	-	-	-		
86	OHX	Q2	502	-	0,6,6	-	-	-		
86	OHX	1	3507	-	0,6,6	-	-	-		
86	OHX	5	3455	-	0,6,6	-	-	-		
86	OHX	6	2020	-	0,6,6	-	-	-		
86	OHX	5	3669	-	0,6,6	-	-	-		
86	OHX	1	3491	-	0,6,6	-	-	-		
86	OHX	1	3650	-	0,6,6	-	-	-		
86	OHX	6	1911	-	0,6,6	-	-	-		
86	OHX	6	1940	-	0,6,6	-	-	-		
86	OHX	5	3652	-	0,6,6	-	-	-		
86	OHX	8	210	-	0,6,6	-	-	-		
86	OHX	1	3529	-	0,6,6	-	-	-		
86	OHX	1	3654	-	0,6,6	-	-	-		
86	OHX	5	3506	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
86	OHX	1	3450	-	0,6,6	-	-	-		
86	OHX	5	3593	-	0,6,6	-	-	-		
86	OHX	M9	201	-	0,6,6	-	-	-		
86	OHX	5	3419	-	0,6,6	-	-	-		
86	OHX	6	1933	-	0,6,6	-	-	-		
86	OHX	1	3459	-	0,6,6	-	-	-		
86	OHX	5	3634	-	0,6,6	-	-	-		
86	OHX	19	201	-	0,6,6	-	-	-		
86	OHX	8	202	-	0,6,6	-	-	-		
86	OHX	5	3573	-	0,6,6	-	-	-		
86	OHX	1	3658	-	0,6,6	-	-	-		
86	OHX	4	216	-	0,6,6	-	-	-		
86	OHX	6	1929	-	0,6,6	-	-	-		
86	OHX	1	3574	-	0,6,6	-	-	-		
86	OHX	6	2030	-	0,6,6	-	-	-		
86	OHX	1	3482	-	0,6,6	-	-	-		
86	OHX	1	3673	-	0,6,6	-	-	-		
86	OHX	6	1990	-	0,6,6	-	-	-		
86	OHX	2	1957	-	0,6,6	-	-	-		
86	OHX	6	1952	-	0,6,6	-	-	-		
86	OHX	6	1975	-	0,6,6	-	-	-		
86	OHX	5	3703	-	0,6,6	-	-	-		
86	OHX	2	1992	-	0,6,6	-	-	-		
86	OHX	1	3611	-	0,6,6	-	-	-		
86	OHX	1	3696	-	0,6,6	-	-	-		
86	OHX	5	3414	-	0,6,6	-	-	-		
86	OHX	2	1993	-	0,6,6	-	-	-		
86	OHX	5	3644	-	0,6,6	-	-	-		
86	OHX	2	2020	-	0,6,6	-	-	-		
86	OHX	5	3684	-	0,6,6	-	-	-		
86	OHX	13	402	-	0,6,6	-	-	-		
86	OHX	5	3564	-	0,6,6	-	-	-		
86	OHX	2	1917	-	0,6,6	-	-	-		
86	OHX	5	3461	-	0,6,6	-	-	-		
86	OHX	5	3603	-	0,6,6	-	-	-		
86	OHX	1	3481	-	0,6,6	-	-	-		
86	OHX	6	1985	-	0,6,6	-	-	-		
86	OHX	1	3513	-	0,6,6	-	-	-		
86	OHX	6	1909	-	0,6,6	-	-	-		
86	OHX	4	206	-	0,6,6	-	-	-		
86	OHX	6	1994	-	0,6,6	-	-	-		
86	OHX	6	1981	-	0,6,6	-	-	-		
86	OHX	8	208	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
86	OHX	6	1905	-	0,6,6	-	-	-		
86	OHX	1	3591	-	0,6,6	-	-	-		
86	OHX	1	3627	-	0,6,6	-	-	-		
86	OHX	1	3443	-	0,6,6	-	-	-		
86	OHX	1	3617	-	0,6,6	-	-	-		
86	OHX	5	3522	-	0,6,6	-	-	-		
86	OHX	1	3444	-	0,6,6	-	-	-		
86	OHX	1	3465	-	0,6,6	-	-	-		
86	OHX	1	3519	-	0,6,6	-	-	-		
86	OHX	1	3600	-	0,6,6	-	-	-		
86	OHX	1	3469	-	0,6,6	-	-	-		
86	OHX	6	2029	-	0,6,6	-	-	-		
86	OHX	1	3434	-	0,6,6	-	-	-		
86	OHX	1	3531	-	0,6,6	-	-	-		
86	OHX	1	3453	-	0,6,6	-	-	-		
86	OHX	l3	401	-	0,6,6	-	-	-		
86	OHX	6	1988	-	0,6,6	-	-	-		
86	OHX	5	3613	-	0,6,6	-	-	-		
86	OHX	c3	201	-	0,6,6	-	-	-		
86	OHX	1	3629	-	0,6,6	-	-	-		
86	OHX	5	3518	-	0,6,6	-	-	-		

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
89	UAM	6	2134	-	-	14/28/40/40	0/2/2/2

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
89	6	2134	UAM	CAZ-CAN-CAS	2.30	115.82	112.65

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
89	6	2134	UAM	NAQ-CAT-CBA-OAI

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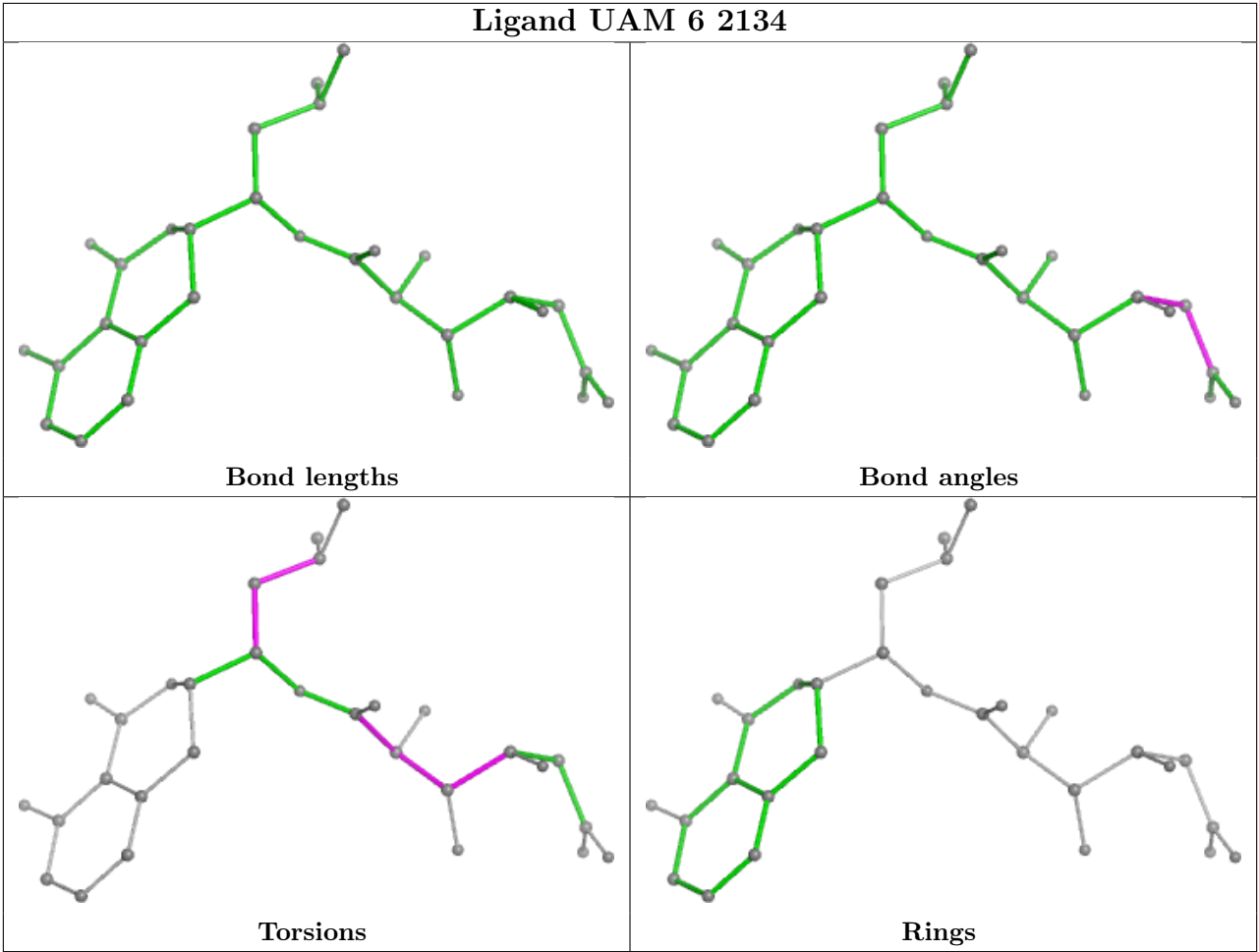
Mol	Chain	Res	Type	Atoms
89	6	2134	UAM	NAQ-CAT-CBA-CBB
89	6	2134	UAM	OAF-CAT-CBA-OAI
89	6	2134	UAM	OAF-CAT-CBA-CBB
89	6	2134	UAM	CAT-CBA-CBB-OAJ
89	6	2134	UAM	CAT-CBA-CBB-CAZ
89	6	2134	UAM	OAI-CBA-CBB-OAJ
89	6	2134	UAM	CBC-CAP-CAY-CAA
89	6	2134	UAM	CBC-CAP-CAY-CAB
89	6	2134	UAM	CAY-CAP-CBC-NAQ
89	6	2134	UAM	OAI-CBA-CBB-CAZ
89	6	2134	UAM	CAN-CAZ-CBB-CBA
89	6	2134	UAM	NAD-CAZ-CBB-OAJ
89	6	2134	UAM	NAD-CAZ-CBB-CBA

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
86	C8	201	OHX	0	1

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 than 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.



5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	2	2
82	m2	2
80	sM	1
68	O2	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	sM	139:UNK	C	155:UNK	N	37.77

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	2	1716:C	O3'	1717:G	P	4.09
1	m2	23:UNK	C	28:UNK	N	3.84
1	m2	52:UNK	C	54:UNK	N	3.47
1	2	1685:G	O3'	1686:C	P	3.06
1	O2	51:SER	C	52:GLN	N	1.19

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

EDS failed to run properly - this section is therefore empty.

### 6.2 Non-standard residues in protein, DNA, RNA chains

EDS failed to run properly - this section is therefore empty.

### 6.3 Carbohydrates

EDS failed to run properly - this section is therefore empty.

### 6.4 Ligands

EDS failed to run properly - this section is therefore empty.

### 6.5 Other polymers

EDS failed to run properly - this section is therefore empty.