Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 04:11 am BST

PDB ID	:	4DR6
Title	:	Crystal structure of the Thermus thermophilus (HB8) 30S ribosomal subunit with codon, near-cognate transfer RNA anticodon stem-loop mismatched at the first codon position and streptomycin bound
Authors	:	Demirci, H.; Murphy IV, F.; Murphy, E.; Gregory, S.T.; Dahlberg, A.E.; Jogl, G.
Deposited on	:	2012-02-16
Resolution	:	3.30 Å(reported)

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

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

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

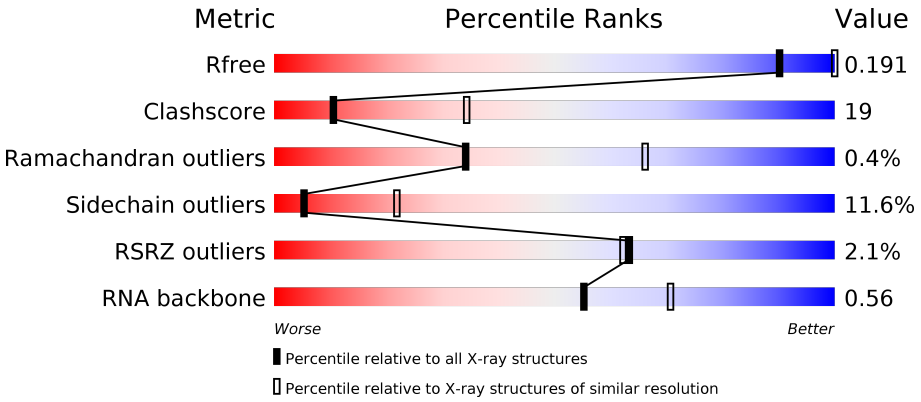
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.30 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1149 (3.34-3.26)
Clashscore	141614	1205 (3.34-3.26)
Ramachandran outliers	138981	1183 (3.34-3.26)
Sidechain outliers	138945	1182 (3.34-3.26)
RSRZ outliers	127900	1115 (3.34-3.26)
RNA backbone	3102	1117 (3.70-2.90)

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

Mol	Chain	Length	Quality of chain
1	A	1522	50% 38% 11%
2	B	256	2% 44% 43% 5% 8%
3	C	239	2% 44% 36% 7% 13%
4	D	209	3% 56% 37% 7%

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Mol	Chain	Length	Quality of chain
5	E	162	49% 35% 9% 7%
6	F	101	% 50% 46% 5%
7	G	156	2% 60% 33% 6%
8	H	138	% 60% 36%
9	I	128	9% 51% 45%
10	J	105	10% 36% 51% 7% 6%
11	K	129	57% 31% 9%
12	L	135	4% 52% 32% 9% 7%
13	M	126	5% 52% 33% 10% 6%
14	N	61	3% 38% 52% 8%
15	O	89	2% 52% 40% 7%
16	P	88	% 64% 28% 5%
17	Q	105	% 52% 38% 5% 5%
18	R	88	% 40% 38% 19%
19	S	93	3% 47% 33% 5% 13%
20	T	106	% 47% 38% 8% 7%
21	U	27	7% 56% 30% 7% 7%
22	V	4	75% 75% 25%
23	W	9	78% 44% 44% 11%
24	a	11	73% 27%
25	b	3	33% 33% 33% 33%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
26	MG	A	1605	-	-	-	X
26	MG	A	1623	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
26	MG	A	1669	-	-	-	X
26	MG	A	1681	-	-	-	X
26	MG	A	1685	-	-	-	X
26	MG	A	1732	-	-	-	X
26	MG	A	1738	-	-	-	X
26	MG	A	1741	-	-	-	X
26	MG	A	1742	-	-	-	X
26	MG	A	1744	-	-	-	X
26	MG	A	1758	-	-	-	X
26	MG	A	1769	-	-	-	X
26	MG	A	1774	-	-	-	X
26	MG	A	1775	-	-	-	X
26	MG	A	1776	-	-	-	X
26	MG	A	1777	-	-	-	X
26	MG	A	1783	-	-	-	X
26	MG	A	1787	-	-	-	X
26	MG	A	1789	-	-	-	X
26	MG	A	1790	-	-	-	X
26	MG	A	1791	-	-	-	X
26	MG	A	1803	-	-	-	X
26	MG	A	1816	-	-	-	X
26	MG	A	1905	-	-	-	X
26	MG	A	1910	-	-	-	X
26	MG	A	1911	-	-	-	X
26	MG	A	1913	-	-	-	X
26	MG	A	1923	-	-	-	X
26	MG	A	1924	-	-	-	X
26	MG	A	1925	-	-	-	X
26	MG	A	1926	-	-	-	X
26	MG	A	1932	-	-	-	X
26	MG	A	1933	-	-	-	X
26	MG	A	1940	-	-	-	X
26	MG	A	1949	-	-	-	X
26	MG	A	1950	-	-	-	X
26	MG	D	302	-	-	-	X
26	MG	G	201[A]	-	-	-	X
26	MG	G	201[B]	-	-	-	X
26	MG	P	101	-	-	-	X

2 Entry composition

There are 29 unique types of molecules in this entry. The entry contains 53550 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
1	A	1514	32546	14496	6020	10517	1513	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1534	C	A	CONFLICT	GB M26923.1
A	1535	A	C	CONFLICT	GB M26923.1

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	236	1896	1211	337	343	5	0	0	1

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	207	1613	1016	315	281	1	0	0	1

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	D	208	1703	1066	339	291	7	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
5	E	151	1147	724	218	201	4	0	0	1

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	101	Total	C	N	O	S	0	0	0
			843	531	155	154	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	G	155	Total	C	N	O	S	0	0	0
			1257	781	252	218	6			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	138	Total	C	N	O	S	0	0	0
			1116	705	215	193	3			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
9	I	127	Total	C	N	O	0	0	0
			1010	639	197	174			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	J	99	Total	C	N	O	S	0	0	1
			793	498	157	137	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	117	Total	C	N	O	S	0	0	0
			873	543	166	161	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	L	125	Total	C	N	O	S	0	0	1
			973	612	196	163	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	M	118	Total	C	N	O	S	0	0	0
			937	579	193	163	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	N	60	Total	C	N	O	S	0	0	0
			492	312	104	72	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	O	88	Total	C	N	O	S	0	0	0
			734	459	147	126	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	P	84	Total	C	N	O	S	0	0	1
			701	443	140	117	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	Q	100	Total	C	N	O	S	0	0	0
			834	534	156	142	2			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Q	96	GLN	GLU	CONFLICT	UNP Q5SHP7

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
18	R	71	Total	C	N	O	0	0	0
			585	373	116	96			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	S	81	Total	C	N	O	S	0	0	1
			648	414	120	112	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	T	99	Total	C	N	O	S	0	0	0
			763	470	162	129	2			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
21	U	25	Total	C	N	O	0	0	1
			209	128	51	30			

- Molecule 22 is a RNA chain called 5'-R(*UP*UP*UP*U)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	V	4	Total	C	N	O	P	0	0	0
			77	36	8	30	3			

- Molecule 23 is a RNA chain called 5'-R(P*UP*UP*GP*AP*GP*GP*(PSU)P*GP*G)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	W	9	Total	C	N	O	P	0	0	0
			197	87	36	65	9			

- Molecule 24 is a RNA chain called 5'-R(P*CP*UP*UP*GP*AP*GP*GP*(PSU)P*GP*GP *U)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	a	11	Total	C	N	O	P	0	0	0
			237	105	41	80	11			

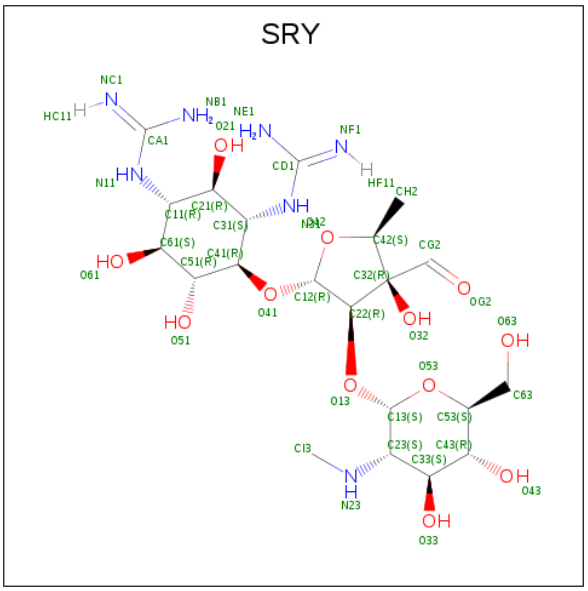
- Molecule 25 is a RNA chain called 5'-R(*UP*UP*U)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	b	2	Total	C	N	O	P	4	0	0
			40	18	4	16	2			

- Molecule 26 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
26	P	3	Total Mg 3 3	0	0
26	G	1	Total Mg 2 2	0	1
26	J	1	Total Mg 1 1	0	0
26	Q	1	Total Mg 1 1	0	0
26	D	3	Total Mg 3 3	0	0
26	E	3	Total Mg 3 3	0	0
26	H	1	Total Mg 1 1	0	0
26	A	355	Total Mg 355 355	0	0
26	T	1	Total Mg 1 1	0	0
26	N	1	Total Mg 1 1	0	0
26	L	1	Total Mg 1 1	0	0
26	S	3	Total Mg 3 3	0	0
26	F	2	Total Mg 2 2	0	0

- Molecule 27 is STREPTOMYCIN (three-letter code: SRY) (formula: $C_{21}H_{39}N_7O_{12}$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
27	A	1	Total	C	N	O	0	0
			40	21	7	12		

- Molecule 28 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
28	D	1	Total	Zn	0	0
			1	1		
28	N	1	Total	Zn	0	0
			1	1		

- Molecule 29 is water.

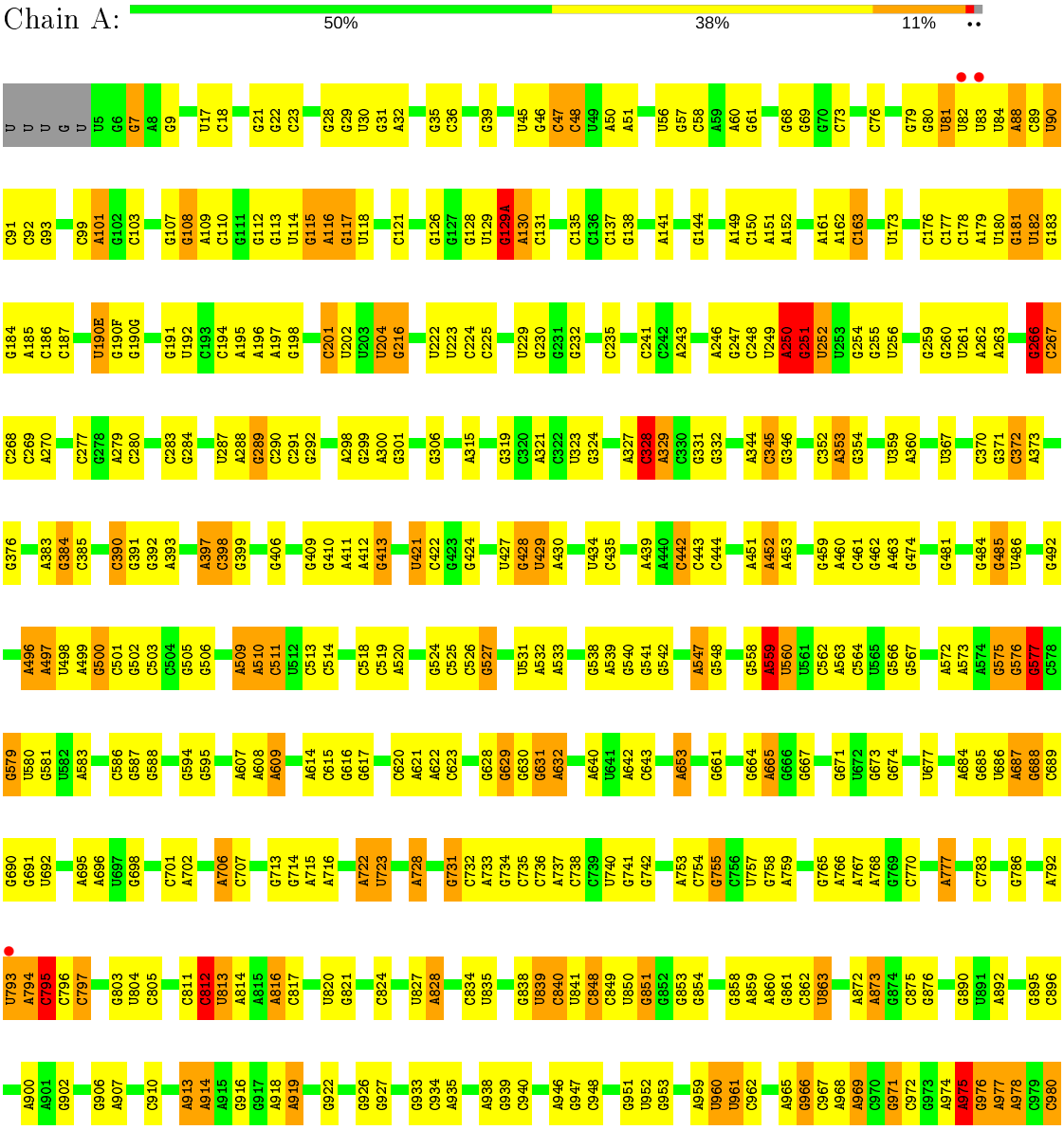
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
29	A	887	Total	O	0	0
			887	887		
29	C	1	Total	O	0	0
			1	1		
29	D	5	Total	O	0	0
			5	5		
29	E	5	Total	O	0	0
			5	5		
29	L	1	Total	O	0	0
			1	1		
29	N	1	Total	O	0	0
			1	1		
29	P	2	Total	O	0	0
			2	2		
29	S	2	Total	O	0	0
			2	2		
29	T	1	Total	O	0	0
			1	1		
29	U	2	Total	O	0	0
			2	2		

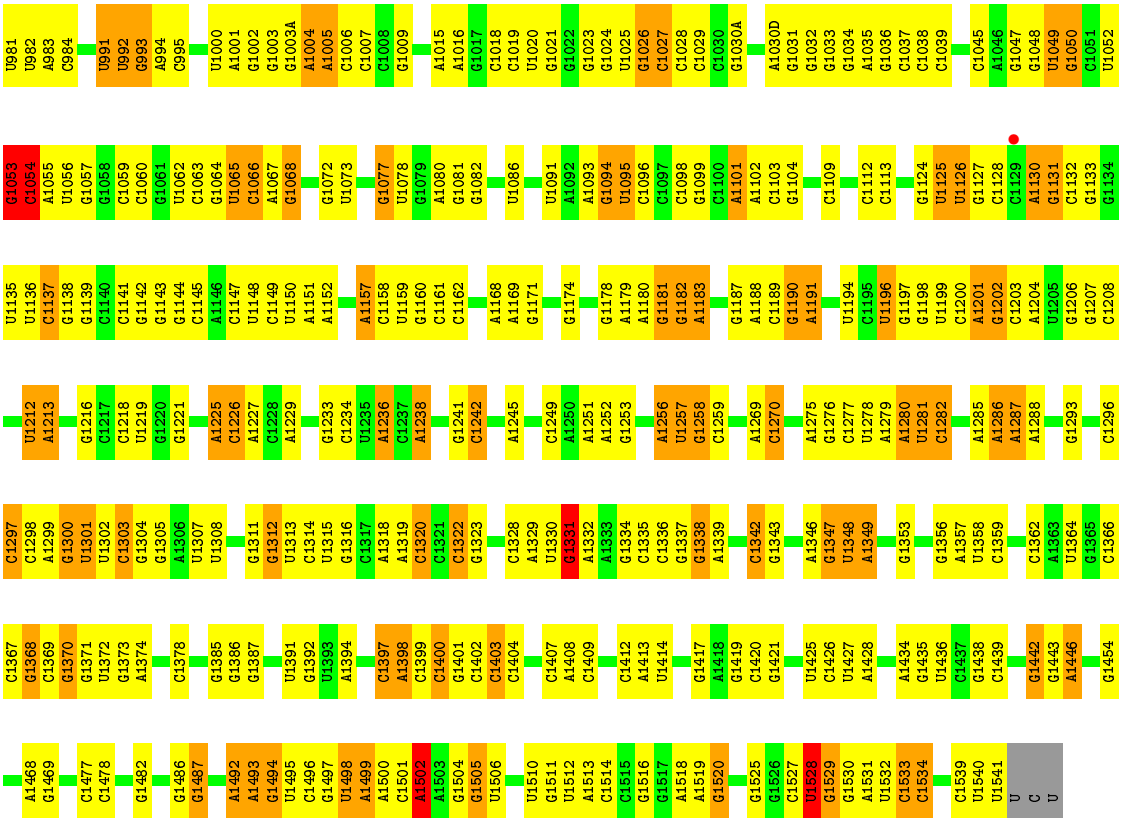
3 Residue-property plots (i)

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

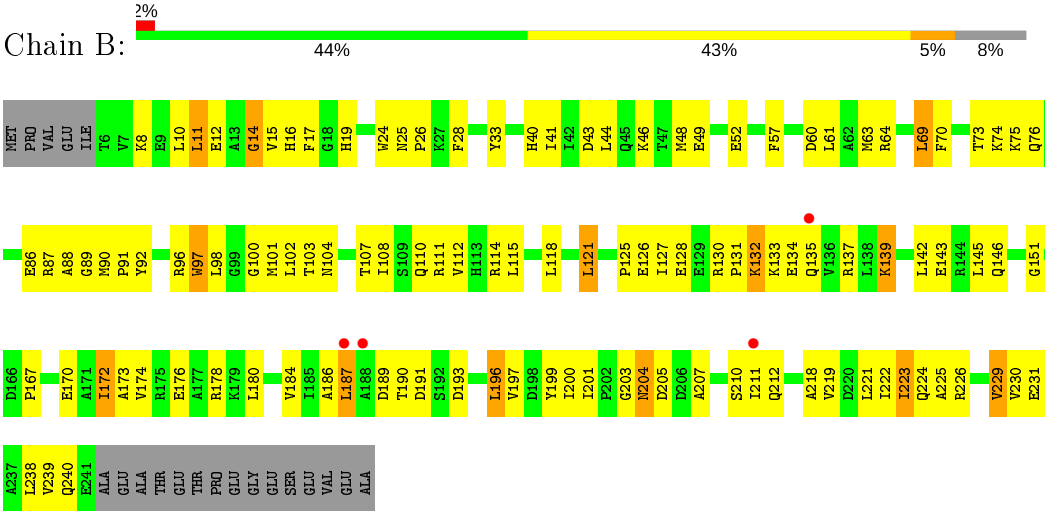
- Molecule 1: 16S rRNA

Chain A:

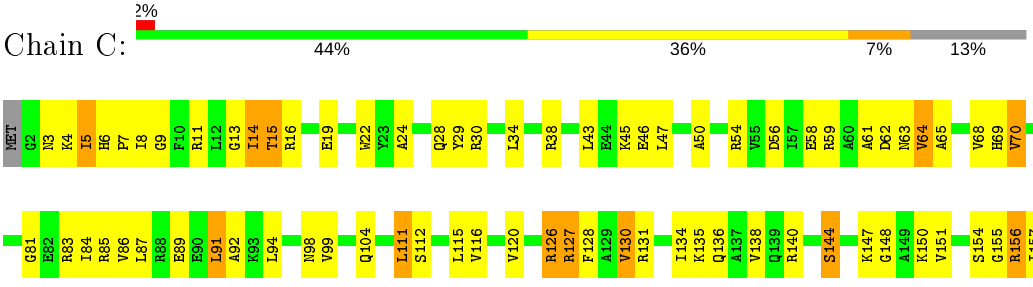


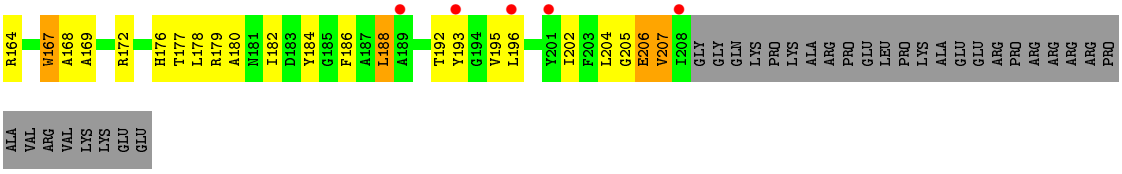


• Molecule 2: 30S ribosomal protein S2

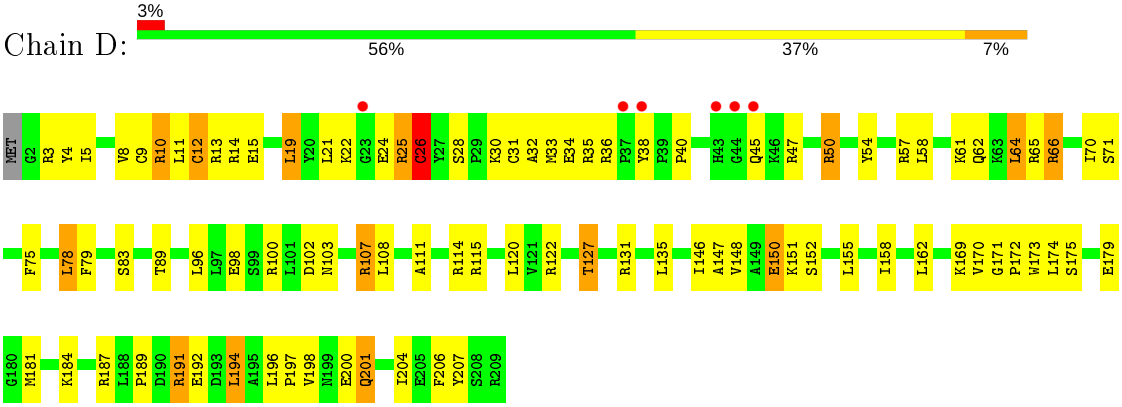


• Molecule 3: 30S ribosomal protein S3

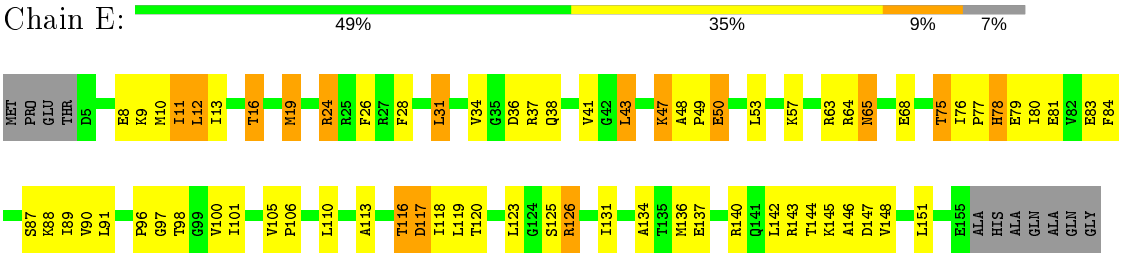




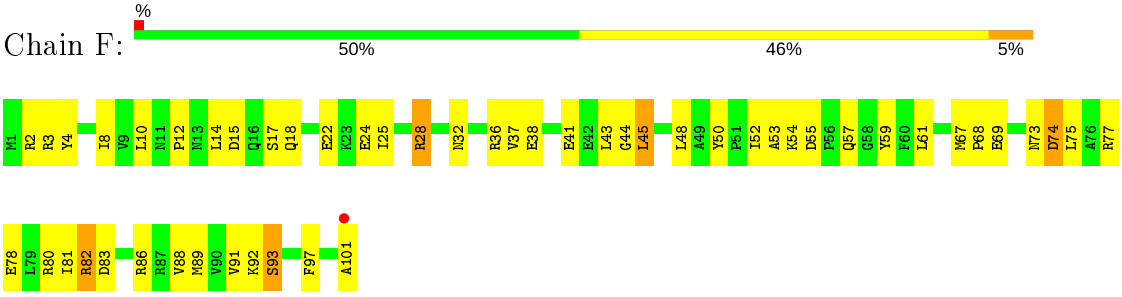
- Molecule 4: 30S ribosomal protein S4



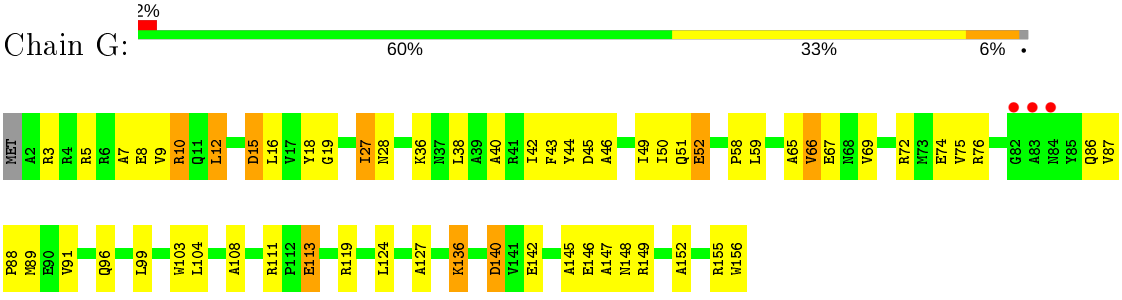
- Molecule 5: 30S ribosomal protein S5



- Molecule 6: 30S ribosomal protein S6

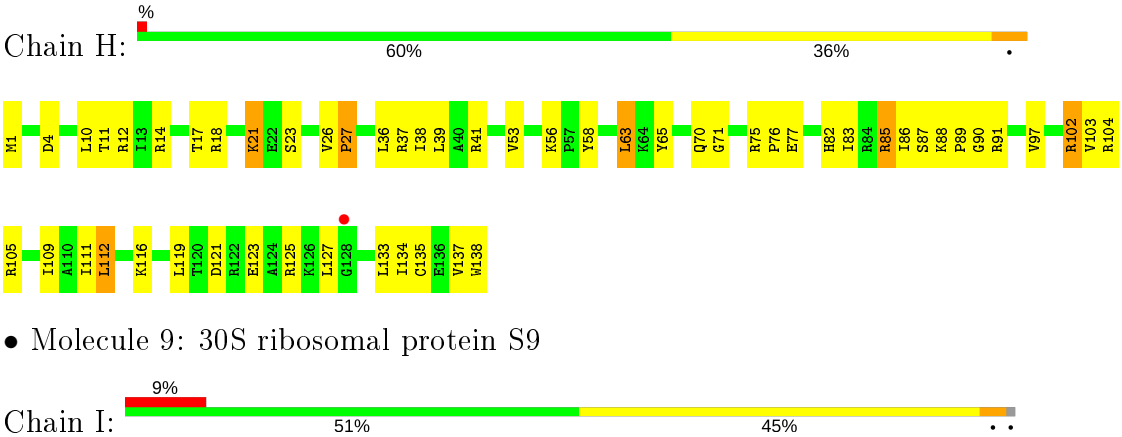


- Molecule 7: 30S ribosomal protein S7



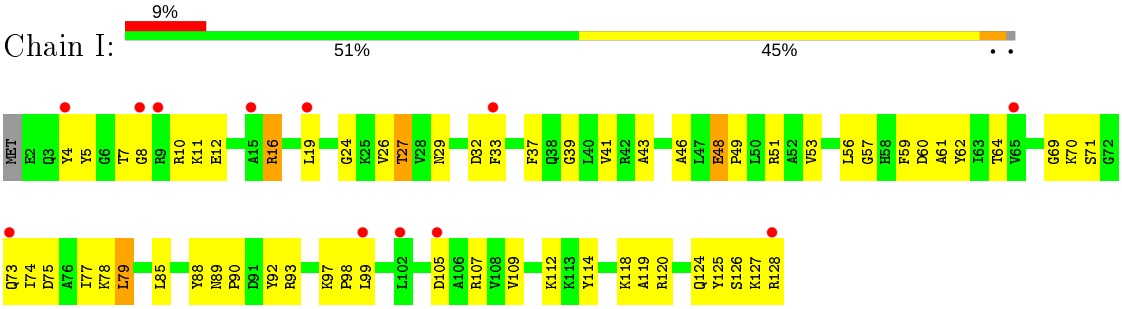
• Molecule 8: 30S ribosomal protein S8

Chain H:



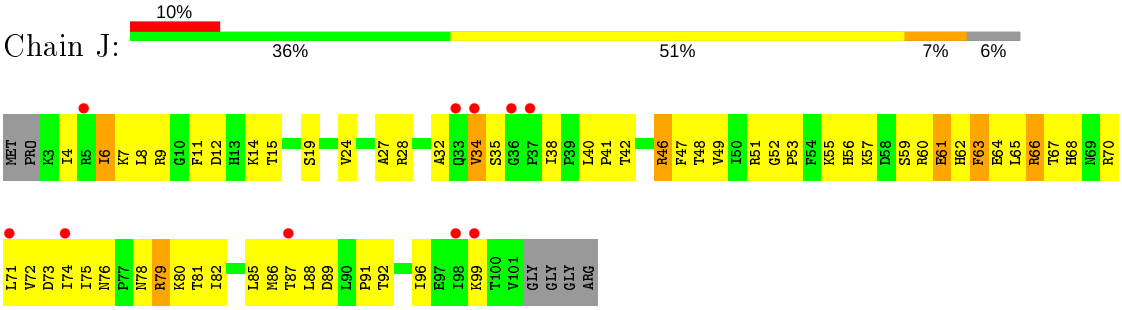
• Molecule 9: 30S ribosomal protein S9

Chain I:



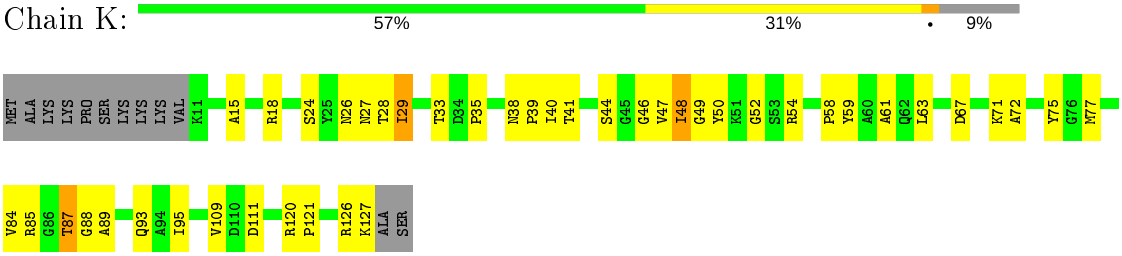
• Molecule 10: 30S ribosomal protein S10

Chain J:



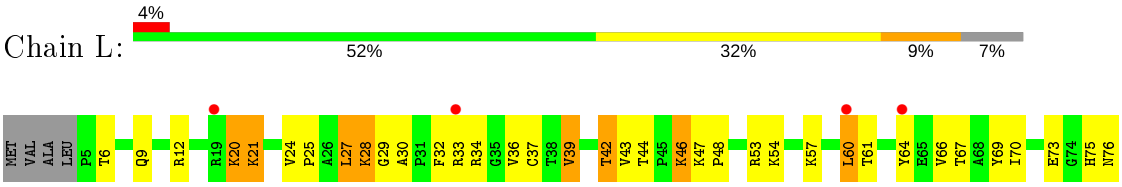
• Molecule 11: 30S ribosomal protein S11

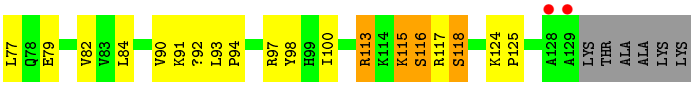
Chain K:



• Molecule 12: 30S ribosomal protein S12

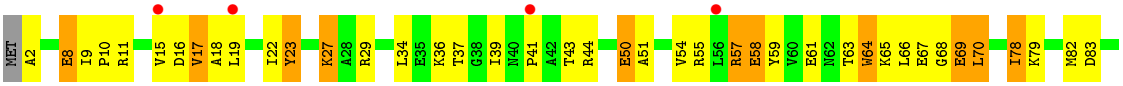
Chain L:

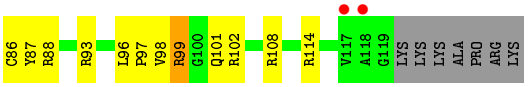




- Molecule 13: 30S ribosomal protein S13

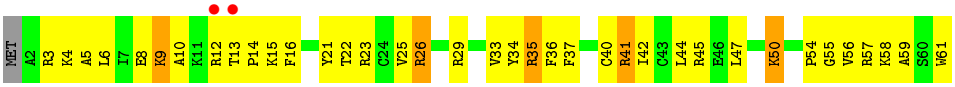
Chain M:





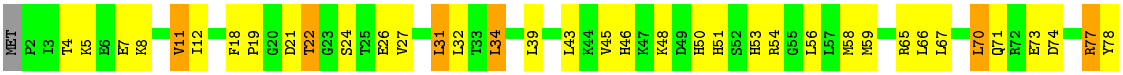
- Molecule 14: 30S ribosomal protein S14

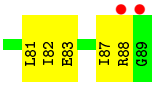
Chain N:



- Molecule 15: 30S ribosomal protein S15

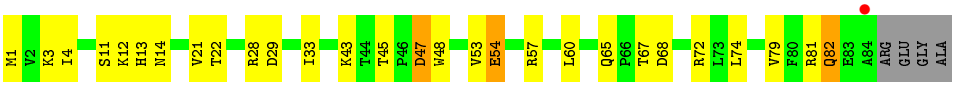
Chain O:





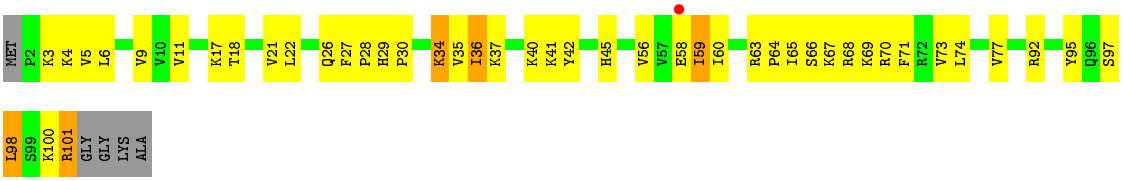
- Molecule 16: 30S ribosomal protein S16

Chain P:



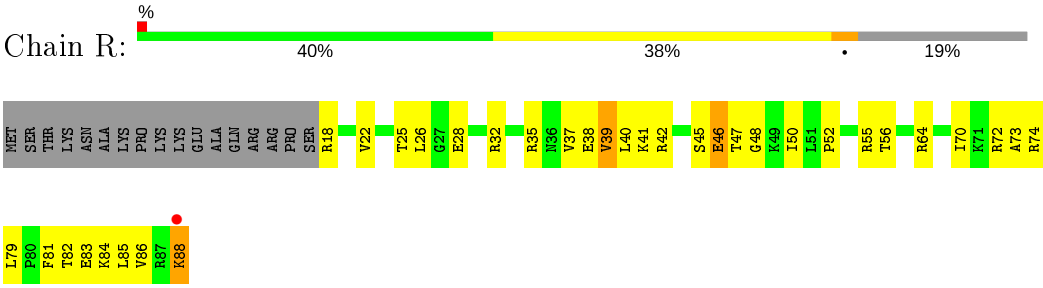
- Molecule 17: 30S ribosomal protein S17

Chain Q:



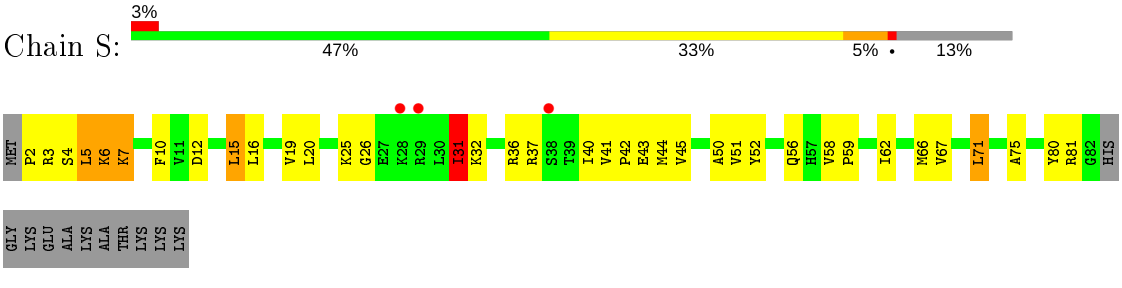
• Molecule 18: 30S ribosomal protein S18

Chain R:



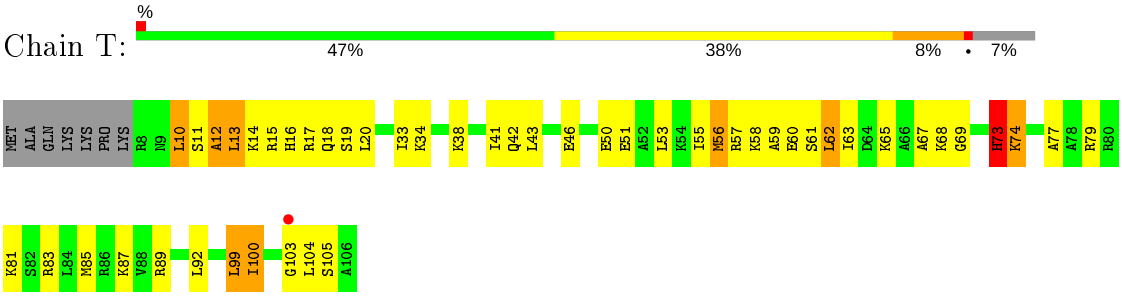
• Molecule 19: 30S ribosomal protein S19

Chain S:



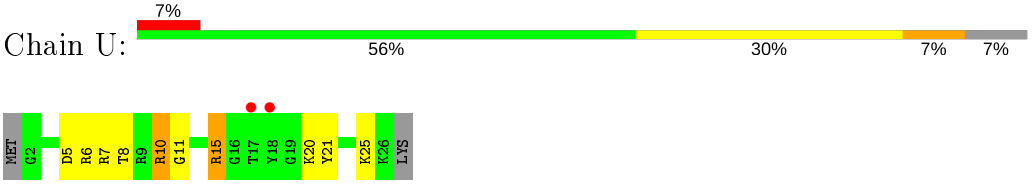
• Molecule 20: 30S ribosomal protein S20

Chain T:



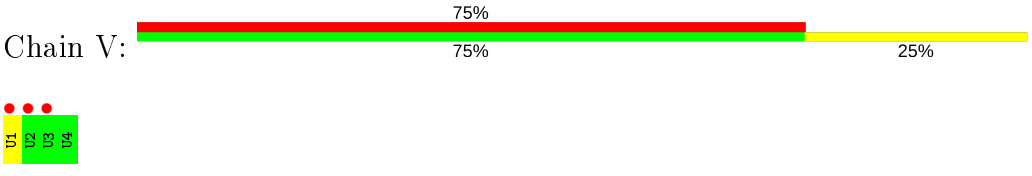
• Molecule 21: 30S ribosomal protein THX

Chain U:



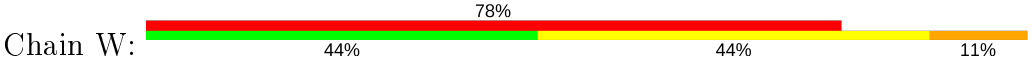
• Molecule 22: 5'-R(*UP*UP*UP*U)-3'

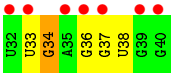
Chain V:



• Molecule 23: 5'-R(P*UP*UP*GP*AP*GP*GP*(PSU)P*GP*G)-3'

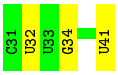
Chain W:





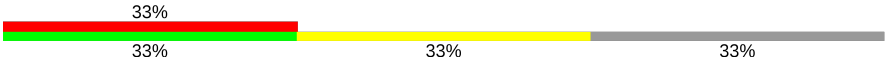
• Molecule 24: 5'-R(P*CP*UP*UP*GP*AP*GP*GP*(PSU)P*GP*GP*U)-3'

Chain a:



• Molecule 25: 5'-R(*UP*UP*U)-3'

Chain b:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α, β, γ	402.60Å 402.60Å 174.90Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.48 – 3.30 49.48 – 3.30	Depositor EDS
% Data completeness (in resolution range)	100.0 (49.48-3.30) 100.0 (49.48-3.30)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.41 (at 3.33Å)	Xtriage
Refinement program	PHENIX dev_978	Depositor
R, R_{free}	0.153 , 0.192 0.152 , 0.191	Depositor DCC
R_{free} test set	10751 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å^2)	112.1	Xtriage
Anisotropy	0.229	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 84.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	53550	wwPDB-VP
Average B, all atoms (Å^2)	120.0	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.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, M2G, MA6, 0TD, MG, 2MG, 5MC, UR3, 4OC, SRY, 7MG, PSU

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	A	0.58	2/36085 (0.0%)	0.99	68/56316 (0.1%)
2	B	0.37	0/1931	0.57	0/2607
3	C	0.34	0/1637	0.55	0/2207
4	D	0.42	1/1733 (0.1%)	0.59	1/2318 (0.0%)
5	E	0.50	0/1163	0.73	0/1566
6	F	0.32	0/856	0.54	0/1154
7	G	0.34	0/1276	0.53	0/1709
8	H	0.52	0/1136	0.71	0/1527
9	I	0.32	0/1029	0.56	1/1379 (0.1%)
10	J	0.35	0/806	0.58	0/1084
11	K	0.40	0/888	0.65	0/1198
12	L	0.47	0/978	0.69	0/1308
13	M	0.33	0/947	0.53	0/1270
14	N	0.38	0/501	0.53	0/664
15	O	0.40	0/745	0.59	0/992
16	P	0.49	0/717	0.69	0/965
17	Q	0.51	0/847	0.72	0/1131
18	R	0.39	0/590	0.59	0/782
19	S	0.30	0/662	0.56	0/892
20	T	0.45	0/765	0.71	0/1007
21	U	0.39	0/213	0.57	0/279
22	V	0.33	0/84	0.75	0/128
23	W	0.34	0/198	0.66	0/308
24	a	0.40	0/242	0.89	0/376
25	b	0.35	0/43	0.59	0/64
All	All	0.53	3/56072 (0.0%)	0.89	70/83231 (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	B	0	2
8	H	0	2
10	J	0	1
12	L	0	1
20	T	0	1
All	All	0	7

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1502	A	N9-C4	-5.33	1.34	1.37
1	A	609	A	N9-C4	-5.14	1.34	1.37
4	D	26	CYS	CB-SG	5.01	1.90	1.82

All (70) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	117	G	N1-C6-O6	11.81	126.99	119.90
1	A	1200	C	N1-C2-O2	7.96	123.67	118.90
1	A	795	C	C6-N1-C2	7.79	123.42	120.30
1	A	117	G	C5-C6-O6	-7.62	124.03	128.60
1	A	251	G	N1-C6-O6	-7.49	115.41	119.90
1	A	1200	C	C2-N1-C1'	7.47	127.02	118.80
1	A	1528	U	C2-N1-C1'	7.39	126.56	117.70
1	A	795	C	N3-C2-O2	7.19	126.93	121.90
1	A	1502	A	C2-N3-C4	-7.08	107.06	110.60
1	A	797	C	C6-N1-C2	6.99	123.10	120.30
1	A	266	G	C5-N7-C8	-6.95	100.83	104.30
1	A	277	C	C6-N1-C2	6.86	123.05	120.30
1	A	117	G	C6-C5-N7	-6.86	126.29	130.40
1	A	266	G	C8-N9-C4	-6.68	103.73	106.40
1	A	559	A	C8-N9-C4	-6.66	103.14	105.80
1	A	266	G	N7-C8-N9	6.42	116.31	113.10
1	A	1403	C	N1-C2-O2	-6.35	115.09	118.90
9	I	39	GLY	N-CA-C	-6.33	97.28	113.10
1	A	1053	G	C8-N9-C4	6.31	108.92	106.40
1	A	795	C	N1-C2-O2	-6.28	115.13	118.90
1	A	722	A	N1-C6-N6	6.06	122.24	118.60
1	A	971	G	C8-N9-C4	6.05	108.82	106.40
1	A	728	A	N1-C6-N6	6.03	122.22	118.60
1	A	129(A)	G	C4-N9-C1'	6.01	134.32	126.50
1	A	824	C	C6-N1-C2	5.92	122.67	120.30
1	A	583	A	C8-N9-C4	5.91	108.16	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1331	G	C8-N9-C4	-5.77	104.09	106.40
1	A	1200	C	C5-C6-N1	5.75	123.87	121.00
1	A	1200	C	C6-N1-C1'	-5.70	113.96	120.80
1	A	559	A	N9-C4-C5	5.68	108.07	105.80
1	A	812	C	C2-N1-C1'	5.66	125.02	118.80
1	A	1342	C	N1-C2-O2	-5.56	115.56	118.90
1	A	1528	U	N3-C2-O2	-5.56	118.31	122.20
1	A	117	G	N9-C4-C5	-5.54	103.18	105.40
1	A	1077	G	C8-N9-C4	5.54	108.61	106.40
1	A	735	C	C6-N1-C2	5.53	122.51	120.30
1	A	783	C	C6-N1-C2	5.53	122.51	120.30
1	A	266	G	N3-C4-N9	-5.52	122.69	126.00
1	A	328	C	C5-C4-N4	5.51	124.06	120.20
1	A	328	C	N3-C4-N4	-5.47	114.17	118.00
1	A	1403	C	N3-C2-O2	5.47	125.73	121.90
1	A	1528	U	N1-C2-O2	5.46	126.62	122.80
1	A	283	C	C5-C6-N1	5.44	123.72	121.00
1	A	251	G	N3-C4-C5	-5.42	125.89	128.60
1	A	1242	C	C6-N1-C2	5.39	122.46	120.30
4	D	12	CYS	CA-CB-SG	5.37	123.67	114.00
1	A	583	A	N1-C6-N6	5.35	121.81	118.60
1	A	753	A	N9-C4-C5	5.32	107.93	105.80
1	A	129(A)	G	C8-N9-C4	-5.31	104.27	106.40
1	A	1417	G	N3-C4-C5	-5.30	125.95	128.60
1	A	306	G	N1-C6-O6	5.27	123.06	119.90
1	A	919	A	C8-N9-C4	5.26	107.90	105.80
1	A	795	C	C2-N1-C1'	-5.21	113.06	118.80
1	A	1525	G	N1-C6-O6	-5.17	116.80	119.90
1	A	117	G	N3-C2-N2	-5.17	116.28	119.90
1	A	135	C	C2-N1-C1'	-5.15	113.14	118.80
1	A	250	A	N1-C6-N6	5.14	121.69	118.60
1	A	1054	C	N1-C2-O2	5.13	121.98	118.90
1	A	241	C	N1-C2-O2	-5.13	115.82	118.90
1	A	559	A	N1-C6-N6	-5.13	115.52	118.60
1	A	284	G	C5-C6-O6	-5.12	125.53	128.60
1	A	577	G	C8-N9-C4	5.10	108.44	106.40
1	A	975	A	C5-N7-C8	-5.09	101.35	103.90
1	A	863	U	C6-N1-C2	5.08	124.05	121.00
1	A	283	C	C6-N1-C2	-5.07	118.27	120.30
1	A	706	A	N1-C6-N6	5.05	121.63	118.60
1	A	753	A	N1-C6-N6	-5.05	115.57	118.60
1	A	1502	A	N1-C6-N6	5.04	121.62	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	117	G	C5-C6-N1	-5.03	108.98	111.50
1	A	722	A	C2-N3-C4	-5.03	108.09	110.60

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	14	GLY	Peptide
2	B	89	GLY	Peptide
8	H	27	PRO	Peptide
8	H	90	GLY	Peptide
10	J	61	GLU	Peptide
12	L	46	LYS	Peptide
20	T	12	ALA	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	32546	0	16456	740	0
2	B	1896	0	1936	103	0
3	C	1613	0	1677	108	0
4	D	1703	0	1763	79	0
5	E	1147	0	1207	75	0
6	F	843	0	857	42	0
7	G	1257	0	1296	51	0
8	H	1116	0	1177	39	0
9	I	1010	0	1037	55	0
10	J	793	0	835	70	0
11	K	873	0	894	35	0
12	L	973	0	1058	50	0
13	M	937	0	995	48	0
14	N	492	0	529	51	0
15	O	734	0	771	37	0
16	P	701	0	720	22	0
17	Q	834	0	906	41	0
18	R	585	0	657	37	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	S	648	0	673	45	0
20	T	763	0	861	63	0
21	U	209	0	221	13	0
22	V	77	0	42	1	0
23	W	197	0	97	6	0
24	a	237	0	118	0	0
25	b	40	0	21	0	0
26	A	355	0	0	0	0
26	D	3	0	0	0	0
26	E	3	0	0	0	0
26	F	2	0	0	0	0
26	G	2	0	0	0	0
26	H	1	0	0	0	0
26	J	1	0	0	0	0
26	L	1	0	0	0	0
26	N	1	0	0	0	0
26	P	3	0	0	0	0
26	Q	1	0	0	0	0
26	S	3	0	0	0	0
26	T	1	0	0	0	0
27	A	40	0	37	9	0
28	D	1	0	0	0	0
28	N	1	0	0	0	0
29	A	887	0	0	41	0
29	C	1	0	0	0	0
29	D	5	0	0	0	0
29	E	5	0	0	0	0
29	L	1	0	0	0	0
29	N	1	0	0	0	0
29	P	2	0	0	0	0
29	S	2	0	0	0	0
29	T	1	0	0	0	0
29	U	2	0	0	0	0
All	All	53550	0	36841	1642	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 19.

All (1642) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:126:ARG:HH11	5:E:126:ARG:HG2	1.10	1.09
13:M:99:ARG:HB2	13:M:101:GLN:HE22	1.14	1.06
5:E:11:ILE:HG22	5:E:31:LEU:HB3	1.41	1.03
17:Q:27:PHE:CE1	17:Q:36:ILE:HD11	1.93	1.02
2:B:88:ALA:HB2	2:B:219:VAL:HG13	1.41	1.00
20:T:67:ALA:O	20:T:73:HIS:HB3	1.61	1.00
11:K:15:ALA:HA	11:K:77:MET:HA	1.42	0.98
1:A:279:A:OP2	17:Q:95:TYR:OH	1.79	0.98
3:C:58:GLU:HB3	10:J:92:THR:HG21	1.44	0.97
10:J:48:THR:HA	10:J:62:HIS:HB3	1.42	0.97
1:A:542:G:OP1	4:D:10:ARG:NH2	1.98	0.96
1:A:413:G:N2	1:A:429:U:OP2	1.99	0.96
13:M:8:GLU:HG2	13:M:22:ILE:HA	1.46	0.95
12:L:27:LEU:O	12:L:29:GLY:N	2.00	0.94
1:A:664:G:H22	1:A:741:G:H1	1.04	0.94
1:A:1256:A:H4'	1:A:1257:U:O5'	1.68	0.93
1:A:975:A:H4'	1:A:976:G:H5"	1.51	0.93
11:K:18:ARG:NH1	11:K:35:PRO:O	2.03	0.91
1:A:298:A:N6	29:A:2233:HOH:O	2.02	0.91
21:U:10:ARG:HG3	21:U:10:ARG:HH11	1.32	0.91
1:A:328:C:O2	1:A:328:C:H2'	1.70	0.89
1:A:834:C:N4	29:A:2826:HOH:O	2.04	0.89
1:A:235:C:H5'	17:Q:70:ARG:HG2	1.55	0.89
1:A:975:A:H5'	1:A:975:A:H8	1.37	0.87
1:A:1124:G:N7	1:A:1145:C:O2'	2.05	0.87
1:A:1147:C:O2	9:I:16:ARG:NH2	2.07	0.87
13:M:37:THR:HG23	13:M:39:ILE:HG13	1.55	0.87
1:A:1054:C:H3'	1:A:1054:C:O2	1.75	0.86
19:S:80:TYR:CE1	19:S:81:ARG:HG2	2.10	0.86
10:J:49:VAL:HG23	14:N:41:ARG:HB2	1.55	0.86
10:J:55:LYS:HG2	10:J:56:HIS:H	1.39	0.86
1:A:372:C:O2'	29:A:2764:HOH:O	1.94	0.85
5:E:144:THR:O	5:E:148:VAL:HG23	1.76	0.85
1:A:1057:G:H5"	3:C:154:SER:HB2	1.58	0.85
1:A:1030(A):G:N2	1:A:1030(D):A:OP2	2.10	0.84
14:N:3:ARG:NH2	14:N:6:LEU:HD21	1.92	0.84
1:A:1314:C:OP2	19:S:6:LYS:HD3	1.78	0.83
7:G:152:ALA:O	7:G:155:ARG:NH1	2.11	0.83
2:B:212:GLN:HE21	2:B:235:SER:HB2	1.44	0.83
20:T:74:LYS:HB3	20:T:74:LYS:NZ	1.91	0.83
1:A:1305:G:N2	1:A:1331:G:H1'	1.93	0.83
5:E:24:ARG:HH11	5:E:24:ARG:HG3	1.42	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:80:ILE:HD12	2:B:80:ILE:H	1.42	0.82
1:A:835:U:OP1	18:R:64:ARG:NH2	2.12	0.82
15:O:26:GLU:OE1	15:O:77:ARG:NH1	2.13	0.82
7:G:38:LEU:O	7:G:42:ILE:HG13	1.79	0.82
1:A:1143:G:H2'	1:A:1144:G:C8	2.14	0.82
1:A:353:A:H5'	1:A:353:A:H8	1.42	0.82
5:E:126:ARG:HG2	5:E:126:ARG:NH1	1.89	0.82
1:A:266:G:O2'	1:A:267:C:OP2	1.98	0.82
12:L:6:THR:OG1	12:L:9:GLN:HG3	1.79	0.81
1:A:1366:C:H2'	1:A:1367:C:H6	1.45	0.81
1:A:499:A:H4'	1:A:500:G:OP1	1.77	0.81
1:A:1347:G:O2'	1:A:1348:U:OP2	1.97	0.81
10:J:63:PHE:HB2	14:N:57:ARG:O	1.80	0.81
1:A:61:G:O2'	29:A:2002:HOH:O	2.00	0.80
1:A:1225:A:H5'	1:A:1226:C:OP2	1.82	0.80
3:C:54:ARG:NH2	3:C:56:ASP:OD1	2.15	0.79
10:J:24:VAL:HG13	10:J:34:VAL:HG11	1.63	0.79
12:L:28:LYS:HE2	12:L:33:ARG:HH12	1.47	0.79
4:D:201:GLN:NE2	5:E:116:THR:HG22	1.98	0.79
1:A:991:U:O2'	1:A:992:U:O5'	1.98	0.78
1:A:1125:U:H3'	1:A:1126:U:C5	2.19	0.78
12:L:27:LEU:C	12:L:29:GLY:H	1.84	0.78
1:A:1412:C:H2'	1:A:1413:A:C8	2.19	0.78
7:G:45:ASP:O	7:G:49:ILE:HG13	1.84	0.78
1:A:953:G:H5'	1:A:965:A:H61	1.49	0.78
19:S:40:ILE:HG22	19:S:67:VAL:HA	1.65	0.78
1:A:1047:G:H5"	14:N:4:LYS:HD3	1.67	0.77
3:C:130:VAL:O	3:C:134:ILE:HG13	1.83	0.77
1:A:580:U:H2'	1:A:581:G:O4'	1.85	0.77
5:E:24:ARG:HH11	5:E:24:ARG:CG	1.96	0.77
15:O:45:VAL:HG12	15:O:46:HIS:N	1.98	0.77
1:A:1148:U:H2'	1:A:1149:C:O4'	1.84	0.77
2:B:130:ARG:HB3	2:B:131:PRO:HD2	1.66	0.77
1:A:1003:G:N2	1:A:1039:C:O2	2.18	0.77
11:K:33:THR:HG22	11:K:39:PRO:HA	1.67	0.77
1:A:1281:U:H4'	1:A:1282:C:OP2	1.85	0.77
1:A:975:A:H5'	1:A:975:A:C8	2.20	0.77
13:M:99:ARG:HB2	13:M:101:GLN:NE2	1.96	0.77
1:A:1196:U:O2'	29:A:2247:HOH:O	2.03	0.76
1:A:793:U:H3'	1:A:794:A:H5"	1.65	0.76
1:A:1314:C:C5	19:S:6:LYS:HE2	2.18	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:Q:68:ARG:H	17:Q:70:ARG:NH1	1.83	0.76
19:S:15:LEU:HD13	19:S:16:LEU:N	2.00	0.76
3:C:155:GLY:O	3:C:196:LEU:HD22	1.86	0.76
1:A:677:U:H3	1:A:713:G:H22	1.33	0.76
1:A:560:U:H5"	1:A:566:G:N2	2.00	0.76
1:A:664:G:OP1	18:R:64:ARG:NH1	2.19	0.76
18:R:47:THR:HG22	18:R:48:GLY:N	2.00	0.75
19:S:40:ILE:HG23	19:S:62:ILE:HD11	1.67	0.75
8:H:102:ARG:H	8:H:102:ARG:CD	1.98	0.75
19:S:36:ARG:NH2	19:S:75:ALA:O	2.19	0.75
2:B:101:MET:HA	2:B:108:ILE:HG13	1.68	0.75
1:A:117:G:OP2	29:A:2018:HOH:O	2.04	0.75
7:G:10:ARG:HH11	7:G:10:ARG:HG2	1.49	0.75
1:A:1003(A):G:N2	1:A:1038:C:O2	2.19	0.75
2:B:75:LYS:HA	2:B:78:GLN:HG3	1.66	0.75
6:F:97:PHE:HB2	18:R:32:ARG:NH1	2.01	0.74
1:A:1347:G:O2'	1:A:1348:U:P	2.45	0.74
1:A:1124:G:H5'	10:J:35:SER:HB2	1.68	0.74
10:J:48:THR:HA	10:J:62:HIS:CB	2.17	0.74
1:A:254:G:OP1	17:Q:67:LYS:O	2.05	0.74
3:C:130:VAL:HG11	3:C:157:ILE:HG23	1.67	0.74
5:E:83:GLU:HG2	5:E:88:LYS:HD2	1.69	0.74
7:G:136:LYS:NZ	7:G:140:ASP:OD1	2.16	0.74
17:Q:101:ARG:HD3	17:Q:101:ARG:H	1.50	0.74
1:A:235:C:N4	29:A:2119:HOH:O	2.20	0.74
1:A:839:U:O2	1:A:839:U:H2'	1.88	0.74
17:Q:67:LYS:O	17:Q:68:ARG:HB2	1.85	0.74
3:C:6:HIS:CD2	3:C:8:ILE:HB	2.23	0.74
10:J:78:ASN:OD1	10:J:79:ARG:NH1	2.21	0.74
1:A:1338:G:H2'	1:A:1339:A:C8	2.24	0.73
1:A:1391:U:H2'	1:A:1392:G:C8	2.23	0.73
1:A:1287:A:H2'	1:A:1288:A:C8	2.22	0.73
1:A:130:A:OP2	1:A:190(E):U:O2'	2.06	0.73
1:A:1502:A:H2	1:A:1505:G:H1	1.34	0.73
5:E:41:VAL:HG13	5:E:113:ALA:HA	1.70	0.73
13:M:78:ILE:HG22	13:M:79:LYS:N	2.03	0.73
10:J:55:LYS:CG	10:J:56:HIS:H	2.01	0.73
13:M:79:LYS:NZ	13:M:83:ASP:OD1	2.21	0.73
20:T:13:LEU:HD12	20:T:14:LYS:N	2.04	0.73
3:C:13:GLY:HA3	14:N:57:ARG:HH22	1.54	0.73
7:G:75:VAL:HG21	7:G:86:GLN:HB3	1.70	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1001:A:H2'	1:A:1002:G:H8	1.52	0.72
1:A:1143:G:H2'	1:A:1144:G:H8	1.55	0.72
2:B:16:HIS:HB3	2:B:44:LEU:HD21	1.72	0.72
1:A:527:7MG:OP2	27:A:1956:SRY:O32	2.05	0.72
17:Q:27:PHE:CZ	17:Q:36:ILE:HD11	2.23	0.72
1:A:1366:C:H2'	1:A:1367:C:C6	2.24	0.72
1:A:1279:A:H5"	1:A:1280:A:OP1	1.90	0.72
2:B:118:LEU:HB3	2:B:142:LEU:HD12	1.72	0.72
13:M:15:VAL:HG23	13:M:43:THR:O	1.90	0.72
1:A:1387:G:O2'	29:A:2237:HOH:O	2.08	0.71
7:G:146:GLU:HA	7:G:149:ARG:HG2	1.72	0.71
1:A:1435:G:H2'	1:A:1436:U:C6	2.24	0.71
4:D:32:ALA:HA	4:D:35:ARG:HB2	1.73	0.71
3:C:134:ILE:HG22	3:C:168:ALA:HB3	1.71	0.71
18:R:47:THR:HG22	18:R:48:GLY:H	1.53	0.71
1:A:640:A:N6	29:A:2098:HOH:O	2.23	0.71
1:A:92:C:O2'	1:A:93:G:H5'	1.90	0.71
4:D:201:GLN:HE22	5:E:116:THR:HG22	1.55	0.70
1:A:353:A:H5'	1:A:353:A:C8	2.26	0.70
10:J:48:THR:CA	10:J:62:HIS:HB3	2.20	0.70
1:A:192:U:O4'	20:T:103:GLY:HA2	1.91	0.70
1:A:1392:G:H21	1:A:1502:A:H8	1.38	0.70
21:U:6:ARG:HB2	21:U:15:ARG:NH1	2.06	0.70
1:A:328:C:O2'	1:A:329:A:OP2	2.10	0.70
12:L:20:LYS:HD2	12:L:20:LYS:H	1.55	0.70
20:T:67:ALA:HA	20:T:73:HIS:H	1.55	0.70
1:A:1304:G:OP2	29:A:2277:HOH:O	2.09	0.70
1:A:1502:A:H2	1:A:1505:G:N1	1.90	0.70
1:A:421:U:H5'	1:A:422:C:C5	2.27	0.70
1:A:914:A:OP1	27:A:1956:SRY:HI33	1.91	0.69
3:C:91:LEU:HD21	3:C:99:VAL:HG22	1.74	0.69
7:G:15:ASP:OD2	7:G:44:TYR:OH	2.10	0.69
1:A:451:A:O2'	29:A:2771:HOH:O	1.63	0.69
2:B:223:ILE:HD13	2:B:230:VAL:H	1.57	0.69
1:A:1002:G:H2'	1:A:1003:G:C8	2.25	0.69
1:A:1190:G:HO2'	1:A:1191:A:P	2.15	0.69
1:A:192:U:C1'	20:T:103:GLY:HA2	2.22	0.69
20:T:83:ARG:O	20:T:87:LYS:HD2	1.92	0.69
6:F:10:LEU:HD12	6:F:59:TYR:HB3	1.74	0.69
1:A:103:C:OP1	20:T:17:ARG:NH1	2.26	0.69
3:C:156:ARG:H	3:C:163:ALA:HA	1.58	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1251:A:H4'	9:I:12:GLU:OE1	1.92	0.69
3:C:77:ILE:HG22	3:C:78:GLY:O	1.93	0.69
2:B:103:THR:HG23	2:B:176:GLU:OE1	1.93	0.69
4:D:70:ILE:HG22	4:D:71:SER:O	1.93	0.69
7:G:65:ALA:HB1	7:G:127:ALA:HB3	1.74	0.69
12:L:60:LEU:HB2	12:L:64:TYR:O	1.93	0.69
1:A:7:G:H5'	1:A:298:A:O4'	1.93	0.68
1:A:299:G:H2'	1:A:300:A:C8	2.28	0.68
4:D:22:LYS:HB2	4:D:26:CYS:SG	2.33	0.68
10:J:7:LYS:HD3	10:J:9:ARG:HH21	1.57	0.68
1:A:453:A:H4'	16:P:72:ARG:HG3	1.76	0.68
2:B:107:THR:O	2:B:110:GLN:HB2	1.92	0.68
1:A:653:A:OP1	8:H:56:LYS:NZ	2.26	0.68
1:A:820:U:H4'	1:A:821:G:OP2	1.92	0.68
1:A:290:C:N4	29:A:2818:HOH:O	2.26	0.68
1:A:409:G:OP1	4:D:24:GLU:O	2.12	0.68
17:Q:40:LYS:HD2	17:Q:42:TYR:CZ	2.29	0.68
19:S:5:LEU:HG	19:S:6:LYS:H	1.59	0.68
16:P:22:THR:HA	16:P:33:ILE:HG13	1.76	0.68
17:Q:63:ARG:HG2	17:Q:64:PRO:HD2	1.76	0.68
1:A:1229:A:OP2	13:M:114:ARG:HD3	1.94	0.67
7:G:27:ILE:HD13	7:G:40:ALA:HA	1.76	0.67
1:A:1510:U:H2'	1:A:1511:G:C8	2.29	0.67
1:A:620:C:N1	4:D:135:LEU:HD13	2.10	0.67
9:I:89:ASN:HB3	9:I:92:TYR:CD1	2.29	0.67
1:A:1497:G:H2'	1:A:1498:UR3:H5'	1.76	0.67
1:A:496:A:H4'	1:A:497:A:OP1	1.92	0.67
19:S:58:VAL:HG12	19:S:59:PRO:HD2	1.75	0.67
9:I:48:GLU:OE1	9:I:48:GLU:HA	1.93	0.67
13:M:51:ALA:O	13:M:54:VAL:HG12	1.94	0.67
9:I:53:VAL:HG21	9:I:85:LEU:HD21	1.77	0.67
17:Q:67:LYS:HA	17:Q:70:ARG:HH12	1.60	0.67
1:A:1300:G:O2'	1:A:1301:U:P	2.52	0.67
8:H:102:ARG:H	8:H:102:ARG:HD2	1.57	0.67
1:A:1049:U:H4'	1:A:1050:G:O5'	1.93	0.67
1:A:1149:C:H2'	1:A:1150:U:C6	2.30	0.67
1:A:509:A:O2'	1:A:510:A:OP1	2.13	0.67
11:K:27:ASN:OD1	11:K:28:THR:N	2.27	0.67
9:I:8:GLY:HA3	9:I:79:LEU:HB3	1.75	0.67
1:A:1392:G:N2	1:A:1502:A:H8	1.93	0.67
10:J:63:PHE:HB3	14:N:58:LYS:HA	1.77	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:89:C:C5	1:A:90:U:C4	2.84	0.67
1:A:951:G:OP2	13:M:102:ARG:NH2	2.28	0.67
1:A:972:C:OP1	10:J:57:LYS:NZ	2.19	0.67
10:J:55:LYS:HG2	10:J:56:HIS:N	2.08	0.67
1:A:129:U:O3'	1:A:129(A):G:H3'	1.95	0.66
2:B:74:LYS:C	2:B:76:GLN:H	1.98	0.66
1:A:1059:C:O3'	14:N:45:ARG:NH2	2.28	0.66
3:C:43:LEU:HD12	3:C:47:LEU:HD13	1.77	0.66
1:A:737:A:H1'	6:F:73:ASN:HD21	1.60	0.66
21:U:6:ARG:HB2	21:U:15:ARG:HH12	1.59	0.66
1:A:442:C:H42	1:A:492:G:H1	1.42	0.66
5:E:81:GLU:HG2	5:E:90:VAL:HG22	1.76	0.66
14:N:41:ARG:HG3	14:N:42:ILE:N	2.10	0.66
1:A:1125:U:H3'	1:A:1126:U:H5	1.59	0.66
1:A:795:C:H5"	1:A:796:C:OP2	1.95	0.66
2:B:239:VAL:O	2:B:240:GLN:HB3	1.95	0.66
1:A:1305:G:H22	1:A:1331:G:H1'	1.58	0.66
1:A:1482:G:N1	29:A:2391:HOH:O	2.17	0.66
9:I:24:GLY:HA3	9:I:57:GLY:HA2	1.76	0.66
1:A:1212:U:H2'	1:A:1212:U:O2	1.95	0.66
2:B:115:LEU:HD13	2:B:145:LEU:HB3	1.78	0.66
3:C:147:LYS:HD3	3:C:205:GLY:H	1.61	0.66
15:O:56:LEU:HA	15:O:59:MET:HE3	1.77	0.66
15:O:74:ASP:HB3	15:O:77:ARG:HG3	1.76	0.66
19:S:51:VAL:HG11	19:S:71:LEU:HD22	1.77	0.66
10:J:32:ALA:O	10:J:34:VAL:HG23	1.95	0.66
17:Q:58:GLU:O	17:Q:59:ILE:HD13	1.95	0.66
19:S:7:LYS:HD2	19:S:7:LYS:O	1.95	0.66
1:A:1101:A:H4'	1:A:1102:A:O5'	1.96	0.66
6:F:28:ARG:O	6:F:32:ASN:ND2	2.29	0.66
8:H:83:ILE:HG13	8:H:137:VAL:HG22	1.78	0.66
12:L:69:TYR:CD1	12:L:90:VAL:HG21	2.30	0.66
1:A:126:G:N7	29:A:2422:HOH:O	2.29	0.66
10:J:27:ALA:HB1	10:J:81:THR:HG23	1.78	0.66
1:A:804:U:H5"	1:A:805:C:OP2	1.95	0.65
1:A:502:G:OP1	12:L:118:SER:OG	2.14	0.65
3:C:151:VAL:O	3:C:167:TRP:O	2.15	0.65
14:N:3:ARG:HH21	14:N:6:LEU:HD21	1.57	0.65
1:A:1005:A:C6	1:A:1026:G:N2	2.65	0.65
12:L:25:PRO:C	12:L:27:LEU:H	1.99	0.65
21:U:10:ARG:NH1	21:U:10:ARG:HG3	2.08	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:134:ILE:O	3:C:138:VAL:HG23	1.96	0.65
20:T:50:GLU:HB2	20:T:99:LEU:HD12	1.77	0.65
8:H:111:ILE:O	8:H:134:ILE:HB	1.97	0.65
1:A:1347:G:C2'	1:A:1348:U:OP2	2.45	0.65
9:I:90:PRO:O	9:I:93:ARG:HG3	1.97	0.65
7:G:50:ILE:HG21	7:G:58:PRO:HA	1.79	0.65
9:I:10:ARG:HG3	9:I:11:LYS:HG2	1.77	0.65
1:A:1368:G:OP2	9:I:112:LYS:HD3	1.96	0.65
13:M:10:PRO:HB2	13:M:18:ALA:HB1	1.78	0.65
1:A:1197:G:OP1	29:A:2249:HOH:O	2.15	0.65
1:A:812:C:H4'	1:A:813:U:O5'	1.97	0.65
5:E:144:THR:HG22	5:E:146:ALA:H	1.62	0.65
10:J:75:ILE:HG22	10:J:76:ASN:H	1.60	0.65
10:J:82:ILE:O	10:J:85:LEU:HB2	1.96	0.65
1:A:1065:U:H1'	1:A:1066:C:OP2	1.97	0.65
1:A:1157:A:H4'	1:A:1158:C:O5'	1.97	0.65
1:A:1212:U:H4'	1:A:1213:A:O5'	1.96	0.64
3:C:34:LEU:O	3:C:38:ARG:HG3	1.97	0.64
5:E:12:LEU:HD23	5:E:13:ILE:N	2.13	0.64
1:A:35:G:H2'	1:A:36:C:C6	2.33	0.64
1:A:1126:U:C4	1:A:1127:G:N2	2.66	0.64
1:A:1425:U:H2'	1:A:1426:C:H6	1.62	0.64
1:A:89:C:H2'	1:A:90:U:O5'	1.98	0.64
10:J:74:ILE:O	10:J:74:ILE:HG13	1.98	0.64
13:M:99:ARG:CB	13:M:101:GLN:HE22	2.00	0.64
13:M:36:LYS:HD2	13:M:59:TYR:OH	1.97	0.64
1:A:1068:G:P	29:A:2237:HOH:O	2.55	0.64
1:A:1136:U:H5"	1:A:1137:C:OP2	1.97	0.64
1:A:1001:A:H2'	1:A:1002:G:C8	2.31	0.64
1:A:1028:C:N3	1:A:1034:G:C2	2.66	0.64
3:C:47:LEU:HG	3:C:76:VAL:HG12	1.79	0.64
1:A:974:A:OP2	14:N:41:ARG:NH1	2.25	0.64
22:V:1:U:H3	23:W:36:G:H1	1.46	0.64
1:A:673:G:H2'	1:A:674:G:C8	2.32	0.64
2:B:170:GLU:HA	2:B:170:GLU:OE2	1.97	0.64
7:G:69:VAL:HG21	7:G:104:LEU:HD21	1.80	0.64
1:A:1328:C:OP1	21:U:20:LYS:NZ	2.28	0.64
3:C:126:ARG:HG2	3:C:128:PHE:HB2	1.78	0.64
3:C:126:ARG:HG3	3:C:128:PHE:H	1.63	0.64
4:D:191:ARG:HH11	4:D:191:ARG:HG3	1.63	0.64
1:A:1152:A:OP1	10:J:68:HIS:ND1	2.28	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:240:GLN:O	2:B:240:GLN:HG2	1.97	0.63
10:J:61:GLU:HG2	10:J:61:GLU:O	1.97	0.63
1:A:977:A:H2'	1:A:978:A:H5'	1.79	0.63
5:E:43:LEU:H	5:E:136:MET:HE2	1.64	0.63
19:S:50:ALA:HA	19:S:58:VAL:O	1.98	0.63
7:G:5:ARG:HG3	7:G:7:ALA:H	1.63	0.63
1:A:1241:G:H2'	1:A:1242:C:C6	2.34	0.63
1:A:1064:G:N2	1:A:1190:G:H2'	2.13	0.63
1:A:1277:C:HO2'	1:A:1279:A:H8	1.46	0.63
1:A:299:G:O6	29:A:2235:HOH:O	2.11	0.63
20:T:74:LYS:HB3	20:T:74:LYS:HZ2	1.63	0.63
3:C:6:HIS:HD2	3:C:9:GLY:H	1.44	0.63
4:D:32:ALA:O	4:D:36:ARG:N	2.29	0.63
1:A:1086:U:H3	1:A:1099:G:H22	1.47	0.62
1:A:1225:A:N3	1:A:1225:A:H2'	2.14	0.62
1:A:1329:A:C2'	1:A:1330:U:H5'	2.30	0.62
1:A:755:G:OP2	15:O:65:ARG:HD2	1.99	0.62
13:M:88:ARG:HD2	19:S:3:ARG:HH21	1.63	0.62
20:T:13:LEU:C	20:T:13:LEU:HD12	2.20	0.62
1:A:1053:G:HO2'	1:A:1199:U:H5	1.44	0.62
3:C:85:ARG:HG2	3:C:85:ARG:HH11	1.63	0.62
1:A:1190:G:O2'	1:A:1191:A:P	2.58	0.62
1:A:229:U:O2'	1:A:230:G:H5'	1.98	0.62
1:A:23:C:N4	29:A:2692:HOH:O	2.33	0.62
1:A:390:C:H2'	1:A:391:G:C8	2.35	0.62
1:A:579:G:H5'	1:A:728:A:H1'	1.79	0.62
8:H:23:SER:HA	8:H:63:LEU:HD22	1.81	0.62
12:L:28:LYS:HE2	12:L:33:ARG:NH1	2.13	0.62
13:M:19:LEU:O	13:M:22:ILE:HG12	1.99	0.62
1:A:1004:A:N7	1:A:1037:C:N3	2.47	0.62
1:A:814:A:H2'	1:A:816:A:C5'	2.30	0.62
3:C:86:VAL:O	3:C:89:GLU:HB3	2.00	0.62
8:H:21:LYS:O	8:H:65:TYR:OH	2.12	0.62
4:D:102:ASP:OD1	4:D:103:ASN:N	2.32	0.62
20:T:16:HIS:O	20:T:19:SER:OG	2.13	0.62
1:A:1112:C:H1'	3:C:179:ARG:HH11	1.63	0.62
1:A:814:A:H2'	1:A:816:A:H5'	1.82	0.62
9:I:5:TYR:OH	9:I:7:THR:OG1	2.17	0.62
1:A:328:C:O2	1:A:328:C:C2'	2.43	0.62
1:A:616:G:O2'	1:A:617:G:H5'	2.00	0.62
3:C:30:ARG:HG2	14:N:36:PHE:O	2.00	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:12:LEU:HD23	5:E:12:LEU:C	2.20	0.62
9:I:8:GLY:HA2	9:I:79:LEU:HD13	1.80	0.62
3:C:46:GLU:HG3	3:C:83:ARG:HH21	1.65	0.62
27:A:1956:SRY:HI32	27:A:1956:SRY:O13	1.99	0.61
1:A:89:C:H6	1:A:89:C:H3'	1.63	0.61
1:A:965:A:H4'	1:A:966:M2G:O5'	1.99	0.61
3:C:180:ALA:HB1	3:C:182:ILE:HG13	1.82	0.61
1:A:1249:C:O2'	9:I:73:GLN:NE2	2.33	0.61
10:J:40:LEU:HB3	10:J:41:PRO:HD2	1.81	0.61
15:O:70:LEU:HD13	15:O:78:TYR:HA	1.82	0.61
5:E:98:THR:HB	5:E:117:ASP:HB3	1.82	0.61
16:P:74:LEU:O	16:P:79:VAL:HG23	2.00	0.61
18:R:47:THR:HA	18:R:83:GLU:HB2	1.80	0.61
1:A:1533:C:HO2'	1:A:1534:C:P	2.22	0.61
3:C:116:VAL:O	3:C:120:VAL:HG23	1.99	0.61
1:A:1278:U:H5"	1:A:1279:A:C8	2.36	0.61
20:T:58:LYS:HE2	20:T:62:LEU:CD2	2.31	0.61
1:A:850:U:H2'	1:A:851:G:H5"	1.81	0.61
2:B:10:LEU:HD22	2:B:15:VAL:HG21	1.81	0.61
13:M:34:LEU:HD13	13:M:41:PRO:HA	1.83	0.61
1:A:1103:C:H5"	2:B:98:LEU:HD12	1.82	0.61
1:A:289:G:P	29:A:2015:HOH:O	2.58	0.61
1:A:539:A:H2'	1:A:540:G:C8	2.36	0.61
3:C:46:GLU:HG2	3:C:87:LEU:HD21	1.83	0.61
1:A:1054:C:C3'	1:A:1054:C:O2	2.48	0.61
10:J:8:LEU:HD23	10:J:96:ILE:HG12	1.82	0.61
1:A:1035:A:H2'	1:A:1036:G:C8	2.36	0.61
1:A:89:C:C4	1:A:90:U:N3	2.69	0.61
1:A:99:C:H2'	1:A:101:A:C8	2.36	0.61
8:H:82:HIS:ND1	8:H:138:TRP:NE1	2.42	0.61
12:L:28:LYS:C	12:L:30:ALA:H	2.05	0.61
14:N:3:ARG:HB2	14:N:6:LEU:HD23	1.82	0.61
6:F:97:PHE:HB2	18:R:32:ARG:HH11	1.65	0.61
1:A:1003:G:N2	1:A:1039:C:C2	2.69	0.60
1:A:1391:U:H2'	1:A:1392:G:H8	1.63	0.60
1:A:972:C:OP1	10:J:57:LYS:HD2	2.01	0.60
1:A:1367:C:H5'	10:J:60:ARG:NH1	2.15	0.60
11:K:50:TYR:HE2	11:K:54:ARG:HH11	1.49	0.60
1:A:1027:C:H5	1:A:1035:A:N1	1.99	0.60
1:A:1269:A:H5"	1:A:1270:C:OP2	2.01	0.60
1:A:1412:C:H2'	1:A:1413:A:H8	1.66	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:126:ARG:CG	3:C:128:PHE:HB2	2.32	0.60
1:A:1316:G:N1	1:A:1319:A:OP2	2.34	0.60
3:C:50:ALA:HB2	3:C:75:VAL:HB	1.83	0.60
4:D:62:GLN:O	4:D:66:ARG:HD3	2.02	0.60
8:H:112:LEU:HD23	8:H:112:LEU:N	2.16	0.60
10:J:6:ILE:HG23	10:J:96:ILE:HG23	1.82	0.60
2:B:139:LYS:HZ3	2:B:143:GLU:HG3	1.66	0.60
1:A:1427:U:H2'	1:A:1428:A:C8	2.37	0.60
2:B:98:LEU:O	2:B:101:MET:HG3	2.02	0.60
17:Q:63:ARG:HG2	17:Q:64:PRO:CD	2.32	0.60
1:A:1256:A:H1'	1:A:1257:U:OP2	2.00	0.60
4:D:25:ARG:O	4:D:25:ARG:HG2	2.02	0.60
1:A:706:A:O4'	11:K:29:ILE:HD11	2.02	0.60
1:A:1004:A:H5'	29:A:2351:HOH:O	2.01	0.59
12:L:53:ARG:HG3	12:L:93:LEU:HD21	1.83	0.59
18:R:40:LEU:HB3	18:R:79:LEU:HD11	1.84	0.59
1:A:1528:U:O2'	1:A:1529:G:OP2	2.13	0.59
16:P:3:LYS:HD2	16:P:65:GLN:O	2.02	0.59
1:A:1313:U:O4	19:S:4:SER:OG	2.19	0.59
10:J:79:ARG:HB2	10:J:80:LYS:HD2	1.83	0.59
20:T:56:MET:HE1	20:T:85:MET:HG2	1.84	0.59
1:A:1131:G:H8	1:A:1131:G:OP2	1.84	0.59
1:A:501:C:H2'	1:A:502:G:C8	2.37	0.59
1:A:88:A:C5	1:A:89:C:N3	2.70	0.59
3:C:195:VAL:C	3:C:196:LEU:HD23	2.23	0.59
3:C:34:LEU:HD22	14:N:25:VAL:HG21	1.84	0.59
17:Q:68:ARG:N	17:Q:70:ARG:NH1	2.51	0.59
1:A:1277:C:O2'	1:A:1279:A:H1'	2.03	0.59
1:A:828:A:H4'	1:A:828:A:OP1	2.00	0.59
1:A:707:C:OP1	11:K:85:ARG:NH1	2.35	0.59
20:T:59:ALA:O	20:T:63:ILE:HG13	2.02	0.59
1:A:89:C:C2'	1:A:90:U:O5'	2.50	0.59
3:C:150:LYS:HG3	3:C:169:ALA:HB2	1.85	0.59
8:H:10:LEU:HD22	8:H:83:ILE:HD11	1.85	0.59
10:J:47:PHE:O	10:J:62:HIS:HB2	2.02	0.59
12:L:70:ILE:HG21	12:L:75:HIS:CD2	2.37	0.59
17:Q:101:ARG:N	17:Q:101:ARG:HD3	2.16	0.59
1:A:1125:U:C3'	1:A:1126:U:H5	2.15	0.59
1:A:1356:G:H2'	1:A:1357:A:C8	2.37	0.59
1:A:1399:C:O2	1:A:1401:G:C5	2.56	0.59
1:A:397:A:H5'	1:A:398:C:OP1	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:594:G:C2'	1:A:595:G:H5'	2.33	0.59
1:A:79:G:C2	1:A:91:C:C2	2.91	0.59
6:F:3:ARG:O	6:F:93:SER:HB2	2.01	0.59
1:A:1004:A:H62	1:A:1037:C:H42	1.50	0.59
1:A:45:U:H2'	1:A:46:G:C8	2.38	0.59
1:A:73:C:N4	29:A:2482:HOH:O	2.34	0.58
1:A:667:G:H4'	15:O:51:HIS:ND1	2.19	0.58
3:C:180:ALA:CB	3:C:182:ILE:HG13	2.34	0.58
5:E:11:ILE:HD11	5:E:105:VAL:HA	1.85	0.58
1:A:1027:C:OP1	1:A:1027:C:C4'	2.51	0.58
1:A:1126:U:O4	1:A:1127:G:N2	2.36	0.58
4:D:150:GLU:N	4:D:150:GLU:OE2	2.36	0.58
7:G:108:ALA:O	7:G:119:ARG:HB3	2.02	0.58
13:M:8:GLU:CG	13:M:22:ILE:HA	2.27	0.58
13:M:2:ALA:O	13:M:9:ILE:HA	2.03	0.58
1:A:1052:U:H2'	1:A:1055:A:OP1	2.03	0.58
1:A:1179:A:H2'	1:A:1180:A:O4'	2.02	0.58
1:A:141:A:H1'	1:A:182:U:O2	2.03	0.58
1:A:251:G:H4'	1:A:252:U:O5'	2.03	0.58
2:B:172:ILE:H	2:B:172:ILE:HD13	1.68	0.58
3:C:91:LEU:HD23	3:C:92:ALA:N	2.19	0.58
1:A:427:U:OP1	4:D:13:ARG:NH2	2.36	0.58
5:E:144:THR:HG22	5:E:145:LYS:N	2.17	0.58
8:H:112:LEU:HD23	8:H:112:LEU:H	1.68	0.58
1:A:914:A:P	27:A:1956:SRY:HI33	2.42	0.58
1:A:31:G:N2	1:A:48:C:OP1	2.27	0.58
4:D:170:VAL:HG13	4:D:171:GLY:N	2.18	0.58
14:N:9:LYS:HD2	14:N:9:LYS:O	2.04	0.58
1:A:1047:G:C2'	1:A:1048:G:H5'	2.32	0.58
1:A:1131:G:H2'	1:A:1132:C:C6	2.38	0.58
6:F:22:GLU:OE2	6:F:82:ARG:HD3	2.04	0.58
6:F:67:MET:HB2	6:F:68:PRO:HD2	1.84	0.58
9:I:26:VAL:HG12	9:I:61:ALA:HB3	1.84	0.58
15:O:45:VAL:CG1	15:O:46:HIS:N	2.66	0.58
1:A:976:G:H5'	1:A:1358:U:O2'	2.03	0.58
6:F:80:ARG:NH1	6:F:88:VAL:O	2.36	0.58
20:T:10:LEU:HG	20:T:12:ALA:H	1.69	0.58
2:B:80:ILE:CD1	2:B:80:ILE:H	2.14	0.58
1:A:35:G:H2'	1:A:36:C:H6	1.66	0.58
3:C:14:ILE:O	3:C:16:ARG:N	2.36	0.58
1:A:421:U:H5'	1:A:422:C:H5	1.68	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:125:PRO:HG2	2:B:126:GLU:OE1	2.04	0.58
10:J:19:SER:OG	10:J:91:PRO:HG2	2.04	0.58
11:K:48:ILE:HG22	11:K:49:GLY:H	1.68	0.58
1:A:1035:A:C6	1:A:1036:G:C6	2.92	0.57
1:A:501:C:H2'	1:A:502:G:H8	1.69	0.57
5:E:126:ARG:CG	5:E:126:ARG:HH11	2.00	0.57
8:H:82:HIS:ND1	8:H:138:TRP:CE2	2.71	0.57
12:L:24:VAL:HG13	12:L:98:TYR:HE2	1.69	0.57
12:L:36:VAL:HG22	12:L:82:VAL:HG22	1.85	0.57
19:S:5:LEU:HG	19:S:6:LYS:N	2.19	0.57
1:A:1004:A:O2'	1:A:1005:A:OP1	2.14	0.57
1:A:1300:G:O2'	1:A:1301:U:OP2	2.21	0.57
6:F:28:ARG:HG2	6:F:32:ASN:HD21	1.67	0.57
8:H:103:VAL:HG21	8:H:109:ILE:O	2.04	0.57
9:I:32:ASP:OD1	9:I:33:PHE:N	2.37	0.57
1:A:1057:G:C5'	3:C:154:SER:HB2	2.33	0.57
1:A:1112:C:N4	3:C:178:LEU:HD23	2.19	0.57
4:D:172:PRO:HD2	4:D:173:TRP:CZ3	2.39	0.57
15:O:11:VAL:HG11	15:O:34:LEU:HD12	1.86	0.57
7:G:75:VAL:CG2	7:G:86:GLN:HB3	2.34	0.57
1:A:972:C:P	10:J:57:LYS:HD2	2.44	0.57
13:M:86:CYS:SG	13:M:87:TYR:N	2.76	0.57
20:T:51:GLU:O	20:T:55:ILE:HG12	2.04	0.57
20:T:69:GLY:O	20:T:73:HIS:CE1	2.57	0.57
1:A:714:G:H2'	1:A:715:A:C8	2.39	0.57
1:A:860:A:H2'	1:A:861:G:O4'	2.04	0.57
2:B:212:GLN:HE21	2:B:235:SER:CB	2.14	0.57
4:D:150:GLU:N	4:D:150:GLU:CD	2.57	0.57
15:O:45:VAL:HG12	15:O:46:HIS:H	1.69	0.57
19:S:41:VAL:HB	19:S:42:PRO:HD2	1.84	0.57
21:U:10:ARG:HH11	21:U:10:ARG:CG	2.11	0.57
1:A:1054:C:O2'	1:A:1055:A:H5"	2.04	0.57
1:A:17:U:H2'	1:A:18:C:C6	2.40	0.57
9:I:97:LYS:HB3	9:I:98:PRO:HD3	1.86	0.57
13:M:16:ASP:OD2	13:M:17:VAL:N	2.34	0.57
1:A:1072:G:H2'	1:A:1073:U:C6	2.39	0.57
1:A:250:A:H1'	1:A:251:G:OP2	2.04	0.57
14:N:41:ARG:HG3	14:N:42:ILE:H	1.69	0.57
1:A:757:U:H2'	1:A:758:G:O4'	2.04	0.57
1:A:895:G:H2'	1:A:896:C:H6	1.70	0.57
3:C:127:ARG:NH2	3:C:193:TYR:HE2	2.03	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:12:ASP:OD2	10:J:15:THR:HG23	2.05	0.57
12:L:24:VAL:HG12	12:L:24:VAL:O	2.04	0.57
18:R:26:LEU:HD11	18:R:42:ARG:HH11	1.70	0.57
19:S:58:VAL:CG1	19:S:59:PRO:HD2	2.35	0.57
20:T:74:LYS:HZ3	20:T:74:LYS:HB3	1.68	0.57
1:A:1015:A:N3	1:A:1218:C:O2'	2.37	0.57
1:A:1407:5MC:C2'	1:A:1408:A:H5'	2.35	0.57
1:A:144:G:H1	1:A:178:C:H42	1.52	0.57
1:A:628:G:C2'	1:A:629:G:H5'	2.35	0.57
5:E:143:ARG:NH1	8:H:77:GLU:OE2	2.38	0.57
1:A:1178:G:N2	1:A:1180:A:H3'	2.20	0.56
1:A:1497:G:C2'	1:A:1498:UR3:H5'	2.35	0.56
13:M:57:ARG:HD3	13:M:61:GLU:OE2	2.05	0.56
19:S:16:LEU:O	19:S:20:LEU:HG	2.05	0.56
4:D:8:VAL:HG11	4:D:21:LEU:HB2	1.88	0.56
1:A:501:C:OP1	12:L:117:ARG:NH2	2.38	0.56
18:R:37:VAL:O	18:R:40:LEU:N	2.38	0.56
1:A:1027:C:O4'	1:A:1027:C:OP1	2.23	0.56
9:I:105:ASP:OD2	9:I:107:ARG:HG3	2.05	0.56
18:R:47:THR:CG2	18:R:48:GLY:N	2.68	0.56
1:A:1064:G:H22	1:A:1190:G:H2'	1.70	0.56
1:A:664:G:N2	1:A:741:G:H1	1.88	0.56
2:B:184:VAL:HG12	2:B:197:VAL:HG13	1.87	0.56
2:B:97:TRP:HZ3	2:B:176:GLU:OE2	1.89	0.56
10:J:34:VAL:HG13	10:J:74:ILE:HG22	1.88	0.56
1:A:1004:A:H5"	29:A:2349:HOH:O	2.06	0.56
1:A:1053:G:C3'	1:A:1054:C:H5'	2.35	0.56
1:A:149:A:H2'	1:A:150:C:C6	2.41	0.56
1:A:628:G:O2'	1:A:629:G:H5'	2.04	0.56
2:B:97:TRP:CZ3	2:B:176:GLU:OE2	2.57	0.56
1:A:187:C:N3	20:T:105:SER:CB	2.69	0.56
2:B:134:GLU:HA	2:B:137:ARG:CG	2.36	0.56
11:K:84:VAL:HG21	11:K:95:ILE:HD11	1.87	0.56
1:A:1277:C:H2'	1:A:1279:A:H8	1.71	0.56
2:B:87:ARG:HG2	2:B:88:ALA:H	1.70	0.56
3:C:127:ARG:HH22	3:C:193:TYR:HE2	1.52	0.56
12:L:20:LYS:CD	12:L:20:LYS:H	2.17	0.56
12:L:54:LYS:HD2	12:L:54:LYS:N	2.19	0.56
10:J:63:PHE:HA	14:N:59:ALA:HB3	1.86	0.56
19:S:7:LYS:HD2	19:S:7:LYS:C	2.25	0.56
1:A:1286:A:H3'	1:A:1287:A:H5"	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:975:A:H4'	1:A:976:G:C5'	2.33	0.56
3:C:188:LEU:HD11	3:C:195:VAL:HG13	1.88	0.56
7:G:28:ASN:OD1	7:G:36:LYS:HE3	2.05	0.56
1:A:777:A:OP1	29:A:2573:HOH:O	2.17	0.56
2:B:132:LYS:NZ	2:B:132:LYS:HB3	2.21	0.56
10:J:47:PHE:CZ	14:N:37:PHE:CE1	2.94	0.56
1:A:428:G:H1'	1:A:429:U:OP2	2.06	0.56
1:A:1442:G:C6	1:A:1446:A:N6	2.73	0.56
1:A:250:A:H4'	1:A:251:G:O5'	2.06	0.56
1:A:503:C:OP2	12:L:116:SER:HB3	2.06	0.56
1:A:946:A:H2'	1:A:947:G:C8	2.41	0.56
2:B:14:GLY:HA3	2:B:210:SER:HB2	1.87	0.56
1:A:1026:G:N7	1:A:1027:C:N3	2.53	0.55
3:C:14:ILE:C	3:C:16:ARG:H	2.09	0.55
7:G:12:LEU:H	7:G:12:LEU:HD12	1.69	0.55
8:H:53:VAL:HB	8:H:58:TYR:CD1	2.40	0.55
11:K:15:ALA:CA	11:K:77:MET:HA	2.27	0.55
17:Q:68:ARG:H	17:Q:70:ARG:HH11	1.54	0.55
1:A:1054:C:N3	23:W:34:G:O4'	2.40	0.55
1:A:983:A:O2'	1:A:1050:G:OP2	2.23	0.55
10:J:24:VAL:O	10:J:28:ARG:HB2	2.06	0.55
1:A:1495:U:H2'	1:A:1496:C:O4'	2.06	0.55
1:A:539:A:H2'	1:A:540:G:H8	1.70	0.55
1:A:187:C:N3	20:T:105:SER:HB2	2.21	0.55
1:A:1027:C:N4	29:A:2347:HOH:O	2.39	0.55
1:A:1498:UR3:O2'	1:A:1499:A:OP2	2.20	0.55
1:A:895:G:H2'	1:A:896:C:C6	2.41	0.55
1:A:91:C:H2'	1:A:92:C:H6	1.71	0.55
2:B:90:MET:HB3	2:B:91:PRO:HD2	1.87	0.55
5:E:76:ILE:HG23	5:E:142:LEU:CD1	2.37	0.55
16:P:47:ASP:O	16:P:47:ASP:CG	2.44	0.55
1:A:1181:G:C2	1:A:1182:G:N2	2.75	0.55
1:A:1160:G:C6	1:A:1181:G:O6	2.60	0.55
14:N:9:LYS:HG3	14:N:10:ALA:N	2.20	0.55
19:S:43:GLU:OE2	19:S:43:GLU:N	2.24	0.55
1:A:1002:G:C6	1:A:1003:G:C6	2.95	0.55
1:A:1003:G:N2	1:A:1003(A):G:C6	2.74	0.55
1:A:1275:A:H2'	1:A:1276:G:O4'	2.06	0.55
1:A:129(A):G:H1'	1:A:190(E):U:H2'	1.88	0.55
12:L:73:GLU:OE1	12:L:73:GLU:HA	2.07	0.55
1:A:620:C:H2'	1:A:621:A:O4'	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:102:ARG:N	8:H:102:ARG:CD	2.65	0.55
9:I:43:ALA:HA	9:I:74:ILE:HD13	1.89	0.55
9:I:70:LYS:O	9:I:74:ILE:HG13	2.06	0.55
1:A:1065:U:H5"	1:A:1190:G:N2	2.22	0.55
1:A:421:U:O2	1:A:421:U:O4'	2.23	0.55
3:C:116:VAL:HG21	3:C:202:ILE:HD11	1.88	0.55
5:E:97:GLY:N	5:E:117:ASP:OD1	2.40	0.55
13:M:59:TYR:O	13:M:63:THR:HB	2.07	0.55
1:A:1532:U:H2'	1:A:1533:C:C6	2.41	0.55
1:A:459:G:H1'	1:A:463:A:H61	1.71	0.55
1:A:526:C:O3'	27:A:1956:SRY:HI31	2.06	0.55
3:C:127:ARG:NH2	3:C:193:TYR:CE2	2.75	0.55
10:J:63:PHE:HA	14:N:59:ALA:CB	2.37	0.55
15:O:8:LYS:O	15:O:12:ILE:HG12	2.06	0.55
19:S:80:TYR:CD1	19:S:81:ARG:N	2.76	0.55
1:A:192:U:H1'	20:T:103:GLY:HA2	1.89	0.55
3:C:156:ARG:NH1	3:C:193:TYR:O	2.40	0.54
4:D:175:SER:HB2	4:D:184:LYS:HB2	1.90	0.54
21:U:7:ARG:O	21:U:21:TYR:CD2	2.61	0.54
11:K:67:ASP:O	11:K:71:LYS:HG3	2.08	0.54
14:N:14:PRO:HB2	14:N:16:PHE:O	2.07	0.54
17:Q:29:HIS:CG	17:Q:30:PRO:HD2	2.42	0.54
1:A:1312:G:N7	19:S:4:SER:HB3	2.21	0.54
1:A:1286:A:H8	1:A:1287:A:H5"	1.71	0.54
1:A:353:A:H8	1:A:353:A:C5'	2.15	0.54
1:A:56:U:H2'	1:A:57:G:C8	2.41	0.54
2:B:115:LEU:HD11	2:B:146:GLN:HG3	1.89	0.54
3:C:46:GLU:HG2	3:C:87:LEU:CD2	2.37	0.54
3:C:6:HIS:CD2	3:C:9:GLY:H	2.25	0.54
5:E:88:LYS:HB3	5:E:123:LEU:HB2	1.89	0.54
7:G:72:ARG:HD3	7:G:142:GLU:OE1	2.07	0.54
9:I:118:LYS:O	9:I:120:ARG:N	2.39	0.54
20:T:67:ALA:HA	20:T:73:HIS:N	2.21	0.54
1:A:594:G:H2'	1:A:595:G:H5'	1.88	0.54
1:A:960:U:H4'	1:A:961:U:C5'	2.37	0.54
17:Q:27:PHE:HB2	17:Q:28:PRO:HD2	1.90	0.54
18:R:47:THR:CG2	18:R:48:GLY:H	2.18	0.54
1:A:1256:A:N6	1:A:1277:C:C5	2.76	0.54
12:L:28:LYS:C	12:L:30:ALA:N	2.61	0.54
19:S:25:LYS:HG3	19:S:26:GLY:H	1.73	0.54
1:A:722:A:O2'	1:A:723:U:C2	2.61	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:T:89:ARG:HB2	20:T:104:LEU:HD11	1.90	0.54
2:B:224:GLN:HG2	2:B:229:VAL:HG22	1.89	0.54
3:C:8:ILE:HG23	3:C:16:ARG:HG2	1.90	0.54
6:F:50:TYR:CE1	18:R:77:GLY:HA2	2.43	0.54
1:A:1533:C:O2'	1:A:1534:C:OP1	2.21	0.54
1:A:179:A:O2'	1:A:180:U:H5'	2.08	0.54
1:A:60:A:H4'	1:A:61:G:O5'	2.08	0.54
1:A:838:G:N2	1:A:849:C:C2	2.75	0.54
9:I:11:LYS:O	9:I:12:GLU:HB2	2.07	0.54
17:Q:59:ILE:CD1	17:Q:73:VAL:HA	2.38	0.54
18:R:39:VAL:O	18:R:42:ARG:HB2	2.08	0.54
18:R:46:GLU:CD	18:R:46:GLU:H	2.11	0.54
3:C:22:TRP:CD1	3:C:59:ARG:HD2	2.43	0.54
12:L:27:LEU:C	12:L:29:GLY:N	2.49	0.54
1:A:1151:A:HO2'	1:A:1152:A:H8	1.57	0.53
1:A:1277:C:C2'	1:A:1279:A:H8	2.21	0.53
1:A:667:G:H4'	15:O:51:HIS:CE1	2.43	0.53
1:A:981:U:H5'	14:N:21:TYR:CE1	2.42	0.53
2:B:189:ASP:HB2	2:B:205:ASP:OD2	2.08	0.53
2:B:16:HIS:CB	2:B:44:LEU:HD21	2.37	0.53
4:D:98:GLU:HG2	4:D:189:PRO:HG3	1.90	0.53
5:E:105:VAL:HG12	5:E:106:PRO:N	2.23	0.53
9:I:27:THR:HG23	9:I:62:TYR:HA	1.89	0.53
19:S:15:LEU:HD13	19:S:16:LEU:H	1.73	0.53
1:A:1003(A):G:C6	1:A:1004:A:H1'	2.43	0.53
1:A:1003(A):G:C2	1:A:1004:A:H1'	2.44	0.53
1:A:1095:U:H2'	1:A:1096:C:O4'	2.08	0.53
1:A:1168:A:H2'	1:A:1169:A:C8	2.43	0.53
1:A:1241:G:H2'	1:A:1242:C:H6	1.72	0.53
4:D:173:TRP:CD1	4:D:189:PRO:HD3	2.43	0.53
10:J:55:LYS:CG	10:J:56:HIS:N	2.71	0.53
1:A:620:C:C2	4:D:135:LEU:HD13	2.44	0.53
1:A:684:A:N6	1:A:685:G:C6	2.77	0.53
1:A:792:A:H4'	1:A:793:U:H5"	1.91	0.53
2:B:80:ILE:HD12	2:B:80:ILE:N	2.16	0.53
9:I:128:ARG:HG3	9:I:128:ARG:OXT	2.07	0.53
10:J:51:ARG:HG3	10:J:59:SER:O	2.08	0.53
17:Q:26:GLN:HG2	17:Q:37:LYS:HB2	1.90	0.53
1:A:509:A:H5'	4:D:54:TYR:HD2	1.73	0.53
12:L:47:LYS:N	12:L:48:PRO:HD2	2.23	0.53
1:A:1142:G:H5'	1:A:1143:G:OP2	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1402:4OC:O2	1:A:1500:A:N1	2.42	0.53
2:B:133:LYS:O	2:B:137:ARG:HG2	2.09	0.53
2:B:24:TRP:CZ3	2:B:26:PRO:HA	2.44	0.53
9:I:53:VAL:CG2	9:I:85:LEU:HD21	2.38	0.53
19:S:51:VAL:O	19:S:58:VAL:HG23	2.08	0.53
1:A:1486:G:H2'	1:A:1487:G:O4'	2.09	0.53
8:H:4:ASP:CG	8:H:85:ARG:HH21	2.11	0.53
3:C:29:TYR:OH	14:N:54:PRO:HD2	2.09	0.53
1:A:204:U:H4'	1:A:216:G:OP1	2.06	0.53
1:A:421:U:H4'	1:A:422:C:OP2	2.09	0.53
6:F:41:GLU:OE1	18:R:35:ARG:NH1	2.35	0.53
20:T:74:LYS:CB	20:T:74:LYS:NZ	2.68	0.53
1:A:609:A:N6	29:A:2344:HOH:O	2.40	0.53
1:A:538:G:OP2	12:L:115:LYS:HG3	2.08	0.53
17:Q:100:LYS:HB2	17:Q:101:ARG:HH11	1.74	0.53
1:A:112:G:C2'	1:A:113:G:H5'	2.39	0.52
1:A:1329:A:H5'	13:M:29:ARG:HD2	1.91	0.52
27:A:1956:SRY:O51	12:L:46:LYS:HE3	2.10	0.52
1:A:630:G:H5'	1:A:631:G:OP2	2.09	0.52
1:A:1073:U:OP2	5:E:57:LYS:HE2	2.08	0.52
17:Q:34:LYS:HG3	17:Q:35:VAL:N	2.24	0.52
20:T:13:LEU:C	20:T:13:LEU:CD1	2.77	0.52
2:B:108:ILE:O	2:B:111:ARG:HB2	2.09	0.52
3:C:59:ARG:HG2	3:C:64:VAL:HG13	1.90	0.52
11:K:85:ARG:HE	11:K:111:ASP:HB3	1.74	0.52
1:A:1296:C:H5"	1:A:1297:C:OP2	2.09	0.52
1:A:1533:C:O2'	1:A:1534:C:P	2.66	0.52
1:A:248:C:C2'	1:A:249:U:H5'	2.39	0.52
1:A:983:A:H1'	1:A:1049:U:O2	2.09	0.52
5:E:76:ILE:HG23	5:E:142:LEU:HD13	1.89	0.52
7:G:74:GLU:HG2	7:G:91:VAL:HG22	1.91	0.52
12:L:76:ASN:O	12:L:77:LEU:HD23	2.09	0.52
13:M:58:GLU:OE2	13:M:58:GLU:HA	2.09	0.52
14:N:5:ALA:O	14:N:8:GLU:HG3	2.09	0.52
1:A:1286:A:C8	1:A:1287:A:H5"	2.44	0.52
1:A:914:A:OP1	27:A:1956:SRY:CI3	2.58	0.52
1:A:315:A:OP1	29:A:2618:HOH:O	2.18	0.52
2:B:11:LEU:HD23	2:B:16:HIS:CE1	2.45	0.52
2:B:197:VAL:HB	2:B:200:ILE:HG12	1.91	0.52
3:C:11:ARG:NH1	3:C:177:THR:O	2.43	0.52
5:E:43:LEU:O	5:E:65:ASN:ND2	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:P:28:ARG:HH11	16:P:28:ARG:HG2	1.75	0.52
1:A:261:U:C5	20:T:79:ARG:NH1	2.78	0.52
20:T:43:LEU:HD13	20:T:51:GLU:HB2	1.91	0.52
1:A:1003:G:C2	1:A:1003(A):G:C6	2.96	0.52
1:A:913:A:H3'	27:A:1956:SRY:HG21	1.91	0.52
4:D:64:LEU:HD23	4:D:198:VAL:HG21	1.91	0.52
1:A:1442:G:C5	1:A:1446:A:N6	2.78	0.52
1:A:192:U:H4'	20:T:57:ARG:HD3	1.92	0.52
2:B:231:GLU:HB3	2:B:232:PRO:HD2	1.91	0.52
3:C:111:LEU:HD21	3:C:144:SER:O	2.10	0.52
6:F:74:ASP:O	6:F:77:ARG:HB3	2.10	0.52
13:M:8:GLU:HG2	13:M:22:ILE:HD13	1.92	0.52
1:A:1068:G:H8	1:A:1068:G:OP2	1.93	0.52
3:C:24:ALA:HB1	3:C:28:GLN:HB2	1.92	0.52
18:R:46:GLU:OE2	18:R:46:GLU:N	2.31	0.52
1:A:1062:U:H2'	1:A:1063:C:C6	2.45	0.52
1:A:992:U:O2'	29:A:2728:HOH:O	2.19	0.52
3:C:130:VAL:HG11	3:C:157:ILE:CG2	2.40	0.52
5:E:117:ASP:OD2	5:E:117:ASP:N	2.43	0.52
1:A:1053:G:O2'	1:A:1199:U:H5	1.92	0.52
1:A:1407:5MC:H2'	1:A:1408:A:H5'	1.90	0.52
1:A:190(F):G:H4'	1:A:190(G):G:OP2	2.09	0.52
2:B:207:ALA:O	2:B:211:ILE:HG13	2.09	0.52
4:D:162:LEU:HD13	4:D:181:MET:HG2	1.91	0.52
5:E:101:ILE:HD12	5:E:101:ILE:N	2.23	0.52
17:Q:100:LYS:CB	17:Q:101:ARG:HH11	2.23	0.52
1:A:1258:G:H2'	1:A:1259:C:C6	2.45	0.51
1:A:1269:A:H2	1:A:1312:G:N3	2.08	0.51
1:A:1434:A:H2'	1:A:1435:G:O4'	2.10	0.51
1:A:983:A:H3'	1:A:983:A:N3	2.25	0.51
1:A:1112:C:N3	3:C:178:LEU:HB2	2.24	0.51
4:D:21:LEU:HD21	4:D:66:ARG:O	2.11	0.51
1:A:984:C:H42	1:A:1221:G:H1	1.58	0.51
3:C:7:PRO:HG2	3:C:184:TYR:HB2	1.92	0.51
3:C:64:VAL:HB	3:C:99:VAL:HB	1.91	0.51
4:D:24:GLU:O	4:D:25:ARG:HB3	2.11	0.51
9:I:8:GLY:CA	9:I:79:LEU:HB3	2.40	0.51
10:J:66:ARG:HH11	10:J:66:ARG:HG3	1.75	0.51
12:L:113:ARG:HH11	12:L:116:SER:H	1.57	0.51
21:U:10:ARG:NH1	21:U:10:ARG:CG	2.72	0.51
1:A:1256:A:H4'	1:A:1257:U:C5'	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:390:C:H2'	1:A:391:G:H8	1.75	0.51
1:A:563:A:H2'	1:A:567:G:C8	2.45	0.51
1:A:737:A:H1'	6:F:73:ASN:ND2	2.25	0.51
10:J:61:GLU:CG	10:J:61:GLU:O	2.59	0.51
20:T:67:ALA:CB	20:T:73:HIS:HA	2.40	0.51
1:A:328:C:H1'	1:A:329:A:OP2	2.11	0.51
1:A:509:A:H3'	1:A:509:A:C8	2.45	0.51
6:F:48:LEU:HD13	6:F:52:ILE:HG13	1.91	0.51
8:H:86:ILE:HG12	8:H:135:CYS:HA	1.91	0.51
19:S:12:ASP:OD2	19:S:37:ARG:NH2	2.40	0.51
1:A:1000:U:H2'	1:A:1001:A:C8	2.46	0.51
6:F:45:LEU:C	6:F:45:LEU:HD12	2.31	0.51
10:J:46:ARG:HG3	10:J:46:ARG:HH11	1.76	0.51
1:A:1126:U:N3	1:A:1127:G:N2	2.58	0.51
4:D:152:SER:O	4:D:155:LEU:HB2	2.11	0.51
5:E:137:GLU:OE2	5:E:140:ARG:HD2	2.11	0.51
1:A:1527:C:C2'	1:A:1528:U:H5'	2.41	0.51
1:A:560:U:C6	1:A:560:U:H5'	2.45	0.51
1:A:910:C:OP2	12:L:21:LYS:NZ	2.31	0.51
12:L:6:THR:HG1	12:L:9:GLN:HG3	1.76	0.51
1:A:179:A:H2'	1:A:180:U:C6	2.45	0.51
4:D:70:ILE:HD11	4:D:100:ARG:CZ	2.41	0.51
13:M:2:ALA:O	13:M:10:PRO:HD2	2.11	0.51
1:A:1206:G:C6	1:A:1207:2MG:C5	2.98	0.51
1:A:1399:C:H4'	1:A:1400:5MC:H5"	1.93	0.51
1:A:991:U:HO2'	1:A:992:U:P	2.33	0.51
3:C:131:ARG:HA	3:C:134:ILE:HD12	1.92	0.51
1:A:1109:C:OP2	3:C:176:HIS:ND1	2.43	0.51
4:D:9:CYS:O	4:D:13:ARG:HG3	2.10	0.51
1:A:687:A:H4'	1:A:688:G:O5'	2.11	0.51
1:A:767:A:H2'	1:A:768:A:O4'	2.10	0.51
18:R:22:VAL:O	18:R:26:LEU:HD13	2.11	0.51
1:A:383:A:C5	1:A:384:G:H1'	2.46	0.50
1:A:510:A:H5"	1:A:511:C:P	2.50	0.50
4:D:65:ARG:HG3	4:D:75:PHE:CD1	2.46	0.50
20:T:56:MET:HE2	20:T:85:MET:HA	1.93	0.50
1:A:1054:C:N4	23:W:34:G:C8	2.79	0.50
1:A:1300:G:C2'	1:A:1301:U:OP2	2.59	0.50
1:A:328:C:C2'	1:A:329:A:OP2	2.59	0.50
3:C:47:LEU:CD2	3:C:68:VAL:HG11	2.42	0.50
13:M:96:LEU:HB3	13:M:97:PRO:CD	2.40	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:21:ASP:OD2	15:O:24:SER:HB3	2.10	0.50
17:Q:5:VAL:HG22	17:Q:60:ILE:HD12	1.94	0.50
1:A:1347:G:H22	1:A:1374:A:P	2.35	0.50
2:B:139:LYS:NZ	2:B:143:GLU:HG3	2.26	0.50
13:M:37:THR:O	13:M:55:ARG:HD2	2.11	0.50
15:O:18:PHE:HB2	15:O:19:PRO:CD	2.41	0.50
20:T:69:GLY:O	20:T:73:HIS:ND1	2.44	0.50
1:A:1226:C:H4'	19:S:80:TYR:CE2	2.47	0.50
5:E:75:THR:HG23	5:E:76:ILE:O	2.10	0.50
12:L:39:VAL:HG23	12:L:57:LYS:HB2	1.93	0.50
1:A:117:G:O5'	1:A:117:G:H8	1.94	0.50
1:A:1233:G:H2'	1:A:1234:C:C6	2.46	0.50
1:A:715:A:H2'	1:A:716:A:C8	2.47	0.50
1:A:83:U:H3'	1:A:83:U:H6	1.76	0.50
2:B:28:PHE:CD2	2:B:190:THR:HA	2.46	0.50
1:A:1189:C:H5"	3:C:5:ILE:HG12	1.94	0.50
9:I:125:TYR:CE1	9:I:127:LYS:HB2	2.47	0.50
13:M:108:ARG:NH2	13:M:114:ARG:HA	2.27	0.50
19:S:15:LEU:O	19:S:19:VAL:HG12	2.11	0.50
2:B:24:TRP:O	2:B:24:TRP:CG	2.64	0.50
21:U:5:ASP:O	21:U:11:GLY:HA3	2.11	0.50
1:A:1190:G:OP1	3:C:4:LYS:HA	2.12	0.50
1:A:1203:C:O5'	1:A:1203:C:H6	1.94	0.50
1:A:1330:U:OP1	13:M:23:TYR:O	2.28	0.50
3:C:58:GLU:HB2	3:C:65:ALA:CB	2.42	0.50
21:U:5:ASP:HB3	21:U:8:THR:OG1	2.12	0.50
1:A:1425:U:H2'	1:A:1426:C:C6	2.45	0.50
1:A:933:G:O6	7:G:3:ARG:NH2	2.45	0.50
16:P:1:MET:O	16:P:1:MET:HG2	2.12	0.50
1:A:1053:G:C4'	1:A:1054:C:H5'	2.42	0.50
2:B:139:LYS:HA	2:B:139:LYS:HE2	1.93	0.50
7:G:9:VAL:HG12	7:G:10:ARG:O	2.11	0.50
14:N:61:TRP:CD1	14:N:61:TRP:O	2.65	0.50
1:A:130:A:C8	17:Q:63:ARG:HG3	2.47	0.50
1:A:112:G:O2'	1:A:113:G:H5'	2.12	0.49
1:A:1202:G:O2'	14:N:29:ARG:HB3	2.12	0.49
1:A:1212:U:H5"	1:A:1213:A:C8	2.47	0.49
1:A:204:U:H4'	1:A:216:G:O4'	2.11	0.49
4:D:170:VAL:CG1	4:D:171:GLY:N	2.75	0.49
11:K:87:THR:O	11:K:87:THR:OG1	2.30	0.49
13:M:65:LYS:O	13:M:70:LEU:HG	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:67:LEU:HD13	15:O:82:ILE:HD11	1.94	0.49
17:Q:40:LYS:HG2	17:Q:41:LYS:N	2.26	0.49
1:A:1004:A:H62	1:A:1037:C:N4	2.10	0.49
1:A:953:G:C5'	1:A:965:A:H61	2.23	0.49
2:B:19:HIS:CD2	2:B:191:ASP:OD1	2.65	0.49
3:C:85:ARG:NH1	3:C:85:ARG:HG2	2.27	0.49
5:E:8:GLU:HB3	5:E:34:VAL:HG12	1.93	0.49
9:I:48:GLU:OE1	9:I:51:ARG:NE	2.42	0.49
1:A:1063:C:H3'	1:A:1064:G:H2'	1.95	0.49
1:A:1403:C:H2'	1:A:1404:5MC:C6	2.47	0.49
6:F:101:ALA:HA	18:R:28:GLU:HB3	1.93	0.49
12:L:28:LYS:HG2	12:L:30:ALA:HB2	1.94	0.49
20:T:33:ILE:O	20:T:34:LYS:C	2.51	0.49
1:A:840:C:H4'	1:A:848:C:O2	2.12	0.49
1:A:980:C:H5"	1:A:981:U:OP2	2.13	0.49
12:L:34:ARG:O	12:L:61:THR:HG23	2.13	0.49
1:A:1277:C:HO2'	1:A:1279:A:H1'	1.77	0.49
1:A:1149:C:O2'	1:A:1280:A:N1	2.42	0.49
1:A:399:G:OP1	29:A:2090:HOH:O	2.20	0.49
1:A:665:A:N3	1:A:732:C:H2'	2.27	0.49
1:A:858:G:O2'	1:A:859:A:H5'	2.12	0.49
9:I:4:TYR:CZ	9:I:88:TYR:HD1	2.30	0.49
1:A:872:A:H4'	1:A:873:A:OP1	2.13	0.49
1:A:961:U:C2'	1:A:962:C:H5'	2.43	0.49
1:A:575:G:O2'	1:A:821:G:H5'	2.11	0.49
2:B:74:LYS:C	2:B:76:GLN:N	2.64	0.49
7:G:111:ARG:HB3	7:G:113:GLU:HG2	1.94	0.49
7:G:15:ASP:O	7:G:19:GLY:HA2	2.12	0.49
8:H:70:GLN:OE1	8:H:70:GLN:HA	2.13	0.49
2:B:48:MET:O	2:B:52:GLU:HG3	2.12	0.49
4:D:83:SER:HA	4:D:89:THR:HG23	1.94	0.49
6:F:82:ARG:HE	6:F:82:ARG:HA	1.76	0.49
7:G:16:LEU:H	7:G:16:LEU:HD22	1.76	0.49
7:G:65:ALA:HB1	7:G:127:ALA:CB	2.40	0.49
20:T:50:GLU:HG3	20:T:100:ILE:HG12	1.93	0.49
1:A:524:G:H2'	1:A:525:C:C6	2.48	0.49
1:A:741:G:H2'	1:A:742:G:O4'	2.13	0.49
4:D:31:CYS:O	4:D:32:ALA:HB3	2.13	0.49
7:G:43:PHE:O	7:G:46:ALA:HB3	2.13	0.49
7:G:51:GLN:O	7:G:52:GLU:CD	2.52	0.49
7:G:5:ARG:HH12	7:G:8:GLU:HG2	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1047:G:H5"	14:N:4:LYS:CD	2.39	0.49
1:A:1095:U:H2'	1:A:1096:C:C6	2.48	0.49
3:C:126:ARG:O	3:C:127:ARG:CB	2.60	0.49
3:C:136:GLN:O	3:C:140:ARG:HG3	2.13	0.49
1:A:1073:U:P	5:E:57:LYS:HE2	2.53	0.48
1:A:1198:G:H2'	1:A:1199:U:C6	2.48	0.48
1:A:1540:PSU:C2	1:A:1541:PSU:C2	3.01	0.48
1:A:88:A:C6	1:A:89:C:N3	2.81	0.48
2:B:75:LYS:CA	2:B:78:GLN:HG3	2.39	0.48
9:I:69:GLY:O	9:I:73:GLN:HG3	2.13	0.48
19:S:5:LEU:O	19:S:6:LYS:HB2	2.13	0.48
1:A:1047:G:O2'	1:A:1048:G:H5'	2.13	0.48
1:A:1281:U:H5'	1:A:1282:C:H5	1.77	0.48
1:A:1378:C:O2	7:G:76:ARG:NH1	2.42	0.48
1:A:461:C:H4'	1:A:462:G:OP2	2.13	0.48
1:A:608:A:OP2	29:A:2345:HOH:O	2.20	0.48
1:A:959:A:H3'	1:A:960:U:H5"	1.94	0.48
3:C:6:HIS:HD2	3:C:8:ILE:HB	1.75	0.48
4:D:50:ARG:HH22	5:E:9:LYS:NZ	2.11	0.48
1:A:1216:G:H5"	14:N:5:ALA:HB2	1.95	0.48
15:O:22:THR:O	15:O:27:VAL:HG11	2.13	0.48
1:A:1065:U:C1'	1:A:1066:C:OP2	2.62	0.48
1:A:1072:G:C5	1:A:1073:U:C4	3.02	0.48
1:A:1112:C:C2	3:C:178:LEU:HB2	2.48	0.48
1:A:56:U:H2'	1:A:57:G:H8	1.78	0.48
3:C:126:ARG:HG3	3:C:128:PHE:N	2.27	0.48
1:A:1103:C:C5'	2:B:98:LEU:HD12	2.43	0.48
1:A:1300:G:C6	1:A:1335:C:C5	3.01	0.48
1:A:1495:U:H2'	1:A:1496:C:C6	2.48	0.48
1:A:519:C:H2'	1:A:520:A:C8	2.49	0.48
1:A:80:G:C2	1:A:81:U:N3	2.79	0.48
4:D:79:PHE:HE1	4:D:204:ILE:HD12	1.79	0.48
5:E:98:THR:N	5:E:117:ASP:OD1	2.42	0.48
6:F:8:ILE:HB	6:F:61:LEU:HB2	1.96	0.48
7:G:99:LEU:HD22	7:G:103:TRP:CZ2	2.49	0.48
9:I:26:VAL:HG23	9:I:33:PHE:HB2	1.94	0.48
9:I:75:ASP:O	9:I:78:LYS:HB3	2.14	0.48
1:A:1064:G:H22	1:A:1190:G:C2'	2.26	0.48
1:A:179:A:H2'	1:A:180:U:H6	1.78	0.48
1:A:256:U:OP1	17:Q:17:LYS:NZ	2.46	0.48
5:E:11:ILE:O	5:E:12:LEU:HB2	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:99:LYS:HG3	10:J:99:LYS:O	2.13	0.48
16:P:74:LEU:N	16:P:74:LEU:HD23	2.28	0.48
1:A:250:A:C4'	1:A:251:G:O5'	2.61	0.48
1:A:452:A:HO2'	1:A:453:A:H8	1.61	0.48
10:J:6:ILE:HB	10:J:72:VAL:HG21	1.94	0.48
1:A:89:C:H3'	1:A:89:C:C6	2.47	0.48
3:C:58:GLU:HB2	3:C:65:ALA:HB2	1.94	0.48
5:E:78:HIS:HE1	5:E:142:LEU:HD23	1.78	0.48
10:J:38:ILE:O	10:J:70:ARG:HA	2.14	0.48
1:A:1018:C:H2'	1:A:1019:C:C6	2.48	0.48
1:A:359:U:H2'	1:A:360:A:C8	2.49	0.48
1:A:376:G:P	16:P:67:THR:HG21	2.53	0.48
1:A:918:A:H2'	1:A:919:A:C8	2.48	0.48
10:J:47:PHE:HD2	14:N:34:TYR:CD2	2.32	0.48
11:K:29:ILE:HB	11:K:44:SER:HB3	1.95	0.48
14:N:26:ARG:HE	14:N:47:LEU:HD11	1.79	0.48
14:N:5:ALA:O	14:N:8:GLU:CG	2.62	0.48
17:Q:68:ARG:N	17:Q:70:ARG:HH11	2.11	0.48
17:Q:95:TYR:O	17:Q:98:LEU:HD12	2.13	0.48
1:A:118:U:H3'	1:A:288:A:H61	1.78	0.48
1:A:976:G:C8	1:A:1358:U:O2	2.67	0.48
1:A:1499:A:H1'	1:A:1520:G:H5'	1.96	0.48
1:A:502:G:H2'	1:A:503:C:O4'	2.14	0.48
3:C:112:SER:O	3:C:116:VAL:HG23	2.14	0.48
4:D:4:TYR:O	4:D:4:TYR:CD2	2.66	0.48
6:F:3:ARG:NH1	6:F:38:GLU:OE2	2.47	0.48
18:R:40:LEU:HD23	18:R:40:LEU:HA	1.65	0.48
1:A:991:U:O2'	1:A:992:U:P	2.71	0.47
4:D:78:LEU:HA	4:D:78:LEU:HD23	1.56	0.47
5:E:90:VAL:O	5:E:91:LEU:HD23	2.13	0.47
9:I:4:TYR:CE2	9:I:88:TYR:HD1	2.32	0.47
10:J:48:THR:O	14:N:34:TYR:OH	2.31	0.47
12:L:24:VAL:HG13	12:L:98:TYR:CE2	2.49	0.47
10:J:47:PHE:CZ	14:N:37:PHE:HE1	2.31	0.47
16:P:28:ARG:NH1	16:P:29:ASP:OD2	2.47	0.47
1:A:1064:G:N2	1:A:1190:G:C2'	2.77	0.47
1:A:1493:A:H5"	1:A:1494:G:OP2	2.15	0.47
1:A:738:C:OP1	6:F:92:LYS:HD3	2.14	0.47
1:A:983:A:H5'	1:A:984:C:OP2	2.14	0.47
2:B:229:VAL:O	2:B:229:VAL:HG12	2.14	0.47
11:K:33:THR:HG22	11:K:39:PRO:CA	2.41	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:695:A:OP1	11:K:52:GLY:HA3	2.14	0.47
12:L:28:LYS:HB3	12:L:30:ALA:HB2	1.96	0.47
13:M:10:PRO:O	13:M:11:ARG:HB2	2.15	0.47
18:R:22:VAL:HG23	18:R:55:ARG:O	2.14	0.47
1:A:1190:G:O2'	1:A:1191:A:OP2	2.17	0.47
1:A:89:C:C3'	1:A:89:C:C6	2.97	0.47
4:D:169:LYS:HE2	4:D:169:LYS:HB2	1.62	0.47
11:K:72:ALA:HB1	11:K:77:MET:HE2	1.95	0.47
14:N:9:LYS:C	14:N:9:LYS:HD2	2.35	0.47
15:O:39:LEU:HD12	15:O:56:LEU:HB2	1.97	0.47
19:S:5:LEU:CG	19:S:6:LYS:N	2.77	0.47
1:A:191:G:N2	20:T:103:GLY:O	2.42	0.47
1:A:1133:G:H1	1:A:1141:C:H42	1.62	0.47
1:A:1346:A:N1	1:A:1374:A:H5"	2.29	0.47
1:A:1397:C:H4'	1:A:1398:A:OP2	2.14	0.47
1:A:510:A:P	29:A:2174:HOH:O	2.71	0.47
1:A:862:C:H5"	29:A:2651:HOH:O	2.14	0.47
5:E:81:GLU:OE2	5:E:88:LYS:NZ	2.40	0.47
6:F:25:ILE:HD13	6:F:82:ARG:HD2	1.96	0.47
7:G:5:ARG:NH1	7:G:8:GLU:HG2	2.30	0.47
17:Q:18:THR:HG23	17:Q:69:LYS:HD3	1.97	0.47
1:A:1281:U:H5'	1:A:1282:C:C5	2.50	0.47
1:A:180:U:H2'	1:A:181:G:H5'	1.96	0.47
4:D:111:ALA:HB2	4:D:120:LEU:HD12	1.97	0.47
5:E:8:GLU:CB	5:E:34:VAL:HG12	2.45	0.47
13:M:66:LEU:O	13:M:69:GLU:HG2	2.13	0.47
15:O:87:ILE:HG22	15:O:88:ARG:HG2	1.97	0.47
1:A:47:C:H4'	1:A:48:C:OP1	2.14	0.47
1:A:890:G:O2'	1:A:906:G:O6	2.22	0.47
1:A:993:G:H4'	1:A:994:A:OP2	2.14	0.47
2:B:41:ILE:HD12	2:B:41:ILE:N	2.29	0.47
3:C:134:ILE:CG2	3:C:168:ALA:HB3	2.43	0.47
3:C:19:GLU:HG2	3:C:54:ARG:HE	1.79	0.47
5:E:36:ASP:CG	5:E:38:GLN:HB2	2.35	0.47
6:F:78:GLU:O	6:F:81:ILE:HG12	2.15	0.47
10:J:82:ILE:O	10:J:82:ILE:HG22	2.15	0.47
13:M:16:ASP:HB3	13:M:34:LEU:HD12	1.97	0.47
14:N:21:TYR:HE2	14:N:23:ARG:NE	2.12	0.47
1:A:1236:A:H4'	1:A:1304:G:H4'	1.95	0.47
1:A:1435:G:H2'	1:A:1436:U:H6	1.77	0.47
3:C:155:GLY:HA2	3:C:164:ARG:O	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:70:ILE:HD11	4:D:100:ARG:NE	2.29	0.47
7:G:10:ARG:HG2	7:G:10:ARG:NH1	2.25	0.47
9:I:10:ARG:NH1	9:I:75:ASP:OD2	2.47	0.47
1:A:1372:U:H5"	9:I:71:SER:HB2	1.95	0.47
13:M:96:LEU:HB3	13:M:97:PRO:HD2	1.97	0.47
20:T:20:LEU:HD13	20:T:20:LEU:HA	1.65	0.47
1:A:1098:C:H2'	1:A:1099:G:O4'	2.15	0.47
1:A:1494:G:OP2	1:A:1494:G:H8	1.98	0.47
1:A:577:G:H1'	1:A:816:A:C4	2.50	0.47
1:A:689:C:OP1	11:K:27:ASN:ND2	2.48	0.47
4:D:28:SER:O	4:D:30:LYS:N	2.44	0.47
8:H:116:LYS:HD3	8:H:127:LEU:HD13	1.97	0.47
11:K:59:TYR:CE2	11:K:63:LEU:HD11	2.49	0.47
13:M:88:ARG:HG2	13:M:98:VAL:HG12	1.97	0.47
15:O:26:GLU:CD	15:O:77:ARG:HH12	2.18	0.47
6:F:89:MET:HE2	18:R:76:LEU:HG	1.96	0.47
20:T:57:ARG:NH2	20:T:100:ILE:HD12	2.30	0.47
1:A:1035:A:N6	1:A:1036:G:O6	2.48	0.47
1:A:1349:A:C2	1:A:1374:A:C4	3.03	0.47
2:B:100:GLY:O	2:B:104:ASN:N	2.44	0.47
2:B:186:ALA:HB3	2:B:197:VAL:HG11	1.95	0.47
3:C:64:VAL:HG12	3:C:65:ALA:H	1.80	0.47
4:D:146:ILE:HD12	4:D:146:ILE:N	2.29	0.47
1:A:922:G:H1'	5:E:19:MET:HB3	1.95	0.47
7:G:10:ARG:HH11	7:G:10:ARG:CG	2.19	0.47
11:K:33:THR:HB	11:K:38:ASN:O	2.14	0.47
1:A:58:C:H6	1:A:58:C:O5'	1.97	0.47
1:A:695:A:H61	1:A:797:C:H1'	1.80	0.47
1:A:90:U:C2'	1:A:91:C:O5'	2.63	0.47
3:C:54:ARG:HB2	3:C:54:ARG:HH11	1.79	0.47
4:D:57:ARG:HB3	4:D:206:PHE:HB2	1.97	0.47
7:G:91:VAL:HG12	7:G:96:GLN:HG3	1.96	0.47
8:H:27:PRO:HA	8:H:58:TYR:CD2	2.50	0.47
1:A:1358:U:OP1	14:N:35:ARG:HG3	2.14	0.47
19:S:31:ILE:O	19:S:50:ALA:HB3	2.14	0.47
1:A:1529:G:OP2	1:A:1529:G:H3'	2.15	0.47
1:A:558:G:H3'	1:A:559:A:H3'	1.97	0.47
2:B:44:LEU:N	2:B:44:LEU:HD22	2.30	0.47
14:N:13:THR:N	14:N:14:PRO:HD3	2.30	0.47
1:A:1091:U:O2	1:A:1093:A:C8	2.68	0.46
1:A:1207:2MG:HM23	1:A:1208:C:H1'	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1347:G:N2	1:A:1373:G:H2'	2.30	0.46
1:A:1392:G:N2	1:A:1502:A:C8	2.80	0.46
1:A:1477:C:H2'	1:A:1478:C:H6	1.80	0.46
1:A:344:A:H5"	1:A:345:C:H5	1.80	0.46
1:A:499:A:C4'	1:A:500:G:OP1	2.56	0.46
1:A:736:C:H2'	1:A:737:A:C8	2.50	0.46
2:B:132:LYS:HB3	2:B:132:LYS:HZ2	1.80	0.46
4:D:206:PHE:CE2	4:D:207:TYR:CE2	3.03	0.46
4:D:8:VAL:O	4:D:11:LEU:N	2.41	0.46
6:F:12:PRO:HG3	6:F:57:GLN:O	2.15	0.46
10:J:48:THR:OG1	10:J:62:HIS:CD2	2.69	0.46
16:P:43:LYS:HG2	16:P:48:TRP:CD2	2.50	0.46
1:A:187:C:O2	20:T:105:SER:HB3	2.15	0.46
1:A:1077:G:N2	1:A:1080:A:OP2	2.43	0.46
1:A:853:G:C2'	1:A:854:G:H5'	2.46	0.46
2:B:128:GLU:HA	2:B:135:GLN:NE2	2.30	0.46
3:C:61:ALA:C	3:C:63:ASN:H	2.17	0.46
1:A:115:G:H1'	1:A:116:A:N7	2.31	0.46
1:A:960:U:H2'	1:A:960:U:O2	2.13	0.46
2:B:46:LYS:HD3	2:B:49:GLU:OE1	2.15	0.46
20:T:79:ARG:HD2	20:T:83:ARG:NH1	2.31	0.46
1:A:1329:A:OP2	21:U:7:ARG:NH2	2.47	0.46
1:A:126:G:N1	29:A:2119:HOH:O	2.34	0.46
1:A:1420:C:H2'	1:A:1421:G:O4'	2.15	0.46
1:A:1112:C:C4	3:C:178:LEU:HD23	2.50	0.46
4:D:127:THR:HG23	4:D:147:ALA:O	2.15	0.46
6:F:14:LEU:HD22	6:F:18:GLN:CB	2.45	0.46
6:F:14:LEU:HD22	6:F:18:GLN:HB3	1.96	0.46
6:F:80:ARG:NH1	6:F:88:VAL:HB	2.31	0.46
19:S:40:ILE:CG2	19:S:62:ILE:HD11	2.43	0.46
1:A:586:C:C2'	1:A:587:G:H5'	2.45	0.46
3:C:179:ARG:HD2	3:C:207:VAL:HG22	1.97	0.46
5:E:48:ALA:HB1	5:E:49:PRO:HD2	1.96	0.46
6:F:4:TYR:CE1	6:F:92:LYS:HG2	2.50	0.46
7:G:124:LEU:HA	7:G:124:LEU:HD23	1.69	0.46
15:O:43:LEU:HD11	15:O:53:HIS:HA	1.97	0.46
17:Q:4:LYS:HD2	17:Q:6:LEU:HD21	1.98	0.46
1:A:1311:G:N7	19:S:2:PRO:HA	2.30	0.46
20:T:53:LEU:HD13	20:T:100:ILE:HG22	1.96	0.46
20:T:60:GLU:HG3	20:T:81:LYS:HD2	1.98	0.46
1:A:1468:A:H2'	1:A:1469:G:O4'	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:186:C:H2'	1:A:187:C:C6	2.51	0.46
1:A:1080:A:H4'	5:E:16:THR:HG21	1.97	0.46
5:E:84:PHE:HB3	5:E:134:ALA:HB2	1.96	0.46
9:I:48:GLU:N	9:I:49:PRO:CD	2.78	0.46
11:K:121:PRO:HB2	11:K:126:ARG:HG3	1.98	0.46
16:P:4:ILE:HG12	16:P:21:VAL:HG22	1.97	0.46
1:A:235:C:C5'	17:Q:70:ARG:HG2	2.37	0.46
18:R:39:VAL:CG1	18:R:40:LEU:N	2.79	0.46
19:S:12:ASP:CG	19:S:37:ARG:HH21	2.19	0.46
1:A:1439:C:OP1	20:T:38:LYS:HE3	2.15	0.46
20:T:67:ALA:HB1	20:T:73:HIS:HA	1.98	0.46
2:B:230:VAL:HG12	2:B:231:GLU:O	2.15	0.46
6:F:45:LEU:HD12	6:F:45:LEU:O	2.15	0.46
1:A:1251:A:C4'	9:I:12:GLU:OE1	2.63	0.46
1:A:984:C:N4	1:A:1221:G:H1	2.14	0.46
1:A:262:A:C6	1:A:263:A:C6	3.03	0.46
1:A:629:G:H2'	1:A:630:G:O4'	2.16	0.46
2:B:112:VAL:O	2:B:115:LEU:HB3	2.16	0.46
2:B:204:ASN:C	2:B:204:ASN:OD1	2.52	0.46
3:C:112:SER:HB3	3:C:115:LEU:HD12	1.97	0.46
5:E:144:THR:HB	5:E:147:ASP:OD1	2.16	0.46
16:P:57:ARG:HD3	16:P:79:VAL:O	2.16	0.46
1:A:1320:C:O2	19:S:36:ARG:NH1	2.49	0.46
1:A:1032:G:H2'	1:A:1033:G:C8	2.50	0.46
1:A:1126:U:C4	1:A:1127:G:C2	3.04	0.46
1:A:1540:PSU:H6	1:A:1540:PSU:O5'	1.99	0.46
1:A:614:A:H2'	1:A:615:C:H6	1.81	0.46
6:F:2:ARG:CZ	6:F:69:GLU:HG2	2.45	0.46
7:G:10:ARG:CG	7:G:10:ARG:NH1	2.77	0.46
13:M:82:MET:HE3	13:M:93:ARG:HG2	1.97	0.46
14:N:14:PRO:O	14:N:15:LYS:HB3	2.16	0.46
19:S:10:PHE:CD2	19:S:10:PHE:C	2.89	0.46
1:A:1201:A:H4'	1:A:1202:G:O5'	2.15	0.46
1:A:1427:U:H2'	1:A:1428:A:H8	1.81	0.46
1:A:151:A:H2'	1:A:152:A:O4'	2.15	0.46
1:A:1329:A:O2'	1:A:1330:U:H5'	2.15	0.45
1:A:184:G:H2'	1:A:185:A:H8	1.81	0.45
1:A:614:A:H2'	1:A:615:C:C6	2.50	0.45
7:G:18:TYR:CE2	7:G:59:LEU:HB2	2.51	0.45
9:I:126:SER:C	9:I:128:ARG:H	2.19	0.45
12:L:76:ASN:O	12:L:76:ASN:OD1	2.34	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1112:C:H1'	3:C:179:ARG:NH1	2.31	0.45
1:A:21:G:H2'	1:A:22:G:C8	2.51	0.45
1:A:411:A:C6	1:A:429:U:C5	3.04	0.45
1:A:68:G:C2'	1:A:69:G:O5'	2.65	0.45
2:B:165:VAL:O	2:B:187:LEU:O	2.34	0.45
3:C:134:ILE:HG22	3:C:168:ALA:CB	2.42	0.45
3:C:8:ILE:HG13	3:C:184:TYR:HB3	1.98	0.45
5:E:96:PRO:HA	5:E:117:ASP:OD1	2.17	0.45
5:E:24:ARG:CG	5:E:24:ARG:NH1	2.64	0.45
9:I:16:ARG:HD3	9:I:64:THR:HB	1.97	0.45
10:J:48:THR:CB	10:J:62:HIS:HB3	2.46	0.45
13:M:67:GLU:HB3	13:M:68:GLY:H	1.48	0.45
19:S:52:TYR:HA	19:S:56:GLN:O	2.17	0.45
1:A:1029:C:N3	1:A:1033:G:N2	2.64	0.45
1:A:130:A:OP2	1:A:190(E):U:C2'	2.64	0.45
1:A:176:C:O2'	1:A:177:C:H5'	2.16	0.45
1:A:22:G:H2'	1:A:23:C:C6	2.52	0.45
2:B:73:THR:HG22	2:B:73:THR:O	2.16	0.45
5:E:144:THR:CG2	5:E:145:LYS:N	2.79	0.45
8:H:104:ARG:O	8:H:105:ARG:C	2.55	0.45
10:J:99:LYS:HB2	10:J:99:LYS:HE3	1.85	0.45
11:K:39:PRO:O	11:K:40:ILE:HD13	2.16	0.45
15:O:31:LEU:HA	15:O:31:LEU:HD12	1.74	0.45
1:A:1053:G:H4'	1:A:1054:C:H5'	1.98	0.45
1:A:114:U:H1'	1:A:353:A:H1'	1.97	0.45
1:A:162:A:H5"	1:A:163:C:OP2	2.16	0.45
1:A:547:A:H4'	1:A:548:G:O5'	2.16	0.45
1:A:811:C:H4'	1:A:900:A:N6	2.31	0.45
7:G:145:ALA:C	7:G:147:ALA:H	2.19	0.45
10:J:71:LEU:HA	10:J:71:LEU:HD23	1.74	0.45
1:A:1003(A):G:C2	1:A:1038:C:O2	2.69	0.45
1:A:107:G:H2'	1:A:108:G:H5"	1.99	0.45
1:A:1277:C:H2'	1:A:1279:A:C8	2.51	0.45
1:A:737:A:H2'	1:A:738:C:C6	2.51	0.45
1:A:981:U:H2'	1:A:982:U:C5	2.51	0.45
6:F:44:GLY:HA2	6:F:59:TYR:CE1	2.52	0.45
7:G:69:VAL:O	7:G:69:VAL:HG12	2.16	0.45
8:H:75:ARG:HA	8:H:76:PRO:HD3	1.71	0.45
9:I:37:PHE:HB3	9:I:43:ALA:HB2	1.98	0.45
11:K:58:PRO:O	11:K:61:ALA:HB3	2.16	0.45
10:J:47:PHE:CE2	14:N:37:PHE:HE1	2.34	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:128:G:H4'	17:Q:3:LYS:HG3	1.99	0.45
21:U:25:LYS:HB3	21:U:25:LYS:NZ	2.32	0.45
1:A:1065:U:C2'	1:A:1066:C:OP2	2.64	0.45
1:A:922:G:N3	1:A:1398:A:H2	2.15	0.45
1:A:560:U:C5'	1:A:566:G:N2	2.77	0.45
1:A:961:U:H2'	1:A:962:C:H5'	1.97	0.45
2:B:167:PRO:HG3	2:B:186:ALA:HB1	1.97	0.45
2:B:174:VAL:O	2:B:178:ARG:HG3	2.17	0.45
4:D:12:CYS:HA	4:D:19:LEU:CD2	2.46	0.45
4:D:38:TYR:CE1	4:D:45:GLN:HG3	2.51	0.45
15:O:56:LEU:HA	15:O:59:MET:CE	2.46	0.45
19:S:40:ILE:CG2	19:S:67:VAL:HA	2.41	0.45
1:A:1055:A:C2	1:A:1056:U:H1'	2.51	0.45
1:A:1128:C:O2'	1:A:1130:A:C8	2.65	0.45
1:A:1493:A:H4'	1:A:1494:G:OP1	2.15	0.45
1:A:243:A:C2	1:A:246:A:C8	3.04	0.45
1:A:793:U:H3'	1:A:794:A:C5'	2.39	0.45
1:A:1003(A):G:N1	1:A:1004:A:H1'	2.32	0.45
1:A:1047:G:H2'	1:A:1048:G:H5'	1.97	0.45
1:A:229:U:H5"	16:P:33:ILE:HD13	1.99	0.45
2:B:212:GLN:NE2	2:B:235:SER:HB2	2.23	0.45
2:B:239:VAL:O	2:B:240:GLN:CB	2.65	0.45
2:B:57:PHE:CD1	2:B:199:TYR:CZ	3.05	0.45
2:B:97:TRP:CH2	2:B:176:GLU:CD	2.90	0.45
3:C:91:LEU:HD21	3:C:99:VAL:HG13	1.99	0.45
4:D:172:PRO:HD2	4:D:173:TRP:CE3	2.51	0.45
5:E:100:VAL:C	5:E:101:ILE:HD12	2.37	0.45
18:R:25:THR:C	18:R:26:LEU:HD12	2.37	0.45
1:A:1298:C:H4'	1:A:1299:A:O4'	2.16	0.45
3:C:180:ALA:HB1	3:C:182:ILE:CG1	2.45	0.45
3:C:94:LEU:HD12	3:C:94:LEU:O	2.17	0.45
4:D:62:GLN:HA	4:D:62:GLN:OE1	2.17	0.45
8:H:85:ARG:HD2	8:H:87:SER:O	2.17	0.45
10:J:75:ILE:HG22	10:J:76:ASN:N	2.27	0.45
12:L:70:ILE:HD13	12:L:77:LEU:HD12	1.97	0.45
13:M:63:THR:HG23	13:M:64:TRP:N	2.32	0.45
1:A:1258:G:H2'	1:A:1259:C:H6	1.79	0.45
3:C:34:LEU:HG	3:C:38:ARG:NE	2.32	0.45
4:D:50:ARG:HH22	5:E:9:LYS:HZ3	1.63	0.45
7:G:87:VAL:HA	7:G:88:PRO:HD3	1.85	0.45
9:I:118:LYS:C	9:I:120:ARG:H	2.19	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:99:LEU:HD22	9:I:99:LEU:H	1.82	0.45
1:A:1006:C:H2'	1:A:1007:C:H6	1.82	0.44
1:A:1300:G:C5	1:A:1335:C:C5	3.04	0.44
1:A:392:G:H2'	1:A:393:A:C8	2.52	0.44
3:C:148:GLY:HA3	3:C:172:ARG:O	2.17	0.44
4:D:107:ARG:NH1	4:D:114:ARG:HH22	2.15	0.44
4:D:206:PHE:HE2	4:D:207:TYR:CE2	2.35	0.44
5:E:101:ILE:CD1	5:E:101:ILE:N	2.80	0.44
7:G:51:GLN:O	7:G:52:GLU:OE2	2.35	0.44
13:M:102:ARG:HG3	13:M:102:ARG:O	2.17	0.44
20:T:10:LEU:HD23	20:T:13:LEU:H	1.82	0.44
1:A:1158:C:O2	1:A:1158:C:H3'	2.16	0.44
1:A:1413:A:H2'	1:A:1414:U:O4'	2.17	0.44
1:A:266:G:H5"	1:A:268:C:H41	1.82	0.44
1:A:814:A:H2'	1:A:816:A:H5"	1.99	0.44
3:C:167:TRP:HZ3	3:C:169:ALA:HB3	1.82	0.44
9:I:89:ASN:O	9:I:92:TYR:HB2	2.17	0.44
13:M:65:LYS:HE3	13:M:65:LYS:HB2	1.72	0.44
1:A:114:U:O2'	1:A:115:G:H5'	2.18	0.44
1:A:259:G:O2'	1:A:260:G:H5'	2.18	0.44
1:A:540:G:H2'	1:A:541:G:O4'	2.17	0.44
1:A:661:G:H8	1:A:661:G:H5"	1.82	0.44
2:B:92:TYR:CD1	2:B:92:TYR:O	2.71	0.44
2:B:97:TRP:CE3	2:B:98:LEU:O	2.71	0.44
3:C:156:ARG:NE	3:C:160:ALA:O	2.50	0.44
3:C:81:GLY:O	3:C:84:ILE:HG22	2.17	0.44
15:O:45:VAL:CG1	15:O:46:HIS:H	2.29	0.44
16:P:12:LYS:C	16:P:14:ASN:H	2.20	0.44
1:A:1054:C:C2'	1:A:1055:A:H5"	2.48	0.44
1:A:1130:A:OP1	1:A:1131:G:OP2	2.34	0.44
1:A:1404:5MC:HM51	1:A:1404:5MC:OP2	2.18	0.44
1:A:1518:MA6:H2'	1:A:1519:MA6:C8	2.47	0.44
1:A:463:A:H2'	1:A:474:G:O4'	2.17	0.44
1:A:913:A:OP1	12:L:91:LYS:HE2	2.17	0.44
2:B:102:LEU:HB3	2:B:180:LEU:HD12	1.98	0.44
1:A:1373:G:H5"	7:G:36:LYS:CG	2.47	0.44
12:L:46:LYS:C	12:L:48:PRO:HD2	2.37	0.44
12:L:53:ARG:HH12	12:L:92:0TD:CG	2.25	0.44
15:O:18:PHE:HB2	15:O:19:PRO:HD2	1.98	0.44
1:A:187:C:C2	20:T:105:SER:HB3	2.52	0.44
20:T:12:ALA:O	20:T:15:ARG:HB2	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1316:G:N2	1:A:1318:A:H3'	2.32	0.44
1:A:229:U:C2'	1:A:230:G:H5'	2.47	0.44
1:A:685:G:C2	1:A:686:U:C4	3.06	0.44
1:A:587:G:N2	1:A:754:C:OP2	2.49	0.44
6:F:69:GLU:CD	6:F:69:GLU:H	2.21	0.44
1:A:526:C:OP1	12:L:91:LYS:HE3	2.18	0.44
13:M:63:THR:HG23	13:M:64:TRP:H	1.83	0.44
15:O:74:ASP:HB3	15:O:77:ARG:CG	2.46	0.44
1:A:1314:C:C6	19:S:6:LYS:HE2	2.53	0.44
20:T:57:ARG:HH21	20:T:100:ILE:HG21	1.83	0.44
1:A:262:A:H5'	20:T:74:LYS:HD3	2.00	0.44
1:A:1202:G:C2	14:N:42:ILE:HG21	2.53	0.44
1:A:162:A:C5	1:A:163:C:H1'	2.53	0.44
1:A:765:G:H5"	1:A:766:A:OP1	2.16	0.44
1:A:89:C:C5	1:A:90:U:N3	2.86	0.44
1:A:1112:C:H5"	1:A:1113:C:OP2	2.18	0.44
1:A:1307:U:H2'	1:A:1308:U:O4'	2.18	0.44
1:A:201:C:H42	1:A:216:G:H1	1.64	0.44
1:A:269:C:H2'	1:A:270:A:C8	2.52	0.44
1:A:57:G:H2'	1:A:58:C:C6	2.51	0.44
1:A:952:U:H2'	1:A:953:G:H8	1.82	0.44
9:I:127:LYS:O	9:I:127:LYS:HG2	2.17	0.44
9:I:7:THR:HG22	9:I:8:GLY:N	2.32	0.44
18:R:76:LEU:HD23	18:R:76:LEU:HA	1.58	0.44
1:A:1125:U:O2'	1:A:1126:U:P	2.76	0.44
4:D:108:LEU:HA	4:D:108:LEU:HD23	1.83	0.44
7:G:113:GLU:HG2	7:G:113:GLU:H	1.55	0.44
7:G:18:TYR:CD2	7:G:59:LEU:HD13	2.52	0.44
9:I:93:ARG:HB3	9:I:93:ARG:NH1	2.33	0.44
10:J:52:GLY:HA2	10:J:53:PRO:HD3	1.85	0.44
23:W:37:G:H2'	23:W:38:PSU:O4'	2.18	0.44
1:A:1003(A):G:C5	1:A:1004:A:H1'	2.53	0.44
1:A:1162:C:H42	1:A:1174:G:H1	1.64	0.44
1:A:1245:A:C2	1:A:1293:G:C2	3.05	0.44
1:A:1511:G:H2'	1:A:1512:U:O4'	2.18	0.44
1:A:161:A:H2'	1:A:162:A:C8	2.53	0.44
1:A:353:A:C5'	1:A:353:A:C8	2.97	0.44
1:A:384:G:H2'	1:A:385:C:C6	2.53	0.44
1:A:444:C:H2'	1:A:444:C:O2	2.18	0.44
1:A:559:A:H4'	1:A:560:U:O5'	2.18	0.44
20:T:14:LYS:O	20:T:18:GLN:HG3	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:184:G:H2'	1:A:185:A:C8	2.53	0.43
1:A:575:G:H4'	1:A:576:G:OP1	2.16	0.43
1:A:968:A:H4'	1:A:969:A:OP2	2.18	0.43
5:E:36:ASP:C	5:E:38:GLN:H	2.19	0.43
5:E:76:ILE:CG2	5:E:77:PRO:HD2	2.48	0.43
1:A:974:A:P	14:N:41:ARG:HH12	2.39	0.43
1:A:1337:G:H5"	1:A:1338:G:OP1	2.18	0.43
1:A:1369:C:H2'	1:A:1370:G:C8	2.53	0.43
27:A:1956:SRY:HI32	27:A:1956:SRY:C22	2.47	0.43
4:D:170:VAL:CG1	4:D:174:LEU:HB2	2.48	0.43
5:E:41:VAL:HG13	5:E:113:ALA:CA	2.43	0.43
9:I:51:ARG:HA	9:I:56:LEU:HG	2.00	0.43
19:S:41:VAL:HG22	19:S:44:MET:HG3	1.99	0.43
1:A:1493:A:C2	23:W:37:G:O4'	2.71	0.43
1:A:1005:A:N1	1:A:1026:G:N2	2.58	0.43
2:B:193:ASP:HB3	2:B:196:LEU:HD11	1.99	0.43
3:C:11:ARG:O	3:C:14:ILE:O	2.37	0.43
11:K:40:ILE:HG22	11:K:41:THR:HG23	1.99	0.43
15:O:7:GLU:O	15:O:11:VAL:HG12	2.18	0.43
15:O:32:LEU:HD23	15:O:32:LEU:HA	1.73	0.43
15:O:74:ASP:OD2	15:O:77:ARG:HD3	2.17	0.43
1:A:1285:A:H4'	1:A:1286:A:O5'	2.18	0.43
1:A:289:G:OP2	29:A:2017:HOH:O	2.21	0.43
1:A:474:G:H5"	16:P:81:ARG:NH1	2.33	0.43
1:A:631:G:H5'	1:A:632:A:P	2.58	0.43
1:A:722:A:H4'	1:A:723:U:C5	2.53	0.43
1:A:948:C:N4	29:A:2306:HOH:O	2.50	0.43
5:E:31:LEU:HA	5:E:31:LEU:HD23	1.60	0.43
6:F:53:ALA:C	6:F:54:LYS:HG2	2.39	0.43
7:G:113:GLU:HG3	7:G:119:ARG:HA	2.00	0.43
10:J:35:SER:OG	10:J:73:ASP:O	2.30	0.43
11:K:24:SER:C	11:K:26:ASN:N	2.71	0.43
12:L:60:LEU:CD2	12:L:66:VAL:HG22	2.48	0.43
1:A:1126:U:H6	1:A:1126:U:P	2.41	0.43
1:A:1187:G:C2	1:A:1188:A:C4	3.07	0.43
1:A:1419:G:C6	1:A:1420:C:C4	3.07	0.43
1:A:1477:C:H2'	1:A:1478:C:C6	2.53	0.43
1:A:1539:C:H2'	1:A:1540:PSU:O4'	2.18	0.43
1:A:939:G:H2'	1:A:940:C:C6	2.53	0.43
5:E:16:THR:O	5:E:26:PHE:HA	2.18	0.43
7:G:46:ALA:O	7:G:50:ILE:HG12	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:88:GLY:O	11:K:89:ALA:C	2.57	0.43
1:A:1533:C:C2'	1:A:1534:C:O5'	2.66	0.43
1:A:255:G:O6	1:A:266:G:O6	2.37	0.43
1:A:345:C:OP2	1:A:345:C:H6	2.01	0.43
1:A:740:U:O3'	15:O:39:LEU:HD23	2.19	0.43
1:A:581:G:N1	1:A:759:A:OP2	2.35	0.43
1:A:84:U:C4	1:A:88:A:C2	3.07	0.43
9:I:19:LEU:HB3	9:I:59:PHE:CD2	2.54	0.43
13:M:97:PRO:HB3	13:M:101:GLN:OE1	2.18	0.43
16:P:12:LYS:O	16:P:13:HIS:HB2	2.19	0.43
18:R:85:LEU:HD23	18:R:88:LYS:HD2	2.00	0.43
1:A:1009:G:C6	1:A:1021:G:C6	3.06	0.43
1:A:1030(D):A:H2'	1:A:1031:G:H5'	2.00	0.43
1:A:187:C:N3	20:T:105:SER:HB3	2.33	0.43
1:A:510:A:H5"	1:A:511:C:OP2	2.19	0.43
5:E:147:ASP:OD1	5:E:147:ASP:N	2.52	0.43
8:H:88:LYS:O	8:H:89:PRO:C	2.56	0.43
13:M:59:TYR:C	13:M:59:TYR:CD2	2.92	0.43
3:C:34:LEU:CD2	14:N:25:VAL:HG21	2.48	0.43
14:N:33:VAL:HG12	14:N:40:CYS:HB3	2.00	0.43
17:Q:45:HIS:HB2	17:Q:65:ILE:HG13	2.00	0.43
18:R:74:ARG:HB3	18:R:81:PHE:CE1	2.53	0.43
20:T:56:MET:CE	20:T:85:MET:HA	2.48	0.43
1:A:103:C:P	20:T:17:ARG:NH1	2.92	0.43
1:A:1130:A:OP2	1:A:1130:A:H3'	2.19	0.43
1:A:1494:G:C8	1:A:1494:G:OP2	2.72	0.43
1:A:509:A:HO2'	1:A:510:A:P	2.38	0.43
2:B:239:VAL:HG12	2:B:239:VAL:O	2.18	0.43
7:G:40:ALA:HB3	9:I:41:VAL:HG21	2.00	0.43
9:I:24:GLY:CA	9:I:57:GLY:HA2	2.45	0.43
9:I:93:ARG:HB3	9:I:93:ARG:HH11	1.84	0.43
11:K:50:TYR:HE2	11:K:54:ARG:NH1	2.14	0.43
12:L:92:0TD:C	12:L:92:0TD:OD1	2.66	0.43
1:A:1023:G:C6	1:A:1024:G:C5	3.07	0.43
1:A:976:G:C8	1:A:1358:U:C2	3.06	0.43
1:A:194:C:OP1	20:T:61:SER:OG	2.35	0.43
1:A:250:A:H4'	1:A:251:G:C5'	2.49	0.43
1:A:410:G:OP2	4:D:25:ARG:HG3	2.19	0.43
1:A:76:C:H42	1:A:93:G:H1	1.65	0.43
1:A:977:A:C2'	1:A:978:A:H5'	2.48	0.43
8:H:103:VAL:HG21	8:H:109:ILE:C	2.39	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:88:LEU:O	10:J:89:ASP:HB3	2.19	0.43
15:O:39:LEU:CD1	15:O:56:LEU:HB2	2.49	0.43
6:F:91:VAL:HG13	18:R:72:ARG:NH2	2.34	0.43
20:T:63:ILE:HG22	20:T:77:ALA:HB1	2.00	0.43
1:A:1168:A:C6	1:A:1169:A:C6	3.07	0.43
1:A:1182:G:H1'	1:A:1183:A:OP2	2.19	0.43
1:A:1314:C:H2'	1:A:1315:U:C6	2.54	0.43
1:A:1357:A:C8	1:A:1358:U:C5	3.07	0.43
1:A:29:G:O2'	1:A:30:U:H5'	2.18	0.43
1:A:328:C:O2'	1:A:329:A:P	2.77	0.43
3:C:179:ARG:HG3	3:C:206:GLU:HG2	1.99	0.43
4:D:61:LYS:HD2	4:D:207:TYR:OH	2.19	0.43
4:D:62:GLN:O	4:D:66:ARG:HB2	2.18	0.43
10:J:86:MET:HG3	10:J:87:THR:H	1.84	0.43
18:R:70:ILE:O	18:R:73:ALA:HB3	2.19	0.43
20:T:74:LYS:HZ3	20:T:74:LYS:CB	2.32	0.43
1:A:1064:G:H1'	1:A:1190:G:H21	1.84	0.42
1:A:1438:G:H2'	1:A:1439:C:C6	2.53	0.42
1:A:1513:A:H2'	1:A:1514:C:C6	2.54	0.42
1:A:235:C:N3	29:A:2119:HOH:O	2.52	0.42
1:A:28:G:C5	29:A:2696:HOH:O	2.71	0.42
1:A:323:U:H2'	1:A:324:G:O4'	2.18	0.42
1:A:947:G:H2'	1:A:948:C:O4'	2.18	0.42
3:C:14:ILE:C	3:C:15:THR:HG23	2.39	0.42
3:C:43:LEU:HD21	3:C:68:VAL:CG2	2.48	0.42
5:E:75:THR:HG23	5:E:76:ILE:N	2.33	0.42
7:G:16:LEU:N	7:G:16:LEU:HD22	2.34	0.42
17:Q:100:LYS:HB2	17:Q:101:ARG:NH1	2.33	0.42
20:T:65:LYS:O	20:T:68:LYS:HB2	2.19	0.42
1:A:1028:C:C2	1:A:1034:G:N2	2.88	0.42
1:A:1218:C:H2'	1:A:1219:U:C6	2.54	0.42
1:A:1238:A:OP1	1:A:1336:C:H5	2.02	0.42
1:A:1368:G:OP2	9:I:114:TYR:N	2.52	0.42
1:A:287:U:C2'	1:A:288:A:H5'	2.49	0.42
1:A:92:C:H2'	1:A:93:G:H8	1.85	0.42
8:H:38:ILE:HD13	8:H:41:ARG:NH2	2.34	0.42
9:I:51:ARG:CD	9:I:56:LEU:HD21	2.48	0.42
10:J:65:LEU:HB2	14:N:56:VAL:HG22	2.01	0.42
13:M:63:THR:HG23	13:M:64:TRP:CD2	2.54	0.42
18:R:45:SER:O	18:R:47:THR:O	2.37	0.42
23:W:33:U:C5'	23:W:34:G:OP2	2.67	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1032:G:H2'	1:A:1033:G:H8	1.84	0.42
1:A:1065:U:O2'	1:A:1066:C:OP2	2.26	0.42
1:A:1094:G:OP1	29:A:2239:HOH:O	2.21	0.42
1:A:1347:G:H1'	1:A:1348:U:H5	1.83	0.42
1:A:266:G:C5'	1:A:268:C:H41	2.32	0.42
1:A:560:U:C5'	1:A:566:G:C2	3.02	0.42
2:B:63:MET:HB3	2:B:225:ALA:HB1	2.00	0.42
4:D:150:GLU:OE1	4:D:151:LYS:HG2	2.19	0.42
4:D:194:LEU:HB3	4:D:196:LEU:HG	2.01	0.42
5:E:105:VAL:HG12	5:E:106:PRO:CD	2.49	0.42
5:E:76:ILE:HG22	5:E:78:HIS:H	1.84	0.42
8:H:112:LEU:CD2	8:H:112:LEU:N	2.83	0.42
8:H:41:ARG:NH1	8:H:123:GLU:OE2	2.52	0.42
13:M:50:GLU:HG3	13:M:51:ALA:N	2.34	0.42
13:M:8:GLU:HG2	13:M:22:ILE:CA	2.33	0.42
16:P:60:LEU:HD23	16:P:60:LEU:HA	1.66	0.42
1:A:1015:A:N6	1:A:1016:A:C6	2.87	0.42
1:A:1233:G:H2'	1:A:1234:C:H6	1.84	0.42
1:A:1342:C:O2'	1:A:1343:G:H5'	2.19	0.42
1:A:442:C:N4	1:A:492:G:H1	2.12	0.42
1:A:690:G:H2'	1:A:691:G:O4'	2.19	0.42
4:D:150:GLU:CD	4:D:150:GLU:H	2.19	0.42
2:B:178:ARG:O	8:H:71:GLY:HA2	2.20	0.42
10:J:11:PHE:CD1	14:N:55:GLY:HA3	2.54	0.42
17:Q:9:VAL:O	17:Q:21:VAL:HA	2.18	0.42
1:A:1329:A:H2'	1:A:1330:U:H5'	1.99	0.42
1:A:291:C:O2'	1:A:292:G:H5'	2.20	0.42
1:A:738:C:OP2	6:F:92:LYS:NZ	2.35	0.42
2:B:97:TRP:HH2	2:B:176:GLU:CD	2.22	0.42
4:D:191:ARG:HD2	4:D:200:GLU:OE2	2.19	0.42
8:H:121:ASP:HB2	8:H:125:ARG:NH2	2.34	0.42
8:H:36:LEU:O	8:H:37:ARG:C	2.56	0.42
10:J:51:ARG:HG2	10:J:61:GLU:HB2	2.01	0.42
10:J:64:GLU:N	14:N:59:ALA:HB2	2.35	0.42
11:K:24:SER:C	11:K:26:ASN:H	2.22	0.42
11:K:50:TYR:CD2	11:K:54:ARG:HB3	2.54	0.42
15:O:54:ARG:O	15:O:58:MET:HG3	2.20	0.42
19:S:31:ILE:HG23	19:S:32:LYS:N	2.34	0.42
19:S:80:TYR:CZ	19:S:81:ARG:HG2	2.53	0.42
20:T:10:LEU:O	20:T:13:LEU:HG	2.20	0.42
1:A:1303:C:N4	1:A:1304:G:C6	2.88	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:232:G:H1'	1:A:262:A:N1	2.33	0.42
1:A:665:A:H2'	1:A:732:C:O2	2.19	0.42
1:A:875:C:O2'	8:H:14:ARG:NH1	2.53	0.42
2:B:134:GLU:HA	2:B:137:ARG:HG2	2.00	0.42
2:B:25:ASN:ND2	2:B:193:ASP:HB2	2.34	0.42
2:B:43:ASP:OD2	2:B:46:LYS:HB2	2.20	0.42
2:B:61:LEU:HD22	2:B:64:ARG:HH12	1.84	0.42
3:C:155:GLY:HA3	3:C:163:ALA:HB1	2.02	0.42
11:K:38:ASN:HA	11:K:39:PRO:HD3	1.91	0.42
12:L:113:ARG:NH1	12:L:116:SER:H	2.18	0.42
15:O:66:LEU:HD23	15:O:66:LEU:HA	1.88	0.42
16:P:82:GLN:HE21	16:P:82:GLN:HB3	1.74	0.42
1:A:1256:A:N6	1:A:1277:C:C6	2.86	0.42
1:A:1277:C:O2'	1:A:1279:A:H8	2.02	0.42
1:A:1279:A:C5'	1:A:1280:A:OP1	2.63	0.42
1:A:434:U:H2'	1:A:435:C:C6	2.55	0.42
6:F:36:ARG:HB3	6:F:36:ARG:NH1	2.35	0.42
10:J:61:GLU:OE1	14:N:45:ARG:NH1	2.53	0.42
17:Q:66:SER:O	17:Q:70:ARG:NH1	2.53	0.42
13:M:27:LYS:HZ3	21:U:21:TYR:HE2	1.67	0.42
1:A:1157:A:C1'	1:A:1181:G:N2	2.83	0.42
1:A:485:G:O2'	1:A:486:U:OP2	2.38	0.42
1:A:548:G:OP1	29:A:2609:HOH:O	2.22	0.42
4:D:179:GLU:HA	4:D:179:GLU:OE2	2.19	0.42
6:F:89:MET:CE	18:R:76:LEU:HG	2.50	0.42
8:H:102:ARG:NE	8:H:102:ARG:H	2.17	0.42
8:H:119:LEU:HB3	8:H:123:GLU:HB2	2.01	0.42
1:A:1125:U:C3'	1:A:1126:U:C5	2.92	0.42
1:A:1203:C:H2'	1:A:1204:A:O4'	2.20	0.42
1:A:371:G:H2'	1:A:372:C:O4'	2.20	0.42
1:A:620:C:C1'	4:D:135:LEU:HD13	2.50	0.42
1:A:695:A:H2'	1:A:696:A:C8	2.55	0.42
2:B:223:ILE:HG13	2:B:223:ILE:H	1.68	0.42
3:C:186:PHE:CD2	3:C:186:PHE:C	2.93	0.42
4:D:4:TYR:O	4:D:4:TYR:CG	2.71	0.42
5:E:91:LEU:HD22	5:E:120:THR:HG22	2.02	0.42
1:A:1359:C:OP1	14:N:22:THR:CG2	2.67	0.42
1:A:622:A:C8	1:A:623:C:C6	3.08	0.42
4:D:3:ARG:HG3	4:D:5:ILE:HD12	2.01	0.42
5:E:151:LEU:HD11	8:H:77:GLU:OE2	2.20	0.42
7:G:66:VAL:HG12	7:G:67:GLU:N	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:37:CYS:O	12:L:79:GLU:O	2.37	0.42
1:A:1527:C:O2'	1:A:1528:U:H5'	2.19	0.41
15:O:77:ARG:HG2	15:O:77:ARG:H	1.46	0.41
17:Q:59:ILE:HD13	17:Q:73:VAL:HA	2.02	0.41
20:T:67:ALA:HA	20:T:73:HIS:CA	2.49	0.41
1:A:1130:A:OP1	1:A:1131:G:P	2.78	0.41
1:A:1144:G:C6	1:A:1145:C:N4	2.89	0.41
1:A:201:C:O2	1:A:201:C:H2'	2.19	0.41
1:A:509:A:C3'	1:A:509:A:C8	3.02	0.41
1:A:665:A:H1'	1:A:733:A:O4'	2.20	0.41
1:A:754:C:H3'	1:A:754:C:O2	2.20	0.41
1:A:994:A:C2	1:A:995:C:C6	3.08	0.41
2:B:201:ILE:O	2:B:203:GLY:N	2.49	0.41
11:K:111:ASP:OD1	18:R:84:LYS:HG2	2.20	0.41
1:A:1408:A:H2'	1:A:1409:C:C6	2.56	0.41
1:A:692:U:H1'	1:A:695:A:N7	2.35	0.41
1:A:88:A:C5	1:A:89:C:C2	3.08	0.41
2:B:10:LEU:HD23	2:B:10:LEU:HA	1.94	0.41
4:D:196:LEU:HA	4:D:197:PRO:HD2	1.89	0.41
4:D:204:ILE:HD13	4:D:204:ILE:N	2.35	0.41
6:F:74:ASP:OD2	6:F:74:ASP:N	2.53	0.41
10:J:42:THR:HG23	10:J:67:THR:O	2.20	0.41
1:A:1060:C:P	14:N:45:ARG:HH22	2.42	0.41
11:K:109:VAL:HA	18:R:85:LEU:O	2.19	0.41
1:A:1034:G:H2'	1:A:1035:A:C8	2.56	0.41
1:A:397:A:N3	1:A:397:A:H3'	2.35	0.41
1:A:840:C:H4'	1:A:848:C:C2	2.54	0.41
1:A:892:A:C2	1:A:907:A:C4	3.08	0.41
1:A:966:M2G:HM22	1:A:967:5MC:O2	2.21	0.41
4:D:13:ARG:NH2	4:D:40:PRO:HA	2.35	0.41
4:D:64:LEU:HD12	4:D:75:PHE:HZ	1.86	0.41
4:D:11:LEU:HD22	4:D:66:ARG:HG2	2.01	0.41
7:G:66:VAL:CG1	7:G:67:GLU:N	2.83	0.41
9:I:24:GLY:N	9:I:60:ASP:OD1	2.35	0.41
12:L:28:LYS:HB3	12:L:30:ALA:CB	2.50	0.41
15:O:48:LYS:HA	15:O:48:LYS:HD3	1.80	0.41
16:P:28:ARG:NH1	16:P:28:ARG:HG2	2.35	0.41
1:A:1003(A):G:N7	1:A:1004:A:N3	2.68	0.41
1:A:1080:A:H5"	5:E:16:THR:HG21	2.02	0.41
1:A:1371:G:C5	1:A:1372:U:C5	3.08	0.41
1:A:22:G:H2'	1:A:23:C:H6	1.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:235:C:N4	29:A:2120:HOH:O	2.54	0.41
1:A:803:G:C5	1:A:804:U:C4	3.08	0.41
1:A:993:G:N3	1:A:993:G:H2'	2.35	0.41
2:B:92:TYR:CE1	2:B:151:GLY:HA3	2.55	0.41
2:B:236:TYR:HD2	2:B:236:TYR:HA	1.69	0.41
5:E:76:ILE:HG23	5:E:77:PRO:HD2	2.02	0.41
5:E:87:SER:HB3	5:E:131:ILE:HD13	2.02	0.41
6:F:48:LEU:HG	6:F:57:GLN:HA	2.02	0.41
8:H:134:ILE:HA	8:H:134:ILE:HD13	1.80	0.41
18:R:52:PRO:O	18:R:56:THR:HG23	2.21	0.41
1:A:1081:G:C2'	1:A:1082:G:H5'	2.50	0.41
1:A:1194:U:H2'	1:A:1194:U:O2	2.20	0.41
1:A:1492:A:H2'	1:A:1493:A:C8	2.56	0.41
1:A:1516:G:H1'	1:A:1519:MA6:H101	2.03	0.41
1:A:182:U:OP2	1:A:182:U:H6	2.03	0.41
1:A:196:A:OP1	20:T:68:LYS:NZ	2.48	0.41
1:A:370:C:C2	1:A:392:G:N2	2.89	0.41
1:A:421:U:OP2	1:A:422:C:N4	2.49	0.41
1:A:88:A:N7	1:A:89:C:N3	2.69	0.41
2:B:135:GLN:O	2:B:139:LYS:HB2	2.21	0.41
3:C:150:LYS:CG	3:C:169:ALA:HB2	2.50	0.41
3:C:22:TRP:CG	3:C:59:ARG:HD2	2.56	0.41
5:E:28:PHE:O	5:E:47:LYS:HA	2.21	0.41
14:N:50:LYS:HD3	14:N:50:LYS:HA	1.89	0.41
16:P:67:THR:HG22	16:P:68:ASP:N	2.35	0.41
1:A:1130:A:H5"	9:I:62:TYR:CE2	2.55	0.41
1:A:1143:G:O5'	1:A:1143:G:H8	2.04	0.41
1:A:1157:A:H4'	1:A:1158:C:C5'	2.51	0.41
2:B:193:ASP:C	2:B:193:ASP:OD1	2.59	0.41
2:B:193:ASP:O	2:B:196:LEU:HD12	2.21	0.41
4:D:14:ARG:O	4:D:14:ARG:HD3	2.20	0.41
5:E:81:GLU:HA	5:E:89:ILE:O	2.21	0.41
8:H:17:THR:HG22	8:H:63:LEU:HG	2.01	0.41
10:J:86:MET:HA	10:J:86:MET:CE	2.50	0.41
1:A:1359:C:OP1	14:N:22:THR:HG22	2.21	0.41
1:A:1303:C:P	29:A:2278:HOH:O	2.79	0.41
1:A:137:C:O2'	1:A:138:G:H5'	2.21	0.41
1:A:938:A:O5'	1:A:938:A:H8	2.04	0.41
2:B:40:HIS:CD2	2:B:190:THR:HG21	2.55	0.41
2:B:69:LEU:C	2:B:69:LEU:CD2	2.89	0.41
3:C:135:LYS:HE2	5:E:50:GLU:HG2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:14:ILE:C	3:C:16:ARG:N	2.74	0.41
4:D:170:VAL:HG13	4:D:174:LEU:HB2	2.02	0.41
4:D:19:LEU:O	4:D:19:LEU:HD23	2.21	0.41
5:E:110:LEU:HD13	5:E:118:ILE:HG21	2.02	0.41
5:E:43:LEU:N	5:E:136:MET:HE2	2.31	0.41
5:E:36:ASP:O	5:E:37:ARG:HB2	2.21	0.41
15:O:70:LEU:HD23	15:O:70:LEU:HA	1.84	0.41
19:S:62:ILE:HG13	19:S:66:MET:HE2	2.03	0.41
20:T:67:ALA:HA	20:T:73:HIS:HA	2.02	0.41
1:A:1160:G:C6	1:A:1161:C:C4	3.08	0.41
1:A:1346:A:C4	7:G:10:ARG:NH2	2.88	0.41
1:A:28:G:N7	29:A:2696:HOH:O	2.53	0.41
1:A:642:A:C6	1:A:643:C:C4	3.08	0.41
1:A:79:G:H2'	1:A:80:G:H8	1.86	0.41
12:L:124:LYS:HA	12:L:125:PRO:HD3	1.85	0.41
12:L:46:LYS:HD3	12:L:94:PRO:HG3	2.01	0.41
18:R:18:ARG:HD3	18:R:18:ARG:HA	1.85	0.41
1:A:577:G:H1'	1:A:816:A:N3	2.36	0.41
1:A:872:A:N3	1:A:872:A:H2'	2.35	0.41
3:C:115:LEU:HA	3:C:115:LEU:HD23	1.85	0.41
17:Q:56:VAL:HG12	17:Q:77:VAL:HB	2.03	0.41
20:T:50:GLU:HG3	20:T:100:ILE:CG1	2.51	0.41
1:A:109:A:H4'	1:A:110:C:OP2	2.21	0.41
1:A:1252:A:H2'	1:A:1253:G:O4'	2.21	0.41
1:A:978:A:O2'	1:A:1322:C:N3	2.51	0.41
1:A:1330:U:H2'	1:A:1331:G:H5'	2.02	0.41
1:A:173:U:H6	1:A:198:G:HO2'	1.65	0.41
1:A:621:A:H2'	1:A:622:A:C8	2.56	0.41
6:F:28:ARG:HG2	6:F:32:ASN:ND2	2.33	0.41
9:I:46:ALA:HB1	9:I:77:ILE:CG2	2.51	0.41
10:J:12:ASP:OD2	10:J:14:LYS:HB2	2.21	0.41
11:K:48:ILE:HG13	11:K:48:ILE:H	1.63	0.41
11:K:58:PRO:HB2	11:K:93:GLN:HG3	2.02	0.41
14:N:3:ARG:CZ	14:N:6:LEU:HD21	2.51	0.41
16:P:54:GLU:HG3	16:P:54:GLU:H	1.58	0.41
17:Q:22:LEU:HA	17:Q:22:LEU:HD12	1.88	0.41
20:T:92:LEU:HA	20:T:92:LEU:HD23	1.89	0.41
1:A:1103:C:H2'	1:A:1104:G:O4'	2.21	0.40
1:A:1300:G:C6	1:A:1334:G:C5	3.09	0.40
1:A:1385:G:H2'	1:A:1386:G:O4'	2.22	0.40
1:A:689:C:P	11:K:46:GLY:HA3	2.60	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:731:G:OP1	1:A:766:A:H1'	2.21	0.40
1:A:786:G:C2	1:A:797:C:C2	3.09	0.40
1:A:862:C:O2'	1:A:863:U:H5'	2.21	0.40
2:B:40:HIS:HD2	2:B:190:THR:HG21	1.86	0.40
3:C:54:ARG:NH1	3:C:54:ARG:CB	2.84	0.40
4:D:31:CYS:C	4:D:33:MET:H	2.24	0.40
10:J:46:ARG:NH1	10:J:46:ARG:HG3	2.36	0.40
19:S:42:PRO:O	19:S:45:VAL:HG23	2.20	0.40
1:A:513:C:H2'	1:A:514:C:C6	2.57	0.40
2:B:79:ASP:HB3	2:B:238:LEU:HD13	2.04	0.40
4:D:79:PHE:HE1	4:D:204:ILE:CD1	2.34	0.40
5:E:80:ILE:HG22	8:H:104:ARG:HH12	1.85	0.40
1:A:1124:G:H4'	10:J:38:ILE:HD11	2.02	0.40
18:R:50:ILE:HG12	18:R:70:ILE:HD13	2.03	0.40
20:T:42:GLN:OE1	20:T:46:GLU:HG3	2.22	0.40
1:A:1394:A:C5	1:A:1501:C:H4'	2.56	0.40
2:B:170:GLU:O	2:B:173:ALA:N	2.54	0.40
2:B:60:ASP:O	2:B:64:ARG:HB2	2.22	0.40
3:C:50:ALA:O	3:C:70:VAL:HG12	2.21	0.40
5:E:118:ILE:HG12	5:E:119:LEU:N	2.37	0.40
10:J:7:LYS:CD	10:J:9:ARG:HH21	2.30	0.40
15:O:12:ILE:CD1	15:O:31:LEU:HD11	2.51	0.40
1:A:109:A:C6	1:A:327:A:C6	3.09	0.40
1:A:1497:G:C3'	1:A:1498:UR3:H5'	2.52	0.40
1:A:222:U:H2'	1:A:223:U:C6	2.56	0.40
1:A:224:C:H2'	1:A:225:C:H6	1.87	0.40
1:A:505:G:H2'	1:A:506:G:C8	2.57	0.40
2:B:121:LEU:HD22	2:B:127:ILE:HG23	2.03	0.40
2:B:16:HIS:NE2	2:B:17:PHE:HE2	2.20	0.40
2:B:218:ALA:O	2:B:222:ILE:HG13	2.21	0.40
2:B:69:LEU:HD23	2:B:70:PHE:N	2.36	0.40
2:B:86:GLU:HG3	2:B:92:TYR:HE2	1.87	0.40
5:E:83:GLU:CG	5:E:88:LYS:HD2	2.47	0.40
12:L:32:PHE:HB3	12:L:84:LEU:HD11	2.02	0.40
18:R:38:GLU:HA	18:R:41:LYS:HD3	2.03	0.40
19:S:7:LYS:CD	19:S:7:LYS:C	2.90	0.40
1:A:738:C:H5"	6:F:69:GLU:HB3	2.04	0.40
3:C:69:HIS:HA	3:C:104:GLN:O	2.21	0.40
4:D:148:VAL:HG11	4:D:158:ILE:HG21	2.03	0.40
12:L:42:THR:HA	12:L:53:ARG:O	2.22	0.40
15:O:50:HIS:O	15:O:53:HIS:HB3	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:Q:59:ILE:HG23	17:Q:71:PHE:HB3	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
2	B	234/256 (91%)	213 (91%)	20 (8%)	1 (0%)	34 66
3	C	205/239 (86%)	186 (91%)	19 (9%)	0	100 100
4	D	206/209 (99%)	197 (96%)	9 (4%)	0	100 100
5	E	149/162 (92%)	142 (95%)	7 (5%)	0	100 100
6	F	99/101 (98%)	95 (96%)	4 (4%)	0	100 100
7	G	153/156 (98%)	135 (88%)	18 (12%)	0	100 100
8	H	136/138 (99%)	130 (96%)	6 (4%)	0	100 100
9	I	125/128 (98%)	112 (90%)	12 (10%)	1 (1%)	19 51
10	J	97/105 (92%)	78 (80%)	18 (19%)	1 (1%)	15 46
11	K	115/129 (89%)	103 (90%)	12 (10%)	0	100 100
12	L	122/135 (90%)	112 (92%)	7 (6%)	3 (2%)	5 27
13	M	116/126 (92%)	107 (92%)	8 (7%)	1 (1%)	17 48
14	N	58/61 (95%)	53 (91%)	5 (9%)	0	100 100
15	O	86/89 (97%)	76 (88%)	10 (12%)	0	100 100
16	P	82/88 (93%)	77 (94%)	5 (6%)	0	100 100
17	Q	98/105 (93%)	91 (93%)	7 (7%)	0	100 100
18	R	69/88 (78%)	61 (88%)	8 (12%)	0	100 100
19	S	79/93 (85%)	71 (90%)	6 (8%)	2 (2%)	5 27
20	T	97/106 (92%)	86 (89%)	10 (10%)	1 (1%)	15 46

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
21	U	23/27 (85%)	22 (96%)	1 (4%)	0	100 100
All	All	2349/2541 (92%)	2147 (91%)	192 (8%)	10 (0%)	34 66

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
12	L	28	LYS
20	T	73	HIS
19	S	31	ILE
12	L	115	LYS
13	M	23	TYR
9	I	119	ALA
12	L	27	LEU
19	S	6	LYS
2	B	229	VAL
10	J	34	VAL

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	B	201/220 (91%)	181 (90%)	20 (10%)	7 27
3	C	160/188 (85%)	138 (86%)	22 (14%)	3 16
4	D	180/181 (99%)	156 (87%)	24 (13%)	4 17
5	E	115/123 (94%)	93 (81%)	22 (19%)	1 6
6	F	90/90 (100%)	76 (84%)	14 (16%)	2 12
7	G	126/127 (99%)	114 (90%)	12 (10%)	8 29
8	H	119/119 (100%)	105 (88%)	14 (12%)	5 21
9	I	98/99 (99%)	91 (93%)	7 (7%)	14 42
10	J	87/92 (95%)	81 (93%)	6 (7%)	15 44
11	K	89/99 (90%)	82 (92%)	7 (8%)	12 37
12	L	103/110 (94%)	89 (86%)	14 (14%)	3 16

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
13	M	94/101 (93%)	82 (87%)	12 (13%)	4 18
14	N	49/50 (98%)	42 (86%)	7 (14%)	3 15
15	O	79/80 (99%)	67 (85%)	12 (15%)	3 13
16	P	72/74 (97%)	66 (92%)	6 (8%)	11 36
17	Q	95/97 (98%)	86 (90%)	9 (10%)	8 29
18	R	62/77 (80%)	57 (92%)	5 (8%)	11 36
19	S	71/80 (89%)	66 (93%)	5 (7%)	15 43
20	T	76/82 (93%)	66 (87%)	10 (13%)	4 17
21	U	19/22 (86%)	17 (90%)	2 (10%)	7 25
All	All	1985/2111 (94%)	1755 (88%)	230 (12%)	5 22

All (230) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	8	LYS
2	B	11	LEU
2	B	12	GLU
2	B	33	TYR
2	B	69	LEU
2	B	96	ARG
2	B	97	TRP
2	B	114	ARG
2	B	121	LEU
2	B	132	LYS
2	B	139	LYS
2	B	163	PHE
2	B	172	ILE
2	B	187	LEU
2	B	196	LEU
2	B	204	ASN
2	B	221	LEU
2	B	223	ILE
2	B	226	ARG
2	B	236	TYR
3	C	3	ASN
3	C	5	ILE
3	C	14	ILE
3	C	15	THR
3	C	45	LYS

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Mol	Chain	Res	Type
3	C	62	ASP
3	C	64	VAL
3	C	70	VAL
3	C	91	LEU
3	C	98	ASN
3	C	111	LEU
3	C	126	ARG
3	C	127	ARG
3	C	130	VAL
3	C	144	SER
3	C	156	ARG
3	C	167	TRP
3	C	188	LEU
3	C	192	THR
3	C	204	LEU
3	C	206	GLU
3	C	207	VAL
4	D	10	ARG
4	D	15	GLU
4	D	19	LEU
4	D	25	ARG
4	D	26	CYS
4	D	34	GLU
4	D	47	ARG
4	D	50	ARG
4	D	58	LEU
4	D	64	LEU
4	D	66	ARG
4	D	78	LEU
4	D	96	LEU
4	D	107	ARG
4	D	115	ARG
4	D	122	ARG
4	D	127	THR
4	D	131	ARG
4	D	150	GLU
4	D	187	ARG
4	D	191	ARG
4	D	192	GLU
4	D	194	LEU
4	D	201	GLN
5	E	10	MET

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Mol	Chain	Res	Type
5	E	11	ILE
5	E	12	LEU
5	E	16	THR
5	E	19	MET
5	E	24	ARG
5	E	31	LEU
5	E	43	LEU
5	E	47	LYS
5	E	50	GLU
5	E	53	LEU
5	E	63	ARG
5	E	64	ARG
5	E	65	ASN
5	E	68	GLU
5	E	75	THR
5	E	78	HIS
5	E	79	GLU
5	E	116	THR
5	E	117	ASP
5	E	125	SER
5	E	126	ARG
6	F	15	ASP
6	F	17	SER
6	F	24	GLU
6	F	28	ARG
6	F	37	VAL
6	F	43	LEU
6	F	45	LEU
6	F	55	ASP
6	F	74	ASP
6	F	75	LEU
6	F	82	ARG
6	F	83	ASP
6	F	86	ARG
6	F	93	SER
7	G	10	ARG
7	G	12	LEU
7	G	15	ASP
7	G	27	ILE
7	G	52	GLU
7	G	66	VAL
7	G	89	MET

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Mol	Chain	Res	Type
7	G	113	GLU
7	G	136	LYS
7	G	140	ASP
7	G	148	ASN
7	G	156	TRP
8	H	1	MET
8	H	11	THR
8	H	12	ARG
8	H	18	ARG
8	H	21	LYS
8	H	26	VAL
8	H	39	LEU
8	H	63	LEU
8	H	85	ARG
8	H	91	ARG
8	H	97	VAL
8	H	102	ARG
8	H	112	LEU
8	H	133	LEU
9	I	16	ARG
9	I	27	THR
9	I	29	ASN
9	I	48	GLU
9	I	79	LEU
9	I	109	VAL
9	I	124	GLN
10	J	4	ILE
10	J	6	ILE
10	J	46	ARG
10	J	63	PHE
10	J	66	ARG
10	J	79	ARG
11	K	29	ILE
11	K	47	VAL
11	K	48	ILE
11	K	75	TYR
11	K	87	THR
11	K	120	ARG
11	K	127	LYS
12	L	12	ARG
12	L	20	LYS
12	L	21	LYS

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Mol	Chain	Res	Type
12	L	39	VAL
12	L	42	THR
12	L	43	VAL
12	L	44	THR
12	L	60	LEU
12	L	67	THR
12	L	97	ARG
12	L	100	ILE
12	L	113	ARG
12	L	116	SER
12	L	118	SER
13	M	8	GLU
13	M	17	VAL
13	M	27	LYS
13	M	44	ARG
13	M	50	GLU
13	M	57	ARG
13	M	58	GLU
13	M	64	TRP
13	M	69	GLU
13	M	70	LEU
13	M	78	ILE
13	M	99	ARG
14	N	9	LYS
14	N	12	ARG
14	N	26	ARG
14	N	35	ARG
14	N	41	ARG
14	N	44	LEU
14	N	50	LYS
15	O	4	THR
15	O	5	LYS
15	O	11	VAL
15	O	22	THR
15	O	31	LEU
15	O	34	LEU
15	O	70	LEU
15	O	71	GLN
15	O	73	GLU
15	O	77	ARG
15	O	81	LEU
15	O	83	GLU

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Mol	Chain	Res	Type
16	P	11	SER
16	P	45	THR
16	P	47	ASP
16	P	53	VAL
16	P	54	GLU
16	P	82	GLN
17	Q	11	VAL
17	Q	34	LYS
17	Q	36	ILE
17	Q	59	ILE
17	Q	74	LEU
17	Q	92	ARG
17	Q	97	SER
17	Q	98	LEU
17	Q	101	ARG
18	R	39	VAL
18	R	46	GLU
18	R	82	THR
18	R	86	VAL
18	R	88	LYS
19	S	5	LEU
19	S	7	LYS
19	S	15	LEU
19	S	31	ILE
19	S	71	LEU
20	T	10	LEU
20	T	11	SER
20	T	13	LEU
20	T	41	ILE
20	T	56	MET
20	T	62	LEU
20	T	73	HIS
20	T	74	LYS
20	T	99	LEU
20	T	100	ILE
21	U	10	ARG
21	U	15	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	40	HIS

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Mol	Chain	Res	Type
2	B	212	GLN
3	C	6	HIS
4	D	201	GLN
5	E	78	HIS
6	F	32	ASN
9	I	73	GLN
13	M	101	GLN

5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	1510/1522 (99%)	237 (15%)	38 (2%)
22	V	3/4 (75%)	0	0
23	W	8/9 (88%)	1 (12%)	0
24	a	10/11 (90%)	3 (30%)	0
25	b	1/3 (33%)	1 (100%)	0
All	All	1532/1549 (98%)	242 (15%)	38 (2%)

All (242) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	7	G
1	A	9	G
1	A	32	A
1	A	39	G
1	A	47	C
1	A	48	C
1	A	50	A
1	A	51	A
1	A	81	U
1	A	82	U
1	A	88	A
1	A	90	U
1	A	101	A
1	A	108	G
1	A	115	G
1	A	116	A
1	A	121	C
1	A	129(A)	G
1	A	130	A
1	A	131	C

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Mol	Chain	Res	Type
1	A	163	C
1	A	182	U
1	A	183	G
1	A	190(E)	U
1	A	195	A
1	A	197	A
1	A	201	C
1	A	202	U
1	A	204	U
1	A	216	G
1	A	247	G
1	A	250	A
1	A	251	G
1	A	252	U
1	A	266	G
1	A	267	C
1	A	280	C
1	A	289	G
1	A	301	G
1	A	319	G
1	A	321	A
1	A	328	C
1	A	329	A
1	A	331	G
1	A	332	G
1	A	345	C
1	A	346	G
1	A	352	C
1	A	353	A
1	A	354	G
1	A	367	U
1	A	372	C
1	A	373	A
1	A	384	G
1	A	390	C
1	A	397	A
1	A	398	C
1	A	406	G
1	A	412	A
1	A	413	G
1	A	421	U
1	A	424	G

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Mol	Chain	Res	Type
1	A	429	U
1	A	430	A
1	A	439	A
1	A	442	C
1	A	443	C
1	A	452	A
1	A	460	A
1	A	481	G
1	A	485	G
1	A	497	A
1	A	498	U
1	A	500	G
1	A	509	A
1	A	510	A
1	A	511	C
1	A	518	C
1	A	527	7MG
1	A	531	U
1	A	532	A
1	A	533	A
1	A	547	A
1	A	559	A
1	A	560	U
1	A	562	C
1	A	564	C
1	A	572	A
1	A	573	A
1	A	576	G
1	A	577	G
1	A	579	G
1	A	588	G
1	A	607	A
1	A	629	G
1	A	631	G
1	A	632	A
1	A	653	A
1	A	665	A
1	A	671	G
1	A	687	A
1	A	688	G
1	A	698	G
1	A	702	A

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Mol	Chain	Res	Type
1	A	723	U
1	A	731	G
1	A	734	G
1	A	755	G
1	A	770	C
1	A	777	A
1	A	793	U
1	A	794	A
1	A	795	C
1	A	812	C
1	A	813	U
1	A	816	A
1	A	817	C
1	A	827	U
1	A	828	A
1	A	839	U
1	A	840	C
1	A	841	U
1	A	848	C
1	A	851	G
1	A	873	A
1	A	876	G
1	A	902	G
1	A	914	A
1	A	916	G
1	A	926	G
1	A	927	G
1	A	934	C
1	A	935	A
1	A	960	U
1	A	961	U
1	A	966	M2G
1	A	969	A
1	A	971	G
1	A	975	A
1	A	976	G
1	A	977	A
1	A	978	A
1	A	980	C
1	A	991	U
1	A	992	U
1	A	993	G

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Mol	Chain	Res	Type
1	A	1004	A
1	A	1005	A
1	A	1020	U
1	A	1025	U
1	A	1026	G
1	A	1027	C
1	A	1045	C
1	A	1050	G
1	A	1053	G
1	A	1054	C
1	A	1065	U
1	A	1066	C
1	A	1068	G
1	A	1078	U
1	A	1094	G
1	A	1095	U
1	A	1101	A
1	A	1125	U
1	A	1126	U
1	A	1130	A
1	A	1131	G
1	A	1135	U
1	A	1137	C
1	A	1138	G
1	A	1139	G
1	A	1157	A
1	A	1159	U
1	A	1171	G
1	A	1181	G
1	A	1182	G
1	A	1183	A
1	A	1190	G
1	A	1191	A
1	A	1196	U
1	A	1201	A
1	A	1202	G
1	A	1212	U
1	A	1213	A
1	A	1225	A
1	A	1226	C
1	A	1227	A
1	A	1236	A

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Mol	Chain	Res	Type
1	A	1238	A
1	A	1256	A
1	A	1257	U
1	A	1258	G
1	A	1270	C
1	A	1280	A
1	A	1281	U
1	A	1282	C
1	A	1286	A
1	A	1287	A
1	A	1297	C
1	A	1300	G
1	A	1301	U
1	A	1302	U
1	A	1303	C
1	A	1312	G
1	A	1320	C
1	A	1322	C
1	A	1323	G
1	A	1332	A
1	A	1338	G
1	A	1348	U
1	A	1349	A
1	A	1353	G
1	A	1362	C
1	A	1364	U
1	A	1368	G
1	A	1370	G
1	A	1398	A
1	A	1400	5MC
1	A	1442	G
1	A	1443	G
1	A	1446	A
1	A	1454	G
1	A	1487	G
1	A	1492	A
1	A	1494	G
1	A	1498	UR3
1	A	1499	A
1	A	1502	A
1	A	1504	G
1	A	1505	G

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Mol	Chain	Res	Type
1	A	1506	U
1	A	1520	G
1	A	1528	U
1	A	1529	G
1	A	1530	G
1	A	1531	A
1	A	1534	C
23	W	34	G
24	a	32	U
24	a	34	G
24	a	41	U
25	b	2	U

All (38) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	115	G
1	A	129(A)	G
1	A	181	G
1	A	204	U
1	A	250	A
1	A	251	G
1	A	266	G
1	A	328	C
1	A	428	G
1	A	429	U
1	A	484	G
1	A	496	A
1	A	509	A
1	A	559	A
1	A	575	G
1	A	687	A
1	A	701	C
1	A	812	C
1	A	913	A
1	A	960	U
1	A	991	U
1	A	1004	A
1	A	1049	U
1	A	1065	U
1	A	1067	A
1	A	1182	G

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Mol	Chain	Res	Type
1	A	1190	G
1	A	1201	A
1	A	1212	U
1	A	1256	A
1	A	1281	U
1	A	1300	G
1	A	1331	G
1	A	1347	G
1	A	1397	C
1	A	1493	A
1	A	1528	U
1	A	1533	C

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
1	5MC	A	1404	1	15,22,23	1.02	1 (6%)	19,32,35	0.84	0
24	PSU	a	38	24	17,21,22	1.14	2 (11%)	20,30,33	3.29	6 (30%)
1	5MC	A	967	1	15,22,23	1.12	2 (13%)	19,32,35	0.96	1 (5%)
1	M2G	A	966	1	20,27,28	1.62	4 (20%)	22,40,43	2.47	4 (18%)
1	5MC	A	1407	1	15,22,23	1.07	1 (6%)	19,32,35	1.23	2 (10%)
1	2MG	A	1207	1	19,26,27	2.69	4 (21%)	21,38,41	2.21	4 (19%)
1	PSU	A	516	1	17,21,22	1.00	2 (11%)	20,30,33	3.24	6 (30%)
1	UR3	A	1498	1	14,22,23	0.63	0	15,32,35	1.07	1 (6%)
1	PSU	A	1540	1	17,21,22	1.07	1 (5%)	20,30,33	3.25	6 (30%)
1	4OC	A	1402	1	16,23,24	0.95	0	17,32,35	0.74	0
1	MA6	A	1518	1	19,26,27	1.21	2 (10%)	18,38,41	0.91	1 (5%)
1	PSU	A	1541	1	17,21,22	1.06	1 (5%)	20,30,33	3.18	7 (35%)
1	7MG	A	527	1	22,26,27	2.06	6 (27%)	28,39,42	1.73	5 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
1	MA6	A	1519	1	19,26,27	1.64	4 (21%)	18,38,41	0.69	0
23	PSU	W	38	23	17,21,22	1.10	1 (5%)	20,30,33	3.29	6 (30%)
12	0TD	L	92	12	4,9,10	1.18	0	3,11,13	3.33	2 (66%)
1	5MC	A	1400	1	15,22,23	1.01	2 (13%)	19,32,35	1.16	3 (15%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	5MC	A	1404	1	-	0/5/25/26	0/2/2/2
24	PSU	a	38	24	-	0/7/25/26	0/2/2/2
1	5MC	A	967	1	-	0/5/25/26	0/2/2/2
1	M2G	A	966	1	-	5/7/29/30	0/3/3/3
1	5MC	A	1407	1	-	0/5/25/26	0/2/2/2
1	2MG	A	1207	1	-	2/5/27/28	0/3/3/3
1	PSU	A	516	1	-	0/7/25/26	0/2/2/2
1	UR3	A	1498	1	-	4/5/25/26	0/2/2/2
1	PSU	A	1540	1	-	0/7/25/26	0/2/2/2
1	4OC	A	1402	1	-	5/9/29/30	0/2/2/2
1	MA6	A	1518	1	-	0/7/29/30	0/3/3/3
1	PSU	A	1541	1	-	0/7/25/26	0/2/2/2
1	7MG	A	527	1	-	2/7/37/38	0/3/3/3
1	MA6	A	1519	1	-	3/7/29/30	0/3/3/3
23	PSU	W	38	23	-	0/7/25/26	0/2/2/2
12	0TD	L	92	12	-	1/3/12/14	-
1	5MC	A	1400	1	-	2/5/25/26	0/2/2/2

All (33) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1207	2MG	C2-N2	9.01	1.41	1.34
1	A	1207	2MG	C6-N1	5.95	1.43	1.33
1	A	966	M2G	C6-N1	5.04	1.41	1.33
1	A	527	7MG	C4-N3	4.78	1.40	1.34
1	A	527	7MG	C8-N9	-4.64	1.34	1.45
1	A	1519	MA6	C6-N1	4.56	1.39	1.33
1	A	527	7MG	C2-N2	4.29	1.42	1.33
1	A	1518	MA6	C6-N1	3.63	1.38	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1540	PSU	C4-N3	3.36	1.38	1.33
1	A	1519	MA6	C4-N3	3.33	1.40	1.35
23	W	38	PSU	C4-N3	3.32	1.38	1.33
1	A	1541	PSU	C4-N3	3.27	1.38	1.33
1	A	516	PSU	C4-N3	3.10	1.38	1.33
24	a	38	PSU	C4-N3	2.97	1.38	1.33
1	A	1519	MA6	C2-N1	2.93	1.39	1.33
1	A	966	M2G	C2-N2	2.80	1.39	1.34
1	A	1407	5MC	C5-C4	2.80	1.45	1.41
1	A	527	7MG	C6-N1	2.70	1.37	1.33
1	A	1207	2MG	C4-N3	2.65	1.39	1.35
1	A	966	M2G	C2-N1	2.63	1.39	1.34
1	A	1207	2MG	C2-N1	2.59	1.42	1.34
24	a	38	PSU	C5-C1'	-2.50	1.50	1.52
1	A	527	7MG	CM7-N7	-2.47	1.41	1.46
1	A	527	7MG	C6-C5	2.40	1.44	1.41
1	A	1518	MA6	C2-N3	2.38	1.35	1.32
1	A	1519	MA6	C2-N3	2.34	1.35	1.32
1	A	967	5MC	C5-C4	2.33	1.45	1.41
1	A	967	5MC	C4-N4	2.31	1.39	1.34
1	A	966	M2G	C4-N3	2.16	1.39	1.35
1	A	1400	5MC	C2-N3	2.12	1.42	1.38
1	A	1404	5MC	C2-N3	2.04	1.42	1.38
1	A	1400	5MC	C4-N4	2.04	1.39	1.34
1	A	516	PSU	O4'-C1'	-2.02	1.41	1.44

All (54) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	516	PSU	N1-C2-N3	-11.44	119.34	128.43
23	W	38	PSU	N1-C2-N3	-11.10	119.61	128.43
1	A	1540	PSU	N1-C2-N3	-10.91	119.76	128.43
1	A	1541	PSU	N1-C2-N3	-10.74	119.89	128.43
24	a	38	PSU	N1-C2-N3	-10.24	120.29	128.43
1	A	966	M2G	C5-C6-N1	-8.40	111.94	123.43
1	A	1207	2MG	C5-C6-N1	-8.15	112.28	123.43
1	A	1540	PSU	C4-N3-C2	6.38	120.53	115.14
1	A	1541	PSU	C4-N3-C2	5.90	120.12	115.14
1	A	516	PSU	C4-N3-C2	5.87	120.10	115.14
23	W	38	PSU	C4-N3-C2	5.79	120.03	115.14
1	A	966	M2G	C6-N1-C2	5.62	122.88	116.18
24	a	38	PSU	C4-N3-C2	5.56	119.83	115.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	a	38	PSU	C5-C1'-C2'	-5.26	105.93	115.32
1	A	527	7MG	N3-C4-N9	4.78	133.05	126.91
12	L	92	0TD	CSB-SB-CB	-4.77	92.46	101.85
24	a	38	PSU	C5-C4-N3	-4.70	119.31	125.36
1	A	1540	PSU	C5-C4-N3	-4.57	119.47	125.36
1	A	1541	PSU	C5-C4-N3	-4.48	119.59	125.36
1	A	527	7MG	C5-C4-N3	-4.44	119.24	126.49
23	W	38	PSU	C5-C4-N3	-4.25	119.88	125.36
1	A	1207	2MG	C6-N1-C2	4.17	122.65	115.18
1	A	516	PSU	C5-C4-N3	-3.92	120.31	125.36
1	A	527	7MG	N7-C8-N9	3.69	108.66	103.38
24	a	38	PSU	C5-C6-N1	-3.49	120.14	124.44
1	A	516	PSU	C6-N1-C2	3.41	120.99	115.36
23	W	38	PSU	C5-C6-N1	-3.29	120.39	124.44
23	W	38	PSU	C6-N1-C2	3.29	120.79	115.36
1	A	966	M2G	N1-C2-N2	-3.19	113.96	117.19
1	A	1540	PSU	C5-C1'-C2'	-3.18	109.64	115.32
1	A	1407	5MC	N4-C4-N3	-3.11	112.64	117.03
1	A	516	PSU	C5-C6-N1	-3.05	120.69	124.44
24	a	38	PSU	C6-N1-C2	3.04	120.37	115.36
1	A	1541	PSU	C6-N1-C2	3.02	120.35	115.36
23	W	38	PSU	C5-C1'-C2'	-3.02	109.94	115.32
1	A	1541	PSU	C5-C6-N1	-2.98	120.77	124.44
12	L	92	0TD	CB-CA-N	-2.91	102.90	109.10
1	A	966	M2G	N3-C2-N2	2.83	120.05	117.18
1	A	1540	PSU	C6-N1-C2	2.82	120.02	115.36
1	A	1400	5MC	C2-N3-C4	2.74	119.33	116.02
1	A	527	7MG	C2-N3-C4	2.58	121.03	113.89
1	A	1518	MA6	C1'-N9-C4	-2.54	122.18	126.64
1	A	1498	UR3	C3'-C2'-C1'	2.42	104.63	100.98
1	A	527	7MG	C6-C5-C4	2.31	117.67	115.20
1	A	1400	5MC	CM5-C5-C4	-2.30	119.40	121.72
1	A	1400	5MC	CM5-C5-C6	2.27	123.48	118.68
1	A	1540	PSU	C5-C6-N1	-2.26	121.66	124.44
1	A	1207	2MG	N2-C2-N3	2.23	119.10	116.96
1	A	1407	5MC	C5-C4-N3	2.22	124.76	121.26
1	A	1541	PSU	C5-C1'-C2'	-2.19	111.42	115.32
1	A	516	PSU	O4'-C1'-C2'	2.11	108.08	104.66
1	A	1541	PSU	O4'-C1'-C2'	2.01	107.92	104.66
1	A	1207	2MG	C4-C5-N7	2.01	111.49	109.40
1	A	967	5MC	CM5-C5-C6	2.00	122.91	118.68

There are no chirality outliers.

All (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	1207	2MG	N1-C2-N2-CM2
1	A	1207	2MG	N3-C2-N2-CM2
1	A	1498	UR3	O4'-C1'-N1-C6
1	A	1498	UR3	C2'-C1'-N1-C6
1	A	1402	4OC	O4'-C4'-C5'-O5'
1	A	1402	4OC	O4'-C1'-N1-C6
1	A	1402	4OC	N3-C4-N4-CM4
1	A	1402	4OC	C5-C4-N4-CM4
1	A	527	7MG	O4'-C4'-C5'-O5'
1	A	527	7MG	C3'-C4'-C5'-O5'
1	A	1519	MA6	C5-C6-N6-C9
1	A	1519	MA6	C5-C6-N6-C10
12	L	92	0TD	CG-CB-SB-CSB
1	A	1402	4OC	C3'-C4'-C5'-O5'
1	A	1400	5MC	O4'-C4'-C5'-O5'
1	A	1498	UR3	C3'-C4'-C5'-O5'
1	A	1400	5MC	C3'-C4'-C5'-O5'
1	A	1519	MA6	N1-C6-N6-C9
1	A	1498	UR3	O4'-C4'-C5'-O5'
1	A	966	M2G	C4'-C5'-O5'-P
1	A	966	M2G	N1-C2-N2-CM1
1	A	966	M2G	N3-C2-N2-CM2
1	A	966	M2G	N3-C2-N2-CM1
1	A	966	M2G	N1-C2-N2-CM2

There are no ring outliers.

15 monomers are involved in 23 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	1404	5MC	2	0
1	A	967	5MC	1	0
1	A	966	M2G	2	0
1	A	1407	5MC	2	0
1	A	1207	2MG	2	0
1	A	1498	UR3	4	0
1	A	1540	PSU	3	0
1	A	1402	4OC	1	0
1	A	1518	MA6	1	0
1	A	1541	PSU	1	0
1	A	527	7MG	1	0
1	A	1519	MA6	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	W	38	PSU	1	0
12	L	92	0TD	2	0
1	A	1400	5MC	1	0

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 380 ligands modelled in this entry, 379 are monoatomic - leaving 1 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	$\#\|Z\| > 2$
27	SRY	A	1956	-	40,42,42	2.39	10 (25%)	49,63,63	2.13	10 (20%)

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
27	SRY	A	1956	-	-	2/20/87/87	0/3/3/3

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	A	1956	SRY	CD1-N31	9.70	1.50	1.33
27	A	1956	SRY	CA1-N11	6.65	1.44	1.33
27	A	1956	SRY	O53-C53	-3.30	1.36	1.44
27	A	1956	SRY	C23-N23	-3.02	1.42	1.47
27	A	1956	SRY	C21-C11	-2.92	1.47	1.53
27	A	1956	SRY	CD1-NE1	2.44	1.44	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	A	1956	SRY	CA1-NB1	2.43	1.44	1.34
27	A	1956	SRY	O32-C32	-2.36	1.40	1.44
27	A	1956	SRY	O51-C51	-2.31	1.37	1.43
27	A	1956	SRY	C32-CG2	-2.14	1.48	1.52

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	A	1956	SRY	C12-O42-C42	-7.39	96.75	108.38
27	A	1956	SRY	C13-O13-C22	-5.55	106.61	116.25
27	A	1956	SRY	O41-C12-O42	-4.87	106.16	111.43
27	A	1956	SRY	O13-C13-C23	4.06	115.25	108.24
27	A	1956	SRY	O42-C12-C22	-3.85	103.14	107.30
27	A	1956	SRY	CI3-N23-C23	-3.70	109.00	114.38
27	A	1956	SRY	C61-C11-N11	-3.47	104.06	110.62
27	A	1956	SRY	C43-C33-C23	-2.91	106.08	110.34
27	A	1956	SRY	C13-O53-C53	-2.53	108.73	113.69
27	A	1956	SRY	C41-C31-N31	2.43	114.95	110.91

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
27	A	1956	SRY	C13-C23-N23-CI3
27	A	1956	SRY	C33-C23-N23-CI3

There are no ring outliers.

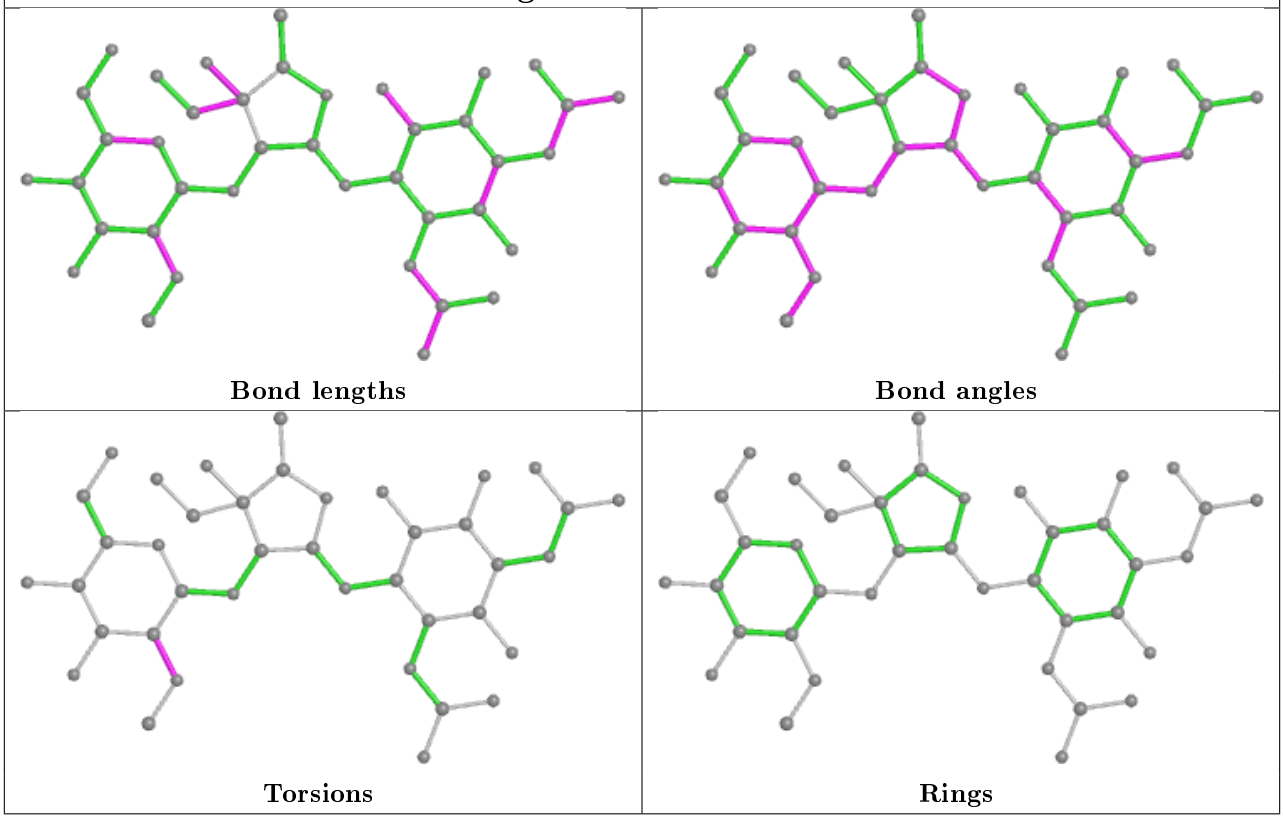
1 monomer is involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
27	A	1956	SRY	9	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and

any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand SRY A 1956



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	1500/1522 (98%)	-0.39	4 (0%) 94 94	63, 101, 198, 295	4 (0%)
2	B	236/256 (92%)	0.01	4 (1%) 70 68	72, 130, 193, 213	0
3	C	207/239 (86%)	-0.04	5 (2%) 59 56	79, 157, 196, 214	0
4	D	208/209 (99%)	-0.05	6 (2%) 51 50	75, 114, 162, 193	0
5	E	151/162 (93%)	-0.33	0 100 100	64, 93, 130, 174	0
6	F	101/101 (100%)	-0.38	1 (0%) 82 82	97, 134, 166, 197	0
7	G	155/156 (99%)	-0.29	3 (1%) 66 65	95, 138, 197, 213	0
8	H	138/138 (100%)	-0.14	1 (0%) 87 88	61, 84, 113, 137	0
9	I	127/128 (99%)	0.42	12 (9%) 8 9	100, 162, 201, 225	0
10	J	99/105 (94%)	0.69	10 (10%) 7 6	84, 191, 266, 285	0
11	K	117/129 (90%)	-0.21	0 100 100	80, 106, 142, 160	0
12	L	124/135 (91%)	0.14	6 (4%) 30 28	70, 102, 139, 224	0
13	M	118/126 (93%)	0.26	6 (5%) 28 26	99, 131, 163, 208	0
14	N	60/61 (98%)	0.07	2 (3%) 46 44	121, 142, 179, 239	0
15	O	88/89 (98%)	0.00	2 (2%) 60 59	73, 102, 145, 195	0
16	P	84/88 (95%)	0.14	1 (1%) 79 78	80, 103, 128, 221	0
17	Q	100/105 (95%)	0.07	1 (1%) 82 82	72, 94, 131, 157	0
18	R	71/88 (80%)	-0.09	1 (1%) 75 75	78, 113, 160, 215	0
19	S	81/93 (87%)	0.21	3 (3%) 41 38	72, 158, 210, 238	0
20	T	99/106 (93%)	-0.11	1 (1%) 82 82	76, 106, 145, 181	0
21	U	25/27 (92%)	0.79	2 (8%) 12 11	90, 144, 162, 196	0
22	V	4/4 (100%)	3.06	3 (75%) 0 0	187, 188, 199, 201	0
23	W	8/9 (88%)	3.32	7 (87%) 0 0	192, 214, 258, 287	0
24	a	10/11 (90%)	0.60	0 100 100	155, 188, 323, 325	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å^2)	Q<0.9
25	b	2/3 (66%)	2.32	1 (50%)	0	116, 116, 116, 187	2 (100%)
All	All	3913/4090 (95%)	-0.13	82 (2%)	63	61, 116, 196, 325	6 (0%)

All (82) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
10	J	34	VAL	8.6
15	O	89	GLY	8.0
1	A	1129	C	7.9
10	J	33	GLN	6.9
12	L	129	ALA	6.9
1	A	82	U	6.5
14	N	12	ARG	6.3
6	F	101	ALA	5.7
3	C	208	ILE	5.6
12	L	128	ALA	5.3
23	W	37	G	5.0
14	N	13	THR	4.9
23	W	33	U	4.5
19	S	29	ARG	4.3
21	U	18	TYR	4.2
23	W	32	U	4.2
10	J	36	GLY	4.1
7	G	83	ALA	4.0
22	V	3	U	3.7
22	V	2	U	3.7
15	O	88	ARG	3.7
3	C	196	LEU	3.7
9	I	15	ALA	3.5
9	I	99	LEU	3.5
10	J	37	PRO	3.5
23	W	36	G	3.3
13	M	15	VAL	3.3
9	I	128	ARG	3.2
12	L	64	TYR	3.1
22	V	1	U	3.1
13	M	117	VAL	3.0
7	G	84	ASN	3.0
23	W	39	G	3.0
23	W	35	A	2.9
2	B	188	ALA	2.9
25	b	2	U	2.9

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Mol	Chain	Res	Type	RSRZ
9	I	9	ARG	2.8
9	I	65	VAL	2.8
16	P	84	ALA	2.8
10	J	71	LEU	2.8
4	D	44	GLY	2.8
9	I	4	TYR	2.7
1	A	793	U	2.7
19	S	28	LYS	2.6
3	C	201	TYR	2.6
4	D	37	PRO	2.6
3	C	193	TYR	2.6
23	W	40	G	2.6
12	L	33	ARG	2.5
19	S	38	SER	2.5
9	I	33	PHE	2.5
4	D	38	TYR	2.5
7	G	82	GLY	2.5
18	R	88	LYS	2.4
10	J	5	ARG	2.4
10	J	74	ILE	2.4
13	M	19	LEU	2.3
21	U	17	THR	2.3
13	M	56	LEU	2.3
2	B	187	LEU	2.3
9	I	105	ASP	2.3
4	D	45	GLN	2.3
3	C	189	ALA	2.2
10	J	99	LYS	2.2
13	M	41	PRO	2.2
8	H	128	GLY	2.2
4	D	23	GLY	2.2
12	L	60	LEU	2.1
2	B	135	GLN	2.1
17	Q	58	GLU	2.1
9	I	102	LEU	2.1
4	D	43	HIS	2.1
10	J	98	ILE	2.1
1	A	83	U	2.0
9	I	8	GLY	2.0
9	I	19	LEU	2.0
10	J	87	THR	2.0
9	I	73	GLN	2.0

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Mol	Chain	Res	Type	RSRZ
2	B	211	ILE	2.0
13	M	118	ALA	2.0
20	T	103	GLY	2.0
12	L	19	ARG	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
1	PSU	A	1541	20/21	0.81	0.24	176,205,227,228	1
23	PSU	W	38	20/21	0.88	0.49	205,221,227,228	0
1	PSU	A	1540	20/21	0.91	0.26	152,168,179,180	2
1	2MG	A	1207	24/25	0.93	0.13	130,139,151,155	0
24	PSU	a	38	20/21	0.94	0.22	158,164,169,169	0
1	MA6	A	1518	24/25	0.94	0.14	85,106,116,122	0
1	4OC	A	1402	22/23	0.95	0.22	82,89,99,102	0
1	UR3	A	1498	21/22	0.95	0.20	89,97,116,118	0
1	5MC	A	1407	21/22	0.96	0.14	109,120,126,130	0
1	5MC	A	1404	21/22	0.96	0.20	89,93,103,111	0
1	MA6	A	1519	24/25	0.96	0.20	82,107,115,116	0
1	PSU	A	516	20/21	0.96	0.12	111,121,127,131	0
1	5MC	A	1400	21/22	0.96	0.16	77,102,129,132	0
1	5MC	A	967	21/22	0.97	0.15	97,105,118,120	0
1	M2G	A	966	25/26	0.97	0.14	92,112,125,128	0
1	7MG	A	527	24/25	0.97	0.19	70,87,95,97	0
12	0TD	L	92	10/11	0.98	0.22	77,93,111,233	0

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
26	MG	A	1941	1/1	0.31	0.27	112,112,112,112	0
26	MG	A	1915	1/1	0.43	0.22	120,120,120,120	0
26	MG	A	1905	1/1	0.45	0.68	105,105,105,105	0
26	MG	A	1744	1/1	0.45	0.51	111,111,111,111	0
26	MG	A	1785	1/1	0.49	0.34	108,108,108,108	0
26	MG	A	1605	1/1	0.50	0.59	100,100,100,100	0
26	MG	A	1913	1/1	0.50	0.91	102,102,102,102	0
26	MG	A	1954	1/1	0.51	0.30	86,86,86,86	0
26	MG	A	1742	1/1	0.52	0.45	102,102,102,102	0
26	MG	A	1774	1/1	0.52	0.69	101,101,101,101	0
26	MG	A	1936	1/1	0.56	0.23	101,101,101,101	0
26	MG	A	1790	1/1	0.56	0.76	112,112,112,112	0
26	MG	A	1685	1/1	0.56	0.66	335,335,335,335	0
26	MG	A	1669	1/1	0.62	0.49	106,106,106,106	0
26	MG	A	1791	1/1	0.64	0.96	91,91,91,91	0
26	MG	A	1940	1/1	0.65	0.45	102,102,102,102	0
26	MG	A	1769	1/1	0.66	0.53	98,98,98,98	0
26	MG	A	1933	1/1	0.67	0.63	94,94,94,94	0
26	MG	A	1803	1/1	0.68	0.67	91,91,91,91	0
26	MG	A	1758	1/1	0.69	0.52	105,105,105,105	0
26	MG	P	102	1/1	0.69	0.27	117,117,117,117	0
26	MG	A	1932	1/1	0.69	0.48	102,102,102,102	0
26	MG	A	1924	1/1	0.69	0.58	109,109,109,109	0
26	MG	A	1921	1/1	0.69	0.24	134,134,134,134	0
26	MG	A	1920	1/1	0.69	0.37	113,113,113,113	0
26	MG	A	1922	1/1	0.70	0.40	104,104,104,104	0
26	MG	D	302	1/1	0.71	0.42	92,92,92,92	0
26	MG	A	1949	1/1	0.71	0.48	88,88,88,88	0
26	MG	A	1681	1/1	0.72	0.83	114,114,114,114	0
26	MG	A	1816	1/1	0.72	0.42	495,495,495,495	0
26	MG	A	1911	1/1	0.73	0.55	99,99,99,99	0
26	MG	A	1923	1/1	0.73	0.76	99,99,99,99	0
26	MG	A	1678	1/1	0.73	0.39	95,95,95,95	0
26	MG	A	1755	1/1	0.74	0.12	119,119,119,119	0
26	MG	A	1925	1/1	0.74	0.65	82,82,82,82	0
26	MG	A	1793	1/1	0.74	0.21	105,105,105,105	0
26	MG	A	1928	1/1	0.74	0.35	94,94,94,94	0
26	MG	A	1789	1/1	0.74	0.51	124,124,124,124	0
26	MG	A	1919	1/1	0.74	0.13	101,101,101,101	0
26	MG	A	1776	1/1	0.75	0.92	110,110,110,110	0
26	MG	A	1775	1/1	0.75	0.79	84,84,84,84	0
26	MG	G	201[A]	1/1	0.75	0.77	62,62,62,62	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
26	MG	G	201[B]	1/1	0.75	0.77	50,50,50,50	1
26	MG	A	1869	1/1	0.75	0.25	412,412,412,412	0
26	MG	Q	201	1/1	0.75	0.16	91,91,91,91	0
26	MG	A	1738	1/1	0.76	0.56	85,85,85,85	0
26	MG	A	1625	1/1	0.76	0.17	89,89,89,89	0
26	MG	A	1910	1/1	0.76	0.42	114,114,114,114	0
26	MG	S	102	1/1	0.77	0.13	99,99,99,99	0
26	MG	A	1787	1/1	0.77	0.60	132,132,132,132	0
26	MG	A	1926	1/1	0.77	0.44	111,111,111,111	0
26	MG	A	1623	1/1	0.77	0.42	85,85,85,85	0
26	MG	A	1783	1/1	0.77	0.42	96,96,96,96	1
26	MG	A	1838	1/1	0.77	0.38	462,462,462,462	0
26	MG	A	1741	1/1	0.77	0.70	119,119,119,119	0
26	MG	A	1732	1/1	0.77	0.47	95,95,95,95	0
26	MG	A	1754	1/1	0.78	0.26	92,92,92,92	0
26	MG	A	1870	1/1	0.78	0.24	456,456,456,456	0
26	MG	A	1643	1/1	0.78	0.31	140,140,140,140	0
26	MG	A	1950	1/1	0.78	0.41	90,90,90,90	0
26	MG	A	1852	1/1	0.79	0.28	426,426,426,426	0
26	MG	A	1865	1/1	0.79	0.35	476,476,476,476	1
26	MG	A	1811	1/1	0.79	0.11	411,411,411,411	0
26	MG	A	1862	1/1	0.79	0.35	463,463,463,463	1
26	MG	A	1764	1/1	0.79	0.17	62,62,62,62	0
26	MG	H	201	1/1	0.80	0.38	73,73,73,73	0
26	MG	A	1952	1/1	0.80	0.34	79,79,79,79	0
26	MG	A	1777	1/1	0.80	0.42	81,81,81,81	0
26	MG	A	1613	1/1	0.80	0.12	170,170,170,170	0
26	MG	A	1621	1/1	0.80	0.38	130,130,130,130	0
26	MG	P	101	1/1	0.80	0.56	75,75,75,75	0
26	MG	A	1904	1/1	0.81	0.27	397,397,397,397	0
26	MG	A	1707	1/1	0.81	0.17	437,437,437,437	0
26	MG	T	201	1/1	0.81	0.32	129,129,129,129	0
26	MG	A	1908	1/1	0.81	0.65	117,117,117,117	0
26	MG	A	1866	1/1	0.81	0.42	425,425,425,425	1
26	MG	A	1938	1/1	0.81	0.96	100,100,100,100	0
26	MG	A	1917	1/1	0.81	0.87	103,103,103,103	0
26	MG	A	1805	1/1	0.81	0.30	79,79,79,79	0
26	MG	A	1929	1/1	0.81	0.39	87,87,87,87	0
26	MG	A	1878	1/1	0.81	0.17	389,389,389,389	0
26	MG	F	201	1/1	0.81	0.36	101,101,101,101	0
26	MG	A	1640	1/1	0.82	0.40	203,203,203,203	0
26	MG	A	1824	1/1	0.82	0.16	404,404,404,404	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
26	MG	A	1748	1/1	0.82	0.69	109,109,109,109	0
26	MG	A	1767	1/1	0.82	0.55	107,107,107,107	0
26	MG	A	1652	1/1	0.82	0.55	77,77,77,77	0
26	MG	A	1930	1/1	0.82	0.20	107,107,107,107	0
26	MG	A	1901	1/1	0.82	0.24	399,399,399,399	0
26	MG	A	1820	1/1	0.83	0.12	427,427,427,427	0
26	MG	A	1815	1/1	0.83	0.18	368,368,368,368	0
26	MG	A	1692	1/1	0.83	0.74	128,128,128,128	0
26	MG	P	103	1/1	0.83	0.28	89,89,89,89	0
26	MG	A	1821	1/1	0.83	0.15	356,356,356,356	0
26	MG	A	1734	1/1	0.83	0.20	114,114,114,114	0
26	MG	A	1823	1/1	0.83	0.28	435,435,435,435	0
26	MG	A	1953	1/1	0.84	0.63	104,104,104,104	0
26	MG	A	1746	1/1	0.84	0.55	120,120,120,120	0
26	MG	A	1697	1/1	0.84	0.35	122,122,122,122	0
26	MG	A	1731	1/1	0.84	1.19	117,117,117,117	0
26	MG	A	1888	1/1	0.84	0.34	347,347,347,347	0
26	MG	A	1675	1/1	0.84	0.11	153,153,153,153	0
26	MG	A	1837	1/1	0.84	0.23	429,429,429,429	0
26	MG	A	1876	1/1	0.85	0.16	289,289,289,289	0
26	MG	A	1682	1/1	0.85	0.39	133,133,133,133	0
26	MG	A	1861	1/1	0.85	0.34	428,428,428,428	0
26	MG	A	1695	1/1	0.85	0.23	123,123,123,123	0
26	MG	A	1708	1/1	0.85	0.22	284,284,284,284	0
26	MG	N	102	1/1	0.85	0.40	87,87,87,87	0
26	MG	A	1846	1/1	0.85	0.18	390,390,390,390	0
26	MG	A	1798	1/1	0.85	0.27	96,96,96,96	0
26	MG	A	1817	1/1	0.85	0.50	378,378,378,378	0
26	MG	A	1733	1/1	0.85	0.23	90,90,90,90	0
26	MG	A	1914	1/1	0.85	0.11	118,118,118,118	0
26	MG	A	1834	1/1	0.85	0.86	364,364,364,364	0
26	MG	A	1939	1/1	0.85	0.32	88,88,88,88	0
26	MG	A	1786	1/1	0.85	0.30	120,120,120,120	0
26	MG	A	1848	1/1	0.85	0.12	361,361,361,361	0
26	MG	A	1927	1/1	0.85	0.40	100,100,100,100	0
26	MG	A	1841	1/1	0.86	0.12	387,387,387,387	0
26	MG	A	1718	1/1	0.86	0.13	160,160,160,160	0
26	MG	A	1934	1/1	0.86	0.43	79,79,79,79	0
26	MG	A	1771	1/1	0.86	0.38	63,63,63,63	0
26	MG	E	203	1/1	0.86	0.10	115,115,115,115	0
26	MG	A	1867	1/1	0.86	0.26	170,170,170,170	1
26	MG	A	1673	1/1	0.86	0.33	179,179,179,179	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
26	MG	A	1645	1/1	0.86	0.20	84,84,84,84	0
26	MG	A	1795	1/1	0.86	1.03	108,108,108,108	0
26	MG	A	1665	1/1	0.86	0.23	189,189,189,189	0
26	MG	A	1943	1/1	0.86	1.06	92,92,92,92	0
26	MG	A	1836	1/1	0.86	0.12	409,409,409,409	0
26	MG	A	1935	1/1	0.87	0.70	108,108,108,108	0
26	MG	A	1945	1/1	0.87	0.58	129,129,129,129	0
26	MG	A	1722	1/1	0.87	0.26	100,100,100,100	0
26	MG	A	1797	1/1	0.87	0.32	84,84,84,84	0
26	MG	A	1729	1/1	0.87	0.32	78,78,78,78	0
26	MG	A	1779	1/1	0.87	0.57	65,65,65,65	0
26	MG	A	1737	1/1	0.87	0.63	104,104,104,104	0
26	MG	A	1679	1/1	0.87	0.26	98,98,98,98	0
26	MG	A	1906	1/1	0.87	0.31	118,118,118,118	0
26	MG	A	1887	1/1	0.87	0.14	365,365,365,365	0
26	MG	A	1828	1/1	0.87	0.56	439,439,439,439	0
26	MG	A	1864	1/1	0.87	0.25	407,407,407,407	1
26	MG	A	1877	1/1	0.88	0.23	430,430,430,430	0
26	MG	A	1634	1/1	0.88	0.25	240,240,240,240	0
26	MG	A	1757	1/1	0.88	0.35	91,91,91,91	0
26	MG	A	1944	1/1	0.88	0.45	100,100,100,100	0
26	MG	A	1931	1/1	0.88	0.23	76,76,76,76	0
26	MG	A	1806	1/1	0.88	0.08	100,100,100,100	0
26	MG	A	1751	1/1	0.88	0.42	82,82,82,82	0
26	MG	A	1642	1/1	0.88	0.25	118,118,118,118	0
26	MG	A	1802	1/1	0.88	0.33	118,118,118,118	0
26	MG	A	1889	1/1	0.88	0.34	401,401,401,401	0
26	MG	A	1792	1/1	0.88	0.69	94,94,94,94	0
26	MG	A	1881	1/1	0.88	0.34	316,316,316,316	0
26	MG	A	1647	1/1	0.88	0.36	133,133,133,133	0
26	MG	A	1728	1/1	0.89	0.66	109,109,109,109	0
26	MG	A	1715	1/1	0.89	0.37	176,176,176,176	0
26	MG	A	1736	1/1	0.89	0.21	97,97,97,97	0
26	MG	A	1761	1/1	0.89	0.34	115,115,115,115	0
26	MG	A	1611	1/1	0.89	0.11	131,131,131,131	0
26	MG	A	1659	1/1	0.89	0.34	105,105,105,105	0
26	MG	A	1749	1/1	0.89	0.27	105,105,105,105	0
26	MG	A	1814	1/1	0.89	0.33	384,384,384,384	0
26	MG	A	1753	1/1	0.89	0.33	93,93,93,93	0
26	MG	A	1863	1/1	0.89	0.09	414,414,414,414	0
26	MG	A	1831	1/1	0.89	0.21	438,438,438,438	0
26	MG	A	1727	1/1	0.89	0.11	222,222,222,222	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
26	MG	A	1730	1/1	0.89	0.57	103,103,103,103	0
26	MG	A	1843	1/1	0.90	0.10	346,346,346,346	0
26	MG	A	1688	1/1	0.90	0.05	130,130,130,130	0
26	MG	A	1630	1/1	0.90	0.29	105,105,105,105	0
26	MG	A	1745	1/1	0.90	0.36	89,89,89,89	0
26	MG	A	1809	1/1	0.90	0.10	268,268,268,268	0
26	MG	L	201	1/1	0.90	0.13	86,86,86,86	0
26	MG	A	1946	1/1	0.90	0.99	111,111,111,111	0
26	MG	A	1778	1/1	0.90	0.27	83,83,83,83	0
26	MG	A	1784	1/1	0.90	0.21	121,121,121,121	0
26	MG	A	1631	1/1	0.90	0.21	159,159,159,159	0
26	MG	A	1909	1/1	0.90	0.28	95,95,95,95	0
26	MG	A	1813	1/1	0.90	0.14	461,461,461,461	0
26	MG	A	1948	1/1	0.91	0.29	115,115,115,115	0
26	MG	J	201	1/1	0.91	0.25	87,87,87,87	0
26	MG	A	1855	1/1	0.91	0.08	315,315,315,315	0
26	MG	A	1819	1/1	0.91	0.31	488,488,488,488	0
26	MG	A	1873	1/1	0.91	0.22	424,424,424,424	0
26	MG	A	1829	1/1	0.91	0.28	387,387,387,387	0
26	MG	D	303	1/1	0.91	0.15	83,83,83,83	0
26	MG	A	1619	1/1	0.91	0.28	80,80,80,80	0
26	MG	A	1650	1/1	0.91	0.44	93,93,93,93	0
26	MG	A	1759	1/1	0.91	0.41	83,83,83,83	0
26	MG	A	1912	1/1	0.91	0.28	97,97,97,97	0
26	MG	A	1719	1/1	0.91	0.38	141,141,141,141	0
26	MG	A	1710	1/1	0.91	0.14	247,247,247,247	0
26	MG	A	1739	1/1	0.91	0.23	105,105,105,105	0
26	MG	A	1788	1/1	0.91	0.36	82,82,82,82	0
26	MG	A	1897	1/1	0.91	0.05	235,235,235,235	0
26	MG	A	1672	1/1	0.91	0.14	91,91,91,91	0
26	MG	A	1947	1/1	0.91	0.14	126,126,126,126	0
26	MG	A	1907	1/1	0.91	0.21	89,89,89,89	0
26	MG	A	1773	1/1	0.91	0.33	78,78,78,78	0
26	MG	A	1804	1/1	0.92	0.11	130,130,130,130	0
26	MG	A	1617	1/1	0.92	0.37	111,111,111,111	0
26	MG	A	1942	1/1	0.92	0.16	92,92,92,92	0
26	MG	A	1890	1/1	0.92	0.21	423,423,423,423	0
26	MG	A	1691	1/1	0.92	0.14	130,130,130,130	0
26	MG	F	202	1/1	0.92	0.18	98,98,98,98	0
26	MG	A	1686	1/1	0.92	0.04	210,210,210,210	0
26	MG	A	1651	1/1	0.92	0.24	109,109,109,109	0
26	MG	A	1900	1/1	0.92	0.18	409,409,409,409	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
26	MG	A	1646	1/1	0.92	0.07	47,47,47,47	0
26	MG	A	1839	1/1	0.92	0.08	375,375,375,375	0
26	MG	A	1699	1/1	0.92	0.15	117,117,117,117	0
26	MG	A	1637	1/1	0.92	0.15	99,99,99,99	0
26	MG	A	1918	1/1	0.92	0.84	114,114,114,114	0
26	MG	A	1706	1/1	0.93	0.17	99,99,99,99	0
26	MG	A	1702	1/1	0.93	0.60	91,91,91,91	0
26	MG	A	1875	1/1	0.93	0.06	151,151,151,151	0
26	MG	A	1661	1/1	0.93	0.18	158,158,158,158	0
26	MG	A	1847	1/1	0.93	0.17	335,335,335,335	0
26	MG	A	1951	1/1	0.93	0.08	122,122,122,122	0
26	MG	A	1827	1/1	0.93	0.14	376,376,376,376	0
26	MG	A	1780	1/1	0.93	1.17	116,116,116,116	0
26	MG	A	1835	1/1	0.93	0.47	448,448,448,448	0
26	MG	A	1740	1/1	0.93	0.71	90,90,90,90	0
26	MG	A	1807	1/1	0.93	0.09	100,100,100,100	0
26	MG	A	1781	1/1	0.93	0.41	72,72,72,72	0
26	MG	A	1799	1/1	0.93	0.45	100,100,100,100	1
26	MG	A	1851	1/1	0.93	0.14	259,259,259,259	0
26	MG	A	1735	1/1	0.93	0.65	116,116,116,116	0
26	MG	A	1714	1/1	0.93	0.14	202,202,202,202	0
26	MG	A	1833	1/1	0.93	1.10	455,455,455,455	1
26	MG	A	1832	1/1	0.93	0.44	421,421,421,421	0
26	MG	A	1760	1/1	0.93	0.15	123,123,123,123	0
26	MG	A	1694	1/1	0.94	0.32	113,113,113,113	0
26	MG	A	1662	1/1	0.94	0.28	122,122,122,122	0
26	MG	A	1687	1/1	0.94	0.30	155,155,155,155	0
26	MG	A	1782	1/1	0.94	0.13	92,92,92,92	0
26	MG	A	1916	1/1	0.94	0.08	121,121,121,121	0
26	MG	A	1849	1/1	0.94	0.05	301,301,301,301	0
26	MG	A	1857	1/1	0.94	0.21	254,254,254,254	0
26	MG	A	1616	1/1	0.94	0.27	76,76,76,76	0
26	MG	A	1796	1/1	0.94	0.10	74,74,74,74	0
26	MG	A	1842	1/1	0.94	0.44	460,460,460,460	0
26	MG	A	1810	1/1	0.94	0.13	277,277,277,277	0
26	MG	A	1765	1/1	0.94	0.32	77,77,77,77	0
26	MG	A	1880	1/1	0.94	0.07	402,402,402,402	0
26	MG	D	304	1/1	0.94	0.09	467,467,467,467	0
26	MG	A	1766	1/1	0.94	0.13	109,109,109,109	0
26	MG	A	1725	1/1	0.94	0.31	119,119,119,119	0
26	MG	A	1895	1/1	0.94	0.16	364,364,364,364	0
26	MG	A	1629	1/1	0.94	0.22	123,123,123,123	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
26	MG	A	1891	1/1	0.94	0.89	398,398,398,398	1
26	MG	A	1608	1/1	0.94	0.07	125,125,125,125	0
28	ZN	D	301	1/1	0.94	0.31	116,116,116,116	0
26	MG	A	1639	1/1	0.94	0.18	124,124,124,124	0
26	MG	E	202	1/1	0.94	0.14	107,107,107,107	0
26	MG	A	1794	1/1	0.94	0.19	87,87,87,87	0
26	MG	A	1684	1/1	0.95	0.15	137,137,137,137	0
26	MG	A	1667	1/1	0.95	0.18	121,121,121,121	0
26	MG	A	1800	1/1	0.95	0.12	87,87,87,87	0
26	MG	A	1644	1/1	0.95	0.17	80,80,80,80	0
26	MG	A	1899	1/1	0.95	0.10	422,422,422,422	0
26	MG	A	1705	1/1	0.95	0.28	98,98,98,98	0
26	MG	A	1801	1/1	0.95	0.38	96,96,96,96	0
26	MG	A	1844	1/1	0.95	0.07	330,330,330,330	0
26	MG	A	1768	1/1	0.95	0.26	115,115,115,115	0
26	MG	A	1763	1/1	0.95	0.15	89,89,89,89	0
26	MG	A	1663	1/1	0.95	0.17	146,146,146,146	0
26	MG	A	1614	1/1	0.95	0.09	92,92,92,92	0
26	MG	A	1713	1/1	0.95	0.34	116,116,116,116	0
26	MG	A	1690	1/1	0.95	0.15	189,189,189,189	0
26	MG	A	1853	1/1	0.95	0.16	395,395,395,395	0
26	MG	A	1872	1/1	0.95	0.23	287,287,287,287	0
26	MG	S	103	1/1	0.95	0.14	92,92,92,92	0
26	MG	A	1830	1/1	0.95	0.11	426,426,426,426	0
26	MG	A	1668	1/1	0.95	0.11	122,122,122,122	0
26	MG	A	1689	1/1	0.96	0.05	273,273,273,273	0
26	MG	A	1860	1/1	0.96	0.15	303,303,303,303	0
26	MG	A	1902	1/1	0.96	0.33	326,326,326,326	0
26	MG	A	1892	1/1	0.96	0.50	354,354,354,354	0
26	MG	A	1893	1/1	0.96	0.31	304,304,304,304	0
26	MG	A	1856	1/1	0.96	0.08	156,156,156,156	0
26	MG	A	1717	1/1	0.96	0.23	197,197,197,197	0
26	MG	A	1903	1/1	0.96	0.10	268,268,268,268	0
26	MG	A	1858	1/1	0.96	0.35	255,255,255,255	1
26	MG	A	1658	1/1	0.96	0.27	115,115,115,115	0
26	MG	A	1601	1/1	0.96	0.57	63,63,63,63	1
26	MG	A	1664	1/1	0.96	0.19	167,167,167,167	0
26	MG	A	1693	1/1	0.96	0.38	129,129,129,129	0
26	MG	A	1854	1/1	0.96	0.13	134,134,134,134	1
26	MG	A	1704	1/1	0.96	0.06	205,205,205,205	0
26	MG	A	1898	1/1	0.96	0.19	370,370,370,370	0
26	MG	A	1653	1/1	0.96	0.15	116,116,116,116	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
26	MG	A	1762	1/1	0.96	0.22	100,100,100,100	0
26	MG	A	1822	1/1	0.96	0.21	281,281,281,281	0
26	MG	A	1884	1/1	0.96	0.11	345,345,345,345	0
26	MG	A	1871	1/1	0.96	0.24	346,346,346,346	0
26	MG	A	1772	1/1	0.96	0.10	116,116,116,116	0
26	MG	A	1874	1/1	0.96	0.07	197,197,197,197	0
26	MG	A	1698	1/1	0.97	0.11	108,108,108,108	0
26	MG	A	1894	1/1	0.97	0.27	340,340,340,340	0
28	ZN	N	101	1/1	0.97	0.16	138,138,138,138	0
26	MG	A	1609	1/1	0.97	0.30	85,85,85,85	0
26	MG	S	101	1/1	0.97	0.17	82,82,82,82	0
26	MG	A	1882	1/1	0.97	0.07	247,247,247,247	0
26	MG	A	1602	1/1	0.97	0.13	124,124,124,124	0
26	MG	A	1632	1/1	0.97	0.42	110,110,110,110	0
26	MG	A	1618	1/1	0.97	0.31	89,89,89,89	0
26	MG	A	1770	1/1	0.97	0.17	79,79,79,79	0
26	MG	A	1825	1/1	0.97	0.18	188,188,188,188	0
26	MG	A	1896	1/1	0.97	0.45	378,378,378,378	0
26	MG	A	1859	1/1	0.97	0.18	278,278,278,278	0
26	MG	A	1636	1/1	0.97	0.08	94,94,94,94	0
26	MG	A	1826	1/1	0.97	0.48	382,382,382,382	0
26	MG	A	1868	1/1	0.97	0.10	435,435,435,435	0
26	MG	A	1720	1/1	0.97	0.15	126,126,126,126	0
26	MG	A	1603	1/1	0.97	0.32	105,105,105,105	0
27	SRY	A	1956	40/40	0.97	0.20	55,83,98,109	0
26	MG	A	1840	1/1	0.97	0.08	119,119,119,119	0
26	MG	A	1879	1/1	0.97	0.12	406,406,406,406	0
26	MG	A	1726	1/1	0.97	0.13	293,293,293,293	0
26	MG	A	1747	1/1	0.97	0.26	75,75,75,75	0
26	MG	A	1709	1/1	0.97	0.32	93,93,93,93	0
26	MG	A	1701	1/1	0.97	0.21	83,83,83,83	0
26	MG	A	1676	1/1	0.97	0.07	121,121,121,121	0
26	MG	A	1724	1/1	0.97	0.19	103,103,103,103	0
26	MG	A	1670	1/1	0.97	0.10	189,189,189,189	0
26	MG	A	1660	1/1	0.97	0.18	118,118,118,118	0
26	MG	A	1818	1/1	0.97	0.15	329,329,329,329	0
26	MG	A	1885	1/1	0.97	0.11	316,316,316,316	0
26	MG	A	1703	1/1	0.98	0.07	117,117,117,117	0
26	MG	A	1657	1/1	0.98	0.17	131,131,131,131	0
26	MG	A	1648	1/1	0.98	0.38	139,139,139,139	0
26	MG	A	1743	1/1	0.98	0.24	72,72,72,72	0
26	MG	A	1808	1/1	0.98	0.14	486,486,486,486	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
26	MG	A	1624	1/1	0.98	0.15	79,79,79,79	0
26	MG	A	1604	1/1	0.98	0.07	134,134,134,134	0
26	MG	A	1756	1/1	0.98	0.48	101,101,101,101	0
26	MG	A	1627	1/1	0.98	0.41	229,229,229,229	0
26	MG	A	1750	1/1	0.98	0.24	109,109,109,109	0
26	MG	A	1654	1/1	0.98	0.16	78,78,78,78	0
26	MG	E	201	1/1	0.98	0.41	111,111,111,111	0
26	MG	A	1620	1/1	0.98	0.13	81,81,81,81	0
26	MG	A	1937	1/1	0.98	0.11	60,60,60,60	0
26	MG	A	1635	1/1	0.98	0.16	73,73,73,73	0
26	MG	A	1955	1/1	0.98	0.14	69,69,69,69	0
26	MG	A	1812	1/1	0.98	0.11	180,180,180,180	0
26	MG	A	1680	1/1	0.98	0.09	258,258,258,258	0
26	MG	A	1677	1/1	0.98	0.10	99,99,99,99	0
26	MG	A	1607	1/1	0.98	0.32	76,76,76,76	0
26	MG	A	1845	1/1	0.98	0.07	98,98,98,98	0
26	MG	A	1641	1/1	0.98	0.15	70,70,70,70	0
26	MG	A	1716	1/1	0.98	0.17	111,111,111,111	1
26	MG	A	1655	1/1	0.99	0.09	64,64,64,64	0
26	MG	A	1606	1/1	0.99	0.07	75,75,75,75	0
26	MG	A	1656	1/1	0.99	0.50	94,94,94,94	0
26	MG	A	1674	1/1	0.99	0.13	98,98,98,98	0
26	MG	A	1612	1/1	0.99	0.15	112,112,112,112	0
26	MG	A	1628	1/1	0.99	0.20	89,89,89,89	0
26	MG	A	1721	1/1	0.99	0.20	175,175,175,175	0
26	MG	A	1683	1/1	0.99	0.15	113,113,113,113	0
26	MG	A	1638	1/1	0.99	0.14	72,72,72,72	0
26	MG	A	1649	1/1	0.99	0.28	93,93,93,93	0
26	MG	A	1610	1/1	0.99	0.10	66,66,66,66	0
26	MG	A	1666	1/1	0.99	0.09	80,80,80,80	0
26	MG	A	1615	1/1	0.99	0.29	72,72,72,72	0
26	MG	A	1886	1/1	0.99	0.16	224,224,224,224	0
26	MG	A	1711	1/1	0.99	0.14	86,86,86,86	0
26	MG	A	1626	1/1	0.99	0.11	94,94,94,94	0
26	MG	A	1752	1/1	0.99	0.24	85,85,85,85	0
26	MG	A	1622	1/1	0.99	0.15	112,112,112,112	0
26	MG	A	1712	1/1	0.99	0.19	109,109,109,109	0
26	MG	A	1696	1/1	0.99	0.15	132,132,132,132	0
26	MG	A	1883	1/1	0.99	0.17	426,426,426,426	0
26	MG	A	1671	1/1	0.99	0.21	99,99,99,99	0
26	MG	A	1850	1/1	0.99	0.07	199,199,199,199	0
26	MG	A	1723	1/1	0.99	0.12	116,116,116,116	0

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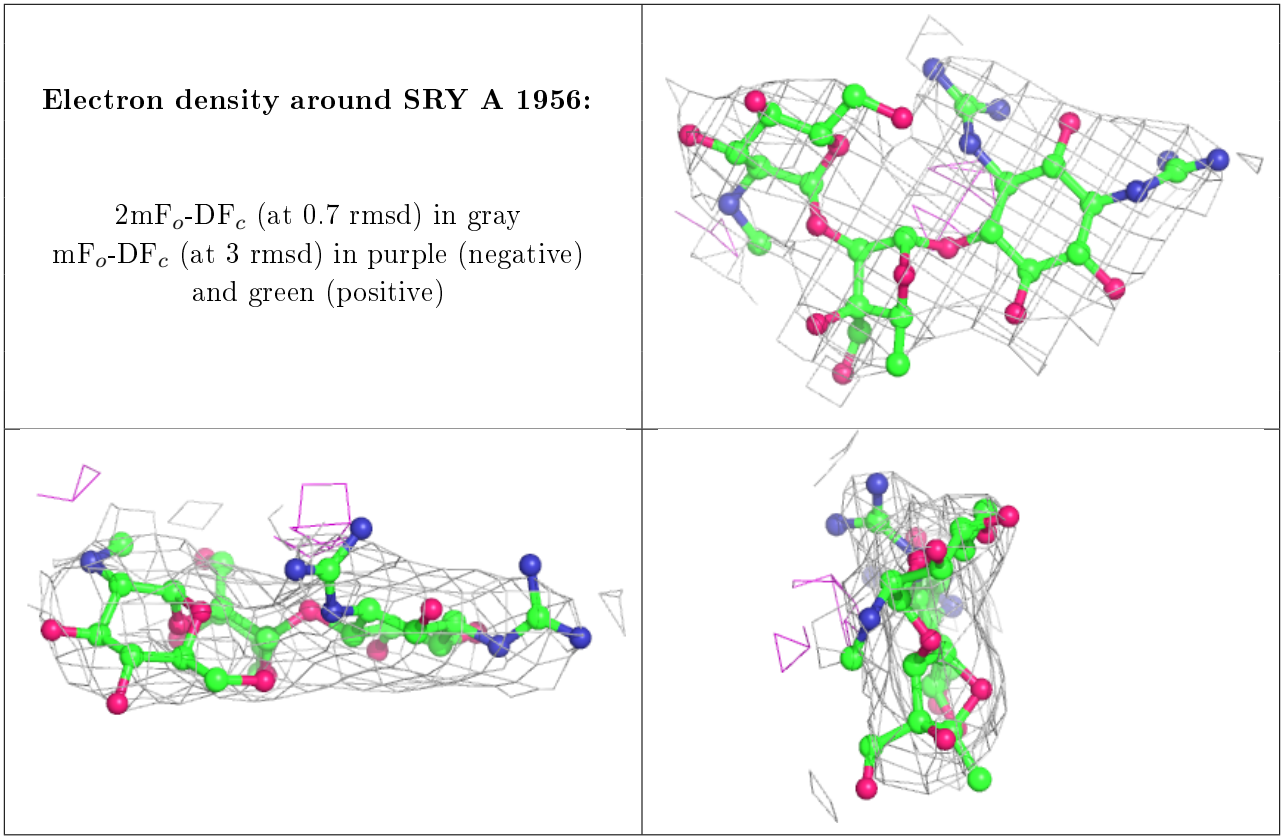
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
26	MG	A	1633	1/1	0.99	0.18	148,148,148,148	0
26	MG	A	1700	1/1	1.00	0.19	167,167,167,167	0

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

Electron density around SRY A 1956:

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



6.5 Other polymers

There are no such residues in this entry.