Full wwPDB X-ray Structure Validation Report ⓘ

Apr 7, 2025 – 08:22 PM JST

PDB ID	:	8WRC / pdb_00008wrc
Title	:	Time-Resolved Ambient Temperature Kineto-Crystallographic Structure of Initiation Factor in Complex with Ribosome
Authors	:	DeMirci, H.; Yapici, I.
Deposited on	:	2023-10-13
Resolution	:	3.59 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 types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

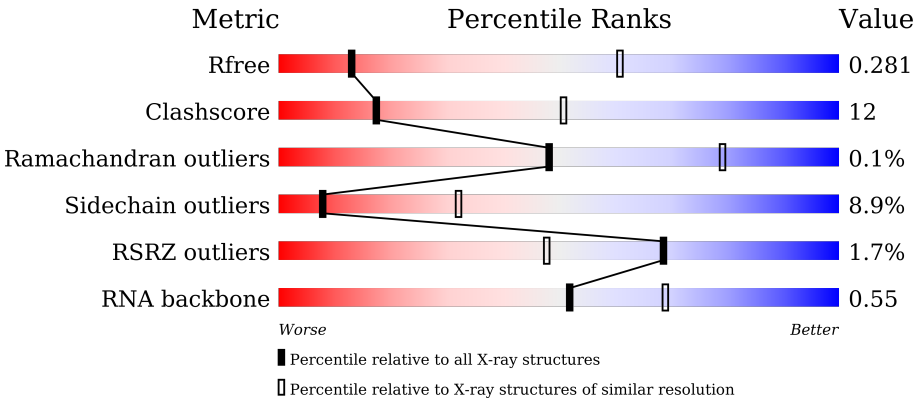
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	2.0rc1
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.006 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.42

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 3.59 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}	164625	1563 (3.70-3.50)
Clashscore	180529	1665 (3.70-3.50)
Ramachandran outliers	177936	1641 (3.70-3.50)
Sidechain outliers	177891	1640 (3.70-3.50)
RSRZ outliers	164620	1562 (3.70-3.50)
RNA backbone	3690	1108 (4.20-3.00)

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

Mol	Chain	Length	Quality of chain
1	A	1522	47% 43% 9%
2	B	256	56% 30% 5% 9%
3	C	239	2% 54% 28% 14%
4	D	209	2% 66% 32%

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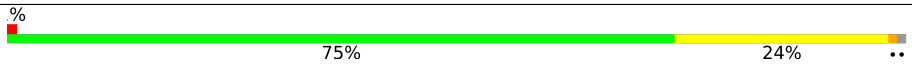
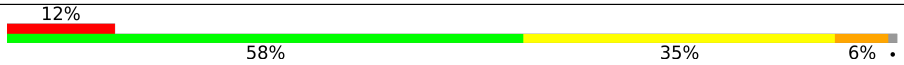
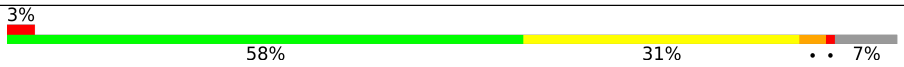
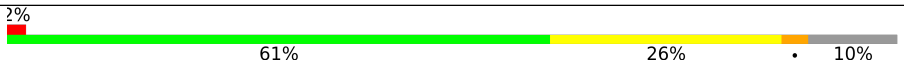
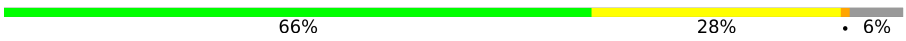
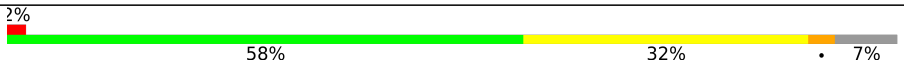
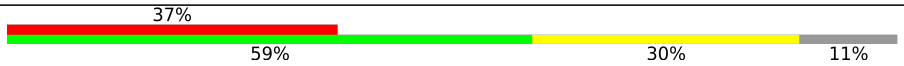
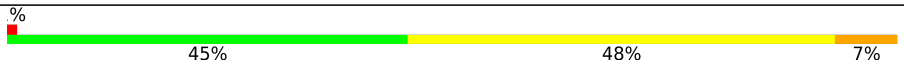
Mol	Chain	Length	Quality of chain
5	E	162	
6	F	101	
7	G	156	
8	H	138	
9	I	128	
10	J	105	
11	K	129	
12	L	135	
13	M	126	
14	N	61	
15	O	89	
16	P	88	
17	Q	105	
18	R	88	
19	S	93	
20	T	106	
21	U	27	
22	W	71	

2 Entry composition (i)

There are 25 unique types of molecules in this entry. The entry contains 52786 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	1511	32623	14530	6037	10539	1517	0	6	0

There are 11 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	U	-	conflict	GB NR_037066
A	13	C	U	conflict	GB NR_037066
A	1027	C	-	insertion	GB NR_037066
A	1031	G	-	insertion	GB NR_037066
A	1244	C	-	insertion	GB NR_037066
A	1245	A	-	insertion	GB NR_037066
A	1534	C	A	conflict	GB NR_037066
A	1535	A	C	conflict	GB NR_037066
A	1540	PSU	-	insertion	GB NR_037066
A	1541	PSU	-	insertion	GB NR_037066
A	1543	C	U	conflict	GB NR_037066

- Molecule 2 is a protein called 30S 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 30S 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 30S ribosomal protein S4.

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

- Molecule 5 is a protein called 30S 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 30S ribosomal protein S6.

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

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

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

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

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

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

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

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

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

- Molecule 11 is a protein called 30S 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 Small ribosomal subunit protein uS12.

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 30S ribosomal protein S13.

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

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

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

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

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

- Molecule 16 is a protein called 30S 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 30S 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			

- Molecule 18 is a protein called 30S 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 30S 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 30S 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 30S 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 a protein called Translation initiation factor IF-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	W	71	Total 570	C 362	N 103	O 103	S 2	0	0	0

- Molecule 23 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
23	A	233	Total 233	Mg 233	0	0
23	B	1	Total 1	Mg 1	0	0
23	C	3	Total 3	Mg 3	0	0
23	D	3	Total 3	Mg 3	0	0
23	E	2	Total 2	Mg 2	0	0
23	F	1	Total 1	Mg 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
23	H	1	Total Mg 1 1	0	0
23	I	3	Total Mg 3 3	0	0
23	L	1	Total Mg 1 1	0	0
23	N	1	Total Mg 1 1	0	0
23	P	2	Total Mg 2 2	0	0
23	Q	1	Total Mg 1 1	0	0
23	S	1	Total Mg 1 1	0	0
23	W	1	Total Mg 1 1	0	0

- Molecule 24 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

- Molecule 25 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
25	A	237	Total O 237 237	0	0
25	C	1	Total O 1 1	0	0
25	D	3	Total O 3 3	0	0
25	E	1	Total O 1 1	0	0
25	L	2	Total O 2 2	0	0
25	N	3	Total O 3 3	0	0
25	O	1	Total O 1 1	0	0

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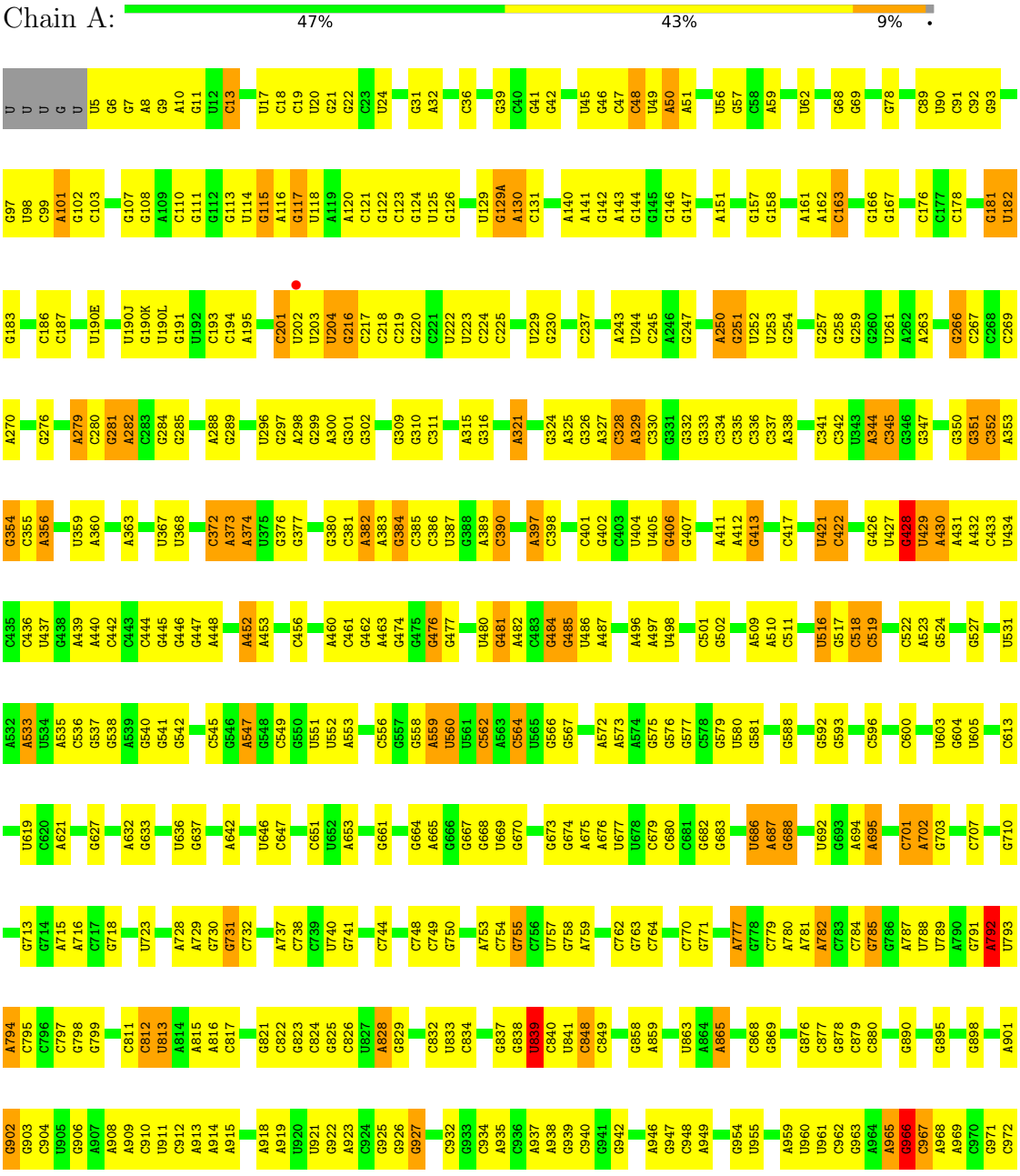
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
25	T	1	Total O 1 1	0	0

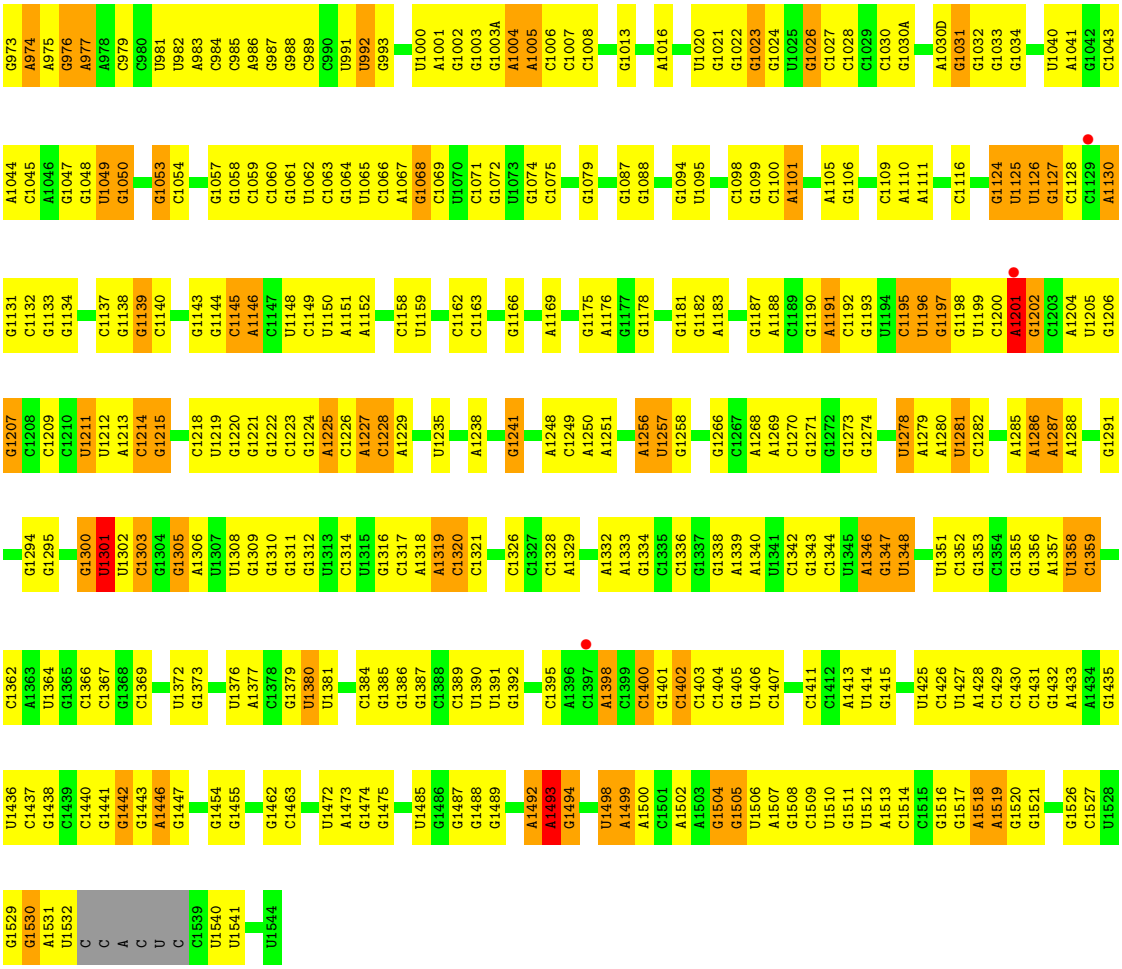
3 Residue-property plots (i)

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

- Molecule 1: 16S rRNA

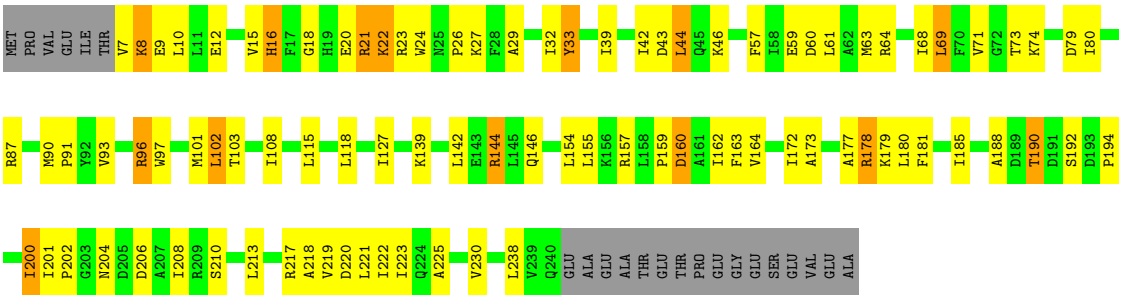
Chain A:





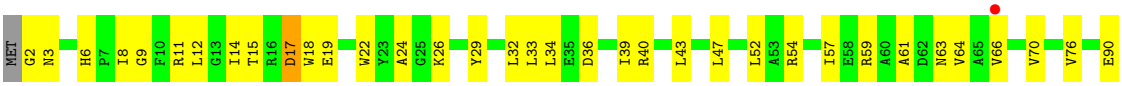
• Molecule 2: 30S ribosomal protein S2

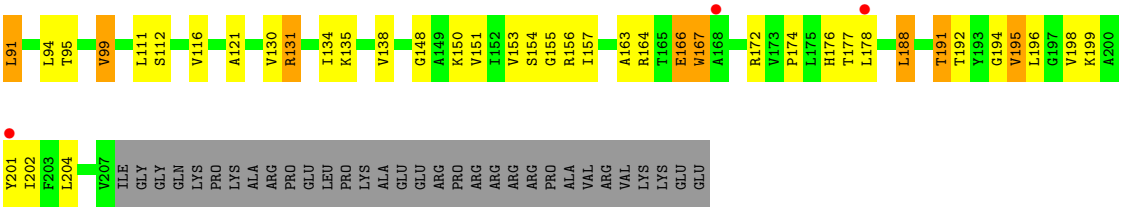
Chain B:



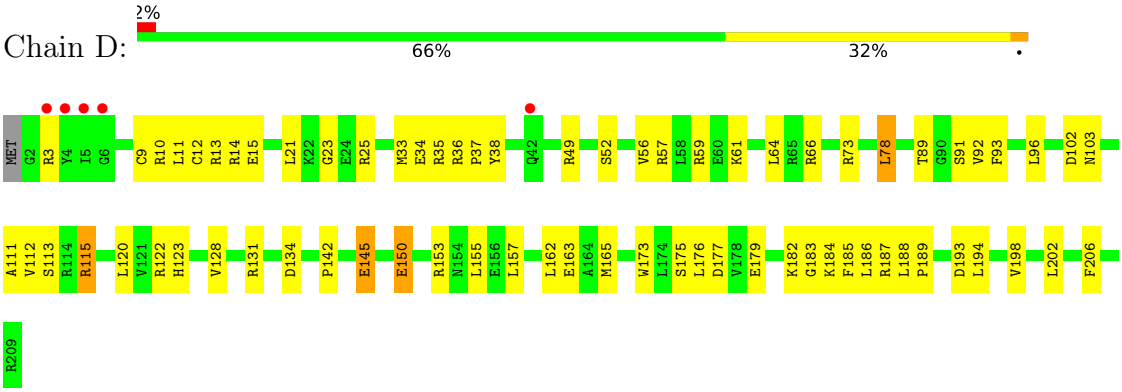
• Molecule 3: 30S ribosomal protein S3

Chain C:

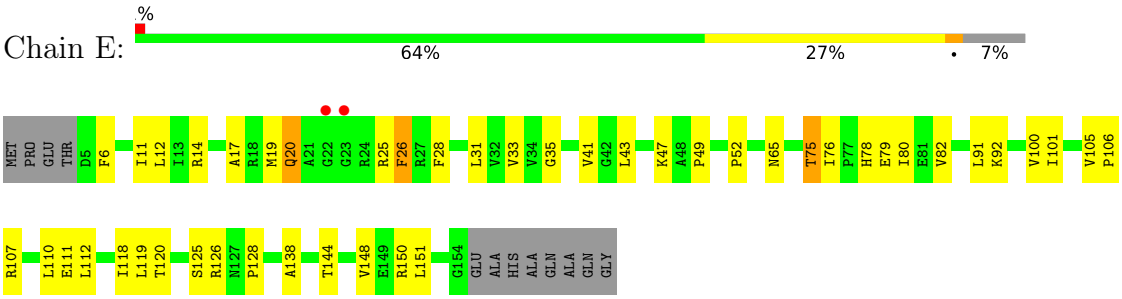




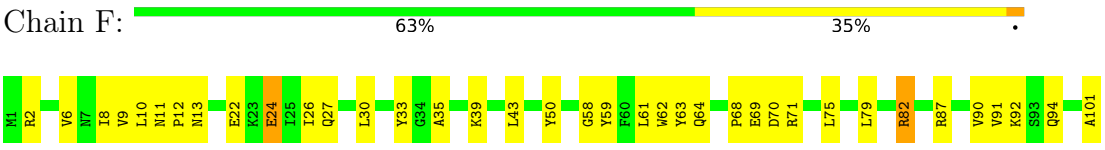
• Molecule 4: 30S ribosomal protein S4



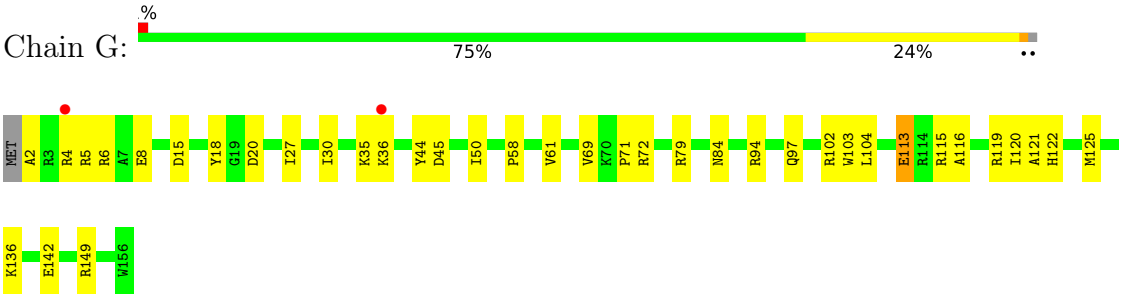
• Molecule 5: 30S ribosomal protein S5



• Molecule 6: 30S ribosomal protein S6

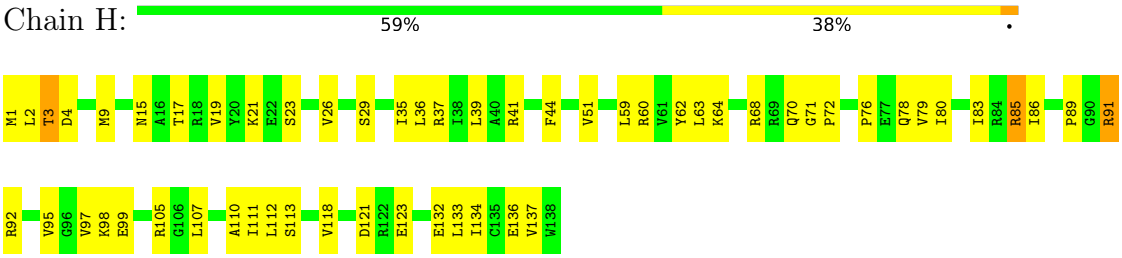


• Molecule 7: 30S ribosomal protein S7



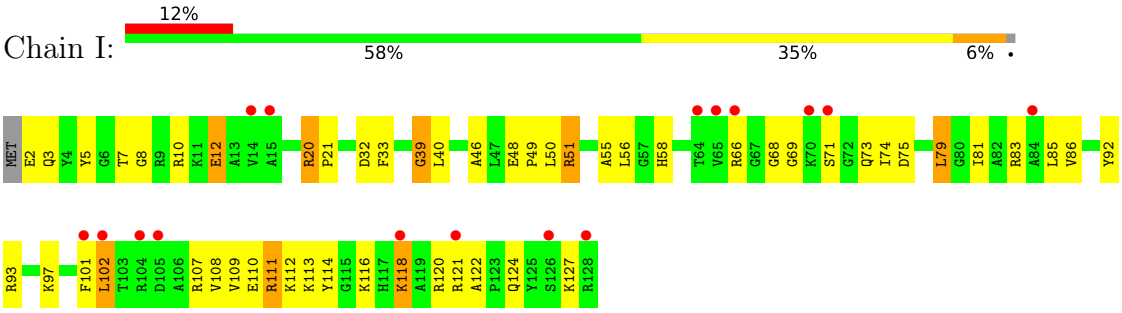
• Molecule 8: 30S ribosomal protein S8

Chain H:



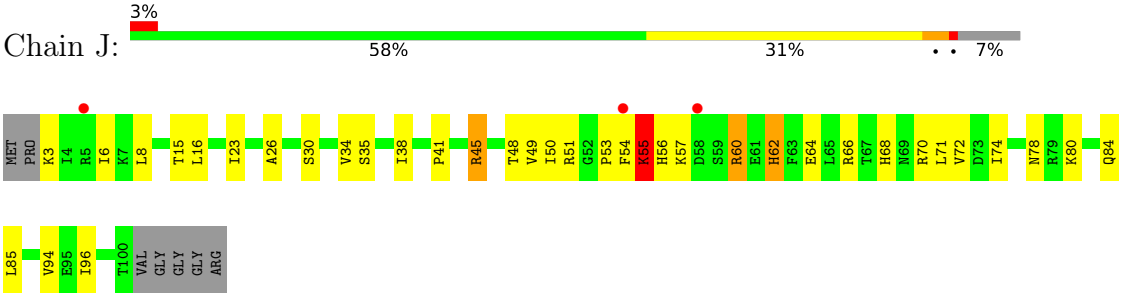
• Molecule 9: 30S ribosomal protein S9

Chain I:



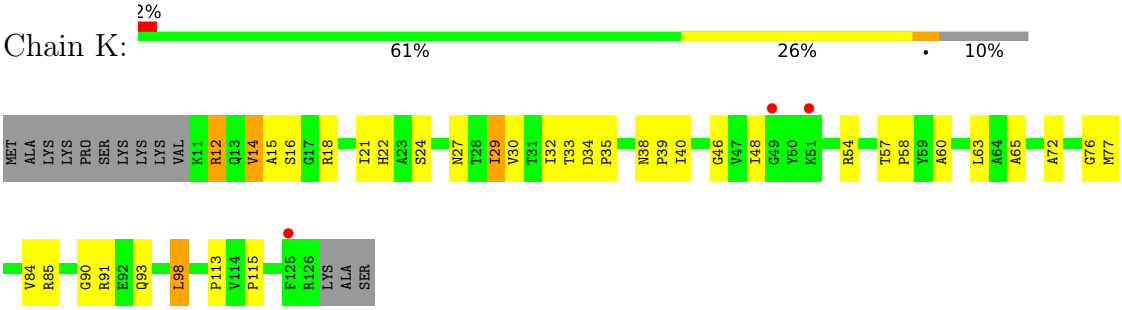
• Molecule 10: 30S ribosomal protein S10

Chain J:



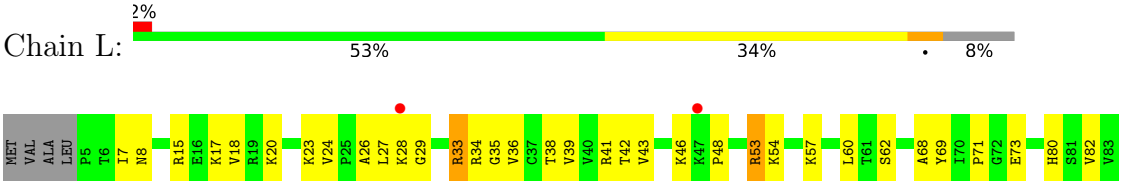
• Molecule 11: 30S ribosomal protein S11

Chain K:



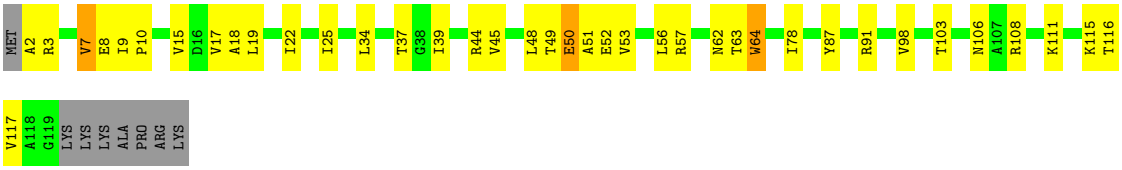
• Molecule 12: Small ribosomal subunit protein uS12

Chain L:



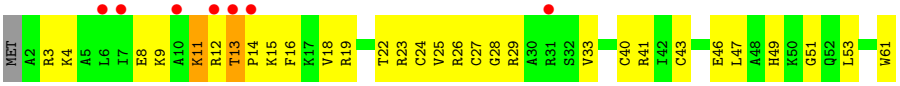
• Molecule 13: 30S ribosomal protein S13

Chain M:



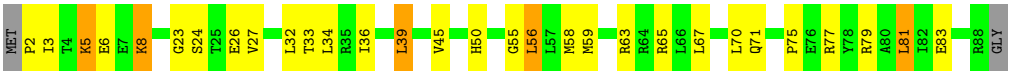
• Molecule 14: 30S ribosomal protein S14 type Z

Chain N:



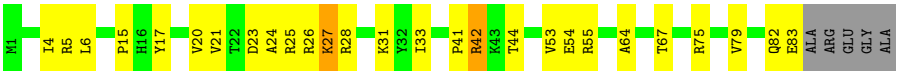
• Molecule 15: 30S ribosomal protein S15

Chain O:



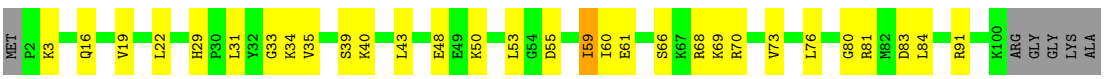
• Molecule 16: 30S ribosomal protein S16

Chain P:



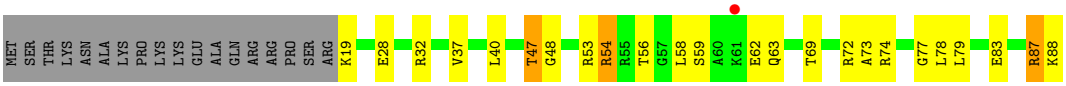
• Molecule 17: 30S ribosomal protein S17

Chain Q:



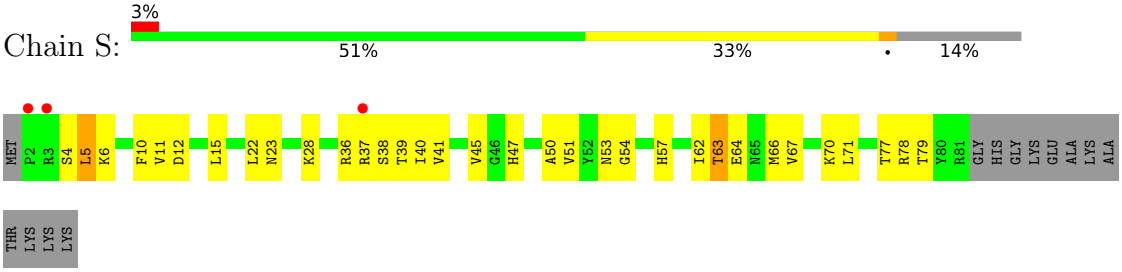
• Molecule 18: 30S ribosomal protein S18

Chain R:



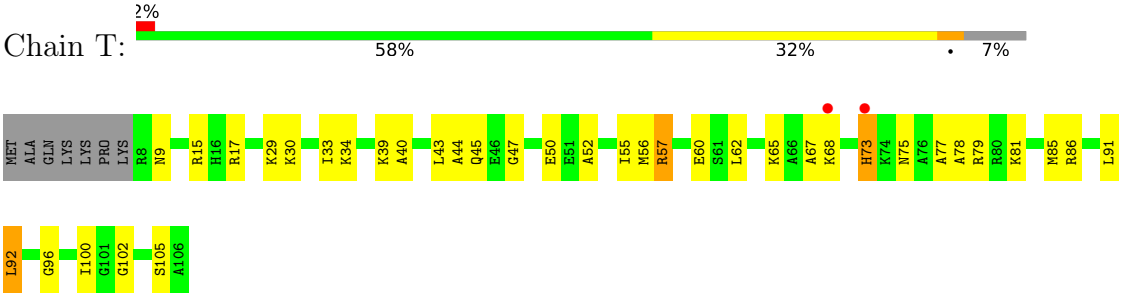
• Molecule 19: 30S ribosomal protein S19

Chain S:



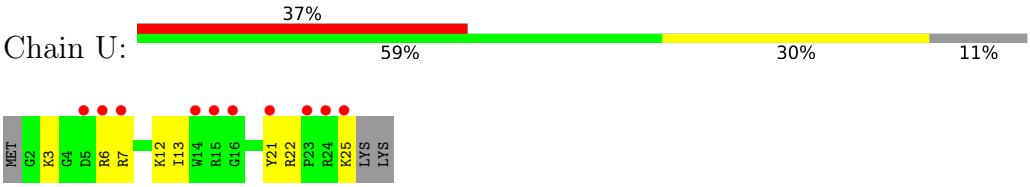
• Molecule 20: 30S ribosomal protein S20

Chain T:



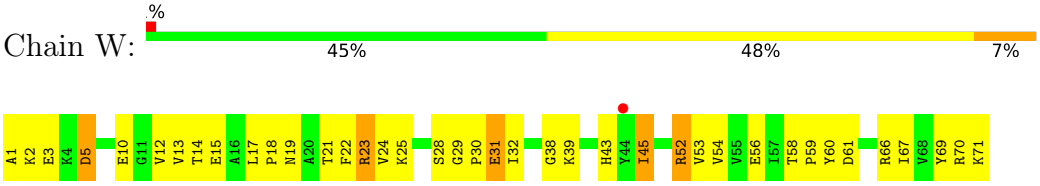
• Molecule 21: 30S ribosomal protein Thx

Chain U:



• Molecule 22: Translation initiation factor IF-1

Chain W:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α, β, γ	402.60Å 402.60Å 175.90Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	51.91 – 3.59 51.91 – 3.59	Depositor EDS
% Data completeness (in resolution range)	98.2 (51.91-3.59) 98.1 (51.91-3.59)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.98 (at 3.57Å)	Xtriage
Refinement program	PHENIX (1.20.1_4487: ???)	Depositor
R, R_{free}	0.233 , 0.282 0.234 , 0.281	Depositor DCC
R_{free} test set	166856 reflections (0.32%)	wwPDB-VP
Wilson B-factor (Å^2)	138.5	Xtriage
Anisotropy	0.172	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 210.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.33$, $< L^2 > = 0.16$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	52786	wwPDB-VP
Average B, all atoms (Å^2)	181.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.42% 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: 4OC, 5MC, G7M, MA6, MG, 0TD, ZN, 2MG, UR3, M2G, 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	0.22	0/36114	0.77	18/56355 (0.0%)
2	B	0.25	0/1935	0.52	0/2609
3	C	0.25	0/1636	0.56	0/2205
4	D	0.25	0/1733	0.55	0/2318
5	E	0.26	0/1162	0.56	0/1564
6	F	0.25	0/856	0.53	0/1154
7	G	0.24	0/1276	0.52	0/1709
8	H	0.27	0/1136	0.59	0/1527
9	I	0.26	0/1029	0.58	1/1379 (0.1%)
10	J	0.24	0/805	0.56	0/1082
11	K	0.26	0/879	0.51	0/1187
12	L	0.26	0/977	0.59	0/1306
13	M	0.25	0/947	0.60	0/1270
14	N	0.25	0/501	0.62	0/664
15	O	0.24	0/740	0.53	0/987
16	P	0.25	0/716	0.58	0/963
17	Q	0.25	0/836	0.55	0/1117
18	R	0.25	0/579	0.57	0/768
19	S	0.24	0/661	0.54	0/890
20	T	0.25	0/765	0.53	0/1007
21	U	0.24	0/212	0.65	0/277
22	W	0.24	0/580	0.54	0/782
All	All	0.23	0/56075	0.71	19/83120 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
3	C	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
8	H	0	1
13	M	0	1
All	All	0	3

There are no bond length outliers.

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1158	C	N1-C2-O2	7.24	123.25	118.90
1	A	328	C	C2-N1-C1'	6.33	125.76	118.80
1	A	839	U	C2-N1-C1'	6.30	125.26	117.70
1	A	1493	A	OP1-P-O3'	6.09	118.59	105.20
1	A	1158	C	N3-C2-O2	-6.08	117.65	121.90
1	A	1158	C	C2-N1-C1'	6.04	125.44	118.80
1	A	1301	U	P-O3'-C3'	5.74	126.59	119.70
1	A	328	C	N1-C2-O2	5.63	122.28	118.90
1	A	839	U	N1-C2-O2	5.61	126.73	122.80
1	A	754	C	C2-N1-C1'	5.60	124.96	118.80
1	A	792	A	P-O3'-C3'	5.51	126.31	119.70
1	A	1301	U	OP1-P-O3'	5.36	116.99	105.20
9	I	39	GLY	N-CA-C	-5.33	99.77	113.10
1	A	1305	G	P-O3'-C3'	5.28	126.04	119.70
1	A	839	U	N3-C2-O2	-5.23	118.54	122.20
1	A	1380	U	P-O3'-C3'	5.23	125.98	119.70
1	A	428	G	P-O3'-C3'	5.17	125.91	119.70
1	A	1346	A	P-O3'-C3'	5.12	125.84	119.70
1	A	1201	A	P-O3'-C3'	5.00	125.71	119.70

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	C	166	GLU	Peptide
8	H	71	GLY	Peptide
13	M	111	LYS	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	32623	0	16486	586	1
2	B	1900	0	1951	62	0
3	C	1612	0	1677	60	0
4	D	1703	0	1763	41	0
5	E	1146	0	1207	36	0
6	F	843	0	857	24	0
7	G	1257	0	1296	26	0
8	H	1116	0	1177	44	0
9	I	1010	0	1037	38	0
10	J	792	0	835	30	0
11	K	864	0	881	25	0
12	L	972	0	1058	47	0
13	M	937	0	995	26	0
14	N	492	0	529	34	0
15	O	729	0	768	16	0
16	P	700	0	720	17	0
17	Q	823	0	893	20	0
18	R	574	0	644	21	0
19	S	647	0	673	23	0
20	T	763	0	861	30	0
21	U	208	0	221	4	0
22	W	570	0	599	28	0
23	A	233	0	0	0	0
23	B	1	0	0	0	0
23	C	3	0	0	0	0
23	D	3	0	0	0	0
23	E	2	0	0	0	0
23	F	1	0	0	0	0
23	H	1	0	0	0	0
23	I	3	0	0	0	0
23	L	1	0	0	0	0
23	N	1	0	0	0	0
23	P	2	0	0	0	0
23	Q	1	0	0	0	0
23	S	1	0	0	0	0
23	W	1	0	0	0	0
24	D	1	0	0	0	0
24	N	1	0	0	0	0
25	A	237	0	0	0	0
25	C	1	0	0	0	0
25	D	3	0	0	0	0
25	E	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
25	L	2	0	0	0	0
25	N	3	0	0	0	0
25	O	1	0	0	0	0
25	T	1	0	0	0	0
All	All	52786	0	37128	1060	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 12.

All (1060) 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:1377:A:HO2'	7:G:2:ALA:N	1.63	0.97
1:A:481:G:HO2'	1:A:482:A:H8	1.01	0.94
1:A:664:G:H22	1:A:741:G:H1	1.09	0.93
1:A:955:U:H1'	1:A:1227:A:H61	1.32	0.92
1:A:463:A:OP1	16:P:75:ARG:NH1	2.13	0.82
20:T:100:ILE:HG22	20:T:102:GLY:H	1.44	0.80
1:A:1372:U:H5"	9:I:71:SER:HB3	1.63	0.79
11:K:91:ARG:HH12	18:R:88:LYS:HD3	1.46	0.79
1:A:448:A:OP2	1:A:485:G:N2	2.13	0.78
7:G:122:HIS:HA	7:G:125:MET:HE2	1.66	0.78
4:D:78:LEU:HB3	4:D:93:PHE:HE1	1.46	0.78
1:A:1443:G:H5"	1:A:1446:A:H5'	1.65	0.78
1:A:1057:G:H5"	3:C:154:SER:HB2	1.64	0.78
1:A:1516[B]:G:N2	1:A:1519[B]:MA6:OP2	2.18	0.77
1:A:1392:G:H21	1:A:1502:A:H8	1.33	0.76
1:A:1125:U:OP2	1:A:1145:C:N4	2.19	0.76
1:A:437:U:HO2'	4:D:123:HIS:HD1	1.34	0.75
1:A:1020:U:H2'	1:A:1021:G:H8	1.52	0.75
9:I:97:LYS:HG3	9:I:102:LEU:HD11	1.69	0.75
1:A:407:G:OP1	4:D:115:ARG:NH1	2.19	0.74
16:P:15:PRO:HD2	16:P:42:ARG:HD3	1.69	0.74
12:L:33:ARG:HD3	12:L:62:SER:HB3	1.67	0.74
1:A:1134:G:H1	1:A:1140:C:H42	1.36	0.73
1:A:1266:G:N2	1:A:1269:A:OP2	2.22	0.73
1:A:1474:G:H2'	1:A:1475:G:C8	2.22	0.73
1:A:1222:G:H5"	19:S:78:ARG:HE	1.54	0.73
1:A:677:U:H3	1:A:713:G:H22	1.37	0.73
12:L:53:ARG:NH1	12:L:92:0TD:OD2	2.22	0.72
1:A:1314:C:N4	19:S:4:SER:OG	2.21	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:10:PRO:HB2	13:M:18:ALA:HB1	1.69	0.72
17:Q:66:SER:O	17:Q:70:ARG:NH1	2.22	0.72
1:A:1205:U:H4'	3:C:195:VAL:HG21	1.72	0.71
1:A:979:C:OP1	1:A:1223:C:N4	2.23	0.71
1:A:1493:A:H4'	1:A:1494:G:OP1	1.89	0.71
1:A:1128:C:O2'	1:A:1130:A:N7	2.23	0.71
1:A:401:C:O2'	1:A:621:A:N3	2.21	0.71
8:H:83:ILE:HG12	8:H:137:VAL:HG22	1.73	0.70
15:O:5:LYS:HA	15:O:8:LYS:HB2	1.74	0.70
3:C:17:ASP:O	3:C:54:ARG:NH2	2.24	0.69
4:D:15:GLU:OE1	4:D:59:ARG:NH2	2.25	0.69
20:T:60:GLU:HG3	20:T:81:LYS:HE3	1.75	0.69
11:K:90:GLY:HA2	11:K:93:GLN:HB2	1.72	0.69
15:O:56:LEU:HA	15:O:59:MET:HE2	1.74	0.69
1:A:921:U:O2'	5:E:19:MET:O	2.09	0.69
1:A:946:A:O2'	1:A:1333:A:N3	2.25	0.69
1:A:1049:U:O2'	14:N:3:ARG:NH1	2.25	0.69
9:I:10:ARG:HG2	9:I:75:ASP:HB2	1.73	0.68
1:A:1030(A):G:N2	1:A:1030(D):A:OP2	2.26	0.68
2:B:63:MET:HB3	2:B:225:ALA:HB1	1.74	0.68
9:I:51:ARG:HG3	9:I:56:LEU:HD21	1.74	0.68
10:J:26:ALA:O	10:J:84:GLN:NE2	2.27	0.68
1:A:1144:G:H21	1:A:1146:A:H62	1.42	0.67
12:L:36:VAL:HG22	12:L:82:VAL:HG12	1.76	0.67
17:Q:22:LEU:HD11	17:Q:39:SER:HB2	1.76	0.67
1:A:201:C:H42	1:A:216:G:H1	1.39	0.67
1:A:1020:U:H2'	1:A:1021:G:C8	2.30	0.67
18:R:32:ARG:HA	18:R:69:THR:HG21	1.77	0.67
1:A:1214:C:H3'	1:A:1215:G:H8	1.59	0.67
4:D:57:ARG:HB3	4:D:206:PHE:HB2	1.77	0.67
1:A:176:C:OP1	20:T:29:LYS:NZ	2.27	0.66
1:A:276:G:O2'	17:Q:68:ARG:NH1	2.29	0.66
1:A:1143:G:H2'	1:A:1144:G:C8	2.31	0.66
1:A:1058:G:H5"	3:C:199:LYS:HE3	1.78	0.66
20:T:43:LEU:HB2	20:T:52:ALA:HB2	1.79	0.65
1:A:976:G:OP2	1:A:1358:U:O2'	2.14	0.65
1:A:13:C:H42	1:A:915:A:H62	1.45	0.65
18:R:47:THR:HA	18:R:83:GLU:HB2	1.78	0.65
1:A:718:G:O6	18:R:74:ARG:NH1	2.30	0.64
22:W:14:THR:HB	22:W:23:ARG:HB3	1.79	0.64
1:A:750:G:N3	15:O:23:GLY:HA3	2.11	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:3:ARG:O	13:M:57:ARG:NH2	2.30	0.64
8:H:9:MET:HG3	8:H:26:VAL:HG21	1.79	0.64
13:M:3:ARG:HE	13:M:7:VAL:HG12	1.62	0.64
7:G:113:GLU:HB2	7:G:119:ARG:HG2	1.78	0.64
1:A:1127:G:H1	1:A:1145:C:H42	1.46	0.64
13:M:49:THR:HG22	13:M:51:ALA:H	1.64	0.63
1:A:126:G:OP1	1:A:605:U:O2'	2.16	0.63
1:A:321:A:N6	1:A:329:A:OP2	2.31	0.63
1:A:664:G:N2	1:A:741:G:H1	1.90	0.63
1:A:1251:A:N3	1:A:1369:C:O2'	2.30	0.63
1:A:1356:G:H2'	1:A:1357:A:C8	2.33	0.63
1:A:1031:G:H2'	1:A:1032:G:H8	1.62	0.63
1:A:1150:U:O4	1:A:1151:A:N6	2.32	0.63
22:W:54:VAL:HB	22:W:69:TYR:HB2	1.80	0.63
1:A:538:G:H5"	12:L:114:LYS:HB2	1.80	0.63
1:A:902:G:H2'	1:A:903:G:H8	1.63	0.63
11:K:84:VAL:HG11	11:K:91:ARG:HD3	1.80	0.63
15:O:26:GLU:OE1	15:O:77:ARG:NH1	2.32	0.63
1:A:826:C:O2	8:H:15:ASN:ND2	2.31	0.63
1:A:922:G:H1	1:A:1395:C:H42	1.44	0.63
2:B:80:ILE:HD11	2:B:208:ILE:HG23	1.81	0.63
11:K:22:HIS:HB3	11:K:29:ILE:HD13	1.79	0.63
1:A:1105:A:H2'	1:A:1106:G:C8	2.34	0.62
2:B:97:TRP:HZ2	2:B:102:LEU:HD22	1.64	0.62
3:C:91:LEU:HD21	3:C:99:VAL:HG22	1.80	0.62
8:H:110:ALA:HB3	8:H:121:ASP:HB3	1.81	0.62
1:A:59:A:H5"	1:A:387:U:H5"	1.81	0.62
1:A:1502:A:H2	1:A:1505:G:H1	1.46	0.62
1:A:579:G:H5'	1:A:728:A:H1'	1.82	0.62
1:A:1057:G:H5"	3:C:154:SER:CB	2.29	0.62
1:A:62:U:OP1	1:A:385:C:O2'	2.16	0.62
1:A:1314:C:C5	19:S:6:LYS:HD3	2.35	0.62
20:T:45:GLN:HA	20:T:91:LEU:HD12	1.82	0.62
1:A:1132:C:H2'	1:A:1133:G:H8	1.65	0.62
1:A:1268:A:N3	1:A:1326:C:O2'	2.33	0.62
1:A:1391:U:H2'	1:A:1392:G:C8	2.33	0.62
3:C:70:VAL:HG21	3:C:76:VAL:HG21	1.80	0.62
1:A:1139:G:H4'	1:A:1140:C:H5'	1.81	0.61
1:A:190(J):U:H2'	1:A:190(K):G:C8	2.36	0.61
19:S:12:ASP:H	19:S:38:SER:HB3	1.64	0.61
1:A:537:G:OP1	12:L:113:ARG:NH2	2.34	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:545:C:O2'	1:A:549:C:OP1	2.19	0.61
9:I:86:VAL:HG22	9:I:93:ARG:HG2	1.81	0.61
10:J:54:PHE:O	10:J:55:LYS:HB2	2.01	0.61
2:B:178:ARG:HB3	8:H:72:PRO:HG3	1.81	0.61
1:A:1213:A:N6	1:A:1215:G:N3	2.48	0.60
1:A:237:C:OP2	17:Q:40:LYS:NZ	2.33	0.60
1:A:501:C:H2'	1:A:502:G:C8	2.36	0.60
1:A:636:U:H2'	1:A:637:G:C8	2.36	0.60
1:A:1126:U:O4	1:A:1127:G:N2	2.34	0.60
1:A:1510:U:H2'	1:A:1511:G:C8	2.36	0.60
8:H:91:ARG:HG3	12:L:7:ILE:HG13	1.82	0.60
10:J:6:ILE:HB	10:J:72:VAL:HB	1.84	0.60
20:T:57:ARG:HE	20:T:102:GLY:HA3	1.66	0.60
17:Q:48:GLU:HB2	17:Q:50:LYS:HG3	1.83	0.60
1:A:372:C:H4'	1:A:373:A:O5'	2.01	0.60
1:A:559:A:OP1	5:E:126:ARG:NH2	2.34	0.60
1:A:880:C:OP1	12:L:8:ASN:ND2	2.34	0.60
1:A:103:C:OP1	20:T:17:ARG:NH1	2.35	0.60
1:A:380:G:N2	1:A:383:A:OP2	2.35	0.60
10:J:8:LEU:HD23	10:J:96:ILE:HG12	1.82	0.59
2:B:32:ILE:HD11	2:B:190:THR:HG23	1.84	0.59
8:H:17:THR:O	8:H:78:GLN:NE2	2.34	0.59
1:A:558:G:OP2	1:A:559:A:O2'	2.19	0.59
3:C:19:GLU:N	14:N:51:GLY:O	2.33	0.59
1:A:91:C:H2'	1:A:92:C:C6	2.38	0.59
1:A:1105:A:H2'	1:A:1106:G:H8	1.67	0.59
1:A:1300:G:H4'	1:A:1301:U:O5'	2.02	0.59
1:A:296:U:O2'	1:A:556:C:O2'	2.16	0.58
1:A:1492:A:H5"	22:W:19:ASN:ND2	2.18	0.58
1:A:413:G:H2'	1:A:428:G:N2	2.18	0.58
1:A:1241:G:OP1	7:G:35:LYS:NZ	2.37	0.58
12:L:41:ARG:NH1	22:W:61:ASP:OD1	2.36	0.58
1:A:603:U:H2'	1:A:604:G:C8	2.38	0.58
1:A:1003(A):G:C5	1:A:1004:A:H1'	2.38	0.58
1:A:110:C:H2'	1:A:111:G:O4'	2.04	0.58
12:L:41:ARG:HH21	12:L:43:VAL:HG22	1.68	0.58
1:A:757:U:O2'	1:A:879:C:O2	2.19	0.58
4:D:176:LEU:HA	4:D:183:GLY:HA2	1.86	0.58
10:J:53:PRO:HA	14:N:41:ARG:HH21	1.68	0.58
21:U:12:LYS:HB3	21:U:22:ARG:HD2	1.85	0.58
1:A:1195:C:H3'	1:A:1196:U:H5"	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:816:A:OP1	1:A:1526:G:O2'	2.22	0.58
1:A:1053:G:HO2'	1:A:1199:U:H5	1.50	0.58
1:A:1487:G:H2'	1:A:1488:G:H8	1.68	0.58
6:F:30:LEU:HB3	6:F:35:ALA:HB3	1.86	0.58
1:A:1049:U:H4'	1:A:1050:G:O5'	2.04	0.58
2:B:188:ALA:HB1	2:B:192:SER:HB2	1.85	0.58
1:A:91:C:H2'	1:A:92:C:H6	1.69	0.57
1:A:390:C:O3'	16:P:28:ARG:NH2	2.37	0.57
1:A:397:A:N7	1:A:547:A:O2'	2.37	0.57
1:A:1027:C:H42	1:A:1034:G:H1	1.51	0.57
1:A:110:C:O2'	16:P:25:ARG:O	2.18	0.57
1:A:107:G:N7	20:T:15:ARG:NH2	2.48	0.57
1:A:1166:G:N2	1:A:1169:A:OP2	2.38	0.57
22:W:5:ASP:HB2	22:W:59:PRO:HG3	1.85	0.57
2:B:118:LEU:HB2	2:B:142:LEU:HD21	1.85	0.57
11:K:85:ARG:HD3	11:K:113:PRO:HD3	1.85	0.57
22:W:10:GLU:HG2	22:W:54:VAL:HG22	1.86	0.57
9:I:110:GLU:OE2	9:I:113:LYS:NZ	2.38	0.57
2:B:15:VAL:HG12	2:B:210:SER:HB3	1.86	0.57
1:A:130:A:OP2	1:A:190(E):U:O2'	2.10	0.57
1:A:1047:G:H5"	14:N:4:LYS:HD2	1.87	0.57
1:A:782:A:OP1	1:A:1521:G:N2	2.38	0.56
1:A:1338:G:H2'	1:A:1339:A:C8	2.40	0.56
12:L:73:GLU:OE1	22:W:1:ALA:N	2.27	0.56
1:A:123:C:OP1	1:A:311:C:O2'	2.24	0.56
2:B:204:ASN:H	2:B:204:ASN:HD22	1.51	0.56
8:H:19:VAL:HG23	8:H:21:LYS:HG2	1.87	0.56
14:N:23:ARG:NH1	14:N:28:GLY:O	2.38	0.56
1:A:144:G:H1	1:A:178:C:H42	1.52	0.56
1:A:411:A:OP2	4:D:25:ARG:NH2	2.39	0.56
2:B:101:MET:HA	2:B:108:ILE:HG13	1.87	0.56
1:A:619:U:N3	4:D:134:ASP:OD1	2.34	0.56
11:K:14:VAL:HG21	11:K:40:ILE:HD13	1.87	0.56
1:A:542:G:OP1	4:D:10:ARG:NH2	2.38	0.56
1:A:982:U:OP2	14:N:23:ARG:NH2	2.39	0.56
8:H:91:ARG:HH12	17:Q:33:GLY:HA3	1.70	0.56
1:A:45:U:H2'	1:A:46:G:C8	2.40	0.56
1:A:426:G:OP1	4:D:38:TYR:OH	2.17	0.56
5:E:35:GLY:HA3	5:E:112:LEU:HB3	1.88	0.56
6:F:94:GLN:HB3	18:R:32:ARG:HH11	1.69	0.56
9:I:8:GLY:HA2	9:I:79:LEU:HD13	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:113:SER:HB2	8:H:134:ILE:HD11	1.87	0.56
1:A:1028:C:H42	1:A:1033:G:H1	1.53	0.56
1:A:910:C:H4'	1:A:1413:A:H4'	1.87	0.56
3:C:156:ARG:H	3:C:163:ALA:HA	1.70	0.56
1:A:972:C:OP1	10:J:57:LYS:NZ	2.23	0.55
1:A:1454:G:H2'	1:A:1455:G:H8	1.71	0.55
8:H:36:LEU:HD23	8:H:39:LEU:HD12	1.88	0.55
1:A:1379:G:O6	7:G:2:ALA:N	2.40	0.55
2:B:162:ILE:HD12	2:B:177:ALA:HB2	1.87	0.55
11:K:58:PRO:HB2	11:K:93:GLN:HG3	1.89	0.55
8:H:86:ILE:HD12	8:H:133:LEU:HD22	1.88	0.55
4:D:57:ARG:NH2	5:E:111:GLU:OE2	2.39	0.55
12:L:97:ARG:NH1	12:L:98:TYR:OH	2.39	0.55
13:M:91:ARG:HH22	13:M:103:THR:HG21	1.71	0.55
1:A:1196:U:OP1	1:A:1197:G:H5'	2.06	0.55
10:J:26:ALA:HB1	10:J:84:GLN:HB2	1.87	0.55
1:A:1316:G:N2	1:A:1319:A:OP2	2.40	0.55
3:C:14:ILE:HG22	3:C:15:THR:HG23	1.89	0.55
14:N:33:VAL:HA	14:N:40:CYS:HA	1.88	0.55
1:A:217:C:H2'	1:A:218:C:C6	2.42	0.55
1:A:812:C:H4'	1:A:813:U:O5'	2.06	0.55
3:C:11:ARG:HG2	3:C:178:LEU:HG	1.88	0.55
7:G:18:TYR:OH	7:G:58:PRO:HG2	2.07	0.55
20:T:75:ASN:OD1	20:T:75:ASN:N	2.40	0.55
1:A:99:C:H2'	1:A:101:A:C8	2.42	0.55
1:A:250:A:H4'	1:A:251:G:O5'	2.06	0.55
1:A:281:G:H4'	1:A:282:A:O5'	2.07	0.55
1:A:299:G:H2'	1:A:300:A:C8	2.41	0.55
1:A:1441:G:H4'	1:A:1442:G:C5	2.42	0.55
1:A:1454:G:H2'	1:A:1455:G:C8	2.42	0.55
13:M:3:ARG:NE	13:M:7:VAL:HG12	2.21	0.55
1:A:157:G:H2'	1:A:158:G:H8	1.71	0.55
1:A:667:G:H2'	1:A:668:G:C8	2.42	0.55
1:A:908:A:H2'	1:A:909:A:C8	2.42	0.55
1:A:1079:G:O3'	5:E:14:ARG:NH2	2.40	0.55
5:E:28:PHE:O	5:E:47:LYS:HA	2.07	0.55
13:M:39:ILE:HD12	13:M:56:LEU:HG	1.89	0.55
22:W:45:ILE:HD13	22:W:70:ARG:HD3	1.89	0.55
8:H:51:VAL:HG11	8:H:60:ARG:HG2	1.88	0.54
1:A:376:G:H5"	16:P:5:ARG:HB2	1.90	0.54
1:A:560:U:H5'	1:A:566:G:N2	2.22	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1286:A:H2'	1:A:1287:A:H4'	1.88	0.54
14:N:16:PHE:HB2	14:N:19:ARG:HG3	1.88	0.54
1:A:501:C:OP1	12:L:117:ARG:NH2	2.40	0.54
4:D:162:LEU:HA	4:D:165:MET:HB2	1.89	0.54
1:A:254:G:H5"	17:Q:69:LYS:HD2	1.90	0.54
1:A:1008:C:N4	1:A:1021:G:H1	2.05	0.54
1:A:1031:G:H2'	1:A:1032:G:C8	2.42	0.54
3:C:9:GLY:HA3	14:N:49:HIS:HA	1.88	0.54
12:L:27:LEU:HG	12:L:28:LYS:H	1.72	0.54
1:A:146:G:H2'	1:A:147:G:H8	1.73	0.54
1:A:757:U:H2'	1:A:758:G:O4'	2.08	0.54
1:A:1100:C:OP1	2:B:96:ARG:NH1	2.40	0.54
6:F:22:GLU:OE1	6:F:82:ARG:NH1	2.40	0.54
3:C:134:ILE:HG23	3:C:151:VAL:HB	1.90	0.54
8:H:95:VAL:HG11	8:H:133:LEU:HD12	1.90	0.54
22:W:15:GLU:HB3	22:W:23:ARG:HB2	1.90	0.54
1:A:517:G:N1	1:A:533:A:OP2	2.41	0.54
1:A:553:A:O2'	12:L:29:GLY:O	2.25	0.54
1:A:1074:G:O2'	1:A:1101:A:N1	2.31	0.54
1:A:463:A:H3'	1:A:474:G:H8	1.73	0.54
1:A:1048:G:H1	1:A:1209:C:H42	1.55	0.54
2:B:181:PHE:CD2	8:H:70:GLN:HB3	2.43	0.54
11:K:57:THR:HG23	11:K:60:ALA:H	1.72	0.54
1:A:918:A:H2'	1:A:919:A:C8	2.43	0.53
1:A:1188:A:OP1	9:I:114:TYR:OH	2.15	0.53
1:A:1519[B]:MA6:O5'	1:A:1519[B]:MA6:H8	2.08	0.53
3:C:157:ILE:HD11	3:C:166:GLU:HB2	1.89	0.53
11:K:65:ALA:HB1	11:K:98:LEU:HD23	1.91	0.53
12:L:104:VAL:HG22	12:L:105:TYR:H	1.72	0.53
1:A:13:C:H42	1:A:915:A:N6	2.06	0.53
1:A:1405:G:O2'	1:A:1518[A]:MA6:O2'	2.27	0.53
1:A:1427:U:H2'	1:A:1428:A:C8	2.43	0.53
4:D:177:ASP:HB3	4:D:182:LYS:HB2	1.90	0.53
14:N:24:CYS:HB3	14:N:29:ARG:HB3	1.89	0.53
1:A:411:A:H62	1:A:413:G:H21	1.57	0.53
1:A:902:G:H2'	1:A:903:G:C8	2.44	0.53
14:N:9:LYS:HD2	14:N:23:ARG:HB2	1.90	0.53
1:A:114:U:H2'	1:A:115:G:C8	2.43	0.53
1:A:157:G:H2'	1:A:158:G:C8	2.43	0.53
1:A:406:G:H2'	1:A:407:G:C8	2.44	0.53
1:A:1256:A:H4'	1:A:1257:U:O5'	2.07	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:7:G:H5'	1:A:298:A:O4'	2.09	0.53
1:A:674:G:H2'	1:A:675:A:C8	2.44	0.53
1:A:36:C:H5"	12:L:123:LYS:HD3	1.89	0.53
1:A:217:C:H2'	1:A:218:C:H6	1.74	0.53
1:A:335:C:H2'	1:A:336:C:C6	2.43	0.53
1:A:344:A:H5'	1:A:345:C:C5	2.44	0.53
2:B:8:LYS:O	2:B:217:ARG:NH1	2.42	0.53
16:P:42:ARG:HB2	16:P:44:THR:HG23	1.91	0.53
1:A:19:C:OP1	5:E:125:SER:OG	2.19	0.53
6:F:8:ILE:HB	6:F:61:LEU:HB2	1.90	0.53
20:T:92:LEU:O	20:T:96:GLY:HA2	2.08	0.53
1:A:949:A:H62	13:M:106:ASN:HD21	1.57	0.53
1:A:1504:G:OP1	1:A:1507:A:H4'	2.07	0.53
3:C:36:ASP:HB3	3:C:40:ARG:HH12	1.74	0.53
4:D:12:CYS:HB3	4:D:33:MET:HG2	1.90	0.53
5:E:31:LEU:HD22	5:E:43:LEU:HD11	1.91	0.53
5:E:75:THR:OG1	5:E:76:ILE:N	2.42	0.53
1:A:92:C:H2'	1:A:93:G:C8	2.44	0.53
1:A:297:G:N2	1:A:300:A:OP2	2.42	0.53
11:K:21:ILE:HG12	11:K:30:VAL:HG22	1.91	0.53
19:S:23:ASN:OD1	19:S:47:HIS:NE2	2.31	0.53
20:T:43:LEU:HD11	20:T:55:ILE:HD12	1.91	0.53
22:W:56:GLU:OE1	22:W:66:ARG:NH1	2.41	0.53
1:A:417:C:H42	1:A:426:G:H1	1.57	0.52
1:A:1000:U:H2'	1:A:1001:A:C8	2.44	0.52
1:A:1192:C:O2	5:E:25:ARG:NH2	2.32	0.52
18:R:47:THR:HG22	18:R:83:GLU:H	1.75	0.52
1:A:1414:U:H2'	1:A:1415:G:H8	1.74	0.52
3:C:36:ASP:HA	3:C:39:ILE:HD12	1.91	0.52
8:H:37:ARG:HD3	8:H:41:ARG:HH21	1.73	0.52
15:O:39:LEU:HD13	15:O:56:LEU:HB2	1.89	0.52
1:A:1200:C:H1'	1:A:1204:A:H61	1.74	0.52
1:A:1494:G:OP2	22:W:18:PRO:HA	2.09	0.52
12:L:69:TYR:O	12:L:100:ILE:HB	2.10	0.52
21:U:13:ILE:HG22	21:U:22:ARG:CZ	2.40	0.52
4:D:23:GLY:HA3	4:D:112:VAL:HG12	1.92	0.52
9:I:3:GLN:HG3	9:I:20:ARG:HG3	1.91	0.52
1:A:938:A:N3	1:A:1376:U:O2'	2.39	0.52
2:B:139:LYS:O	2:B:139:LYS:NZ	2.41	0.52
4:D:11:LEU:HD13	4:D:66:ARG:HD3	1.91	0.52
5:E:33:VAL:HG12	5:E:112:LEU:HD12	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:R:53:ARG:NH1	18:R:58:LEU:O	2.38	0.52
5:E:11:ILE:HB	5:E:31:LEU:HB3	1.92	0.52
5:E:78:HIS:HD2	8:H:107:LEU:HD12	1.75	0.52
22:W:13:VAL:HG22	22:W:24:VAL:HG22	1.92	0.52
1:A:682:G:H2'	1:A:683:G:H8	1.74	0.52
1:A:1030:C:H2'	1:A:1030(A):G:C8	2.44	0.52
1:A:1206:G:O2'	3:C:192:THR:O	2.23	0.52
1:A:1516[A]:G:H2'	1:A:1518[A]:MA6:OP2	2.10	0.52
3:C:172:ARG:NH2	3:C:174:PRO:HG3	2.24	0.52
13:M:19:LEU:HB3	13:M:25:ILE:HG21	1.91	0.52
1:A:261:U:OP2	20:T:79:ARG:NH2	2.43	0.52
1:A:552:U:H2'	1:A:553:A:H8	1.75	0.52
2:B:21:ARG:HA	2:B:39:ILE:HA	1.90	0.52
12:L:35:GLY:HA3	12:L:60:LEU:HD13	1.91	0.52
1:A:551:U:H2'	1:A:552:U:C6	2.44	0.52
1:A:1193:G:OP1	3:C:167:TRP:NE1	2.43	0.52
1:A:24:U:OP1	12:L:23:LYS:HE3	2.10	0.51
4:D:78:LEU:HB3	4:D:93:PHE:CE1	2.37	0.51
13:M:39:ILE:HD13	13:M:52:GLU:HB3	1.91	0.51
1:A:90:U:H2'	1:A:91:C:C6	2.45	0.51
1:A:677:U:H3	1:A:713:G:N2	2.08	0.51
1:A:1411:C:H42	1:A:1489:G:H1	1.59	0.51
6:F:6:VAL:HA	6:F:90:VAL:HG22	1.92	0.51
20:T:100:ILE:HG22	20:T:102:GLY:N	2.20	0.51
1:A:421:U:H5'	1:A:422:C:C5	2.46	0.51
1:A:651:C:N4	1:A:753:A:OP2	2.38	0.51
1:A:1251:A:H5'	9:I:12:GLU:HG2	1.92	0.51
1:A:1499:A:H1'	1:A:1520[A]:G:H5'	1.92	0.51
13:M:50:GLU:HA	13:M:53:VAL:HB	1.92	0.51
5:E:105:VAL:HG21	5:E:128:PRO:HB3	1.91	0.51
6:F:68:PRO:HG2	6:F:71:ARG:HG3	1.93	0.51
1:A:17:U:H2'	1:A:18:C:C6	2.46	0.51
1:A:384:G:H2'	1:A:385:C:C6	2.45	0.51
1:A:791:G:O6	1:A:792:A:N6	2.43	0.51
1:A:1002:G:H2'	1:A:1003:G:C8	2.45	0.51
1:A:1221:G:O3'	19:S:77:THR:HG21	2.11	0.51
9:I:21:PRO:HA	9:I:58:HIS:O	2.11	0.51
11:K:48:ILE:HD13	11:K:63:LEU:HB2	1.93	0.51
14:N:27:CYS:SG	14:N:29:ARG:HB2	2.51	0.51
1:A:501:C:O3'	12:L:118:SER:OG	2.27	0.51
1:A:701:C:H4'	1:A:702:A:O5'	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:105:VAL:HB	5:E:106:PRO:HD3	1.93	0.51
15:O:24:SER:HB2	15:O:27:VAL:HG23	1.93	0.51
1:A:1248:A:H2'	1:A:1249:C:H6	1.76	0.51
3:C:12:LEU:HD11	14:N:51:GLY:HA2	1.92	0.51
5:E:80:ILE:HD11	5:E:91:LEU:HD12	1.92	0.51
12:L:89:ARG:CZ	12:L:97:ARG:HG2	2.41	0.51
17:Q:29:HIS:HB3	17:Q:33:GLY:N	2.26	0.51
5:E:106:PRO:O	5:E:110:LEU:HG	2.11	0.50
1:A:187:C:N3	20:T:105:SER:OG	2.39	0.50
1:A:974:A:OP2	14:N:29:ARG:NH2	2.44	0.50
1:A:1225:A:OP1	13:M:103:THR:N	2.34	0.50
1:A:161:A:N1	1:A:347:G:O2'	2.32	0.50
1:A:838:G:H1	1:A:848:C:H42	1.59	0.50
1:A:922:G:O2'	1:A:1398:A:N1	2.34	0.50
1:A:1235:U:H5"	21:U:3:LYS:HB2	1.93	0.50
1:A:1441:G:H4'	1:A:1442:G:C6	2.46	0.50
11:K:18:ARG:NH2	11:K:35:PRO:O	2.31	0.50
19:S:62:ILE:HD12	19:S:66:MET:HG3	1.93	0.50
1:A:518:C:O2'	22:W:38:GLY:HA3	2.12	0.50
1:A:1022:G:N2	1:A:1023:G:N7	2.59	0.50
1:A:1512:U:H2'	1:A:1513:A:C8	2.46	0.50
1:A:219:C:O2'	1:A:381:C:H5'	2.12	0.50
1:A:1071:C:H2'	1:A:1072:G:H8	1.76	0.50
1:A:1294:G:H2'	1:A:1295:G:C8	2.46	0.50
1:A:1319:A:O5'	19:S:70:LYS:NZ	2.43	0.50
3:C:24:ALA:HB3	3:C:29:TYR:HD1	1.77	0.50
10:J:50:ILE:HD12	10:J:50:ILE:H	1.75	0.50
1:A:280:C:N3	17:Q:39:SER:OG	2.42	0.50
1:A:939:G:H5"	7:G:102:ARG:HH12	1.77	0.50
1:A:985:C:H2'	1:A:986:A:C8	2.46	0.50
1:A:1162:C:H2'	1:A:1163:C:C6	2.46	0.50
1:A:1288:A:N3	1:A:1352:C:O2'	2.37	0.50
10:J:16:LEU:HD12	10:J:68:HIS:HB2	1.94	0.50
16:P:53:VAL:HG12	16:P:79:VAL:HG22	1.93	0.50
1:A:309:G:H2'	1:A:310:G:H8	1.77	0.50
1:A:1013:G:N2	1:A:1016:A:OP2	2.45	0.50
1:A:1027:C:N4	1:A:1034:G:H1	2.10	0.50
1:A:1310:G:H2'	1:A:1311:G:H8	1.77	0.50
1:A:1498:UR3:O5'	1:A:1498:UR3:H6	2.11	0.50
1:A:1504:G:H4'	1:A:1505:G:O5'	2.11	0.50
1:A:118:U:H3'	1:A:288:A:H61	1.77	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:822:C:H2'	1:A:823:G:H8	1.77	0.50
1:A:946:A:H2'	1:A:947:G:C8	2.47	0.50
1:A:501:C:H2'	1:A:502:G:H8	1.76	0.50
1:A:1301:U:O2'	1:A:1303:C:OP2	2.30	0.50
8:H:64:LYS:HG3	8:H:79:VAL:HG21	1.93	0.50
15:O:55:GLY:HA2	15:O:58:MET:HE2	1.92	0.50
1:A:452:A:O2'	1:A:453:A:O4'	2.29	0.49
1:A:939:G:H1	1:A:1344:C:H42	1.58	0.49
1:A:1087:G:N2	1:A:1099:G:H1'	2.26	0.49
1:A:1098:C:OP2	2:B:144:ARG:NH2	2.38	0.49
12:L:38:THR:HB	12:L:57:LYS:HB2	1.94	0.49
1:A:715:A:H2'	1:A:716:A:C8	2.46	0.49
1:A:762:C:H2'	1:A:763:G:C8	2.47	0.49
1:A:1278:U:H5'	1:A:1279:A:O4'	2.12	0.49
1:A:1309:G:H5'	13:M:78:ILE:HD11	1.94	0.49
2:B:74:LYS:NZ	2:B:206:ASP:OD1	2.44	0.49
3:C:188:LEU:HD11	3:C:195:VAL:HG22	1.94	0.49
18:R:37:VAL:HG22	18:R:78:LEU:HB3	1.94	0.49
1:A:411:A:H62	1:A:413:G:N2	2.10	0.49
1:A:833:U:H2'	1:A:834:C:C6	2.46	0.49
1:A:949:A:N7	13:M:106:ASN:ND2	2.60	0.49
1:A:1250:A:H4'	9:I:68:GLY:H	1.77	0.49
17:Q:81:ARG:NH2	17:Q:83:ASP:OD2	2.45	0.49
22:W:39:LYS:O	22:W:43:HIS:ND1	2.44	0.49
1:A:1145:C:O2'	1:A:1146:A:O5'	2.30	0.49
1:A:1281:U:H5'	1:A:1282:C:H5	1.78	0.49
10:J:48:THR:HA	10:J:62:HIS:HB3	1.94	0.49
14:N:9:LYS:NZ	14:N:12:ARG:HH21	2.10	0.49
22:W:13:VAL:HG13	22:W:22:PHE:HB3	1.93	0.49
22:W:53:VAL:HB	22:W:67:ILE:HG23	1.94	0.49
1:A:31:G:N2	1:A:48:C:OP1	2.46	0.49
1:A:566:G:H4'	1:A:567:G:OP1	2.12	0.49
1:A:963:G:H1	1:A:972:C:H42	1.59	0.49
1:A:1294:G:H2'	1:A:1295:G:H8	1.77	0.49
1:A:1427:U:H2'	1:A:1428:A:H8	1.77	0.49
6:F:62:TRP:CH2	6:F:64:GLN:HB2	2.48	0.49
9:I:118:LYS:O	9:I:120:ARG:N	2.43	0.49
1:A:363:A:OP2	12:L:34:ARG:NE	2.46	0.49
1:A:411:A:N3	1:A:413:G:O2'	2.35	0.49
1:A:687:A:H4'	1:A:688:G:O5'	2.13	0.49
3:C:64:VAL:HG12	3:C:66:VAL:HG23	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:150:GLU:HA	4:D:153:ARG:HG3	1.93	0.49
16:P:17:TYR:HE2	16:P:41:PRO:HG3	1.78	0.49
6:F:11:ASN:HD21	6:F:13:ASN:HB2	1.78	0.49
15:O:36:ILE:HD13	15:O:59:MET:HE3	1.94	0.49
1:A:401:C:H2'	1:A:402:G:C8	2.48	0.49
1:A:1509:C:H2'	1:A:1510:U:O4'	2.13	0.49
2:B:71:VAL:HB	2:B:164:VAL:HG12	1.95	0.49
9:I:79:LEU:HD22	9:I:83:ARG:HG3	1.95	0.49
1:A:815:A:N3	1:A:1527:C:O2'	2.36	0.49
1:A:1376:U:H2'	1:A:1377:A:C8	2.48	0.49
2:B:223:ILE:HD13	2:B:230:VAL:HG21	1.94	0.49
10:J:15:THR:HG22	10:J:94:VAL:HB	1.95	0.49
1:A:263:A:OP2	20:T:79:ARG:NH1	2.46	0.48
1:A:269:C:H2'	1:A:270:A:C8	2.48	0.48
1:A:580:U:H2'	1:A:581:G:O4'	2.13	0.48
6:F:26:ILE:HG21	6:F:63:TYR:HE2	1.78	0.48
7:G:116:ALA:O	7:G:120:ILE:HG12	2.13	0.48
13:M:10:PRO:O	13:M:45:VAL:HG11	2.12	0.48
1:A:603:U:H2'	1:A:604:G:H8	1.78	0.48
1:A:1405:G:O2'	1:A:1518[B]:MA6:O2'	2.31	0.48
1:A:1502:A:H2	1:A:1505:G:N1	2.11	0.48
2:B:87:ARG:HH21	2:B:219:VAL:HB	1.77	0.48
11:K:32:ILE:HD13	11:K:72:ALA:HB2	1.95	0.48
1:A:142:G:H2'	1:A:143:A:H8	1.78	0.48
1:A:932:C:H5'	7:G:4:ARG:HG3	1.95	0.48
1:A:983:A:N1	1:A:1222:G:N2	2.61	0.48
1:A:1061:G:N7	3:C:2:GLY:HA3	2.28	0.48
1:A:1373:G:H5"	7:G:36:LYS:HE3	1.94	0.48
1:A:1530:G:H2'	1:A:1531:A:C8	2.48	0.48
3:C:36:ASP:OD1	3:C:59:ARG:NH2	2.29	0.48
1:A:1087:G:H2'	1:A:1088:G:C8	2.48	0.48
11:K:34:ASP:OD1	11:K:38:ASN:N	2.46	0.48
1:A:356:A:N3	1:A:368:U:O2'	2.34	0.48
1:A:562:C:H1'	12:L:15:ARG:HD2	1.94	0.48
1:A:939:G:H2'	1:A:940:C:C6	2.47	0.48
1:A:1071:C:H5"	5:E:49:PRO:HG3	1.95	0.48
1:A:1425:U:H2'	1:A:1426:C:C6	2.48	0.48
1:A:8:A:H8	5:E:101:ILE:HG23	1.78	0.48
1:A:253:U:H2'	1:A:254:G:H8	1.79	0.48
1:A:911:U:H2'	1:A:912:C:C6	2.48	0.48
1:A:1221:G:OP2	19:S:37:ARG:NH2	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1513:A:H2'	1:A:1514:C:C6	2.48	0.48
16:P:26:ARG:HD2	16:P:31:LYS:O	2.14	0.48
1:A:592:G:H2'	1:A:593:G:C8	2.48	0.48
1:A:1213:A:N1	1:A:1215:G:H1'	2.29	0.48
2:B:20:GLU:OE1	2:B:23:ARG:NH1	2.45	0.48
3:C:57:ILE:HG12	3:C:66:VAL:HG22	1.95	0.48
4:D:187:ARG:NH2	4:D:188:LEU:HB2	2.29	0.48
1:A:191:G:O2'	20:T:102:GLY:O	2.13	0.48
1:A:1109:C:H2'	1:A:1110:A:O4'	2.14	0.48
1:A:632:A:H2'	1:A:633:G:O4'	2.14	0.48
2:B:12:GLU:HG3	2:B:213:LEU:HD21	1.95	0.48
12:L:84:LEU:HD23	12:L:101:VAL:HG21	1.95	0.48
1:A:352:C:H4'	1:A:354:G:OP1	2.12	0.48
1:A:1124:G:H5'	10:J:35:SER:O	2.14	0.48
1:A:1472:U:H2'	1:A:1473:A:C8	2.49	0.48
2:B:87:ARG:NH2	2:B:220:ASP:OD1	2.38	0.48
15:O:55:GLY:O	15:O:59:MET:HG3	2.14	0.48
1:A:216:G:H2'	1:A:217:C:C6	2.49	0.47
1:A:674:G:H2'	1:A:675:A:H8	1.78	0.47
14:N:29:ARG:HH22	14:N:41:ARG:HH12	1.61	0.47
1:A:101:A:H2'	1:A:102:G:C8	2.49	0.47
1:A:315:A:O2'	1:A:330:C:O2'	2.26	0.47
5:E:100:VAL:O	5:E:107:ARG:NH2	2.47	0.47
18:R:59:SER:H	18:R:62:GLU:HB2	1.79	0.47
1:A:456:C:H42	1:A:476:G:H1	1.62	0.47
1:A:833:U:H2'	1:A:834:C:H6	1.79	0.47
3:C:11:ARG:HH12	3:C:178:LEU:HA	1.79	0.47
13:M:63:THR:HG23	13:M:64:TRP:CD2	2.48	0.47
1:A:1358:U:O2'	1:A:1359:C:OP1	2.32	0.47
3:C:33:LEU:HD21	14:N:53:LEU:HD22	1.96	0.47
8:H:44:PHE:HD1	8:H:80:ILE:HG12	1.79	0.47
13:M:91:ARG:HB2	13:M:98:VAL:HG22	1.96	0.47
17:Q:29:HIS:HB3	17:Q:33:GLY:H	1.80	0.47
1:A:673:G:H5"	6:F:87:ARG:CZ	2.44	0.47
1:A:686:U:HO2'	1:A:687:A:H8	1.57	0.47
1:A:1228:C:H4'	13:M:116:THR:HA	1.95	0.47
1:A:1437:C:H2'	1:A:1438:G:C8	2.49	0.47
3:C:43:LEU:O	3:C:47:LEU:HB2	2.15	0.47
3:C:188:LEU:HD11	3:C:195:VAL:HG13	1.96	0.47
11:K:21:ILE:HB	11:K:84:VAL:HG22	1.96	0.47
17:Q:59:ILE:HD12	17:Q:73:VAL:HA	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:R:73:ALA:HB1	18:R:78:LEU:HB2	1.97	0.47
19:S:40:ILE:HB	19:S:67:VAL:O	2.15	0.47
1:A:812:C:OP1	1:A:903:G:H1'	2.14	0.47
1:A:987:G:H2'	1:A:988:G:C8	2.50	0.47
1:A:1064:G:N2	1:A:1191:A:OP2	2.41	0.47
1:A:1178:G:N2	1:A:1181:G:OP2	2.47	0.47
1:A:1202:G:N1	14:N:46:GLU:OE2	2.45	0.47
2:B:178:ARG:O	8:H:72:PRO:HD3	2.15	0.47
3:C:19:GLU:HG2	3:C:54:ARG:HE	1.79	0.47
9:I:46:ALA:HB2	9:I:74:ILE:HG23	1.96	0.47
10:J:53:PRO:HA	14:N:41:ARG:NH2	2.29	0.47
1:A:41:G:H2'	1:A:42:G:C8	2.49	0.47
1:A:193:C:H2'	1:A:194:C:H6	1.79	0.47
1:A:279:A:H5"	1:A:281:G:H5'	1.96	0.47
1:A:878:G:H5"	8:H:89:PRO:O	2.14	0.47
1:A:1332:A:H2'	1:A:1333:A:C8	2.50	0.47
1:A:1474:G:H2'	1:A:1475:G:H8	1.74	0.47
2:B:44:LEU:H	2:B:44:LEU:HG	1.51	0.47
7:G:121:ALA:O	7:G:125:MET:HG3	2.14	0.47
8:H:111:ILE:HG22	8:H:134:ILE:HD12	1.95	0.47
15:O:26:GLU:HA	15:O:81:LEU:HD11	1.97	0.47
18:R:56:THR:HB	18:R:58:LEU:HG	1.97	0.47
19:S:36:ARG:NH1	19:S:53:ASN:HA	2.29	0.47
1:A:21:G:O5'	1:A:21:G:H8	1.98	0.47
1:A:89:C:H2'	1:A:90:U:O4'	2.15	0.47
1:A:101:A:H2'	1:A:102:G:H8	1.80	0.47
1:A:433:C:H2'	1:A:434:U:C6	2.49	0.47
1:A:676:A:H1'	11:K:115:PRO:HB3	1.95	0.47
1:A:939:G:H5"	7:G:102:ARG:NH1	2.29	0.47
1:A:1512:U:H2'	1:A:1513:A:H8	1.80	0.47
3:C:148:GLY:HA3	3:C:172:ARG:O	2.15	0.47
10:J:8:LEU:HB2	10:J:70:ARG:HB2	1.97	0.47
10:J:30:SER:HB3	10:J:80:LYS:HB2	1.97	0.47
12:L:24:VAL:HG12	12:L:26:ALA:H	1.80	0.47
12:L:68:ALA:HB1	12:L:100:ILE:HG13	1.96	0.47
12:L:82:VAL:HG23	12:L:105:TYR:HB2	1.97	0.47
1:A:325:A:H2'	1:A:326:G:O4'	2.15	0.47
1:A:972:C:H4'	10:J:57:LYS:HD3	1.97	0.47
2:B:218:ALA:O	2:B:222:ILE:HG13	2.14	0.47
4:D:13:ARG:HH11	4:D:36:ARG:HG2	1.78	0.47
8:H:35:ILE:HD13	8:H:118:VAL:HG11	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:447:G:N1	1:A:485:G:H2'	2.29	0.47
1:A:518:C:H4'	1:A:519:C:O5'	2.14	0.47
1:A:1048:G:H1	1:A:1209:C:N4	2.13	0.47
12:L:117:ARG:NH2	12:L:124:LYS:HD3	2.30	0.47
1:A:124:G:H2'	1:A:125:U:O4'	2.15	0.46
1:A:244:U:H4'	1:A:245:C:H5"	1.98	0.46
1:A:1148:U:H2'	1:A:1149:C:O4'	2.16	0.46
1:A:1339:A:H2'	1:A:1340:A:O4'	2.16	0.46
2:B:24:TRP:CZ3	2:B:26:PRO:HA	2.51	0.46
4:D:13:ARG:NH1	4:D:36:ARG:HG2	2.30	0.46
9:I:85:LEU:HG	9:I:92:TYR:CD2	2.50	0.46
14:N:24:CYS:SG	14:N:40:CYS:N	2.81	0.46
19:S:11:VAL:HG21	19:S:41:VAL:HG13	1.96	0.46
1:A:428:G:H1'	1:A:429:U:OP2	2.15	0.46
1:A:646:U:H2'	1:A:647:C:C6	2.51	0.46
1:A:1273:G:H2'	1:A:1274:G:O4'	2.14	0.46
2:B:115:LEU:HD11	2:B:146:GLN:HG3	1.97	0.46
10:J:49:VAL:HG13	14:N:41:ARG:HD2	1.96	0.46
15:O:39:LEU:HB3	15:O:56:LEU:HD12	1.97	0.46
1:A:898:G:N2	1:A:901:A:OP2	2.44	0.46
1:A:977:A:O2'	1:A:981:U:N3	2.48	0.46
1:A:1248:A:H2'	1:A:1249:C:C6	2.51	0.46
1:A:737:A:H2'	1:A:738:C:C6	2.50	0.46
1:A:1348:U:H4'	9:I:120:ARG:HG3	1.98	0.46
1:A:1366:C:H2'	1:A:1367:C:C6	2.50	0.46
1:A:1518[B]:MA6:H102	1:A:1519[B]:MA6:H103	1.98	0.46
3:C:155:GLY:HA3	3:C:163:ALA:HB1	1.96	0.46
1:A:385:C:H2'	1:A:386:C:C6	2.50	0.46
1:A:677:U:O2	1:A:777:A:O2'	2.26	0.46
1:A:1175:G:H2'	1:A:1176:A:C8	2.50	0.46
1:A:129:U:O3'	1:A:129(A):G:H3'	2.16	0.46
1:A:324:G:N1	1:A:327:A:OP2	2.49	0.46
1:A:335:C:O2'	1:A:1433:A:N3	2.49	0.46
1:A:762:C:H2'	1:A:763:G:H8	1.80	0.46
1:A:1270:C:H2'	1:A:1271:G:C8	2.51	0.46
1:A:462:G:H21	16:P:82:GLN:HE21	1.62	0.46
1:A:939:G:H5"	7:G:102:ARG:HH22	1.80	0.46
1:A:1062:U:H2'	1:A:1063:C:C6	2.51	0.46
1:A:1087:G:H22	1:A:1099:G:H1'	1.81	0.46
1:A:1151:A:C5'	10:J:41:PRO:HA	2.46	0.46
2:B:102:LEU:HB3	2:B:180:LEU:HD12	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:131:ARG:HH22	3:C:164:ARG:HH22	1.63	0.46
6:F:101:ALA:HA	18:R:28:GLU:HG3	1.97	0.46
12:L:46:LYS:HB2	12:L:92:0TD:H5	1.96	0.46
1:A:374:A:H5'	1:A:452:A:N1	2.30	0.46
1:A:384:G:H2'	1:A:385:C:H6	1.81	0.46
1:A:542:G:O3'	4:D:14:ARG:NH2	2.42	0.46
1:A:1059:C:H2'	1:A:1060:C:C6	2.51	0.46
1:A:1143:G:H2'	1:A:1144:G:H8	1.79	0.46
1:A:1435:G:H2'	1:A:1436:U:C6	2.51	0.46
7:G:72:ARG:NH1	7:G:142:GLU:OE1	2.49	0.46
19:S:45:VAL:HA	19:S:62:ILE:HG13	1.96	0.46
1:A:1057:G:H2'	1:A:1058:G:O4'	2.15	0.46
1:A:1328:C:H2'	1:A:1329:A:C8	2.51	0.46
1:A:341:C:H2'	1:A:342:C:C6	2.51	0.45
1:A:680:C:H42	1:A:710:G:H1	1.64	0.45
1:A:1425:U:H2'	1:A:1426:C:H6	1.82	0.45
7:G:69:VAL:HG21	7:G:104:LEU:HD21	1.98	0.45
1:A:243:A:H2	1:A:245:C:H2'	1.81	0.45
1:A:552:U:H2'	1:A:553:A:C8	2.51	0.45
1:A:922:G:H4'	5:E:20:GLN:HA	1.97	0.45
1:A:1043:C:H2'	1:A:1044:A:H8	1.81	0.45
1:A:1218:C:H2'	1:A:1219:U:C6	2.51	0.45
3:C:134:ILE:O	3:C:138:VAL:HG23	2.17	0.45
6:F:70:ASP:OD1	6:F:70:ASP:N	2.47	0.45
18:R:53:ARG:HD3	18:R:63:GLN:HB2	1.98	0.45
20:T:67:ALA:HB2	20:T:77:ALA:HB2	1.97	0.45
1:A:146:G:H2'	1:A:147:G:C8	2.51	0.45
1:A:979:C:H42	14:N:18:VAL:HB	1.82	0.45
1:A:1402:4OC:H2'	1:A:1403:C:O4'	2.17	0.45
2:B:172:ILE:HD12	2:B:173:ALA:N	2.30	0.45
4:D:173:TRP:CD2	4:D:189:PRO:HB3	2.52	0.45
8:H:86:ILE:HD11	8:H:136:GLU:HG3	1.98	0.45
12:L:82:VAL:O	12:L:106:ASP:HB2	2.17	0.45
20:T:43:LEU:O	20:T:47:GLY:N	2.49	0.45
1:A:463:A:H3'	1:A:474:G:C8	2.52	0.45
1:A:559:A:H4'	1:A:560:U:O5'	2.16	0.45
1:A:728:A:H2'	1:A:729:A:C8	2.51	0.45
1:A:797:C:H2'	1:A:798:G:H8	1.81	0.45
1:A:987:G:H2'	1:A:988:G:H8	1.81	0.45
3:C:11:ARG:NH1	3:C:178:LEU:HA	2.32	0.45
9:I:49:PRO:HB2	9:I:81:ILE:HG22	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:453:A:N6	1:A:480:U:O2	2.50	0.45
1:A:1198:G:H2'	1:A:1199:U:C6	2.52	0.45
1:A:1431:C:H2'	1:A:1432:G:O4'	2.17	0.45
2:B:57:PHE:HE2	2:B:185:ILE:HD11	1.80	0.45
4:D:142:PRO:HA	4:D:185:PHE:HD1	1.80	0.45
5:E:101:ILE:O	5:E:120:THR:HB	2.16	0.45
1:A:140:A:H2'	1:A:141:A:C8	2.51	0.45
1:A:341:C:H2'	1:A:342:C:H6	1.82	0.45
1:A:376:G:H5"	16:P:5:ARG:HD2	1.99	0.45
1:A:535:A:OP1	1:A:536:C:H5	1.99	0.45
1:A:1201:A:H4'	1:A:1202:G:O5'	2.17	0.45
1:A:1250:A:H4'	9:I:68:GLY:N	2.31	0.45
2:B:59:GLU:HB2	2:B:221:LEU:HD11	1.98	0.45
5:E:82:VAL:HG21	5:E:138:ALA:HA	1.98	0.45
8:H:132:GLU:O	8:H:134:ILE:HG13	2.17	0.45
12:L:24:VAL:HG13	12:L:98:TYR:CE2	2.52	0.45
1:A:56:U:H2'	1:A:57:G:C8	2.52	0.45
1:A:254:G:O2'	17:Q:16:GLN:O	2.34	0.45
1:A:413:G:H2'	1:A:428:G:H22	1.81	0.45
1:A:779:C:H2'	1:A:780:A:O4'	2.17	0.45
1:A:922:G:H2'	1:A:923:A:C8	2.52	0.45
1:A:1318:A:O2'	19:S:37:ARG:HB3	2.17	0.45
9:I:8:GLY:H	9:I:83:ARG:NH1	2.15	0.45
11:K:12:ARG:HD2	11:K:14:VAL:HG13	1.97	0.45
1:A:193:C:H2'	1:A:194:C:C6	2.52	0.45
1:A:837:G:H1	1:A:849:C:H42	1.65	0.45
4:D:184:LYS:HE3	4:D:184:LYS:HB2	1.78	0.45
5:E:17:ALA:HA	5:E:26:PHE:HB3	1.99	0.45
18:R:40:LEU:HB3	18:R:79:LEU:HD11	1.99	0.45
2:B:160:ASP:N	2:B:160:ASP:OD1	2.50	0.45
4:D:57:ARG:HG2	4:D:202:LEU:O	2.17	0.45
8:H:68:ARG:HA	8:H:76:PRO:HG3	1.98	0.45
22:W:25:LYS:HE3	22:W:29:GLY:O	2.16	0.45
1:A:669:U:H2'	1:A:670:G:C8	2.51	0.45
4:D:185:PHE:CE1	4:D:188:LEU:HD23	2.52	0.45
6:F:33:TYR:CG	6:F:75:LEU:HD23	2.51	0.45
8:H:44:PHE:HB3	8:H:80:ILE:HD11	1.99	0.45
1:A:575:G:HO2'	1:A:821:G:H5'	1.82	0.44
1:A:1516[A]:G:N2	1:A:1519[A]:MA6:OP2	2.43	0.44
2:B:68:ILE:O	2:B:90:MET:HB3	2.17	0.44
9:I:5:TYR:HE2	9:I:7:THR:HG1	1.65	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:P:4:ILE:HG13	16:P:64:ALA:HB1	1.98	0.44
1:A:142:G:H2'	1:A:143:A:C8	2.52	0.44
1:A:1195:C:H3'	1:A:1196:U:C5'	2.46	0.44
1:A:1317:C:H2'	1:A:1318:A:O4'	2.17	0.44
1:A:1319:A:OP1	19:S:5:LEU:HD22	2.16	0.44
2:B:142:LEU:HD23	2:B:142:LEU:HA	1.79	0.44
7:G:71:PRO:HG3	7:G:103:TRP:CH2	2.52	0.44
8:H:41:ARG:NH1	8:H:123:GLU:OE2	2.47	0.44
1:A:302:G:H5"	12:L:17:LYS:NZ	2.32	0.44
1:A:939:G:H5"	7:G:102:ARG:NH2	2.31	0.44
14:N:23:ARG:HA	14:N:23:ARG:HD3	1.69	0.44
15:O:2:PRO:HB2	15:O:3:ILE:H	1.59	0.44
1:A:1075:C:H5"	2:B:179:LYS:NZ	2.32	0.44
3:C:12:LEU:HD23	3:C:12:LEU:HA	1.75	0.44
3:C:52:LEU:HA	3:C:70:VAL:HA	1.99	0.44
4:D:175:SER:OG	4:D:186:LEU:HD21	2.17	0.44
8:H:23:SER:HB2	8:H:62:TYR:CD1	2.53	0.44
14:N:8:GLU:HB2	14:N:11:LYS:HE3	1.99	0.44
1:A:251:G:C6	1:A:266:G:C6	3.05	0.44
1:A:564:C:C2	17:Q:31:LEU:HD11	2.53	0.44
1:A:794:A:H2'	1:A:795:C:C6	2.53	0.44
1:A:868:C:H2'	1:A:869:G:O4'	2.18	0.44
6:F:39:LYS:HB2	6:F:39:LYS:HE3	1.75	0.44
11:K:54:ARG:O	11:K:57:THR:HG22	2.17	0.44
14:N:12:ARG:HG3	14:N:13:THR:H	1.82	0.44
14:N:24:CYS:H	14:N:33:VAL:HG21	1.83	0.44
19:S:50:ALA:HB1	19:S:57:HIS:HB3	1.99	0.44
1:A:1308:U:OP1	13:M:98:VAL:N	2.50	0.44
1:A:1462:G:H2'	1:A:1463:C:C6	2.53	0.44
1:A:600:C:OP1	8:H:97:VAL:HG12	2.17	0.44
1:A:1498:UR3:O4'	1:A:1519[A]:MA6:H2	2.18	0.44
2:B:59:GLU:HG3	2:B:225:ALA:HB2	2.00	0.44
3:C:135:LYS:NZ	5:E:52:PRO:HG2	2.31	0.44
10:J:23:ILE:HG23	10:J:85:LEU:HD11	2.00	0.44
13:M:15:VAL:HG12	13:M:34:LEU:HD21	2.00	0.44
20:T:39:LYS:O	20:T:43:LEU:HG	2.16	0.44
22:W:45:ILE:HG21	22:W:70:ARG:HB2	2.00	0.44
1:A:966:M2G:HM22	1:A:967:5MC:C2	2.53	0.44
1:A:1384:C:H2'	1:A:1385:G:C8	2.52	0.44
1:A:1414:U:O2'	1:A:1415:G:O4'	2.30	0.44
1:A:97:G:H2'	1:A:98:U:O4'	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:421:U:OP2	1:A:422:C:N4	2.51	0.44
1:A:787:A:N6	1:A:792:A:O2'	2.51	0.44
1:A:959:A:O2'	1:A:984:C:O2'	2.29	0.44
1:A:1111:A:N1	3:C:177:THR:HB	2.33	0.44
1:A:1517[A]:G:N7	1:A:1518[A]:MA6:H103	2.33	0.44
13:M:2:ALA:O	13:M:9:ILE:HA	2.17	0.44
1:A:166:G:H2'	1:A:167:G:H8	1.83	0.43
1:A:427:U:O4'	1:A:541:G:H5"	2.18	0.43
1:A:613:C:H42	1:A:627:G:H1	1.66	0.43
1:A:679:C:H2'	1:A:680:C:C6	2.53	0.43
2:B:179:LYS:HB2	2:B:179:LYS:HE3	1.79	0.43
3:C:150:LYS:HB3	3:C:201:TYR:HB2	2.00	0.43
1:A:41:G:H2'	1:A:42:G:H8	1.82	0.43
1:A:973:G:H3'	1:A:974:A:H5"	1.99	0.43
1:A:1187:G:H4'	9:I:111:ARG:NH1	2.33	0.43
2:B:181:PHE:CE2	8:H:70:GLN:HB3	2.52	0.43
1:A:440:A:H3'	1:A:442:C:C6	2.53	0.43
1:A:1347:G:O2'	9:I:109:VAL:HA	2.18	0.43
3:C:26:LYS:NZ	10:J:45:ARG:HE	2.15	0.43
5:E:65:ASN:ND2	5:E:65:ASN:O	2.51	0.43
8:H:37:ARG:HD3	8:H:41:ARG:NH2	2.34	0.43
8:H:105:ARG:HD3	8:H:105:ARG:HA	1.82	0.43
9:I:69:GLY:O	9:I:73:GLN:HG3	2.19	0.43
16:P:23:ASP:OD2	16:P:25:ARG:NE	2.41	0.43
1:A:359:U:H2'	1:A:360:A:C8	2.54	0.43
1:A:688:G:H5'	11:K:46:GLY:C	2.39	0.43
1:A:986:A:H2'	1:A:987:G:O4'	2.18	0.43
1:A:986:A:H1'	19:S:54:GLY:O	2.18	0.43
1:A:1318:A:H4'	19:S:10:PHE:CD2	2.53	0.43
1:A:1440:C:H2'	1:A:1441:G:O4'	2.18	0.43
2:B:9:GLU:OE1	2:B:10:LEU:N	2.51	0.43
2:B:69:LEU:HD21	2:B:93:VAL:HG23	2.00	0.43
2:B:79:ASP:HB3	2:B:238:LEU:HD13	2.00	0.43
6:F:9:VAL:HA	6:F:59:TYR:O	2.18	0.43
10:J:62:HIS:CD2	10:J:62:HIS:H	2.36	0.43
16:P:27:LYS:H	16:P:27:LYS:HG3	1.55	0.43
1:A:476:G:H2'	1:A:477:G:C8	2.53	0.43
1:A:770:C:H2'	1:A:771:G:H8	1.83	0.43
1:A:1048:G:O4'	1:A:1215:G:H4'	2.19	0.43
3:C:26:LYS:HZ3	10:J:45:ARG:HE	1.67	0.43
9:I:93:ARG:CZ	9:I:93:ARG:HB3	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:49:VAL:HG13	14:N:41:ARG:HB2	2.01	0.43
12:L:41:ARG:O	12:L:54:LYS:HA	2.18	0.43
1:A:669:U:H2'	1:A:670:G:H8	1.83	0.43
2:B:102:LEU:HD21	2:B:162:ILE:HD11	1.99	0.43
6:F:50:TYR:CE1	18:R:77:GLY:HA2	2.53	0.43
8:H:112:LEU:HD23	8:H:133:LEU:HA	2.01	0.43
20:T:29:LYS:O	20:T:33:ILE:HG12	2.19	0.43
20:T:44:ALA:HA	20:T:92:LEU:HD22	2.01	0.43
1:A:186:C:H2'	1:A:187:C:C6	2.54	0.43
1:A:373:A:H1'	1:A:481:G:N3	2.34	0.43
1:A:484:G:H4'	1:A:485:G:O5'	2.18	0.43
1:A:764:C:H5"	15:O:50:HIS:CD2	2.54	0.43
1:A:1291:G:H5"	9:I:39:GLY:O	2.19	0.43
2:B:18:GLY:HA2	2:B:42:ILE:HD12	2.01	0.43
5:E:118:ILE:HG12	5:E:119:LEU:N	2.34	0.43
12:L:38:THR:N	12:L:57:LYS:O	2.36	0.43
12:L:42:THR:HG23	22:W:61:ASP:HB2	2.00	0.43
15:O:75:PRO:O	15:O:79:ARG:HG3	2.18	0.43
22:W:17:LEU:HB2	22:W:21:THR:HB	2.01	0.43
1:A:162:A:C5	1:A:163:C:H1'	2.54	0.43
1:A:229:U:H2'	1:A:230:G:C8	2.54	0.43
1:A:695:A:H61	1:A:797:C:H1'	1.83	0.43
1:A:1007:C:O2	1:A:1023:G:N1	2.52	0.43
1:A:1149:C:H2'	1:A:1150:U:C6	2.53	0.43
1:A:1200:C:H1'	1:A:1204:A:N6	2.33	0.43
1:A:1386:G:H2'	1:A:1387:G:C8	2.54	0.43
6:F:33:TYR:CD1	6:F:75:LEU:HD23	2.54	0.43
6:F:75:LEU:O	6:F:79:LEU:HG	2.19	0.43
17:Q:55:ASP:HA	17:Q:80:GLY:H	1.83	0.43
20:T:43:LEU:HD12	20:T:52:ALA:HA	2.00	0.43
1:A:49:U:O2'	1:A:50:A:H2'	2.19	0.43
1:A:433:C:H2'	1:A:434:U:H6	1.84	0.43
1:A:824:C:H2'	1:A:825:G:H8	1.83	0.43
1:A:937:A:H2'	1:A:938:A:H8	1.84	0.43
1:A:1069:C:O2'	1:A:1192:C:H1'	2.18	0.43
2:B:43:ASP:HB3	2:B:46:LYS:HB2	2.01	0.43
5:E:150:ARG:HE	5:E:150:ARG:HB2	1.57	0.43
5:E:151:LEU:HD23	5:E:151:LEU:HA	1.85	0.43
7:G:15:ASP:HB3	7:G:20:ASP:H	1.83	0.43
7:G:94:ARG:O	7:G:97:GLN:HB3	2.18	0.43
9:I:127:LYS:HE3	9:I:127:LYS:HB3	1.74	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:P:6:LEU:HB3	16:P:17:TYR:HB3	2.01	0.43
1:A:10:A:H2'	1:A:11:G:C8	2.54	0.43
1:A:102:G:O2'	1:A:151:A:N3	2.40	0.43
1:A:117:G:H2'	1:A:118:U:O4'	2.18	0.43
1:A:452:A:O2'	1:A:453:A:O5'	2.35	0.43
1:A:592:G:H2'	1:A:593:G:H8	1.83	0.43
1:A:642:A:N3	8:H:113:SER:OG	2.49	0.43
1:A:824:C:H2'	1:A:825:G:C8	2.53	0.43
1:A:954:G:H2'	1:A:955:U:O4'	2.19	0.43
2:B:24:TRP:HZ3	2:B:29:ALA:HB2	1.84	0.43
17:Q:43:LEU:HD23	17:Q:43:LEU:HA	1.84	0.43
17:Q:48:GLU:OE1	17:Q:50:LYS:HD2	2.19	0.43
1:A:1128:C:H1'	1:A:1146:A:H61	1.82	0.42
2:B:33:TYR:HB2	2:B:43:ASP:HA	2.01	0.42
2:B:103:THR:HA	2:B:180:LEU:HD11	2.00	0.42
4:D:64:LEU:HD23	4:D:198:VAL:HG21	2.01	0.42
1:A:1048:G:O3'	1:A:1049:U:H3'	2.19	0.42
1:A:1291:G:O3'	9:I:39:GLY:HA3	2.18	0.42
1:A:1492:A:H5"	22:W:19:ASN:HD22	1.82	0.42
6:F:2:ARG:CZ	6:F:69:GLU:HG2	2.49	0.42
10:J:64:GLU:CD	10:J:66:ARG:HH21	2.21	0.42
14:N:26:ARG:HB3	14:N:43:CYS:SG	2.59	0.42
20:T:56:MET:HE2	20:T:85:MET:HA	2.02	0.42
1:A:8:A:C8	5:E:101:ILE:HG23	2.53	0.42
1:A:190(K):G:H2'	1:A:190(L):U:C6	2.54	0.42
1:A:1060:C:H5"	10:J:51:ARG:HB3	2.01	0.42
2:B:155:LEU:HD11	2:B:159:PRO:HG3	2.02	0.42
12:L:48:PRO:HD2	12:L:92:0TD:H8	2.01	0.42
17:Q:3:LYS:HB3	17:Q:61:GLU:HB3	2.01	0.42
18:R:19:LYS:HE3	18:R:19:LYS:HB2	1.74	0.42
1:A:682:G:H2'	1:A:683:G:C8	2.53	0.42
1:A:890:G:O2'	1:A:906:G:O6	2.27	0.42
2:B:22:LYS:HD2	2:B:22:LYS:HA	1.82	0.42
2:B:60:ASP:O	2:B:64:ARG:NH1	2.52	0.42
4:D:59:ARG:HH22	4:D:66:ARG:HH12	1.66	0.42
9:I:111:ARG:HG3	14:N:61:TRP:NE1	2.34	0.42
22:W:12:VAL:HG22	22:W:52:ARG:NH1	2.35	0.42
1:A:447:G:O2'	1:A:487:A:N6	2.51	0.42
1:A:738:C:OP2	6:F:92:LYS:NZ	2.48	0.42
1:A:1429:C:H2'	1:A:1430:C:C6	2.54	0.42
2:B:97:TRP:CZ2	2:B:102:LEU:HD22	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:111:ALA:HB2	4:D:120:LEU:HD12	2.00	0.42
9:I:10:ARG:NH1	9:I:75:ASP:OD2	2.52	0.42
9:I:50:LEU:HD22	9:I:55:ALA:HB3	2.01	0.42
1:A:13:C:N4	1:A:20:U:H3	2.18	0.42
1:A:130:A:H1'	1:A:263:A:O2'	2.20	0.42
1:A:316:G:OP2	1:A:351:G:O2'	2.37	0.42
1:A:755:G:H1'	8:H:1:MET:HE1	2.01	0.42
1:A:877:C:O2	8:H:3:THR:HG21	2.20	0.42
1:A:1333:A:H3'	1:A:1334:G:H8	1.84	0.42
1:A:1342:C:H2'	1:A:1343:G:C8	2.55	0.42
3:C:130:VAL:HG21	3:C:153:VAL:HG11	2.01	0.42
5:E:92:LYS:HB3	5:E:119:LEU:HB2	2.02	0.42
9:I:32:ASP:OD1	9:I:33:PHE:N	2.52	0.42
11:K:33:THR:HA	11:K:39:PRO:HA	2.01	0.42
19:S:22:LEU:HD13	19:S:28:LYS:HB3	2.02	0.42
20:T:50:GLU:HG3	20:T:100:ILE:HG13	2.02	0.42
21:U:7:ARG:HB2	21:U:21:TYR:CE2	2.54	0.42
1:A:113:G:H1'	1:A:354:G:H5'	2.02	0.42
1:A:222:U:H2'	1:A:223:U:C6	2.55	0.42
1:A:284:G:H2'	1:A:285:G:H8	1.83	0.42
1:A:839:U:O2	1:A:839:U:H2'	2.19	0.42
1:A:1206:G:O4'	3:C:194:GLY:HA2	2.20	0.42
1:A:1517[B]:G:N7	1:A:1518[B]:MA6:H103	2.35	0.42
3:C:26:LYS:H	3:C:26:LYS:HG2	1.72	0.42
3:C:112:SER:O	3:C:116:VAL:HG23	2.20	0.42
4:D:57:ARG:NH2	5:E:107:ARG:HE	2.16	0.42
8:H:85:ARG:HD3	8:H:86:ILE:N	2.34	0.42
15:O:6:GLU:H	15:O:6:GLU:HG2	1.66	0.42
22:W:3:GLU:HB3	22:W:5:ASP:OD1	2.20	0.42
1:A:21:G:H2'	1:A:22:G:C8	2.54	0.42
1:A:523:A:H61	12:L:92:0TD:CG	2.33	0.42
1:A:1220:G:H2'	1:A:1221:G:C8	2.55	0.42
2:B:16:HIS:CG	2:B:210:SER:HB2	2.55	0.42
3:C:43:LEU:HA	3:C:47:LEU:HD13	2.00	0.42
3:C:130:VAL:O	3:C:134:ILE:N	2.51	0.42
4:D:102:ASP:OD1	4:D:103:ASN:N	2.53	0.42
7:G:5:ARG:HG2	7:G:6:ARG:H	1.84	0.42
8:H:36:LEU:HD12	8:H:59:LEU:HD13	2.02	0.42
9:I:116:LYS:HD2	9:I:122:ALA:HA	2.01	0.42
11:K:24:SER:OG	11:K:27:ASN:O	2.29	0.42
14:N:14:PRO:O	14:N:15:LYS:HB3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:S:51:VAL:HG22	19:S:71:LEU:HD23	2.02	0.42
22:W:52:ARG:HH11	22:W:52:ARG:HB2	1.85	0.42
22:W:58:THR:HG22	22:W:60:TYR:H	1.85	0.42
1:A:190(J):U:H2'	1:A:190(K):G:H8	1.80	0.42
1:A:302:G:H21	1:A:556:C:H4'	1.85	0.42
1:A:444:C:H2'	1:A:445:G:C8	2.54	0.42
1:A:523:A:C2	12:L:91:LYS:HB3	2.55	0.42
1:A:692:U:H2'	1:A:694:A:OP2	2.20	0.42
1:A:1384:C:H2'	1:A:1385:G:H8	1.85	0.42
1:A:1392:G:N2	1:A:1502:A:H8	2.09	0.42
5:E:144:THR:O	5:E:148:VAL:HG23	2.19	0.42
8:H:95:VAL:HB	8:H:99:GLU:HB2	2.02	0.42
12:L:46:LYS:HB2	12:L:92:0TD:CSB	2.49	0.42
13:M:62:ASN:OD1	13:M:62:ASN:N	2.51	0.42
15:O:63:ARG:O	15:O:67:LEU:HG	2.20	0.42
1:A:430:A:OP1	4:D:9:CYS:N	2.52	0.42
1:A:828:A:H2'	1:A:829:G:O4'	2.20	0.42
1:A:1060:C:O2'	10:J:56:HIS:ND1	2.37	0.42
3:C:121:ALA:HB2	3:C:198:VAL:HG21	2.01	0.42
3:C:188:LEU:HD22	3:C:188:LEU:HA	1.89	0.42
7:G:113:GLU:CB	7:G:119:ARG:HG2	2.48	0.42
9:I:48:GLU:HB3	9:I:101:PHE:CE2	2.55	0.42
10:J:50:ILE:HA	10:J:60:ARG:HA	2.02	0.42
17:Q:81:ARG:HE	17:Q:84:LEU:HG	1.84	0.42
22:W:25:LYS:HA	22:W:31:GLU:HB3	2.01	0.42
1:A:381:C:H2'	1:A:382:A:O4'	2.19	0.41
1:A:406:G:H1	1:A:436:C:H42	1.66	0.41
1:A:661:G:H1	1:A:744:C:H42	1.67	0.41
1:A:731:G:H2'	1:A:732:C:H6	1.85	0.41
1:A:863:U:H2'	1:A:865:A:OP2	2.20	0.41
1:A:1367:C:H4'	10:J:48:THR:HG21	2.02	0.41
3:C:18:TRP:NE1	14:N:53:LEU:O	2.53	0.41
3:C:24:ALA:HB3	3:C:29:TYR:CD1	2.55	0.41
11:K:16:SER:O	11:K:35:PRO:HD3	2.20	0.41
12:L:24:VAL:HG13	12:L:98:TYR:HE2	1.84	0.41
19:S:63:THR:HG22	19:S:64:GLU:H	1.85	0.41
1:A:140:A:H2'	1:A:141:A:H8	1.85	0.41
1:A:299:G:C6	1:A:300:A:C6	3.08	0.41
1:A:540:G:H2'	1:A:541:G:O4'	2.18	0.41
1:A:811:C:O2'	1:A:901:A:N1	2.53	0.41
1:A:895:G:H1	1:A:904:C:H42	1.68	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:965:A:H4'	1:A:966:M2G:OP1	2.19	0.41
1:A:1389:C:H2'	1:A:1390:U:O4'	2.20	0.41
2:B:27:LYS:HB2	2:B:194:PRO:HD2	2.01	0.41
4:D:61:LYS:HD3	4:D:206:PHE:CE2	2.55	0.41
7:G:15:ASP:OD1	7:G:44:TYR:OH	2.38	0.41
1:A:822:C:H2'	1:A:823:G:C8	2.55	0.41
1:A:962:C:H2'	1:A:963:G:C8	2.55	0.41
1:A:1116:C:O2'	9:I:108:VAL:HG21	2.20	0.41
1:A:1348:U:OP2	1:A:1373:G:N2	2.51	0.41
2:B:91:PRO:HG2	2:B:155:LEU:HG	2.02	0.41
20:T:67:ALA:O	20:T:73:HIS:ND1	2.53	0.41
1:A:740:U:H2'	1:A:741:G:H8	1.86	0.41
1:A:858:G:O2'	1:A:859:A:H5'	2.20	0.41
1:A:865:A:H2	1:A:918:A:H4'	1.84	0.41
1:A:948:C:H2'	1:A:949:A:C8	2.56	0.41
1:A:992:U:H3	1:A:1044:A:H62	1.67	0.41
1:A:1211:U:H1'	1:A:1213:A:C2	2.56	0.41
1:A:1225:A:H2'	1:A:1225:A:N3	2.35	0.41
1:A:1318:A:H4'	19:S:10:PHE:CE2	2.56	0.41
2:B:200:ILE:HG13	2:B:201:ILE:N	2.34	0.41
3:C:202:ILE:HG22	3:C:204:LEU:HD23	2.01	0.41
7:G:113:GLU:HG3	7:G:119:ARG:HA	2.03	0.41
8:H:91:ARG:NH1	17:Q:33:GLY:HA3	2.34	0.41
12:L:104:VAL:HG12	12:L:107:ALA:HB3	2.02	0.41
13:M:15:VAL:O	13:M:19:LEU:HG	2.20	0.41
13:M:22:ILE:HB	13:M:25:ILE:HB	2.01	0.41
20:T:40:ALA:HB2	20:T:55:ILE:HG22	2.02	0.41
1:A:120:A:C6	1:A:122:G:C2	3.09	0.41
1:A:125:U:H2'	1:A:126:G:C8	2.55	0.41
1:A:204:U:H4'	1:A:216:G:OP1	2.21	0.41
1:A:1500:A:H5"	1:A:1508:G:H5"	2.01	0.41
2:B:59:GLU:O	2:B:63:MET:HG2	2.20	0.41
14:N:24:CYS:SG	14:N:40:CYS:HB3	2.60	0.41
16:P:21:VAL:HG12	16:P:33:ILE:HD12	2.02	0.41
1:A:181:G:H4'	1:A:182:U:C5'	2.50	0.41
1:A:257:G:H1	1:A:269:C:H42	1.68	0.41
1:A:404:U:H2'	1:A:405:U:C6	2.56	0.41
1:A:431:A:H2'	1:A:432:A:O4'	2.20	0.41
1:A:516:PSU:O2'	22:W:2:LYS:HD2	2.20	0.41
1:A:522:C:OP2	12:L:69:TYR:OH	2.31	0.41
1:A:925:G:O2'	1:A:927:G:OP1	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:6:HIS:CE1	3:C:8:ILE:HB	2.56	0.41
6:F:24:GLU:HA	6:F:27:GLN:HG2	2.01	0.41
12:L:42:THR:HA	12:L:53:ARG:O	2.20	0.41
1:A:298:A:H2'	1:A:299:G:O4'	2.20	0.41
1:A:333:G:H2'	1:A:334:C:C6	2.56	0.41
1:A:355:C:H5'	1:A:389:A:OP2	2.20	0.41
1:A:575:G:O2'	1:A:821:G:H5'	2.21	0.41
1:A:784:C:H2'	1:A:785:G:O4'	2.21	0.41
1:A:948:C:H2'	1:A:949:A:H8	1.86	0.41
1:A:1134:G:N2	1:A:1140:C:N3	2.53	0.41
1:A:1351:U:O4	9:I:118:LYS:NZ	2.32	0.41
4:D:128:VAL:HA	4:D:145:GLU:O	2.19	0.41
18:R:54:ARG:H	18:R:54:ARG:HG3	1.56	0.41
22:W:29:GLY:HA3	22:W:30:PRO:HD3	1.90	0.41
1:A:1069:C:O2'	5:E:25:ARG:NH1	2.50	0.41
1:A:1206:G:H2'	1:A:1207:2MG:C8	2.55	0.41
1:A:1369:C:OP2	9:I:112:LYS:N	2.44	0.41
4:D:3:ARG:HA	4:D:3:ARG:HD3	1.88	0.41
11:K:15:ALA:HA	11:K:76:GLY:O	2.20	0.41
18:R:87:ARG:HD2	18:R:87:ARG:HA	1.84	0.41
1:A:68:G:H2'	1:A:69:G:O4'	2.21	0.41
1:A:377:G:H5"	16:P:24:ALA:HB1	2.03	0.41
1:A:673:G:H2'	1:A:674:G:C8	2.56	0.41
1:A:715:A:H2'	1:A:716:A:H8	1.86	0.41
1:A:878:G:H5'	8:H:89:PRO:HG2	2.02	0.41
1:A:1068:G:H8	1:A:1068:G:OP2	2.04	0.41
1:A:1320:C:O2	19:S:36:ARG:NH2	2.40	0.41
1:A:1401:G:C2	1:A:1402:4OC:H1'	2.55	0.41
3:C:24:ALA:HB2	3:C:32:LEU:HD12	2.03	0.41
3:C:61:ALA:C	3:C:63:ASN:H	2.25	0.41
4:D:36:ARG:N	4:D:37:PRO:HD3	2.36	0.41
4:D:92:VAL:O	4:D:96:LEU:HD13	2.21	0.41
10:J:34:VAL:HG13	10:J:74:ILE:HA	2.02	0.41
1:A:144:G:H1	1:A:178:C:N4	2.18	0.41
1:A:186:C:H5'	20:T:78:ALA:HB1	2.03	0.41
1:A:224:C:H2'	1:A:225:C:C6	2.56	0.41
1:A:1206:G:H4'	3:C:191:THR:O	2.21	0.41
1:A:1287:A:H2'	1:A:1288:A:C8	2.56	0.41
4:D:21:LEU:O	4:D:113:SER:HB2	2.21	0.41
18:R:87:ARG:O	18:R:88:LYS:HB2	2.20	0.41
1:A:258:G:H2'	1:A:259:G:H8	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:309:G:H2'	1:A:310:G:C8	2.55	0.40
1:A:337:C:H2'	1:A:338:A:C8	2.56	0.40
1:A:363:A:P	12:L:34:ARG:HG2	2.61	0.40
1:A:406:G:H2'	1:A:407:G:H8	1.84	0.40
1:A:1005:A:N3	1:A:1026:G:N2	2.69	0.40
1:A:1040:U:H2'	1:A:1041:A:H8	1.85	0.40
1:A:1406:U:O2	1:A:1517[A]:G:N2	2.48	0.40
6:F:12:PRO:HD3	6:F:58:GLY:HA2	2.02	0.40
7:G:113:GLU:H	7:G:113:GLU:HG2	1.44	0.40
13:M:3:ARG:HA	13:M:8:GLU:O	2.20	0.40
1:A:187:C:H5"	20:T:86:ARG:HG3	2.02	0.40
1:A:194:C:H5"	20:T:65:LYS:HG3	2.03	0.40
1:A:730:G:C5	1:A:731:G:H1'	2.56	0.40
1:A:1367:C:H5'	10:J:60:ARG:HE	1.87	0.40
1:A:1520[B]:G:H2'	1:A:1521:G:H8	1.86	0.40
2:B:90:MET:HA	2:B:91:PRO:HD3	1.97	0.40
3:C:6:HIS:HE1	3:C:8:ILE:HB	1.86	0.40
11:K:15:ALA:HA	11:K:77:MET:HA	2.03	0.40
12:L:69:TYR:O	12:L:71:PRO:HD3	2.21	0.40
1:A:397:A:N3	1:A:397:A:H3'	2.37	0.40
2:B:42:ILE:HG21	2:B:202:PRO:HB2	2.02	0.40
5:E:31:LEU:HA	5:E:31:LEU:HD23	1.85	0.40
1:A:445:G:H2'	1:A:446:G:H8	1.86	0.40
1:A:788:U:H2'	1:A:789:U:O4'	2.22	0.40
1:A:832:C:H2'	1:A:833:U:O4'	2.21	0.40
1:A:1071:C:H2'	1:A:1072:G:C8	2.55	0.40
1:A:1321:C:H4'	13:M:87:TYR:CZ	2.57	0.40
4:D:52:SER:O	4:D:56:VAL:HG23	2.21	0.40
7:G:27:ILE:HA	7:G:30:ILE:HD12	2.03	0.40
7:G:50:ILE:HD11	7:G:61:VAL:HG11	2.03	0.40
8:H:4:ASP:OD1	8:H:85:ARG:NH1	2.54	0.40
14:N:9:LYS:HZ1	14:N:12:ARG:HH21	1.69	0.40
14:N:47:LEU:HB3	14:N:53:LEU:HD21	2.02	0.40
1:A:300:A:H8	1:A:300:A:O5'	2.03	0.40
1:A:707:C:O2	11:K:39:PRO:HD3	2.21	0.40
1:A:1059:C:H2'	1:A:1060:C:H6	1.86	0.40
1:A:1347:G:O6	9:I:107:ARG:NH2	2.55	0.40
1:A:1355:G:H2'	1:A:1356:G:C8	2.56	0.40
2:B:16:HIS:ND1	2:B:210:SER:HB2	2.35	0.40
2:B:97:TRP:CZ2	2:B:101:MET:HB2	2.57	0.40
3:C:130:VAL:HG13	3:C:131:ARG:N	2.37	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:148:VAL:HG21	8:H:107:LEU:HD13	2.04	0.40
6:F:8:ILE:HB	6:F:61:LEU:HD12	2.04	0.40
6:F:91:VAL:HG11	18:R:72:ARG:NH1	2.36	0.40
12:L:7:ILE:HD13	12:L:7:ILE:HA	1.87	0.40
18:R:47:THR:HG22	18:R:48:GLY:H	1.85	0.40
20:T:30:LYS:O	20:T:34:LYS:HG3	2.22	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:78:G:OP1	1:A:1229:A:O2'[3_655]	2.14	0.06

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%)	211 (91%)	21 (9%)	0	100	100
3	C	204/239 (85%)	182 (89%)	22 (11%)	0	100	100
4	D	206/209 (99%)	197 (96%)	9 (4%)	0	100	100
5	E	148/162 (91%)	139 (94%)	9 (6%)	0	100	100
6	F	99/101 (98%)	98 (99%)	1 (1%)	0	100	100
7	G	153/156 (98%)	146 (95%)	7 (5%)	0	100	100
8	H	136/138 (99%)	128 (94%)	8 (6%)	0	100	100
9	I	125/128 (98%)	113 (90%)	12 (10%)	0	100	100
10	J	96/105 (91%)	82 (85%)	13 (14%)	1 (1%)	13	46
11	K	114/129 (88%)	106 (93%)	8 (7%)	0	100	100
12	L	121/135 (90%)	113 (93%)	8 (7%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
13	M	116/126 (92%)	101 (87%)	15 (13%)	0	100 100
14	N	58/61 (95%)	52 (90%)	6 (10%)	0	100 100
15	O	85/89 (96%)	83 (98%)	2 (2%)	0	100 100
16	P	81/88 (92%)	78 (96%)	3 (4%)	0	100 100
17	Q	97/105 (92%)	91 (94%)	6 (6%)	0	100 100
18	R	68/88 (77%)	63 (93%)	5 (7%)	0	100 100
19	S	78/93 (84%)	70 (90%)	8 (10%)	0	100 100
20	T	97/106 (92%)	88 (91%)	9 (9%)	0	100 100
21	U	22/27 (82%)	21 (96%)	1 (4%)	0	100 100
22	W	69/71 (97%)	57 (83%)	11 (16%)	1 (1%)	9 40
All	All	2405/2612 (92%)	2219 (92%)	184 (8%)	2 (0%)	48 79

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
10	J	55	LYS
22	W	45	ILE

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	B	202/220 (92%)	181 (90%)	21 (10%)	5 26
3	C	160/188 (85%)	143 (89%)	17 (11%)	5 26
4	D	180/181 (99%)	162 (90%)	18 (10%)	6 28
5	E	115/123 (94%)	108 (94%)	7 (6%)	15 44
6	F	90/90 (100%)	86 (96%)	4 (4%)	24 53
7	G	126/127 (99%)	118 (94%)	8 (6%)	15 44
8	H	119/119 (100%)	111 (93%)	8 (7%)	13 41
9	I	98/99 (99%)	86 (88%)	12 (12%)	4 21

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
10	J	87/92 (95%)	79 (91%)	8 (9%)	7 31
11	K	88/99 (89%)	84 (96%)	4 (4%)	23 53
12	L	103/110 (94%)	94 (91%)	9 (9%)	8 33
13	M	94/101 (93%)	84 (89%)	10 (11%)	5 26
14	N	49/50 (98%)	45 (92%)	4 (8%)	9 34
15	O	79/80 (99%)	66 (84%)	13 (16%)	2 12
16	P	72/74 (97%)	65 (90%)	7 (10%)	6 29
17	Q	94/97 (97%)	86 (92%)	8 (8%)	8 33
18	R	61/77 (79%)	58 (95%)	3 (5%)	21 50
19	S	71/80 (89%)	66 (93%)	5 (7%)	12 40
20	T	76/82 (93%)	70 (92%)	6 (8%)	10 35
21	U	19/22 (86%)	17 (90%)	2 (10%)	5 26
22	W	62/62 (100%)	55 (89%)	7 (11%)	4 24
All	All	2045/2173 (94%)	1864 (91%)	181 (9%)	8 32

All (181) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	7	VAL
2	B	8	LYS
2	B	16	HIS
2	B	21	ARG
2	B	22	LYS
2	B	33	TYR
2	B	44	LEU
2	B	61	LEU
2	B	69	LEU
2	B	73	THR
2	B	96	ARG
2	B	102	LEU
2	B	127	ILE
2	B	144	ARG
2	B	154	LEU
2	B	157	ARG
2	B	160	ASP
2	B	163	PHE
2	B	178	ARG

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Mol	Chain	Res	Type
2	B	190	THR
2	B	200	ILE
3	C	3	ASN
3	C	17	ASP
3	C	22	TRP
3	C	34	LEU
3	C	90	GLU
3	C	91	LEU
3	C	94	LEU
3	C	95	THR
3	C	99	VAL
3	C	111	LEU
3	C	131	ARG
3	C	167	TRP
3	C	176	HIS
3	C	188	LEU
3	C	191	THR
3	C	195	VAL
3	C	196	LEU
4	D	34	GLU
4	D	35	ARG
4	D	49	ARG
4	D	73	ARG
4	D	78	LEU
4	D	89	THR
4	D	91	SER
4	D	115	ARG
4	D	122	ARG
4	D	131	ARG
4	D	145	GLU
4	D	150	GLU
4	D	155	LEU
4	D	157	LEU
4	D	163	GLU
4	D	179	GLU
4	D	193	ASP
4	D	194	LEU
5	E	6	PHE
5	E	12	LEU
5	E	20	GLN
5	E	26	PHE
5	E	41	VAL

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Mol	Chain	Res	Type
5	E	75	THR
5	E	79	GLU
6	F	10	LEU
6	F	24	GLU
6	F	43	LEU
6	F	82	ARG
7	G	8	GLU
7	G	45	ASP
7	G	79	ARG
7	G	84	ASN
7	G	113	GLU
7	G	115	ARG
7	G	136	LYS
7	G	149	ARG
8	H	2	LEU
8	H	3	THR
8	H	29	SER
8	H	63	LEU
8	H	85	ARG
8	H	91	ARG
8	H	92	ARG
8	H	98	LYS
9	I	2	GLU
9	I	12	GLU
9	I	20	ARG
9	I	40	LEU
9	I	51	ARG
9	I	66	ARG
9	I	79	LEU
9	I	102	LEU
9	I	111	ARG
9	I	118	LYS
9	I	121	ARG
9	I	124	GLN
10	J	3	LYS
10	J	38	ILE
10	J	45	ARG
10	J	55	LYS
10	J	60	ARG
10	J	62	HIS
10	J	71	LEU
10	J	78	ASN

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Mol	Chain	Res	Type
11	K	12	ARG
11	K	14	VAL
11	K	29	ILE
11	K	98	LEU
12	L	18	VAL
12	L	20	LYS
12	L	33	ARG
12	L	39	VAL
12	L	53	ARG
12	L	80	HIS
12	L	97	ARG
12	L	100	ILE
12	L	113	ARG
13	M	7	VAL
13	M	17	VAL
13	M	37	THR
13	M	44	ARG
13	M	48	LEU
13	M	50	GLU
13	M	64	TRP
13	M	108	ARG
13	M	115	LYS
13	M	117	VAL
14	N	11	LYS
14	N	13	THR
14	N	22	THR
14	N	25	VAL
15	O	5	LYS
15	O	8	LYS
15	O	32	LEU
15	O	33	THR
15	O	34	LEU
15	O	39	LEU
15	O	45	VAL
15	O	56	LEU
15	O	65	ARG
15	O	70	LEU
15	O	71	GLN
15	O	81	LEU
15	O	83	GLU
16	P	20	VAL
16	P	27	LYS

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Mol	Chain	Res	Type
16	P	42	ARG
16	P	54	GLU
16	P	55	ARG
16	P	67	THR
16	P	83	GLU
17	Q	19	VAL
17	Q	34	LYS
17	Q	35	VAL
17	Q	53	LEU
17	Q	59	ILE
17	Q	60	ILE
17	Q	76	LEU
17	Q	91	ARG
18	R	47	THR
18	R	54	ARG
18	R	87	ARG
19	S	5	LEU
19	S	15	LEU
19	S	39	THR
19	S	63	THR
19	S	79	THR
20	T	9	ASN
20	T	57	ARG
20	T	62	LEU
20	T	68	LYS
20	T	73	HIS
20	T	92	LEU
21	U	6	ARG
21	U	25	LYS
22	W	5	ASP
22	W	23	ARG
22	W	28	SER
22	W	31	GLU
22	W	32	ILE
22	W	52	ARG
22	W	71	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	204	ASN
10	J	84	GLN

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Mol	Chain	Res	Type
13	M	106	ASN
16	P	82	GLN
22	W	19	ASN

5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	1502/1522 (98%)	233 (15%)	48 (3%)

All (233) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	6	G
1	A	9	G
1	A	13	C
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	101	A
1	A	108	G
1	A	116	A
1	A	117	G
1	A	121	C
1	A	129(A)	G
1	A	130	A
1	A	131	C
1	A	163	C
1	A	182	U
1	A	183	G
1	A	195	A
1	A	201	C
1	A	202	U
1	A	203	U
1	A	204	U
1	A	216	G
1	A	220	G
1	A	247	G
1	A	251	G

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Mol	Chain	Res	Type
1	A	252	U
1	A	266	G
1	A	267	C
1	A	279	A
1	A	282	A
1	A	289	G
1	A	301	G
1	A	321	A
1	A	328	C
1	A	329	A
1	A	332	G
1	A	344	A
1	A	345	C
1	A	350	G
1	A	351	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	374	A
1	A	382	A
1	A	384	G
1	A	390	C
1	A	397	A
1	A	398	C
1	A	406	G
1	A	412	A
1	A	413	G
1	A	421	U
1	A	422	C
1	A	429	U
1	A	430	A
1	A	439	A
1	A	452	A
1	A	460	A
1	A	461	C
1	A	476	G
1	A	481	G
1	A	485	G

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Mol	Chain	Res	Type
1	A	486	U
1	A	497	A
1	A	498	U
1	A	509	A
1	A	510	A
1	A	511	C
1	A	518	C
1	A	519	C
1	A	524	G
1	A	531	U
1	A	533	A
1	A	547	A
1	A	559	A
1	A	560	U
1	A	562	C
1	A	564	C
1	A	572	A
1	A	573	A
1	A	576	G
1	A	577	G
1	A	588	G
1	A	596	C
1	A	653	A
1	A	665	A
1	A	686	U
1	A	687	A
1	A	688	G
1	A	695	A
1	A	701	C
1	A	702	A
1	A	703	G
1	A	723	U
1	A	731	G
1	A	749	C
1	A	755	G
1	A	759	A
1	A	777	A
1	A	781	A
1	A	782	A
1	A	785	G
1	A	792	A
1	A	793	U

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Mol	Chain	Res	Type
1	A	794	A
1	A	799	G
1	A	812	C
1	A	813	U
1	A	817	C
1	A	828	A
1	A	839	U
1	A	840	C
1	A	841	U
1	A	848	C
1	A	876	G
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	942	G
1	A	960	U
1	A	961	U
1	A	966	M2G
1	A	968	A
1	A	969	A
1	A	971	G
1	A	974	A
1	A	975	A
1	A	976	G
1	A	977	A
1	A	989	C
1	A	991	U
1	A	992	U
1	A	993	G
1	A	1004	A
1	A	1005	A
1	A	1006	C
1	A	1023	G
1	A	1024	G
1	A	1026	G
1	A	1031	G
1	A	1045	C
1	A	1050	G
1	A	1053	G

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Mol	Chain	Res	Type
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	1101	A
1	A	1124	G
1	A	1125	U
1	A	1126	U
1	A	1127	G
1	A	1130	A
1	A	1131	G
1	A	1137	C
1	A	1138	G
1	A	1139	G
1	A	1146	A
1	A	1152	A
1	A	1159	U
1	A	1183	A
1	A	1191	A
1	A	1195	C
1	A	1196	U
1	A	1197	G
1	A	1201	A
1	A	1202	G
1	A	1211	U
1	A	1212	U
1	A	1214	C
1	A	1215	G
1	A	1224	G
1	A	1225	A
1	A	1226	C
1	A	1227	A
1	A	1228	C
1	A	1238	A
1	A	1241	G
1	A	1256	A
1	A	1257	U
1	A	1258	G
1	A	1278	U
1	A	1280	A

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Mol	Chain	Res	Type
1	A	1281	U
1	A	1286	A
1	A	1287	A
1	A	1300	G
1	A	1301	U
1	A	1302	U
1	A	1303	C
1	A	1306	A
1	A	1312	G
1	A	1319	A
1	A	1320	C
1	A	1336	C
1	A	1346	A
1	A	1347	G
1	A	1348	U
1	A	1353	G
1	A	1359	C
1	A	1362	C
1	A	1364	U
1	A	1381	U
1	A	1398	A
1	A	1400	5MC
1	A	1442	G
1	A	1446	A
1	A	1447	G
1	A	1485	U
1	A	1492	A
1	A	1493	A
1	A	1494	G
1	A	1499	A
1	A	1504	G
1	A	1505	G
1	A	1506	U
1	A	1529	G
1	A	1530	G
1	A	1532	U

All (48) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	5	U
1	A	115	G

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Mol	Chain	Res	Type
1	A	129(A)	G
1	A	181	G
1	A	204	U
1	A	250	A
1	A	251	G
1	A	281	G
1	A	328	C
1	A	372	C
1	A	428	G
1	A	429	U
1	A	484	G
1	A	485	G
1	A	496	A
1	A	509	A
1	A	518	C
1	A	559	A
1	A	687	A
1	A	701	C
1	A	748	C
1	A	792	A
1	A	812	C
1	A	865	A
1	A	913	A
1	A	960	U
1	A	965	A
1	A	992	U
1	A	1049	U
1	A	1065	U
1	A	1067	A
1	A	1126	U
1	A	1145	C
1	A	1182	G
1	A	1190	G
1	A	1201	A
1	A	1256	A
1	A	1257	U
1	A	1285	A
1	A	1300	G
1	A	1301	U
1	A	1305	G
1	A	1346	A
1	A	1347	G

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Mol	Chain	Res	Type
1	A	1358	U
1	A	1380	U
1	A	1493	A
1	A	1504	G

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

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	M2G	A	966	1	20,27,28	1.67	4 (20%)	22,40,43	1.36	3 (13%)
1	5MC	A	967	1	18,22,23	1.16	2 (11%)	26,32,35	0.95	1 (3%)
1	2MG	A	1207	1	18,26,27	1.55	4 (22%)	16,38,41	1.38	2 (12%)
1	5MC	A	1400	1	18,22,23	1.13	3 (16%)	26,32,35	1.00	2 (7%)
1	MA6	A	1518[A]	1	18,26,27	1.00	1 (5%)	19,38,41	0.72	0
1	MA6	A	1518[B]	1	18,26,27	1.21	2 (11%)	19,38,41	0.74	0
1	MA6	A	1519[B]	1	18,26,27	1.19	2 (11%)	19,38,41	0.56	0
1	5MC	A	1407	1	18,22,23	1.24	2 (11%)	26,32,35	1.09	1 (3%)
12	0TD	L	92	12	7,9,10	1.03	0	6,11,13	1.96	2 (33%)
1	PSU	A	1540	1	18,21,22	1.07	1 (5%)	22,30,33	1.74	3 (13%)
1	PSU	A	516	1,23	18,21,22	1.11	1 (5%)	22,30,33	1.78	6 (27%)
1	5MC	A	1404	1	18,22,23	1.15	3 (16%)	26,32,35	0.92	1 (3%)
1	UR3	A	1498	1,23	19,22,23	0.81	1 (5%)	26,32,35	0.88	1 (3%)
1	4OC	A	1402	1	20,23,24	1.18	2 (10%)	26,32,35	0.78	1 (3%)
1	G7M	A	527	1	20,26,27	1.27	2 (10%)	17,39,42	0.79	1 (5%)
1	MA6	A	1519[A]	1	18,26,27	1.03	2 (11%)	19,38,41	0.60	0
1	PSU	A	1541	1	18,21,22	1.12	1 (5%)	22,30,33	1.62	3 (13%)

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	M2G	A	966	1	-	7/7/29/30	0/3/3/3
1	5MC	A	967	1	-	2/7/25/26	0/2/2/2
1	2MG	A	1207	1	-	0/5/27/28	0/3/3/3
1	5MC	A	1400	1	-	2/7/25/26	0/2/2/2
1	MA6	A	1518[A]	1	-	0/7/29/30	0/3/3/3
1	MA6	A	1518[B]	1	-	0/7/29/30	0/3/3/3
1	MA6	A	1519[B]	1	-	3/7/29/30	0/3/3/3
1	5MC	A	1407	1	-	0/7/25/26	0/2/2/2
12	0TD	L	92	12	-	3/7/12/14	-
1	PSU	A	1540	1	-	1/7/25/26	0/2/2/2
1	PSU	A	516	1,23	-	0/7/25/26	0/2/2/2
1	5MC	A	1404	1	-	0/7/25/26	0/2/2/2
1	UR3	A	1498	1,23	-	0/7/25/26	0/2/2/2
1	4OC	A	1402	1	-	2/9/29/30	0/2/2/2
1	G7M	A	527	1	-	2/3/25/26	0/3/3/3
1	MA6	A	1519[A]	1	-	5/7/29/30	0/3/3/3
1	PSU	A	1541	1	-	1/7/25/26	0/2/2/2

All (33) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	966	M2G	C2-N3	4.25	1.35	1.30
1	A	527	G7M	C2-N2	4.11	1.44	1.34
1	A	1207	2MG	C6-N1	3.88	1.43	1.37
1	A	966	M2G	C6-N1	3.79	1.43	1.37
1	A	1541	PSU	C6-C5	3.73	1.39	1.35
1	A	516	PSU	C6-C5	3.65	1.39	1.35
1	A	1540	PSU	C6-C5	3.53	1.39	1.35
1	A	966	M2G	C2-N2	3.50	1.41	1.35
1	A	1518[B]	MA6	C6-N1	3.36	1.38	1.33
1	A	1407	5MC	C6-C5	3.22	1.39	1.34
1	A	1519[B]	MA6	C6-N1	3.22	1.37	1.33
1	A	1207	2MG	C2-N1	3.16	1.41	1.36
1	A	1402	4OC	C2-N1	3.14	1.46	1.40
1	A	1207	2MG	C2-N2	3.07	1.40	1.33
1	A	1519[A]	MA6	C6-N1	2.87	1.37	1.33
1	A	1400	5MC	C2-N1	2.81	1.46	1.40
1	A	1518[A]	MA6	C6-N1	2.81	1.37	1.33
1	A	967	5MC	C2-N1	2.69	1.45	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1402	4OC	C2-N3	2.64	1.41	1.36
1	A	1404	5MC	C2-N1	2.56	1.45	1.40
1	A	967	5MC	C2-N3	2.55	1.41	1.36
1	A	1407	5MC	C4-N4	2.52	1.40	1.34
1	A	1404	5MC	C2-N3	2.48	1.41	1.36
1	A	1498	UR3	C2-N1	2.42	1.42	1.38
1	A	527	G7M	CN7-N7	-2.38	1.42	1.47
1	A	1519[B]	MA6	C2-N1	2.30	1.38	1.33
1	A	1207	2MG	C5-C6	-2.25	1.42	1.47
1	A	1400	5MC	C2-N3	2.19	1.40	1.36
1	A	1404	5MC	C6-C5	2.17	1.38	1.34
1	A	966	M2G	C5-C6	-2.13	1.43	1.47
1	A	1518[B]	MA6	C2-N1	2.13	1.37	1.33
1	A	1519[A]	MA6	C2-N1	2.06	1.37	1.33
1	A	1400	5MC	C6-C5	2.04	1.37	1.34

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1540	PSU	C4-N3-C2	-4.58	119.74	126.34
1	A	516	PSU	N1-C2-N3	4.57	120.31	115.13
1	A	516	PSU	C4-N3-C2	-4.51	119.85	126.34
1	A	1541	PSU	C4-N3-C2	-4.35	120.08	126.34
1	A	1540	PSU	N1-C2-N3	4.25	119.94	115.13
1	A	1541	PSU	N1-C2-N3	3.98	119.64	115.13
1	A	1207	2MG	O6-C6-N1	-3.98	115.95	120.65
1	A	966	M2G	N1-C2-N2	-3.44	115.10	118.04
1	A	1207	2MG	O6-C6-C5	3.23	130.68	124.37
12	L	92	0TD	CSB-SB-CB	-3.23	96.61	102.44
1	A	966	M2G	O6-C6-C5	3.09	130.40	124.37
1	A	1407	5MC	N4-C4-N3	-3.01	112.99	118.48
1	A	966	M2G	O6-C6-N1	-2.95	117.17	120.65
1	A	527	G7M	C2-N1-C6	-2.63	120.26	125.10
1	A	1540	PSU	O2-C2-N1	-2.60	119.93	122.79
1	A	1400	5MC	N4-C4-N3	-2.53	113.85	118.48
1	A	967	5MC	N4-C4-N3	-2.46	113.98	118.48
1	A	516	PSU	O2-C2-N1	-2.39	120.16	122.79
1	A	1404	5MC	N4-C4-N3	-2.37	114.15	118.48
12	L	92	0TD	OD1-CG-CB	-2.35	117.53	122.44
1	A	516	PSU	C6-N1-C2	-2.30	120.33	122.68
1	A	1541	PSU	O2-C2-N1	-2.23	120.33	122.79
1	A	1402	4OC	C5-C4-N4	-2.12	118.30	122.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1400	5MC	C5-C4-N3	2.08	123.91	121.67
1	A	516	PSU	O4'-C1'-C2'	2.07	108.06	105.14
1	A	516	PSU	C6-C5-C4	2.05	119.63	118.20
1	A	1498	UR3	C6-N1-C2	-2.04	119.96	121.79

There are no chirality outliers.

All (28) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	966	M2G	C4'-C5'-O5'-P
1	A	966	M2G	N1-C2-N2-CM1
1	A	966	M2G	N3-C2-N2-CM1
1	A	1400	5MC	O4'-C4'-C5'-O5'
1	A	1519[A]	MA6	C3'-C4'-C5'-O5'
1	A	1519[A]	MA6	C5-C6-N6-C9
1	A	1519[A]	MA6	C5-C6-N6-C10
1	A	1519[B]	MA6	C5-C6-N6-C9
1	A	1519[B]	MA6	C5-C6-N6-C10
12	L	92	0TD	O-C-CA-CB
1	A	967	5MC	O4'-C4'-C5'-O5'
1	A	1400	5MC	C3'-C4'-C5'-O5'
1	A	1402	4OC	O4'-C4'-C5'-O5'
1	A	1519[A]	MA6	O4'-C4'-C5'-O5'
1	A	967	5MC	C3'-C4'-C5'-O5'
1	A	1402	4OC	C3'-C4'-C5'-O5'
1	A	1519[A]	MA6	N1-C6-N6-C9
1	A	1519[B]	MA6	N1-C6-N6-C9
1	A	527	G7M	C3'-C4'-C5'-O5'
1	A	966	M2G	O4'-C4'-C5'-O5'
1	A	966	M2G	C3'-C4'-C5'-O5'
1	A	966	M2G	N3-C2-N2-CM2
12	L	92	0TD	CG-CB-SB-CSB
12	L	92	0TD	SB-CB-CG-OD1
1	A	1541	PSU	O4'-C1'-C5-C4
1	A	527	G7M	O4'-C4'-C5'-O5'
1	A	966	M2G	N1-C2-N2-CM2
1	A	1540	PSU	O4'-C4'-C5'-O5'

There are no ring outliers.

11 monomers are involved in 22 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	966	M2G	2	0
1	A	967	5MC	1	0
1	A	1207	2MG	1	0
1	A	1518[A]	MA6	3	0
1	A	1518[B]	MA6	3	0
1	A	1519[B]	MA6	3	0
12	L	92	0TD	5	0
1	A	516	PSU	1	0
1	A	1498	UR3	2	0
1	A	1402	4OC	2	0
1	A	1519[A]	MA6	2	0

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 256 ligands modelled in this entry, 256 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

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	1497/1522 (98%)	-0.34	4 (0%) 90 79	67, 163, 304, 482	4 (0%)
2	B	234/256 (91%)	-0.38	0 100 100	114, 177, 251, 306	0
3	C	206/239 (86%)	0.03	4 (1%) 66 45	202, 257, 322, 353	0
4	D	208/209 (99%)	-0.03	5 (2%) 59 39	109, 166, 247, 301	0
5	E	150/162 (92%)	-0.30	2 (1%) 74 53	90, 133, 188, 216	0
6	F	101/101 (100%)	-0.42	0 100 100	133, 170, 203, 216	0
7	G	155/156 (99%)	-0.26	2 (1%) 74 53	137, 199, 268, 298	0
8	H	138/138 (100%)	-0.39	0 100 100	76, 117, 159, 238	0
9	I	127/128 (99%)	0.75	16 (12%) 9 8	164, 258, 332, 373	0
10	J	98/105 (93%)	0.13	3 (3%) 51 33	158, 253, 340, 363	0
11	K	116/129 (89%)	-0.45	3 (2%) 57 37	112, 151, 191, 218	0
12	L	123/135 (91%)	0.05	3 (2%) 59 39	100, 171, 206, 258	0
13	M	118/126 (93%)	-0.15	0 100 100	149, 188, 239, 319	0
14	N	60/61 (98%)	0.70	7 (11%) 10 9	179, 223, 289, 324	0
15	O	87/89 (97%)	-0.27	0 100 100	103, 143, 196, 219	0
16	P	83/88 (94%)	-0.30	0 100 100	115, 152, 190, 239	0
17	Q	99/105 (94%)	-0.19	0 100 100	99, 129, 164, 181	0
18	R	70/88 (79%)	-0.31	1 (1%) 73 52	102, 150, 218, 239	0
19	S	80/93 (86%)	0.03	3 (3%) 44 29	203, 239, 294, 312	0
20	T	99/106 (93%)	-0.14	2 (2%) 64 44	127, 152, 214, 238	0
21	U	24/27 (88%)	1.67	10 (41%) 1 1	152, 213, 278, 302	0
22	W	71/71 (100%)	-0.08	1 (1%) 73 52	91, 171, 228, 245	41 (57%)
All	All	3944/4134 (95%)	-0.19	66 (1%) 69 48	67, 172, 292, 482	45 (1%)

All (66) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
21	U	6	ARG	7.3
4	D	4	TYR	4.9
19	S	2	PRO	4.6
9	I	71	SER	4.5
9	I	105	ASP	4.3
4	D	5	ILE	4.2
21	U	7	ARG	4.0
20	T	73	HIS	4.0
11	K	51	LYS	4.0
11	K	49	GLY	3.9
14	N	13	THR	3.9
4	D	6	GLY	3.7
10	J	54	PHE	3.5
14	N	10	ALA	3.4
14	N	12	ARG	3.4
12	L	28	LYS	3.4
3	C	168	ALA	3.3
9	I	70	LYS	3.3
9	I	126	SER	3.3
14	N	7	ILE	3.1
7	G	4	ARG	3.1
9	I	64	THR	3.0
12	L	89	ARG	3.0
21	U	16	GLY	2.9
20	T	68	LYS	2.9
5	E	23	GLY	2.9
4	D	3	ARG	2.8
21	U	25	LYS	2.8
14	N	31	ARG	2.8
9	I	104	ARG	2.7
21	U	15	ARG	2.7
3	C	178	LEU	2.6
9	I	15	ALA	2.6
1	A	1129	C	2.5
21	U	23	PRO	2.5
7	G	36	LYS	2.5
9	I	84	ALA	2.4
19	S	3	ARG	2.4
21	U	24	ARG	2.4
18	R	61	LYS	2.4
9	I	121	ARG	2.4
9	I	66	ARG	2.3
1	A	1201	A	2.3

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Mol	Chain	Res	Type	RSRZ
21	U	5	ASP	2.3
5	E	22	GLY	2.3
1	A	1397	C	2.3
9	I	118	LYS	2.3
9	I	14	VAL	2.2
9	I	128	ARG	2.2
9	I	102	LEU	2.2
14	N	6	LEU	2.2
12	L	47	LYS	2.2
14	N	14	PRO	2.2
9	I	65	VAL	2.2
21	U	14	TRP	2.2
4	D	42	GLN	2.1
22	W	44	TYR	2.1
3	C	201	TYR	2.1
11	K	125	PHE	2.1
21	U	21	TYR	2.1
3	C	66	VAL	2.1
10	J	5	ARG	2.1
9	I	101	PHE	2.1
1	A	202	U	2.0
10	J	58	ASP	2.0
19	S	37	ARG	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
1	PSU	A	1541	20/21	0.83	0.23	362,405,482,541	0
1	PSU	A	1540	20/21	0.88	0.19	274,296,321,345	0
1	2MG	A	1207	24/25	0.89	0.11	262,276,288,300	0
1	PSU	A	516	20/21	0.92	0.07	183,200,205,207	0
1	5MC	A	1407	21/22	0.94	0.08	169,180,191,196	0
1	5MC	A	1404	21/22	0.95	0.11	114,141,154,158	0
1	5MC	A	967	21/22	0.95	0.12	165,179,199,201	0
1	UR3	A	1498	21/22	0.96	0.12	134,148,155,162	0
1	MA6	A	1518[A]	24/25	0.96	0.13	121,125,132,133	24
1	MA6	A	1518[B]	24/25	0.96	0.13	125,131,138,139	24

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
1	G7M	A	527	24/25	0.96	0.09	137,149,162,167	0
1	5MC	A	1400	21/22	0.96	0.11	150,172,187,191	0
1	4OC	A	1402	22/23	0.97	0.09	113,158,174,180	0
1	M2G	A	966	25/26	0.97	0.10	147,187,194,201	0
1	MA6	A	1519[A]	24/25	0.98	0.10	116,125,141,143	24
1	MA6	A	1519[B]	24/25	0.98	0.10	118,135,139,150	24
12	0TD	L	92	10/11	0.99	0.07	154,164,189,189	0

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
23	MG	A	1622	1/1	0.53	0.18	191,191,191,191	0
23	MG	A	1795	1/1	0.58	0.24	200,200,200,200	0
23	MG	A	1602	1/1	0.65	0.18	164,164,164,164	0
23	MG	A	1683	1/1	0.66	0.14	143,143,143,143	0
23	MG	A	1770	1/1	0.68	0.22	153,153,153,153	0
23	MG	A	1776	1/1	0.71	0.13	147,147,147,147	0
23	MG	A	1730	1/1	0.72	0.06	135,135,135,135	0
23	MG	A	1812	1/1	0.72	0.13	71,71,71,71	0
23	MG	A	1700	1/1	0.74	0.18	111,111,111,111	0
23	MG	A	1780	1/1	0.75	0.11	146,146,146,146	0
23	MG	C	302	1/1	0.75	0.13	180,180,180,180	0
23	MG	L	201	1/1	0.75	0.15	128,128,128,128	0
23	MG	A	1686	1/1	0.76	0.09	182,182,182,182	0
23	MG	A	1669	1/1	0.76	0.16	119,119,119,119	0
23	MG	A	1827	1/1	0.77	0.13	109,109,109,109	0
23	MG	A	1688	1/1	0.77	0.16	131,131,131,131	0
23	MG	D	303	1/1	0.77	0.10	87,87,87,87	0
23	MG	A	1817	1/1	0.77	0.23	120,120,120,120	0
23	MG	A	1668	1/1	0.78	0.09	134,134,134,134	0
23	MG	A	1739	1/1	0.78	0.17	123,123,123,123	0
23	MG	A	1757	1/1	0.79	0.17	156,156,156,156	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
23	MG	A	1675	1/1	0.80	0.15	139,139,139,139	0
23	MG	A	1704	1/1	0.80	0.14	86,86,86,86	0
23	MG	C	301	1/1	0.80	0.09	137,137,137,137	0
23	MG	A	1777	1/1	0.81	0.13	150,150,150,150	0
23	MG	A	1822	1/1	0.81	0.14	97,97,97,97	0
23	MG	A	1749	1/1	0.81	0.34	128,128,128,128	0
23	MG	A	1831	1/1	0.81	0.13	133,133,133,133	0
23	MG	A	1653	1/1	0.82	0.32	83,83,83,83	0
23	MG	A	1717	1/1	0.82	0.10	88,88,88,88	0
23	MG	A	1719	1/1	0.82	0.11	132,132,132,132	0
23	MG	S	101	1/1	0.82	0.10	114,114,114,114	0
23	MG	A	1665	1/1	0.83	0.30	164,164,164,164	0
23	MG	A	1703	1/1	0.83	0.15	96,96,96,96	0
23	MG	A	1752	1/1	0.83	0.12	109,109,109,109	0
23	MG	F	201	1/1	0.83	0.14	148,148,148,148	0
23	MG	A	1672	1/1	0.83	0.11	140,140,140,140	0
23	MG	A	1762	1/1	0.83	0.10	94,94,94,94	0
23	MG	A	1684	1/1	0.84	0.14	136,136,136,136	0
23	MG	A	1734	1/1	0.84	0.14	170,170,170,170	0
23	MG	A	1758	1/1	0.84	0.07	127,127,127,127	0
23	MG	A	1825	1/1	0.84	0.15	96,96,96,96	0
23	MG	A	1716	1/1	0.85	0.23	98,98,98,98	0
23	MG	A	1604	1/1	0.85	0.18	145,145,145,145	0
23	MG	A	1677	1/1	0.85	0.12	143,143,143,143	0
23	MG	A	1682	1/1	0.85	0.21	135,135,135,135	0
23	MG	A	1805	1/1	0.85	0.23	202,202,202,202	0
23	MG	A	1808	1/1	0.85	0.27	172,172,172,172	0
23	MG	A	1761	1/1	0.85	0.36	110,110,110,110	0
23	MG	I	202	1/1	0.85	0.07	151,151,151,151	0
23	MG	A	1657	1/1	0.85	0.08	123,123,123,123	0
23	MG	A	1633	1/1	0.85	0.13	117,117,117,117	0
23	MG	A	1634	1/1	0.86	0.10	65,65,65,65	0
23	MG	A	1708	1/1	0.86	0.14	142,142,142,142	0
23	MG	A	1742	1/1	0.86	0.18	70,70,70,70	0
23	MG	A	1748	1/1	0.86	0.23	92,92,92,92	0
23	MG	A	1689	1/1	0.86	0.09	155,155,155,155	0
23	MG	A	1796	1/1	0.86	0.13	169,169,169,169	0
23	MG	A	1800	1/1	0.86	0.14	145,145,145,145	0
23	MG	A	1828	1/1	0.86	0.08	172,172,172,172	0
23	MG	A	1632	1/1	0.87	0.15	103,103,103,103	0
23	MG	A	1711	1/1	0.87	0.08	189,189,189,189	0
23	MG	A	1656	1/1	0.87	0.10	136,136,136,136	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
23	MG	B	301	1/1	0.87	0.08	145,145,145,145	0
23	MG	A	1609	1/1	0.87	0.16	109,109,109,109	0
23	MG	A	1662	1/1	0.87	0.19	102,102,102,102	0
23	MG	A	1721	1/1	0.87	0.14	101,101,101,101	0
23	MG	A	1680	1/1	0.87	0.15	87,87,87,87	0
23	MG	A	1631	1/1	0.87	0.11	150,150,150,150	0
23	MG	A	1644	1/1	0.87	0.19	129,129,129,129	0
23	MG	A	1706	1/1	0.87	0.11	116,116,116,116	0
23	MG	W	101	1/1	0.87	0.14	176,176,176,176	1
23	MG	A	1674	1/1	0.88	0.12	85,85,85,85	0
23	MG	A	1648	1/1	0.88	0.07	61,61,61,61	0
23	MG	A	1649	1/1	0.88	0.13	89,89,89,89	0
23	MG	A	1818	1/1	0.88	0.10	149,149,149,149	0
23	MG	A	1616	1/1	0.88	0.07	118,118,118,118	0
23	MG	A	1664	1/1	0.88	0.06	190,190,190,190	0
23	MG	A	1760	1/1	0.88	0.11	85,85,85,85	0
23	MG	A	1696	1/1	0.88	0.15	126,126,126,126	0
23	MG	A	1699	1/1	0.88	0.10	153,153,153,153	0
23	MG	A	1826	1/1	0.89	0.17	54,54,54,54	0
23	MG	D	302	1/1	0.89	0.16	152,152,152,152	0
23	MG	A	1619	1/1	0.89	0.07	72,72,72,72	0
23	MG	A	1701	1/1	0.89	0.11	72,72,72,72	0
23	MG	A	1830	1/1	0.89	0.11	82,82,82,82	0
23	MG	A	1802	1/1	0.89	0.08	205,205,205,205	0
23	MG	A	1660	1/1	0.89	0.11	103,103,103,103	0
23	MG	A	1673	1/1	0.89	0.09	127,127,127,127	0
23	MG	A	1618	1/1	0.90	0.13	109,109,109,109	0
23	MG	A	1756	1/1	0.90	0.16	100,100,100,100	0
23	MG	A	1685	1/1	0.90	0.12	90,90,90,90	0
23	MG	A	1725	1/1	0.90	0.14	84,84,84,84	0
23	MG	A	1666	1/1	0.90	0.09	154,154,154,154	0
23	MG	A	1623	1/1	0.90	0.12	101,101,101,101	0
23	MG	A	1809	1/1	0.90	0.08	121,121,121,121	0
23	MG	A	1810	1/1	0.90	0.21	102,102,102,102	0
23	MG	A	1679	1/1	0.90	0.11	136,136,136,136	0
23	MG	A	1765	1/1	0.90	0.09	160,160,160,160	0
23	MG	A	1601	1/1	0.90	0.12	100,100,100,100	0
23	MG	A	1746	1/1	0.90	0.09	142,142,142,142	0
23	MG	A	1640	1/1	0.90	0.12	142,142,142,142	0
23	MG	A	1655	1/1	0.90	0.15	91,91,91,91	0
23	MG	A	1736	1/1	0.91	0.06	58,58,58,58	0
23	MG	A	1813	1/1	0.91	0.06	115,115,115,115	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
23	MG	A	1798	1/1	0.91	0.14	104,104,104,104	0
23	MG	A	1728	1/1	0.91	0.12	125,125,125,125	0
23	MG	A	1821	1/1	0.91	0.14	105,105,105,105	0
23	MG	A	1714	1/1	0.91	0.05	61,61,61,61	0
23	MG	A	1804	1/1	0.91	0.30	162,162,162,162	0
23	MG	A	1779	1/1	0.91	0.10	138,138,138,138	0
23	MG	A	1743	1/1	0.91	0.08	113,113,113,113	0
23	MG	A	1788	1/1	0.91	0.10	58,58,58,58	0
23	MG	A	1678	1/1	0.91	0.13	157,157,157,157	0
23	MG	A	1816	1/1	0.92	0.26	83,83,83,83	0
23	MG	A	1784	1/1	0.92	0.09	90,90,90,90	0
23	MG	A	1654	1/1	0.92	0.06	107,107,107,107	0
23	MG	A	1790	1/1	0.92	0.17	131,131,131,131	0
23	MG	A	1792	1/1	0.92	0.06	116,116,116,116	0
23	MG	A	1793	1/1	0.92	0.10	86,86,86,86	0
23	MG	A	1747	1/1	0.92	0.50	140,140,140,140	0
23	MG	A	1612	1/1	0.92	0.07	142,142,142,142	0
23	MG	A	1764	1/1	0.92	0.07	134,134,134,134	0
23	MG	A	1799	1/1	0.92	0.21	110,110,110,110	0
23	MG	A	1629	1/1	0.92	0.11	85,85,85,85	0
23	MG	A	1750	1/1	0.92	0.15	104,104,104,104	0
23	MG	A	1803	1/1	0.92	0.08	102,102,102,102	0
23	MG	A	1670	1/1	0.92	0.09	116,116,116,116	0
23	MG	A	1692	1/1	0.92	0.11	146,146,146,146	0
23	MG	A	1806	1/1	0.92	0.08	149,149,149,149	0
23	MG	A	1695	1/1	0.92	0.09	135,135,135,135	0
23	MG	A	1630	1/1	0.92	0.10	62,62,62,62	0
23	MG	A	1781	1/1	0.92	0.07	110,110,110,110	0
23	MG	N	102	1/1	0.92	0.08	176,176,176,176	0
23	MG	P	101	1/1	0.92	0.26	89,89,89,89	0
23	MG	A	1782	1/1	0.92	0.06	92,92,92,92	0
23	MG	A	1783	1/1	0.92	0.05	109,109,109,109	0
23	MG	A	1646	1/1	0.93	0.09	119,119,119,119	0
23	MG	A	1731	1/1	0.93	0.29	144,144,144,144	0
23	MG	A	1815	1/1	0.93	0.10	88,88,88,88	0
23	MG	A	1636	1/1	0.93	0.25	113,113,113,113	0
23	MG	A	1801	1/1	0.93	0.11	120,120,120,120	0
23	MG	A	1620	1/1	0.93	0.14	92,92,92,92	0
23	MG	E	202	1/1	0.93	0.06	81,81,81,81	0
23	MG	A	1643	1/1	0.93	0.09	154,154,154,154	0
23	MG	H	201	1/1	0.93	0.10	104,104,104,104	0
23	MG	A	1767	1/1	0.93	0.06	125,125,125,125	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
23	MG	A	1753	1/1	0.93	0.15	83,83,83,83	0
23	MG	A	1772	1/1	0.93	0.13	88,88,88,88	0
23	MG	A	1707	1/1	0.93	0.07	102,102,102,102	0
23	MG	Q	201	1/1	0.93	0.08	113,113,113,113	0
23	MG	A	1687	1/1	0.93	0.08	138,138,138,138	0
23	MG	A	1627	1/1	0.93	0.11	170,170,170,170	0
23	MG	A	1769	1/1	0.94	0.19	106,106,106,106	0
23	MG	A	1744	1/1	0.94	0.09	108,108,108,108	0
23	MG	A	1645	1/1	0.94	0.06	139,139,139,139	0
23	MG	A	1775	1/1	0.94	0.07	118,118,118,118	0
23	MG	A	1652	1/1	0.94	0.08	122,122,122,122	0
23	MG	A	1709	1/1	0.94	0.08	126,126,126,126	0
23	MG	A	1778	1/1	0.94	0.05	100,100,100,100	0
23	MG	A	1638	1/1	0.94	0.08	121,121,121,121	0
23	MG	A	1611	1/1	0.94	0.08	132,132,132,132	0
23	MG	A	1763	1/1	0.94	0.07	109,109,109,109	0
23	MG	A	1715	1/1	0.94	0.10	91,91,91,91	0
23	MG	A	1729	1/1	0.94	0.09	144,144,144,144	0
23	MG	A	1755	1/1	0.94	0.08	134,134,134,134	0
23	MG	A	1768	1/1	0.94	0.14	74,74,74,74	0
23	MG	A	1829	1/1	0.94	0.12	89,89,89,89	0
23	MG	A	1789	1/1	0.94	0.18	182,182,182,182	0
23	MG	A	1726	1/1	0.95	0.10	124,124,124,124	0
23	MG	A	1727	1/1	0.95	0.07	110,110,110,110	0
23	MG	A	1713	1/1	0.95	0.17	117,117,117,117	0
23	MG	A	1671	1/1	0.95	0.06	95,95,95,95	0
23	MG	A	1650	1/1	0.95	0.30	118,118,118,118	0
23	MG	A	1751	1/1	0.95	0.04	111,111,111,111	0
23	MG	A	1603	1/1	0.95	0.06	119,119,119,119	0
23	MG	A	1791	1/1	0.95	0.07	61,61,61,61	0
23	MG	A	1647	1/1	0.95	0.13	69,69,69,69	0
23	MG	A	1754	1/1	0.95	0.08	74,74,74,74	0
23	MG	A	1773	1/1	0.95	0.12	168,168,168,168	0
23	MG	A	1718	1/1	0.95	0.08	72,72,72,72	0
23	MG	A	1797	1/1	0.95	0.09	151,151,151,151	0
23	MG	A	1819	1/1	0.95	0.12	64,64,64,64	0
23	MG	A	1639	1/1	0.95	0.09	100,100,100,100	0
23	MG	A	1710	1/1	0.95	0.04	108,108,108,108	0
23	MG	A	1724	1/1	0.95	0.15	139,139,139,139	0
23	MG	A	1610	1/1	0.95	0.08	141,141,141,141	0
23	MG	A	1745	1/1	0.95	0.10	83,83,83,83	0
24	ZN	N	101	1/1	0.95	0.10	276,276,276,276	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
23	MG	A	1823	1/1	0.96	0.18	167,167,167,167	0
23	MG	A	1607	1/1	0.96	0.04	138,138,138,138	0
23	MG	A	1774	1/1	0.96	0.10	101,101,101,101	0
23	MG	A	1624	1/1	0.96	0.11	85,85,85,85	0
23	MG	A	1712	1/1	0.96	0.12	90,90,90,90	0
23	MG	A	1625	1/1	0.96	0.14	98,98,98,98	0
23	MG	A	1697	1/1	0.96	0.06	154,154,154,154	0
23	MG	A	1735	1/1	0.96	0.11	61,61,61,61	0
23	MG	A	1681	1/1	0.96	0.08	131,131,131,131	0
23	MG	A	1759	1/1	0.96	0.08	127,127,127,127	0
23	MG	A	1608	1/1	0.96	0.07	80,80,80,80	0
23	MG	A	1606	1/1	0.96	0.09	108,108,108,108	0
23	MG	A	1659	1/1	0.96	0.13	153,153,153,153	0
23	MG	D	304	1/1	0.96	0.05	118,118,118,118	0
23	MG	A	1811	1/1	0.96	0.16	107,107,107,107	0
23	MG	A	1613	1/1	0.96	0.05	114,114,114,114	0
23	MG	A	1720	1/1	0.96	0.25	114,114,114,114	0
23	MG	A	1705	1/1	0.96	0.15	127,127,127,127	0
23	MG	A	1722	1/1	0.96	0.18	145,145,145,145	0
23	MG	A	1614	1/1	0.96	0.11	109,109,109,109	0
23	MG	A	1641	1/1	0.96	0.07	109,109,109,109	0
23	MG	A	1676	1/1	0.96	0.13	78,78,78,78	0
23	MG	A	1820	1/1	0.96	0.33	89,89,89,89	0
23	MG	A	1771	1/1	0.96	0.06	104,104,104,104	0
23	MG	A	1642	1/1	0.96	0.09	114,114,114,114	0
23	MG	A	1615	1/1	0.97	0.16	113,113,113,113	0
23	MG	A	1794	1/1	0.97	0.04	124,124,124,124	0
23	MG	A	1807	1/1	0.97	0.12	158,158,158,158	0
23	MG	A	1626	1/1	0.97	0.08	104,104,104,104	0
23	MG	A	1733	1/1	0.97	0.05	102,102,102,102	0
23	MG	A	1663	1/1	0.97	0.07	119,119,119,119	0
23	MG	A	1658	1/1	0.97	0.10	174,174,174,174	0
23	MG	I	201	1/1	0.97	0.06	106,106,106,106	0
23	MG	A	1786	1/1	0.97	0.04	75,75,75,75	0
23	MG	I	203	1/1	0.97	0.08	95,95,95,95	0
23	MG	A	1605	1/1	0.97	0.06	115,115,115,115	0
23	MG	A	1814	1/1	0.97	0.21	159,159,159,159	0
23	MG	A	1766	1/1	0.97	0.08	89,89,89,89	0
23	MG	A	1738	1/1	0.97	0.06	115,115,115,115	0
23	MG	A	1832	1/1	0.97	0.05	80,80,80,80	0
23	MG	A	1723	1/1	0.97	0.07	73,73,73,73	0
23	MG	A	1741	1/1	0.97	0.08	138,138,138,138	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
23	MG	A	1690	1/1	0.98	0.07	123,123,123,123	0
23	MG	A	1691	1/1	0.98	0.06	192,192,192,192	0
23	MG	A	1824	1/1	0.98	0.07	44,44,44,44	0
23	MG	E	201	1/1	0.98	0.04	70,70,70,70	0
23	MG	A	1651	1/1	0.98	0.04	55,55,55,55	0
23	MG	A	1693	1/1	0.98	0.03	176,176,176,176	0
23	MG	A	1694	1/1	0.98	0.09	122,122,122,122	0
23	MG	A	1635	1/1	0.98	0.06	133,133,133,133	0
23	MG	A	1621	1/1	0.98	0.07	86,86,86,86	0
23	MG	A	1637	1/1	0.98	0.05	124,124,124,124	0
23	MG	A	1698	1/1	0.98	0.12	139,139,139,139	0
23	MG	A	1737	1/1	0.98	0.04	104,104,104,104	0
23	MG	A	1833	1/1	0.98	0.06	82,82,82,82	0
23	MG	A	1628	1/1	0.98	0.06	90,90,90,90	0
23	MG	A	1667	1/1	0.98	0.10	101,101,101,101	0
23	MG	A	1661	1/1	0.98	0.05	100,100,100,100	0
23	MG	C	303	1/1	0.98	0.04	93,93,93,93	0
23	MG	A	1702	1/1	0.99	0.06	106,106,106,106	0
23	MG	A	1740	1/1	0.99	0.06	46,46,46,46	0
23	MG	P	102	1/1	0.99	0.05	75,75,75,75	0
23	MG	A	1785	1/1	0.99	0.04	92,92,92,92	0
23	MG	A	1617	1/1	0.99	0.04	93,93,93,93	0
23	MG	A	1787	1/1	0.99	0.04	94,94,94,94	0
24	ZN	D	301	1/1	0.99	0.12	168,168,168,168	0
23	MG	A	1732	1/1	0.99	0.04	77,77,77,77	0

6.5 Other polymers (i)

There are no such residues in this entry.