Full wwPDB X-ray Structure Validation Report (i)

Jun 18, 2024 – 02:06 PM EDT

PDB ID	:	4NXM
Title	:	Crystal Structure of the 30S ribosomal subunit from a GidB (RsmG) mutant of Thermus thermophilus (HB8)
Authors	:	Demirci, H.; Murphy IV, F.; Murphy, E.; Gregory, S.T.; Dahlberg, A.E.; Jogl, G.
Deposited on	:	2013-12-09
Resolution	:	3.65 Å(reported)

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

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

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

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

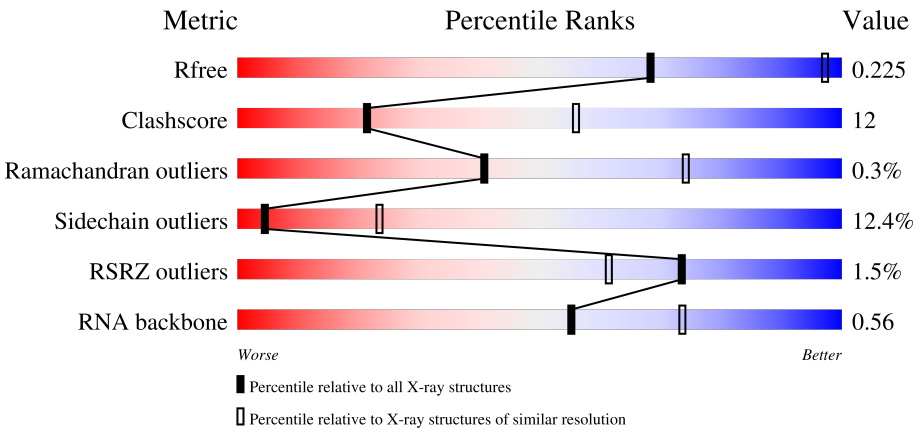
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.65 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	1557 (3.82-3.50)
Clashscore	141614	1037 (3.80-3.52)
Ramachandran outliers	138981	1004 (3.80-3.52)
Sidechain outliers	138945	1002 (3.80-3.52)
RSRZ outliers	127900	1441 (3.82-3.50)
RNA backbone	3102	1024 (4.30-3.00)

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

Mol	Chain	Length	Quality of chain
1	A	1522	% 48% 40% 10% ••
2	B	256	51% 36% 5% 9%
3	C	239	4% 48% 33% 6% 14%
4	D	209	65% 30% 5%

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Mol	Chain	Length	Quality of chain
5	E	162	62% 25% 6% 7%
6	F	101	71% 25% •
7	G	156	% 66% 31% • •
8	H	138	64% 30% 6%
9	I	128	2% 53% 38% 8% •
10	J	105	7% 48% 42% • 7%
11	K	129	64% 24% • 10%
12	L	135	61% 23% 8% 8%
13	M	126	2% 61% 29% • 6%
14	N	61	8% 41% 48% 10% •
15	O	89	72% 24% • •
16	P	88	64% 28% • 6%
17	Q	105	64% 30% • 6%
18	R	88	56% 24% 20%
19	S	93	4% 60% 20% 5% 14%
20	T	106	% 58% 30% 6% 7%
21	U	27	15% 63% 15% 11% 11%

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
22	MG	A	1695	-	-	-	X
22	MG	A	1713	-	-	-	X
22	MG	A	1728	-	-	-	X
22	MG	A	1761	-	-	-	X
22	MG	A	1773	-	-	-	X
22	MG	A	1796	-	-	-	X
22	MG	A	1812	-	-	-	X

2 Entry composition (i)

There are 24 unique types of molecules in this entry. The entry contains 52194 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	1512	32643	14539	6039	10547	1518	0	6	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1534	C	A	SEE REMARK 999	GB M26923.1
A	1535	A	C	SEE REMARK 999	GB M26923.1

- Molecule 2 is a protein called ribosomal protein S2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	234	1900	1213	341	341	5	0	0	0

- Molecule 3 is a protein called ribosomal protein S3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	206	1612	1016	314	281	1	0	0	0

- Molecule 4 is a protein called 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 ribosomal protein S5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
5	E	150	1146	724	217	201	4	0	0	0

- Molecule 6 is a protein called ribosomal protein S6.

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

- Molecule 7 is a protein called ribosomal protein S7.

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

- Molecule 8 is a protein called ribosomal protein S8.

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

- Molecule 9 is a protein called ribosomal protein S9.

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

- Molecule 10 is a protein called ribosomal protein S10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
10	J	98	792	498	156	137	1	0	0	0

- Molecule 11 is a protein called ribosomal protein S11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
11	K	116	864	537	164	160	3	0	0	0

- Molecule 12 is a protein called ribosomal protein S12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
12	L	124	972	612	195	163	2	0	0	0

- Molecule 13 is a protein called ribosomal protein S13.

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

- Molecule 14 is a protein called ribosomal protein S14.

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

- Molecule 15 is a protein called ribosomal protein S15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
15	O	87	729	457	146	124	2	0	0	0

- Molecule 16 is a protein called ribosomal protein S16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
16	P	83	700	443	139	117	1	0	0	0

- Molecule 17 is a protein called ribosomal protein S17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
17	Q	99	823	528	151	142	2	0	0	0

- Molecule 18 is a protein called ribosomal protein S18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
18	R	70	574	367	112	95	0	0	0

- Molecule 19 is a protein called ribosomal protein S19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
19	S	80	647	414	119	112	2	0	0	0

- Molecule 20 is a protein called ribosomal protein S20.

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

- Molecule 21 is a protein called ribosomal protein THX.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
21	U	24	208	128	50	30	0	0	0

- Molecule 22 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
22	A	212	212	212	0	0
22	B	1	1	1	0	0
22	C	2	2	2	0	0
22	D	3	3	3	0	0
22	E	1	1	1	0	0
22	F	1	1	1	0	0
22	P	2	2	2	0	0
22	Q	1	1	1	0	0
22	U	1	1	1	0	0

- Molecule 23 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 24 is water.

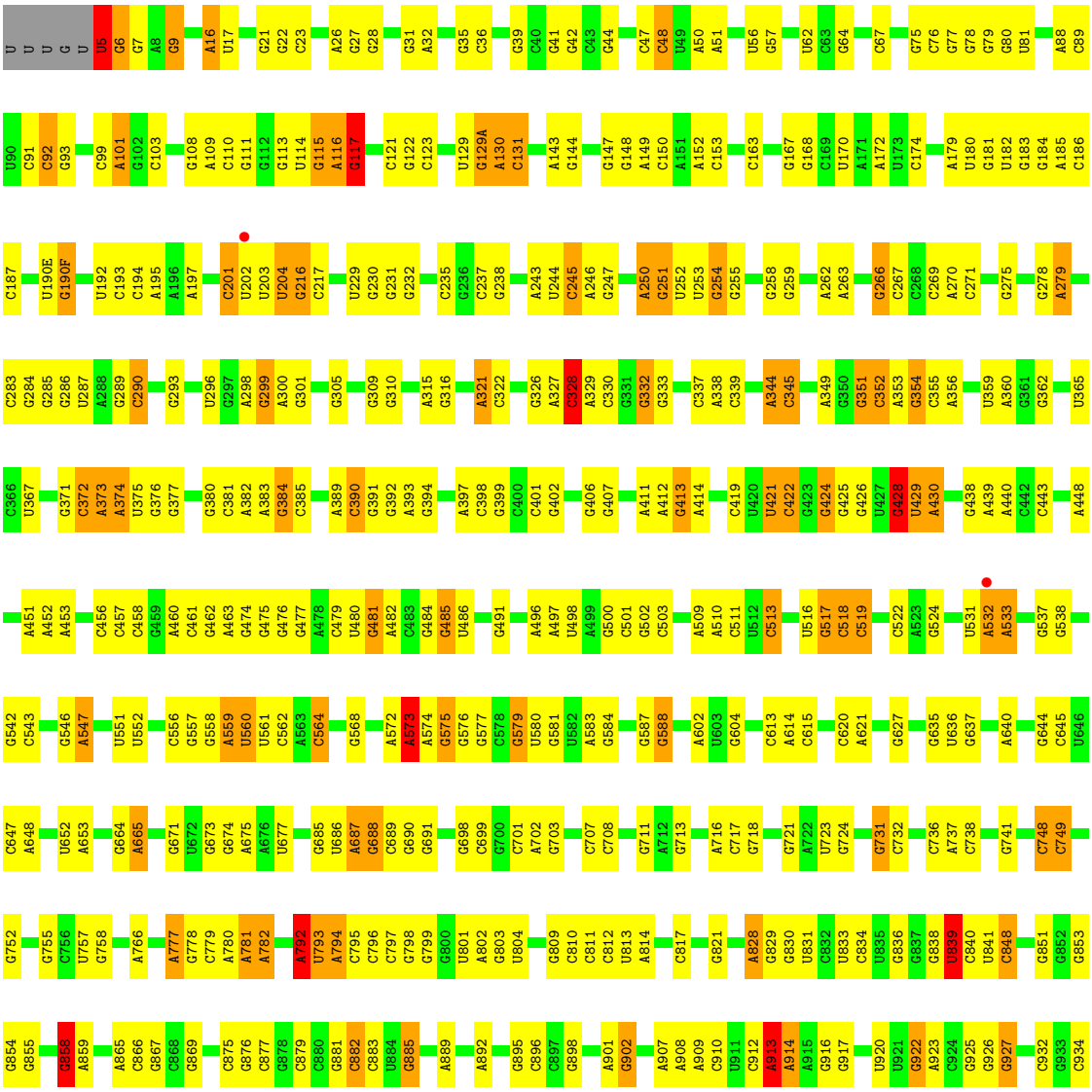
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
24	A	228	228	228	0	0
			Total	O		
24	C	1	1	1	0	0
			Total	O		
24	D	1	1	1	0	0
			Total	O		
24	E	3	3	3	0	0
			Total	O		
24	N	1	1	1	0	0
			Total	O		
24	Q	2	2	2	0	0
			Total	O		
24	T	1	1	1	0	0

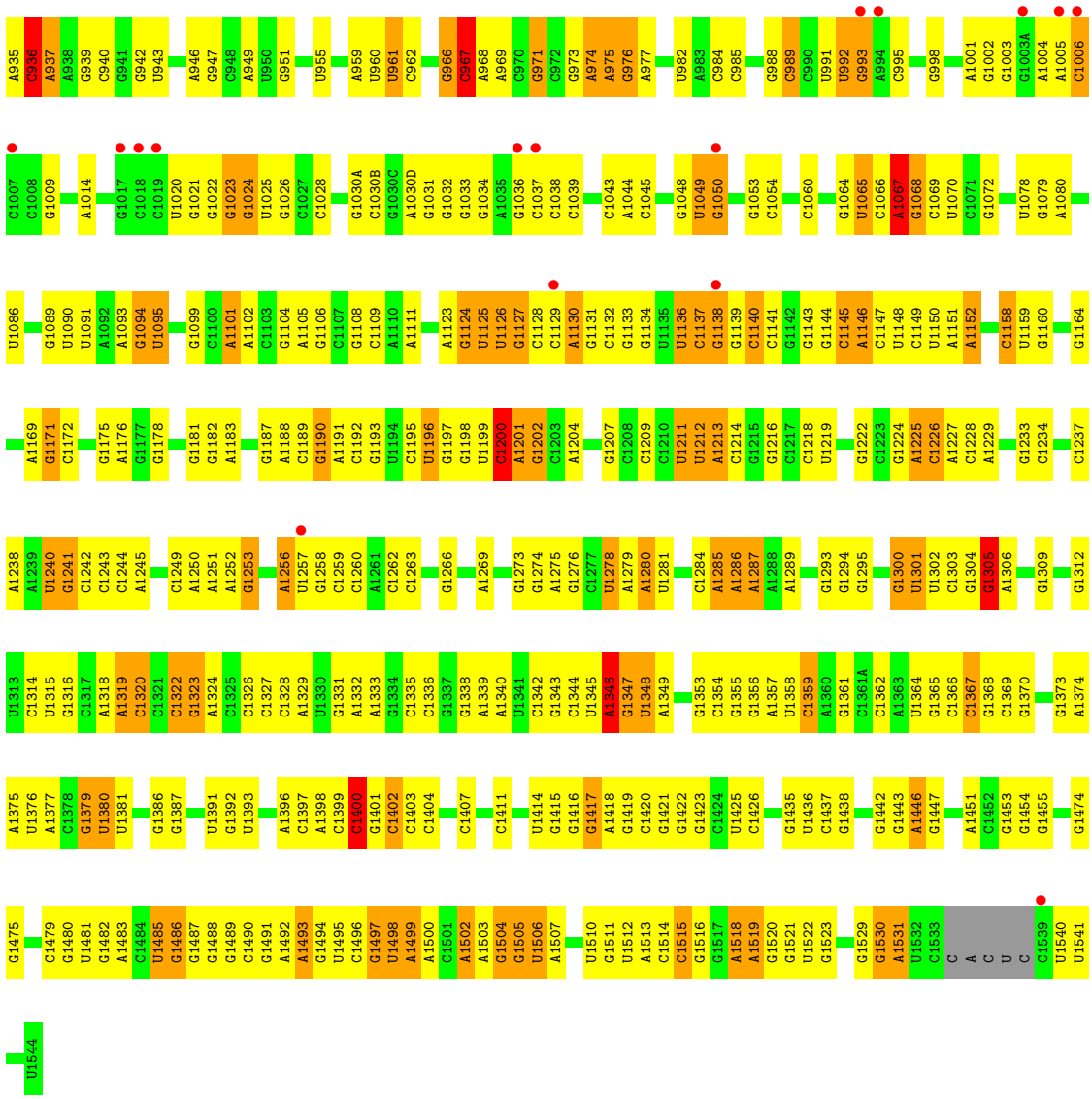
3 Residue-property plots (i)

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

- Molecule 1: 16S rRNA

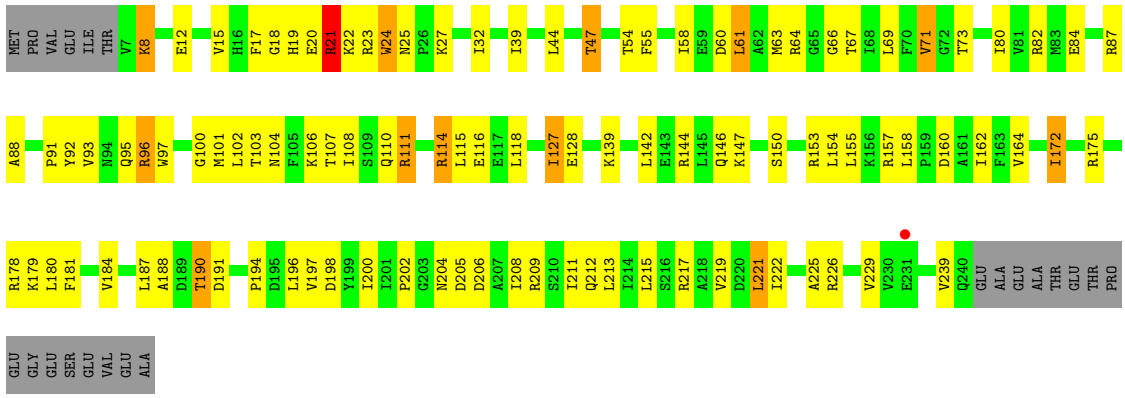
Chain A:





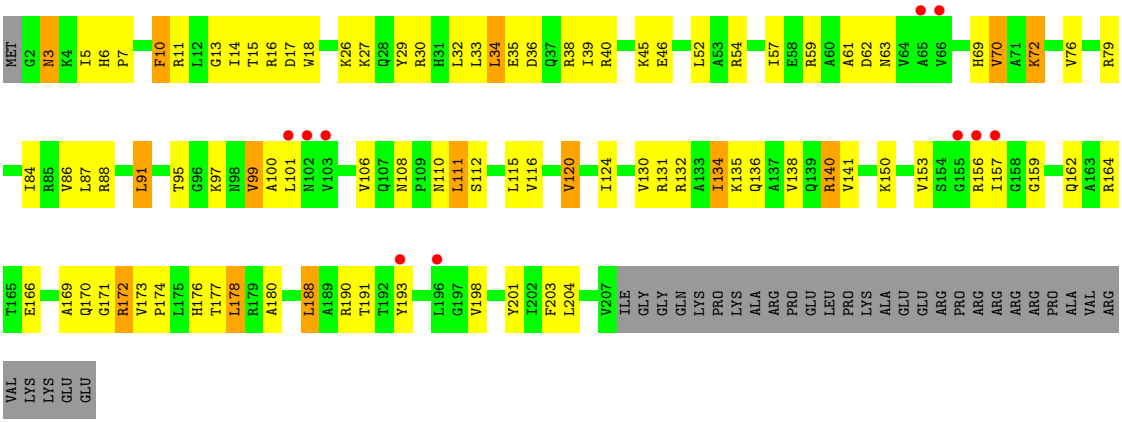
• Molecule 2: ribosomal protein S2

Chain B: 51% 36% 5% 9%



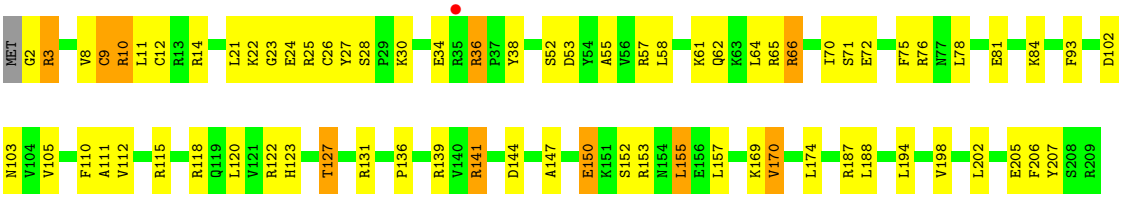
• Molecule 3: ribosomal protein S3

Chain C:



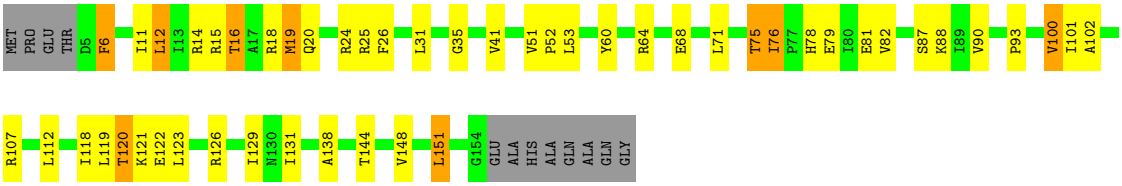
- Molecule 4: ribosomal protein S4

Chain D:



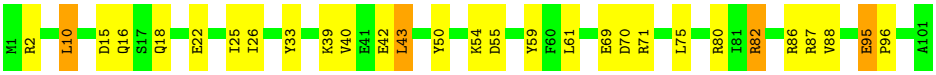
- Molecule 5: ribosomal protein S5

Chain E:



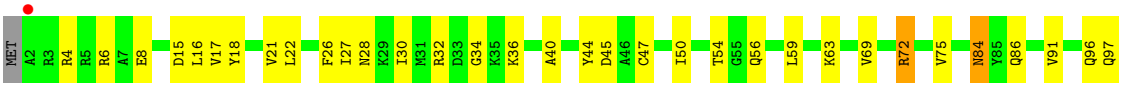
- Molecule 6: ribosomal protein S6

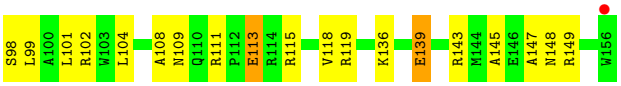
Chain F:



- Molecule 7: ribosomal protein S7

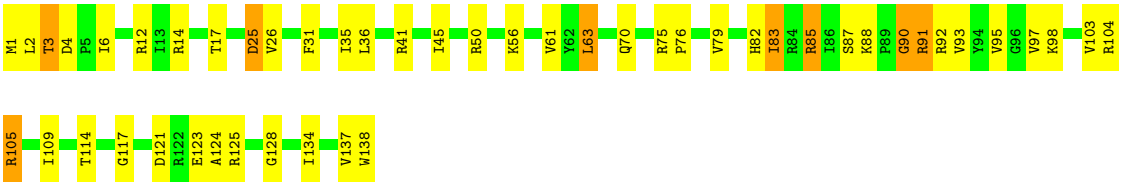
Chain G:





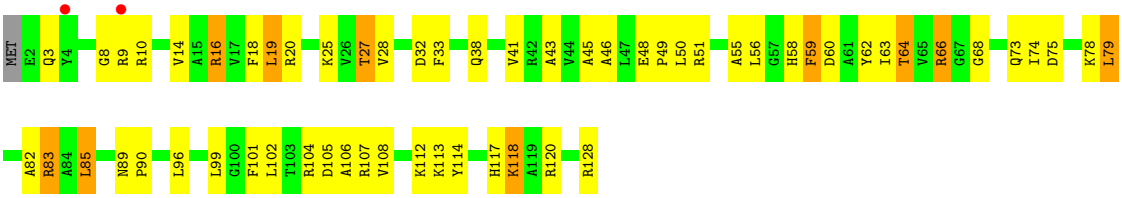
• Molecule 8: ribosomal protein S8

Chain H:



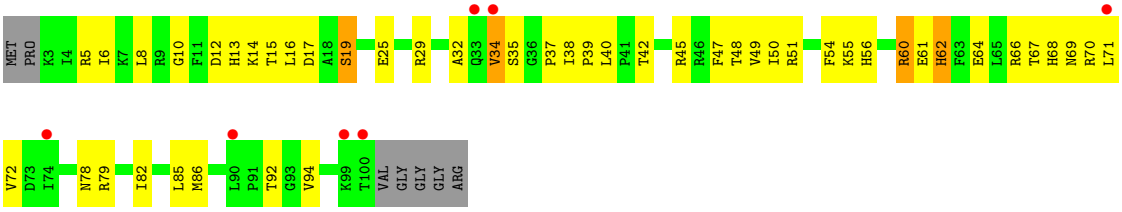
• Molecule 9: ribosomal protein S9

Chain I:



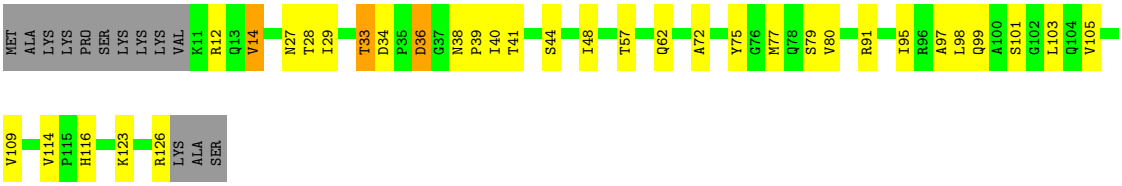
• Molecule 10: ribosomal protein S10

Chain J:



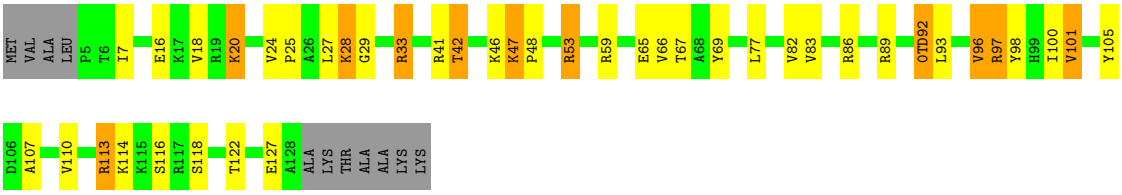
• Molecule 11: ribosomal protein S11

Chain K:



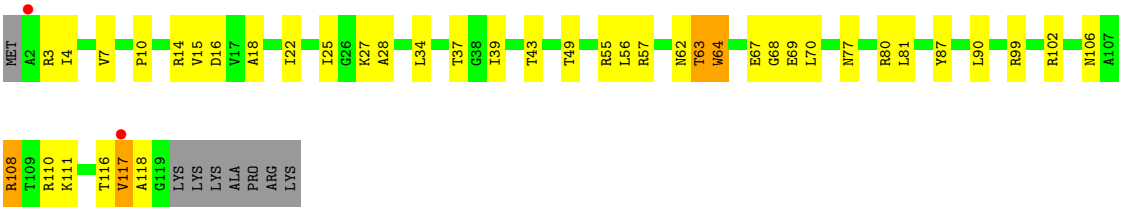
• Molecule 12: ribosomal protein S12

Chain L:



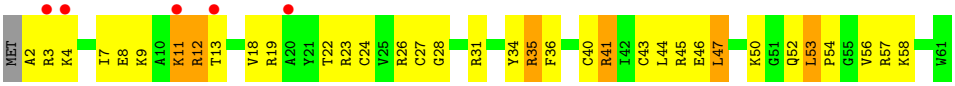
• Molecule 13: ribosomal protein S13

Chain M:



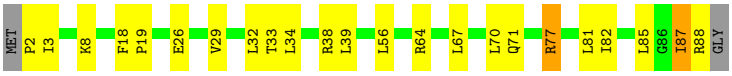
• Molecule 14: ribosomal protein S14

Chain N:



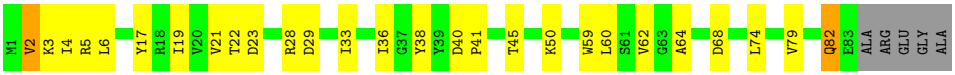
• Molecule 15: ribosomal protein S15

Chain O:



• Molecule 16: ribosomal protein S16

Chain P:



• Molecule 17: ribosomal protein S17

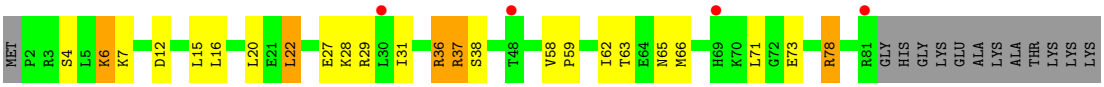
Chain Q:

• Molecule 18: ribosomal protein S18

Chain R:

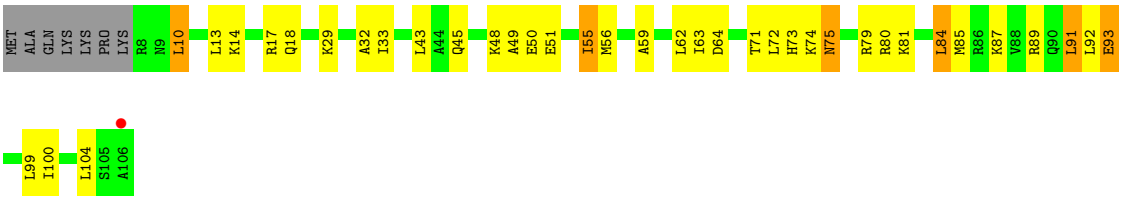
- Molecule 19: ribosomal protein S19

Chain S:



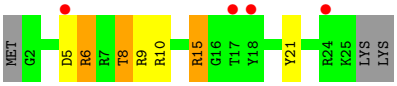
- Molecule 20: ribosomal protein S20

Chain T:



- Molecule 21: ribosomal protein THX

Chain U:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α, β, γ	402.92Å 402.92Å 174.34Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	34.62 – 3.65 34.62 – 3.65	Depositor EDS
% Data completeness (in resolution range)	98.2 (34.62-3.65) 98.0 (34.62-3.65)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.84 (at 3.66Å)	Xtriage
Refinement program	PHENIX dev_1555	Depositor
R, R_{free}	0.180 , 0.226 0.182 , 0.225	Depositor DCC
R_{free} test set	7764 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	130.3	Xtriage
Anisotropy	0.198	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.23 , 105.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	52194	wwPDB-VP
Average B, all atoms (Å^2)	146.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.92% 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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: M2G, 2MG, MG, UR3, MA6, 5MC, 0TD, ZN, 4OC, 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	0.81	3/36165 (0.0%)	0.98	49/56437 (0.1%)
2	B	0.45	0/1935	0.58	0/2609
3	C	0.32	0/1636	0.53	0/2205
4	D	0.41	0/1733	0.52	0/2318
5	E	0.61	0/1162	0.66	0/1564
6	F	0.36	0/856	0.48	0/1154
7	G	0.35	0/1276	0.47	0/1709
8	H	0.71	0/1136	0.64	0/1527
9	I	0.34	0/1029	0.52	0/1379
10	J	0.28	0/805	0.53	0/1082
11	K	0.48	0/879	0.54	0/1187
12	L	0.50	0/977	0.60	0/1306
13	M	0.32	0/947	0.50	0/1270
14	N	0.34	0/501	0.49	0/664
15	O	0.48	0/740	0.56	0/987
16	P	0.56	0/716	0.59	0/963
17	Q	0.61	0/836	0.67	0/1117
18	R	0.44	0/579	0.54	0/768
19	S	0.26	0/661	0.55	0/890
20	T	0.43	0/765	0.56	0/1007
21	U	0.35	0/212	0.44	0/277
All	All	0.70	3/55546 (0.0%)	0.87	49/82420 (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	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
20	T	0	1
All	All	0	4

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	16	A	N9-C4	-6.37	1.34	1.37
1	A	279	A	N9-C4	-6.01	1.34	1.37
1	A	16	A	N3-C4	-5.15	1.31	1.34

All (49) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	573	A	C8-N9-C4	-8.21	102.52	105.80
1	A	254	G	O5'-P-OP1	-7.98	98.52	105.70
1	A	858	G	C4-C5-N7	7.48	113.79	110.80
1	A	328	C	C2-N1-C1'	7.27	126.80	118.80
1	A	1237	C	C6-N1-C2	-7.05	117.48	120.30
1	A	1305	G	C8-N9-C4	-7.04	103.58	106.40
1	A	1158	C	N1-C2-O2	6.95	123.07	118.90
1	A	328	C	C6-N1-C2	-6.88	117.55	120.30
1	A	1158	C	C2-N1-C1'	6.70	126.17	118.80
1	A	1158	C	C6-N1-C2	-6.66	117.64	120.30
1	A	1158	C	N3-C2-O2	-6.58	117.29	121.90
1	A	839	U	N1-C2-O2	6.55	127.39	122.80
1	A	1354	C	C6-N1-C2	-6.48	117.71	120.30
1	A	266	G	C4-C5-N7	6.33	113.33	110.80
1	A	839	U	C2-N1-C1'	6.32	125.29	117.70
1	A	328	C	C5-C6-N1	6.18	124.09	121.00
1	A	858	G	C5-N7-C8	-6.10	101.25	104.30
1	A	1301	U	P-O3'-C3'	6.00	126.89	119.70
1	A	117	G	N1-C6-O6	5.99	123.50	119.90
1	A	279	A	C5-N7-C8	-5.96	100.92	103.90
1	A	1305	G	N3-C4-C5	-5.95	125.63	128.60
1	A	882	C	C6-N1-C2	-5.94	117.92	120.30
1	A	724	G	C5-C6-O6	-5.65	125.21	128.60
1	A	1300	G	P-O3'-C3'	5.61	126.43	119.70
1	A	839	U	N3-C2-O2	-5.57	118.30	122.20
1	A	1367	C	C6-N1-C2	-5.57	118.07	120.30
1	A	117	G	C6-C5-N7	-5.47	127.12	130.40
1	A	1200	C	C2-N1-C1'	5.47	124.81	118.80
1	A	1502	A	N1-C6-N6	5.44	121.87	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	5	U	P-O3'-C3'	5.41	126.19	119.70
1	A	1301	U	OP1-P-O3'	5.36	116.99	105.20
1	A	328	C	N1-C2-O2	5.35	122.11	118.90
1	A	266	G	O4'-C1'-N9	-5.31	103.95	108.20
1	A	1515[A]	C	C6-N1-C2	-5.28	118.19	120.30
1	A	1515[B]	C	C6-N1-C2	-5.28	118.19	120.30
1	A	16	A	C2-N3-C4	-5.25	107.97	110.60
1	A	16	A	N1-C2-N3	5.24	131.92	129.30
1	A	1346	A	P-O3'-C3'	5.24	125.99	119.70
1	A	1380	U	P-O3'-C3'	5.23	125.98	119.70
1	A	573	A	N7-C8-N9	5.13	116.37	113.80
1	A	328	C	N3-C2-O2	-5.13	118.31	121.90
1	A	1067	A	P-O3'-C3'	5.12	125.84	119.70
1	A	913	A	P-O3'-C3'	5.12	125.84	119.70
1	A	640	A	C8-N9-C4	-5.12	103.75	105.80
1	A	792	A	P-O3'-C3'	5.11	125.83	119.70
1	A	117	G	C5-C6-O6	-5.09	125.55	128.60
1	A	936	C	C6-N1-C2	5.04	122.32	120.30
1	A	428	G	P-O3'-C3'	5.03	125.73	119.70
1	A	1502	A	C6-C5-N7	-5.01	128.79	132.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	71	VAL	Peptide
2	B	8	LYS	Peptide
8	H	90	GLY	Peptide
20	T	93	GLU	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	32643	0	16503	570	0
2	B	1900	0	1951	64	0
3	C	1612	0	1676	63	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	D	1703	0	1763	48	0
5	E	1146	0	1207	31	0
6	F	843	0	857	20	0
7	G	1257	0	1296	30	0
8	H	1116	0	1177	34	0
9	I	1010	0	1037	45	0
10	J	792	0	835	36	0
11	K	864	0	881	17	0
12	L	972	0	1058	35	0
13	M	937	0	995	23	0
14	N	492	0	529	25	0
15	O	729	0	768	13	0
16	P	700	0	720	20	0
17	Q	823	0	891	28	0
18	R	574	0	644	16	0
19	S	647	0	673	19	0
20	T	763	0	861	24	0
21	U	208	0	221	6	0
22	A	212	0	0	0	0
22	B	1	0	0	0	0
22	C	2	0	0	0	0
22	D	3	0	0	0	0
22	E	1	0	0	0	0
22	F	1	0	0	0	0
22	P	2	0	0	0	0
22	Q	1	0	0	0	0
22	U	1	0	0	0	0
23	D	1	0	0	0	0
23	N	1	0	0	0	0
24	A	228	0	0	4	0
24	C	1	0	0	0	0
24	D	1	0	0	0	0
24	E	3	0	0	0	0
24	N	1	0	0	0	0
24	Q	2	0	0	0	0
24	T	1	0	0	0	0
All	All	52194	0	36543	1048	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 12.

All (1048) 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)
1:A:1443:G:H5"	1:A:1446:A:H5'	1.51	0.89
1:A:235:C:H5'	17:Q:70:ARG:HG2	1.55	0.85
1:A:279:A:OP2	17:Q:95:TYR:OH	1.99	0.79
9:I:50:LEU:HB3	9:I:55:ALA:HB3	1.64	0.78
1:A:1009:G:H1	1:A:1020:U:H3	1.31	0.78
1:A:1125:U:OP2	1:A:1145:C:N4	2.17	0.77
1:A:9:G:OP2	5:E:121:LYS:NZ	2.17	0.76
1:A:1195:C:H3'	1:A:1196:U:H5"	1.66	0.76
1:A:237:C:OP2	17:Q:40:LYS:NZ	2.19	0.75
3:C:134:ILE:HD11	3:C:153:VAL:HG23	1.69	0.75
4:D:150:GLU:HA	4:D:153:ARG:HB2	1.68	0.75
1:A:1240:U:OP1	7:G:119:ARG:NH2	2.13	0.75
3:C:88:ARG:HH21	3:C:100:ALA:HB1	1.52	0.75
11:K:40:ILE:HG22	11:K:41:THR:HG23	1.69	0.74
10:J:15:THR:HG22	10:J:94:VAL:HG13	1.68	0.74
1:A:299:G:N1	24:A:2057:HOH:O	2.19	0.74
1:A:1415:G:H1	1:A:1485:U:H3	1.34	0.74
11:K:27:ASN:OD1	11:K:28:THR:N	2.21	0.73
1:A:652:U:O4	1:A:752:G:O2'	2.04	0.73
1:A:103:C:OP1	20:T:17:ARG:NH1	2.21	0.73
12:L:24:VAL:HG13	12:L:98:TYR:HE2	1.52	0.73
1:A:269:C:H2'	1:A:270:A:H8	1.54	0.72
1:A:1349:A:OP1	9:I:118:LYS:NZ	2.19	0.72
10:J:61:GLU:OE2	14:N:58:LYS:NZ	2.23	0.72
1:A:269:C:H2'	1:A:270:A:C8	2.24	0.71
1:A:973:G:H3'	1:A:974:A:H5"	1.73	0.71
8:H:114:THR:OG1	8:H:117:GLY:O	2.08	0.71
1:A:564:C:O2'	8:H:91:ARG:NH2	2.23	0.71
1:A:1295:G:O2'	13:M:14:ARG:NH1	2.24	0.71
4:D:23:GLY:HA3	4:D:112:VAL:HG12	1.73	0.71
1:A:1347:G:O6	9:I:10:ARG:NH2	2.21	0.70
1:A:1048:G:H5"	14:N:3:ARG:HD2	1.73	0.70
3:C:174:PRO:HB2	3:C:177:THR:HG22	1.74	0.70
1:A:1498:UR3:O2'	1:A:1499:A:OP2	2.08	0.70
4:D:61:LYS:NZ	4:D:72:GLU:OE2	2.25	0.70
1:A:255:G:O3'	17:Q:17:LYS:NZ	2.25	0.69
1:A:1403:C:O2	1:A:1499:A:N6	2.19	0.69
6:F:10:LEU:HD12	6:F:59:TYR:HB3	1.73	0.69
16:P:21:VAL:HG21	16:P:59:TRP:CD1	2.27	0.69
8:H:4:ASP:OD2	8:H:85:ARG:NH1	2.24	0.69
15:O:26:GLU:HG3	15:O:81:LEU:HD12	1.74	0.69
1:A:1417:G:O2'	1:A:1483:A:N6	2.26	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:254:G:OP1	17:Q:66:SER:OG	2.11	0.68
1:A:998:G:N2	1:A:1043:C:O2	2.26	0.68
1:A:559:A:OP1	5:E:126:ARG:NH2	2.27	0.68
3:C:164:ARG:NH1	3:C:166:GLU:OE1	2.27	0.68
12:L:47:LYS:HG2	12:L:48:PRO:HD3	1.75	0.68
3:C:150:LYS:HB2	3:C:173:VAL:HG21	1.75	0.68
1:A:501:C:H2'	1:A:502:G:C8	2.29	0.68
12:L:24:VAL:HG13	12:L:98:TYR:CE2	2.28	0.68
14:N:8:GLU:HA	14:N:11:LYS:HD3	1.76	0.68
17:Q:66:SER:O	17:Q:70:ARG:NH1	2.27	0.67
1:A:1134:G:H1	1:A:1140:C:H42	1.42	0.67
1:A:1345:U:OP1	9:I:120:ARG:NH1	2.28	0.67
1:A:1286:A:H2'	1:A:1287:A:H4'	1.77	0.67
3:C:17:ASP:O	3:C:54:ARG:NH2	2.27	0.67
1:A:1049:U:O2'	14:N:3:ARG:NH1	2.27	0.67
1:A:1130:A:O2'	9:I:3:GLN:NE2	2.28	0.66
6:F:22:GLU:OE1	6:F:82:ARG:NH1	2.28	0.66
12:L:77:LEU:HD21	12:L:107:ALA:HB2	1.76	0.66
17:Q:12:SER:HB3	17:Q:20:THR:HB	1.78	0.66
1:A:1147:C:O2	9:I:16:ARG:NH2	2.29	0.66
12:L:27:LEU:O	12:L:29:GLY:N	2.29	0.66
1:A:413:G:O6	4:D:36:ARG:NH1	2.29	0.66
4:D:127:THR:HG22	4:D:147:ALA:HB3	1.77	0.66
1:A:664:G:H22	1:A:741:G:H1	1.44	0.65
1:A:946:A:H2'	1:A:947:G:C8	2.31	0.65
1:A:1126:U:O4	1:A:1127:G:N2	2.29	0.65
1:A:1030(A):G:N2	1:A:1030(D):A:OP2	2.27	0.65
21:U:5:ASP:O	21:U:8:THR:OG1	2.15	0.65
1:A:992:U:H3	1:A:1044:A:H62	1.45	0.65
1:A:1256:A:N6	1:A:1278:U:O2	2.29	0.65
9:I:46:ALA:HB2	9:I:74:ILE:HG23	1.79	0.65
2:B:91:PRO:HG3	2:B:154:LEU:HB2	1.79	0.65
1:A:1520[B]:G:H2'	1:A:1521:G:H8	1.61	0.65
1:A:1252:A:H61	1:A:1285:A:H61	1.44	0.64
1:A:1259:C:H42	1:A:1276:G:H1	1.45	0.64
5:E:11:ILE:HD12	5:E:31:LEU:HD13	1.79	0.64
1:A:542:G:OP1	4:D:10:ARG:NH2	2.31	0.64
1:A:673:G:H2'	1:A:674:G:C8	2.32	0.64
3:C:14:ILE:HG22	3:C:15:THR:HG23	1.79	0.64
10:J:61:GLU:OE1	14:N:45:ARG:NH1	2.31	0.64
14:N:40:CYS:O	14:N:44:LEU:N	2.20	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:27:THR:HG23	9:I:62:TYR:HA	1.79	0.64
1:A:989:C:H42	1:A:1216:G:H1	1.45	0.64
2:B:60:ASP:OD2	2:B:64:ARG:NH1	2.31	0.64
19:S:22:LEU:HD21	19:S:28:LYS:HB2	1.80	0.63
1:A:372:C:H4'	1:A:373:A:O5'	1.99	0.63
1:A:1145:C:O2'	1:A:1146:A:O5'	2.17	0.63
6:F:50:TYR:CE1	18:R:77:GLY:HA2	2.34	0.63
1:A:426:G:OP1	4:D:38:TYR:OH	2.16	0.63
10:J:49:VAL:HG13	14:N:41:ARG:HB2	1.79	0.63
1:A:989:C:N3	1:A:1216:G:N2	2.43	0.63
1:A:235:C:N4	24:A:1985:HOH:O	2.32	0.62
20:T:50:GLU:H	20:T:99:LEU:HD12	1.64	0.62
15:O:64:ARG:HG2	15:O:88:ARG:HH11	1.63	0.62
2:B:71:VAL:HB	2:B:164:VAL:HG12	1.81	0.62
16:P:4:ILE:HG12	16:P:21:VAL:HG22	1.81	0.62
1:A:1262:C:H42	1:A:1273:G:H1	1.46	0.62
1:A:1422:G:H2'	1:A:1423:G:H8	1.64	0.62
1:A:462:G:H21	16:P:82:GLN:HE21	1.48	0.62
1:A:1191:A:OP1	3:C:3:ASN:ND2	2.31	0.62
1:A:1391:U:H2'	1:A:1392:G:H8	1.64	0.62
1:A:263:A:OP2	20:T:79:ARG:NH1	2.32	0.62
1:A:1376:U:OP1	7:G:98:SER:OG	2.12	0.61
1:A:1065:U:H5"	1:A:1190:G:N2	2.15	0.61
4:D:22:LYS:HB2	4:D:26:CYS:SG	2.39	0.61
1:A:1150:U:O4	1:A:1151:A:N6	2.33	0.61
1:A:1391:U:H2'	1:A:1392:G:C8	2.35	0.61
1:A:1515[B]:C:H42	1:A:1520[B]:G:H1	1.49	0.61
1:A:1090:U:H2'	1:A:1091:U:H6	1.66	0.61
1:A:1399:C:H4'	1:A:1400:5MC:H5"	1.81	0.61
4:D:61:LYS:HD2	4:D:207:TYR:OH	2.01	0.61
17:Q:40:LYS:HD2	17:Q:42:TYR:CZ	2.34	0.61
1:A:298:A:N6	24:A:2057:HOH:O	2.23	0.61
13:M:10:PRO:HB2	13:M:18:ALA:HB1	1.83	0.61
1:A:184:G:H2'	1:A:185:A:H8	1.66	0.61
1:A:532:A:N6	3:C:159:GLY:O	2.34	0.60
1:A:685:G:N2	1:A:686:U:C4	2.69	0.60
1:A:793:U:O2	1:A:1516[A]:G:O2'	2.16	0.60
1:A:1518[A]:MA6:H8	1:A:1518[A]:MA6:O5'	2.02	0.60
1:A:925:G:C2	1:A:927:G:C8	2.89	0.60
1:A:1080:A:O3'	5:E:16:THR:OG1	2.18	0.60
10:J:8:LEU:HB2	10:J:70:ARG:HB2	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:150:LYS:HB3	3:C:201:TYR:HB2	1.83	0.60
16:P:28:ARG:NH1	16:P:29:ASP:OD2	2.34	0.60
1:A:201:C:N3	1:A:216:G:N2	2.45	0.60
9:I:48:GLU:OE1	9:I:51:ARG:NH1	2.35	0.60
1:A:501:C:H2'	1:A:502:G:H8	1.65	0.60
2:B:184:VAL:N	2:B:198:ASP:OD2	2.33	0.60
1:A:1222:G:OP2	1:A:1322:C:N4	2.24	0.59
1:A:1504:G:OP1	1:A:1507:A:H4'	2.02	0.59
1:A:1060:C:HO2'	10:J:56:HIS:HD1	1.50	0.59
12:L:20:LYS:NZ	12:L:20:LYS:H	2.00	0.59
1:A:795:C:H5"	1:A:796:C:OP2	2.03	0.59
10:J:51:ARG:NE	10:J:61:GLU:HB3	2.18	0.59
1:A:1415:G:H2'	1:A:1416:G:H8	1.66	0.59
1:A:542:G:O3'	4:D:14:ARG:NH2	2.32	0.59
1:A:103:C:P	20:T:17:ARG:HH12	2.26	0.59
5:E:76:ILE:HD12	5:E:118:ILE:HD11	1.83	0.59
1:A:976:G:OP2	1:A:1358:U:H1'	2.03	0.59
1:A:1144:G:H21	1:A:1146:A:H62	1.50	0.59
1:A:28:G:O2'	1:A:296:U:OP1	2.19	0.59
20:T:45:GLN:HA	20:T:91:LEU:HD12	1.83	0.59
1:A:1518[B]:MA6:H102	1:A:1519[B]:MA6:H103	1.85	0.58
17:Q:67:LYS:HA	17:Q:70:ARG:HH12	1.69	0.58
1:A:1523:G:OP1	11:K:123:LYS:HD2	2.03	0.58
9:I:16:ARG:HB2	9:I:64:THR:HG23	1.84	0.58
1:A:677:U:H3	1:A:713:G:H22	1.51	0.58
3:C:150:LYS:HG3	3:C:169:ALA:HB2	1.84	0.58
6:F:33:TYR:HA	6:F:71:ARG:HH21	1.68	0.58
1:A:1369:C:H2'	1:A:1370:G:C8	2.39	0.58
5:E:60:TYR:OH	5:E:64:ARG:NH2	2.37	0.58
1:A:179:A:H2'	1:A:180:U:C6	2.39	0.58
1:A:1278:U:H5'	1:A:1279:A:H5'	1.85	0.58
10:J:50:ILE:HD12	10:J:50:ILE:H	1.69	0.58
1:A:424:G:H2'	1:A:425:G:H8	1.68	0.58
1:A:1356:G:H2'	1:A:1357:A:C8	2.38	0.58
2:B:21:ARG:HB3	2:B:39:ILE:HG12	1.86	0.58
12:L:25:PRO:C	12:L:27:LEU:H	2.06	0.58
1:A:1305:G:N2	1:A:1331:G:H1'	2.18	0.57
10:J:50:ILE:HA	10:J:60:ARG:HB3	1.86	0.57
15:O:87:ILE:HG22	15:O:88:ARG:H	1.69	0.57
1:A:123:C:O2'	1:A:290:C:O2	2.22	0.57
20:T:50:GLU:HA	20:T:100:ILE:HG13	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:558:G:H5"	1:A:559:A:H3'	1.87	0.57
10:J:48:THR:HA	10:J:62:HIS:HB3	1.85	0.57
18:R:59:SER:H	18:R:62:GLU:HB2	1.68	0.57
1:A:152:A:N6	1:A:170:U:C2	2.73	0.57
1:A:1105:A:H2'	1:A:1106:G:H8	1.69	0.57
1:A:1349:A:P	9:I:118:LYS:HZ1	2.27	0.57
1:A:1419:G:H2'	1:A:1420:C:C6	2.39	0.57
1:A:811:C:O2'	1:A:901:A:N1	2.35	0.57
3:C:26:LYS:O	3:C:30:ARG:NH1	2.38	0.57
1:A:337:C:H2'	1:A:338:A:H8	1.70	0.57
1:A:975:A:H4'	1:A:976:G:O5'	2.04	0.57
1:A:1158:C:N3	1:A:1181:G:N2	2.53	0.57
1:A:1420:C:H2'	1:A:1421:G:H8	1.69	0.57
1:A:216:G:H2'	1:A:217:C:C6	2.39	0.57
1:A:1022:G:N2	1:A:1023:G:O6	2.35	0.57
1:A:1320:C:H1'	19:S:73:GLU:HG2	1.86	0.57
18:R:36:ASN:OD1	18:R:39:VAL:HG12	2.05	0.57
7:G:21:VAL:HG23	7:G:22:LEU:HD23	1.87	0.57
1:A:390:C:O3'	16:P:28:ARG:NH2	2.38	0.56
1:A:1028:C:H42	1:A:1033:G:H22	1.53	0.56
1:A:1020:U:H2'	1:A:1021:G:C8	2.40	0.56
1:A:951:G:OP2	13:M:102:ARG:NH2	2.38	0.56
4:D:102:ASP:OD1	4:D:103:ASN:N	2.39	0.56
1:A:1065:U:H5"	1:A:1190:G:H22	1.70	0.56
1:A:1079:G:O3'	5:E:14:ARG:NH2	2.38	0.56
4:D:62:GLN:OE1	4:D:65:ARG:NH1	2.39	0.56
1:A:686:U:C2	1:A:687:A:N7	2.74	0.56
4:D:187:ARG:HH22	4:D:188:LEU:HD12	1.71	0.56
14:N:26:ARG:NH1	14:N:47:LEU:HD23	2.20	0.56
1:A:908:A:C2	1:A:909:A:C4	2.93	0.56
1:A:1510:U:H2'	1:A:1511:G:C8	2.41	0.56
5:E:75:THR:OG1	5:E:76:ILE:N	2.39	0.56
6:F:55:ASP:HB3	6:F:86:ARG:HH12	1.70	0.56
1:A:250:A:H4'	1:A:251:G:O5'	2.06	0.56
1:A:1026:G:O6	1:A:1036:G:N2	2.39	0.56
2:B:21:ARG:HA	2:B:39:ILE:HA	1.86	0.55
3:C:35:GLU:HB3	3:C:59:ARG:HH22	1.71	0.55
12:L:53:ARG:HG2	12:L:93:LEU:HD11	1.88	0.55
12:L:28:LYS:HG3	12:L:33:ARG:CZ	2.37	0.55
3:C:157:ILE:HD13	3:C:166:GLU:HG2	1.89	0.55
7:G:28:ASN:OD1	7:G:36:LYS:NZ	2.39	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:47:LEU:HD13	14:N:52:GLN:HB2	1.89	0.55
20:T:89:ARG:NH2	20:T:104:LEU:HB3	2.21	0.55
1:A:407:G:OP1	4:D:115:ARG:NH1	2.40	0.55
1:A:538:G:O3'	12:L:114:LYS:HD3	2.06	0.55
13:M:63:THR:HG23	13:M:64:TRP:H	1.70	0.55
20:T:51:GLU:O	20:T:55:ILE:HG13	2.06	0.55
2:B:71:VAL:HG22	2:B:93:VAL:HB	1.89	0.55
3:C:91:LEU:HD21	3:C:99:VAL:HG22	1.88	0.55
1:A:674:G:H2'	1:A:675:A:H8	1.72	0.55
1:A:1260:C:OP1	1:A:1284:C:O2'	2.23	0.55
1:A:939:G:H2'	1:A:940:C:C6	2.42	0.54
2:B:17:PHE:HD1	2:B:18:GLY:N	2.05	0.54
4:D:24:GLU:HA	4:D:27:TYR:HD1	1.71	0.54
5:E:16:THR:OG1	5:E:16:THR:O	2.23	0.54
16:P:28:ARG:HG3	16:P:29:ASP:OD2	2.06	0.54
1:A:1425:U:H2'	1:A:1426:C:C6	2.42	0.54
19:S:28:LYS:HG2	19:S:29:ARG:H	1.72	0.54
1:A:959:A:O2'	1:A:984:C:O2'	2.26	0.54
1:A:1133:G:H1	1:A:1141:C:H42	1.55	0.54
20:T:75:ASN:OD1	20:T:75:ASN:N	2.41	0.54
1:A:88:A:H2'	1:A:89:C:O4'	2.08	0.54
1:A:1418:A:H61	1:A:1482:G:H1'	1.71	0.54
1:A:1049:U:H4'	1:A:1050:G:O5'	2.06	0.54
4:D:8:VAL:HG11	4:D:21:LEU:HB2	1.89	0.54
5:E:101:ILE:O	5:E:120:THR:HB	2.08	0.54
9:I:3:GLN:OE1	9:I:20:ARG:NH2	2.41	0.54
1:A:1414:U:H3	1:A:1486:G:H1	1.55	0.54
10:J:10:GLY:HA3	10:J:16:LEU:HD21	1.90	0.54
11:K:80:VAL:HG21	11:K:103:LEU:HD13	1.89	0.54
1:A:193:C:H2'	1:A:194:C:H6	1.73	0.54
1:A:149:A:H2'	1:A:150:C:H6	1.72	0.54
1:A:448:A:P	1:A:485:G:H22	2.31	0.54
7:G:16:LEU:HD11	9:I:45:ALA:HB2	1.90	0.54
12:L:27:LEU:C	12:L:29:GLY:H	2.11	0.54
14:N:2:ALA:N	14:N:28:GLY:O	2.41	0.54
1:A:21:G:H2'	1:A:22:G:C8	2.43	0.54
1:A:352:C:N3	1:A:356:A:N6	2.56	0.54
15:O:39:LEU:HD13	15:O:56:LEU:HB2	1.90	0.54
15:O:85:LEU:HB3	15:O:87:ILE:HD11	1.89	0.54
1:A:910:C:OP1	12:L:97:ARG:NH2	2.39	0.54
8:H:87:SER:HA	8:H:93:VAL:HG13	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:476:G:H2'	1:A:477:G:C8	2.43	0.53
1:A:1125:U:O4	10:J:5:ARG:NE	2.27	0.53
2:B:158:LEU:HD12	2:B:158:LEU:H	1.72	0.53
1:A:299:G:C6	1:A:300:A:C6	2.96	0.53
1:A:1250:A:H4'	9:I:68:GLY:N	2.24	0.53
2:B:205:ASP:OD1	2:B:206:ASP:N	2.41	0.53
3:C:156:ARG:NH1	3:C:193:TYR:O	2.37	0.53
16:P:21:VAL:HG12	16:P:33:ILE:HD12	1.89	0.53
1:A:443:C:H42	1:A:491:G:H1	1.56	0.53
3:C:13:GLY:HA3	14:N:57:ARG:HH21	1.73	0.53
5:E:12:LEU:HD13	5:E:31:LEU:HB2	1.89	0.53
1:A:1148:U:H2'	1:A:1149:C:O4'	2.09	0.53
3:C:116:VAL:O	3:C:120:VAL:HG22	2.09	0.53
13:M:16:ASP:OD1	13:M:16:ASP:N	2.41	0.53
15:O:29:VAL:HG11	15:O:67:LEU:HD21	1.89	0.53
1:A:838:G:H1	1:A:848:C:H42	1.55	0.53
1:A:966:M2G:HM13	1:A:967:5MC:H1'	1.90	0.53
3:C:3:ASN:OD1	3:C:3:ASN:N	2.41	0.53
10:J:12:ASP:OD2	10:J:15:THR:OG1	2.23	0.53
1:A:192:U:H2'	1:A:193:C:H6	1.73	0.53
3:C:84:ILE:HG12	3:C:88:ARG:HH11	1.74	0.53
1:A:56:U:H2'	1:A:57:G:H8	1.73	0.53
1:A:757:U:O2'	1:A:879:C:O2	2.24	0.53
1:A:1435:G:H2'	1:A:1436:U:C6	2.44	0.53
1:A:1491:G:H21	1:A:1492:A:H62	1.57	0.53
1:A:686:U:HO2'	1:A:687:A:H8	1.57	0.53
1:A:1143:G:H2'	1:A:1144:G:C8	2.43	0.53
19:S:12:ASP:H	19:S:38:SER:HB3	1.74	0.53
20:T:87:LYS:O	20:T:91:LEU:HB2	2.08	0.53
1:A:7:G:H5'	1:A:298:A:O4'	2.09	0.53
1:A:664:G:OP1	18:R:64:ARG:NH1	2.33	0.53
1:A:1090:U:H2'	1:A:1091:U:C6	2.44	0.53
2:B:61:LEU:HD11	2:B:160:ASP:HB2	1.91	0.53
3:C:170:GLN:HG2	3:C:171:GLY:H	1.74	0.53
1:A:1031:G:H2'	1:A:1032:G:C8	2.43	0.52
5:E:88:LYS:HB3	5:E:123:LEU:HB2	1.91	0.52
7:G:69:VAL:HG21	7:G:104:LEU:HD21	1.91	0.52
1:A:939:G:H5"	7:G:102:ARG:NH2	2.23	0.52
2:B:32:ILE:HD11	2:B:190:THR:HG23	1.92	0.52
4:D:3:ARG:NH2	4:D:70:ILE:HG23	2.24	0.52
7:G:47:CYS:O	7:G:50:ILE:HG22	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:537:G:OP1	12:L:113:ARG:NH2	2.42	0.52
1:A:1200:C:H1'	1:A:1204:A:N6	2.25	0.52
1:A:186:C:H2'	1:A:187:C:C6	2.44	0.52
1:A:731:G:OP1	1:A:766:A:H1'	2.10	0.52
1:A:877:C:O2	8:H:3:THR:HG21	2.09	0.52
8:H:85:ARG:NE	8:H:87:SER:O	2.42	0.52
9:I:19:LEU:HD23	9:I:60:ASP:O	2.10	0.52
1:A:946:A:H2'	1:A:947:G:H8	1.75	0.52
2:B:17:PHE:HD1	2:B:18:GLY:H	1.56	0.52
3:C:27:LYS:HA	3:C:30:ARG:HH12	1.75	0.52
11:K:12:ARG:HD2	11:K:14:VAL:HG13	1.92	0.52
1:A:522:C:OP2	12:L:69:TYR:OH	2.21	0.52
1:A:955:U:H1'	1:A:1227:A:H61	1.74	0.52
1:A:966:M2G:C5	1:A:967:5MC:HM52	2.45	0.52
1:A:982:U:OP2	14:N:23:ARG:NH2	2.43	0.52
1:A:1368:G:H5"	9:I:112:LYS:HB3	1.91	0.52
1:A:1516[A]:G:H2'	1:A:1518[A]:MA6:OP2	2.09	0.52
3:C:39:ILE:HD12	3:C:57:ILE:HD13	1.91	0.52
4:D:141:ARG:N	4:D:144:ASP:OD2	2.43	0.52
12:L:28:LYS:HG3	12:L:33:ARG:NH1	2.25	0.52
21:U:5:ASP:HB3	21:U:8:THR:OG1	2.09	0.52
2:B:101:MET:HA	2:B:108:ILE:HG13	1.92	0.52
17:Q:67:LYS:O	17:Q:68:ARG:HB2	2.09	0.52
1:A:122:G:C2	1:A:123:C:C2	2.98	0.52
1:A:1347:G:O2'	1:A:1348:U:P	2.68	0.52
1:A:1111:A:N1	3:C:177:THR:OG1	2.40	0.52
1:A:1498:UR3:O4'	1:A:1519[A]:MA6:H2	2.10	0.52
2:B:24:TRP:CG	2:B:25:ASN:N	2.77	0.52
1:A:129:U:O3'	1:A:129(A):G:H3'	2.09	0.51
1:A:1366:C:H2'	1:A:1367:C:H6	1.76	0.51
2:B:19:HIS:ND1	2:B:20:GLU:HG2	2.25	0.51
6:F:33:TYR:CG	6:F:75:LEU:HD23	2.45	0.51
18:R:37:VAL:HG12	18:R:41:LYS:HD2	1.92	0.51
1:A:332:G:H2'	1:A:333:G:H8	1.76	0.51
1:A:543:C:P	4:D:14:ARG:HH21	2.33	0.51
1:A:1105:A:H2'	1:A:1106:G:C8	2.45	0.51
1:A:1474:G:H2'	1:A:1475:G:H8	1.75	0.51
4:D:105:VAL:HG13	4:D:110:PHE:HB2	1.92	0.51
1:A:109:A:H2'	1:A:326:G:N2	2.25	0.51
1:A:1266:G:N2	1:A:1269:A:OP2	2.39	0.51
1:A:1368:G:OP2	9:I:112:LYS:HD3	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:93:PRO:HG2	8:H:105:ARG:NH2	2.25	0.51
10:J:47:PHE:HB3	14:N:34:TYR:HE2	1.74	0.51
13:M:22:ILE:HB	13:M:25:ILE:HB	1.93	0.51
1:A:41:G:C2	1:A:42:G:C5	2.99	0.51
1:A:476:G:H2'	1:A:477:G:H8	1.75	0.51
1:A:581:G:O6	1:A:758:G:C8	2.63	0.51
1:A:869:G:N7	24:A:2107:HOH:O	2.34	0.51
1:A:77:G:H1	1:A:92:C:H42	1.58	0.51
1:A:532:A:O2'	1:A:533:A:OP1	2.22	0.51
3:C:36:ASP:HB3	3:C:40:ARG:HH12	1.76	0.51
5:E:51:VAL:HB	5:E:52:PRO:HD3	1.93	0.51
1:A:110:C:H2'	1:A:111:G:O4'	2.11	0.51
1:A:167:G:H2'	1:A:168:G:C8	2.46	0.51
1:A:337:C:H2'	1:A:338:A:C8	2.45	0.51
1:A:392:G:H2'	1:A:393:A:C8	2.46	0.51
1:A:1495:U:H2'	1:A:1496:C:C6	2.46	0.51
9:I:118:LYS:NZ	9:I:118:LYS:O	2.27	0.51
1:A:782:A:C6	1:A:801:U:C2	2.99	0.51
1:A:1454:G:H2'	1:A:1455:G:H8	1.76	0.51
1:A:113:G:C2	1:A:114:U:C2	2.98	0.51
4:D:118:ARG:HG3	4:D:136:PRO:HB3	1.93	0.51
12:L:59:ARG:HG3	12:L:65:GLU:HG3	1.92	0.51
1:A:1043:C:H2'	1:A:1044:A:H8	1.76	0.51
1:A:1314:C:H2'	1:A:1315:U:C6	2.46	0.51
1:A:1520[B]:G:H2'	1:A:1521:G:C8	2.45	0.51
10:J:19:SER:HB2	10:J:94:VAL:HG11	1.92	0.51
1:A:413:G:H2'	1:A:428:G:N2	2.26	0.51
1:A:580:U:H2'	1:A:581:G:O4'	2.11	0.51
1:A:424:G:H2'	1:A:425:G:C8	2.46	0.50
1:A:429:U:H1'	1:A:430:A:H5"	1.93	0.50
1:A:737:A:H2'	1:A:738:C:C6	2.46	0.50
1:A:1347:G:H1'	1:A:1348:U:H5	1.76	0.50
1:A:1516[A]:G:N2	1:A:1519[A]:MA6:OP2	2.34	0.50
12:L:93:LEU:O	12:L:96:VAL:HG23	2.11	0.50
20:T:81:LYS:O	20:T:85:MET:HG3	2.11	0.50
1:A:1164:G:H1	1:A:1172:C:H42	1.59	0.50
1:A:1228:C:H2'	1:A:1229:A:H8	1.75	0.50
1:A:1127:G:O6	1:A:1144:G:N1	2.44	0.50
1:A:1402:4OC:H2'	1:A:1403:C:O4'	2.10	0.50
13:M:106:ASN:O	13:M:106:ASN:ND2	2.44	0.50
18:R:46:GLU:CD	18:R:46:GLU:H	2.15	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:538:G:H5"	12:L:114:LYS:HB2	1.93	0.50
1:A:1355:G:H2'	1:A:1356:G:H8	1.76	0.50
3:C:70:VAL:HG21	3:C:76:VAL:HG21	1.94	0.50
1:A:518:C:H4'	1:A:519:C:O5'	2.11	0.50
1:A:1095:U:OP1	1:A:1108:G:N2	2.43	0.50
5:E:18:ARG:HG2	5:E:19:MET:N	2.26	0.50
7:G:115:ARG:HB2	7:G:118:VAL:HG23	1.94	0.50
12:L:41:ARG:HG2	12:L:42:THR:N	2.27	0.50
19:S:4:SER:O	19:S:6:LYS:NZ	2.41	0.50
20:T:14:LYS:O	20:T:18:GLN:HG3	2.12	0.50
1:A:244:U:H4'	1:A:245:C:H5"	1.92	0.50
1:A:781:A:C5	1:A:802:A:C2	3.00	0.50
1:A:839:U:O2	1:A:839:U:H2'	2.12	0.50
8:H:104:ARG:HG3	8:H:138:TRP:CD2	2.46	0.50
1:A:41:G:H2'	1:A:42:G:H8	1.76	0.50
1:A:452:A:O2'	1:A:453:A:O4'	2.29	0.50
1:A:513:C:H42	1:A:538:G:H1	1.59	0.50
1:A:1347:G:C8	9:I:107:ARG:HB3	2.47	0.50
7:G:72:ARG:HB3	7:G:72:ARG:HH11	1.75	0.50
2:B:64:ARG:HB2	2:B:64:ARG:HH11	1.76	0.50
1:A:502:G:P	12:L:118:SER:HG	2.35	0.50
1:A:556:C:H2'	1:A:557:G:O4'	2.12	0.50
1:A:858:G:O2'	1:A:859:A:H5'	2.12	0.50
1:A:922:G:C2	1:A:1396:A:C6	3.00	0.50
1:A:1192:C:O2	5:E:25:ARG:NH2	2.41	0.49
6:F:22:GLU:O	6:F:26:ILE:HG13	2.12	0.49
1:A:430:A:P	4:D:8:VAL:H	2.34	0.49
1:A:1189:C:P	10:J:51:ARG:HH22	2.35	0.49
1:A:1347:G:N2	1:A:1373:G:H2'	2.26	0.49
16:P:38:TYR:CE2	16:P:50:LYS:HD2	2.48	0.49
1:A:41:G:H2'	1:A:42:G:C8	2.47	0.49
1:A:103:C:O2'	1:A:172:A:N1	2.36	0.49
1:A:113:G:H1'	1:A:354:G:H5'	1.94	0.49
6:F:80:ARG:NH1	6:F:88:VAL:O	2.46	0.49
1:A:481:G:O2'	1:A:482:A:H8	1.95	0.49
1:A:766:A:C8	1:A:814:A:N6	2.81	0.49
1:A:1094:G:O2'	1:A:1108:G:N2	2.45	0.49
1:A:1228:C:H4'	13:M:116:THR:HA	1.94	0.49
16:P:74:LEU:O	16:P:79:VAL:HG23	2.13	0.49
1:A:22:G:H2'	1:A:23:C:C6	2.47	0.49
1:A:27:G:C5	1:A:557:G:N2	2.81	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:238:G:OP1	17:Q:25:ARG:NH2	2.45	0.49
1:A:371:G:O2'	1:A:372:C:H5'	2.13	0.49
1:A:1505:G:O2'	1:A:1506:U:OP2	2.23	0.49
2:B:172:ILE:HD12	2:B:172:ILE:H	1.77	0.49
1:A:613:C:H42	1:A:627:G:H1	1.59	0.49
1:A:1195:C:H3'	1:A:1196:U:C5'	2.40	0.49
1:A:1320:C:H42	19:S:36:ARG:HG3	1.77	0.49
12:L:46:LYS:HE3	12:L:47:LYS:NZ	2.28	0.49
1:A:401:C:H2'	1:A:402:G:C8	2.47	0.49
1:A:932:C:H5'	7:G:4:ARG:HG2	1.95	0.49
4:D:111:ALA:HB2	4:D:120:LEU:HD12	1.93	0.49
8:H:17:THR:HG22	8:H:63:LEU:HG	1.95	0.49
10:J:16:LEU:HD23	10:J:94:VAL:HG12	1.95	0.49
10:J:32:ALA:O	10:J:34:VAL:HG23	2.13	0.49
15:O:39:LEU:HB3	15:O:56:LEU:HD12	1.95	0.49
19:S:62:ILE:HA	19:S:66:MET:SD	2.52	0.49
1:A:451:A:N6	1:A:481:G:C4	2.80	0.49
1:A:988:G:H4'	1:A:1014:A:H61	1.78	0.49
1:A:1101:A:H4'	1:A:1102:A:O5'	2.13	0.49
1:A:1175:G:H2'	1:A:1176:A:H8	1.78	0.49
4:D:152:SER:O	4:D:155:LEU:HB2	2.12	0.49
11:K:34:ASP:OD1	11:K:38:ASN:N	2.45	0.49
17:Q:29:HIS:CG	17:Q:30:PRO:HD2	2.47	0.49
1:A:380:G:C2	1:A:384:G:C6	3.00	0.49
1:A:1067:A:O2'	1:A:1093:A:O3'	2.19	0.49
2:B:12:GLU:HG3	2:B:213:LEU:HD21	1.95	0.48
2:B:15:VAL:HG13	2:B:209:ARG:HG2	1.95	0.48
20:T:49:ALA:HB3	20:T:99:LEU:HG	1.95	0.48
1:A:401:C:H2'	1:A:402:G:H8	1.78	0.48
1:A:1152:A:H5'	10:J:13:HIS:HB2	1.94	0.48
1:A:1328:C:OP1	21:U:21:TYR:OH	2.21	0.48
1:A:1422:G:H2'	1:A:1423:G:C8	2.48	0.48
1:A:44:G:N2	1:A:399:G:C4	2.81	0.48
1:A:167:G:H2'	1:A:168:G:H8	1.77	0.48
1:A:780:A:OP1	11:K:123:LYS:HB2	2.14	0.48
1:A:792:A:H4'	1:A:793:U:O5'	2.13	0.48
1:A:1137:C:H4'	1:A:1138:G:C2	2.48	0.48
1:A:1474:G:H2'	1:A:1475:G:C8	2.47	0.48
4:D:57:ARG:HG3	4:D:202:LEU:HD12	1.95	0.48
15:O:70:LEU:HD21	15:O:77:ARG:HB2	1.95	0.48
2:B:82:ARG:HG3	2:B:92:TYR:CZ	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:52:LEU:HA	3:C:70:VAL:HA	1.96	0.48
8:H:2:LEU:HD23	8:H:3:THR:N	2.28	0.48
12:L:46:LYS:HB3	12:L:92:0TD:H5	1.95	0.48
1:A:77:G:H2'	1:A:78:G:H8	1.78	0.48
1:A:382:A:H2'	1:A:383:A:H8	1.78	0.48
1:A:665:A:C2	1:A:732:C:C2	3.01	0.48
1:A:673:G:O3'	6:F:87:ARG:NH2	2.45	0.48
1:A:1149:C:O2'	1:A:1280:A:N1	2.40	0.48
2:B:102:LEU:HD11	2:B:162:ILE:HD11	1.94	0.48
3:C:84:ILE:O	3:C:88:ARG:HD3	2.13	0.48
9:I:79:LEU:O	9:I:83:ARG:HG2	2.14	0.48
1:A:262:A:C6	1:A:263:A:C6	3.01	0.48
1:A:1152:A:OP1	10:J:68:HIS:ND1	2.46	0.48
4:D:8:VAL:O	4:D:11:LEU:N	2.28	0.48
8:H:31:PHE:O	8:H:35:ILE:HG12	2.14	0.48
10:J:40:LEU:HB2	10:J:69:ASN:HB2	1.96	0.48
1:A:858:G:O6	1:A:869:G:C8	2.67	0.48
2:B:208:ILE:HA	2:B:211:ILE:HD12	1.96	0.48
3:C:130:VAL:HG21	3:C:157:ILE:HG23	1.96	0.48
7:G:40:ALA:HB3	9:I:41:VAL:HG21	1.95	0.48
1:A:62:U:OP1	1:A:385:C:O2'	2.30	0.48
1:A:359:U:H2'	1:A:360:A:C8	2.49	0.48
1:A:1106:G:H5"	3:C:172:ARG:HB3	1.96	0.48
1:A:99:C:H2'	1:A:101:A:C8	2.49	0.48
1:A:1037:C:N3	1:A:1038:C:N4	2.62	0.48
3:C:136:GLN:O	3:C:140:ARG:HG2	2.13	0.48
9:I:10:ARG:HG2	9:I:75:ASP:HB2	1.96	0.48
16:P:6:LEU:HD23	16:P:17:TYR:CG	2.48	0.48
1:A:602:A:C2	1:A:637:G:C2	3.01	0.48
1:A:803:G:C6	1:A:804:U:C4	3.02	0.48
1:A:975:A:H5'	1:A:975:A:H8	1.79	0.48
1:A:1415:G:H2'	1:A:1416:G:C8	2.45	0.48
2:B:116:GLU:HG2	2:B:153:ARG:HH11	1.79	0.48
8:H:104:ARG:HG3	8:H:138:TRP:CE3	2.48	0.48
9:I:28:VAL:HA	9:I:63:ILE:O	2.14	0.48
10:J:45:ARG:NH1	10:J:45:ARG:HB3	2.29	0.48
1:A:149:A:H2'	1:A:150:C:C6	2.49	0.47
1:A:1244:C:H42	1:A:1293:G:H1	1.62	0.47
3:C:108:ASN:HB3	3:C:111:LEU:HB2	1.96	0.47
4:D:25:ARG:CZ	4:D:30:LYS:HB3	2.44	0.47
8:H:31:PHE:CE1	8:H:35:ILE:HD11	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:121:ASP:HB2	8:H:125:ARG:HH22	1.78	0.47
1:A:1316:G:N1	1:A:1319:A:OP2	2.47	0.47
19:S:15:LEU:HD21	19:S:38:SER:OG	2.13	0.47
1:A:21:G:C2	1:A:22:G:C6	3.02	0.47
1:A:374:A:C6	1:A:375:U:C4	3.02	0.47
4:D:78:LEU:HB3	4:D:93:PHE:HE2	1.79	0.47
6:F:15:ASP:OD2	6:F:16:GLN:N	2.47	0.47
1:A:35:G:H2'	1:A:36:C:C6	2.50	0.47
1:A:689:C:OP1	11:K:44:SER:OG	2.17	0.47
1:A:974:A:H4'	1:A:975:A:H3'	1.96	0.47
2:B:19:HIS:CD2	2:B:20:GLU:H	2.31	0.47
2:B:88:ALA:HB2	2:B:219:VAL:HG13	1.95	0.47
17:Q:83:ASP:OD1	17:Q:83:ASP:N	2.45	0.47
1:A:949:A:C2	1:A:1233:G:N3	2.83	0.47
1:A:1328:C:H2'	1:A:1329:A:C8	2.50	0.47
1:A:1513:A:H2'	1:A:1514:C:C6	2.50	0.47
16:P:2:VAL:O	16:P:64:ALA:HA	2.14	0.47
1:A:481:G:HO2'	1:A:482:A:H8	1.59	0.47
1:A:690:G:O6	1:A:691:G:N1	2.48	0.47
1:A:1109:C:P	3:C:176:HIS:HD1	2.37	0.47
1:A:1125:U:H3	10:J:5:ARG:HH21	1.62	0.47
1:A:1201:A:H4'	1:A:1202:G:O5'	2.15	0.47
1:A:1328:C:H2'	1:A:1329:A:H8	1.78	0.47
5:E:102:ALA:O	5:E:107:ARG:NH1	2.48	0.47
9:I:50:LEU:HD23	9:I:85:LEU:HD21	1.96	0.47
10:J:48:THR:OG1	10:J:62:HIS:HB3	2.14	0.47
13:M:4:ILE:HG23	13:M:57:ARG:HA	1.96	0.47
1:A:9:G:C2	1:A:26:A:N1	2.83	0.47
1:A:16:A:C2	1:A:920:U:O2	2.67	0.47
1:A:31:G:N2	1:A:48:C:OP1	2.46	0.47
1:A:116:A:H2'	1:A:117:G:H8	1.80	0.47
1:A:143:A:O3'	1:A:144:G:H8	1.96	0.47
1:A:382:A:H2'	1:A:383:A:C8	2.49	0.47
1:A:1414:U:H2'	1:A:1415:G:C8	2.48	0.47
2:B:27:LYS:O	2:B:194:PRO:HG2	2.14	0.47
5:E:82:VAL:HG21	5:E:138:ALA:HA	1.96	0.47
8:H:41:ARG:NH1	8:H:123:GLU:OE2	2.47	0.47
9:I:106:ALA:O	9:I:108:VAL:HG23	2.15	0.47
13:M:4:ILE:HD13	13:M:56:LEU:HB3	1.96	0.47
14:N:18:VAL:HG23	14:N:19:ARG:HD2	1.96	0.47
15:O:2:PRO:O	15:O:38:ARG:NH1	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:Q:74:LEU:HG	17:Q:75:ARG:HG3	1.96	0.47
5:E:122:GLU:O	5:E:123:LEU:HD23	2.15	0.47
8:H:103:VAL:HG21	8:H:109:ILE:O	2.15	0.47
11:K:98:LEU:HA	11:K:101:SER:HB2	1.97	0.47
1:A:707:C:H2'	1:A:708:C:H6	1.80	0.47
1:A:925:G:C6	1:A:927:G:N7	2.83	0.47
1:A:1258:G:H2'	1:A:1259:C:C6	2.49	0.47
2:B:17:PHE:CD1	2:B:18:GLY:N	2.82	0.47
2:B:19:HIS:CG	2:B:20:GLU:HG2	2.50	0.47
6:F:2:ARG:CZ	6:F:69:GLU:HG2	2.44	0.47
16:P:19:ILE:HG22	16:P:36:ILE:HD11	1.97	0.47
20:T:92:LEU:HD23	20:T:92:LEU:HA	1.82	0.47
1:A:130:A:OP2	1:A:190(E):U:O2'	2.22	0.47
1:A:258:G:H2'	1:A:259:G:H8	1.80	0.47
5:E:144:THR:O	5:E:148:VAL:HG23	2.15	0.47
12:L:89:ARG:HG2	12:L:97:ARG:HA	1.95	0.47
1:A:309:G:C2	1:A:310:G:N7	2.83	0.46
1:A:502:G:H2'	1:A:503:C:O4'	2.15	0.46
1:A:686:U:O2'	1:A:687:A:H8	1.99	0.46
2:B:84:GLU:HB3	2:B:219:VAL:HG21	1.97	0.46
8:H:124:ALA:O	8:H:128:GLY:N	2.48	0.46
14:N:53:LEU:HD12	14:N:56:VAL:HG21	1.98	0.46
1:A:193:C:H2'	1:A:194:C:C6	2.49	0.46
1:A:898:G:C2	1:A:902:G:C6	3.03	0.46
1:A:1345:U:C2	1:A:1377:A:C2	3.03	0.46
1:A:1392:G:N2	1:A:1502:A:H8	2.14	0.46
4:D:81:GLU:OE2	4:D:139:ARG:NH2	2.48	0.46
7:G:18:TYR:HD2	7:G:59:LEU:HD13	1.79	0.46
13:M:62:ASN:OD1	13:M:62:ASN:N	2.48	0.46
1:A:1187:G:C2	1:A:1188:A:C4	3.03	0.46
3:C:88:ARG:NH2	3:C:100:ALA:HB1	2.23	0.46
1:A:344:A:H5'	1:A:345:C:C5	2.50	0.46
1:A:575:G:C8	1:A:881:G:N2	2.84	0.46
1:A:923:A:O2'	1:A:1399:C:OP2	2.25	0.46
14:N:4:LYS:HA	14:N:7:ILE:HG13	1.97	0.46
1:A:243:A:C2	1:A:246:A:C8	3.03	0.46
1:A:452:A:O2'	1:A:453:A:O5'	2.32	0.46
1:A:620:C:H2'	1:A:621:A:O4'	2.16	0.46
1:A:687:A:H4'	1:A:688:G:O5'	2.15	0.46
1:A:1305:G:H22	1:A:1331:G:H1'	1.79	0.46
2:B:20:GLU:OE1	2:B:23:ARG:NH1	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:34:LEU:O	3:C:38:ARG:HG2	2.16	0.46
9:I:75:ASP:O	9:I:78:LYS:HB3	2.16	0.46
1:A:736:C:H2'	1:A:737:A:C8	2.50	0.46
1:A:793:U:H4'	1:A:794:A:OP2	2.15	0.46
1:A:1048:G:H1	1:A:1209:C:H42	1.64	0.46
1:A:1211:U:H5'	1:A:1212:U:OP1	2.15	0.46
1:A:1262:C:N4	1:A:1273:G:H1	2.13	0.46
8:H:63:LEU:H	8:H:63:LEU:HD22	1.81	0.46
18:R:22:VAL:HG12	18:R:26:LEU:HD22	1.98	0.46
1:A:229:U:C2	1:A:230:G:C8	3.03	0.46
4:D:187:ARG:HD2	4:D:187:ARG:HA	1.64	0.46
1:A:110:C:C4	1:A:111:G:C5	3.04	0.46
2:B:24:TRP:HB2	2:B:190:THR:HG22	1.97	0.46
4:D:62:GLN:O	4:D:66:ARG:HB2	2.15	0.46
5:E:78:HIS:ND1	8:H:104:ARG:HD2	2.31	0.46
9:I:8:GLY:HA3	9:I:79:LEU:HB3	1.97	0.46
1:A:285:G:C2	1:A:286:G:C8	3.03	0.46
1:A:479:C:H2'	1:A:480:U:O4'	2.16	0.46
3:C:46:GLU:HG3	3:C:87:LEU:HD22	1.97	0.46
4:D:25:ARG:HA	4:D:28:SER:OG	2.16	0.46
6:F:22:GLU:OE2	6:F:82:ARG:HD3	2.15	0.46
7:G:26:PHE:HD1	7:G:101:LEU:HD22	1.81	0.46
8:H:105:ARG:HA	8:H:105:ARG:HD3	1.79	0.46
12:L:110:VAL:O	12:L:122:THR:HG21	2.16	0.46
1:A:56:U:H2'	1:A:57:G:C8	2.51	0.46
1:A:1241:G:H2'	1:A:1242:C:C6	2.51	0.46
1:A:1323:G:H2'	1:A:1324:A:C8	2.51	0.46
2:B:191:ASP:OD1	2:B:191:ASP:N	2.48	0.46
7:G:86:GLN:HB2	7:G:148:ASN:ND2	2.30	0.46
1:A:517:G:N1	1:A:533:A:OP2	2.47	0.45
1:A:836:G:C6	1:A:851:G:C6	3.04	0.45
4:D:9:CYS:O	4:D:12:CYS:HB2	2.17	0.45
5:E:151:LEU:HD13	8:H:79:VAL:HG22	1.99	0.45
6:F:42:GLU:HG3	6:F:61:LEU:HD23	1.98	0.45
11:K:62:GLN:HG3	11:K:97:ALA:HB2	1.97	0.45
11:K:72:ALA:HB1	11:K:77:MET:HG3	1.98	0.45
1:A:315:A:O2'	1:A:330:C:O2'	2.34	0.45
1:A:1507:A:C8	1:A:1530:G:N2	2.84	0.45
2:B:222:ILE:O	2:B:226:ARG:HG3	2.16	0.45
4:D:150:GLU:HB3	4:D:153:ARG:NH2	2.31	0.45
7:G:18:TYR:CD2	7:G:59:LEU:HD13	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:83:ILE:HG12	8:H:137:VAL:HG22	1.97	0.45
9:I:66:ARG:HE	9:I:66:ARG:HB2	1.32	0.45
17:Q:12:SER:HB3	17:Q:20:THR:CB	2.45	0.45
1:A:148:G:H2'	1:A:149:A:H8	1.80	0.45
1:A:1189:C:H4'	3:C:10:PHE:HE1	1.81	0.45
1:A:1386:G:H2'	1:A:1387:G:H8	1.80	0.45
1:A:1136:U:H5"	1:A:1137:C:OP2	2.17	0.45
1:A:1488:G:H2'	1:A:1489:G:C8	2.52	0.45
1:A:1521:G:H2'	1:A:1522:U:C6	2.51	0.45
2:B:23:ARG:O	2:B:24:TRP:HD1	2.00	0.45
2:B:127:ILE:H	2:B:127:ILE:HG13	1.53	0.45
7:G:84:ASN:OD1	7:G:84:ASN:N	2.50	0.45
8:H:1:MET:HG2	8:H:2:LEU:N	2.32	0.45
11:K:36:ASP:OD2	11:K:38:ASN:ND2	2.49	0.45
20:T:29:LYS:O	20:T:33:ILE:HG13	2.17	0.45
1:A:79:G:N1	1:A:80:G:C5	2.85	0.45
3:C:174:PRO:O	3:C:177:THR:HG22	2.17	0.45
4:D:70:ILE:HG22	4:D:71:SER:O	2.16	0.45
7:G:27:ILE:HD12	7:G:40:ALA:HA	1.98	0.45
9:I:79:LEU:HD23	9:I:79:LEU:HA	1.84	0.45
1:A:438:G:H4'	4:D:123:HIS:CD2	2.52	0.45
1:A:647:C:H2'	1:A:648:A:H8	1.81	0.45
1:A:664:G:OP1	18:R:64:ARG:HD2	2.17	0.45
1:A:866:C:H2'	1:A:867:G:O4'	2.16	0.45
1:A:967:5MC:O2'	9:I:128:ARG:NH2	2.50	0.45
1:A:1060:C:OP1	14:N:45:ARG:NH2	2.50	0.45
2:B:63:MET:HB3	2:B:225:ALA:HB1	1.97	0.45
18:R:39:VAL:HG13	18:R:40:LEU:HD23	1.98	0.45
19:S:37:ARG:HD2	19:S:37:ARG:N	2.32	0.45
20:T:43:LEU:HG	20:T:55:ILE:HD11	1.98	0.45
1:A:362:G:N2	1:A:365:U:OP2	2.48	0.45
1:A:1392:G:H2'	1:A:1393:U:H6	1.81	0.45
4:D:64:LEU:HD23	4:D:198:VAL:HG21	1.98	0.45
16:P:60:LEU:HD23	16:P:60:LEU:HA	1.70	0.45
1:A:16:A:O2'	1:A:17:U:H5'	2.17	0.45
1:A:411:A:N3	1:A:413:G:O2'	2.39	0.45
1:A:1189:C:H4'	3:C:10:PHE:CE1	2.52	0.45
1:A:1342:C:H2'	1:A:1343:G:C8	2.51	0.45
1:A:1343:G:C5	1:A:1344:C:C4	3.05	0.45
2:B:215:LEU:HD23	2:B:215:LEU:HA	1.63	0.45
4:D:205:GLU:OE1	5:E:100:VAL:HG23	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:82:HIS:ND1	8:H:138:TRP:NE1	2.64	0.45
19:S:78:ARG:H	19:S:78:ARG:HG2	1.48	0.45
1:A:77:G:C6	1:A:93:G:N1	2.85	0.45
1:A:204:U:H4'	1:A:216:G:OP1	2.16	0.45
1:A:270:A:H2'	1:A:271:C:C6	2.51	0.45
1:A:316:G:OP2	1:A:351:G:O2'	2.35	0.45
1:A:376:G:C4	1:A:389:A:C2	3.05	0.45
1:A:936:C:N4	1:A:937:A:C6	2.85	0.45
1:A:1437:C:H2'	1:A:1438:G:H8	1.82	0.45
4:D:52:SER:O	4:D:55:ALA:HB3	2.17	0.45
9:I:112:LYS:HE3	9:I:117:HIS:O	2.16	0.45
1:A:153:C:H42	1:A:168:G:H1	1.64	0.45
1:A:293:G:C6	1:A:305:G:C2	3.06	0.45
1:A:355:C:H5'	1:A:389:A:OP2	2.17	0.45
1:A:707:C:H2'	1:A:708:C:C6	2.52	0.45
2:B:146:GLN:O	2:B:150:SER:HB3	2.16	0.45
7:G:26:PHE:CE2	7:G:30:ILE:HD11	2.52	0.45
8:H:25:ASP:N	8:H:25:ASP:OD1	2.50	0.45
13:M:3:ARG:NH2	13:M:7:VAL:HA	2.32	0.45
1:A:644:G:C5	1:A:645:C:C5	3.05	0.44
1:A:830:G:C6	1:A:831:U:C4	3.04	0.44
1:A:1089:G:C6	1:A:1090:U:C4	3.05	0.44
7:G:139:GLU:HB3	7:G:143:ARG:NH1	2.33	0.44
16:P:36:ILE:H	16:P:36:ILE:HG13	1.65	0.44
1:A:1343:G:C6	1:A:1344:C:C4	3.05	0.44
1:A:1358:U:H5"	14:N:35:ARG:HG3	2.00	0.44
3:C:54:ARG:HB3	3:C:69:HIS:HD2	1.81	0.44
2:B:54:THR:O	2:B:58:ILE:HG13	2.17	0.44
7:G:75:VAL:HG11	7:G:86:GLN:HB3	1.99	0.44
9:I:49:PRO:HG3	9:I:101:PHE:HD2	1.82	0.44
11:K:95:ILE:H	11:K:95:ILE:HG13	1.39	0.44
1:A:64:G:C2	1:A:67:C:N4	2.85	0.44
1:A:279:A:H5'	1:A:279:A:H8	1.83	0.44
1:A:1269:A:N1	1:A:1312:G:O2'	2.44	0.44
11:K:33:THR:HG22	11:K:39:PRO:HA	1.99	0.44
1:A:153:C:N4	1:A:168:G:H1	2.16	0.44
1:A:172:A:C8	1:A:174:C:C5	3.06	0.44
1:A:456:C:H2'	1:A:457:C:C6	2.52	0.44
2:B:196:LEU:HD23	2:B:196:LEU:HA	1.78	0.44
3:C:180:ALA:HB1	3:C:203:PHE:CD1	2.52	0.44
1:A:419:C:H42	1:A:424:G:H1	1.65	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1009:G:N2	1:A:1020:U:O2	2.32	0.44
1:A:1069:C:O2'	1:A:1192:C:H1'	2.18	0.44
1:A:1124:G:H5'	10:J:35:SER:O	2.17	0.44
1:A:1294:G:H2'	1:A:1295:G:H8	1.82	0.44
4:D:150:GLU:H	4:D:150:GLU:HG3	1.56	0.44
1:A:283:C:C2	1:A:284:G:C8	3.06	0.44
1:A:392:G:H2'	1:A:393:A:H8	1.83	0.44
1:A:828:A:H2'	1:A:829:G:O4'	2.18	0.44
1:A:1198:G:H2'	1:A:1199:U:C6	2.53	0.44
2:B:114:ARG:HH11	2:B:118:LEU:HD11	1.82	0.44
13:M:15:VAL:HG23	13:M:43:THR:O	2.18	0.44
21:U:6:ARG:CZ	21:U:15:ARG:HH12	2.31	0.44
21:U:6:ARG:NH1	21:U:15:ARG:HH22	2.16	0.44
1:A:5:U:H4'	1:A:6:G:O5'	2.18	0.44
9:I:43:ALA:HA	9:I:74:ILE:HD13	1.99	0.44
17:Q:13:ASP:HB2	17:Q:53:LEU:HD12	2.00	0.44
1:A:636:U:H2'	1:A:637:G:C8	2.53	0.44
1:A:1218:C:H2'	1:A:1219:U:C6	2.53	0.44
1:A:1314:C:H41	19:S:6:LYS:HE2	1.83	0.44
2:B:179:LYS:HB2	2:B:179:LYS:HE3	1.85	0.44
9:I:99:LEU:HB3	9:I:101:PHE:CD1	2.52	0.44
10:J:25:GLU:O	10:J:29:ARG:HG2	2.18	0.44
12:L:46:LYS:HG2	12:L:47:LYS:HD3	2.00	0.44
1:A:278:G:C6	17:Q:95:TYR:HD2	2.35	0.43
1:A:537:G:H2'	1:A:538:G:H8	1.83	0.43
1:A:971:G:H1'	1:A:1365:G:O2'	2.18	0.43
1:A:1175:G:H2'	1:A:1176:A:C8	2.53	0.43
1:A:1347:G:HO2'	1:A:1348:U:P	2.41	0.43
2:B:103:THR:HA	2:B:180:LEU:HD11	1.99	0.43
14:N:50:LYS:HB3	14:N:52:GLN:HG3	1.99	0.43
1:A:895:G:H2'	1:A:896:C:C6	2.53	0.43
1:A:912:C:H5"	12:L:46:LYS:HE2	1.99	0.43
1:A:1006:C:N4	1:A:1024:G:H1'	2.33	0.43
6:F:43:LEU:HD22	6:F:43:LEU:HA	1.82	0.43
1:A:575:G:C6	1:A:821:G:N7	2.87	0.43
1:A:895:G:H2'	1:A:896:C:H6	1.84	0.43
7:G:15:ASP:OD1	7:G:44:TYR:OH	2.37	0.43
10:J:14:LYS:HA	10:J:17:ASP:HB2	2.00	0.43
13:M:37:THR:HG23	13:M:55:ARG:HB3	2.00	0.43
13:M:77:ASN:O	13:M:80:ARG:HB3	2.18	0.43
17:Q:5:VAL:O	17:Q:6:LEU:HD23	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:R:44:LEU:HD21	18:R:70:ILE:HD13	2.00	0.43
1:A:78:G:N2	1:A:79:G:H1'	2.33	0.43
1:A:381:C:H2'	1:A:382:A:O4'	2.19	0.43
1:A:501:C:O3'	12:L:118:SER:OG	2.36	0.43
1:A:547:A:OP2	4:D:2:GLY:N	2.51	0.43
1:A:716:A:C6	1:A:717:C:C4	3.06	0.43
1:A:809:G:C6	1:A:810:C:C5	3.06	0.43
1:A:1349:A:C2	1:A:1374:A:C4	3.07	0.43
4:D:64:LEU:HD12	4:D:75:PHE:HZ	1.82	0.43
4:D:194:LEU:HD13	4:D:194:LEU:HA	1.75	0.43
8:H:45:ILE:HD12	8:H:61:VAL:HG13	2.01	0.43
10:J:54:PHE:CD2	10:J:55:LYS:HG2	2.54	0.43
1:A:428:G:C5	1:A:430:A:C6	3.06	0.43
1:A:1355:G:H2'	1:A:1356:G:C8	2.53	0.43
3:C:11:ARG:O	3:C:16:ARG:HB3	2.19	0.43
10:J:45:ARG:HB3	10:J:45:ARG:CZ	2.48	0.43
14:N:40:CYS:H	14:N:43:CYS:HB2	1.83	0.43
1:A:560:U:H4'	1:A:561:U:H5"	1.99	0.43
1:A:913:A:H4'	1:A:914:A:O5'	2.18	0.43
1:A:942:G:N2	1:A:943:U:C2	2.86	0.43
3:C:11:ARG:HG2	3:C:178:LEU:HD21	2.00	0.43
3:C:140:ARG:HG2	3:C:140:ARG:H	1.70	0.43
20:T:29:LYS:O	20:T:32:ALA:HB3	2.18	0.43
1:A:390:C:H2'	1:A:391:G:C8	2.53	0.43
1:A:614:A:H2'	1:A:615:C:C6	2.54	0.43
1:A:778:G:H2'	1:A:779:C:O4'	2.18	0.43
2:B:221:LEU:HD23	2:B:221:LEU:HA	1.86	0.43
3:C:61:ALA:C	3:C:63:ASN:H	2.22	0.43
8:H:75:ARG:HA	8:H:76:PRO:HD3	1.72	0.43
1:A:711:G:OP2	6:F:54:LYS:NZ	2.51	0.43
1:A:1025:U:O2	1:A:1026:G:N2	2.51	0.43
1:A:1104:G:O3'	2:B:111:ARG:NH2	2.51	0.43
1:A:1225:A:H2'	1:A:1225:A:N3	2.32	0.43
1:A:1243:C:H42	1:A:1294:G:H1	1.67	0.43
1:A:1314:C:H41	19:S:6:LYS:NZ	2.17	0.43
2:B:204:ASN:H	2:B:204:ASN:HD22	1.66	0.43
5:E:31:LEU:HD23	5:E:31:LEU:HA	1.76	0.43
9:I:96:LEU:HB3	9:I:102:LEU:HG	2.00	0.43
10:J:39:PRO:HA	10:J:70:ARG:HD3	2.00	0.43
11:K:33:THR:HB	11:K:38:ASN:C	2.39	0.43
12:L:27:LEU:C	12:L:29:GLY:N	2.69	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:59:ARG:CZ	12:L:65:GLU:HG2	2.49	0.43
20:T:73:HIS:HB3	20:T:74:LYS:H	1.59	0.43
1:A:854:G:C2	1:A:855:G:C8	3.07	0.43
17:Q:59:ILE:HG22	17:Q:71:PHE:CD1	2.54	0.43
19:S:22:LEU:HD22	19:S:27:GLU:HA	2.01	0.43
1:A:457:C:H2'	1:A:458:C:C6	2.54	0.43
1:A:674:G:H2'	1:A:675:A:C8	2.53	0.43
1:A:1212:U:O2'	1:A:1213:A:H8	2.02	0.43
1:A:1326:C:H2'	1:A:1327:C:C6	2.53	0.43
2:B:204:ASN:HD22	2:B:204:ASN:N	2.17	0.43
3:C:110:ASN:O	3:C:141:VAL:HG22	2.19	0.43
3:C:120:VAL:O	3:C:124:ILE:HG13	2.19	0.43
4:D:57:ARG:HB3	4:D:206:PHE:HB2	2.00	0.43
7:G:17:VAL:HG12	7:G:18:TYR:HD1	1.84	0.43
10:J:13:HIS:CD2	10:J:14:LYS:HG3	2.54	0.43
14:N:53:LEU:HA	14:N:54:PRO:HD2	1.81	0.43
18:R:22:VAL:HG23	18:R:55:ARG:O	2.18	0.43
18:R:26:LEU:HA	18:R:26:LEU:HD12	1.77	0.43
19:S:58:VAL:HA	19:S:59:PRO:HD3	1.86	0.43
1:A:376:G:H5"	16:P:5:ARG:HD2	2.01	0.42
1:A:559:A:H4'	1:A:560:U:O5'	2.18	0.42
1:A:885:G:C2	1:A:913:A:N1	2.87	0.42
1:A:1241:G:C2	1:A:1242:C:C4	3.07	0.42
1:A:1252:A:H61	1:A:1285:A:N6	2.15	0.42
2:B:73:THR:HG23	2:B:95:GLN:O	2.19	0.42
3:C:112:SER:HB3	3:C:115:LEU:HD12	2.00	0.42
1:A:231:G:H2'	1:A:232:G:H8	1.85	0.42
1:A:1126:U:O2'	1:A:1127:G:OP1	2.33	0.42
1:A:1332:A:C2	1:A:1333:A:C4	3.07	0.42
1:A:1401:G:O6	1:A:1504:G:N2	2.52	0.42
10:J:42:THR:HG23	10:J:67:THR:O	2.18	0.42
10:J:79:ARG:O	10:J:82:ILE:N	2.52	0.42
18:R:59:SER:N	18:R:62:GLU:OE1	2.52	0.42
1:A:275:G:H5'	17:Q:14:LYS:HD3	2.01	0.42
1:A:327:A:O2'	1:A:328:C:O4'	2.33	0.42
1:A:376:G:N3	1:A:389:A:C2	2.88	0.42
1:A:875:C:O2'	8:H:14:ARG:NH1	2.48	0.42
1:A:992:U:O2'	1:A:993:G:OP2	2.31	0.42
1:A:1128:C:O2'	1:A:1130:A:N7	2.45	0.42
1:A:1171:G:H2'	1:A:1172:C:C6	2.54	0.42
1:A:1274:G:H2'	1:A:1275:A:H8	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1497:G:H2'	1:A:1498:UR3:H5'	2.01	0.42
1:A:1499:A:H2'	1:A:1500:A:H8	1.85	0.42
1:A:1511:G:H2'	1:A:1512:U:O4'	2.19	0.42
3:C:62:ASP:HA	3:C:97:LYS:NZ	2.33	0.42
3:C:188:LEU:HD22	3:C:188:LEU:HA	1.86	0.42
5:E:35:GLY:HA3	5:E:112:LEU:HB3	2.00	0.42
12:L:82:VAL:HG23	12:L:105:TYR:HB3	2.00	0.42
13:M:108:ARG:NH2	13:M:111:LYS:HD2	2.34	0.42
16:P:74:LEU:HD22	16:P:79:VAL:HG21	2.01	0.42
20:T:10:LEU:HA	20:T:10:LEU:HD22	1.81	0.42
20:T:59:ALA:O	20:T:63:ILE:HG13	2.19	0.42
1:A:537:G:H2'	1:A:538:G:C8	2.54	0.42
1:A:916:G:H2'	1:A:917:G:H8	1.83	0.42
1:A:1225:A:H5'	1:A:1226:C:OP2	2.19	0.42
5:E:129:ILE:HD12	5:E:129:ILE:H	1.84	0.42
7:G:99:LEU:HD23	7:G:99:LEU:HA	1.89	0.42
8:H:6:ILE:HB	8:H:85:ARG:NH1	2.34	0.42
1:A:673:G:H5"	6:F:87:ARG:NH1	2.34	0.42
1:A:1064:G:N2	1:A:1190:G:H2'	2.34	0.42
1:A:1347:G:N2	1:A:1374:A:OP2	2.38	0.42
1:A:1399:C:O2	1:A:1401:G:C5	2.72	0.42
2:B:144:ARG:O	2:B:147:LYS:HB3	2.19	0.42
3:C:72:LYS:HE2	3:C:72:LYS:HB2	1.83	0.42
4:D:84:LYS:HE2	4:D:84:LYS:HB3	1.83	0.42
5:E:81:GLU:HG2	5:E:90:VAL:HG22	2.01	0.42
16:P:22:THR:OG1	16:P:23:ASP:N	2.52	0.42
1:A:377:G:OP1	16:P:3:LYS:NZ	2.49	0.42
1:A:865:A:H2'	1:A:866:C:C6	2.54	0.42
1:A:992:U:H3	1:A:1044:A:N6	2.13	0.42
1:A:1359:C:O2'	1:A:1361:G:N7	2.52	0.42
1:A:1374:A:H2'	1:A:1375:A:H8	1.84	0.42
9:I:9:ARG:HG2	9:I:14:VAL:HG22	2.01	0.42
10:J:6:ILE:HD13	10:J:72:VAL:HB	2.02	0.42
13:M:117:VAL:HG12	13:M:118:ALA:H	1.85	0.42
20:T:71:THR:O	20:T:72:LEU:HD23	2.19	0.42
1:A:114:U:H2'	1:A:115:G:C8	2.55	0.42
1:A:309:G:H2'	1:A:310:G:H8	1.84	0.42
1:A:1036:G:H2'	1:A:1037:C:O4'	2.19	0.42
2:B:95:GLN:O	2:B:96:ARG:HD2	2.20	0.42
2:B:107:THR:O	2:B:110:GLN:HB2	2.19	0.42
2:B:181:PHE:CD2	8:H:70:GLN:HB3	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:18:TRP:CD1	14:N:54:PRO:HA	2.54	0.42
3:C:135:LYS:HB3	3:C:135:LYS:HE2	1.91	0.42
12:L:127:GLU:H	12:L:127:GLU:HG2	1.65	0.42
17:Q:63:ARG:HG2	17:Q:64:PRO:HD2	2.02	0.42
19:S:16:LEU:O	19:S:20:LEU:HG	2.20	0.42
1:A:79:G:C2	1:A:80:G:C8	3.08	0.42
1:A:1091:U:O2	1:A:1093:A:C8	2.73	0.42
1:A:1346:A:C4	1:A:1348:U:C4	3.08	0.42
1:A:1531:A:O5'	1:A:1531:A:H8	2.03	0.42
2:B:55:PHE:CD2	2:B:58:ILE:HD12	2.55	0.42
3:C:11:ARG:HA	3:C:178:LEU:HD11	2.01	0.42
15:O:85:LEU:HD23	15:O:85:LEU:HA	1.85	0.42
1:A:1131:G:H2'	1:A:1132:C:C6	2.54	0.42
5:E:131:ILE:HD13	5:E:131:ILE:HA	1.67	0.42
18:R:79:LEU:HA	18:R:80:PRO:HD3	1.86	0.42
1:A:109:A:C6	1:A:327:A:C6	3.08	0.42
1:A:757:U:O2'	1:A:879:C:H1'	2.20	0.42
1:A:838:G:H1	1:A:848:C:N4	2.18	0.42
1:A:937:A:C2	1:A:1379:G:C6	3.08	0.42
1:A:1329:A:P	13:M:28:ALA:HB3	2.60	0.42
1:A:1347:G:H1'	1:A:1348:U:C5	2.55	0.42
1:A:1515[B]:C:N4	1:A:1520[B]:G:H1	2.14	0.42
2:B:61:LEU:HD13	2:B:66:GLY:HA3	2.01	0.42
2:B:100:GLY:O	2:B:104:ASN:N	2.53	0.42
3:C:120:VAL:HG23	3:C:198:VAL:HG11	2.02	0.42
5:E:119:LEU:HA	5:E:119:LEU:HD23	1.77	0.42
7:G:32:ARG:C	7:G:34:GLY:H	2.24	0.42
7:G:145:ALA:C	7:G:147:ALA:H	2.23	0.42
17:Q:48:GLU:C	17:Q:50:LYS:H	2.22	0.42
1:A:551:U:H2'	1:A:552:U:C6	2.55	0.41
1:A:1245:A:C2	1:A:1293:G:C2	3.08	0.41
1:A:1262:C:H2'	1:A:1263:C:C6	2.55	0.41
1:A:1338:G:H2'	1:A:1339:A:C8	2.54	0.41
2:B:188:ALA:O	2:B:202:PRO:HA	2.20	0.41
6:F:25:ILE:HD12	6:F:82:ARG:HD2	2.01	0.41
7:G:108:ALA:O	7:G:111:ARG:HB2	2.20	0.41
7:G:113:GLU:H	7:G:113:GLU:HG2	1.33	0.41
12:L:25:PRO:C	12:L:27:LEU:N	2.70	0.41
1:A:451:A:N6	1:A:481:G:N3	2.67	0.41
1:A:573:A:C6	1:A:574:A:N1	2.87	0.41
1:A:1178:G:N2	1:A:1181:G:OP2	2.52	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1251:A:H2'	1:A:1252:A:C8	2.55	0.41
1:A:1309:G:OP2	13:M:99:ARG:NH1	2.52	0.41
1:A:1314:C:H41	19:S:6:LYS:HZ3	1.68	0.41
3:C:6:HIS:HA	3:C:7:PRO:HD3	1.90	0.41
3:C:29:TYR:HE2	3:C:33:LEU:HD22	1.84	0.41
9:I:8:GLY:HA2	9:I:79:LEU:HD13	2.02	0.41
9:I:32:ASP:OD1	9:I:33:PHE:N	2.48	0.41
16:P:40:ASP:HA	16:P:41:PRO:HD2	1.87	0.41
1:A:75:G:C2	1:A:76:C:C4	3.08	0.41
1:A:583:A:H2'	1:A:584:G:O4'	2.21	0.41
1:A:1425:U:H2'	1:A:1426:C:H6	1.83	0.41
3:C:5:ILE:HD11	3:C:10:PHE:HD1	1.85	0.41
12:L:83:VAL:HG21	12:L:100:ILE:HD13	2.01	0.41
16:P:68:ASP:N	16:P:68:ASP:OD1	2.53	0.41
1:A:748:C:H1'	1:A:749:C:OP2	2.21	0.41
1:A:833:U:H2'	1:A:834:C:C6	2.56	0.41
1:A:1273:G:H2'	1:A:1274:G:O4'	2.19	0.41
3:C:69:HIS:HB3	3:C:106:VAL:HG23	2.03	0.41
8:H:134:ILE:HD13	8:H:134:ILE:HA	1.89	0.41
9:I:79:LEU:O	9:I:82:ALA:HB3	2.21	0.41
15:O:2:PRO:HB2	15:O:3:ILE:H	1.64	0.41
15:O:18:PHE:HB2	15:O:19:PRO:HD2	2.02	0.41
19:S:6:LYS:HE3	19:S:6:LYS:N	2.34	0.41
1:A:130:A:H5'	17:Q:63:ARG:HE	1.84	0.41
1:A:216:G:C2	1:A:217:C:N3	2.88	0.41
1:A:338:A:C6	1:A:339:C:C4	3.09	0.41
1:A:463:A:H2'	1:A:474:G:O4'	2.21	0.41
1:A:604:G:C2	1:A:635:G:C5	3.08	0.41
1:A:1249:C:O2'	9:I:73:GLN:NE2	2.54	0.41
8:H:90:GLY:O	17:Q:34:LYS:HE2	2.21	0.41
13:M:67:GLU:HB3	13:M:68:GLY:H	1.64	0.41
13:M:87:TYR:HA	13:M:90:LEU:HD12	2.02	0.41
17:Q:59:ILE:HD13	17:Q:59:ILE:HA	1.76	0.41
20:T:84:LEU:HD22	20:T:84:LEU:HA	1.79	0.41
21:U:6:ARG:NH1	21:U:15:ARG:HH12	2.17	0.41
1:A:797:C:H2'	1:A:798:G:H8	1.86	0.41
1:A:803:G:C5	1:A:804:U:C5	3.08	0.41
1:A:892:A:C6	1:A:907:A:C8	3.09	0.41
1:A:1072:G:O6	1:A:1102:A:N6	2.53	0.41
1:A:1252:A:H2'	1:A:1253:G:O4'	2.20	0.41
1:A:1314:C:N4	19:S:6:LYS:HZ3	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:22:LYS:HE2	2:B:22:LYS:HB3	1.80	0.41
2:B:47:THR:OG1	2:B:202:PRO:HB2	2.21	0.41
2:B:155:LEU:HD23	2:B:155:LEU:HA	1.87	0.41
5:E:6:PHE:HD2	5:E:6:PHE:HA	1.76	0.41
6:F:95:GLU:HA	6:F:96:PRO:HD3	1.79	0.41
8:H:36:LEU:HD23	8:H:36:LEU:HA	1.88	0.41
10:J:64:GLU:OE2	10:J:66:ARG:NH2	2.54	0.41
1:A:411:A:H62	1:A:413:G:N2	2.19	0.41
1:A:443:C:N4	1:A:491:G:H1	2.19	0.41
1:A:909:A:H2'	1:A:910:C:O4'	2.20	0.41
1:A:993:G:H2'	1:A:995:C:H41	1.85	0.41
1:A:1070:U:O2	1:A:1106:G:C2	2.74	0.41
1:A:1123:A:H4'	10:J:37:PRO:HG2	2.03	0.41
1:A:1309:G:C6	1:A:1329:A:C2	3.08	0.41
1:A:1342:C:H2'	1:A:1343:G:H8	1.85	0.41
1:A:1345:U:O2	1:A:1377:A:C6	2.74	0.41
2:B:103:THR:H	2:B:103:THR:HG1	1.59	0.41
3:C:35:GLU:OE2	3:C:59:ARG:NH1	2.53	0.41
4:D:3:ARG:CZ	4:D:71:SER:H	2.34	0.41
8:H:12:ARG:HH11	8:H:12:ARG:HD3	1.75	0.41
11:K:109:VAL:HG13	18:R:85:LEU:O	2.20	0.41
1:A:853:G:C2	1:A:854:G:C8	3.08	0.41
1:A:1003:G:N2	1:A:1039:C:O2	2.54	0.41
6:F:39:LYS:HE3	6:F:39:LYS:HB2	1.82	0.41
9:I:19:LEU:HD22	9:I:59:PHE:CD2	2.56	0.41
9:I:104:ARG:NH1	9:I:105:ASP:O	2.47	0.41
1:A:27:G:C6	1:A:557:G:C2	3.09	0.41
1:A:35:G:H2'	1:A:36:C:H6	1.86	0.41
1:A:321:A:H2'	1:A:322:C:C6	2.55	0.41
1:A:393:A:C2	1:A:394:G:C8	3.09	0.41
1:A:690:G:N2	1:A:698:G:C6	2.89	0.41
1:A:698:G:C2	1:A:699:C:C2	3.09	0.41
1:A:777:A:C6	1:A:778:G:C5	3.09	0.41
1:A:1068:G:OP2	1:A:1068:G:H8	2.03	0.41
1:A:1274:G:H2'	1:A:1275:A:C8	2.56	0.41
1:A:1314:C:H41	19:S:6:LYS:CE	2.34	0.41
1:A:1347:G:O2'	1:A:1348:U:O5'	2.35	0.41
1:A:1437:C:H2'	1:A:1438:G:C8	2.56	0.41
1:A:1493:A:H2'	1:A:1494:G:H8	1.86	0.41
1:A:1496:C:H2'	1:A:1497:G:O4'	2.20	0.41
3:C:30:ARG:HG2	14:N:36:PHE:O	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:170:VAL:HG13	4:D:174:LEU:HB2	2.02	0.41
4:D:187:ARG:NH2	4:D:188:LEU:HB2	2.36	0.41
6:F:15:ASP:HB3	6:F:18:GLN:HG3	2.03	0.41
12:L:7:ILE:HD13	12:L:7:ILE:HA	1.80	0.41
1:A:235:C:C5'	17:Q:70:ARG:HG2	2.39	0.41
1:A:286:G:N2	1:A:287:U:H1'	2.36	0.41
1:A:327:A:O2'	1:A:328:C:H6	2.04	0.41
1:A:974:A:OP2	14:N:41:ARG:NH1	2.53	0.41
1:A:1345:U:C2	1:A:1377:A:N1	2.89	0.41
1:A:1454:G:N3	1:A:1455:G:C8	2.89	0.41
2:B:19:HIS:CG	2:B:20:GLU:N	2.89	0.41
3:C:30:ARG:H	3:C:30:ARG:HG3	1.63	0.41
3:C:108:ASN:CB	3:C:111:LEU:HB2	2.51	0.41
7:G:91:VAL:CG1	7:G:96:GLN:HG3	2.51	0.41
9:I:18:PHE:CD1	9:I:62:TYR:HD2	2.39	0.41
1:A:372:C:H1'	1:A:373:A:OP2	2.21	0.40
1:A:384:G:H2'	1:A:385:C:C6	2.56	0.40
1:A:421:U:H5"	1:A:422:C:H5	1.85	0.40
1:A:500:G:C6	1:A:546:G:C2	3.09	0.40
1:A:690:G:H2'	1:A:691:G:O4'	2.20	0.40
1:A:829:G:C6	1:A:858:G:N2	2.90	0.40
1:A:1001:A:H2'	1:A:1002:G:H8	1.87	0.40
1:A:1086:U:H3	1:A:1099:G:H22	1.70	0.40
1:A:1399:C:C2	1:A:1401:G:C5	3.09	0.40
1:A:1435:G:H8	1:A:1435:G:O5'	2.04	0.40
1:A:1480:G:C2	1:A:1481:U:C2	3.09	0.40
1:A:1481:U:H2'	1:A:1482:G:O4'	2.21	0.40
2:B:217:ARG:HD3	2:B:217:ARG:HA	1.80	0.40
5:E:87:SER:HB3	5:E:131:ILE:HD13	2.03	0.40
18:R:36:ASN:O	18:R:40:LEU:HG	2.21	0.40
1:A:147:G:C2	1:A:148:G:C8	3.09	0.40
1:A:690:G:C6	1:A:691:G:C2	3.09	0.40
1:A:961:U:H2'	1:A:962:C:O4'	2.22	0.40
1:A:1234:C:H1'	1:A:1364:U:O2	2.21	0.40
1:A:1399:C:C2	1:A:1502:A:N6	2.89	0.40
7:G:50:ILE:O	7:G:54:THR:HG22	2.20	0.40
13:M:34:LEU:HD13	13:M:39:ILE:HB	2.03	0.40
15:O:38:ARG:HD3	15:O:38:ARG:HA	1.89	0.40
1:A:114:U:O2'	1:A:115:G:H5'	2.21	0.40
1:A:131:C:OP2	1:A:190(F):G:O2'	2.40	0.40
1:A:587:G:O2'	1:A:588:G:OP2	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:794:A:C5	1:A:795:C:C4	3.10	0.40
1:A:882:C:O2'	1:A:883:C:H5'	2.21	0.40
1:A:1505:G:C8	1:A:1505:G:H3'	2.56	0.40
11:K:33:THR:HB	11:K:38:ASN:O	2.22	0.40
13:M:27:LYS:HA	13:M:27:LYS:HD2	1.87	0.40
17:Q:59:ILE:HG23	17:Q:71:PHE:HB3	2.04	0.40
20:T:50:GLU:HG3	20:T:100:ILE:HD11	2.02	0.40
1:A:579:G:C6	1:A:580:U:C4	3.09	0.40
12:L:86:ARG:HB2	12:L:101:VAL:HG13	2.03	0.40
14:N:12:ARG:HB3	14:N:13:THR:H	1.53	0.40
20:T:55:ILE:HG13	20:T:55:ILE:H	1.41	0.40
1:A:321:A:H2'	1:A:322:C:H6	1.86	0.40
1:A:411:A:N7	1:A:413:G:N3	2.70	0.40
1:A:474:G:H2'	1:A:475:G:H8	1.86	0.40
1:A:778:G:C6	1:A:779:C:C4	3.10	0.40
1:A:907:A:C4	1:A:908:A:C8	3.09	0.40
1:A:1067:A:H8	1:A:1067:A:H2'	1.82	0.40
1:A:1188:A:OP1	9:I:114:TYR:OH	2.34	0.40
1:A:1454:G:C2	1:A:1455:G:C8	3.10	0.40
2:B:204:ASN:HB3	2:B:206:ASP:O	2.21	0.40
9:I:89:ASN:HA	9:I:90:PRO:HD2	1.98	0.40
17:Q:63:ARG:HA	17:Q:64:PRO:HD3	1.96	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	232/256 (91%)	207 (89%)	23 (10%)	2 (1%)	17 54
3	C	204/239 (85%)	175 (86%)	28 (14%)	1 (0%)	29 66
4	D	206/209 (99%)	192 (93%)	14 (7%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	E	148/162 (91%)	137 (93%)	11 (7%)	0	100	100
6	F	99/101 (98%)	96 (97%)	3 (3%)	0	100	100
7	G	153/156 (98%)	139 (91%)	14 (9%)	0	100	100
8	H	136/138 (99%)	133 (98%)	3 (2%)	0	100	100
9	I	125/128 (98%)	113 (90%)	12 (10%)	0	100	100
10	J	96/105 (91%)	85 (88%)	9 (9%)	2 (2%)	7	38
11	K	114/129 (88%)	105 (92%)	9 (8%)	0	100	100
12	L	121/135 (90%)	110 (91%)	10 (8%)	1 (1%)	19	56
13	M	116/126 (92%)	103 (89%)	13 (11%)	0	100	100
14	N	58/61 (95%)	53 (91%)	5 (9%)	0	100	100
15	O	85/89 (96%)	75 (88%)	10 (12%)	0	100	100
16	P	81/88 (92%)	76 (94%)	5 (6%)	0	100	100
17	Q	97/105 (92%)	90 (93%)	7 (7%)	0	100	100
18	R	68/88 (77%)	61 (90%)	7 (10%)	0	100	100
19	S	78/93 (84%)	72 (92%)	5 (6%)	1 (1%)	12	47
20	T	97/106 (92%)	86 (89%)	11 (11%)	0	100	100
21	U	22/27 (82%)	20 (91%)	2 (9%)	0	100	100
All	All	2336/2541 (92%)	2128 (91%)	201 (9%)	7 (0%)	41	74

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
19	S	31	ILE
2	B	21	ARG
12	L	28	LYS
10	J	86	MET
10	J	34	VAL
2	B	229	VAL
3	C	86	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	202/220 (92%)	171 (85%)	31 (15%)	2	17
3	C	160/188 (85%)	134 (84%)	26 (16%)	2	14
4	D	180/181 (99%)	162 (90%)	18 (10%)	7	32
5	E	115/123 (94%)	97 (84%)	18 (16%)	2	16
6	F	90/90 (100%)	84 (93%)	6 (7%)	16	48
7	G	126/127 (99%)	113 (90%)	13 (10%)	7	31
8	H	119/119 (100%)	104 (87%)	15 (13%)	4	23
9	I	98/99 (99%)	83 (85%)	15 (15%)	2	17
10	J	87/92 (95%)	79 (91%)	8 (9%)	9	36
11	K	88/99 (89%)	74 (84%)	14 (16%)	2	15
12	L	103/110 (94%)	89 (86%)	14 (14%)	3	21
13	M	94/101 (93%)	85 (90%)	9 (10%)	8	34
14	N	49/50 (98%)	37 (76%)	12 (24%)	0	5
15	O	79/80 (99%)	71 (90%)	8 (10%)	7	31
16	P	72/74 (97%)	68 (94%)	4 (6%)	21	53
17	Q	94/97 (97%)	89 (95%)	5 (5%)	22	54
18	R	61/77 (79%)	58 (95%)	3 (5%)	25	56
19	S	71/80 (89%)	62 (87%)	9 (13%)	4	23
20	T	76/82 (93%)	64 (84%)	12 (16%)	2	16
21	U	19/22 (86%)	14 (74%)	5 (26%)	0	4
All	All	1983/2111 (94%)	1738 (88%)	245 (12%)	4	23

All (245) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	8	LYS
2	B	21	ARG
2	B	24	TRP
2	B	44	LEU
2	B	47	THR
2	B	61	LEU
2	B	67	THR
2	B	69	LEU

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Mol	Chain	Res	Type
2	B	80	ILE
2	B	87	ARG
2	B	96	ARG
2	B	97	TRP
2	B	106	LYS
2	B	111	ARG
2	B	114	ARG
2	B	115	LEU
2	B	127	ILE
2	B	128	GLU
2	B	139	LYS
2	B	142	LEU
2	B	157	ARG
2	B	172	ILE
2	B	175	ARG
2	B	178	ARG
2	B	187	LEU
2	B	190	THR
2	B	197	VAL
2	B	200	ILE
2	B	212	GLN
2	B	221	LEU
2	B	239	VAL
3	C	3	ASN
3	C	10	PHE
3	C	32	LEU
3	C	34	LEU
3	C	45	LYS
3	C	70	VAL
3	C	72	LYS
3	C	79	ARG
3	C	91	LEU
3	C	95	THR
3	C	99	VAL
3	C	101	LEU
3	C	111	LEU
3	C	120	VAL
3	C	131	ARG
3	C	132	ARG
3	C	134	ILE
3	C	138	VAL
3	C	140	ARG

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Mol	Chain	Res	Type
3	C	162	GLN
3	C	172	ARG
3	C	178	LEU
3	C	188	LEU
3	C	190	ARG
3	C	191	THR
3	C	204	LEU
4	D	3	ARG
4	D	9	CYS
4	D	10	ARG
4	D	34	GLU
4	D	36	ARG
4	D	53	ASP
4	D	58	LEU
4	D	66	ARG
4	D	76	ARG
4	D	122	ARG
4	D	127	THR
4	D	131	ARG
4	D	141	ARG
4	D	150	GLU
4	D	155	LEU
4	D	157	LEU
4	D	169	LYS
4	D	170	VAL
5	E	6	PHE
5	E	12	LEU
5	E	15	ARG
5	E	16	THR
5	E	19	MET
5	E	20	GLN
5	E	24	ARG
5	E	26	PHE
5	E	41	VAL
5	E	53	LEU
5	E	68	GLU
5	E	71	LEU
5	E	75	THR
5	E	76	ILE
5	E	79	GLU
5	E	100	VAL
5	E	120	THR

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Mol	Chain	Res	Type
5	E	151	LEU
6	F	10	LEU
6	F	40	VAL
6	F	43	LEU
6	F	70	ASP
6	F	82	ARG
6	F	95	GLU
7	G	6	ARG
7	G	8	GLU
7	G	45	ASP
7	G	56	GLN
7	G	63	LYS
7	G	72	ARG
7	G	84	ASN
7	G	97	GLN
7	G	109	ASN
7	G	113	GLU
7	G	136	LYS
7	G	139	GLU
7	G	149	ARG
8	H	3	THR
8	H	25	ASP
8	H	26	VAL
8	H	50	ARG
8	H	56	LYS
8	H	63	LEU
8	H	83	ILE
8	H	85	ARG
8	H	88	LYS
8	H	91	ARG
8	H	92	ARG
8	H	95	VAL
8	H	97	VAL
8	H	98	LYS
8	H	105	ARG
9	I	16	ARG
9	I	19	LEU
9	I	25	LYS
9	I	27	THR
9	I	38	GLN
9	I	56	LEU
9	I	58	HIS

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Mol	Chain	Res	Type
9	I	59	PHE
9	I	64	THR
9	I	66	ARG
9	I	79	LEU
9	I	83	ARG
9	I	85	LEU
9	I	113	LYS
9	I	118	LYS
10	J	19	SER
10	J	38	ILE
10	J	60	ARG
10	J	62	HIS
10	J	71	LEU
10	J	78	ASN
10	J	85	LEU
10	J	92	THR
11	K	14	VAL
11	K	29	ILE
11	K	33	THR
11	K	36	ASP
11	K	48	ILE
11	K	57	THR
11	K	75	TYR
11	K	79	SER
11	K	91	ARG
11	K	99	GLN
11	K	105	VAL
11	K	114	VAL
11	K	116	HIS
11	K	126	ARG
12	L	16	GLU
12	L	18	VAL
12	L	20	LYS
12	L	33	ARG
12	L	42	THR
12	L	47	LYS
12	L	53	ARG
12	L	66	VAL
12	L	67	THR
12	L	96	VAL
12	L	97	ARG
12	L	101	VAL

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Mol	Chain	Res	Type
12	L	113	ARG
12	L	116	SER
13	M	49	THR
13	M	63	THR
13	M	64	TRP
13	M	69	GLU
13	M	70	LEU
13	M	81	LEU
13	M	108	ARG
13	M	110	ARG
13	M	117	VAL
14	N	9	LYS
14	N	11	LYS
14	N	12	ARG
14	N	22	THR
14	N	24	CYS
14	N	27	CYS
14	N	31	ARG
14	N	35	ARG
14	N	41	ARG
14	N	46	GLU
14	N	47	LEU
14	N	53	LEU
15	O	8	LYS
15	O	32	LEU
15	O	33	THR
15	O	34	LEU
15	O	71	GLN
15	O	77	ARG
15	O	82	ILE
15	O	87	ILE
16	P	2	VAL
16	P	45	THR
16	P	62	VAL
16	P	82	GLN
17	Q	34	LYS
17	Q	38	ARG
17	Q	60	ILE
17	Q	76	LEU
17	Q	92	ARG
18	R	19	LYS
18	R	35	ARG

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Mol	Chain	Res	Type
18	R	47	THR
19	S	6	LYS
19	S	7	LYS
19	S	22	LEU
19	S	36	ARG
19	S	37	ARG
19	S	63	THR
19	S	65	ASN
19	S	71	LEU
19	S	78	ARG
20	T	10	LEU
20	T	13	LEU
20	T	48	LYS
20	T	55	ILE
20	T	56	MET
20	T	62	LEU
20	T	64	ASP
20	T	75	ASN
20	T	80	ARG
20	T	84	LEU
20	T	91	LEU
20	T	93	GLU
21	U	6	ARG
21	U	8	THR
21	U	9	ARG
21	U	10	ARG
21	U	15	ARG

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

Mol	Chain	Res	Type
2	B	204	ASN
4	D	45	GLN
4	D	74	GLN
4	D	123	HIS
9	I	73	GLN
11	K	26	ASN
16	P	82	GLN
19	S	14	HIS

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	1504/1522 (98%)	268 (17%)	46 (3%)

All (268) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	6	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	91	C
1	A	92	C
1	A	101	A
1	A	108	G
1	A	116	A
1	A	117	G
1	A	121	C
1	A	129(A)	G
1	A	130	A
1	A	131	C
1	A	163	C
1	A	182	U
1	A	183	G
1	A	190(F)	G
1	A	195	A
1	A	197	A
1	A	201	C
1	A	202	U
1	A	203	U
1	A	204	U
1	A	216	G
1	A	245	C
1	A	247	G
1	A	251	G
1	A	252	U
1	A	253	U
1	A	266	G
1	A	267	C
1	A	289	G

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Mol	Chain	Res	Type
1	A	290	C
1	A	299	G
1	A	301	G
1	A	321	A
1	A	328	C
1	A	329	A
1	A	332	G
1	A	344	A
1	A	345	C
1	A	349	A
1	A	351	G
1	A	352	C
1	A	353	A
1	A	354	G
1	A	367	U
1	A	373	A
1	A	374	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	414	A
1	A	421	U
1	A	422	C
1	A	424	G
1	A	429	U
1	A	430	A
1	A	439	A
1	A	440	A
1	A	460	A
1	A	461	C
1	A	481	G
1	A	485	G
1	A	486	U
1	A	497	A
1	A	498	U
1	A	509	A
1	A	510	A
1	A	511	C

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Mol	Chain	Res	Type
1	A	513	C
1	A	517	G
1	A	518	C
1	A	519	C
1	A	524	G
1	A	531	U
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	568	G
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	653	A
1	A	665	A
1	A	671	G
1	A	687	A
1	A	688	G
1	A	701	C
1	A	702	A
1	A	703	G
1	A	718	G
1	A	721	G
1	A	723	U
1	A	731	G
1	A	749	C
1	A	755	G
1	A	777	A
1	A	781	A
1	A	782	A
1	A	792	A
1	A	793	U
1	A	794	A
1	A	799	G
1	A	813	U
1	A	817	C

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Mol	Chain	Res	Type
1	A	828	A
1	A	839	U
1	A	840	C
1	A	841	U
1	A	848	C
1	A	858	G
1	A	876	G
1	A	885	G
1	A	889	A
1	A	902	G
1	A	914	A
1	A	922	G
1	A	926	G
1	A	927	G
1	A	934	C
1	A	935	A
1	A	936	C
1	A	937	A
1	A	960	U
1	A	961	U
1	A	967	5MC
1	A	968	A
1	A	969	A
1	A	971	G
1	A	974	A
1	A	975	A
1	A	976	G
1	A	977	A
1	A	985	C
1	A	989	C
1	A	991	U
1	A	992	U
1	A	993	G
1	A	1004	A
1	A	1005	A
1	A	1006	C
1	A	1023	G
1	A	1024	G
1	A	1030(B)	C
1	A	1034	G
1	A	1045	C
1	A	1050	G

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Mol	Chain	Res	Type
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	1124	G
1	A	1125	U
1	A	1126	U
1	A	1127	G
1	A	1129	C
1	A	1130	A
1	A	1136	U
1	A	1137	C
1	A	1138	G
1	A	1139	G
1	A	1140	C
1	A	1145	C
1	A	1146	A
1	A	1152	A
1	A	1159	U
1	A	1160	G
1	A	1169	A
1	A	1171	G
1	A	1183	A
1	A	1190	G
1	A	1193	G
1	A	1196	U
1	A	1197	G
1	A	1200	C
1	A	1201	A
1	A	1202	G
1	A	1211	U
1	A	1212	U
1	A	1213	A
1	A	1214	C
1	A	1224	G
1	A	1225	A
1	A	1226	C

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Mol	Chain	Res	Type
1	A	1238	A
1	A	1240	U
1	A	1241	G
1	A	1253	G
1	A	1256	A
1	A	1257	U
1	A	1278	U
1	A	1280	A
1	A	1281	U
1	A	1285	A
1	A	1286	A
1	A	1287	A
1	A	1289	A
1	A	1300	G
1	A	1301	U
1	A	1302	U
1	A	1303	C
1	A	1304	G
1	A	1305	G
1	A	1306	A
1	A	1318	A
1	A	1319	A
1	A	1320	C
1	A	1322	C
1	A	1323	G
1	A	1335	C
1	A	1336	C
1	A	1340	A
1	A	1346	A
1	A	1347	G
1	A	1348	U
1	A	1353	G
1	A	1359	C
1	A	1362	C
1	A	1379	G
1	A	1381	U
1	A	1397	C
1	A	1398	A
1	A	1400	5MC
1	A	1411	C
1	A	1417	G
1	A	1442	G

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Mol	Chain	Res	Type
1	A	1446	A
1	A	1447	G
1	A	1451	A
1	A	1453	G
1	A	1479	C
1	A	1485	U
1	A	1486	G
1	A	1487	G
1	A	1490	C
1	A	1493	A
1	A	1497	G
1	A	1498	UR3
1	A	1499	A
1	A	1503	A
1	A	1504	G
1	A	1505	G
1	A	1506	U
1	A	1529	G
1	A	1530	G
1	A	1531	A

All (46) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	5	U
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	328	C
1	A	372	C
1	A	428	G
1	A	429	U
1	A	484	G
1	A	485	G
1	A	496	A
1	A	509	A
1	A	518	C
1	A	532	A
1	A	559	A

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Mol	Chain	Res	Type
1	A	575	G
1	A	687	A
1	A	701	C
1	A	748	C
1	A	792	A
1	A	793	U
1	A	812	C
1	A	913	A
1	A	960	U
1	A	975	A
1	A	992	U
1	A	1049	U
1	A	1065	U
1	A	1067	A
1	A	1126	U
1	A	1139	G
1	A	1145	C
1	A	1182	G
1	A	1201	A
1	A	1285	A
1	A	1300	G
1	A	1301	U
1	A	1305	G
1	A	1346	A
1	A	1347	G
1	A	1380	U
1	A	1397	C
1	A	1505	G

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

16 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	PSU	A	516	22,1	18,21,22	1.08	2 (11%)	21,30,33	1.78	4 (19%)
1	MA6	A	1519[B]	1	19,26,27	1.31	3 (15%)	18,38,41	0.61	0
1	PSU	A	1541	22,1	18,21,22	1.10	1 (5%)	21,30,33	1.92	4 (19%)
1	M2G	A	966	1	20,27,28	1.30	4 (20%)	19,40,43	1.15	2 (10%)
1	5MC	A	1400	1	19,22,23	1.15	2 (10%)	26,32,35	1.09	3 (11%)
1	2MG	A	1207	1	18,26,27	1.50	4 (22%)	16,38,41	1.41	2 (12%)
1	UR3	A	1498	1	19,22,23	0.57	0	26,32,35	0.96	0
1	5MC	A	967	1	19,22,23	1.15	3 (15%)	26,32,35	0.94	1 (3%)
1	5MC	A	1407	1	19,22,23	0.90	2 (10%)	26,32,35	1.02	2 (7%)
1	MA6	A	1518[A]	1	19,26,27	0.95	1 (5%)	18,38,41	0.91	1 (5%)
1	MA6	A	1518[B]	1	19,26,27	1.27	2 (10%)	18,38,41	0.69	0
1	PSU	A	1540	1	18,21,22	1.10	1 (5%)	21,30,33	1.77	4 (19%)
1	4OC	A	1402	1	20,23,24	0.90	1 (5%)	25,32,35	0.87	1 (4%)
1	MA6	A	1519[A]	1	19,26,27	1.01	1 (5%)	18,38,41	0.68	0
12	0TD	L	92	12	8,9,10	1.13	0	6,11,13	2.53	2 (33%)
1	5MC	A	1404	1	19,22,23	1.08	1 (5%)	26,32,35	0.97	2 (7%)

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	PSU	A	516	22,1	-	0/7/25/26	0/2/2/2
1	MA6	A	1519[B]	1	-	4/7/29/30	0/3/3/3
1	PSU	A	1541	22,1	-	0/7/25/26	0/2/2/2
1	M2G	A	966	1	-	2/7/29/30	0/3/3/3
1	5MC	A	1400	1	-	2/7/25/26	0/2/2/2
1	2MG	A	1207	1	-	0/5/27/28	0/3/3/3
1	UR3	A	1498	1	-	2/7/25/26	0/2/2/2
1	5MC	A	967	1	-	3/7/25/26	0/2/2/2
1	5MC	A	1407	1	-	0/7/25/26	0/2/2/2
1	MA6	A	1518[A]	1	-	0/7/29/30	0/3/3/3
1	MA6	A	1518[B]	1	-	0/7/29/30	0/3/3/3
1	PSU	A	1540	1	-	0/7/25/26	0/2/2/2
1	4OC	A	1402	1	-	2/9/29/30	0/2/2/2
1	MA6	A	1519[A]	1	-	3/7/29/30	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	0TD	L	92	12	-	2/7/12/14	-
1	5MC	A	1404	1	-	0/7/25/26	0/2/2/2

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1518[B]	MA6	C6-N1	3.98	1.38	1.32
1	A	1519[B]	MA6	C6-N1	3.78	1.37	1.32
1	A	1540	PSU	C6-C5	3.72	1.39	1.35
1	A	1207	2MG	C6-N1	3.65	1.43	1.37
1	A	1541	PSU	C6-C5	3.54	1.39	1.35
1	A	516	PSU	C6-C5	3.37	1.39	1.35
1	A	966	M2G	C5-C6	-3.18	1.41	1.47
1	A	1207	2MG	C2-N2	3.04	1.39	1.33
1	A	966	M2G	C2-N3	2.72	1.34	1.30
1	A	1207	2MG	C2-N1	2.70	1.41	1.36
1	A	1519[A]	MA6	C6-N1	2.66	1.36	1.32
1	A	1518[A]	MA6	C6-N1	2.64	1.36	1.32
1	A	1400	5MC	C2-N1	2.57	1.45	1.40
1	A	967	5MC	C2-N3	2.54	1.41	1.36
1	A	1207	2MG	C5-C6	-2.51	1.42	1.47
1	A	1519[B]	MA6	C2-N1	2.39	1.38	1.33
1	A	1404	5MC	C5-C4	-2.30	1.42	1.44
1	A	966	M2G	C2-N2	2.26	1.39	1.35
1	A	1400	5MC	C5-C4	-2.26	1.42	1.44
1	A	966	M2G	C6-N1	2.25	1.41	1.37
1	A	967	5MC	C2-N1	2.20	1.44	1.40
1	A	1519[B]	MA6	C2-N3	2.17	1.35	1.32
1	A	967	5MC	C6-C5	2.13	1.38	1.34
1	A	1402	4OC	O2-C2	-2.11	1.19	1.23
1	A	1407	5MC	C2-N3	2.05	1.40	1.36
1	A	516	PSU	C4-C5	-2.05	1.38	1.44
1	A	1518[B]	MA6	C2-N1	2.04	1.37	1.33
1	A	1407	5MC	C2-N1	2.01	1.44	1.40

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	L	92	0TD	CSB-SB-CB	-4.82	93.70	102.36
1	A	1541	PSU	C4-N3-C2	-4.78	119.79	126.37
1	A	1541	PSU	N1-C2-N3	4.68	120.10	115.17
1	A	1540	PSU	C4-N3-C2	-4.52	120.14	126.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	516	PSU	C4-N3-C2	-4.52	120.15	126.37
1	A	516	PSU	N1-C2-N3	4.43	119.84	115.17
1	A	1540	PSU	N1-C2-N3	4.40	119.80	115.17
1	A	1207	2MG	O6-C6-N1	-3.99	115.88	120.62
1	A	1207	2MG	O6-C6-C5	3.32	130.91	124.32
1	A	966	M2G	O6-C6-C5	3.17	130.60	124.32
1	A	966	M2G	O6-C6-N1	-3.03	117.02	120.62
1	A	1541	PSU	O2-C2-N1	-3.02	119.67	122.79
1	A	1407	5MC	N4-C4-N3	-2.77	113.50	118.51
1	A	1540	PSU	O2-C2-N1	-2.54	120.17	122.79
1	A	516	PSU	C6-N1-C2	-2.52	120.35	122.69
1	A	1541	PSU	C6-N1-C2	-2.44	120.42	122.69
1	A	1400	5MC	C5-C4-N3	2.36	124.17	121.75
12	L	92	0TD	OD1-CG-CB	-2.34	117.54	122.44
1	A	1404	5MC	N4-C4-N3	-2.32	114.30	118.51
1	A	516	PSU	O2-C2-N1	-2.31	120.41	122.79
1	A	1540	PSU	C6-N1-C2	-2.26	120.59	122.69
1	A	1407	5MC	C5-C4-N3	2.22	124.03	121.75
1	A	1404	5MC	C5-C4-N3	2.19	124.00	121.75
1	A	1400	5MC	O2-C2-N3	-2.17	118.91	122.33
1	A	1400	5MC	N4-C4-N3	-2.16	114.59	118.51
1	A	967	5MC	N4-C4-N3	-2.12	114.67	118.51
1	A	1402	4OC	C5-C4-N4	-2.06	117.88	122.40
1	A	1518[A]	MA6	N1-C6-N6	-2.04	114.47	116.83

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	967	5MC	O4'-C4'-C5'-O5'
1	A	1400	5MC	O4'-C4'-C5'-O5'
1	A	1402	4OC	O4'-C4'-C5'-O5'
1	A	1519[A]	MA6	C5-C6-N6-C10
1	A	1519[B]	MA6	C5-C6-N6-C9
1	A	967	5MC	C3'-C4'-C5'-O5'
1	A	1519[B]	MA6	N1-C6-N6-C9
1	A	1400	5MC	C3'-C4'-C5'-O5'
1	A	1402	4OC	C3'-C4'-C5'-O5'
1	A	1519[A]	MA6	C3'-C4'-C5'-O5'
1	A	1519[B]	MA6	C3'-C4'-C5'-O5'
1	A	1498	UR3	O4'-C4'-C5'-O5'
1	A	1519[A]	MA6	O4'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
1	A	966	M2G	C3'-C4'-C5'-O5'
12	L	92	0TD	CG-CB-SB-CSB
1	A	1498	UR3	C3'-C4'-C5'-O5'
1	A	1519[B]	MA6	O4'-C4'-C5'-O5'
12	L	92	0TD	SB-CB-CG-OD1
1	A	966	M2G	O4'-C4'-C5'-O5'
1	A	967	5MC	C2'-C1'-N1-C2

There are no ring outliers.

10 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	1519[B]	MA6	1	0
1	A	966	M2G	2	0
1	A	1400	5MC	1	0
1	A	1498	UR3	3	0
1	A	967	5MC	3	0
1	A	1518[A]	MA6	2	0
1	A	1518[B]	MA6	1	0
1	A	1402	4OC	1	0
1	A	1519[A]	MA6	2	0
12	L	92	0TD	1	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 226 ligands modelled in this entry, 226 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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 (i)

6.1 Protein, DNA and RNA chains (i)

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, 95th 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	1499/1522 (98%)	-0.40	18 (1%)	79	68	83, 131, 266, 392	0
2	B	234/256 (91%)	-0.53	1 (0%)	92	88	103, 141, 230, 267	0
3	C	206/239 (86%)	-0.05	10 (4%)	29	21	164, 199, 241, 275	0
4	D	208/209 (99%)	-0.51	1 (0%)	91	85	88, 130, 174, 240	0
5	E	150/162 (92%)	-0.58	0	100	100	69, 103, 137, 197	0
6	F	101/101 (100%)	-0.71	0	100	100	106, 141, 171, 194	0
7	G	155/156 (99%)	-0.44	2 (1%)	77	65	130, 162, 216, 232	0
8	H	138/138 (100%)	-0.72	0	100	100	73, 90, 118, 162	0
9	I	127/128 (99%)	-0.17	2 (1%)	72	59	141, 195, 240, 281	0
10	J	98/105 (93%)	0.41	7 (7%)	16	10	154, 216, 300, 311	0
11	K	116/129 (89%)	-0.51	0	100	100	98, 123, 165, 192	0
12	L	123/135 (91%)	-0.43	0	100	100	78, 129, 154, 235	0
13	M	118/126 (93%)	-0.19	2 (1%)	70	57	130, 158, 194, 319	0
14	N	60/61 (98%)	0.22	5 (8%)	11	8	164, 182, 231, 299	0
15	O	87/89 (97%)	-0.58	0	100	100	84, 111, 146, 167	0
16	P	83/88 (94%)	-0.56	0	100	100	105, 125, 151, 189	0
17	Q	99/105 (94%)	-0.59	0	100	100	82, 103, 134, 162	0
18	R	70/88 (79%)	-0.61	0	100	100	85, 123, 173, 195	0
19	S	80/93 (86%)	0.24	4 (5%)	28	20	157, 200, 249, 276	0
20	T	99/106 (93%)	-0.60	1 (1%)	82	72	104, 129, 176, 205	0
21	U	24/27 (88%)	1.18	4 (16%)	1	1	136, 164, 196, 209	0
All	All	3875/4063 (95%)	-0.38	57 (1%)	73	61	69, 138, 238, 392	0

All (57) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1129	C	5.3
4	D	35	ARG	5.2
21	U	17	THR	5.0
21	U	18	TYR	4.8
3	C	157	ILE	4.5
1	A	993	G	4.2
1	A	1018	C	4.0
10	J	34	VAL	3.9
10	J	33	GLN	3.7
7	G	2	ALA	3.4
1	A	1050	G	3.3
1	A	1257	U	3.2
3	C	156	ARG	3.2
1	A	1019	C	3.1
14	N	4	LYS	3.0
3	C	193	TYR	3.0
1	A	1007	C	3.0
14	N	20	ALA	3.0
1	A	1006	C	2.9
1	A	1539	C	2.9
3	C	102	ASN	2.9
1	A	1037	C	2.7
10	J	74	ILE	2.6
3	C	66	VAL	2.6
10	J	99	LYS	2.6
9	I	9	ARG	2.6
3	C	103	VAL	2.6
20	T	106	ALA	2.6
19	S	69	HIS	2.5
9	I	4	TYR	2.5
1	A	994	A	2.5
10	J	90	LEU	2.5
7	G	156	TRP	2.5
1	A	1005	A	2.4
13	M	2	ALA	2.4
1	A	1017	G	2.4
19	S	48	THR	2.4
19	S	81	ARG	2.3
3	C	101	LEU	2.3
1	A	1003(A)	G	2.2
2	B	231	GLU	2.2
21	U	24	ARG	2.2
1	A	202	U	2.2

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Mol	Chain	Res	Type	RSRZ
13	M	117	VAL	2.2
3	C	155	GLY	2.2
1	A	1036	G	2.2
10	J	100	THR	2.2
14	N	13	THR	2.1
21	U	5	ASP	2.1
3	C	196	LEU	2.1
10	J	71	LEU	2.1
19	S	30	LEU	2.1
14	N	11	LYS	2.1
1	A	532	A	2.0
1	A	1138	G	2.0
3	C	65	ALA	2.0
14	N	3	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, 95th 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	1540	20/21	0.86	0.60	230,237,250,253	0
1	2MG	A	1207	24/25	0.90	0.18	193,202,214,223	0
1	PSU	A	1541	20/21	0.92	0.35	232,244,251,253	0
12	0TD	L	92	10/11	0.92	0.42	128,129,132,295	0
1	5MC	A	1400	21/22	0.93	0.19	117,120,123,125	0
1	PSU	A	516	20/21	0.93	0.10	140,148,158,159	0
1	UR3	A	1498	21/22	0.94	0.25	109,117,125,146	0
1	MA6	A	1518[B]	24/25	0.95	0.24	113,118,121,127	24
1	MA6	A	1519[A]	24/25	0.95	0.22	109,112,113,113	24
1	MA6	A	1519[B]	24/25	0.95	0.22	109,112,114,115	24
1	5MC	A	967	21/22	0.95	0.11	127,132,139,142	0
1	M2G	A	966	25/26	0.95	0.14	129,148,165,166	0
1	MA6	A	1518[A]	24/25	0.95	0.24	115,118,119,120	24
1	5MC	A	1404	21/22	0.96	0.18	113,117,122,123	0
1	5MC	A	1407	21/22	0.96	0.21	128,142,148,156	0
1	4OC	A	1402	22/23	0.97	0.20	118,123,135,138	0

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th 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
22	MG	A	1801	1/1	0.71	0.32	87,87,87,87	0
22	MG	A	1765	1/1	0.72	0.37	71,71,71,71	0
22	MG	A	1796	1/1	0.74	0.46	68,68,68,68	0
22	MG	A	1795	1/1	0.74	0.15	75,75,75,75	0
22	MG	A	1773	1/1	0.75	0.44	63,63,63,63	0
22	MG	A	1728	1/1	0.76	0.52	83,83,83,83	0
22	MG	A	1695	1/1	0.77	0.42	59,59,59,59	0
22	MG	A	1812	1/1	0.77	0.56	112,112,112,112	0
22	MG	A	1761	1/1	0.78	0.45	83,83,83,83	0
22	MG	A	1787	1/1	0.79	0.21	120,120,120,120	0
22	MG	A	1797	1/1	0.79	0.30	92,92,92,92	0
22	MG	A	1713	1/1	0.80	0.53	116,116,116,116	0
22	MG	A	1689	1/1	0.80	0.38	100,100,100,100	0
22	MG	A	1740	1/1	0.80	0.29	85,85,85,85	0
22	MG	A	1610	1/1	0.81	0.35	77,77,77,77	0
22	MG	A	1724	1/1	0.81	0.94	102,102,102,102	0
22	MG	A	1747	1/1	0.81	0.25	111,111,111,111	0
22	MG	A	1626	1/1	0.82	0.26	81,81,81,81	0
22	MG	A	1664	1/1	0.82	0.32	90,90,90,90	0
22	MG	A	1704	1/1	0.82	0.53	94,94,94,94	0
22	MG	A	1764	1/1	0.82	0.44	100,100,100,100	0
22	MG	A	1737	1/1	0.83	0.30	73,73,73,73	0
22	MG	A	1807	1/1	0.83	0.17	76,76,76,76	0
22	MG	A	1749	1/1	0.83	0.30	84,84,84,84	0
22	MG	D	304	1/1	0.83	0.15	88,88,88,88	0
22	MG	A	1601	1/1	0.84	0.38	107,107,107,107	0
22	MG	A	1669	1/1	0.84	0.11	129,129,129,129	0
22	MG	A	1785	1/1	0.85	0.30	86,86,86,86	0
22	MG	A	1661	1/1	0.85	0.21	71,71,71,71	0
22	MG	A	1752	1/1	0.85	0.34	91,91,91,91	0
22	MG	Q	201	1/1	0.85	0.10	75,75,75,75	0
22	MG	A	1706	1/1	0.86	0.09	68,68,68,68	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
22	MG	A	1762	1/1	0.86	0.53	103,103,103,103	0
22	MG	A	1712	1/1	0.86	0.13	238,238,238,238	0
22	MG	A	1729	1/1	0.86	0.28	87,87,87,87	0
22	MG	A	1674	1/1	0.86	0.18	90,90,90,90	0
22	MG	A	1717	1/1	0.87	0.24	72,72,72,72	0
22	MG	A	1656	1/1	0.87	0.20	59,59,59,59	0
22	MG	A	1681	1/1	0.87	0.19	97,97,97,97	0
22	MG	A	1682	1/1	0.88	0.58	86,86,86,86	0
22	MG	A	1684	1/1	0.88	0.77	94,94,94,94	0
22	MG	A	1804	1/1	0.88	0.25	94,94,94,94	0
22	MG	A	1756	1/1	0.88	0.32	73,73,73,73	0
22	MG	A	1627	1/1	0.88	0.10	125,125,125,125	0
22	MG	A	1630	1/1	0.88	0.23	92,92,92,92	0
22	MG	A	1632	1/1	0.88	0.47	79,79,79,79	0
22	MG	A	1742	1/1	0.89	0.25	82,82,82,82	0
22	MG	A	1628	1/1	0.89	0.37	104,104,104,104	0
22	MG	A	1748	1/1	0.89	0.45	69,69,69,69	0
22	MG	A	1697	1/1	0.89	0.23	93,93,93,93	0
22	MG	A	1774	1/1	0.89	0.30	94,94,94,94	0
22	MG	A	1809	1/1	0.89	0.18	130,130,130,130	0
22	MG	A	1700	1/1	0.89	0.83	78,78,78,78	0
22	MG	A	1666	1/1	0.89	0.14	90,90,90,90	0
22	MG	A	1722	1/1	0.89	0.39	97,97,97,97	0
22	MG	A	1734	1/1	0.90	0.26	111,111,111,111	0
22	MG	A	1735	1/1	0.90	0.33	65,65,65,65	0
22	MG	A	1625	1/1	0.90	0.67	78,78,78,78	0
22	MG	A	1659	1/1	0.90	0.17	203,203,203,203	0
22	MG	A	1702	1/1	0.90	0.20	192,192,192,192	0
22	MG	A	1745	1/1	0.90	0.13	105,105,105,105	0
22	MG	A	1771	1/1	0.90	0.22	90,90,90,90	0
22	MG	A	1605	1/1	0.90	1.00	79,79,79,79	0
22	MG	A	1691	1/1	0.90	0.14	121,121,121,121	0
22	MG	C	301	1/1	0.90	0.11	103,103,103,103	0
22	MG	A	1780	1/1	0.90	0.09	95,95,95,95	0
22	MG	A	1641	1/1	0.90	0.23	107,107,107,107	0
22	MG	A	1767	1/1	0.91	0.48	69,69,69,69	0
22	MG	A	1750	1/1	0.91	0.08	112,112,112,112	0
22	MG	A	1676	1/1	0.91	0.20	103,103,103,103	0
22	MG	A	1731	1/1	0.91	0.24	97,97,97,97	0
22	MG	A	1806	1/1	0.91	0.16	92,92,92,92	0
22	MG	A	1777	1/1	0.91	0.18	111,111,111,111	0
22	MG	A	1688	1/1	0.91	0.20	67,67,67,67	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
22	MG	A	1783	1/1	0.91	0.47	66,66,66,66	0
22	MG	A	1671	1/1	0.91	0.18	95,95,95,95	0
22	MG	A	1736	1/1	0.91	0.68	104,104,104,104	0
22	MG	A	1667	1/1	0.91	0.27	86,86,86,86	0
22	MG	A	1665	1/1	0.92	0.19	100,100,100,100	0
22	MG	A	1660	1/1	0.92	0.32	92,92,92,92	0
22	MG	A	1685	1/1	0.92	0.08	160,160,160,160	0
22	MG	A	1770	1/1	0.92	0.27	112,112,112,112	0
22	MG	A	1617	1/1	0.92	0.25	58,58,58,58	0
22	MG	A	1678	1/1	0.92	0.29	88,88,88,88	0
22	MG	A	1679	1/1	0.92	0.22	83,83,83,83	0
22	MG	A	1644	1/1	0.92	0.13	115,115,115,115	0
22	MG	A	1759	1/1	0.93	0.15	74,74,74,74	0
22	MG	A	1657	1/1	0.93	0.19	103,103,103,103	0
22	MG	A	1608	1/1	0.93	0.10	109,109,109,109	0
22	MG	A	1687	1/1	0.93	0.21	117,117,117,117	0
22	MG	A	1781	1/1	0.93	0.18	86,86,86,86	0
22	MG	A	1623	1/1	0.93	0.58	47,47,47,47	0
22	MG	A	1784	1/1	0.93	0.14	105,105,105,105	0
22	MG	A	1715	1/1	0.93	0.11	72,72,72,72	0
22	MG	A	1755	1/1	0.93	0.25	95,95,95,95	0
22	MG	A	1788	1/1	0.93	0.19	104,104,104,104	0
22	MG	P	102	1/1	0.93	0.34	72,72,72,72	0
22	MG	A	1637	1/1	0.93	0.15	84,84,84,84	0
23	ZN	N	101	1/1	0.93	0.13	246,246,246,246	0
22	MG	A	1786	1/1	0.94	0.22	84,84,84,84	0
22	MG	A	1766	1/1	0.94	0.55	57,57,57,57	0
22	MG	A	1732	1/1	0.94	0.38	53,53,53,53	0
22	MG	A	1769	1/1	0.94	0.19	80,80,80,80	0
22	MG	A	1640	1/1	0.94	0.15	87,87,87,87	0
22	MG	A	1622	1/1	0.94	0.18	79,79,79,79	0
22	MG	A	1754	1/1	0.94	0.12	59,59,59,59	0
22	MG	A	1720	1/1	0.94	0.16	112,112,112,112	0
22	MG	A	1775	1/1	0.94	0.33	69,69,69,69	0
22	MG	A	1776	1/1	0.94	0.39	86,86,86,86	0
22	MG	A	1808	1/1	0.94	0.14	103,103,103,103	0
22	MG	A	1638	1/1	0.94	0.14	195,195,195,195	0
22	MG	A	1810	1/1	0.94	0.07	79,79,79,79	0
22	MG	A	1811	1/1	0.94	0.19	90,90,90,90	0
22	MG	A	1778	1/1	0.94	0.13	87,87,87,87	0
22	MG	B	301	1/1	0.94	0.33	102,102,102,102	0
22	MG	A	1709	1/1	0.94	0.16	79,79,79,79	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
22	MG	A	1727	1/1	0.94	0.14	81,81,81,81	0
22	MG	A	1680	1/1	0.94	0.17	129,129,129,129	0
22	MG	A	1651	1/1	0.94	0.15	86,86,86,86	0
22	MG	A	1714	1/1	0.94	0.17	77,77,77,77	0
22	MG	A	1634	1/1	0.95	0.15	154,154,154,154	0
22	MG	A	1805	1/1	0.95	0.10	97,97,97,97	0
22	MG	A	1693	1/1	0.95	0.21	137,137,137,137	0
22	MG	A	1675	1/1	0.95	0.10	90,90,90,90	0
22	MG	A	1603	1/1	0.95	0.12	78,78,78,78	0
22	MG	A	1677	1/1	0.95	0.09	221,221,221,221	0
22	MG	A	1686	1/1	0.95	0.14	167,167,167,167	0
22	MG	A	1721	1/1	0.95	0.13	75,75,75,75	0
22	MG	A	1703	1/1	0.95	0.09	114,114,114,114	0
22	MG	A	1793	1/1	0.95	0.16	284,284,284,284	0
22	MG	A	1649	1/1	0.95	0.17	79,79,79,79	0
22	MG	D	303	1/1	0.95	0.08	90,90,90,90	0
22	MG	A	1612	1/1	0.95	0.07	107,107,107,107	0
22	MG	A	1763	1/1	0.95	0.30	150,150,150,150	0
22	MG	A	1800	1/1	0.95	0.14	95,95,95,95	0
22	MG	A	1616	1/1	0.95	0.11	62,62,62,62	0
22	MG	A	1692	1/1	0.96	0.10	124,124,124,124	0
22	MG	A	1799	1/1	0.96	0.12	113,113,113,113	0
22	MG	A	1639	1/1	0.96	0.12	72,72,72,72	0
22	MG	A	1730	1/1	0.96	0.60	99,99,99,99	0
22	MG	A	1802	1/1	0.96	0.33	98,98,98,98	0
22	MG	A	1650	1/1	0.96	0.14	48,48,48,48	0
22	MG	A	1604	1/1	0.96	0.15	91,91,91,91	0
22	MG	A	1733	1/1	0.96	0.13	101,101,101,101	0
22	MG	A	1779	1/1	0.96	0.29	67,67,67,67	0
22	MG	A	1760	1/1	0.96	0.14	65,65,65,65	0
22	MG	A	1614	1/1	0.96	0.08	101,101,101,101	0
22	MG	A	1716	1/1	0.96	0.12	93,93,93,93	0
22	MG	A	1701	1/1	0.96	0.10	153,153,153,153	0
22	MG	A	1642	1/1	0.96	0.09	79,79,79,79	0
22	MG	A	1607	1/1	0.96	0.17	75,75,75,75	0
22	MG	A	1645	1/1	0.96	0.19	82,82,82,82	0
22	MG	D	302	1/1	0.96	0.64	85,85,85,85	0
22	MG	A	1723	1/1	0.96	0.17	111,111,111,111	0
22	MG	A	1791	1/1	0.96	0.19	202,202,202,202	0
22	MG	A	1705	1/1	0.96	0.22	276,276,276,276	0
22	MG	A	1725	1/1	0.96	0.14	167,167,167,167	0
22	MG	U	1300	1/1	0.96	0.19	90,90,90,90	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
22	MG	A	1672	1/1	0.96	0.20	105,105,105,105	0
22	MG	A	1668	1/1	0.97	0.14	101,101,101,101	0
22	MG	A	1690	1/1	0.97	0.13	138,138,138,138	0
22	MG	A	1803	1/1	0.97	0.38	62,62,62,62	0
22	MG	A	1658	1/1	0.97	0.11	107,107,107,107	0
22	MG	A	1739	1/1	0.97	0.12	100,100,100,100	0
22	MG	A	1648	1/1	0.97	0.18	91,91,91,91	0
22	MG	A	1710	1/1	0.97	0.38	166,166,166,166	0
22	MG	A	1744	1/1	0.97	0.18	74,74,74,74	0
22	MG	A	1618	1/1	0.97	0.20	93,93,93,93	0
22	MG	A	1683	1/1	0.97	0.39	62,62,62,62	0
22	MG	A	1643	1/1	0.97	0.43	67,67,67,67	0
22	MG	A	1768	1/1	0.97	0.11	79,79,79,79	0
22	MG	A	1790	1/1	0.97	0.14	117,117,117,117	0
22	MG	A	1624	1/1	0.97	0.14	124,124,124,124	0
22	MG	C	302	1/1	0.97	0.07	121,121,121,121	0
22	MG	A	1652	1/1	0.97	0.06	96,96,96,96	0
22	MG	A	1794	1/1	0.97	0.16	127,127,127,127	0
22	MG	A	1751	1/1	0.97	0.39	112,112,112,112	0
22	MG	A	1633	1/1	0.97	0.38	173,173,173,173	0
22	MG	A	1753	1/1	0.97	0.13	94,94,94,94	0
22	MG	A	1719	1/1	0.97	0.13	115,115,115,115	0
22	MG	A	1647	1/1	0.97	0.11	111,111,111,111	0
22	MG	A	1646	1/1	0.98	0.10	159,159,159,159	0
22	MG	A	1746	1/1	0.98	0.10	109,109,109,109	0
22	MG	A	1673	1/1	0.98	0.11	89,89,89,89	0
22	MG	A	1726	1/1	0.98	0.15	74,74,74,74	0
22	MG	A	1772	1/1	0.98	0.25	96,96,96,96	0
22	MG	A	1615	1/1	0.98	0.06	79,79,79,79	0
22	MG	A	1629	1/1	0.98	0.30	68,68,68,68	0
22	MG	A	1609	1/1	0.98	0.14	75,75,75,75	0
22	MG	A	1711	1/1	0.98	0.22	343,343,343,343	0
22	MG	A	1662	1/1	0.98	0.06	93,93,93,93	0
22	MG	A	1663	1/1	0.98	0.12	72,72,72,72	0
22	MG	A	1631	1/1	0.98	0.09	85,85,85,85	0
22	MG	A	1613	1/1	0.98	0.05	123,123,123,123	0
22	MG	A	1757	1/1	0.98	0.09	97,97,97,97	0
22	MG	A	1782	1/1	0.98	0.19	89,89,89,89	0
22	MG	A	1758	1/1	0.98	0.16	53,53,53,53	0
22	MG	A	1602	1/1	0.98	0.15	118,118,118,118	0
22	MG	A	1698	1/1	0.98	0.21	128,128,128,128	0
22	MG	A	1699	1/1	0.98	0.18	111,111,111,111	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
22	MG	A	1653	1/1	0.98	0.20	100,100,100,100	0
22	MG	A	1655	1/1	0.98	0.12	136,136,136,136	0
22	MG	A	1789	1/1	0.98	0.34	135,135,135,135	0
22	MG	A	1741	1/1	0.98	0.06	78,78,78,78	0
22	MG	F	201	1/1	0.98	0.45	104,104,104,104	0
22	MG	A	1619	1/1	0.98	0.10	59,59,59,59	0
22	MG	A	1792	1/1	0.98	0.21	229,229,229,229	0
22	MG	A	1743	1/1	0.98	0.11	83,83,83,83	0
23	ZN	D	301	1/1	0.98	0.33	79,79,79,79	0
22	MG	A	1620	1/1	0.98	0.28	120,120,120,120	0
22	MG	A	1738	1/1	0.99	0.20	69,69,69,69	0
22	MG	A	1611	1/1	0.99	0.24	83,83,83,83	0
22	MG	A	1707	1/1	0.99	0.12	126,126,126,126	0
22	MG	A	1718	1/1	0.99	0.27	80,80,80,80	0
22	MG	A	1708	1/1	0.99	0.15	154,154,154,154	0
22	MG	A	1635	1/1	0.99	0.12	70,70,70,70	0
22	MG	A	1606	1/1	0.99	0.08	94,94,94,94	0
22	MG	E	201	1/1	0.99	0.09	94,94,94,94	0
22	MG	A	1654	1/1	0.99	0.07	95,95,95,95	0
22	MG	P	101	1/1	0.99	0.12	54,54,54,54	0
22	MG	A	1694	1/1	0.99	0.16	249,249,249,249	0
22	MG	A	1670	1/1	0.99	0.07	120,120,120,120	0
22	MG	A	1696	1/1	0.99	0.12	102,102,102,102	0
22	MG	A	1621	1/1	0.99	0.11	57,57,57,57	0
22	MG	A	1798	1/1	0.99	0.18	114,114,114,114	0
22	MG	A	1636	1/1	1.00	0.28	97,97,97,97	0

6.5 Other polymers (i)

There are no such residues in this entry.