Full wwPDB X-ray Structure Validation Report ⓘ

May 17, 2020 – 12:21 am BST

PDB ID	:	4DUY
Title	:	Crystal structure of the Thermus thermophilus 30S ribosomal subunit with a 16S rRNA mutation, U13C
Authors	:	Demirci, H.; Murphy IV, F.; Murphy, E.; Gregory, S.T.; Dahlberg, A.E.; Jogl, G.
Deposited on	:	2012-02-22
Resolution	:	3.39 Å(reported)

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

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

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

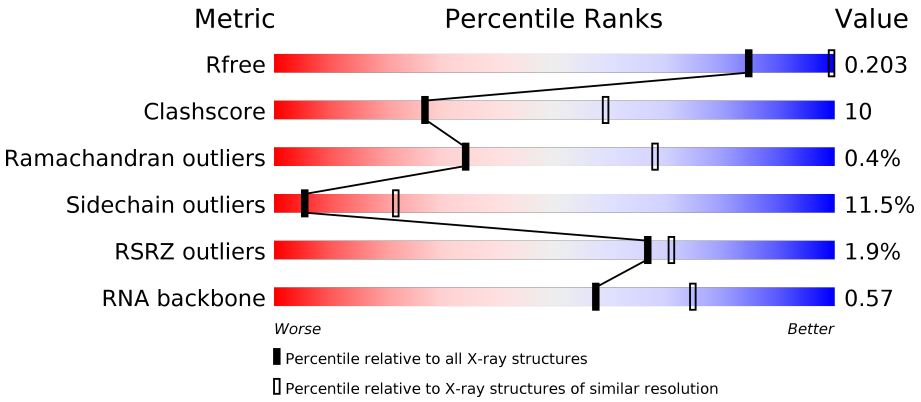
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA,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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.39 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	1691 (3.46-3.30)
Clashscore	141614	1762 (3.46-3.30)
Ramachandran outliers	138981	1732 (3.46-3.30)
Sidechain outliers	138945	1731 (3.46-3.30)
RSRZ outliers	127900	1635 (3.46-3.30)
RNA backbone	3102	1001 (3.80-2.96)

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

Mol	Chain	Length	Quality of chain
1	A	1522	56% 33% 9%
2	B	256	2% 59% 28% 9%
3	C	239	3% 50% 31% 5% 14%
4	D	209	3% 71% 26%

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Mol	Chain	Length	Quality of chain
5	E	162	60% 27% 5% 7%
6	F	101	69% 27%
7	G	156	4% 71% 28%
8	H	138	69% 26% 5%
9	I	128	3% 58% 38%
10	J	105	11% 48% 39% 7% 7%
11	K	129	64% 22% 10%
12	L	135	% 56% 31% 8%
13	M	126	4% 60% 29% 5% 6%
14	N	61	7% 57% 34% 7%
15	O	89	60% 35%
16	P	88	42% 47% 6% 6%
17	Q	105	70% 22% 6%
18	R	88	51% 26% 20%
19	S	93	5% 52% 29% 5% 14%
20	T	106	64% 24% 6% 7%
21	U	27	22% 59% 22% 7% 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	1624	-	-	-	X
22	MG	A	1628	-	-	-	X
22	MG	A	1638	-	-	-	X
22	MG	A	1656	-	-	-	X
22	MG	A	1686	-	-	-	X
22	MG	A	1698	-	-	-	X
22	MG	A	1712	-	-	-	X
22	MG	A	1719	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
22	MG	A	1736	-	-	-	X
22	MG	A	1739	-	-	-	X
22	MG	A	1745	-	-	-	X
22	MG	A	1751	-	-	-	X
22	MG	A	1756	-	-	-	X
22	MG	A	1768	-	-	-	X
22	MG	A	1771	-	-	-	X
22	MG	A	1845	-	-	-	X
22	MG	A	1873	-	-	-	X
22	MG	A	1880	-	-	-	X
22	MG	A	1882	-	-	-	X
22	MG	A	1884	-	-	-	X
22	MG	A	1888	-	-	-	X
22	MG	A	1890	-	-	-	X
22	MG	J	201	-	-	-	X
22	MG	P	104	-	-	-	X
22	MG	Q	202	-	-	-	X

2 Entry composition

There are 24 unique types of molecules in this entry. The entry contains 52584 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	32644	14540	6040	10546	1518	0	6	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	13	C	U	ENGINEERED MUTATION	GB M26923.1
A	1534	C	A	CONFLICT	GB M26923.1
A	1535	A	C	CONFLICT	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
5	E	150	Total	C	N	O	S	0	0	0
			1146	724	217	201	4			

- Molecule 6 is a protein called ribosomal protein S6.

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

- Molecule 7 is a protein called ribosomal protein S7.

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

- Molecule 8 is a protein called ribosomal protein S8.

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

- Molecule 9 is a protein called ribosomal protein S9.

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

- Molecule 10 is a protein called ribosomal protein S10.

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

- Molecule 11 is a protein called ribosomal protein S11.

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

- Molecule 12 is a protein called ribosomal protein S12.

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

- Molecule 13 is a protein called ribosomal protein S13.

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

- Molecule 14 is a protein called ribosomal protein S14.

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

- Molecule 15 is a protein called ribosomal protein S15.

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

- Molecule 16 is a protein called ribosomal protein S16.

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

- Molecule 17 is a protein called ribosomal protein S17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	Q	99	Total	C	N	O	S	0	0	0
			823	528	152	141	2			

There is a discrepancy between the modelled and reference sequences:

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

- Molecule 18 is a protein called ribosomal protein S18.

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

- Molecule 19 is a protein called ribosomal protein S19.

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

- Molecule 20 is a protein called ribosomal protein S20.

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

- Molecule 21 is a protein called ribosomal protein THX.

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

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
22	P	4	Total 4	Mg 4	0	0
22	G	1	Total 1	Mg 1	0	0
22	J	1	Total 1	Mg 1	0	0
22	Q	2	Total 2	Mg 2	0	0
22	D	4	Total 4	Mg 4	0	0
22	E	1	Total 1	Mg 1	0	0
22	B	2	Total 2	Mg 2	0	0
22	C	1	Total 1	Mg 1	0	0
22	A	293	Total 293	Mg 293	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
22	N	1	Total Mg 1 1	0	0
22	S	1	Total Mg 1 1	0	0
22	F	1	Total Mg 1 1	0	0

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

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

- Molecule 24 is water.

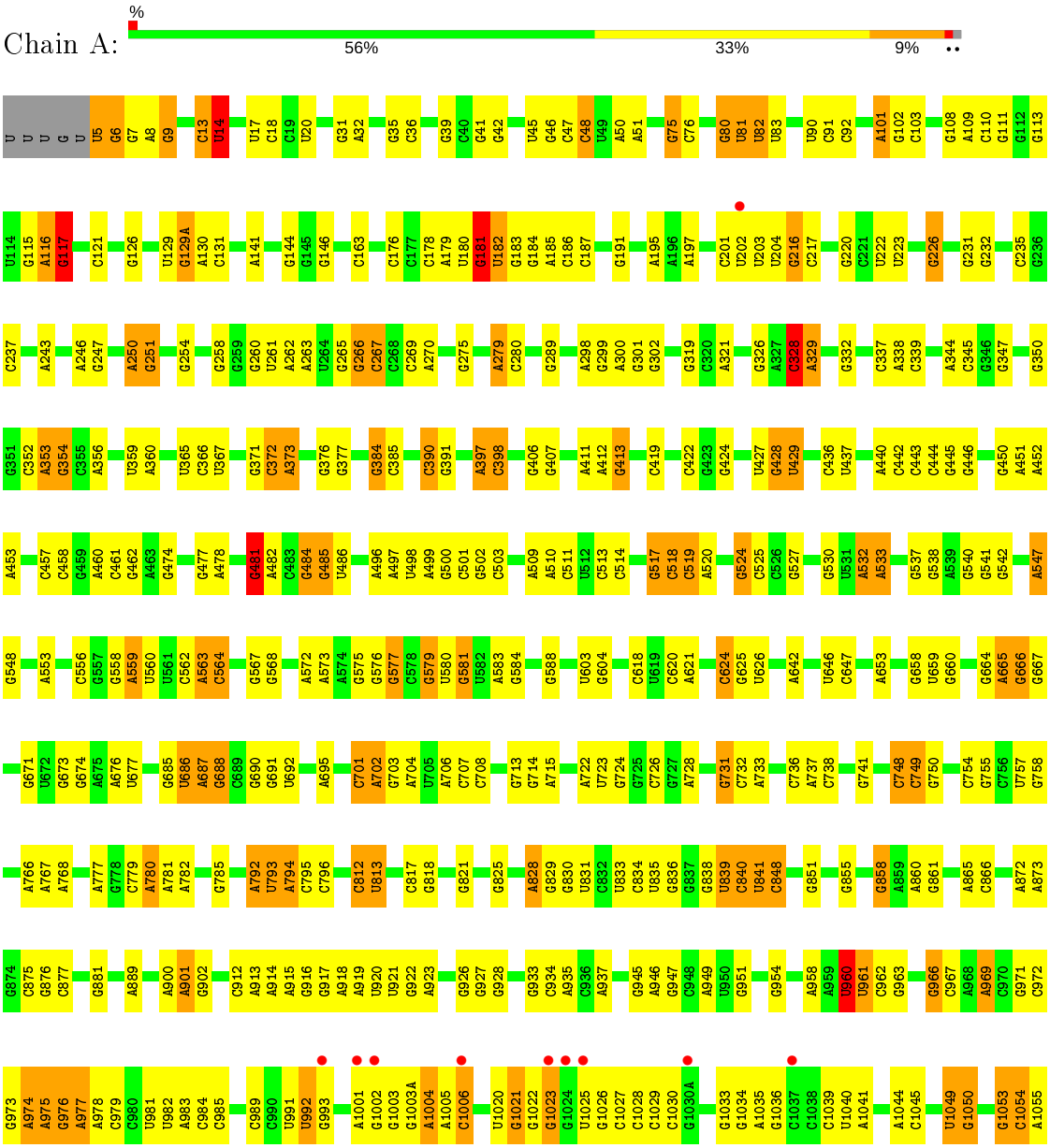
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
24	A	501	Total O 501 501	0	0
24	D	3	Total O 3 3	0	0
24	E	2	Total O 2 2	0	0
24	J	3	Total O 3 3	0	0
24	L	5	Total O 5 5	0	0
24	M	9	Total O 9 9	0	0
24	N	3	Total O 3 3	0	0
24	P	7	Total O 7 7	0	0
24	Q	1	Total O 1 1	0	0
24	S	3	Total O 3 3	0	0
24	T	1	Total O 1 1	0	0

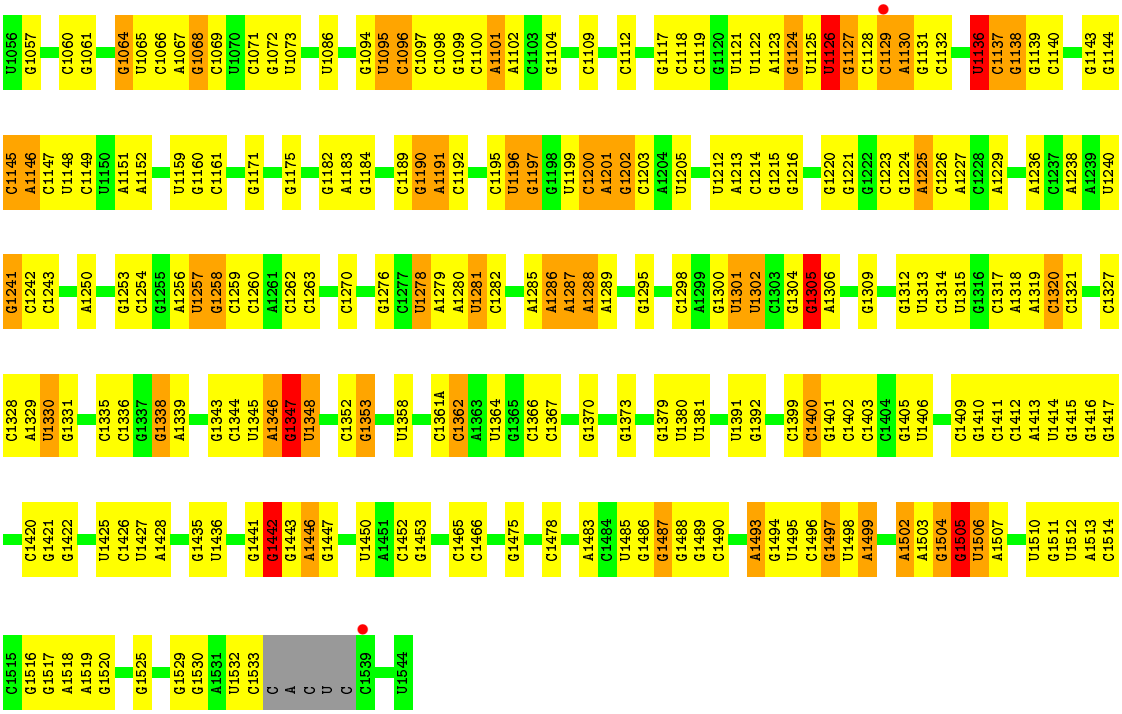
3 Residue-property plots (i)

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

- Molecule 1: 16S rRNA

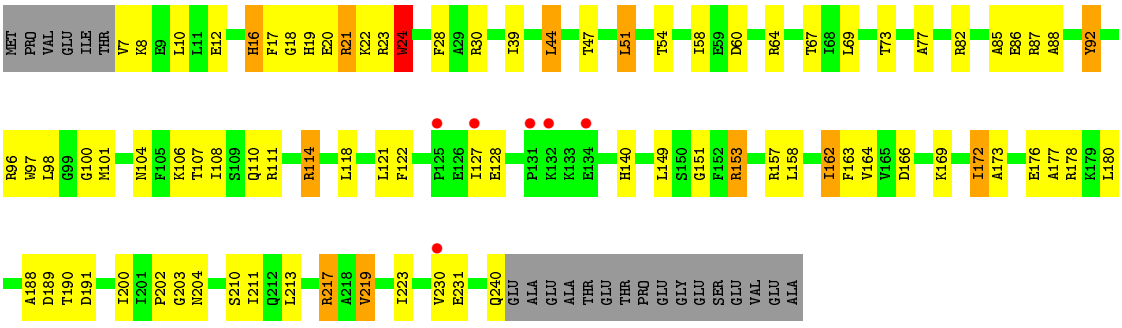
Chain A:





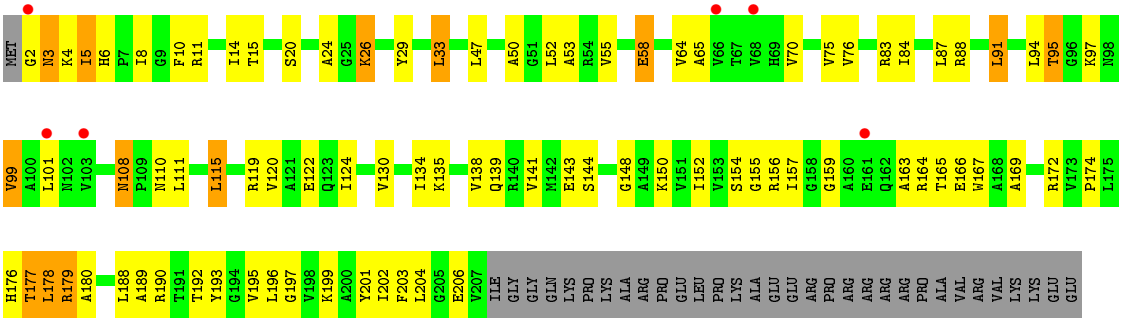
- Molecule 2: ribosomal protein S2

Chain B:



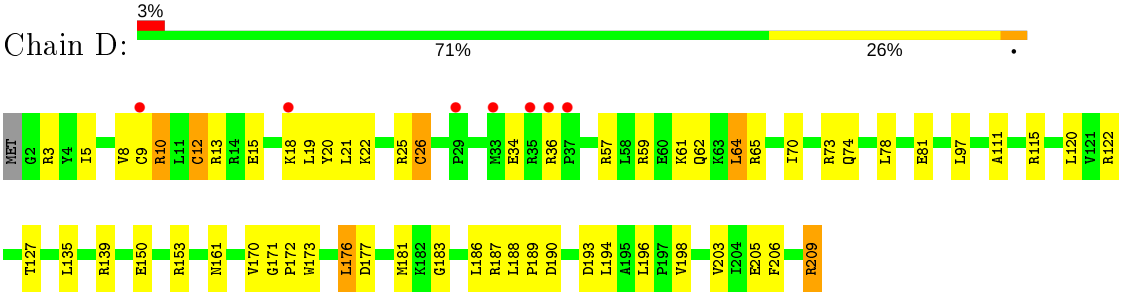
- Molecule 3: ribosomal protein S3

Chain C:



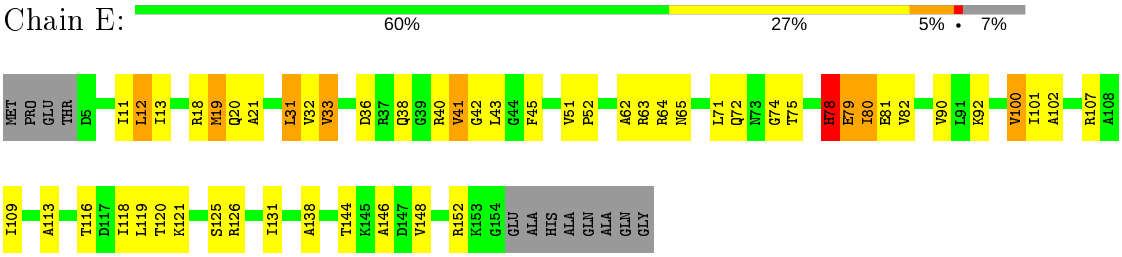
- Molecule 4: ribosomal protein S4

Chain D:



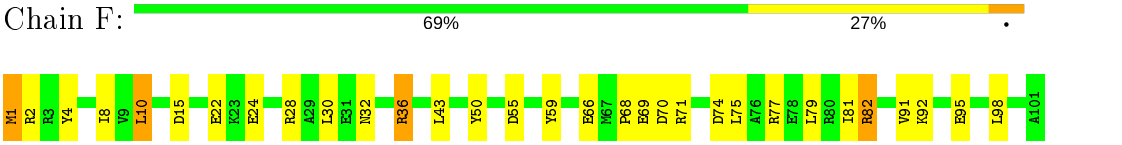
- Molecule 5: ribosomal protein S5

Chain E:



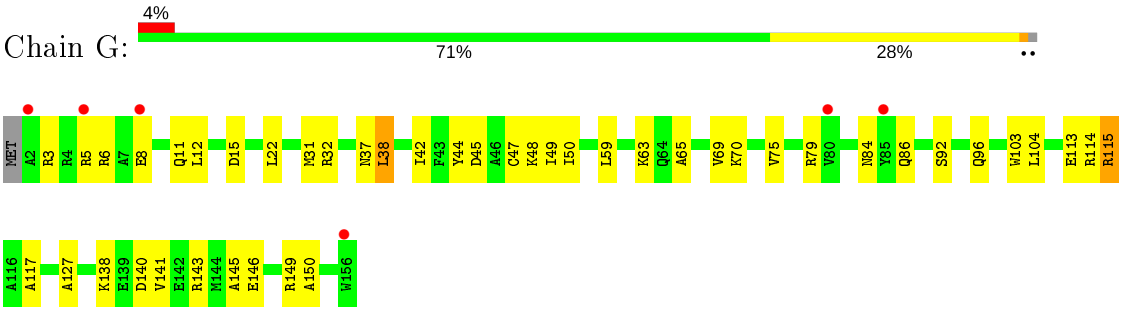
- Molecule 6: ribosomal protein S6

Chain F:



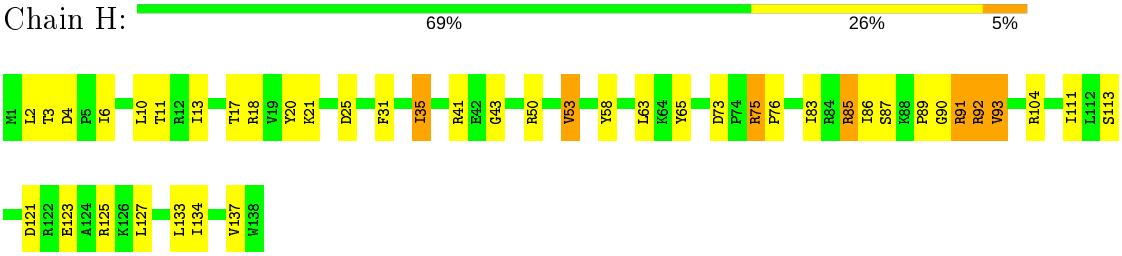
- Molecule 7: ribosomal protein S7

Chain G:



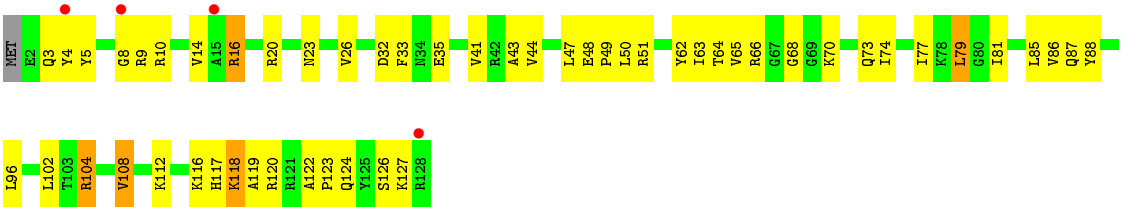
- Molecule 8: ribosomal protein S8

Chain H:



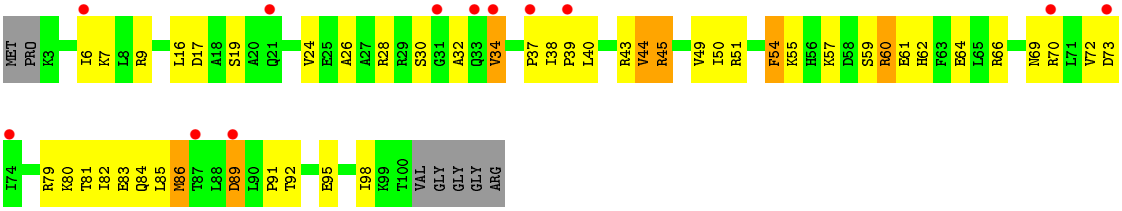
- Molecule 9: ribosomal protein S9

Chain I:



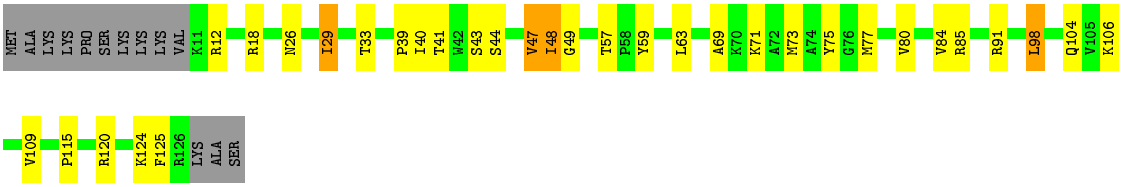
• Molecule 10: ribosomal protein S10

Chain J:



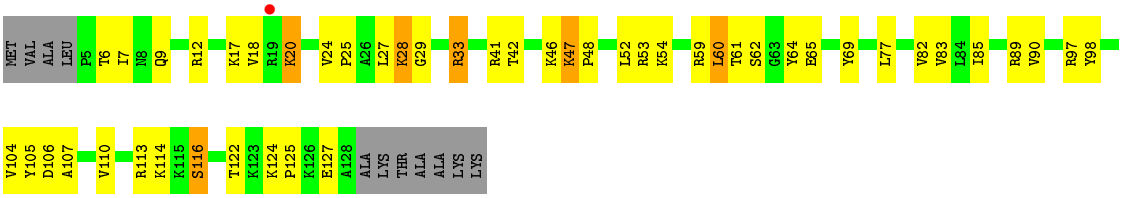
• Molecule 11: ribosomal protein S11

Chain K:



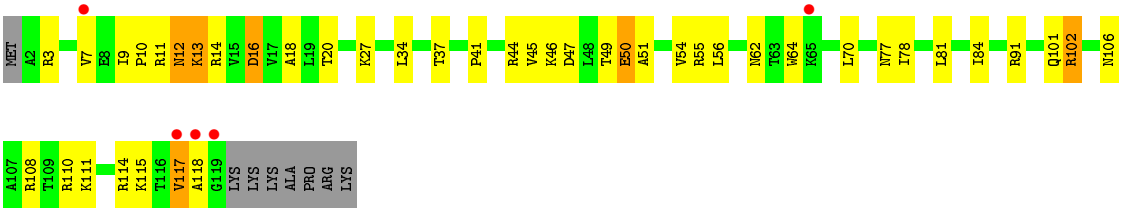
• Molecule 12: ribosomal protein S12

Chain L:



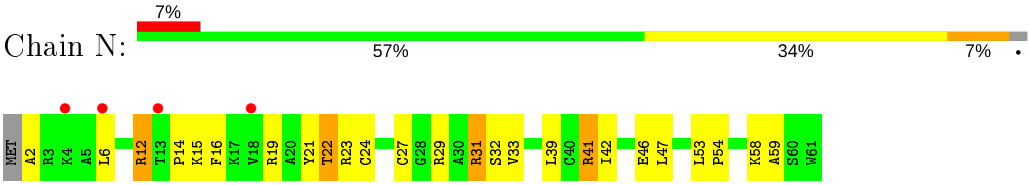
• Molecule 13: ribosomal protein S13

Chain M:



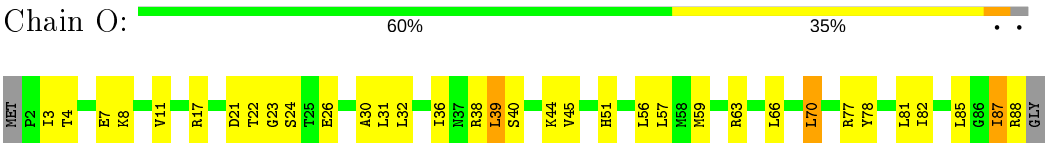
• Molecule 14: ribosomal protein S14

Chain N:



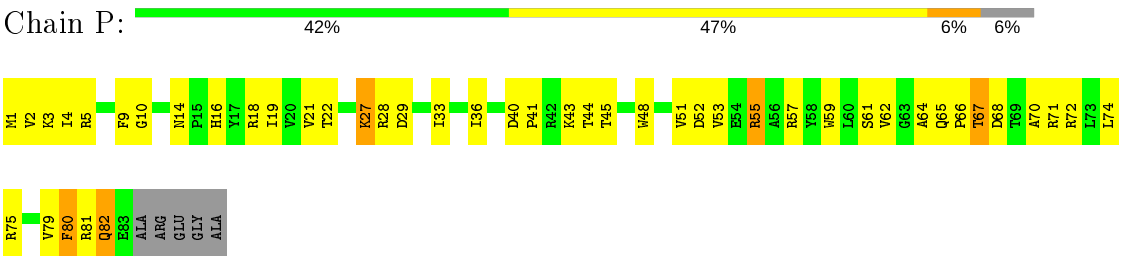
• Molecule 15: ribosomal protein S15

Chain O:



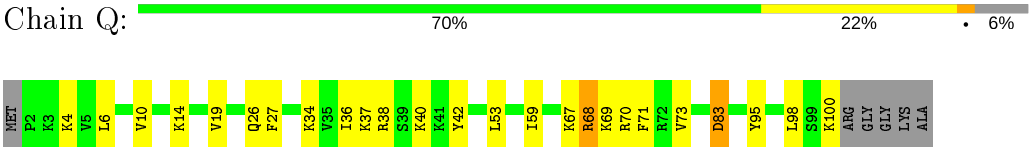
• Molecule 16: ribosomal protein S16

Chain P:



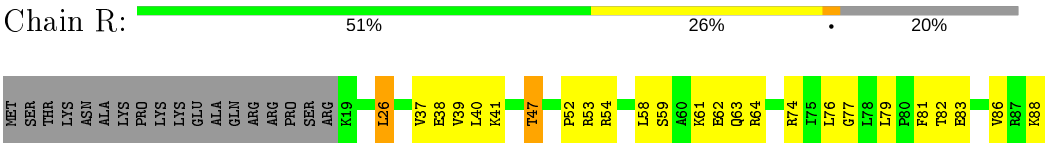
• Molecule 17: ribosomal protein S17

Chain Q:



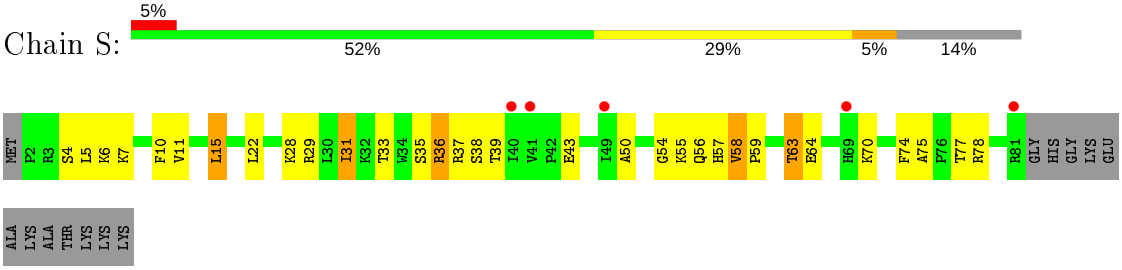
• Molecule 18: ribosomal protein S18

Chain R:



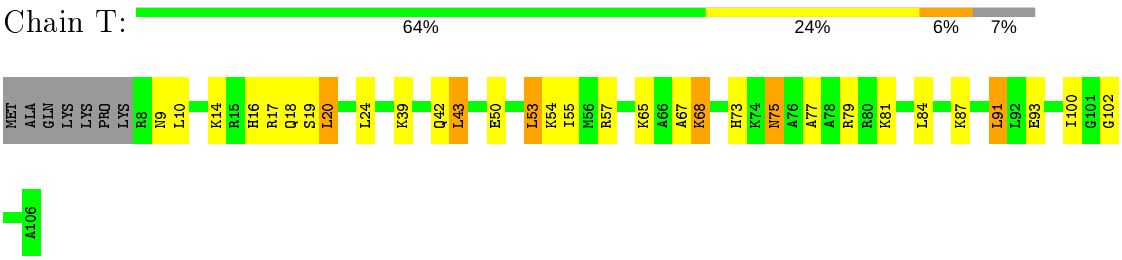
• Molecule 19: ribosomal protein S19

Chain S:



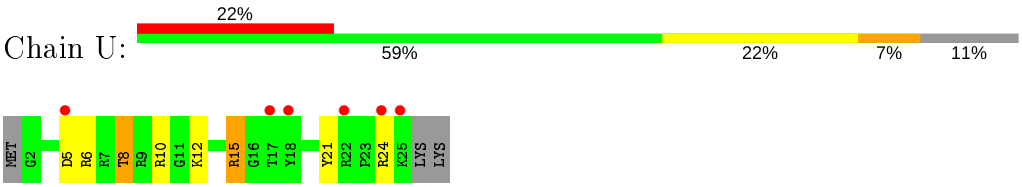
• Molecule 20: ribosomal protein S20

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	402.52Å 402.52Å 175.89Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	34.87 – 3.39 34.87 – 3.39	Depositor EDS
% Data completeness (in resolution range)	97.0 (34.87-3.39) 96.8 (34.87-3.39)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.90 (at 3.39Å)	Xtriage
Refinement program	PHENIX dev_978	Depositor
R, R_{free}	0.159 , 0.202 0.160 , 0.203	Depositor DCC
R_{free} test set	9698 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å^2)	124.2	Xtriage
Anisotropy	0.219	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.26 , 101.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	52584	wwPDB-VP
Average B, all atoms (Å^2)	141.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.56% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.51	1/36139 (0.0%)	0.91	46/56396 (0.1%)
2	B	0.36	0/1935	0.62	0/2609
3	C	0.31	0/1636	0.55	0/2205
4	D	0.41	1/1733 (0.1%)	0.58	1/2318 (0.0%)
5	E	0.48	0/1162	0.72	1/1564 (0.1%)
6	F	0.30	0/856	0.53	0/1154
7	G	0.35	0/1276	0.54	0/1709
8	H	0.46	0/1136	0.66	0/1527
9	I	0.29	0/1029	0.53	0/1379
10	J	0.33	0/805	0.62	0/1082
11	K	0.37	0/879	0.60	0/1187
12	L	0.40	0/977	0.67	0/1306
13	M	0.32	0/947	0.56	0/1270
14	N	0.33	0/501	0.58	0/664
15	O	0.38	0/740	0.57	0/987
16	P	0.40	0/716	0.67	0/963
17	Q	0.43	0/836	0.66	0/1117
18	R	0.37	0/579	0.55	0/768
19	S	0.29	0/661	0.56	0/890
20	T	0.39	0/765	0.66	0/1007
21	U	0.30	0/212	0.53	0/277
All	All	0.47	2/55520 (0.0%)	0.83	48/82379 (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	1
3	C	0	2

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Mol	Chain	#Chirality outliers	#Planarity outliers
5	E	0	1
8	H	0	1
10	J	0	1
20	T	0	1
All	All	0	7

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	279	A	N9-C4	-6.74	1.33	1.37
4	D	12	CYS	CB-SG	5.31	1.91	1.82

All (48) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	14	U	C5-C6-N1	9.14	127.27	122.70
1	A	328	C	N1-C2-O2	8.92	124.25	118.90
1	A	328	C	N3-C2-O2	-8.29	116.10	121.90
1	A	117	G	N1-C6-O6	8.23	124.84	119.90
1	A	1136	U	C2-N1-C1'	8.22	127.57	117.70
1	A	1505	G	C8-N9-C4	-7.66	103.34	106.40
1	A	328	C	C2-N1-C1'	7.49	127.04	118.80
1	A	1136	U	N1-C2-O2	7.29	127.91	122.80
1	A	1126	U	C2-N1-C1'	7.24	126.39	117.70
1	A	279	A	C5-N7-C8	-7.15	100.32	103.90
1	A	1064	G	N3-C4-N9	-6.82	121.91	126.00
1	A	1502	A	C6-C5-N7	-6.67	127.63	132.30
1	A	1502	A	C5-N7-C8	-6.66	100.57	103.90
1	A	279	A	C2-N3-C4	-6.66	107.27	110.60
1	A	624	C	C6-N1-C2	6.61	122.94	120.30
1	A	14	U	C6-N1-C2	-6.35	117.19	121.00
1	A	1502	A	C4-C5-N7	6.11	113.75	110.70
1	A	1502	A	N1-C6-N6	6.08	122.25	118.60
1	A	117	G	C6-C5-N7	-6.02	126.79	130.40
1	A	266	G	C5-N7-C8	-5.99	101.31	104.30
1	A	875	C	C6-N1-C2	5.90	122.66	120.30
1	A	328	C	C6-N1-C2	-5.89	117.94	120.30
1	A	1126	U	N1-C2-O2	5.86	126.90	122.80
1	A	1136	U	N3-C2-O2	-5.81	118.13	122.20
1	A	960	U	N1-C2-O2	5.73	126.81	122.80
1	A	1136	U	C6-N1-C1'	-5.71	113.20	121.20
1	A	722	A	N1-C6-N6	5.59	121.95	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	D	12	CYS	CA-CB-SG	5.57	124.03	114.00
1	A	1064	G	N3-C2-N2	-5.55	116.01	119.90
1	A	1502	A	C2-N3-C4	-5.55	107.83	110.60
1	A	481	G	N3-C4-N9	5.55	129.33	126.00
1	A	1305	G	C4-N9-C1'	5.52	133.67	126.50
1	A	117	G	C5-C6-O6	-5.47	125.32	128.60
1	A	1502	A	N7-C8-N9	5.41	116.51	113.80
1	A	577	G	C8-N9-C4	5.25	108.50	106.40
1	A	266	G	C4-C5-N7	5.21	112.89	110.80
1	A	1126	U	C6-N1-C1'	-5.19	113.94	121.20
1	A	1347	G	C4-N9-C1'	-5.16	119.80	126.50
1	A	1346	A	P-O3'-C3'	5.16	125.89	119.70
1	A	1442	G	C4-N9-C1'	5.11	133.14	126.50
1	A	722	A	C2-N3-C4	-5.09	108.05	110.60
1	A	181	G	N3-C4-C5	-5.08	126.06	128.60
1	A	1136	U	C5-C6-N1	5.06	125.23	122.70
1	A	280	C	C6-N1-C2	5.06	122.32	120.30
1	A	901	A	C2-N3-C4	-5.05	108.08	110.60
1	A	754	C	C2-N1-C1'	5.04	124.35	118.80
1	A	365	U	C2-N1-C1'	5.03	123.73	117.70
5	E	41	VAL	CB-CA-C	-5.02	101.86	111.40

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	16	HIS	Peptide
3	C	166	GLU	Peptide
3	C	179	ARG	Peptide
5	E	78	HIS	Peptide
8	H	90	GLY	Peptide
10	J	86	MET	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	32644	0	16508	437	0
2	B	1900	0	1951	55	0
3	C	1612	0	1677	67	0
4	D	1703	0	1763	35	0
5	E	1146	0	1207	33	0
6	F	843	0	857	19	0
7	G	1257	0	1296	23	0
8	H	1116	0	1177	29	0
9	I	1010	0	1037	33	0
10	J	792	0	835	33	0
11	K	864	0	881	25	0
12	L	972	0	1058	34	0
13	M	937	0	995	24	0
14	N	492	0	529	20	0
15	O	729	0	768	20	0
16	P	700	0	720	36	0
17	Q	823	0	893	19	0
18	R	574	0	644	14	0
19	S	647	0	673	26	0
20	T	763	0	861	22	0
21	U	208	0	221	8	0
22	A	293	0	0	0	0
22	B	2	0	0	0	0
22	C	1	0	0	0	0
22	D	4	0	0	0	0
22	E	1	0	0	0	0
22	F	1	0	0	0	0
22	G	1	0	0	0	0
22	J	1	0	0	0	0
22	N	1	0	0	0	0
22	P	4	0	0	0	0
22	Q	2	0	0	0	0
22	S	1	0	0	0	0
23	D	1	0	0	0	0
23	N	1	0	0	0	0
24	A	501	0	0	12	0
24	D	3	0	0	0	0
24	E	2	0	0	0	0
24	J	3	0	0	1	0
24	L	5	0	0	0	0
24	M	9	0	0	1	0
24	N	3	0	0	0	0
24	P	7	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
24	Q	1	0	0	0	0
24	S	3	0	0	0	0
24	T	1	0	0	0	0
All	All	52584	0	36551	889	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 10.

All (889) 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:481:G:HO2'	1:A:482:A:H8	1.07	0.99
20:T:100:ILE:HG22	20:T:102:GLY:H	1.35	0.89
1:A:235:C:H5'	17:Q:70:ARG:HG3	1.54	0.89
1:A:664:G:H22	1:A:741:G:H1	1.20	0.87
1:A:427:U:OP1	4:D:13:ARG:NH2	2.13	0.82
1:A:1126:U:O4	1:A:1127:G:N2	2.14	0.79
14:N:12:ARG:HH11	14:N:14:PRO:HG3	1.48	0.78
3:C:58:GLU:HB3	10:J:92:THR:HG21	1.65	0.77
1:A:279:A:OP2	17:Q:95:TYR:OH	2.02	0.77
1:A:537:G:OP1	12:L:113:ARG:NH2	2.18	0.76
18:R:47:THR:HA	18:R:83:GLU:HB2	1.68	0.76
1:A:1502:A:H2	1:A:1505:G:H1	1.33	0.75
12:L:27:LEU:O	12:L:29:GLY:N	2.19	0.75
1:A:1195:C:H3'	1:A:1196:U:H5"	1.66	0.75
1:A:928:G:O2'	1:A:1533:C:OP1	2.04	0.75
6:F:2:ARG:HE	6:F:69:GLU:HG2	1.52	0.74
1:A:13:C:O2'	1:A:14:U:O5'	2.06	0.74
1:A:1256:A:H5'	1:A:1258:G:H1'	1.69	0.74
1:A:390:C:O3'	16:P:28:ARG:NH2	2.21	0.74
1:A:298:A:N6	24:A:2044:HOH:O	2.20	0.74
16:P:80:PHE:N	24:P:207:HOH:O	2.20	0.73
1:A:226:G:N2	24:A:2215:HOH:O	2.03	0.73
6:F:8:ILE:HD11	6:F:79:LEU:HD13	1.72	0.72
1:A:250:A:H4'	1:A:251:G:O5'	1.90	0.72
1:A:962:C:O2'	24:A:2129:HOH:O	2.08	0.72
1:A:692:U:OP1	11:K:124:LYS:NZ	2.22	0.72
2:B:16:HIS:HD2	2:B:204:ASN:H	1.35	0.72
13:M:10:PRO:HB2	13:M:18:ALA:HB1	1.72	0.71
1:A:1443:G:H5"	1:A:1446:A:H5'	1.73	0.71
1:A:1205:U:OP1	3:C:190:ARG:NH2	2.22	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:542:G:OP1	4:D:10:ARG:NH2	2.25	0.70
1:A:1525:G:OP1	11:K:120:ARG:NH2	2.23	0.70
1:A:1028:C:N3	1:A:1033:G:N2	2.37	0.70
19:S:33:THR:HG22	19:S:35:SER:H	1.56	0.70
1:A:31:G:N2	1:A:48:C:OP1	2.22	0.70
1:A:20:U:H3	1:A:915:A:H61	1.38	0.70
1:A:912:C:OP1	12:L:46:LYS:NZ	2.25	0.70
10:J:6:ILE:HB	10:J:72:VAL:HB	1.71	0.70
1:A:1504:G:OP1	1:A:1507:A:H4'	1.92	0.70
1:A:835:U:OP1	18:R:64:ARG:NH2	2.25	0.69
19:S:55:LYS:HG3	19:S:56:GLN:HG3	1.73	0.69
12:L:24:VAL:HG13	12:L:98:TYR:HE2	1.57	0.69
1:A:1347:G:O6	9:I:10:ARG:NH2	2.26	0.69
1:A:452:A:O2'	1:A:453:A:O4'	2.06	0.68
1:A:1366:C:O2'	10:J:60:ARG:NH2	2.26	0.68
2:B:16:HIS:CD2	2:B:204:ASN:H	2.10	0.68
7:G:70:LYS:HE2	7:G:96:GLN:HB3	1.74	0.68
7:G:15:ASP:OD2	7:G:44:TYR:OH	2.12	0.67
3:C:130:VAL:HG21	3:C:157:ILE:HG23	1.76	0.67
3:C:88:ARG:HD2	3:C:101:LEU:H	1.60	0.67
1:A:1498:UR3:O2'	1:A:1499:A:OP2	2.07	0.66
6:F:30:LEU:HD23	6:F:75:LEU:HD21	1.78	0.66
10:J:40:LEU:HB2	10:J:69:ASN:HB2	1.77	0.66
1:A:1435:G:H2'	1:A:1436:U:C6	2.30	0.66
9:I:44:VAL:HG22	9:I:51:ARG:HH12	1.61	0.66
2:B:60:ASP:OD1	2:B:64:ARG:NH1	2.27	0.66
1:A:1399:C:H4'	1:A:1400:5MC:H5"	1.76	0.66
1:A:975:A:H5'	1:A:975:A:H8	1.61	0.66
1:A:1006:C:H42	1:A:1022:G:H22	1.43	0.65
10:J:79:ARG:O	10:J:83:GLU:N	2.27	0.65
1:A:1327:C:OP2	21:U:12:LYS:NZ	2.28	0.65
2:B:101:MET:HA	2:B:108:ILE:HG13	1.79	0.65
10:J:80:LYS:H	10:J:80:LYS:HD2	1.62	0.65
12:L:89:ARG:HG2	12:L:97:ARG:HA	1.78	0.65
3:C:14:ILE:HG22	3:C:15:THR:HG23	1.78	0.65
15:O:39:LEU:HB3	15:O:56:LEU:HD12	1.78	0.65
24:A:2335:HOH:O	16:P:75:ARG:HG3	1.96	0.65
1:A:1409:C:H2'	1:A:1410:G:H8	1.62	0.65
2:B:87:ARG:HH21	2:B:219:VAL:HG23	1.62	0.65
1:A:1003:G:N2	1:A:1039:C:O2	2.31	0.64
2:B:122:PHE:HA	2:B:127:ILE:HD11	1.78	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:462:G:H21	16:P:82:GLN:HE21	1.44	0.64
16:P:75:ARG:HA	24:P:206:HOH:O	1.97	0.64
1:A:1060:C:C5	3:C:2:GLY:HA3	2.33	0.64
7:G:79:ARG:HD3	7:G:84:ASN:HB3	1.79	0.64
1:A:1195:C:H3'	1:A:1196:U:C5'	2.28	0.64
10:J:19:SER:HB2	10:J:91:PRO:HG2	1.80	0.64
4:D:150:GLU:CD	4:D:150:GLU:H	2.01	0.64
20:T:67:ALA:HA	20:T:73:HIS:H	1.61	0.64
1:A:13:C:HO2'	1:A:14:U:H6	1.45	0.63
1:A:989:C:O2	1:A:1216:G:N2	2.29	0.63
3:C:150:LYS:HG3	3:C:169:ALA:HB2	1.80	0.63
1:A:975:A:HO2'	14:N:32:SER:HG	1.44	0.63
1:A:45:U:H2'	1:A:46:G:C8	2.34	0.63
5:E:11:ILE:HB	5:E:31:LEU:HB3	1.81	0.63
1:A:1415:G:H2'	1:A:1416:G:H8	1.64	0.63
17:Q:4:LYS:HD3	17:Q:6:LEU:HD21	1.80	0.62
13:M:34:LEU:HD13	13:M:41:PRO:HA	1.82	0.62
16:P:22:THR:HA	16:P:33:ILE:HG13	1.81	0.62
1:A:1347:G:O2'	1:A:1348:U:OP2	2.18	0.62
1:A:1425:U:H3	1:A:1475:G:H1	1.46	0.62
1:A:411:A:N3	1:A:413:G:O2'	2.24	0.62
5:E:101:ILE:O	5:E:120:THR:HB	1.99	0.62
6:F:70:ASP:N	6:F:70:ASP:OD1	2.33	0.62
3:C:156:ARG:H	3:C:163:ALA:HA	1.64	0.62
1:A:1022:G:N2	1:A:1023:G:N7	2.43	0.61
2:B:240:GLN:OE1	2:B:240:GLN:N	2.31	0.61
2:B:85:ALA:HB3	2:B:92:TYR:HD2	1.63	0.61
3:C:33:LEU:HD21	14:N:53:LEU:HD22	1.81	0.61
1:A:973:G:H3'	1:A:974:A:H5"	1.83	0.61
4:D:15:GLU:OE1	4:D:59:ARG:NH2	2.33	0.61
11:K:44:SER:H	11:K:47:VAL:HB	1.65	0.61
1:A:532:A:N6	3:C:159:GLY:O	2.33	0.61
16:P:19:ILE:HG22	16:P:36:ILE:HG13	1.82	0.61
1:A:1392:G:H21	1:A:1502:A:H8	1.46	0.61
1:A:677:U:H3	1:A:713:G:H22	1.47	0.61
1:A:1498:UR3:O4'	1:A:1519[A]:MA6:H2	2.01	0.61
1:A:992:U:H3	1:A:1044:A:H62	1.47	0.61
1:A:8:A:C6	4:D:209:ARG:HB2	2.35	0.61
1:A:1147:C:O2'	9:I:5:TYR:OH	2.19	0.61
6:F:74:ASP:HA	6:F:77:ARG:HH11	1.66	0.61
11:K:69:ALA:O	11:K:73:MET:HG2	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:97:TRP:HH2	2:B:176:GLU:CD	2.04	0.61
1:A:836:G:OP1	18:R:61:LYS:NZ	2.24	0.60
3:C:179:ARG:HD2	3:C:206:GLU:HG3	1.82	0.60
1:A:275:G:H5'	17:Q:14:LYS:HD3	1.83	0.60
1:A:501:C:H2'	1:A:502:G:C8	2.37	0.60
1:A:792:A:H4'	1:A:793:U:O5'	2.01	0.60
10:J:50:ILE:H	10:J:50:ILE:HD12	1.66	0.60
13:M:49:THR:HG22	13:M:51:ALA:H	1.65	0.60
17:Q:59:ILE:HG23	17:Q:71:PHE:HD1	1.67	0.60
1:A:501:C:H2'	1:A:502:G:H8	1.66	0.59
12:L:6:THR:OG1	12:L:9:GLN:HG3	2.01	0.59
1:A:1286:A:H2'	1:A:1287:A:H4'	1.83	0.59
1:A:263:A:OP2	20:T:79:ARG:NH1	2.35	0.59
4:D:64:LEU:HG	4:D:198:VAL:HG11	1.84	0.59
9:I:43:ALA:HA	9:I:74:ILE:HD13	1.84	0.59
15:O:87:ILE:HG22	15:O:88:ARG:H	1.67	0.59
1:A:532:A:O2'	1:A:533:A:OP1	2.15	0.59
1:A:979:C:O2	14:N:19:ARG:NE	2.34	0.59
8:H:85:ARG:NE	8:H:87:SER:O	2.36	0.59
1:A:830:G:H5"	2:B:22:LYS:HE2	1.83	0.59
9:I:26:VAL:HB	9:I:33:PHE:HB2	1.84	0.59
11:K:41:THR:HG21	11:K:71:LYS:HB3	1.84	0.59
1:A:1392:G:N2	1:A:1502:A:H8	2.00	0.58
1:A:673:G:H2'	1:A:674:G:C8	2.37	0.58
1:A:113:G:H1'	1:A:354:G:H5'	1.84	0.58
1:A:1338:G:H2'	1:A:1339:A:C8	2.38	0.58
13:M:16:ASP:OD1	13:M:16:ASP:N	2.35	0.58
1:A:376:G:H5"	16:P:5:ARG:HD2	1.84	0.58
1:A:1254:C:H41	10:J:43:ARG:HH12	1.51	0.58
1:A:975:A:H5'	1:A:975:A:C8	2.39	0.58
6:F:1:MET:SD	6:F:1:MET:N	2.71	0.58
1:A:1505:G:O2'	1:A:1506:U:OP2	2.21	0.58
16:P:79:VAL:N	24:P:207:HOH:O	2.37	0.58
1:A:581:G:N7	24:A:1969:HOH:O	2.32	0.58
1:A:9:G:OP2	5:E:121:LYS:NZ	2.19	0.58
6:F:2:ARG:NE	6:F:69:GLU:HG2	2.17	0.58
1:A:1101:A:H4'	1:A:1102:A:O5'	2.04	0.58
1:A:353:A:H5'	1:A:353:A:H8	1.69	0.58
1:A:748:C:H4'	1:A:749:C:O5'	2.03	0.57
12:L:85:ILE:HG23	12:L:98:TYR:HB3	1.86	0.57
13:M:108:ARG:NH2	13:M:111:LYS:HD2	2.19	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:Q:95:TYR:HA	17:Q:98:LEU:HD13	1.86	0.57
1:A:1049:U:H4'	1:A:1050:G:O5'	2.03	0.57
10:J:49:VAL:HG13	14:N:41:ARG:HB2	1.86	0.57
16:P:28:ARG:NH1	16:P:29:ASP:OD2	2.38	0.57
1:A:1510:U:H2'	1:A:1511:G:C8	2.40	0.57
1:A:1405:G:O2'	1:A:1518[B]:MA6:O2'	2.22	0.57
1:A:1143:G:H2'	1:A:1144:G:C8	2.39	0.57
3:C:155:GLY:HA3	3:C:163:ALA:HB1	1.85	0.57
1:A:191:G:O2'	20:T:102:GLY:O	2.14	0.57
12:L:24:VAL:HG13	12:L:98:TYR:CE2	2.39	0.57
1:A:450:G:H4'	16:P:41:PRO:HB2	1.87	0.57
1:A:1391:U:H2'	1:A:1392:G:C8	2.40	0.57
1:A:126:G:N2	24:A:2343:HOH:O	2.37	0.57
1:A:949:A:OP1	13:M:101:GLN:HB3	2.05	0.57
15:O:39:LEU:HD13	15:O:56:LEU:HB2	1.87	0.57
9:I:8:GLY:HA2	9:I:79:LEU:HD13	1.86	0.57
1:A:666:G:H5'	1:A:726:C:H1'	1.87	0.56
13:M:3:ARG:HH21	13:M:7:VAL:HG12	1.70	0.56
1:A:923:A:OP1	5:E:21:ALA:HB2	2.04	0.56
2:B:86:GLU:HG3	2:B:92:TYR:HE2	1.70	0.56
3:C:26:LYS:HD3	10:J:45:ARG:HH21	1.70	0.56
1:A:1100:C:H3'	24:A:2244:HOH:O	2.05	0.56
1:A:1313:U:O4	19:S:4:SER:OG	2.11	0.56
16:P:21:VAL:HG12	16:P:33:ILE:HD12	1.88	0.56
8:H:10:LEU:HD22	8:H:83:ILE:HD11	1.87	0.56
1:A:1488:G:H2'	1:A:1489:G:C8	2.40	0.56
5:E:81:GLU:HG2	5:E:90:VAL:HG22	1.86	0.56
1:A:1136:U:H2'	1:A:1136:U:O2	2.06	0.56
1:A:1502:A:H2	1:A:1505:G:N1	2.03	0.56
1:A:538:G:H5"	12:L:114:LYS:HB2	1.86	0.56
1:A:840:C:H5"	1:A:841:U:OP1	2.05	0.56
12:L:33:ARG:HD3	12:L:62:SER:HB3	1.88	0.56
1:A:1223:C:OP2	19:S:78:ARG:NH2	2.38	0.56
1:A:390:C:H2'	1:A:391:G:C8	2.40	0.56
20:T:65:LYS:O	20:T:68:LYS:HB3	2.06	0.56
3:C:180:ALA:HB1	3:C:203:PHE:CE1	2.41	0.56
1:A:707:C:OP1	11:K:85:ARG:NH1	2.38	0.56
1:A:13:C:O2'	1:A:14:U:H6	1.88	0.56
3:C:52:LEU:HD13	3:C:55:VAL:HG23	1.87	0.56
1:A:1055:A:O2'	3:C:156:ARG:NH1	2.38	0.55
15:O:36:ILE:HD13	15:O:59:MET:HE3	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:64:GLU:OE2	10:J:66:ARG:NH2	2.38	0.55
10:J:81:THR:O	10:J:85:LEU:HG	2.05	0.55
1:A:1402:4OC:H2'	1:A:1403:C:O4'	2.05	0.55
4:D:173:TRP:CD1	4:D:189:PRO:HG3	2.42	0.55
1:A:110:C:H2'	1:A:111:G:O4'	2.06	0.55
1:A:1412:C:H2'	1:A:1413:A:C8	2.42	0.55
4:D:18:LYS:HE2	4:D:20:TYR:HE2	1.71	0.55
16:P:74:LEU:HB3	16:P:79:VAL:HG21	1.87	0.55
4:D:176:LEU:HA	4:D:183:GLY:HA2	1.88	0.55
1:A:1213:A:N1	1:A:1215:G:H1'	2.22	0.55
1:A:1301:U:O2'	1:A:1302:U:H3'	2.06	0.55
1:A:518:C:H4'	1:A:519:C:O5'	2.07	0.55
2:B:16:HIS:HD2	2:B:204:ASN:HD22	1.55	0.55
1:A:35:G:H2'	1:A:36:C:C6	2.42	0.55
1:A:793:U:H4'	1:A:794:A:OP2	2.05	0.55
6:F:77:ARG:O	6:F:81:ILE:HG13	2.06	0.55
1:A:1147:C:HO2'	9:I:5:TYR:HH	1.48	0.54
3:C:111:LEU:HD21	3:C:144:SER:O	2.07	0.54
1:A:1145:C:O2'	1:A:1146:A:H8	1.90	0.54
1:A:1415:G:H2'	1:A:1416:G:C8	2.42	0.54
1:A:1406:U:O2'	1:A:1517[B]:G:N2	2.39	0.54
14:N:21:TYR:CE2	14:N:23:ARG:HG3	2.41	0.54
1:A:1068:G:H8	1:A:1068:G:OP2	1.91	0.54
2:B:162:ILE:HD12	2:B:177:ALA:HB2	1.89	0.54
1:A:685:G:C2'	1:A:686:U:H5"	2.37	0.54
2:B:16:HIS:CE1	2:B:210:SER:HB2	2.41	0.54
3:C:6:HIS:HD2	3:C:8:ILE:H	1.53	0.54
6:F:10:LEU:HD12	6:F:59:TYR:HB3	1.90	0.54
1:A:1118:C:H2'	1:A:1119:C:C6	2.42	0.54
1:A:1409:C:H2'	1:A:1410:G:C8	2.42	0.54
5:E:152:ARG:HB3	8:H:43:GLY:HA3	1.90	0.54
6:F:68:PRO:HB2	6:F:71:ARG:HG3	1.90	0.54
10:J:62:HIS:HB3	14:N:59:ALA:HB3	1.90	0.54
5:E:80:ILE:HD13	5:E:138:ALA:HB1	1.88	0.54
8:H:121:ASP:HB2	8:H:125:ARG:HH22	1.73	0.54
17:Q:59:ILE:HD12	17:Q:73:VAL:HA	1.88	0.54
1:A:109:A:H2'	1:A:326:G:N2	2.23	0.54
1:A:328:C:O2	1:A:328:C:H2'	2.08	0.54
1:A:372:C:H4'	1:A:373:A:O5'	2.07	0.54
3:C:91:LEU:HD21	3:C:99:VAL:HG22	1.89	0.54
1:A:951:G:OP2	13:M:102:ARG:NH2	2.41	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1137:C:O2'	1:A:1138:G:N2	2.41	0.53
1:A:269:C:H2'	1:A:270:A:C8	2.43	0.53
1:A:524:G:H2'	1:A:525:C:C6	2.42	0.53
1:A:839:U:H5'	1:A:840:C:C5	2.43	0.53
6:F:4:TYR:CE1	6:F:92:LYS:HG2	2.43	0.53
8:H:83:ILE:HG13	8:H:137:VAL:HG22	1.89	0.53
2:B:47:THR:O	2:B:51:LEU:HB2	2.09	0.53
1:A:839:U:H5'	1:A:840:C:H5	1.73	0.53
19:S:11:VAL:HG13	19:S:38:SER:HB2	1.91	0.53
12:L:25:PRO:C	12:L:27:LEU:H	2.08	0.53
5:E:12:LEU:HD13	5:E:31:LEU:HB2	1.91	0.53
1:A:1221:G:OP2	19:S:37:ARG:NH2	2.42	0.53
12:L:113:ARG:NH1	12:L:116:SER:H	2.06	0.53
1:A:1327:C:P	21:U:12:LYS:HZ1	2.31	0.53
1:A:1001:A:H2'	1:A:1002:G:C8	2.44	0.53
1:A:1281:U:O4	10:J:7:LYS:NZ	2.41	0.52
1:A:1305:G:N2	1:A:1331:G:H1'	2.24	0.52
1:A:144:G:H1	1:A:178:C:H42	1.57	0.52
1:A:1495:U:H2'	1:A:1496:C:C6	2.44	0.52
1:A:667:G:H4'	15:O:51:HIS:CE1	2.44	0.52
1:A:91:C:H2'	1:A:92:C:H6	1.73	0.52
13:M:37:THR:O	13:M:55:ARG:NH2	2.42	0.52
10:J:24:VAL:HG13	10:J:34:VAL:HG11	1.91	0.52
10:J:9:ARG:HG3	10:J:95:GLU:HB3	1.91	0.52
11:K:84:VAL:HG11	11:K:91:ARG:HD3	1.91	0.52
1:A:1347:G:O2'	1:A:1348:U:P	2.68	0.52
1:A:812:C:H4'	1:A:813:U:O5'	2.09	0.52
1:A:960:U:H1'	1:A:1223:C:H5'	1.91	0.52
1:A:1191:A:OP1	3:C:3:ASN:ND2	2.43	0.52
11:K:57:THR:HG22	11:K:59:TYR:H	1.74	0.52
1:A:103:C:OP1	20:T:17:ARG:NH1	2.41	0.52
21:U:6:ARG:HD3	21:U:15:ARG:HH22	1.73	0.52
1:A:13:C:O2'	1:A:14:U:C6	2.60	0.52
1:A:757:U:H2'	1:A:758:G:O4'	2.10	0.52
8:H:86:ILE:HG21	8:H:133:LEU:HD22	1.90	0.52
1:A:1236:A:H4'	1:A:1304:G:H4'	1.91	0.52
1:A:559:A:OP1	5:E:126:ARG:NH2	2.43	0.52
9:I:112:LYS:HE3	9:I:117:HIS:O	2.09	0.52
1:A:444:C:H2'	1:A:445:G:C8	2.45	0.52
15:O:39:LEU:HD12	15:O:59:MET:HE2	1.91	0.52
1:A:81:U:H5'	1:A:82:U:OP2	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:838:G:H2'	1:A:839:U:H5"	1.90	0.52
5:E:144:THR:O	5:E:148:VAL:HG23	2.10	0.52
5:E:65:ASN:ND2	5:E:65:ASN:O	2.43	0.52
13:M:84:ILE:HB	19:S:74:PHE:HE2	1.75	0.52
1:A:1200:C:O2'	1:A:1205:U:O4	2.23	0.52
1:A:17:U:H2'	1:A:18:C:C6	2.44	0.52
1:A:1073:U:O2	2:B:104:ASN:ND2	2.42	0.52
1:A:1441:G:H4'	1:A:1442:G:C5	2.45	0.52
3:C:120:VAL:O	3:C:124:ILE:HG13	2.10	0.52
1:A:1196:U:OP1	1:A:1197:G:H5'	2.10	0.52
1:A:1281:U:H5'	1:A:1282:C:H5	1.75	0.52
1:A:1145:C:O2'	1:A:1146:A:O5'	2.25	0.51
1:A:1320:C:H41	19:S:37:ARG:HD3	1.76	0.51
1:A:45:U:H2'	1:A:46:G:H8	1.74	0.51
5:E:144:THR:HG22	5:E:146:ALA:H	1.75	0.51
16:P:43:LYS:HG2	16:P:48:TRP:CD2	2.45	0.51
2:B:23:ARG:O	2:B:24:TRP:HD1	1.93	0.51
19:S:50:ALA:HB1	19:S:57:HIS:HB3	1.92	0.51
1:A:1315:U:OP2	19:S:6:LYS:NZ	2.43	0.51
1:A:945:G:H5"	24:A:2221:HOH:O	2.10	0.51
2:B:100:GLY:O	2:B:104:ASN:N	2.43	0.51
1:A:1020:U:H2'	1:A:1021:G:C8	2.45	0.51
1:A:444:C:H2'	1:A:445:G:H8	1.75	0.51
1:A:517:G:N1	1:A:533:A:OP2	2.36	0.51
3:C:124:ILE:HG21	3:C:196:LEU:HD22	1.93	0.51
3:C:50:ALA:HB2	3:C:75:VAL:HB	1.92	0.51
8:H:121:ASP:HB2	8:H:125:ARG:NH2	2.26	0.51
1:A:116:A:H2'	1:A:117:G:H8	1.74	0.51
1:A:179:A:H2'	1:A:180:U:C6	2.45	0.51
1:A:513:C:H2'	1:A:514:C:O4'	2.10	0.51
1:A:518:C:H2'	1:A:530:G:C8	2.45	0.51
1:A:665:A:N3	1:A:732:C:H2'	2.26	0.51
1:A:731:G:OP1	1:A:766:A:H1'	2.11	0.51
1:A:977:A:H2'	1:A:978:A:H5"	1.93	0.51
10:J:28:ARG:HG3	10:J:34:VAL:HG21	1.92	0.51
1:A:540:G:H2'	1:A:541:G:O4'	2.11	0.51
12:L:27:LEU:C	12:L:29:GLY:H	2.10	0.51
1:A:1516[A]:G:N2	1:A:1519[A]:MA6:OP2	2.43	0.51
1:A:237:C:OP2	17:Q:40:LYS:NZ	2.43	0.51
7:G:12:LEU:H	7:G:12:LEU:HD12	1.76	0.51
20:T:75:ASN:OD1	20:T:75:ASN:N	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:116:A:H2'	1:A:117:G:C8	2.46	0.51
1:A:1443:G:H5"	1:A:1446:A:C5'	2.39	0.51
19:S:50:ALA:HA	19:S:58:VAL:O	2.11	0.51
1:A:1223:C:P	19:S:78:ARG:HH21	2.33	0.51
1:A:1401:G:C2	1:A:1402:4OC:H1'	2.47	0.51
3:C:6:HIS:CD2	3:C:8:ILE:HB	2.46	0.51
20:T:39:LYS:HG2	20:T:55:ILE:HD13	1.93	0.51
1:A:1420:C:H2'	1:A:1421:G:H8	1.76	0.50
7:G:140:ASP:OD1	7:G:143:ARG:NH1	2.44	0.50
19:S:36:ARG:NH2	19:S:75:ALA:O	2.44	0.50
1:A:1257:U:O2'	1:A:1258:G:O5'	2.29	0.50
1:A:825:G:H21	8:H:11:THR:HG21	1.76	0.50
8:H:20:TYR:CE1	8:H:76:PRO:HG2	2.45	0.50
8:H:25:ASP:OD1	8:H:25:ASP:N	2.43	0.50
1:A:1027:C:N4	1:A:1034:G:O6	2.44	0.50
1:A:462:G:H21	16:P:82:GLN:NE2	2.09	0.50
2:B:73:THR:HG21	2:B:96:ARG:HD2	1.93	0.50
12:L:20:LYS:HD2	12:L:20:LYS:H	1.77	0.50
1:A:1004:A:H5"	1:A:1025:U:N3	2.27	0.50
1:A:1497:G:H2'	1:A:1498:UR3:H5'	1.94	0.50
3:C:108:ASN:HD21	3:C:110:ASN:HB2	1.77	0.50
1:A:1071:C:H2'	1:A:1072:G:C8	2.47	0.50
2:B:166:ASP:OD2	2:B:169:LYS:HB2	2.12	0.50
6:F:28:ARG:O	6:F:32:ASN:HB2	2.12	0.50
1:A:1220:G:N2	19:S:54:GLY:O	2.44	0.50
1:A:1427:U:H2'	1:A:1428:A:C8	2.47	0.50
1:A:1034:G:H2'	1:A:1035:A:H8	1.77	0.50
6:F:91:VAL:HG12	6:F:92:LYS:O	2.11	0.50
1:A:1417:G:O2'	1:A:1483:A:N6	2.41	0.50
1:A:377:G:OP1	16:P:3:LYS:NZ	2.27	0.50
1:A:877:C:O2	8:H:3:THR:HG21	2.11	0.50
8:H:89:PRO:HA	8:H:92:ARG:NH1	2.26	0.50
12:L:47:LYS:HD2	12:L:48:PRO:HD3	1.93	0.50
1:A:1309:G:H5'	13:M:78:ILE:HD11	1.94	0.50
1:A:1071:C:H2'	1:A:1072:G:H8	1.77	0.50
1:A:1057:G:H5"	3:C:154:SER:HB2	1.94	0.50
3:C:47:LEU:HB2	3:C:52:LEU:HD23	1.93	0.50
10:J:26:ALA:O	10:J:84:GLN:NE2	2.45	0.50
13:M:20:THR:HG22	24:M:209:HOH:O	2.12	0.50
17:Q:59:ILE:HG23	17:Q:71:PHE:CD1	2.45	0.50
3:C:134:ILE:O	3:C:138:VAL:HG23	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:48:ILE:HD13	11:K:63:LEU:HB3	1.94	0.49
12:L:82:VAL:HG23	12:L:105:TYR:HB3	1.94	0.49
16:P:9:PHE:HD1	16:P:18:ARG:HG3	1.76	0.49
21:U:6:ARG:HD3	21:U:15:ARG:NH2	2.27	0.49
1:A:685:G:H2'	1:A:686:U:H5"	1.94	0.49
14:N:27:CYS:SG	14:N:29:ARG:HB2	2.52	0.49
2:B:60:ASP:CG	2:B:64:ARG:HH12	2.16	0.49
3:C:130:VAL:HG12	3:C:134:ILE:HD11	1.93	0.49
1:A:1345:U:OP1	9:I:120:ARG:NH1	2.45	0.49
9:I:9:ARG:HG2	9:I:14:VAL:HG22	1.95	0.49
19:S:22:LEU:HD21	19:S:28:LYS:HD2	1.94	0.49
1:A:1242:C:OP1	21:U:10:ARG:NH1	2.44	0.49
2:B:158:LEU:HD21	2:B:180:LEU:HD13	1.94	0.49
3:C:108:ASN:ND2	3:C:110:ASN:HB2	2.27	0.49
2:B:204:ASN:HD22	2:B:204:ASN:H	1.60	0.49
2:B:223:ILE:HG21	2:B:230:VAL:HB	1.95	0.49
4:D:150:GLU:HA	4:D:153:ARG:HG3	1.94	0.49
1:A:1298:C:C4	7:G:114:ARG:HD3	2.47	0.49
7:G:6:ARG:HA	7:G:6:ARG:NH1	2.27	0.49
1:A:452:A:O2'	16:P:72:ARG:HD2	2.12	0.49
17:Q:6:LEU:HB2	17:Q:59:ILE:HG22	1.95	0.49
1:A:580:U:H2'	1:A:581:G:O4'	2.13	0.49
9:I:4:TYR:CZ	9:I:88:TYR:HD1	2.31	0.49
12:L:82:VAL:O	12:L:106:ASP:HB2	2.12	0.49
1:A:5:U:H4'	1:A:6:G:O5'	2.13	0.49
1:A:831:U:OP2	2:B:22:LYS:NZ	2.33	0.49
3:C:189:ALA:HB3	3:C:196:LEU:HB2	1.94	0.49
1:A:1518[B]:MA6:H93	1:A:1519[B]:MA6:N1	2.28	0.49
12:L:110:VAL:O	12:L:122:THR:HG21	2.12	0.49
1:A:1320:C:H2'	1:A:1321:C:O4'	2.12	0.49
1:A:918:A:H2'	1:A:919:A:C8	2.47	0.49
9:I:32:ASP:HB3	9:I:35:GLU:HB2	1.95	0.49
1:A:1497:G:C2'	1:A:1498:UR3:H5'	2.42	0.48
1:A:975:A:O2'	14:N:32:SER:OG	2.15	0.48
1:A:1243:C:H5"	21:U:8:THR:HG22	1.95	0.48
1:A:384:G:H2'	1:A:385:C:C6	2.48	0.48
1:A:625:G:H2'	1:A:626:U:H6	1.78	0.48
3:C:148:GLY:HA3	3:C:172:ARG:O	2.13	0.48
8:H:41:ARG:NH1	8:H:123:GLU:OE2	2.45	0.48
1:A:1426:C:H2'	1:A:1427:U:C6	2.48	0.48
1:A:443:C:H2'	1:A:444:C:H6	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:390:C:H2'	1:A:391:G:H8	1.76	0.48
2:B:107:THR:O	2:B:110:GLN:HB2	2.14	0.48
2:B:188:ALA:O	2:B:202:PRO:HA	2.13	0.48
10:J:39:PRO:HA	10:J:70:ARG:HD3	1.94	0.48
11:K:124:LYS:HG3	11:K:125:PHE:CD1	2.48	0.48
1:A:1366:C:H2'	1:A:1367:C:C6	2.49	0.48
1:A:958:A:N3	1:A:985:C:O2'	2.38	0.48
1:A:1262:C:H2'	1:A:1263:C:C6	2.48	0.48
2:B:64:ARG:NH1	2:B:64:ARG:HB2	2.28	0.48
1:A:184:G:H2'	1:A:185:A:H8	1.78	0.48
11:K:29:ILE:HG22	11:K:44:SER:HB2	1.96	0.48
18:R:40:LEU:HB3	18:R:79:LEU:HD11	1.95	0.48
1:A:299:G:H2'	1:A:300:A:C8	2.49	0.48
2:B:17:PHE:HD1	2:B:18:GLY:H	1.62	0.48
12:L:60:LEU:HD11	12:L:85:ILE:HD12	1.96	0.48
20:T:50:GLU:HG3	20:T:100:ILE:HG13	1.96	0.48
1:A:1347:G:H3'	9:I:108:VAL:O	2.14	0.48
1:A:1525:G:P	11:K:120:ARG:HH22	2.36	0.48
16:P:57:ARG:NE	16:P:79:VAL:O	2.40	0.48
1:A:1197:G:H5"	24:A:2052:HOH:O	2.13	0.47
1:A:1415:G:H1	1:A:1485:U:H3	1.61	0.47
1:A:181:G:H4'	1:A:182:U:C5'	2.44	0.47
4:D:62:GLN:OE1	4:D:65:ARG:NH1	2.48	0.47
5:E:36:ASP:OD2	5:E:38:GLN:HB2	2.14	0.47
13:M:13:LYS:O	13:M:45:VAL:HG23	2.14	0.47
1:A:243:A:C2	1:A:246:A:C8	3.02	0.47
1:A:841:U:H3'	1:A:848:C:O4'	2.15	0.47
1:A:1109:C:P	3:C:176:HIS:HD1	2.36	0.47
1:A:1190:G:OP1	3:C:4:LYS:HA	2.15	0.47
1:A:1069:C:O2'	1:A:1192:C:H1'	2.14	0.47
1:A:825:G:N2	8:H:11:THR:HG21	2.29	0.47
3:C:6:HIS:NE2	3:C:8:ILE:HB	2.29	0.47
12:L:77:LEU:HD21	12:L:107:ALA:HB2	1.96	0.47
1:A:1213:A:C5	1:A:1215:G:C4	3.03	0.47
1:A:547:A:H4'	1:A:548:G:O5'	2.15	0.47
1:A:707:C:H2'	1:A:708:C:C6	2.49	0.47
8:H:6:ILE:HB	8:H:85:ARG:NH1	2.30	0.47
1:A:1086:U:H3	1:A:1099:G:H22	1.62	0.47
5:E:82:VAL:HG21	5:E:138:ALA:HA	1.96	0.47
13:M:102:ARG:HH11	13:M:102:ARG:HB2	1.79	0.47
2:B:172:ILE:HD12	2:B:173:ALA:H	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:48:GLU:N	9:I:49:PRO:HD2	2.29	0.47
16:P:66:PRO:HG2	16:P:71:ARG:NH1	2.30	0.47
1:A:117:G:OP2	1:A:117:G:C8	2.67	0.47
1:A:954:G:H21	1:A:1227:A:H62	1.61	0.47
1:A:828:A:H4'	1:A:828:A:OP1	2.13	0.47
2:B:19:HIS:CG	2:B:20:GLU:HG2	2.50	0.47
1:A:1104:G:O5'	2:B:111:ARG:HD2	2.15	0.47
1:A:436:C:H2'	1:A:437:U:H6	1.79	0.47
1:A:701:C:H4'	1:A:702:A:O5'	2.14	0.47
17:Q:83:ASP:OD2	17:Q:83:ASP:N	2.46	0.47
1:A:1361(A):C:HO2'	1:A:1362:C:H6	1.61	0.47
3:C:64:VAL:HB	3:C:99:VAL:HB	1.96	0.47
1:A:1123:A:H4'	10:J:37:PRO:HD2	1.96	0.47
13:M:117:VAL:HG12	13:M:118:ALA:H	1.79	0.47
19:S:39:THR:HA	19:S:70:LYS:HG2	1.97	0.47
1:A:1493:A:HO2'	1:A:1494:G:H8	1.61	0.47
1:A:1511:G:H2'	1:A:1512:U:O4'	2.15	0.47
1:A:141:A:H1'	1:A:182:U:O2	2.15	0.47
1:A:353:A:H5'	1:A:353:A:C8	2.49	0.47
1:A:688:G:O2'	1:A:704:A:N1	2.44	0.47
1:A:706:A:C4'	11:K:29:ILE:HD11	2.44	0.47
1:A:736:C:H2'	1:A:737:A:C8	2.50	0.47
2:B:12:GLU:HG3	2:B:213:LEU:HD21	1.96	0.47
5:E:102:ALA:O	5:E:107:ARG:NH1	2.48	0.47
1:A:1295:G:O2'	13:M:14:ARG:NH1	2.48	0.47
18:R:41:LYS:HB3	18:R:41:LYS:HE2	1.68	0.47
1:A:204:U:H4'	1:A:216:G:C8	2.50	0.47
1:A:858:G:N7	24:A:2231:HOH:O	2.36	0.47
8:H:86:ILE:HG22	8:H:93:VAL:HG11	1.97	0.47
1:A:972:C:H4'	10:J:57:LYS:HB3	1.97	0.46
5:E:74:GLY:HA3	5:E:116:THR:HG22	1.98	0.46
1:A:937:A:N6	1:A:1345:U:O4	2.44	0.46
1:A:46:G:H2'	1:A:366:C:C5	2.50	0.46
19:S:15:LEU:HD23	19:S:33:THR:HG21	1.97	0.46
1:A:976:G:OP2	1:A:1358:U:O2'	2.30	0.46
3:C:141:VAL:HG11	3:C:202:ILE:HG12	1.98	0.46
5:E:78:HIS:CD2	8:H:104:ARG:HG3	2.49	0.46
11:K:48:ILE:HG22	11:K:49:GLY:H	1.80	0.46
4:D:111:ALA:HB2	4:D:120:LEU:HD12	1.97	0.46
7:G:65:ALA:O	7:G:69:VAL:HG23	2.16	0.46
14:N:14:PRO:O	14:N:15:LYS:HB3	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1040:U:H2'	1:A:1041:A:C8	2.51	0.46
1:A:1161:C:H42	1:A:1175:G:H1	1.62	0.46
1:A:1225:A:N3	1:A:1225:A:H2'	2.28	0.46
1:A:1532:U:H2'	1:A:1533:C:H3'	1.98	0.46
1:A:337:C:H2'	1:A:338:A:C8	2.51	0.46
2:B:21:ARG:HG3	2:B:22:LYS:H	1.79	0.46
3:C:155:GLY:HA2	3:C:164:ARG:O	2.15	0.46
4:D:111:ALA:HA	4:D:161:ASN:HD22	1.81	0.46
15:O:39:LEU:CD1	15:O:56:LEU:HB2	2.46	0.46
1:A:1129:C:H4'	1:A:1130:A:OP2	2.15	0.46
1:A:1148:U:H2'	1:A:1149:C:O4'	2.16	0.46
1:A:620:C:H2'	1:A:621:A:O4'	2.15	0.46
12:L:69:TYR:CD1	12:L:90:VAL:HG21	2.51	0.46
16:P:9:PHE:N	16:P:16:HIS:O	2.44	0.46
17:Q:26:GLN:HG2	17:Q:37:LYS:HB2	1.98	0.46
17:Q:27:PHE:CE1	17:Q:36:ILE:HD11	2.51	0.46
1:A:795:C:H5"	1:A:796:C:OP2	2.15	0.46
5:E:71:LEU:HD11	5:E:113:ALA:O	2.15	0.46
15:O:78:TYR:O	15:O:82:ILE:HG12	2.16	0.46
19:S:63:THR:HG22	19:S:64:GLU:H	1.80	0.46
20:T:91:LEU:HD13	20:T:91:LEU:HA	1.83	0.46
1:A:881:G:OP2	12:L:12:ARG:NH2	2.49	0.46
1:A:80:G:N1	1:A:90:U:O2	2.49	0.46
1:A:946:A:H2'	1:A:947:G:C8	2.51	0.46
4:D:153:ARG:HD2	4:D:181:MET:SD	2.55	0.46
5:E:79:GLU:HB3	5:E:92:LYS:HA	1.96	0.46
14:N:31:ARG:HA	14:N:31:ARG:HD2	1.79	0.46
1:A:328:C:H4'	1:A:329:A:O5'	2.16	0.46
5:E:33:VAL:HG11	5:E:109:ILE:HA	1.97	0.46
7:G:31:MET:HG3	7:G:32:ARG:N	2.30	0.46
18:R:58:LEU:HA	18:R:58:LEU:HD23	1.63	0.46
1:A:1250:A:H4'	9:I:68:GLY:N	2.30	0.46
1:A:222:U:H2'	1:A:223:U:C6	2.51	0.46
4:D:187:ARG:NH1	4:D:188:LEU:H	2.14	0.46
7:G:115:ARG:HD2	7:G:117:ALA:HB3	1.97	0.46
12:L:20:LYS:HD2	12:L:20:LYS:N	2.31	0.46
13:M:49:THR:HG22	13:M:51:ALA:N	2.31	0.46
16:P:10:GLY:HA3	16:P:14:ASN:O	2.16	0.46
1:A:337:C:H2'	1:A:338:A:H8	1.82	0.45
9:I:81:ILE:O	9:I:85:LEU:HB2	2.16	0.45
1:A:1118:C:H2'	1:A:1119:C:H6	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1399:C:C2	1:A:1502:A:N6	2.84	0.45
3:C:154:SER:HG	3:C:197:GLY:H	1.62	0.45
18:R:26:LEU:HD21	18:R:39:VAL:HG23	1.98	0.45
20:T:67:ALA:HB2	20:T:77:ALA:HB2	1.98	0.45
1:A:1003(A):G:C5	1:A:1004:A:H1'	2.52	0.45
1:A:1004:A:H5"	1:A:1025:U:C2	2.52	0.45
1:A:1035:A:C6	1:A:1036:G:C6	3.05	0.45
1:A:1347:G:HO2'	1:A:1373:G:H1	1.63	0.45
1:A:232:G:H1'	1:A:262:A:N1	2.31	0.45
2:B:157:ARG:HG2	2:B:158:LEU:N	2.31	0.45
10:J:50:ILE:HA	10:J:60:ARG:HB3	1.97	0.45
1:A:1256:A:O2'	1:A:1257:U:O4'	2.34	0.45
1:A:625:G:H2'	1:A:626:U:C6	2.51	0.45
1:A:642:A:N3	8:H:113:SER:OG	2.47	0.45
5:E:131:ILE:HD13	5:E:131:ILE:HA	1.82	0.45
7:G:38:LEU:O	7:G:42:ILE:HG13	2.17	0.45
9:I:118:LYS:O	9:I:120:ARG:N	2.45	0.45
1:A:1060:C:H2'	1:A:1061:G:H8	1.82	0.45
1:A:1201:A:H4'	1:A:1202:G:O5'	2.17	0.45
1:A:359:U:H2'	1:A:360:A:C8	2.52	0.45
2:B:149:LEU:O	2:B:153:ARG:HG3	2.17	0.45
7:G:75:VAL:HG11	7:G:86:GLN:HB3	1.98	0.45
9:I:65:VAL:HG21	9:I:73:GLN:HB3	1.99	0.45
10:J:51:ARG:HG2	10:J:59:SER:O	2.16	0.45
1:A:1203:C:OP1	14:N:2:ALA:HB3	2.16	0.45
1:A:1352:C:H2'	1:A:1353:G:C8	2.52	0.45
1:A:646:U:H2'	1:A:647:C:C6	2.51	0.45
1:A:692:U:OP2	11:K:26:ASN:ND2	2.48	0.45
1:A:767:A:H2'	1:A:768:A:O4'	2.17	0.45
1:A:900:A:H2'	1:A:901:A:C8	2.51	0.45
3:C:20:SER:O	14:N:54:PRO:HB3	2.17	0.45
4:D:8:VAL:HG11	4:D:21:LEU:HB2	1.98	0.45
1:A:462:G:N2	16:P:82:GLN:HE21	2.14	0.45
20:T:43:LEU:HD22	20:T:43:LEU:HA	1.83	0.45
1:A:109:A:C6	1:A:326:G:C6	3.04	0.45
1:A:371:G:O2'	1:A:372:C:H5'	2.16	0.45
3:C:29:TYR:OH	14:N:54:PRO:O	2.35	0.45
20:T:50:GLU:HA	20:T:100:ILE:HG13	1.98	0.45
2:B:114:ARG:HH11	2:B:118:LEU:HG	1.82	0.45
1:A:1117:G:O3'	9:I:104:ARG:NE	2.49	0.45
13:M:108:ARG:HH22	13:M:111:LYS:HD2	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:30:ALA:HA	15:O:85:LEU:HD11	1.98	0.45
6:F:50:TYR:CE1	18:R:77:GLY:HA2	2.52	0.45
1:A:1001:A:H2'	1:A:1002:G:H8	1.81	0.45
2:B:44:LEU:H	2:B:44:LEU:HD12	1.82	0.45
1:A:1069:C:O3'	5:E:20:GLN:NE2	2.50	0.45
7:G:103:TRP:CH2	7:G:141:VAL:HG21	2.52	0.45
1:A:1518[B]:MA6:H102	1:A:1519[B]:MA6:H103	1.99	0.45
1:A:407:G:OP1	4:D:115:ARG:NH1	2.50	0.45
2:B:19:HIS:CD2	2:B:20:GLU:H	2.35	0.45
4:D:190:ASP:HB3	4:D:193:ASP:OD2	2.17	0.45
1:A:1128:C:H42	1:A:1143:G:H1	1.64	0.44
1:A:583:A:H2'	1:A:584:G:O4'	2.17	0.44
3:C:154:SER:OG	3:C:197:GLY:N	2.37	0.44
5:E:51:VAL:HB	5:E:52:PRO:HD3	1.99	0.44
11:K:33:THR:HG22	11:K:39:PRO:HA	1.99	0.44
1:A:1414:U:H2'	1:A:1415:G:H8	1.81	0.44
1:A:916:G:H2'	1:A:917:G:H8	1.82	0.44
3:C:174:PRO:HB2	3:C:177:THR:HG23	1.98	0.44
5:E:11:ILE:HA	5:E:11:ILE:HD13	1.76	0.44
2:B:223:ILE:HD13	2:B:230:VAL:HG21	1.98	0.44
21:U:5:ASP:O	21:U:8:THR:OG1	2.34	0.44
1:A:1028:C:H42	1:A:1033:G:H1	1.64	0.44
1:A:1040:U:H2'	1:A:1041:A:H8	1.83	0.44
1:A:1053:G:O2'	1:A:1199:U:H5	2.01	0.44
1:A:1112:C:H42	3:C:177:THR:HA	1.81	0.44
1:A:41:G:H2'	1:A:42:G:H8	1.82	0.44
1:A:840:C:H4'	1:A:841:U:O5'	2.16	0.44
2:B:82:ARG:HG3	2:B:92:TYR:CZ	2.52	0.44
7:G:69:VAL:HG21	7:G:104:LEU:HD21	1.98	0.44
20:T:14:LYS:O	20:T:18:GLN:HG3	2.17	0.44
1:A:302:G:N3	1:A:556:C:H4'	2.33	0.44
4:D:205:GLU:OE1	5:E:100:VAL:HG23	2.18	0.44
8:H:111:ILE:O	8:H:134:ILE:HB	2.17	0.44
10:J:79:ARG:O	10:J:82:ILE:N	2.50	0.44
11:K:40:ILE:HG22	11:K:41:THR:HG23	2.00	0.44
1:A:1287:A:H2'	1:A:1288:A:C8	2.53	0.44
1:A:1427:U:H2'	1:A:1428:A:H8	1.82	0.44
1:A:1532:U:H6	1:A:1532:U:O5'	2.01	0.44
1:A:436:C:H2'	1:A:437:U:C6	2.53	0.44
1:A:474:G:OP1	16:P:81:ARG:HB2	2.18	0.44
2:B:106:LYS:O	2:B:110:GLN:HG3	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:217:ARG:HD3	2:B:217:ARG:HA	1.71	0.44
11:K:48:ILE:HG13	11:K:48:ILE:H	1.62	0.44
11:K:98:LEU:HD23	11:K:98:LEU:HA	1.83	0.44
2:B:16:HIS:NE2	2:B:210:SER:HB2	2.32	0.44
2:B:98:LEU:HB2	2:B:101:MET:HG3	2.00	0.44
11:K:12:ARG:HB2	11:K:75:TYR:HD2	1.82	0.44
1:A:1426:C:H2'	1:A:1427:U:H6	1.81	0.44
1:A:1513:A:H2'	1:A:1514:C:C6	2.52	0.44
1:A:624:C:H2'	1:A:625:G:C8	2.52	0.44
3:C:150:LYS:HB3	3:C:201:TYR:HB2	2.00	0.44
3:C:155:GLY:O	3:C:156:ARG:HB2	2.18	0.44
5:E:32:VAL:O	5:E:43:LEU:HD12	2.18	0.44
1:A:933:G:O6	7:G:3:ARG:NH2	2.50	0.44
2:B:28:PHE:CD2	2:B:190:THR:HA	2.53	0.44
4:D:57:ARG:HB3	4:D:206:PHE:HB2	1.99	0.44
4:D:3:ARG:NH2	4:D:74:GLN:OE1	2.36	0.44
10:J:61:GLU:HA	24:J:303:HOH:O	2.17	0.44
10:J:30:SER:OG	10:J:81:THR:OG1	2.21	0.44
11:K:43:SER:HA	11:K:47:VAL:HG21	1.99	0.44
15:O:70:LEU:HD13	15:O:78:TYR:HA	1.99	0.44
1:A:1095:U:H2'	1:A:1096:C:O4'	2.18	0.43
1:A:1130:A:O2'	9:I:3:GLN:NE2	2.40	0.43
1:A:1278:U:H5'	1:A:1279:A:H5'	2.00	0.43
1:A:265:G:H2'	1:A:267:C:H5	1.82	0.43
1:A:413:G:H2'	1:A:428:G:N2	2.33	0.43
1:A:477:G:H2'	1:A:478:A:C8	2.52	0.43
1:A:502:G:H2'	1:A:503:C:O4'	2.18	0.43
1:A:624:C:H2'	1:A:625:G:H8	1.83	0.43
1:A:833:U:H2'	1:A:834:C:C6	2.53	0.43
9:I:118:LYS:C	9:I:120:ARG:H	2.20	0.43
1:A:553:A:O2'	12:L:29:GLY:O	2.36	0.43
12:L:28:LYS:HG3	12:L:33:ARG:CZ	2.48	0.43
17:Q:68:ARG:H	17:Q:70:ARG:HH21	1.64	0.43
1:A:1516[A]:G:H2'	1:A:1518[A]:MA6:OP2	2.18	0.43
1:A:969:A:N6	24:A:2283:HOH:O	2.24	0.43
4:D:61:LYS:HE3	4:D:61:LYS:HB3	1.90	0.43
5:E:40:ARG:HH11	5:E:40:ARG:HG2	1.83	0.43
5:E:72:GLN:O	5:E:75:THR:HG22	2.18	0.43
7:G:47:CYS:O	7:G:50:ILE:HG22	2.19	0.43
16:P:70:ALA:O	16:P:74:LEU:HG	2.18	0.43
18:R:59:SER:H	18:R:62:GLU:HB2	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:603:U:H2'	1:A:604:G:C8	2.52	0.43
1:A:1101:A:N6	2:B:176:GLU:OE2	2.52	0.43
3:C:156:ARG:HH21	3:C:193:TYR:HB2	1.83	0.43
4:D:22:LYS:HB2	4:D:26:CYS:SG	2.59	0.43
8:H:13:ILE:O	8:H:17:THR:HG23	2.18	0.43
10:J:89:ASP:OD2	10:J:91:PRO:HD2	2.19	0.43
12:L:7:ILE:HA	12:L:7:ILE:HD13	1.77	0.43
1:A:1137:C:H4'	1:A:1138:G:C2	2.54	0.43
1:A:1285:A:H4'	1:A:1286:A:O5'	2.18	0.43
1:A:1399:C:C2	1:A:1401:G:C5	3.06	0.43
1:A:860:A:H2'	1:A:861:G:O4'	2.19	0.43
3:C:152:ILE:HB	3:C:199:LYS:HB2	1.99	0.43
4:D:173:TRP:HB2	4:D:187:ARG:O	2.18	0.43
5:E:42:GLY:HA3	5:E:62:ALA:O	2.18	0.43
7:G:65:ALA:HB1	7:G:127:ALA:HB3	2.01	0.43
15:O:17:ARG:CZ	15:O:77:ARG:HH11	2.32	0.43
1:A:1259:C:H42	1:A:1276:G:H1	1.64	0.43
1:A:484:G:H4'	1:A:485:G:O5'	2.18	0.43
14:N:39:LEU:HD11	14:N:47:LEU:HD12	2.01	0.43
18:R:74:ARG:HB3	18:R:81:PHE:CE1	2.53	0.43
20:T:87:LYS:HB2	20:T:87:LYS:HE3	1.83	0.43
1:A:714:G:H2'	1:A:715:A:C8	2.54	0.43
1:A:865:A:H2'	1:A:866:C:C6	2.54	0.43
8:H:73:ASP:OD2	8:H:75:ARG:HB2	2.19	0.43
10:J:16:LEU:HD13	10:J:70:ARG:HG2	2.01	0.43
13:M:11:ARG:HG3	13:M:12:ASN:HB2	2.00	0.43
17:Q:40:LYS:HD3	17:Q:42:TYR:OH	2.19	0.43
20:T:16:HIS:O	20:T:20:LEU:HD12	2.18	0.43
20:T:24:LEU:HD12	20:T:24:LEU:HA	1.80	0.43
1:A:1130:A:OP1	1:A:1130:A:H3'	2.18	0.43
1:A:1450:U:H2'	1:A:1452:C:C5	2.53	0.43
1:A:981:U:H2'	1:A:982:U:C5	2.54	0.43
4:D:97:LEU:HD23	4:D:97:LEU:HA	1.82	0.43
7:G:59:LEU:HD11	7:G:63:LYS:HE2	1.99	0.43
7:G:150:ALA:HB1	11:K:57:THR:HG21	2.00	0.43
14:N:42:ILE:O	14:N:46:GLU:HG3	2.19	0.43
18:R:52:PRO:HG2	18:R:54:ARG:NH2	2.34	0.43
1:A:254:G:OP1	17:Q:67:LYS:O	2.36	0.43
1:A:35:G:H2'	1:A:36:C:H6	1.83	0.43
1:A:499:A:H4'	1:A:500:G:OP1	2.18	0.43
1:A:558:G:H3'	1:A:559:A:H3'	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:88:ALA:HB2	2:B:219:VAL:HG12	2.00	0.43
4:D:61:LYS:HA	4:D:203:VAL:HG22	2.01	0.43
5:E:18:ARG:HG2	5:E:19:MET:N	2.33	0.43
5:E:31:LEU:HA	5:E:31:LEU:HD23	1.78	0.43
16:P:27:LYS:HG3	16:P:27:LYS:H	1.54	0.43
18:R:53:ARG:HG2	18:R:63:GLN:OE1	2.18	0.43
19:S:28:LYS:HG2	19:S:29:ARG:H	1.84	0.43
1:A:1465:C:H2'	1:A:1466:C:O4'	2.19	0.43
1:A:338:A:H2'	1:A:339:C:C6	2.54	0.43
1:A:443:C:H2'	1:A:444:C:C6	2.54	0.43
1:A:737:A:H2'	1:A:738:C:C6	2.54	0.43
1:A:838:G:C2'	1:A:839:U:H5"	2.48	0.43
8:H:53:VAL:HG12	8:H:58:TYR:CD1	2.54	0.43
16:P:43:LYS:HG2	16:P:48:TRP:CE2	2.54	0.43
20:T:53:LEU:HD22	20:T:53:LEU:HA	1.87	0.43
1:A:451:A:N6	1:A:481:G:C4	2.87	0.43
8:H:31:PHE:O	8:H:35:ILE:HG12	2.19	0.43
9:I:118:LYS:H	9:I:118:LYS:HG3	1.57	0.43
12:L:42:THR:OG1	12:L:52:LEU:HB3	2.19	0.43
1:A:1064:G:N2	1:A:1190:G:H2'	2.34	0.42
1:A:1422:G:H1	1:A:1478:C:H42	1.66	0.42
1:A:960:U:H4'	1:A:961:U:C5'	2.49	0.42
3:C:87:LEU:O	3:C:91:LEU:HB3	2.19	0.42
16:P:21:VAL:HG21	16:P:59:TRP:CD1	2.54	0.42
20:T:77:ALA:O	20:T:81:LYS:HG3	2.18	0.42
1:A:1121:U:H2'	1:A:1122:U:C6	2.54	0.42
1:A:41:G:H2'	1:A:42:G:C8	2.54	0.42
7:G:45:ASP:O	7:G:49:ILE:HG13	2.18	0.42
11:K:106:LYS:HD3	11:K:106:LYS:HA	1.82	0.42
13:M:50:GLU:O	13:M:54:VAL:HG23	2.19	0.42
16:P:4:ILE:O	16:P:66:PRO:HA	2.20	0.42
20:T:39:LYS:O	20:T:43:LEU:HB2	2.18	0.42
1:A:701:C:H5"	1:A:703:G:H5'	2.02	0.42
3:C:139:GLN:HB3	3:C:143:GLU:OE2	2.18	0.42
8:H:21:LYS:O	8:H:65:TYR:OH	2.28	0.42
9:I:126:SER:OG	9:I:127:LYS:N	2.53	0.42
14:N:58:LYS:HE3	14:N:58:LYS:HB3	1.88	0.42
16:P:3:LYS:HD2	16:P:65:GLN:O	2.19	0.42
1:A:1347:G:HO2'	1:A:1348:U:P	2.36	0.42
1:A:397:A:H5'	1:A:398:C:OP1	2.19	0.42
1:A:373:A:H1'	1:A:481:G:N3	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:194:LEU:HD13	4:D:194:LEU:HA	1.83	0.42
10:J:32:ALA:O	10:J:34:VAL:HG23	2.19	0.42
1:A:129:U:O3'	1:A:129(A):G:H3'	2.18	0.42
1:A:1317:C:H2'	1:A:1318:A:O4'	2.19	0.42
1:A:81:U:H2'	1:A:83:U:OP2	2.19	0.42
15:O:70:LEU:HA	15:O:70:LEU:HD23	1.80	0.42
16:P:51:VAL:O	16:P:52:ASP:HB3	2.20	0.42
1:A:1124:G:C8	1:A:1145:C:C5	3.06	0.42
1:A:1499:A:H1'	1:A:1520[A]:G:OP1	2.19	0.42
1:A:262:A:C6	1:A:263:A:C6	3.07	0.42
1:A:372:C:H1'	1:A:373:A:OP2	2.19	0.42
1:A:440:A:H5'	1:A:442:C:OP2	2.18	0.42
1:A:690:G:H2'	1:A:691:G:O4'	2.20	0.42
1:A:579:G:H5'	1:A:728:A:H1'	2.00	0.42
1:A:983:A:H5'	1:A:984:C:OP2	2.19	0.42
3:C:24:ALA:HB3	3:C:29:TYR:HD1	1.85	0.42
4:D:3:ARG:HD3	4:D:3:ARG:HA	1.83	0.42
16:P:52:ASP:OD2	16:P:55:ARG:HB2	2.20	0.42
1:A:1287:A:C6	1:A:1288:A:C6	3.08	0.42
2:B:16:HIS:CD2	2:B:204:ASN:HD22	2.36	0.42
2:B:77:ALA:HB2	2:B:211:ILE:HD13	2.01	0.42
4:D:171:GLY:HA2	4:D:172:PRO:HD3	1.87	0.42
9:I:86:VAL:HG21	9:I:102:LEU:HD21	2.01	0.42
1:A:706:A:O4'	11:K:29:ILE:HD11	2.20	0.42
15:O:21:ASP:OD2	15:O:24:SER:OG	2.31	0.42
2:B:189:ASP:HB3	2:B:203:GLY:O	2.19	0.42
1:A:1189:C:H4'	3:C:10:PHE:CE1	2.54	0.42
15:O:26:GLU:OE1	15:O:77:ARG:HB3	2.20	0.42
1:A:1035:A:H2'	1:A:1036:G:C8	2.55	0.42
1:A:1196:U:H4'	1:A:1197:G:OP2	2.19	0.42
1:A:1229:A:OP2	13:M:114:ARG:HD3	2.20	0.42
1:A:519:C:H2'	1:A:520:A:C8	2.55	0.42
3:C:95:THR:C	3:C:97:LYS:H	2.22	0.42
4:D:9:CYS:O	4:D:12:CYS:HB2	2.20	0.42
9:I:70:LYS:O	9:I:74:ILE:HG13	2.20	0.42
12:L:54:LYS:N	12:L:54:LYS:HD2	2.35	0.42
13:M:46:LYS:HG3	13:M:47:ASP:OD2	2.20	0.42
14:N:6:LEU:HD23	14:N:6:LEU:HA	1.85	0.42
17:Q:10:VAL:HG13	17:Q:19:VAL:HB	2.01	0.42
1:A:1121:U:H2'	1:A:1122:U:H6	1.85	0.42
4:D:196:LEU:HA	4:D:196:LEU:HD23	1.64	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:118:ILE:HG12	5:E:119:LEU:N	2.35	0.42
6:F:22:GLU:OE2	6:F:82:ARG:HD3	2.20	0.42
9:I:47:LEU:HB3	9:I:50:LEU:HD12	2.02	0.42
1:A:881:G:P	12:L:12:ARG:HH22	2.43	0.42
1:A:750:G:N3	15:O:23:GLY:HA3	2.34	0.42
15:O:7:GLU:O	15:O:11:VAL:HG23	2.19	0.42
15:O:85:LEU:HD23	15:O:85:LEU:HA	1.72	0.42
1:A:1320:C:O2	19:S:36:ARG:NH1	2.53	0.42
1:A:1518[A]:MA6:H93	1:A:1519[A]:MA6:H92	2.01	0.41
1:A:181:G:H4'	1:A:182:U:H5'	2.01	0.41
1:A:676:A:H1'	11:K:115:PRO:HB3	2.01	0.41
1:A:922:G:C6	1:A:923:A:C6	3.08	0.41
3:C:11:ARG:NH1	3:C:177:THR:O	2.53	0.41
19:S:33:THR:HG22	19:S:35:SER:N	2.28	0.41
19:S:58:VAL:HA	19:S:59:PRO:HD3	1.89	0.41
1:A:1314:C:C5	19:S:6:LYS:HE2	2.54	0.41
1:A:1060:C:H2'	1:A:1061:G:C8	2.55	0.41
6:F:1:MET:HB3	6:F:69:GLU:OE2	2.20	0.41
1:A:1131:G:H2'	1:A:1132:C:C6	2.55	0.41
1:A:1190:G:O2'	1:A:1191:A:P	2.78	0.41
1:A:186:C:H2'	1:A:187:C:C6	2.55	0.41
2:B:54:THR:O	2:B:58:ILE:HG13	2.20	0.41
3:C:135:LYS:HE3	3:C:135:LYS:HB2	1.86	0.41
6:F:36:ARG:NH1	6:F:66:GLU:OE1	2.53	0.41
14:N:22:THR:HB	14:N:33:VAL:HG11	2.01	0.41
1:A:1486:G:H2'	1:A:1487:G:O4'	2.20	0.41
7:G:145:ALA:O	7:G:146:GLU:HB2	2.21	0.41
8:H:127:LEU:HD13	8:H:127:LEU:HA	1.81	0.41
9:I:122:ALA:HA	9:I:123:PRO:HD3	1.93	0.41
17:Q:38:ARG:HA	17:Q:38:ARG:HD3	1.90	0.41
1:A:101:A:H2'	1:A:102:G:H8	1.86	0.41
1:A:1124:G:C8	1:A:1145:C:H5	2.38	0.41
1:A:1320:C:N3	19:S:36:ARG:HG3	2.35	0.41
1:A:457:C:H2'	1:A:458:C:H6	1.85	0.41
1:A:920:U:H2'	1:A:921:U:C6	2.55	0.41
4:D:3:ARG:HH11	4:D:70:ILE:HA	1.86	0.41
14:N:14:PRO:HB2	14:N:16:PHE:O	2.20	0.41
16:P:2:VAL:O	16:P:64:ALA:HA	2.19	0.41
18:R:54:ARG:HE	18:R:54:ARG:HB2	1.57	0.41
1:A:1318:A:H4'	19:S:10:PHE:CE2	2.55	0.41
1:A:1328:C:P	21:U:21:TYR:HH	2.44	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1518[B]:MA6:O2'	1:A:1519[B]:MA6:O5'	2.37	0.41
1:A:687:A:H4'	1:A:688:G:O5'	2.20	0.41
1:A:779:C:H2'	1:A:780:A:O4'	2.20	0.41
3:C:180:ALA:HB1	3:C:203:PHE:CD1	2.55	0.41
10:J:54:PHE:HD2	10:J:55:LYS:HG2	1.86	0.41
12:L:124:LYS:HD2	12:L:125:PRO:HD2	2.03	0.41
12:L:27:LEU:HD23	12:L:28:LYS:HE2	2.02	0.41
1:A:1199:U:H4'	10:J:54:PHE:CD1	2.55	0.41
1:A:1250:A:H4'	9:I:68:GLY:H	1.85	0.41
1:A:411:A:N7	1:A:413:G:N3	2.68	0.41
1:A:564:C:O2'	8:H:91:ARG:NH2	2.48	0.41
3:C:76:VAL:O	3:C:83:ARG:HB3	2.21	0.41
9:I:63:ILE:HG21	9:I:77:ILE:HG12	2.02	0.41
1:A:1029:C:H2'	1:A:1030:C:H6	1.86	0.41
1:A:659:U:H2'	1:A:660:G:C8	2.56	0.41
8:H:18:ARG:HD3	8:H:18:ARG:HA	1.70	0.41
20:T:67:ALA:O	20:T:73:HIS:ND1	2.54	0.41
1:A:1347:G:C2'	1:A:1348:U:OP2	2.69	0.41
1:A:260:G:H2'	1:A:261:U:C6	2.56	0.41
1:A:7:G:H5'	1:A:298:A:O4'	2.21	0.41
1:A:428:G:H4'	1:A:429:U:O5'	2.20	0.41
1:A:563:A:H2'	1:A:567:G:C8	2.56	0.41
1:A:966:M2G:HM22	1:A:967:5MC:O2	2.21	0.41
2:B:24:TRP:HA	2:B:191:ASP:HA	2.01	0.41
3:C:155:GLY:HA2	3:C:164:ARG:H	1.85	0.41
3:C:159:GLY:HA2	3:C:193:TYR:CD1	2.56	0.41
4:D:188:LEU:HD23	4:D:188:LEU:HA	1.84	0.41
12:L:59:ARG:NE	12:L:65:GLU:HG3	2.36	0.41
15:O:3:ILE:HD11	15:O:38:ARG:HG3	2.02	0.41
16:P:40:ASP:OD1	16:P:44:THR:OG1	2.26	0.41
16:P:67:THR:HG22	16:P:68:ASP:H	1.86	0.41
16:P:53:VAL:HG12	16:P:79:VAL:HG22	2.03	0.41
19:S:77:THR:HG22	19:S:78:ARG:N	2.35	0.41
1:A:1097:C:H2'	1:A:1098:C:C6	2.55	0.41
20:T:100:ILE:HG22	20:T:102:GLY:N	2.17	0.41
1:A:1259:C:N4	1:A:1260:C:O2	2.54	0.41
1:A:1329:A:H2'	1:A:1330:U:O4'	2.21	0.41
1:A:13:C:O2'	1:A:14:U:P	2.78	0.41
4:D:187:ARG:NH1	4:D:188:LEU:HB2	2.36	0.41
4:D:81:GLU:CD	4:D:139:ARG:HH22	2.25	0.41
8:H:35:ILE:HG22	8:H:111:ILE:HD13	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:20:ARG:HH12	9:I:62:TYR:HB3	1.85	0.41
1:A:1053:G:H4'	1:A:1054:C:H5'	2.03	0.40
1:A:146:G:H1	1:A:176:C:H42	1.67	0.40
3:C:26:LYS:H	3:C:26:LYS:NZ	2.19	0.40
3:C:58:GLU:H	3:C:65:ALA:HB3	1.86	0.40
3:C:88:ARG:HA	3:C:91:LEU:HD22	2.03	0.40
7:G:37:ASN:OD1	9:I:41:VAL:HG23	2.22	0.40
17:Q:67:LYS:O	17:Q:69:LYS:N	2.55	0.40
1:A:1241:G:H2'	1:A:1242:C:C6	2.56	0.40
1:A:658:G:OP1	15:O:8:LYS:NZ	2.48	0.40
1:A:75:G:C6	1:A:76:C:C4	3.09	0.40
1:A:91:C:H2'	1:A:92:C:C6	2.54	0.40
2:B:92:TYR:CD1	2:B:151:GLY:HA3	2.56	0.40
3:C:11:ARG:HH11	3:C:178:LEU:HA	1.85	0.40
1:A:1061:G:N7	3:C:2:GLY:N	2.70	0.40
1:A:1189:C:H5"	3:C:5:ILE:HD12	2.04	0.40
6:F:15:ASP:N	6:F:15:ASP:OD2	2.50	0.40
1:A:1128:C:OP1	9:I:66:ARG:NH2	2.54	0.40
1:A:1151:A:HO2'	1:A:1152:A:H8	1.68	0.40
1:A:1224:G:O2'	24:A:2318:HOH:O	2.19	0.40
1:A:1343:G:H2'	1:A:1344:C:C6	2.56	0.40
1:A:836:G:C6	1:A:851:G:C6	3.10	0.40
3:C:150:LYS:HD3	3:C:152:ILE:HD11	2.02	0.40
13:M:27:LYS:HA	13:M:27:LYS:HD2	1.63	0.40
15:O:40:SER:O	15:O:44:LYS:HG3	2.21	0.40
1:A:1305:G:H8	1:A:1305:G:H2'	1.70	0.40
1:A:1502:A:C2	1:A:1504:G:C2	3.09	0.40
3:C:53:ALA:HB2	3:C:115:LEU:HD23	2.03	0.40
6:F:82:ARG:HE	6:F:82:ARG:HA	1.86	0.40
7:G:44:TYR:O	7:G:48:LYS:HG2	2.20	0.40
8:H:4:ASP:OD2	8:H:85:ARG:NH1	2.54	0.40
10:J:44:VAL:HG13	10:J:66:ARG:HB3	2.04	0.40
13:M:91:ARG:HD2	13:M:91:ARG:HA	1.85	0.40
18:R:74:ARG:HB3	18:R:81:PHE:CZ	2.56	0.40
2:B:23:ARG:HB2	2:B:24:TRP:H	1.73	0.40
5:E:90:VAL:O	5:E:120:THR:HA	2.21	0.40
9:I:16:ARG:HB2	9:I:64:THR:HG22	2.03	0.40
12:L:25:PRO:HA	12:L:27:LEU:H	1.86	0.40
12:L:60:LEU:HB2	12:L:64:TYR:O	2.22	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%)	208 (90%)	22 (10%)	2 (1%)	17 51
3	C	204/239 (85%)	178 (87%)	26 (13%)	0	100 100
4	D	206/209 (99%)	196 (95%)	10 (5%)	0	100 100
5	E	148/162 (91%)	140 (95%)	8 (5%)	0	100 100
6	F	99/101 (98%)	97 (98%)	2 (2%)	0	100 100
7	G	153/156 (98%)	148 (97%)	5 (3%)	0	100 100
8	H	136/138 (99%)	131 (96%)	5 (4%)	0	100 100
9	I	125/128 (98%)	114 (91%)	10 (8%)	1 (1%)	19 53
10	J	96/105 (91%)	80 (83%)	13 (14%)	3 (3%)	4 25
11	K	114/129 (88%)	105 (92%)	9 (8%)	0	100 100
12	L	121/135 (90%)	108 (89%)	12 (10%)	1 (1%)	19 53
13	M	116/126 (92%)	99 (85%)	17 (15%)	0	100 100
14	N	58/61 (95%)	52 (90%)	6 (10%)	0	100 100
15	O	85/89 (96%)	78 (92%)	7 (8%)	0	100 100
16	P	81/88 (92%)	77 (95%)	4 (5%)	0	100 100
17	Q	97/105 (92%)	91 (94%)	6 (6%)	0	100 100
18	R	68/88 (77%)	65 (96%)	3 (4%)	0	100 100
19	S	78/93 (84%)	72 (92%)	5 (6%)	1 (1%)	12 42
20	T	97/106 (92%)	87 (90%)	10 (10%)	0	100 100
21	U	22/27 (82%)	21 (96%)	0	1 (4%)	2 17
All	All	2336/2541 (92%)	2147 (92%)	180 (8%)	9 (0%)	34 68

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
12	L	28	LYS

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Mol	Chain	Res	Type
19	S	31	ILE
2	B	21	ARG
10	J	54	PHE
10	J	86	MET
2	B	24	TRP
9	I	119	ALA
21	U	24	ARG
10	J	34	VAL

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	B	202/220 (92%)	177 (88%)	25 (12%)	4 18
3	C	160/188 (85%)	137 (86%)	23 (14%)	3 14
4	D	180/181 (99%)	162 (90%)	18 (10%)	7 28
5	E	115/123 (94%)	101 (88%)	14 (12%)	5 19
6	F	90/90 (100%)	81 (90%)	9 (10%)	7 28
7	G	126/127 (99%)	116 (92%)	10 (8%)	12 39
8	H	119/119 (100%)	109 (92%)	10 (8%)	11 37
9	I	98/99 (99%)	88 (90%)	10 (10%)	7 28
10	J	87/92 (95%)	79 (91%)	8 (9%)	9 32
11	K	88/99 (89%)	79 (90%)	9 (10%)	7 28
12	L	103/110 (94%)	90 (87%)	13 (13%)	4 18
13	M	94/101 (93%)	77 (82%)	17 (18%)	1 7
14	N	49/50 (98%)	44 (90%)	5 (10%)	7 28
15	O	79/80 (99%)	67 (85%)	12 (15%)	3 12
16	P	72/74 (97%)	63 (88%)	9 (12%)	4 18
17	Q	94/97 (97%)	89 (95%)	5 (5%)	22 54
18	R	61/77 (79%)	53 (87%)	8 (13%)	4 17

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
19	S	71/80 (89%)	63 (89%)	8 (11%)	6 22
20	T	76/82 (93%)	63 (83%)	13 (17%)	2 9
21	U	19/22 (86%)	17 (90%)	2 (10%)	7 26
All	All	1983/2111 (94%)	1755 (88%)	228 (12%)	5 22

All (228) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	7	VAL
2	B	8	LYS
2	B	10	LEU
2	B	24	TRP
2	B	30	ARG
2	B	39	ILE
2	B	44	LEU
2	B	51	LEU
2	B	67	THR
2	B	69	LEU
2	B	92	TYR
2	B	114	ARG
2	B	121	LEU
2	B	128	GLU
2	B	140	HIS
2	B	153	ARG
2	B	162	ILE
2	B	163	PHE
2	B	164	VAL
2	B	172	ILE
2	B	178	ARG
2	B	200	ILE
2	B	217	ARG
2	B	219	VAL
2	B	231	GLU
3	C	3	ASN
3	C	5	ILE
3	C	26	LYS
3	C	33	LEU
3	C	58	GLU
3	C	70	VAL
3	C	84	ILE
3	C	91	LEU

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Mol	Chain	Res	Type
3	C	94	LEU
3	C	95	THR
3	C	99	VAL
3	C	108	ASN
3	C	115	LEU
3	C	119	ARG
3	C	122	GLU
3	C	165	THR
3	C	167	TRP
3	C	177	THR
3	C	178	LEU
3	C	188	LEU
3	C	192	THR
3	C	195	VAL
3	C	204	LEU
4	D	5	ILE
4	D	10	ARG
4	D	19	LEU
4	D	25	ARG
4	D	26	CYS
4	D	34	GLU
4	D	36	ARG
4	D	64	LEU
4	D	73	ARG
4	D	78	LEU
4	D	122	ARG
4	D	127	THR
4	D	135	LEU
4	D	170	VAL
4	D	176	LEU
4	D	177	ASP
4	D	186	LEU
4	D	209	ARG
5	E	12	LEU
5	E	13	ILE
5	E	19	MET
5	E	31	LEU
5	E	33	VAL
5	E	41	VAL
5	E	45	PHE
5	E	63	ARG
5	E	64	ARG

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Mol	Chain	Res	Type
5	E	78	HIS
5	E	79	GLU
5	E	80	ILE
5	E	100	VAL
5	E	125	SER
6	F	1	MET
6	F	10	LEU
6	F	24	GLU
6	F	36	ARG
6	F	43	LEU
6	F	55	ASP
6	F	82	ARG
6	F	95	GLU
6	F	98	LEU
7	G	5	ARG
7	G	8	GLU
7	G	11	GLN
7	G	22	LEU
7	G	38	LEU
7	G	92	SER
7	G	113	GLU
7	G	115	ARG
7	G	138	LYS
7	G	149	ARG
8	H	2	LEU
8	H	35	ILE
8	H	50	ARG
8	H	53	VAL
8	H	63	LEU
8	H	75	ARG
8	H	85	ARG
8	H	91	ARG
8	H	92	ARG
8	H	93	VAL
9	I	16	ARG
9	I	23	ASN
9	I	79	LEU
9	I	87	GLN
9	I	96	LEU
9	I	104	ARG
9	I	108	VAL
9	I	116	LYS

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Mol	Chain	Res	Type
9	I	118	LYS
9	I	124	GLN
10	J	17	ASP
10	J	38	ILE
10	J	44	VAL
10	J	45	ARG
10	J	60	ARG
10	J	73	ASP
10	J	89	ASP
10	J	98	ILE
11	K	18	ARG
11	K	29	ILE
11	K	47	VAL
11	K	48	ILE
11	K	77	MET
11	K	80	VAL
11	K	98	LEU
11	K	104	GLN
11	K	109	VAL
12	L	17	LYS
12	L	18	VAL
12	L	20	LYS
12	L	33	ARG
12	L	41	ARG
12	L	47	LYS
12	L	53	ARG
12	L	60	LEU
12	L	61	THR
12	L	83	VAL
12	L	104	VAL
12	L	116	SER
12	L	127	GLU
13	M	9	ILE
13	M	12	ASN
13	M	13	LYS
13	M	16	ASP
13	M	44	ARG
13	M	50	GLU
13	M	56	LEU
13	M	62	ASN
13	M	64	TRP
13	M	70	LEU

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Mol	Chain	Res	Type
13	M	77	ASN
13	M	81	LEU
13	M	102	ARG
13	M	106	ASN
13	M	110	ARG
13	M	115	LYS
13	M	117	VAL
14	N	12	ARG
14	N	22	THR
14	N	24	CYS
14	N	31	ARG
14	N	41	ARG
15	O	4	THR
15	O	22	THR
15	O	31	LEU
15	O	32	LEU
15	O	39	LEU
15	O	45	VAL
15	O	57	LEU
15	O	63	ARG
15	O	66	LEU
15	O	70	LEU
15	O	81	LEU
15	O	87	ILE
16	P	1	MET
16	P	27	LYS
16	P	45	THR
16	P	55	ARG
16	P	61	SER
16	P	62	VAL
16	P	67	THR
16	P	80	PHE
16	P	82	GLN
17	Q	34	LYS
17	Q	53	LEU
17	Q	68	ARG
17	Q	83	ASP
17	Q	100	LYS
18	R	26	LEU
18	R	37	VAL
18	R	38	GLU
18	R	47	THR

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Mol	Chain	Res	Type
18	R	76	LEU
18	R	82	THR
18	R	86	VAL
18	R	88	LYS
19	S	5	LEU
19	S	7	LYS
19	S	15	LEU
19	S	31	ILE
19	S	36	ARG
19	S	43	GLU
19	S	58	VAL
19	S	63	THR
20	T	9	ASN
20	T	10	LEU
20	T	19	SER
20	T	20	LEU
20	T	42	GLN
20	T	43	LEU
20	T	53	LEU
20	T	54	LYS
20	T	57	ARG
20	T	68	LYS
20	T	75	ASN
20	T	84	LEU
20	T	91	LEU
21	U	8	THR
21	U	15	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	16	HIS
2	B	204	ASN
3	C	3	ASN
3	C	6	HIS
3	C	108	ASN
15	O	46	HIS
16	P	82	GLN

5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	1504/1522 (98%)	258 (17%)	45 (2%)

All (258) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	6	G
1	A	9	G
1	A	13	C
1	A	14	U
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	75	G
1	A	80	G
1	A	81	U
1	A	82	U
1	A	101	A
1	A	108	G
1	A	115	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	195	A
1	A	197	A
1	A	201	C
1	A	202	U
1	A	203	U
1	A	216	G
1	A	217	C
1	A	220	G
1	A	226	G
1	A	231	G
1	A	247	G
1	A	251	G

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Mol	Chain	Res	Type
1	A	258	G
1	A	266	G
1	A	267	C
1	A	289	G
1	A	301	G
1	A	319	G
1	A	321	A
1	A	328	C
1	A	329	A
1	A	332	G
1	A	344	A
1	A	345	C
1	A	347	G
1	A	350	G
1	A	352	C
1	A	353	A
1	A	354	G
1	A	356	A
1	A	367	U
1	A	372	C
1	A	373	A
1	A	384	G
1	A	390	C
1	A	397	A
1	A	398	C
1	A	406	G
1	A	412	A
1	A	413	G
1	A	419	C
1	A	422	C
1	A	424	G
1	A	429	U
1	A	446	G
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

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Mol	Chain	Res	Type
1	A	511	C
1	A	517	G
1	A	518	C
1	A	519	C
1	A	524	G
1	A	527	7MG
1	A	532	A
1	A	533	A
1	A	547	A
1	A	559	A
1	A	560	U
1	A	562	C
1	A	563	A
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	581	G
1	A	588	G
1	A	618	C
1	A	653	A
1	A	665	A
1	A	666	G
1	A	671	G
1	A	687	A
1	A	688	G
1	A	695	A
1	A	701	C
1	A	702	A
1	A	723	U
1	A	724	G
1	A	731	G
1	A	733	A
1	A	749	C
1	A	755	G
1	A	777	A
1	A	780	A
1	A	781	A
1	A	782	A

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Mol	Chain	Res	Type
1	A	785	G
1	A	792	A
1	A	793	U
1	A	794	A
1	A	813	U
1	A	817	C
1	A	818	G
1	A	821	G
1	A	828	A
1	A	829	G
1	A	839	U
1	A	841	U
1	A	848	C
1	A	855	G
1	A	858	G
1	A	872	A
1	A	873	A
1	A	876	G
1	A	889	A
1	A	902	G
1	A	914	A
1	A	926	G
1	A	927	G
1	A	934	C
1	A	935	A
1	A	960	U
1	A	961	U
1	A	963	G
1	A	966	M2G
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	991	U
1	A	992	U
1	A	993	G
1	A	1004	A
1	A	1005	A
1	A	1006	C
1	A	1021	G

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Mol	Chain	Res	Type
1	A	1023	G
1	A	1026	G
1	A	1045	C
1	A	1050	G
1	A	1053	G
1	A	1054	C
1	A	1065	U
1	A	1066	C
1	A	1068	G
1	A	1094	G
1	A	1095	U
1	A	1096	C
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	1159	U
1	A	1160	G
1	A	1171	G
1	A	1182	G
1	A	1183	A
1	A	1184	G
1	A	1190	G
1	A	1191	A
1	A	1196	U
1	A	1197	G
1	A	1200	C
1	A	1201	A
1	A	1202	G
1	A	1212	U
1	A	1214	C
1	A	1225	A

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Mol	Chain	Res	Type
1	A	1226	C
1	A	1238	A
1	A	1240	U
1	A	1241	G
1	A	1253	G
1	A	1257	U
1	A	1258	G
1	A	1270	C
1	A	1278	U
1	A	1280	A
1	A	1281	U
1	A	1286	A
1	A	1287	A
1	A	1288	A
1	A	1289	A
1	A	1300	G
1	A	1301	U
1	A	1302	U
1	A	1306	A
1	A	1312	G
1	A	1319	A
1	A	1320	C
1	A	1330	U
1	A	1335	C
1	A	1336	C
1	A	1338	G
1	A	1346	A
1	A	1347	G
1	A	1348	U
1	A	1353	G
1	A	1362	C
1	A	1364	U
1	A	1370	G
1	A	1379	G
1	A	1381	U
1	A	1400	5MC
1	A	1411	C
1	A	1442	G
1	A	1446	A
1	A	1447	G
1	A	1453	G
1	A	1487	G

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Mol	Chain	Res	Type
1	A	1490	C
1	A	1493	A
1	A	1497	G
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

All (45) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	5	U
1	A	80	G
1	A	115	G
1	A	129(A)	G
1	A	181	G
1	A	250	A
1	A	328	C
1	A	353	A
1	A	372	C
1	A	428	G
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
1	A	575	G
1	A	686	U
1	A	687	A
1	A	701	C
1	A	748	C
1	A	792	A
1	A	812	C
1	A	840	C
1	A	913	A
1	A	960	U
1	A	991	U

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Mol	Chain	Res	Type
1	A	992	U
1	A	1004	A
1	A	1049	U
1	A	1065	U
1	A	1067	A
1	A	1139	G
1	A	1145	C
1	A	1190	G
1	A	1196	U
1	A	1201	A
1	A	1257	U
1	A	1301	U
1	A	1305	G
1	A	1346	A
1	A	1347	G
1	A	1380	U
1	A	1505	G

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
1	PSU	A	1541	1,22	17,21,22	1.05	2 (11%)	20,30,33	3.08	6 (30%)
1	PSU	A	516	1,22	17,21,22	1.09	2 (11%)	20,30,33	3.06	6 (30%)
1	M2G	A	966	1	20,27,28	1.71	4 (20%)	22,40,43	2.43	5 (22%)
1	UR3	A	1498	1	14,22,23	0.78	0	15,32,35	1.12	1 (6%)
1	MA6	A	1518[B]	1	19,26,27	1.29	3 (15%)	18,38,41	0.87	1 (5%)
1	7MG	A	527	1,22	22,26,27	2.05	5 (22%)	28,39,42	1.69	5 (17%)
1	5MC	A	1407	1	15,22,23	1.03	1 (6%)	19,32,35	1.13	2 (10%)
1	5MC	A	1400	1	15,22,23	0.95	1 (6%)	19,32,35	1.05	1 (5%)
1	4OC	A	1402	1	16,23,24	0.97	1 (6%)	17,32,35	0.74	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
12	0TD	L	92	12	4,9,10	0.95	0	3,11,13	2.95	1 (33%)
1	MA6	A	1518[A]	1	19,26,27	0.88	1 (5%)	18,38,41	0.71	0
1	5MC	A	1404	1	15,22,23	1.15	2 (13%)	19,32,35	0.92	1 (5%)
1	PSU	A	1540	1	17,21,22	1.06	1 (5%)	20,30,33	3.29	6 (30%)
1	MA6	A	1519[B]	1	19,26,27	1.32	3 (15%)	18,38,41	0.62	0
1	MA6	A	1519[A]	1	19,26,27	0.72	0	18,38,41	0.87	0
1	2MG	A	1207	1	19,26,27	2.35	4 (21%)	21,38,41	2.05	3 (14%)
1	5MC	A	967	1	15,22,23	0.94	1 (6%)	19,32,35	1.07	1 (5%)

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	1541	1,22	-	0/7/25/26	0/2/2/2
1	PSU	A	516	1,22	-	0/7/25/26	0/2/2/2
1	M2G	A	966	1	-	4/7/29/30	0/3/3/3
1	UR3	A	1498	1	-	0/5/25/26	0/2/2/2
1	MA6	A	1518[B]	1	-	0/7/29/30	0/3/3/3
1	7MG	A	527	1,22	-	2/7/37/38	0/3/3/3
1	5MC	A	1407	1	-	0/5/25/26	0/2/2/2
1	5MC	A	1400	1	-	2/5/25/26	0/2/2/2
1	4OC	A	1402	1	-	3/9/29/30	0/2/2/2
12	0TD	L	92	12	-	1/3/12/14	-
1	MA6	A	1518[A]	1	-	2/7/29/30	0/3/3/3
1	5MC	A	1404	1	-	0/5/25/26	0/2/2/2
1	PSU	A	1540	1	-	0/7/25/26	0/2/2/2
1	MA6	A	1519[B]	1	-	3/7/29/30	0/3/3/3
1	MA6	A	1519[A]	1	-	2/7/29/30	0/3/3/3
1	2MG	A	1207	1	-	0/5/27/28	0/3/3/3
1	5MC	A	967	1	-	0/5/25/26	0/2/2/2

All (31) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1207	2MG	C2-N2	7.53	1.40	1.34
1	A	1207	2MG	C6-N1	5.49	1.42	1.33
1	A	966	M2G	C6-N1	5.11	1.41	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	527	7MG	C4-N3	4.92	1.40	1.34
1	A	527	7MG	C8-N9	-4.40	1.35	1.45
1	A	527	7MG	C2-N2	4.35	1.42	1.33
1	A	1518[B]	MA6	C6-N1	3.68	1.38	1.33
1	A	1519[B]	MA6	C6-N1	3.61	1.38	1.33
1	A	966	M2G	C2-N2	3.36	1.40	1.34
1	A	1540	PSU	C4-N3	3.28	1.38	1.33
1	A	527	7MG	C6-C5	3.13	1.45	1.41
1	A	1541	PSU	C4-N3	3.10	1.38	1.33
1	A	516	PSU	C4-N3	3.03	1.38	1.33
1	A	966	M2G	C2-N1	2.94	1.39	1.34
1	A	1404	5MC	C5-C4	2.88	1.45	1.41
1	A	1207	2MG	C4-N3	2.73	1.39	1.35
1	A	966	M2G	C4-N3	2.61	1.39	1.35
1	A	1519[B]	MA6	C2-N1	2.51	1.38	1.33
1	A	527	7MG	C6-N1	2.50	1.37	1.33
1	A	1404	5MC	C2-N3	2.44	1.43	1.38
1	A	1518[B]	MA6	C2-N1	2.43	1.38	1.33
1	A	1407	5MC	C5-C4	2.31	1.45	1.41
1	A	1207	2MG	C2-N1	2.27	1.41	1.34
1	A	516	PSU	O4'-C1'	-2.21	1.41	1.44
1	A	1541	PSU	O4'-C1'	-2.20	1.41	1.44
1	A	1400	5MC	C4-N4	2.17	1.39	1.34
1	A	1519[B]	MA6	C2-N3	2.13	1.35	1.32
1	A	1402	4OC	C4-N4	2.12	1.40	1.36
1	A	1518[B]	MA6	C2-N3	2.04	1.35	1.32
1	A	1518[A]	MA6	C6-N1	2.03	1.36	1.33
1	A	967	5MC	C4-N4	2.01	1.39	1.34

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1540	PSU	N1-C2-N3	-11.37	119.39	128.43
1	A	1541	PSU	N1-C2-N3	-10.36	120.19	128.43
1	A	516	PSU	N1-C2-N3	-10.08	120.41	128.43
1	A	966	M2G	C5-C6-N1	-8.35	112.01	123.43
1	A	1207	2MG	C5-C6-N1	-7.55	113.11	123.43
1	A	1540	PSU	C4-N3-C2	5.98	120.19	115.14
1	A	966	M2G	C6-N1-C2	5.93	123.24	116.18
1	A	516	PSU	C4-N3-C2	5.86	120.09	115.14
1	A	1541	PSU	C4-N3-C2	5.19	119.53	115.14
1	A	516	PSU	C5-C4-N3	-4.74	119.26	125.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	L	92	0TD	CSB-SB-CB	-4.67	92.66	101.85
1	A	1541	PSU	C5-C4-N3	-4.46	119.62	125.36
1	A	527	7MG	C5-C4-N3	-4.28	119.50	126.49
1	A	527	7MG	N3-C4-N9	4.28	132.40	126.91
1	A	1540	PSU	C5-C4-N3	-4.17	119.98	125.36
1	A	1207	2MG	C6-N1-C2	3.93	122.21	115.18
1	A	527	7MG	N7-C8-N9	3.71	108.68	103.38
1	A	1541	PSU	C5-C6-N1	-3.49	120.14	124.44
1	A	1540	PSU	C6-N1-C2	3.32	120.84	115.36
1	A	1541	PSU	C6-N1-C2	3.29	120.78	115.36
1	A	516	PSU	C5-C6-N1	-3.19	120.52	124.44
1	A	1540	PSU	C5-C6-N1	-3.08	120.65	124.44
1	A	516	PSU	C6-N1-C2	2.82	120.01	115.36
1	A	966	M2G	N1-C2-N2	-2.76	114.40	117.19
1	A	966	M2G	N3-C2-N2	2.73	119.95	117.18
1	A	527	7MG	C2-N3-C4	2.61	121.11	113.89
1	A	1407	5MC	N4-C4-N3	-2.58	113.39	117.03
1	A	1541	PSU	O4'-C1'-C2'	2.38	108.51	104.66
1	A	1498	UR3	C3'-C2'-C1'	2.35	104.52	100.98
1	A	967	5MC	C2-N3-C4	2.34	118.84	116.02
1	A	1540	PSU	C5-C1'-C2'	-2.29	111.24	115.32
1	A	1407	5MC	C2-N3-C4	2.22	118.70	116.02
1	A	1404	5MC	N4-C4-N3	-2.18	113.95	117.03
1	A	527	7MG	C6-N1-C2	2.18	119.39	115.93
1	A	516	PSU	O4'-C1'-C2'	2.15	108.15	104.66
1	A	1400	5MC	C2-N3-C4	2.11	118.56	116.02
1	A	1207	2MG	N2-C2-N3	2.03	118.91	116.96
1	A	1518[B]	MA6	C3'-C2'-C1'	2.01	104.01	100.98
1	A	966	M2G	C2-N3-C4	-2.01	112.99	115.28

There are no chirality outliers.

All (19) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	527	7MG	O4'-C4'-C5'-O5'
1	A	527	7MG	C3'-C4'-C5'-O5'
1	A	1402	4OC	O4'-C4'-C5'-O5'
12	L	92	0TD	CG-CB-SB-CSB
1	A	1519[B]	MA6	C5-C6-N6-C9
1	A	1519[A]	MA6	O4'-C4'-C5'-O5'
1	A	1400	5MC	O4'-C4'-C5'-O5'
1	A	1402	4OC	C3'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
1	A	1519[A]	MA6	C3'-C4'-C5'-O5'
1	A	1400	5MC	C3'-C4'-C5'-O5'
1	A	1518[A]	MA6	C5-C6-N6-C9
1	A	1519[B]	MA6	C5-C6-N6-C10
1	A	1402	4OC	C3'-C2'-O2'-CM2
1	A	1519[B]	MA6	N1-C6-N6-C9
1	A	1518[A]	MA6	C5-C6-N6-C10
1	A	966	M2G	N1-C2-N2-CM1
1	A	966	M2G	N3-C2-N2-CM1
1	A	966	M2G	N1-C2-N2-CM2
1	A	966	M2G	N3-C2-N2-CM2

There are no ring outliers.

9 monomers are involved in 15 short contacts:

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

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 314 ligands modelled in this entry, 314 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

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	1498/1522 (98%)	-0.33	12 (0%) 86 89	80, 123, 244, 351	0
2	B	234/256 (91%)	-0.24	6 (2%) 56 59	102, 150, 230, 265	0
3	C	206/239 (86%)	-0.04	6 (2%) 51 55	131, 174, 221, 266	0
4	D	208/209 (99%)	-0.17	7 (3%) 45 48	94, 131, 181, 214	0
5	E	150/162 (92%)	-0.31	0 100 100	79, 107, 143, 177	0
6	F	101/101 (100%)	-0.52	0 100 100	114, 154, 176, 221	0
7	G	155/156 (99%)	-0.21	6 (3%) 39 43	109, 151, 196, 223	0
8	H	138/138 (100%)	-0.52	0 100 100	74, 99, 133, 155	0
9	I	127/128 (99%)	-0.04	4 (3%) 49 53	126, 180, 210, 231	0
10	J	98/105 (93%)	0.59	12 (12%) 4 5	153, 205, 281, 312	0
11	K	116/129 (89%)	-0.35	0 100 100	98, 123, 161, 180	0
12	L	123/135 (91%)	-0.21	1 (0%) 86 89	75, 130, 163, 197	0
13	M	118/126 (93%)	-0.18	5 (4%) 36 40	125, 155, 185, 290	0
14	N	60/61 (98%)	0.37	4 (6%) 17 21	140, 168, 203, 246	0
15	O	87/89 (97%)	-0.30	0 100 100	86, 114, 161, 176	0
16	P	83/88 (94%)	-0.24	0 100 100	96, 124, 155, 205	0
17	Q	99/105 (94%)	-0.32	0 100 100	79, 115, 150, 179	0
18	R	70/88 (79%)	-0.32	0 100 100	95, 128, 181, 202	0
19	S	80/93 (86%)	0.26	5 (6%) 20 23	143, 197, 244, 249	0
20	T	99/106 (93%)	-0.41	0 100 100	96, 125, 168, 200	0
21	U	24/27 (88%)	1.32	6 (25%) 0 0	133, 151, 179, 212	0
All	All	3874/4063 (95%)	-0.23	74 (1%) 66 71	74, 136, 221, 351	0

All (74) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1129	C	6.1
4	D	35	ARG	5.7
21	U	18	TYR	5.5
10	J	33	GLN	4.2
7	G	2	ALA	4.1
2	B	132	LYS	4.1
1	A	1001	A	4.1
7	G	156	TRP	4.0
1	A	993	G	3.8
9	I	8	GLY	3.7
10	J	39	PRO	3.5
3	C	103	VAL	3.5
19	S	81	ARG	3.4
10	J	37	PRO	3.4
9	I	4	TYR	3.4
4	D	9	CYS	3.4
9	I	15	ALA	3.3
1	A	1024	G	3.3
1	A	1006	C	3.3
10	J	89	ASP	3.2
10	J	70	ARG	3.2
21	U	25	LYS	3.2
3	C	68	VAL	3.1
13	M	119	GLY	3.1
1	A	1037	C	3.1
3	C	66	VAL	3.1
4	D	33	MET	3.0
14	N	6	LEU	3.0
12	L	19	ARG	3.0
7	G	80	VAL	2.9
1	A	1023	G	2.9
10	J	34	VAL	2.9
21	U	24	ARG	2.9
10	J	74	ILE	2.9
13	M	117	VAL	2.9
10	J	87	THR	2.9
1	A	1539	C	2.8
3	C	101	LEU	2.8
13	M	118	ALA	2.8
13	M	7	VAL	2.8
9	I	128	ARG	2.7
3	C	161	GLU	2.7
21	U	22	ARG	2.6

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Mol	Chain	Res	Type	RSRZ
19	S	49	ILE	2.6
21	U	17	THR	2.6
19	S	40	ILE	2.5
3	C	2	GLY	2.5
2	B	127	ILE	2.4
14	N	13	THR	2.4
1	A	202	U	2.4
2	B	230	VAL	2.4
10	J	21	GLN	2.4
1	A	1025	U	2.3
4	D	36	ARG	2.3
1	A	1002	G	2.3
10	J	73	ASP	2.3
14	N	18	VAL	2.2
21	U	5	ASP	2.2
1	A	1030(A)	G	2.2
19	S	69	HIS	2.2
19	S	41	VAL	2.2
13	M	65	LYS	2.2
4	D	18	LYS	2.2
7	G	8	GLU	2.2
10	J	31	GLY	2.2
2	B	134	GLU	2.1
2	B	131	PRO	2.1
10	J	6	ILE	2.1
4	D	29	PRO	2.0
7	G	5	ARG	2.0
14	N	4	LYS	2.0
2	B	125	PRO	2.0
4	D	37	PRO	2.0
7	G	85	TYR	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
1	PSU	A	1540	20/21	0.85	0.50	184,209,213,215	0
1	PSU	A	1541	20/21	0.89	0.30	157,174,186,187	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
1	MA6	A	1518[A]	24/25	0.94	0.26	96,100,103,110	24
1	MA6	A	1518[B]	24/25	0.94	0.26	97,103,122,125	24
1	5MC	A	1400	21/22	0.95	0.18	93,108,127,129	0
1	2MG	A	1207	24/25	0.95	0.11	165,172,180,183	0
1	UR3	A	1498	21/22	0.96	0.20	95,109,121,123	0
1	PSU	A	516	20/21	0.96	0.09	135,141,155,161	0
1	MA6	A	1519[B]	24/25	0.96	0.28	90,98,101,105	24
1	MA6	A	1519[A]	24/25	0.96	0.28	91,98,105,112	24
1	M2G	A	966	25/26	0.96	0.14	122,138,155,161	0
1	5MC	A	1407	21/22	0.97	0.20	111,137,143,147	0
1	5MC	A	1404	21/22	0.97	0.16	104,112,121,126	0
12	0TD	L	92	10/11	0.97	0.40	111,120,126,312	0
1	5MC	A	967	21/22	0.97	0.13	117,132,145,150	0
1	7MG	A	527	24/25	0.98	0.14	103,114,125,127	0
1	4OC	A	1402	22/23	0.98	0.17	103,111,141,148	0

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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	1882	1/1	0.40	1.17	111,111,111,111	0
22	MG	A	1845	1/1	0.46	0.73	389,389,389,389	0
22	MG	A	1887	1/1	0.50	0.37	108,108,108,108	0
22	MG	A	1675	1/1	0.52	0.33	119,119,119,119	0
22	MG	A	1890	1/1	0.53	0.50	124,124,124,124	0
22	MG	A	1751	1/1	0.55	0.51	116,116,116,116	0
22	MG	A	1745	1/1	0.56	0.82	130,130,130,130	0
22	MG	P	104	1/1	0.56	0.62	136,136,136,136	0
22	MG	A	1653	1/1	0.58	0.26	120,120,120,120	0
22	MG	A	1874	1/1	0.61	0.20	155,155,155,155	0
22	MG	A	1724	1/1	0.62	0.39	99,99,99,99	0
22	MG	Q	202	1/1	0.63	0.72	101,101,101,101	0
22	MG	A	1880	1/1	0.63	0.50	104,104,104,104	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
22	MG	A	1883	1/1	0.65	0.32	117,117,117,117	0
22	MG	A	1884	1/1	0.65	1.31	113,113,113,113	0
22	MG	A	1637	1/1	0.67	0.22	110,110,110,110	0
22	MG	A	1891	1/1	0.68	0.33	140,140,140,140	0
22	MG	A	1888	1/1	0.69	0.48	105,105,105,105	0
22	MG	A	1739	1/1	0.69	0.46	95,95,95,95	0
22	MG	A	1726	1/1	0.70	0.28	128,128,128,128	0
22	MG	A	1863	1/1	0.70	0.15	137,137,137,137	0
22	MG	A	1756	1/1	0.72	0.51	128,128,128,128	0
22	MG	A	1624	1/1	0.73	0.53	114,114,114,114	0
22	MG	A	1768	1/1	0.75	0.76	224,224,224,224	0
22	MG	A	1765	1/1	0.75	0.24	193,193,193,193	0
22	MG	A	1719	1/1	0.75	0.58	105,105,105,105	0
22	MG	A	1873	1/1	0.76	0.60	125,125,125,125	0
22	MG	A	1638	1/1	0.76	0.87	106,106,106,106	0
22	MG	A	1736	1/1	0.76	0.53	94,94,94,94	0
22	MG	J	201	1/1	0.76	0.58	360,360,360,360	0
22	MG	A	1762	1/1	0.76	0.20	152,152,152,152	0
22	MG	A	1771	1/1	0.77	0.45	138,138,138,138	0
22	MG	A	1741	1/1	0.77	0.34	114,114,114,114	0
22	MG	A	1628	1/1	0.77	1.21	111,111,111,111	0
22	MG	D	305	1/1	0.77	0.36	107,107,107,107	0
22	MG	A	1712	1/1	0.77	0.72	102,102,102,102	0
22	MG	A	1686	1/1	0.78	0.89	103,103,103,103	0
22	MG	A	1872	1/1	0.79	0.24	91,91,91,91	0
22	MG	A	1614	1/1	0.79	0.38	134,134,134,134	0
22	MG	A	1656	1/1	0.79	0.45	94,94,94,94	0
22	MG	A	1698	1/1	0.79	0.44	120,120,120,120	0
22	MG	A	1662	1/1	0.81	0.23	109,109,109,109	0
22	MG	A	1760	1/1	0.81	0.41	126,126,126,126	0
22	MG	G	201	1/1	0.81	0.20	121,121,121,121	0
22	MG	A	1856	1/1	0.81	0.40	205,205,205,205	0
22	MG	A	1758	1/1	0.81	0.80	110,110,110,110	0
22	MG	A	1858	1/1	0.82	0.53	332,332,332,332	0
22	MG	A	1795	1/1	0.82	0.38	321,321,321,321	0
22	MG	A	1881	1/1	0.82	0.39	88,88,88,88	0
22	MG	A	1810	1/1	0.82	0.36	273,273,273,273	0
22	MG	A	1834	1/1	0.82	0.21	315,315,315,315	0
22	MG	A	1730	1/1	0.82	0.68	117,117,117,117	0
22	MG	A	1817	1/1	0.82	0.30	264,264,264,264	0
22	MG	A	1860	1/1	0.82	0.80	95,95,95,95	0
22	MG	A	1663	1/1	0.83	0.17	102,102,102,102	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
22	MG	A	1772	1/1	0.83	0.12	134,134,134,134	0
22	MG	A	1709	1/1	0.83	0.14	259,259,259,259	0
22	MG	A	1689	1/1	0.83	0.38	118,118,118,118	0
22	MG	A	1699	1/1	0.84	0.38	216,216,216,216	0
22	MG	A	1705	1/1	0.84	0.54	120,120,120,120	0
22	MG	A	1791	1/1	0.84	0.09	313,313,313,313	0
22	MG	N	102	1/1	0.84	0.36	129,129,129,129	0
22	MG	S	101	1/1	0.84	0.72	136,136,136,136	0
22	MG	A	1669	1/1	0.84	0.34	158,158,158,158	0
22	MG	A	1804	1/1	0.84	1.22	313,313,313,313	0
22	MG	A	1715	1/1	0.84	0.42	116,116,116,116	0
22	MG	A	1850	1/1	0.84	0.17	333,333,333,333	0
22	MG	A	1814	1/1	0.84	0.30	240,240,240,240	0
22	MG	D	304	1/1	0.84	0.85	113,113,113,113	0
22	MG	A	1670	1/1	0.84	0.39	110,110,110,110	0
22	MG	A	1691	1/1	0.84	0.27	115,115,115,115	0
22	MG	A	1750	1/1	0.85	0.30	119,119,119,119	0
22	MG	A	1828	1/1	0.85	0.46	310,310,310,310	0
22	MG	A	1713	1/1	0.85	0.52	117,117,117,117	0
22	MG	A	1652	1/1	0.85	0.36	122,122,122,122	0
22	MG	A	1711	1/1	0.85	0.33	117,117,117,117	0
22	MG	A	1798	1/1	0.86	0.50	297,297,297,297	0
22	MG	A	1746	1/1	0.86	0.32	107,107,107,107	0
22	MG	A	1879	1/1	0.86	0.27	107,107,107,107	0
22	MG	A	1807	1/1	0.86	0.26	200,200,200,200	0
22	MG	A	1776	1/1	0.86	0.13	118,118,118,118	0
22	MG	A	1659	1/1	0.86	0.13	168,168,168,168	0
22	MG	A	1606	1/1	0.87	0.09	143,143,143,143	0
22	MG	A	1701	1/1	0.87	0.60	134,134,134,134	0
22	MG	A	1878	1/1	0.87	0.40	107,107,107,107	0
22	MG	P	102	1/1	0.87	0.16	128,128,128,128	0
22	MG	A	1868	1/1	0.87	0.47	100,100,100,100	0
22	MG	A	1731	1/1	0.87	0.62	92,92,92,92	0
22	MG	P	101	1/1	0.87	0.39	90,90,90,90	0
22	MG	A	1806	1/1	0.87	0.23	232,232,232,232	0
22	MG	A	1838	1/1	0.87	0.33	354,354,354,354	0
22	MG	A	1703	1/1	0.87	0.20	94,94,94,94	0
22	MG	A	1783	1/1	0.88	0.29	224,224,224,224	0
22	MG	A	1728	1/1	0.88	0.32	106,106,106,106	0
22	MG	A	1725	1/1	0.88	0.34	128,128,128,128	0
22	MG	A	1808	1/1	0.88	0.60	242,242,242,242	0
22	MG	A	1865	1/1	0.88	0.32	118,118,118,118	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
22	MG	A	1812	1/1	0.89	0.78	401,401,401,401	0
22	MG	A	1840	1/1	0.89	0.83	200,200,200,200	0
22	MG	A	1759	1/1	0.89	0.25	154,154,154,154	0
22	MG	A	1893	1/1	0.89	0.18	118,118,118,118	0
22	MG	A	1674	1/1	0.89	0.22	161,161,161,161	0
22	MG	A	1744	1/1	0.89	0.88	128,128,128,128	0
22	MG	A	1678	1/1	0.89	0.27	140,140,140,140	0
22	MG	A	1702	1/1	0.89	0.33	101,101,101,101	0
22	MG	A	1740	1/1	0.89	0.49	112,112,112,112	0
22	MG	A	1822	1/1	0.89	0.18	290,290,290,290	0
22	MG	A	1690	1/1	0.89	0.17	126,126,126,126	0
22	MG	B	302	1/1	0.89	0.19	147,147,147,147	0
22	MG	A	1704	1/1	0.89	0.18	110,110,110,110	0
22	MG	A	1683	1/1	0.89	0.20	111,111,111,111	0
22	MG	A	1844	1/1	0.90	0.20	309,309,309,309	0
22	MG	A	1700	1/1	0.90	0.15	223,223,223,223	0
22	MG	A	1619	1/1	0.90	0.50	123,123,123,123	0
22	MG	A	1777	1/1	0.91	0.14	104,104,104,104	0
22	MG	A	1608	1/1	0.91	0.22	93,93,93,93	0
22	MG	A	1802	1/1	0.91	0.12	324,324,324,324	0
22	MG	A	1738	1/1	0.91	0.47	112,112,112,112	0
22	MG	A	1864	1/1	0.91	0.15	155,155,155,155	0
22	MG	A	1602	1/1	0.91	0.09	108,108,108,108	0
22	MG	A	1832	1/1	0.91	0.34	267,267,267,267	0
22	MG	A	1885	1/1	0.91	0.62	124,124,124,124	0
22	MG	A	1687	1/1	0.91	0.57	146,146,146,146	0
22	MG	A	1735	1/1	0.91	0.32	96,96,96,96	0
22	MG	A	1616	1/1	0.91	0.30	125,125,125,125	0
22	MG	A	1870	1/1	0.91	0.10	138,138,138,138	0
22	MG	B	301	1/1	0.91	0.24	117,117,117,117	0
22	MG	A	1757	1/1	0.91	0.25	99,99,99,99	0
22	MG	A	1830	1/1	0.92	0.35	297,297,297,297	0
22	MG	A	1794	1/1	0.92	0.24	346,346,346,346	0
22	MG	A	1673	1/1	0.92	0.15	208,208,208,208	0
22	MG	A	1785	1/1	0.92	0.28	242,242,242,242	0
22	MG	A	1871	1/1	0.92	0.65	136,136,136,136	0
22	MG	A	1667	1/1	0.92	0.25	110,110,110,110	0
22	MG	A	1640	1/1	0.92	0.31	143,143,143,143	0
22	MG	A	1634	1/1	0.92	0.14	174,174,174,174	0
22	MG	A	1661	1/1	0.92	0.22	137,137,137,137	0
22	MG	A	1754	1/1	0.92	0.31	151,151,151,151	0
22	MG	A	1857	1/1	0.92	0.35	287,287,287,287	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
22	MG	A	1820	1/1	0.92	0.20	320,320,320,320	0
22	MG	A	1809	1/1	0.92	0.17	169,169,169,169	0
22	MG	A	1657	1/1	0.93	0.22	124,124,124,124	0
22	MG	A	1645	1/1	0.93	0.18	65,65,65,65	0
22	MG	A	1710	1/1	0.93	0.22	85,85,85,85	0
22	MG	A	1655	1/1	0.93	0.45	96,96,96,96	0
22	MG	A	1646	1/1	0.93	0.27	102,102,102,102	0
22	MG	A	1694	1/1	0.93	0.16	152,152,152,152	0
22	MG	A	1775	1/1	0.93	0.27	107,107,107,107	0
22	MG	A	1633	1/1	0.93	0.47	105,105,105,105	0
22	MG	A	1842	1/1	0.93	0.46	228,228,228,228	0
22	MG	A	1875	1/1	0.93	0.24	99,99,99,99	0
22	MG	A	1796	1/1	0.93	0.34	235,235,235,235	0
22	MG	A	1732	1/1	0.93	0.20	104,104,104,104	0
22	MG	A	1626	1/1	0.93	0.23	106,106,106,106	0
22	MG	A	1773	1/1	0.93	0.33	151,151,151,151	0
22	MG	A	1853	1/1	0.93	0.14	333,333,333,333	0
22	MG	A	1748	1/1	0.94	0.17	114,114,114,114	0
22	MG	A	1604	1/1	0.94	0.87	113,113,113,113	0
22	MG	A	1852	1/1	0.94	0.18	309,309,309,309	0
22	MG	A	1625	1/1	0.94	0.49	120,120,120,120	0
22	MG	A	1886	1/1	0.94	0.16	94,94,94,94	0
22	MG	A	1797	1/1	0.94	0.26	272,272,272,272	0
22	MG	A	1643	1/1	0.94	0.50	128,128,128,128	0
22	MG	A	1855	1/1	0.94	0.17	173,173,173,173	0
22	MG	A	1630	1/1	0.94	0.11	103,103,103,103	0
22	MG	A	1729	1/1	0.94	0.15	67,67,67,67	0
22	MG	A	1805	1/1	0.94	0.09	198,198,198,198	0
22	MG	A	1720	1/1	0.94	0.17	122,122,122,122	0
22	MG	A	1695	1/1	0.94	0.28	104,104,104,104	0
22	MG	A	1769	1/1	0.94	0.18	193,193,193,193	0
22	MG	A	1848	1/1	0.94	0.29	233,233,233,233	0
22	MG	A	1833	1/1	0.94	0.23	207,207,207,207	0
22	MG	A	1664	1/1	0.94	0.07	90,90,90,90	0
22	MG	A	1688	1/1	0.94	0.10	130,130,130,130	0
22	MG	A	1717	1/1	0.94	0.42	72,72,72,72	0
22	MG	A	1869	1/1	0.94	0.31	129,129,129,129	0
22	MG	A	1612	1/1	0.94	0.09	113,113,113,113	0
22	MG	A	1780	1/1	0.94	0.19	131,131,131,131	0
22	MG	A	1892	1/1	0.94	0.46	92,92,92,92	0
22	MG	A	1781	1/1	0.95	0.16	160,160,160,160	0
22	MG	A	1649	1/1	0.95	0.36	121,121,121,121	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
22	MG	A	1819	1/1	0.95	0.29	330,330,330,330	0
22	MG	A	1613	1/1	0.95	0.13	113,113,113,113	0
22	MG	A	1821	1/1	0.95	0.24	230,230,230,230	0
22	MG	A	1672	1/1	0.95	0.08	147,147,147,147	0
22	MG	A	1737	1/1	0.95	0.26	138,138,138,138	0
22	MG	A	1799	1/1	0.95	0.16	185,185,185,185	0
22	MG	A	1621	1/1	0.95	0.22	99,99,99,99	0
22	MG	A	1788	1/1	0.95	0.21	365,365,365,365	0
22	MG	A	1770	1/1	0.95	0.17	120,120,120,120	0
22	MG	A	1784	1/1	0.95	0.37	324,324,324,324	0
22	MG	A	1813	1/1	0.95	0.22	326,326,326,326	0
22	MG	A	1747	1/1	0.95	0.33	100,100,100,100	0
22	MG	A	1727	1/1	0.95	0.46	114,114,114,114	0
22	MG	A	1767	1/1	0.95	0.12	193,193,193,193	0
22	MG	A	1831	1/1	0.95	0.16	288,288,288,288	0
22	MG	A	1837	1/1	0.95	0.16	142,142,142,142	0
22	MG	A	1790	1/1	0.95	0.09	138,138,138,138	0
22	MG	A	1818	1/1	0.96	0.20	242,242,242,242	0
22	MG	A	1603	1/1	0.96	0.20	109,109,109,109	0
22	MG	Q	201	1/1	0.96	0.12	103,103,103,103	0
22	MG	A	1707	1/1	0.96	0.17	69,69,69,69	0
22	MG	A	1761	1/1	0.96	0.12	98,98,98,98	0
22	MG	A	1839	1/1	0.96	0.30	258,258,258,258	0
22	MG	A	1696	1/1	0.96	0.69	150,150,150,150	0
22	MG	A	1877	1/1	0.96	0.33	150,150,150,150	0
22	MG	A	1755	1/1	0.96	0.15	96,96,96,96	0
22	MG	A	1867	1/1	0.96	0.10	115,115,115,115	0
22	MG	A	1763	1/1	0.96	0.18	110,110,110,110	0
22	MG	A	1815	1/1	0.96	0.41	147,147,147,147	0
22	MG	A	1811	1/1	0.96	0.14	325,325,325,325	0
22	MG	A	1826	1/1	0.96	0.27	235,235,235,235	0
22	MG	A	1849	1/1	0.96	0.33	174,174,174,174	0
22	MG	A	1789	1/1	0.96	0.08	229,229,229,229	0
22	MG	A	1639	1/1	0.96	0.15	204,204,204,204	0
22	MG	A	1618	1/1	0.96	0.60	124,124,124,124	0
22	MG	A	1716	1/1	0.96	0.33	80,80,80,80	0
22	MG	A	1787	1/1	0.96	0.14	260,260,260,260	0
22	MG	A	1792	1/1	0.96	0.18	312,312,312,312	0
22	MG	A	1782	1/1	0.96	0.22	127,127,127,127	0
22	MG	A	1859	1/1	0.96	0.28	267,267,267,267	0
22	MG	A	1714	1/1	0.96	0.26	97,97,97,97	0
22	MG	A	1692	1/1	0.96	0.23	352,352,352,352	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
22	MG	A	1647	1/1	0.96	0.25	92,92,92,92	0
22	MG	A	1824	1/1	0.96	0.08	177,177,177,177	0
22	MG	A	1825	1/1	0.96	0.71	271,271,271,271	0
22	MG	A	1861	1/1	0.96	0.18	182,182,182,182	0
22	MG	A	1749	1/1	0.96	0.26	108,108,108,108	0
22	MG	A	1823	1/1	0.96	0.25	246,246,246,246	0
22	MG	A	1835	1/1	0.96	0.22	148,148,148,148	0
22	MG	A	1836	1/1	0.96	0.20	228,228,228,228	0
22	MG	A	1862	1/1	0.96	0.87	130,130,130,130	0
22	MG	A	1889	1/1	0.96	0.09	100,100,100,100	0
22	MG	A	1803	1/1	0.96	0.18	206,206,206,206	0
22	MG	A	1718	1/1	0.96	0.24	108,108,108,108	0
22	MG	A	1846	1/1	0.96	0.24	222,222,222,222	0
22	MG	A	1827	1/1	0.96	0.14	393,393,393,393	0
22	MG	A	1841	1/1	0.97	0.17	278,278,278,278	0
22	MG	P	103	1/1	0.97	0.29	220,220,220,220	0
22	MG	A	1681	1/1	0.97	0.17	146,146,146,146	0
22	MG	A	1778	1/1	0.97	0.14	135,135,135,135	0
22	MG	A	1636	1/1	0.97	0.14	120,120,120,120	0
22	MG	A	1620	1/1	0.97	0.18	86,86,86,86	0
22	MG	A	1876	1/1	0.97	0.55	138,138,138,138	0
22	MG	A	1708	1/1	0.97	0.07	124,124,124,124	0
22	MG	A	1866	1/1	0.97	0.26	110,110,110,110	0
22	MG	A	1601	1/1	0.97	0.34	112,112,112,112	0
22	MG	A	1734	1/1	0.97	0.26	84,84,84,84	0
23	ZN	N	101	1/1	0.97	0.19	160,160,160,160	0
22	MG	A	1854	1/1	0.97	0.10	251,251,251,251	0
22	MG	A	1766	1/1	0.97	0.11	195,195,195,195	0
22	MG	A	1779	1/1	0.97	0.32	101,101,101,101	0
22	MG	A	1697	1/1	0.97	0.14	101,101,101,101	0
22	MG	A	1851	1/1	0.97	0.34	286,286,286,286	0
22	MG	A	1733	1/1	0.97	0.23	102,102,102,102	0
22	MG	A	1693	1/1	0.97	0.23	101,101,101,101	0
22	MG	A	1677	1/1	0.97	0.67	185,185,185,185	0
22	MG	A	1793	1/1	0.97	0.12	159,159,159,159	0
22	MG	A	1622	1/1	0.97	0.81	67,67,67,67	0
22	MG	A	1668	1/1	0.97	0.16	130,130,130,130	0
22	MG	A	1753	1/1	0.97	0.20	99,99,99,99	0
22	MG	A	1610	1/1	0.97	0.16	172,172,172,172	0
22	MG	A	1721	1/1	0.97	0.29	109,109,109,109	0
22	MG	A	1665	1/1	0.97	0.13	253,253,253,253	0
22	MG	A	1644	1/1	0.97	0.31	114,114,114,114	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
22	MG	A	1801	1/1	0.98	0.18	350,350,350,350	0
22	MG	A	1706	1/1	0.98	0.26	128,128,128,128	0
22	MG	A	1671	1/1	0.98	0.49	108,108,108,108	0
22	MG	A	1829	1/1	0.98	0.18	269,269,269,269	0
22	MG	A	1800	1/1	0.98	0.06	297,297,297,297	0
22	MG	A	1658	1/1	0.98	0.14	134,134,134,134	0
22	MG	A	1764	1/1	0.98	0.10	113,113,113,113	0
22	MG	A	1648	1/1	0.98	0.30	157,157,157,157	0
22	MG	A	1609	1/1	0.98	0.32	103,103,103,103	0
22	MG	A	1847	1/1	0.98	0.12	269,269,269,269	0
22	MG	F	201	1/1	0.98	0.42	131,131,131,131	0
22	MG	A	1684	1/1	0.98	0.16	128,128,128,128	0
22	MG	A	1685	1/1	0.98	0.10	97,97,97,97	0
22	MG	A	1786	1/1	0.98	0.40	310,310,310,310	0
22	MG	D	303	1/1	0.98	0.09	98,98,98,98	0
22	MG	E	201	1/1	0.98	0.14	118,118,118,118	0
22	MG	C	301	1/1	0.98	0.44	169,169,169,169	0
22	MG	A	1642	1/1	0.98	0.53	130,130,130,130	0
22	MG	D	302	1/1	0.98	0.49	90,90,90,90	0
22	MG	A	1752	1/1	0.98	0.13	91,91,91,91	0
22	MG	A	1676	1/1	0.98	0.04	132,132,132,132	0
22	MG	A	1623	1/1	0.98	0.17	118,118,118,118	0
22	MG	A	1682	1/1	0.98	0.24	122,122,122,122	0
22	MG	A	1723	1/1	0.98	0.16	122,122,122,122	0
22	MG	A	1635	1/1	0.98	0.16	90,90,90,90	0
22	MG	A	1651	1/1	0.98	0.26	149,149,149,149	0
22	MG	A	1666	1/1	0.98	0.34	108,108,108,108	0
22	MG	A	1615	1/1	0.98	0.16	72,72,72,72	0
22	MG	A	1743	1/1	0.98	0.48	92,92,92,92	0
22	MG	A	1680	1/1	0.98	0.42	144,144,144,144	0
22	MG	A	1611	1/1	0.98	0.10	128,128,128,128	0
22	MG	A	1607	1/1	0.98	0.40	101,101,101,101	0
22	MG	A	1843	1/1	0.98	0.20	401,401,401,401	0
22	MG	A	1654	1/1	0.99	0.12	92,92,92,92	0
22	MG	A	1627	1/1	0.99	0.09	84,84,84,84	0
22	MG	A	1650	1/1	0.99	0.24	99,99,99,99	0
22	MG	A	1617	1/1	0.99	0.26	116,116,116,116	0
22	MG	A	1816	1/1	0.99	0.14	57,57,57,57	0
22	MG	A	1722	1/1	0.99	0.06	97,97,97,97	0
22	MG	A	1641	1/1	0.99	0.20	151,151,151,151	0
22	MG	A	1660	1/1	0.99	0.09	112,112,112,112	0
22	MG	A	1605	1/1	0.99	0.08	105,105,105,105	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
22	MG	A	1742	1/1	0.99	0.06	94,94,94,94	0
22	MG	A	1679	1/1	0.99	0.13	169,169,169,169	0
23	ZN	D	301	1/1	0.99	0.41	118,118,118,118	0
22	MG	A	1632	1/1	0.99	0.40	88,88,88,88	0
22	MG	A	1774	1/1	0.99	0.23	190,190,190,190	0
22	MG	A	1631	1/1	0.99	0.11	95,95,95,95	0
22	MG	A	1629	1/1	1.00	0.36	139,139,139,139	0

6.5 Other polymers

There are no such residues in this entry.