



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 12, 2020 – 10:53 AM EDT

PDB ID : 5WNP  
Title : Crystal Structure of 30S ribosomal subunit from *Thermus thermophilus*  
Authors : DeMirci, H.  
Deposited on : 2017-08-01  
Resolution : 3.30 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.14.6  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.14.6

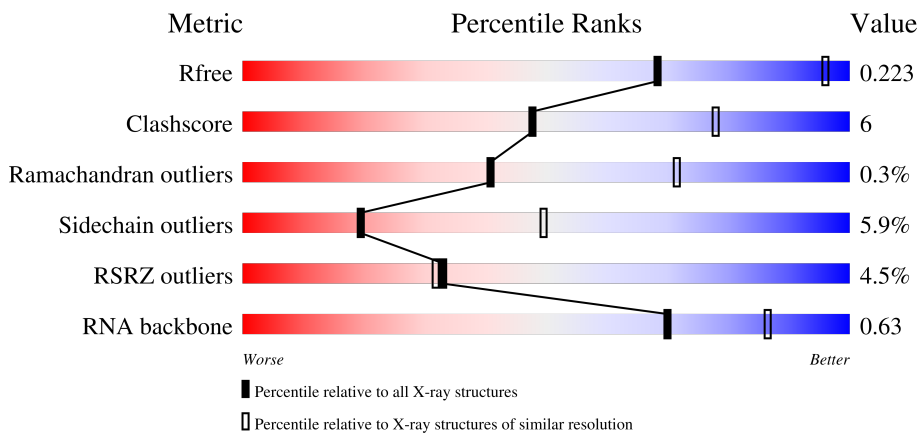
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.30 Å.

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



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . 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	 66% 27% 6%
2	B	236	 79% 20%
3	C	207	 80% 19%
4	D	208	 80% 20%

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Mol	Chain	Length	Quality of chain
5	E	151	
6	F	101	
7	G	155	
8	H	138	
9	I	127	
10	J	99	
11	K	119	
12	L	125	
13	M	118	
14	N	60	
15	O	88	
16	P	84	
17	Q	99	
18	R	73	
19	S	81	
20	T	99	
21	U	25	
22	a	6	
23	b	15	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
23	12A	b	37	X	-	-	-
24	MG	A	1627	-	-	-	X
24	MG	A	1629	-	-	-	X
24	MG	A	1666	-	-	-	X
24	MG	A	1677	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
24	MG	A	1683	-	-	-	X
24	MG	A	1687	-	-	-	X
24	MG	A	1690	-	-	-	X
24	MG	A	1692	-	-	-	X
24	MG	A	1699	-	-	-	X
24	MG	A	1701	-	-	-	X
24	MG	A	1704	-	-	-	X
24	MG	A	1730	-	-	-	X
24	MG	A	1757	-	-	-	X
24	MG	A	1769	-	-	-	X
24	MG	A	1770	-	-	-	X
24	MG	A	1780	-	-	-	X
24	MG	A	1782	-	-	-	X
24	MG	A	1784	-	-	-	X
24	MG	A	1791	-	-	-	X
24	MG	A	1794	-	-	-	X
24	MG	A	1795	-	-	-	X
24	MG	A	1802	-	-	-	X
24	MG	A	1803	-	-	-	X
24	MG	A	1805	-	-	-	X
24	MG	A	1817	-	-	-	X
24	MG	A	1818	-	-	-	X
24	MG	A	1824	-	-	-	X
24	MG	H	201	-	-	-	X
24	MG	P	101	-	-	-	X
24	MG	Q	202	-	-	-	X
25	K	A	1834	-	-	-	X
25	K	A	1839	-	-	-	X
25	K	A	1841	-	-	-	X
25	K	A	1843	-	-	-	X
25	K	A	1844	-	-	-	X
26	ZN	D	301	-	-	-	X

## 2 Entry composition [i](#)

There are 27 unique types of molecules in this entry. The entry contains 52586 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 Ribosomal RNA rRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
1	A	1512	32504	14477	6011	10505	1511	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1534	C	A	conflict	GB 55771382
A	1535	A	C	conflict	GB 55771382

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	236	1874	1195	336	338	5	0	0	1

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
11	K	119	885	549	168	165	3	0	0	0

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
18	R	73	598	381	118	99	0	0	0

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
22	a	6	123	57	21	40	5	0	0	0

- Molecule 23 is a RNA chain called RNA (5'-R(P\*UP\*AP\*GP\*AP\*CP\*UP\*(70U)P\*UP\*U P\*(12A)P\*AP\*(PSU)P\*CP\*UP\*A)-3').

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	P	S			
23	b	15	330	150	51	112	15	2	0	0	0

- Molecule 24 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
24	P	3	Total 3	Mg 3	0	0
24	G	1	Total 1	Mg 1	0	0
24	Q	2	Total 2	Mg 2	0	0
24	D	1	Total 1	Mg 1	0	0
24	E	1	Total 1	Mg 1	0	0
24	H	2	Total 2	Mg 2	0	0
24	A	236	Total 236	Mg 236	0	0
24	T	1	Total 1	Mg 1	0	0
24	N	1	Total 1	Mg 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
24	L	1	Total 1	Mg 1	0	0
24	S	3	Total 3	Mg 3	0	0
24	F	1	Total 1	Mg 1	0	0

- Molecule 25 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
25	A	22	Total 22	K 22	0	0

- Molecule 26 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

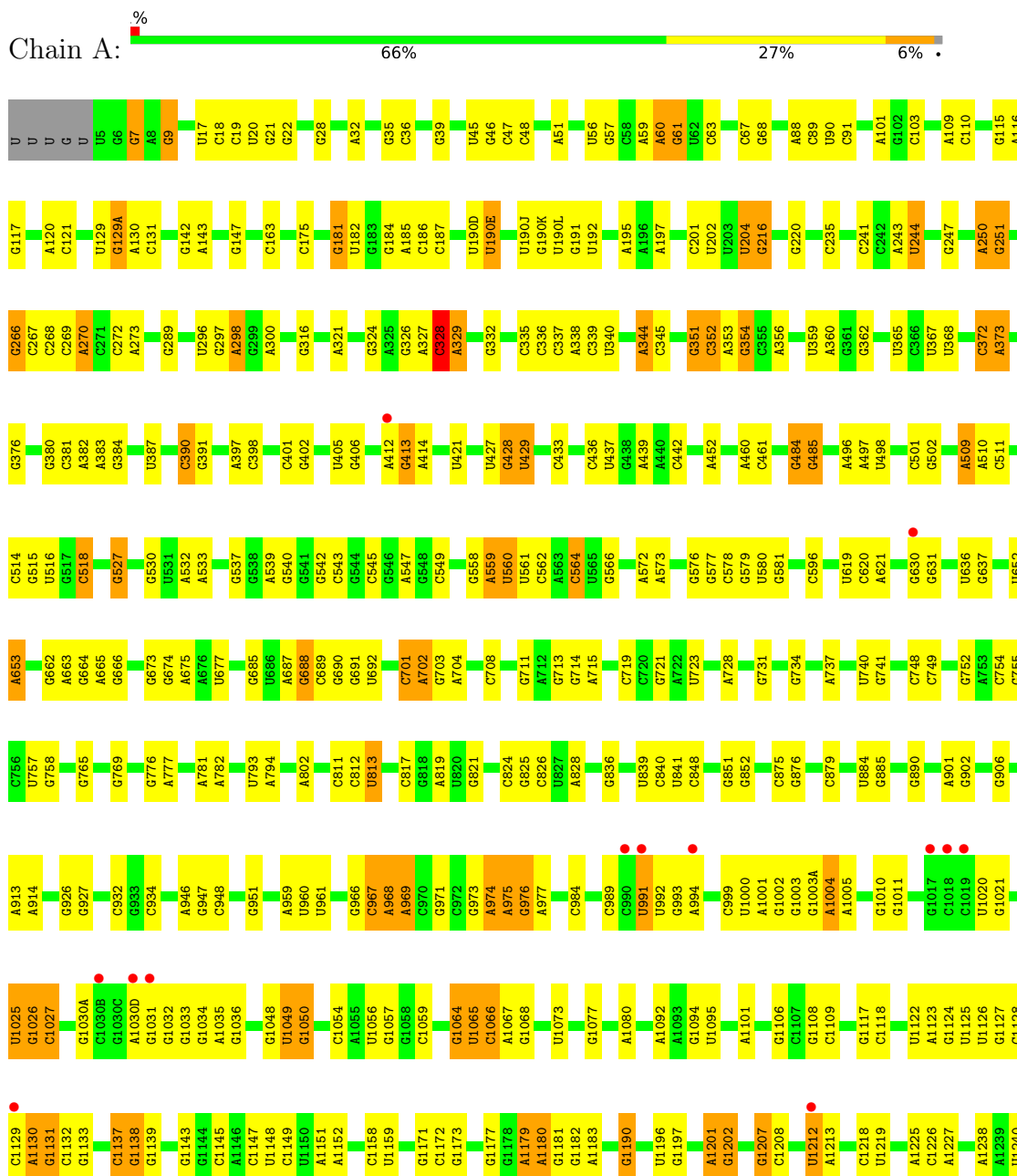
- Molecule 27 is water.

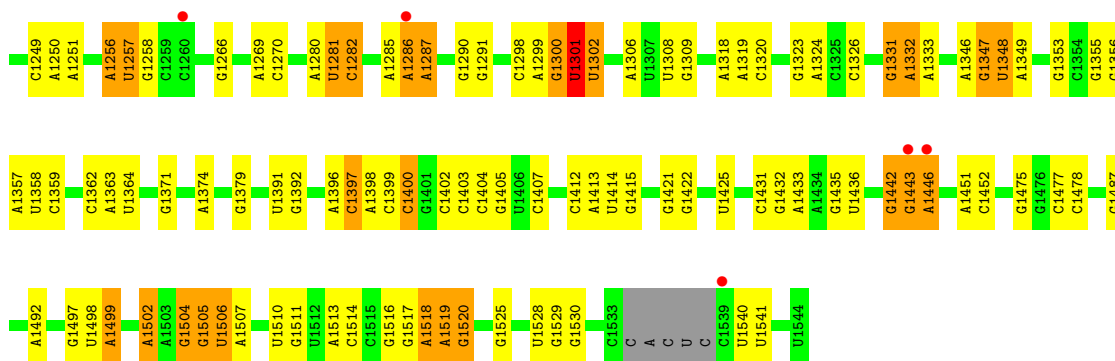
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
27	A	217	Total 217	O 217	0	0
27	D	3	Total 3	O 3	0	0
27	E	5	Total 5	O 5	0	0
27	K	1	Total 1	O 1	0	0
27	L	3	Total 3	O 3	0	0
27	T	1	Total 1	O 1	0	0
27	a	3	Total 3	O 3	0	0

### 3 Residue-property plots

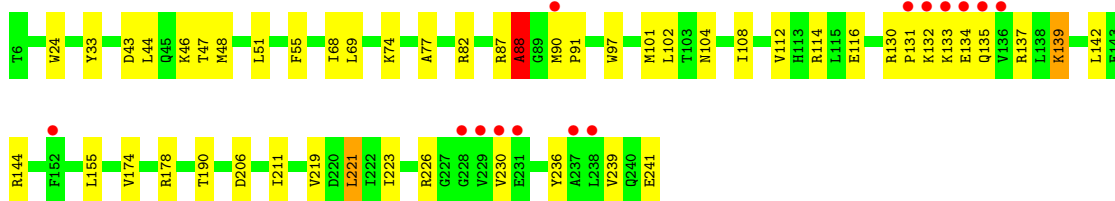
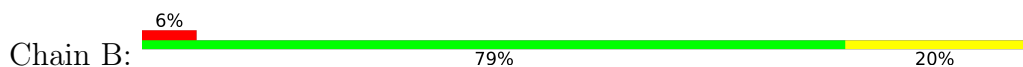
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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 Ribosomal RNA rRNA

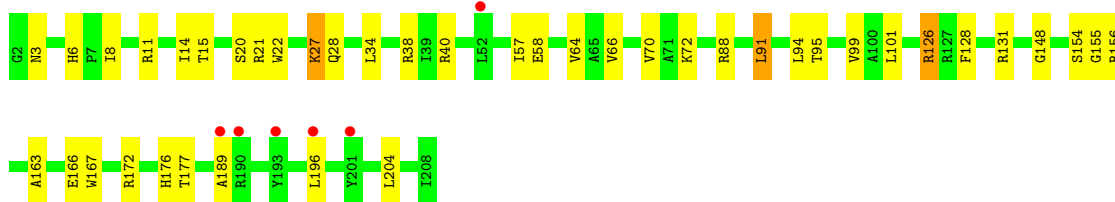
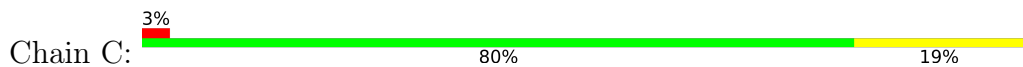




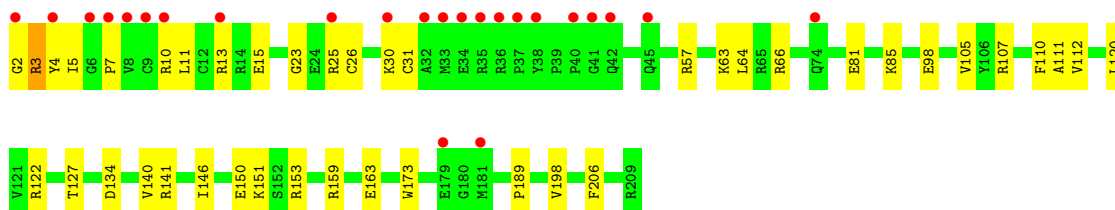
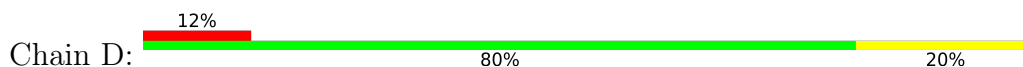
- Molecule 2: 30S ribosomal protein S2



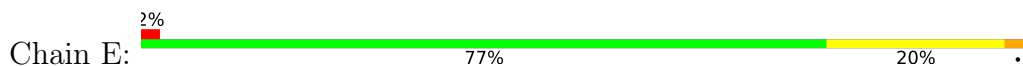
- Molecule 3: 30S ribosomal protein S3



- Molecule 4: 30S ribosomal protein S4

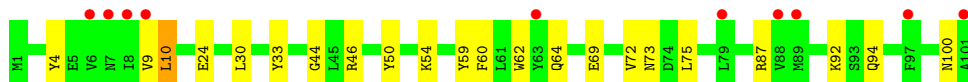
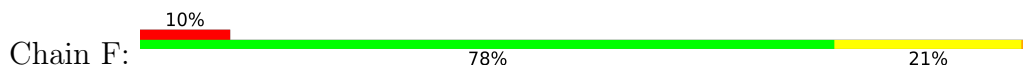


- Molecule 5: 30S ribosomal protein S5

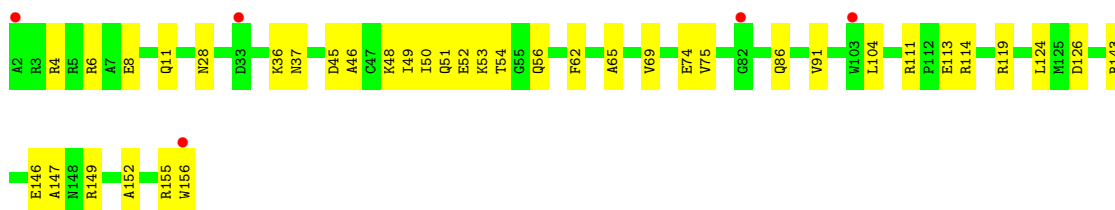
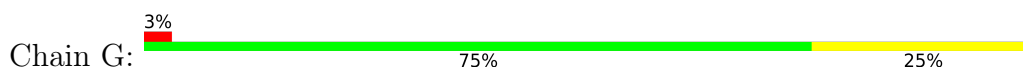




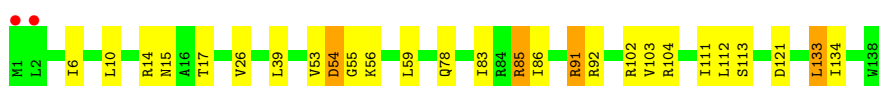
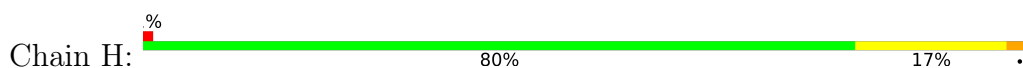
- Molecule 6: 30S ribosomal protein S6



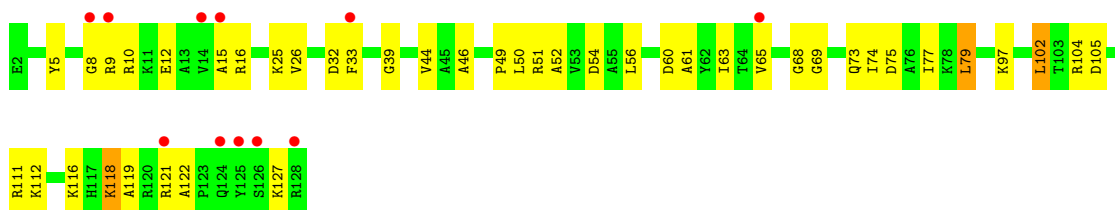
- Molecule 7: 30S ribosomal protein S7



- Molecule 8: 30S ribosomal protein S8



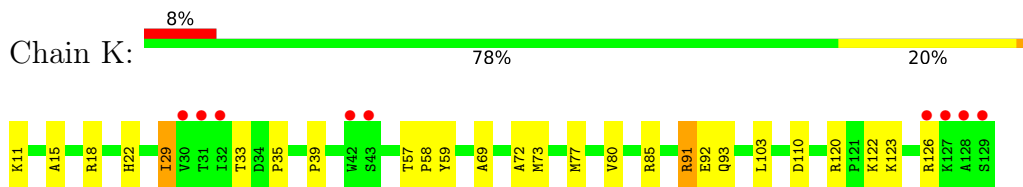
- Molecule 9: 30S ribosomal protein S9



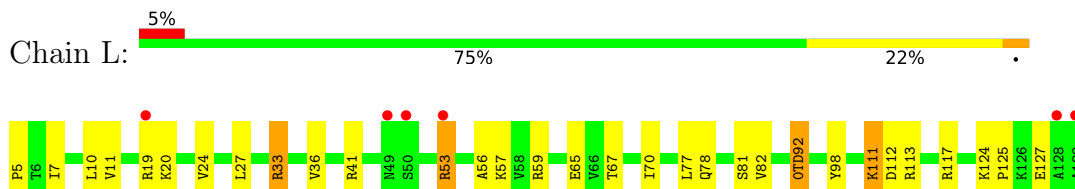
- Molecule 10: 30S ribosomal protein S10



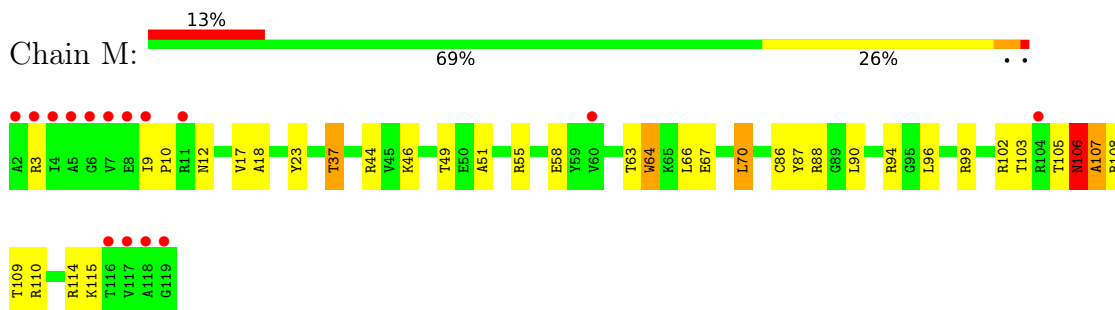
- Molecule 11: 30S ribosomal protein S11



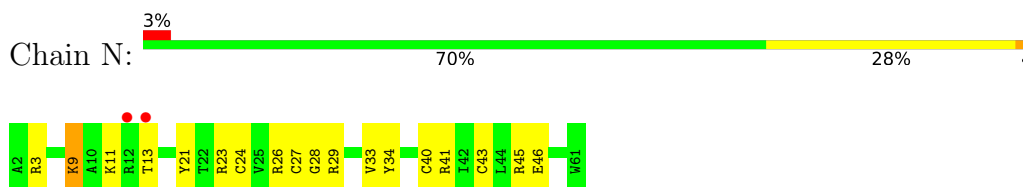
- Molecule 12: 30S ribosomal protein S12



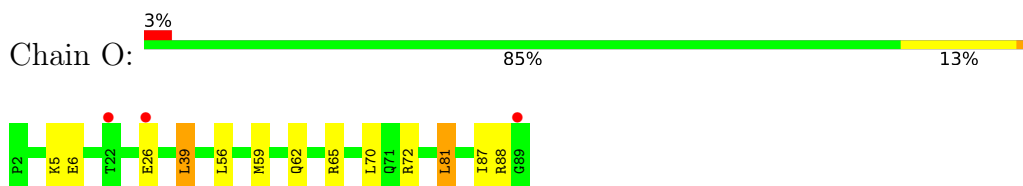
- Molecule 13: 30S ribosomal protein S13



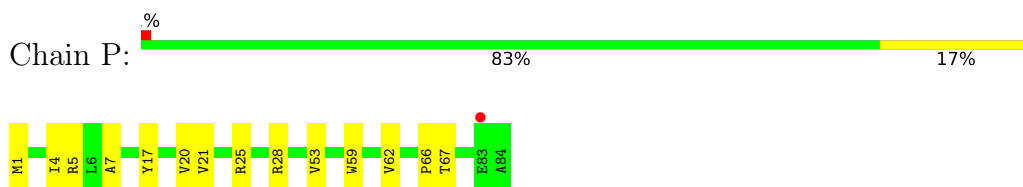
- Molecule 14: 30S ribosomal protein S14 type Z



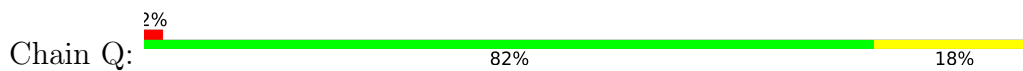
- Molecule 15: 30S ribosomal protein S15



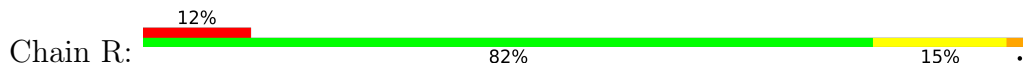
- Molecule 16: 30S ribosomal protein S16



- Molecule 17: 30S ribosomal protein S17



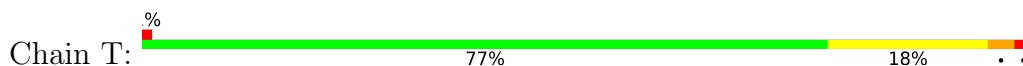
- Molecule 18: 30S ribosomal protein S18



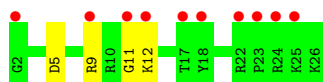
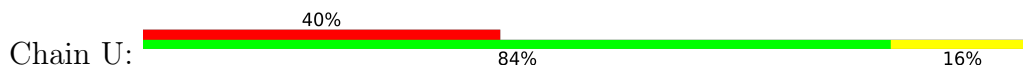
- Molecule 19: 30S ribosomal protein S19



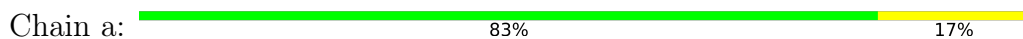
- Molecule 20: 30S ribosomal protein S20



- Molecule 21: 30S ribosomal protein Thx



- Molecule 22: RNA (5'-R(\*AP\*AP\*AP\*UP\*UP\*U)-3')



- Molecule 23: RNA (5'-R(P\*UP\*AP\*GP\*AP\*CP\*UP\*(70U)P\*UP\*UP\*(12A)P\*AP\*(PSU)P\*C P\*UP\*A)-3')



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	400.00Å 400.00Å 173.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.98 – 3.30 39.80 – 2.90	Depositor EDS
% Data completeness (in resolution range)	99.0 (29.98-3.30) 69.4 (39.80-2.90)	Depositor EDS
$R_{merge}$	0.83	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	-0.64 (at 2.90Å)	Xtrriage
Refinement program	PHENIX	Depositor
R, $R_{free}$	0.191 , 0.224 0.193 , 0.223	Depositor DCC
$R_{free}$ test set	2000 reflections (0.67%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	95.7	Xtrriage
Anisotropy	0.165	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.24 , 87.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.28$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	52586	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	162.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.49% of the height of the origin peak. No significant pseudotranslation is detected.*

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

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 12A, ZN, MA6, 70U, K, 0TD, MG, 2MG, 5MC, UR3, 4OC, M2G, 7MG, PSU

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.17	0/36037	0.75	5/56239 (0.0%)
2	B	0.24	0/1909	0.41	0/2579
3	C	0.24	0/1637	0.44	0/2207
4	D	0.24	0/1733	0.40	0/2318
5	E	0.25	0/1163	0.44	0/1566
6	F	0.23	0/856	0.41	0/1154
7	G	0.24	0/1276	0.38	0/1709
8	H	0.24	0/1136	0.43	0/1527
9	I	0.25	0/1029	0.44	0/1379
10	J	0.24	0/806	0.50	0/1084
11	K	0.24	0/900	0.45	0/1213
12	L	0.24	0/978	0.49	0/1308
13	M	0.23	0/947	0.42	0/1270
14	N	0.24	0/501	0.41	0/664
15	O	0.23	0/745	0.38	0/992
16	P	0.23	0/717	0.42	0/965
17	Q	0.23	0/836	0.42	0/1117
18	R	0.24	0/604	0.40	0/801
19	S	0.24	0/662	0.46	0/892
20	T	0.24	0/765	0.39	0/1007
21	U	0.22	0/213	0.40	0/279
22	a	0.17	0/137	0.66	0/211
23	b	0.15	0/276	0.76	1/419 (0.2%)
All	All	0.20	0/55863	0.67	6/82900 (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
2	B	0	1
13	M	0	1
20	T	0	1
23	b	1	0
All	All	1	3

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1301	U	P-O3'-C3'	5.70	126.53	119.70
23	b	29	A	OP1-P-O3'	5.47	117.23	105.20
1	A	1158	C	N1-C2-O2	5.20	122.02	118.90
1	A	328	C	P-O3'-C3'	5.13	125.86	119.70
1	A	181	G	OP2-P-O3'	5.10	116.42	105.20
1	A	1158	C	C2-N1-C1'	5.01	124.31	118.80

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
23	b	37	12A	C1'

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	88	ALA	Peptide
13	M	106	ASN	Peptide
20	T	74	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	32504	0	16434	262	0
2	B	1874	0	1887	26	0
3	C	1613	0	1677	26	0
4	D	1703	0	1763	25	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	E	1147	0	1207	22	0
6	F	843	0	857	14	0
7	G	1257	0	1296	23	0
8	H	1116	0	1177	17	0
9	I	1010	0	1037	31	0
10	J	793	0	835	22	0
11	K	885	0	904	15	0
12	L	973	0	1058	18	0
13	M	937	0	995	19	0
14	N	492	0	529	16	0
15	O	734	0	771	6	0
16	P	701	0	720	7	0
17	Q	823	0	891	10	0
18	R	598	0	670	12	0
19	S	648	0	673	12	0
20	T	763	0	861	13	0
21	U	209	0	221	2	0
22	a	123	0	65	0	0
23	b	330	0	172	0	0
24	A	236	0	0	0	0
24	D	1	0	0	0	0
24	E	1	0	0	0	0
24	F	1	0	0	0	0
24	G	1	0	0	0	0
24	H	2	0	0	0	0
24	L	1	0	0	0	0
24	N	1	0	0	0	0
24	P	3	0	0	0	0
24	Q	2	0	0	0	0
24	S	3	0	0	0	0
24	T	1	0	0	0	0
25	A	22	0	0	0	0
26	D	1	0	0	0	0
26	N	1	0	0	0	0
27	A	217	0	0	2	0
27	D	3	0	0	1	0
27	E	5	0	0	0	0
27	K	1	0	0	1	0
27	L	3	0	0	0	0
27	T	1	0	0	0	0
27	a	3	0	0	0	0
All	All	52586	0	36700	522	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

All (522) 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)
2:B:223:ILE:HD13	2:B:230:VAL:H	1.50	0.77
1:A:1266:G:N2	1:A:1269:A:OP2	2.19	0.75
1:A:1281:U:H5''	1:A:1282:C:H5	1.54	0.72
1:A:1347:G:O6	9:I:10:ARG:NH2	2.23	0.72
5:E:80:ILE:HD12	5:E:138:ALA:HB1	1.71	0.71
1:A:1422:G:H1	1:A:1478:C:H42	1.39	0.71
6:F:9:VAL:HB	6:F:87:ARG:HB2	1.73	0.71
13:M:10:PRO:HB2	13:M:18:ALA:HB1	1.70	0.70
6:F:10:LEU:HD12	6:F:59:TYR:HB3	1.74	0.70
1:A:501:C:OP1	12:L:117:ARG:NH2	2.25	0.70
16:P:4:ILE:HG12	16:P:21:VAL:HG22	1.72	0.70
12:L:57:LYS:HG2	12:L:67:THR:HG22	1.73	0.69
1:A:975:A:H4'	1:A:976:G:H5''	1.74	0.69
7:G:143:ARG:O	7:G:147:ALA:HB2	1.92	0.69
10:J:8:LEU:O	10:J:69:ASN:HA	1.92	0.68
1:A:664:G:H22	1:A:741:G:H1	1.40	0.68
3:C:189:ALA:HB3	3:C:196:LEU:HB2	1.76	0.68
9:I:112:LYS:HA	9:I:119:ALA:HB2	1.76	0.67
9:I:46:ALA:HB2	9:I:74:ILE:HG23	1.77	0.67
3:C:131:ARG:HH11	3:C:166:GLU:HG3	1.60	0.67
8:H:10:LEU:HD22	8:H:83:ILE:HD11	1.77	0.67
3:C:14:ILE:HG22	3:C:15:THR:HG23	1.76	0.66
7:G:113:GLU:HB2	7:G:119:ARG:HG3	1.77	0.66
2:B:134:GLU:HG2	2:B:137:ARG:HH21	1.59	0.66
1:A:1073:U:O2	2:B:104:ASN:ND2	2.28	0.66
20:T:74:LYS:O	20:T:76:ALA:N	2.27	0.66
11:K:15:ALA:HA	11:K:77:MET:HA	1.76	0.65
12:L:53:ARG:NH1	12:L:92:OTD:OD2	2.29	0.65
1:A:1505:G:O2'	1:A:1506:U:OP2	2.13	0.65
5:E:80:ILE:HG13	5:E:91:LEU:HB2	1.79	0.65
1:A:1030(A):G:N2	1:A:1030(D):A:OP2	2.30	0.65
1:A:1326:C:OP1	21:U:12:LYS:NZ	2.30	0.65
19:S:50:ALA:HB1	19:S:57:HIS:HB3	1.78	0.65
2:B:77:ALA:HB2	2:B:211:ILE:HD13	1.79	0.64
1:A:1124:G:N7	1:A:1145:C:O2'	2.28	0.64
1:A:235:C:N4	27:A:1902:HOH:O	2.30	0.64
9:I:15:ALA:HB2	9:I:65:VAL:HG13	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:123:LYS:HA	11:K:126:ARG:HG3	1.79	0.63
4:D:141:ARG:NH2	27:D:401:HOH:O	2.32	0.63
1:A:316:G:OP2	1:A:351:G:O2'	2.16	0.62
1:A:427:U:OP1	4:D:13:ARG:NH2	2.32	0.62
1:A:976:G:OP2	1:A:1358:U:O2'	2.17	0.62
1:A:564:C:O2'	8:H:91:ARG:NH2	2.32	0.62
5:E:140:ARG:O	5:E:143:ARG:NH2	2.32	0.62
1:A:811:C:O2'	1:A:901:A:N1	2.32	0.62
1:A:1443:G:H4'	1:A:1446:A:O5'	1.99	0.62
13:M:23:TYR:HB3	13:M:67:GLU:HG2	1.83	0.61
2:B:174:VAL:O	2:B:178:ARG:HG2	1.99	0.61
1:A:542:G:OP1	4:D:10:ARG:NH2	2.33	0.61
13:M:108:ARG:HD2	13:M:114:ARG:HE	1.66	0.61
3:C:156:ARG:H	3:C:163:ALA:HA	1.66	0.60
9:I:10:ARG:HG2	9:I:75:ASP:HB2	1.83	0.60
1:A:1405:G:O2'	1:A:1518:MA6:O2'	2.19	0.60
1:A:579:G:H5'	1:A:728:A:H1'	1.83	0.60
11:K:122:LYS:NZ	27:K:201:HOH:O	2.34	0.60
1:A:266:G:H5'	1:A:268:C:H41	1.65	0.60
1:A:509:A:N3	1:A:543:C:O2'	2.31	0.60
3:C:6:HIS:HD2	3:C:8:ILE:H	1.49	0.60
7:G:111:ARG:NH2	7:G:126:ASP:OD2	2.35	0.60
2:B:74:LYS:NZ	2:B:206:ASP:OD1	2.32	0.59
8:H:53:VAL:HG12	8:H:54:ASP:H	1.66	0.59
1:A:1391:U:H2'	1:A:1392:G:C8	2.37	0.59
5:E:79:GLU:HG3	5:E:93:PRO:HD2	1.84	0.59
9:I:51:ARG:HG3	9:I:56:LEU:HD21	1.83	0.59
15:O:39:LEU:HD13	15:O:56:LEU:HB2	1.85	0.59
3:C:27:LYS:HD3	3:C:27:LYS:H	1.67	0.59
5:E:102:ALA:HB1	5:E:106:PRO:HG2	1.85	0.59
1:A:335:C:O2'	1:A:1433:A:N3	2.34	0.59
1:A:537:G:OP1	12:L:113:ARG:NH2	2.29	0.59
5:E:102:ALA:O	5:E:107:ARG:NH1	2.35	0.58
11:K:22:HIS:HB3	11:K:29:ILE:HG23	1.84	0.58
7:G:143:ARG:O	7:G:147:ALA:CB	2.50	0.58
1:A:413:G:N2	1:A:429:U:OP2	2.36	0.58
3:C:11:ARG:NH1	3:C:177:THR:O	2.37	0.58
10:J:48:THR:O	14:N:34:TYR:OH	2.22	0.58
1:A:558:G:OP2	1:A:559:A:O2'	2.22	0.58
5:E:88:LYS:HB3	5:E:123:LEU:HB2	1.86	0.58
1:A:362:G:N2	1:A:365:U:OP2	2.36	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:33:VAL:HG22	5:E:43:LEU:HD23	1.85	0.58
1:A:1349:A:OP2	9:I:118:LYS:NZ	2.37	0.58
10:J:8:LEU:HB2	10:J:70:ARG:HB2	1.85	0.57
20:T:75:ASN:N	20:T:75:ASN:OD1	2.36	0.57
10:J:26:ALA:O	10:J:84:GLN:NE2	2.38	0.57
10:J:19:SER:HB3	10:J:91:PRO:HG3	1.85	0.57
18:R:26:LEU:HD21	18:R:39:VAL:HG23	1.86	0.57
18:R:48:GLY:O	18:R:74:ARG:NH2	2.37	0.57
20:T:30:LYS:HE3	20:T:72:LEU:HD23	1.87	0.57
10:J:49:VAL:HG23	14:N:41:ARG:HB2	1.87	0.57
14:N:26:ARG:NH2	14:N:46:GLU:OE1	2.37	0.57
3:C:70:VAL:HG12	3:C:72:LYS:H	1.70	0.56
18:R:32:ARG:HA	18:R:69:THR:HG21	1.86	0.56
4:D:7:PRO:HB2	4:D:10:ARG:HD2	1.86	0.56
10:J:40:LEU:HB3	10:J:69:ASN:HB2	1.86	0.56
1:A:1137:C:H4'	1:A:1138:G:C2	2.40	0.56
2:B:48:MET:HA	2:B:51:LEU:HB2	1.87	0.56
1:A:376:G:H5''	16:P:5:ARG:HB2	1.87	0.56
1:A:390:C:O3'	16:P:28:ARG:NH2	2.39	0.56
1:A:1179:A:O2'	1:A:1180:A:OP1	2.23	0.56
12:L:41:ARG:HE	12:L:57:LYS:HE2	1.71	0.55
13:M:49:THR:HG22	13:M:51:ALA:H	1.71	0.55
1:A:250:A:H4'	1:A:251:G:O5'	2.06	0.55
9:I:44:VAL:HG12	9:I:51:ARG:HH22	1.71	0.55
1:A:1026:G:H3'	1:A:1027:C:H5''	1.89	0.55
15:O:62:GLN:OE1	15:O:65:ARG:NH2	2.39	0.55
1:A:1510:U:H2'	1:A:1511:G:C8	2.41	0.55
1:A:559:A:OP1	5:E:126:ARG:NH2	2.36	0.55
14:N:11:LYS:HG3	14:N:13:THR:H	1.72	0.55
1:A:1301:U:HO2'	1:A:1302:U:P	2.29	0.55
1:A:1498:UR3:H1'	1:A:1499:A:OP2	2.06	0.55
20:T:92:LEU:O	20:T:96:GLY:N	2.34	0.55
1:A:110:C:O2'	16:P:25:ARG:O	2.22	0.55
1:A:1049:U:H4'	1:A:1050:G:O5'	2.06	0.54
2:B:88:ALA:HB1	2:B:226:ARG:HH21	1.72	0.54
1:A:28:G:O2'	1:A:296:U:OP1	2.23	0.54
3:C:91:LEU:HD21	3:C:99:VAL:HG22	1.88	0.54
8:H:113:SER:HB2	8:H:134:ILE:HD11	1.89	0.54
9:I:116:LYS:HD2	9:I:122:ALA:HA	1.88	0.54
1:A:1080:A:H5''	5:E:16:THR:HG21	1.89	0.54
1:A:1399:C:H4'	1:A:1400:5MC:H5''	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1301:U:O2'	1:A:1302:U:O5'	2.25	0.54
1:A:1031:G:H2'	1:A:1032:G:C8	2.42	0.53
7:G:75:VAL:HG21	7:G:86:GLN:HB3	1.90	0.53
1:A:1226:C:OP2	13:M:103:THR:OG1	2.18	0.53
8:H:17:THR:O	8:H:78:GLN:NE2	2.37	0.53
7:G:152:ALA:O	7:G:155:ARG:NH1	2.41	0.53
9:I:32:ASP:OD1	9:I:33:PHE:N	2.41	0.53
1:A:946:A:H2'	1:A:947:G:C8	2.44	0.53
4:D:26:CYS:HA	4:D:31:CYS:HB2	1.90	0.53
1:A:1031:G:H2'	1:A:1032:G:H8	1.74	0.53
1:A:708:C:OP1	11:K:85:ARG:NH2	2.42	0.53
7:G:146:GLU:HA	7:G:149:ARG:HG2	1.89	0.53
1:A:1122:U:O4	1:A:1123:A:N6	2.42	0.53
19:S:12:ASP:HB2	19:S:38:SER:HB3	1.91	0.53
1:A:1128:C:H42	1:A:1143:G:H1	1.56	0.52
2:B:55:PHE:HD2	2:B:221:LEU:HG	1.74	0.52
19:S:55:LYS:HG2	19:S:56:GLN:HG3	1.91	0.52
8:H:112:LEU:HD23	8:H:133:LEU:HA	1.91	0.52
9:I:26:VAL:HG13	9:I:61:ALA:HB3	1.90	0.52
18:R:21:LYS:O	18:R:25:THR:OG1	2.22	0.52
7:G:54:THR:HG22	7:G:56:GLN:H	1.73	0.52
4:D:11:LEU:HD13	4:D:66:ARG:HD3	1.91	0.52
1:A:1309:G:N7	13:M:99:ARG:NH2	2.57	0.52
1:A:652:U:O4	1:A:752:G:O2'	2.22	0.52
1:A:401:C:H2'	1:A:402:G:H8	1.75	0.52
1:A:45:U:H2'	1:A:46:G:C8	2.44	0.52
1:A:1048:G:H5''	14:N:3:ARG:HG3	1.92	0.52
11:K:72:ALA:HB1	11:K:77:MET:HE2	1.91	0.52
1:A:372:C:H4'	1:A:373:A:O5'	2.09	0.52
4:D:63:LYS:HD2	4:D:198:VAL:HG22	1.92	0.52
1:A:1004:A:OP1	1:A:1025:U:N3	2.44	0.51
1:A:951:G:OP2	13:M:102:ARG:NH2	2.43	0.51
6:F:94:GLN:HB3	18:R:32:ARG:HH11	1.75	0.51
13:M:86:CYS:SG	13:M:87:TYR:N	2.83	0.51
17:Q:22:LEU:HD11	17:Q:39:SER:HB2	1.92	0.51
1:A:337:C:H2'	1:A:338:A:C8	2.45	0.51
1:A:60:A:H4'	1:A:61:G:O5'	2.10	0.51
1:A:243:A:H4'	1:A:244:U:H5'	1.93	0.51
10:J:82:ILE:HA	10:J:85:LEU:HB2	1.92	0.51
2:B:112:VAL:O	2:B:116:GLU:HG2	2.11	0.50
2:B:239:VAL:O	2:B:241:GLU:N	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1059:C:O3'	14:N:45:ARG:NH2	2.44	0.50
1:A:1250:A:H4'	9:I:68:GLY:N	2.26	0.50
17:Q:21:VAL:HG21	17:Q:59:ILE:HD11	1.94	0.50
1:A:1392:G:N2	1:A:1502:A:H8	2.08	0.50
1:A:1319:A:H5'	19:S:5:LEU:HD22	1.93	0.50
1:A:776:G:N2	1:A:802:A:OP2	2.40	0.50
1:A:1057:G:H5''	3:C:154:SER:HB2	1.93	0.50
1:A:685:G:N2	1:A:704:A:OP2	2.42	0.50
1:A:1414:U:H2'	1:A:1415:G:H8	1.77	0.50
1:A:967:5MC:H5''	1:A:968:A:OP2	2.11	0.50
11:K:57:THR:HG22	11:K:59:TYR:H	1.77	0.50
14:N:23:ARG:NH1	14:N:28:GLY:O	2.45	0.50
1:A:890:G:O2'	1:A:906:G:O6	2.24	0.50
1:A:56:U:H2'	1:A:57:G:C8	2.47	0.50
9:I:65:VAL:HG11	9:I:73:GLN:HB3	1.92	0.50
19:S:33:THR:HG22	19:S:35:SER:H	1.75	0.50
1:A:1402:4OC:H2'	1:A:1403:C:O4'	2.11	0.50
1:A:352:C:O2'	1:A:354:G:OP1	2.26	0.49
9:I:16:ARG:O	9:I:63:ILE:HA	2.12	0.49
13:M:37:THR:HG22	13:M:55:ARG:HD2	1.94	0.49
13:M:88:ARG:HH11	19:S:3:ARG:HH21	1.60	0.49
1:A:1035:A:H2'	1:A:1036:G:H8	1.76	0.49
1:A:298:A:N6	27:A:1903:HOH:O	2.31	0.49
1:A:1207:2MG:HM23	1:A:1208:C:H1'	1.95	0.49
12:L:124:LYS:HD3	12:L:125:PRO:HD2	1.93	0.49
14:N:9:LYS:HE2	14:N:23:ARG:HB2	1.94	0.49
1:A:192:U:H1'	20:T:103:GLY:HA2	1.93	0.49
2:B:87:ARG:HH21	2:B:219:VAL:HB	1.76	0.49
1:A:1240:U:OP1	7:G:119:ARG:NH1	2.45	0.49
1:A:1435:G:H2'	1:A:1436:U:C6	2.47	0.49
5:E:45:PHE:CE2	5:E:47:LYS:HD2	2.48	0.49
12:L:56:ALA:HB2	12:L:70:ILE:HD11	1.94	0.49
18:R:47:THR:HA	18:R:83:GLU:HB2	1.95	0.49
1:A:1504:G:OP1	1:A:1507:A:H4'	2.12	0.49
3:C:64:VAL:HG23	3:C:99:VAL:HG11	1.94	0.49
1:A:1128:C:HO2'	1:A:1130:A:H8	1.59	0.49
9:I:97:LYS:HA	9:I:102:LEU:HD11	1.94	0.49
1:A:1152:A:OP1	10:J:68:HIS:ND1	2.46	0.49
1:A:1035:A:H2'	1:A:1036:G:C8	2.47	0.49
11:K:80:VAL:HG11	11:K:103:LEU:HD13	1.95	0.49
13:M:12:ASN:OD1	13:M:46:LYS:NZ	2.41	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:235:C:H5'	17:Q:70:ARG:HG2	1.94	0.49
1:A:1256:A:HO2'	1:A:1257:U:P	2.35	0.49
1:A:356:A:N3	1:A:368:U:O2'	2.36	0.49
1:A:372:C:H1'	1:A:373:A:OP2	2.13	0.49
2:B:33:TYR:HB2	2:B:43:ASP:HA	1.94	0.49
1:A:1412:C:H2'	1:A:1413:A:C8	2.47	0.48
3:C:38:ARG:HB3	3:C:94:LEU:HD21	1.95	0.48
19:S:50:ALA:HA	19:S:58:VAL:O	2.13	0.48
1:A:1396:A:H4'	1:A:1397:C:H5''	1.94	0.48
1:A:1405:G:HO2'	1:A:1518:MA6:HO2'	1.49	0.48
1:A:1291:G:H4'	9:I:39:GLY:HA3	1.95	0.48
1:A:1147:C:HO2'	9:I:5:TYR:HH	1.61	0.48
1:A:337:C:H2'	1:A:338:A:H8	1.77	0.48
1:A:875:C:O2'	8:H:14:ARG:NH1	2.47	0.48
1:A:578:C:O2'	1:A:728:A:N3	2.39	0.48
1:A:754:C:OP1	15:O:72:ARG:NH1	2.35	0.48
1:A:973:G:H3'	1:A:974:A:H5''	1.95	0.48
4:D:64:LEU:HB2	4:D:198:VAL:HG11	1.94	0.48
1:A:1109:C:OP2	3:C:176:HIS:ND1	2.45	0.48
9:I:49:PRO:O	9:I:52:ALA:HB3	2.14	0.48
14:N:24:CYS:SG	14:N:40:CYS:N	2.86	0.48
1:A:1402:4OC:HM22	1:A:1403:C:H5'	1.95	0.48
11:K:58:PRO:HB2	11:K:93:GLN:HG3	1.96	0.48
13:M:63:THR:HG23	13:M:64:TRP:CD2	2.49	0.48
1:A:1151:A:H5'	10:J:41:PRO:HA	1.95	0.48
1:A:7:G:H5'	1:A:298:A:O4'	2.14	0.48
8:H:103:VAL:HG12	8:H:104:ARG:HG2	1.95	0.48
1:A:190(L):U:O2	20:T:105:SER:OG	2.25	0.47
1:A:1106:G:H5''	3:C:172:ARG:HG2	1.96	0.47
1:A:559:A:P	5:E:126:ARG:HH22	2.36	0.47
4:D:57:ARG:HB3	4:D:206:PHE:HB2	1.96	0.47
20:T:10:LEU:HG	20:T:12:ALA:H	1.79	0.47
1:A:413:G:H1'	1:A:428:G:N2	2.30	0.47
2:B:130:ARG:HD3	2:B:130:ARG:HA	1.62	0.47
4:D:4:TYR:CG	4:D:4:TYR:O	2.67	0.47
7:G:46:ALA:O	7:G:50:ILE:HG12	2.13	0.47
15:O:26:GLU:HA	15:O:81:LEU:HD11	1.96	0.47
1:A:324:G:N1	1:A:327:A:OP2	2.46	0.47
1:A:501:C:H2'	1:A:502:G:C8	2.49	0.47
8:H:6:ILE:O	8:H:10:LEU:HG	2.14	0.47
8:H:121:ASP:N	8:H:121:ASP:OD1	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1371:G:O3'	9:I:69:GLY:HA3	2.13	0.47
1:A:1218:C:H2'	1:A:1219:U:C6	2.49	0.47
4:D:105:VAL:HG13	4:D:110:PHE:HB2	1.97	0.47
20:T:26:ASN:OD1	20:T:71:THR:OG1	2.26	0.47
1:A:947:G:H4'	1:A:1332:A:H2	1.78	0.47
7:G:111:ARG:HB2	7:G:119:ARG:HG2	1.96	0.47
10:J:15:THR:HG22	10:J:91:PRO:HB3	1.96	0.47
1:A:1001:A:H2'	1:A:1002:G:C8	2.49	0.47
1:A:1065:U:H1'	1:A:1066:C:OP2	2.15	0.47
1:A:1301:U:H1'	1:A:1302:U:OP1	2.14	0.47
1:A:1477:C:H2'	1:A:1478:C:C6	2.50	0.47
3:C:64:VAL:HB	3:C:99:VAL:HG21	1.95	0.47
5:E:142:LEU:O	5:E:143:ARG:NE	2.45	0.47
1:A:1132:C:H2'	1:A:1133:G:H8	1.80	0.47
1:A:1298:C:H4'	1:A:1299:A:C4	2.50	0.47
1:A:67:C:H2'	1:A:68:G:C8	2.49	0.47
6:F:44:GLY:HA2	6:F:59:TYR:CZ	2.50	0.47
1:A:1034:G:H2'	1:A:1035:A:C8	2.50	0.47
1:A:1425:U:H3	1:A:1475:G:H1	1.60	0.47
1:A:969:A:OP1	10:J:55:LYS:NZ	2.36	0.47
17:Q:83:ASP:N	17:Q:83:ASP:OD1	2.48	0.47
1:A:1020:U:H2'	1:A:1021:G:H8	1.79	0.47
5:E:76:ILE:O	5:E:93:PRO:HB3	2.14	0.47
5:E:81:GLU:HG2	5:E:88:LYS:HE2	1.96	0.47
13:M:90:LEU:O	13:M:94:ARG:HG2	2.14	0.47
1:A:1499:A:H1'	1:A:1520:G:H5'	1.97	0.46
10:J:57:LYS:HE2	10:J:60:ARG:NH2	2.30	0.46
1:A:1451:A:H5''	1:A:1452:C:H5	1.79	0.46
1:A:21:G:H2'	1:A:22:G:C8	2.50	0.46
1:A:59:A:H5''	1:A:387:U:H5''	1.97	0.46
1:A:1123:A:H4'	10:J:36:GLY:HA3	1.98	0.46
1:A:1065:U:H4'	1:A:1066:C:O5'	2.15	0.46
1:A:1518:MA6:H93	1:A:1519:MA6:H92	1.97	0.46
2:B:97:TRP:H22	2:B:102:LEU:HD13	1.79	0.46
13:M:96:LEU:O	13:M:110:ARG:NH1	2.48	0.46
15:O:87:ILE:HG22	15:O:88:ARG:H	1.79	0.46
18:R:47:THR:HG22	18:R:83:GLU:H	1.80	0.46
1:A:1148:U:H2'	1:A:1149:C:O4'	2.15	0.46
1:A:740:U:H2'	1:A:741:G:H8	1.80	0.46
1:A:619:U:N3	4:D:134:ASP:OD1	2.44	0.46
6:F:33:TYR:HB2	6:F:75:LEU:HD12	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:344:A:H5'	1:A:345:C:C5	2.50	0.46
1:A:1525:G:OP1	11:K:120:ARG:NH2	2.48	0.46
12:L:36:VAL:HG22	12:L:82:VAL:HG22	1.96	0.46
1:A:946:A:O2'	1:A:1333:A:N3	2.42	0.46
1:A:1502:A:H2	1:A:1505:G:H1	1.63	0.46
1:A:757:U:H2'	1:A:758:G:O4'	2.16	0.46
19:S:23:ASN:OD1	19:S:47:HIS:NE2	2.41	0.46
1:A:1306:A:H61	1:A:1331:G:H1'	1.80	0.46
1:A:184:G:H2'	1:A:185:A:H8	1.80	0.46
1:A:677:U:H3	1:A:713:G:H22	1.62	0.46
10:J:90:LEU:N	10:J:91:PRO:HD2	2.31	0.46
14:N:24:CYS:HB3	14:N:29:ARG:H	1.81	0.46
1:A:390:C:H2'	1:A:391:G:C8	2.51	0.46
1:A:689:C:H2'	1:A:690:G:O4'	2.16	0.46
4:D:98:GLU:OE2	4:D:107:ARG:NE	2.45	0.46
5:E:79:GLU:HG2	5:E:92:LYS:HG3	1.98	0.46
16:P:7:ALA:O	16:P:17:TYR:HA	2.16	0.46
1:A:103:C:OP1	20:T:17:ARG:NH1	2.49	0.46
1:A:539:A:H2'	1:A:540:G:C8	2.51	0.45
7:G:74:GLU:HG2	7:G:91:VAL:HG22	1.96	0.45
1:A:1286:A:H2'	1:A:1287:A:H4'	1.98	0.45
1:A:186:C:H2'	1:A:187:C:C6	2.51	0.45
7:G:45:ASP:O	7:G:49:ILE:HG13	2.15	0.45
7:G:65:ALA:O	7:G:69:VAL:HG23	2.16	0.45
8:H:86:ILE:HD12	8:H:133:LEU:HD22	1.99	0.45
11:K:69:ALA:O	11:K:73:MET:HG2	2.15	0.45
1:A:405:U:O4	4:D:2:GLY:HA2	2.16	0.45
7:G:152:ALA:HB1	7:G:155:ARG:HH12	1.81	0.45
9:I:8:GLY:HA2	9:I:79:LEU:HD13	1.98	0.45
11:K:18:ARG:NH1	11:K:35:PRO:O	2.50	0.45
1:A:580:U:H2'	1:A:581:G:O4'	2.15	0.45
1:A:1034:G:H2'	1:A:1035:A:H8	1.80	0.45
1:A:1355:G:H2'	1:A:1356:G:C8	2.51	0.45
1:A:701:C:H4'	1:A:702:A:O5'	2.16	0.45
3:C:126:ARG:HE	3:C:128:PHE:HD1	1.64	0.45
6:F:46:ARG:HB2	6:F:60:PHE:CE2	2.52	0.45
7:G:69:VAL:HG21	7:G:104:LEU:HD21	1.99	0.45
1:A:1391:U:H2'	1:A:1392:G:H8	1.79	0.45
4:D:3:ARG:CZ	4:D:5:ILE:HD11	2.47	0.45
5:E:81:GLU:HG3	5:E:90:VAL:HG22	1.99	0.45
6:F:30:LEU:HD23	6:F:75:LEU:HD11	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:3:ARG:HA	13:M:9:ILE:HG13	1.98	0.45
20:T:63:ILE:HG21	20:T:81:LYS:HG3	1.98	0.45
1:A:1177:G:O5'	9:I:97:LYS:NZ	2.47	0.45
1:A:653:A:C8	8:H:56:LYS:HG2	2.52	0.45
1:A:272:C:H2'	1:A:273:A:H8	1.82	0.45
1:A:514:C:H2'	1:A:515:G:H8	1.82	0.45
1:A:959:A:HO2'	1:A:984:C:HO2'	1.63	0.45
5:E:90:VAL:O	5:E:120:THR:HA	2.17	0.45
8:H:111:ILE:HG22	8:H:134:ILE:HD12	1.99	0.45
1:A:1300:G:O2'	1:A:1301:U:O5'	2.33	0.44
1:A:17:U:H2'	1:A:18:C:C6	2.52	0.44
1:A:204:U:H4'	1:A:216:G:C8	2.53	0.44
1:A:272:C:H2'	1:A:273:A:C8	2.53	0.44
1:A:380:G:N2	1:A:383:A:OP2	2.36	0.44
1:A:769:G:H4'	1:A:1513:A:H4'	1.99	0.44
3:C:88:ARG:HE	3:C:101:LEU:HB3	1.82	0.44
1:A:1003:G:H2'	1:A:1003(A):G:C8	2.52	0.44
1:A:1010:G:H2'	1:A:1011:G:H8	1.81	0.44
14:N:9:LYS:HD3	14:N:21:TYR:O	2.18	0.44
1:A:1308:U:H2'	1:A:1309:G:C8	2.52	0.44
1:A:560:U:H5'	1:A:566:G:N2	2.31	0.44
10:J:40:LEU:HA	10:J:40:LEU:HD23	1.85	0.44
1:A:269:C:H2'	1:A:270:A:C8	2.52	0.44
4:D:151:LYS:H	4:D:151:LYS:HD2	1.80	0.44
1:A:1323:G:H2'	1:A:1324:A:C8	2.53	0.44
1:A:1356:G:H2'	1:A:1357:A:C8	2.52	0.44
1:A:328:C:H4'	1:A:329:A:O5'	2.18	0.44
1:A:401:C:H2'	1:A:402:G:C8	2.52	0.44
9:I:25:LYS:N	9:I:60:ASP:OD1	2.47	0.44
9:I:50:LEU:O	9:I:54:ASP:N	2.51	0.44
11:K:33:THR:HA	11:K:39:PRO:HA	1.99	0.44
1:A:737:A:N3	6:F:73:ASN:ND2	2.53	0.44
1:A:1505:G:HO2'	1:A:1506:U:P	2.39	0.43
4:D:150:GLU:HG3	4:D:153:ARG:NH1	2.32	0.43
1:A:932:C:H4'	7:G:4:ARG:NH2	2.33	0.43
17:Q:68:ARG:HG3	17:Q:68:ARG:O	2.17	0.43
1:A:1347:G:O2'	1:A:1348:U:P	2.76	0.43
1:A:335:C:H2'	1:A:336:C:C6	2.53	0.43
19:S:28:LYS:HG2	19:S:29:ARG:H	1.83	0.43
20:T:72:LEU:HA	20:T:72:LEU:HD22	1.79	0.43
1:A:1172:C:H2'	1:A:1173:G:H8	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:88:ALA:HB1	2:B:226:ARG:NH2	2.33	0.43
3:C:155:GLY:HA3	3:C:163:ALA:HB1	2.00	0.43
1:A:826:C:O2	8:H:15:ASN:ND2	2.51	0.43
1:A:1049:U:O2'	14:N:3:ARG:NH1	2.51	0.43
6:F:4:TYR:CE2	6:F:92:LYS:HG2	2.53	0.43
8:H:53:VAL:O	8:H:55:GLY:N	2.51	0.43
14:N:26:ARG:HE	14:N:43:CYS:HB3	1.83	0.43
4:D:111:ALA:HB2	4:D:120:LEU:HD12	2.00	0.43
6:F:4:TYR:CZ	6:F:72:VAL:HG21	2.53	0.43
10:J:38:ILE:HB	10:J:71:LEU:HB3	2.00	0.43
14:N:9:LYS:HE3	14:N:9:LYS:HB3	1.77	0.43
1:A:1346:A:N1	1:A:1374:A:H5''	2.34	0.43
1:A:1442:G:O6	1:A:1446:A:N6	2.52	0.43
1:A:142:G:H2'	1:A:143:A:C8	2.54	0.43
1:A:674:G:H2'	1:A:675:A:C8	2.54	0.43
1:A:991:U:O4	1:A:1212:U:O2'	2.25	0.43
11:K:110:ASP:OD2	18:R:88:LYS:NZ	2.50	0.43
12:L:111:LYS:HE3	12:L:112:ASP:H	1.84	0.43
1:A:976:G:H5'	1:A:1358:U:O2'	2.18	0.43
1:A:35:G:H2'	1:A:36:C:C6	2.54	0.43
4:D:23:GLY:HA3	4:D:112:VAL:HG22	1.99	0.43
9:I:10:ARG:HD3	9:I:105:ASP:HB3	2.00	0.43
10:J:66:ARG:HD3	10:J:68:HIS:CE1	2.54	0.43
21:U:5:ASP:O	21:U:11:GLY:HA3	2.17	0.43
1:A:1431:C:H2'	1:A:1432:G:O4'	2.18	0.43
1:A:1513:A:H2'	1:A:1514:C:C6	2.53	0.43
1:A:190(K):G:H2'	1:A:190(L):U:C6	2.53	0.43
1:A:401:C:O2'	1:A:621:A:N3	2.42	0.43
1:A:765:G:N2	1:A:813:U:OP2	2.52	0.43
1:A:90:U:H2'	1:A:91:C:C6	2.54	0.43
2:B:43:ASP:O	2:B:47:THR:OG1	2.35	0.43
9:I:127:LYS:HB3	9:I:127:LYS:HE3	1.84	0.43
1:A:191:G:N2	20:T:103:GLY:O	2.35	0.43
5:E:99:GLY:N	5:E:117:ASP:OD2	2.44	0.43
10:J:51:ARG:CZ	10:J:61:GLU:HG3	2.49	0.43
1:A:190(D):U:O2'	1:A:190(E):U:H5'	2.18	0.42
1:A:514:C:H2'	1:A:515:G:C8	2.54	0.42
1:A:974:A:OP2	14:N:29:ARG:NH2	2.52	0.42
2:B:101:MET:HA	2:B:108:ILE:HG13	2.01	0.42
2:B:68:ILE:O	2:B:90:MET:HB3	2.19	0.42
9:I:69:GLY:O	9:I:73:GLN:HG3	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:6:ILE:HB	8:H:85:ARG:HH12	1.83	0.42
2:B:44:LEU:H	2:B:44:LEU:HD12	1.83	0.42
1:A:1249:C:O2'	9:I:73:GLN:NE2	2.53	0.42
1:A:1064:G:H21	1:A:1190:G:H2'	1.84	0.42
1:A:1516:G:H2'	1:A:1518:MA6:OP2	2.18	0.42
1:A:501:C:H2'	1:A:502:G:H8	1.82	0.42
2:B:87:ARG:O	2:B:88:ALA:C	2.57	0.42
9:I:44:VAL:HG12	9:I:51:ARG:NH2	2.34	0.42
10:J:66:ARG:HD3	10:J:68:HIS:HE1	1.84	0.42
1:A:691:G:H2'	1:A:692:U:C6	2.54	0.42
3:C:148:GLY:HA3	3:C:172:ARG:O	2.20	0.42
1:A:1291:G:OP1	7:G:37:ASN:ND2	2.52	0.42
7:G:62:PHE:HA	7:G:124:LEU:HD12	2.01	0.42
1:A:1379:G:OP1	7:G:6:ARG:NH1	2.52	0.42
2:B:131:PRO:O	2:B:133:LYS:N	2.52	0.42
4:D:159:ARG:O	4:D:163:GLU:HB2	2.19	0.42
4:D:98:GLU:HG2	4:D:189:PRO:HG3	2.01	0.42
6:F:62:TRP:CH2	6:F:64:GLN:HB2	2.55	0.42
1:A:1127:G:O2'	9:I:16:ARG:NH2	2.50	0.42
1:A:142:G:H2'	1:A:143:A:H8	1.84	0.42
1:A:359:U:H2'	1:A:360:A:C8	2.55	0.42
1:A:948:C:OP1	13:M:107:ALA:HA	2.19	0.42
4:D:140:VAL:HG11	4:D:146:ILE:HD11	2.00	0.42
7:G:28:ASN:OD1	7:G:36:LYS:NZ	2.50	0.42
13:M:66:LEU:O	13:M:70:LEU:HB2	2.19	0.42
1:A:1300:G:HO2'	1:A:1301:U:P	2.43	0.42
1:A:884:U:H4'	1:A:885:G:H5''	2.02	0.42
2:B:91:PRO:HG2	2:B:155:LEU:HG	2.02	0.42
1:A:673:G:O3'	6:F:87:ARG:NH2	2.52	0.42
3:C:58:GLU:HB3	10:J:92:THR:HG21	2.01	0.42
15:O:56:LEU:HA	15:O:59:MET:HE2	2.00	0.42
1:A:1092:A:H5''	7:G:4:ARG:CZ	2.50	0.42
1:A:714:G:H2'	1:A:715:A:C8	2.55	0.42
1:A:484:G:H4'	1:A:485:G:O5'	2.20	0.42
3:C:21:ARG:HG3	3:C:58:GLU:HG2	2.02	0.42
3:C:20:SER:HB3	3:C:22:TRP:HE1	1.84	0.42
1:A:1131:G:H2'	1:A:1132:C:C6	2.55	0.41
1:A:184:G:H2'	1:A:185:A:C8	2.55	0.41
1:A:381:C:H2'	1:A:382:A:O4'	2.20	0.41
4:D:81:GLU:O	4:D:85:LYS:HG3	2.19	0.41
12:L:70:ILE:HD13	12:L:77:LEU:HD12	2.00	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:636:U:H5'	17:Q:2:PRO:HG3	2.01	0.41
1:A:9:G:OP2	5:E:121:LYS:NZ	2.36	0.41
12:L:7:ILE:O	12:L:11:VAL:HG23	2.20	0.41
1:A:1318:A:H4'	19:S:10:PHE:CE1	2.55	0.41
19:S:80:TYR:CZ	19:S:81:ARG:HD3	2.53	0.41
1:A:324:G:OP1	20:T:70:SER:OG	2.33	0.41
1:A:501:C:H1'	1:A:549:C:H1'	2.00	0.41
1:A:636:U:H2'	1:A:637:G:C8	2.56	0.41
1:A:673:G:H2'	1:A:674:G:C8	2.54	0.41
1:A:757:U:O2'	1:A:879:C:O2	2.38	0.41
4:D:173:TRP:CD2	4:D:189:PRO:HB3	2.54	0.41
7:G:51:GLN:C	7:G:53:LYS:H	2.23	0.41
17:Q:18:THR:HG23	17:Q:69:LYS:HE3	2.01	0.41
1:A:662:G:H2'	1:A:663:A:C8	2.55	0.41
8:H:26:VAL:HG13	8:H:59:LEU:HB2	2.02	0.41
13:M:115:LYS:HE2	13:M:115:LYS:HB2	1.93	0.41
19:S:31:ILE:HD13	19:S:32:LYS:H	1.85	0.41
1:A:436:C:H2'	1:A:437:U:C6	2.55	0.41
2:B:116:GLU:H	2:B:116:GLU:HG2	1.71	0.41
10:J:71:LEU:HA	10:J:71:LEU:HD22	1.95	0.41
12:L:59:ARG:NH1	12:L:65:GLU:OE2	2.54	0.41
12:L:5:PRO:HG2	12:L:10:LEU:HD21	2.03	0.41
6:F:50:TYR:CE2	18:R:77:GLY:HA2	2.56	0.41
1:A:1077:G:N2	1:A:1080:A:OP2	2.50	0.41
1:A:711:G:P	6:F:54:LYS:HZ3	2.44	0.41
1:A:88:A:H2'	1:A:89:C:O4'	2.21	0.41
9:I:63:ILE:HG21	9:I:77:ILE:HG12	2.03	0.41
12:L:24:VAL:HG13	12:L:98:TYR:CE1	2.56	0.41
1:A:1392:G:H21	1:A:1502:A:H8	1.67	0.41
1:A:560:U:H4'	1:A:561:U:H5''	2.02	0.41
3:C:57:ILE:HG12	3:C:66:VAL:HG22	2.01	0.41
5:E:6:PHE:HA	5:E:6:PHE:HD1	1.75	0.41
16:P:59:TRP:HA	16:P:62:VAL:HG22	2.02	0.41
1:A:1032:G:H2'	1:A:1033:G:C8	2.55	0.41
1:A:518:C:H2'	1:A:530:G:N3	2.35	0.41
1:A:851:G:H2'	1:A:852:G:C8	2.56	0.41
2:B:135:GLN:O	2:B:139:LYS:HB2	2.21	0.41
1:A:1118:C:H1'	1:A:1179:A:C5	2.55	0.41
1:A:1225:A:H5''	1:A:1226:C:OP2	2.21	0.41
1:A:1250:A:H2'	1:A:1251:A:C8	2.56	0.41
1:A:1302:U:C5	13:M:17:VAL:HG21	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:9:ARG:HB3	9:I:104:ARG:NH2	2.36	0.41
12:L:7:ILE:HD13	12:L:10:LEU:HD12	2.02	0.41
17:Q:5:VAL:HA	17:Q:59:ILE:O	2.20	0.41
18:R:26:LEU:HA	18:R:26:LEU:HD12	1.88	0.41
1:A:1201:A:H1'	1:A:1202:G:OP2	2.20	0.41
1:A:147:G:H1	1:A:175:C:H42	1.69	0.41
1:A:484:G:H1'	1:A:485:G:OP2	2.21	0.41
11:K:91:ARG:NE	18:R:88:LYS:HZ3	2.19	0.41
4:D:25:ARG:NH1	4:D:30:LYS:O	2.54	0.41
12:L:78:GLN:N	12:L:81:SER:OG	2.54	0.41
1:A:1308:U:H2'	1:A:1309:G:H8	1.86	0.40
1:A:190(J):U:H2'	1:A:190(K):G:C8	2.56	0.40
1:A:19:C:OP1	5:E:125:SER:OG	2.31	0.40
1:A:620:C:H2'	1:A:621:A:O4'	2.20	0.40
1:A:688:G:H2'	1:A:689:C:C6	2.56	0.40
2:B:88:ALA:O	2:B:90:MET:N	2.52	0.40
3:C:20:SER:OG	3:C:40:ARG:NH2	2.39	0.40
12:L:33:ARG:HA	12:L:33:ARG:HD2	1.76	0.40
16:P:4:ILE:O	16:P:66:PRO:HA	2.21	0.40
17:Q:6:LEU:HB3	17:Q:23:VAL:HG11	2.02	0.40
1:A:129:U:O3'	1:A:129(A):G:H3'	2.22	0.40
1:A:19:C:H2'	1:A:20:U:C6	2.56	0.40
1:A:1306:A:N6	1:A:1331:G:H1'	2.37	0.40
3:C:3:ASN:N	3:C:3:ASN:OD1	2.54	0.40
17:Q:67:LYS:HA	17:Q:70:ARG:HH12	1.86	0.40
1:A:999:C:H2'	1:A:1000:U:C6	2.57	0.40
1:A:109:A:C6	1:A:326:G:C6	3.09	0.40
1:A:241:C:H4'	12:L:19:ARG:NH2	2.37	0.40
1:A:297:G:N2	1:A:300:A:OP2	2.49	0.40
1:A:339:C:H2'	1:A:340:U:C6	2.57	0.40
1:A:824:C:H2'	1:A:825:G:C8	2.57	0.40
1:A:1056:U:H5'	3:C:163:ALA:HB2	2.03	0.40
14:N:27:CYS:SG	14:N:29:ARG:HB2	2.61	0.40
1:A:719:C:O2'	18:R:49:LYS:HB3	2.22	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	234/236 (99%)	214 (92%)	18 (8%)	2 (1%)	17	48
3	C	205/207 (99%)	189 (92%)	16 (8%)	0	100	100
4	D	206/208 (99%)	201 (98%)	5 (2%)	0	100	100
5	E	149/151 (99%)	145 (97%)	4 (3%)	0	100	100
6	F	99/101 (98%)	99 (100%)	0	0	100	100
7	G	153/155 (99%)	148 (97%)	5 (3%)	0	100	100
8	H	136/138 (99%)	129 (95%)	7 (5%)	0	100	100
9	I	125/127 (98%)	114 (91%)	11 (9%)	0	100	100
10	J	97/99 (98%)	78 (80%)	18 (19%)	1 (1%)	15	46
11	K	117/119 (98%)	109 (93%)	8 (7%)	0	100	100
12	L	122/125 (98%)	113 (93%)	9 (7%)	0	100	100
13	M	116/118 (98%)	108 (93%)	6 (5%)	2 (2%)	9	35
14	N	58/60 (97%)	56 (97%)	2 (3%)	0	100	100
15	O	86/88 (98%)	84 (98%)	2 (2%)	0	100	100
16	P	82/84 (98%)	80 (98%)	2 (2%)	0	100	100
17	Q	97/99 (98%)	92 (95%)	5 (5%)	0	100	100
18	R	71/73 (97%)	69 (97%)	2 (3%)	0	100	100
19	S	79/81 (98%)	73 (92%)	6 (8%)	0	100	100
20	T	97/99 (98%)	88 (91%)	6 (6%)	3 (3%)	4	23
21	U	23/25 (92%)	21 (91%)	2 (9%)	0	100	100
All	All	2352/2393 (98%)	2210 (94%)	134 (6%)	8 (0%)	41	71

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
20	T	75	ASN

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Mol	Chain	Res	Type
2	B	132	LYS
13	M	106	ASN
20	T	74	LYS
20	T	73	HIS
10	J	55	LYS
13	M	107	ALA
2	B	88	ALA

### 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	194/204 (95%)	183 (94%)	11 (6%)	20	51
3	C	160/161 (99%)	152 (95%)	8 (5%)	24	55
4	D	180/180 (100%)	176 (98%)	4 (2%)	52	74
5	E	115/116 (99%)	104 (90%)	11 (10%)	8	29
6	F	90/90 (100%)	86 (96%)	4 (4%)	28	59
7	G	126/126 (100%)	120 (95%)	6 (5%)	25	56
8	H	119/119 (100%)	112 (94%)	7 (6%)	19	49
9	I	98/98 (100%)	92 (94%)	6 (6%)	18	48
10	J	87/89 (98%)	80 (92%)	7 (8%)	12	37
11	K	90/90 (100%)	86 (96%)	4 (4%)	28	59
12	L	103/103 (100%)	97 (94%)	6 (6%)	20	50
13	M	94/94 (100%)	86 (92%)	8 (8%)	10	35
14	N	49/49 (100%)	47 (96%)	2 (4%)	30	61
15	O	79/79 (100%)	74 (94%)	5 (6%)	18	47
16	P	72/72 (100%)	68 (94%)	4 (6%)	21	52
17	Q	94/94 (100%)	90 (96%)	4 (4%)	29	59
18	R	64/64 (100%)	62 (97%)	2 (3%)	40	67
19	S	71/71 (100%)	65 (92%)	6 (8%)	10	35

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
20	T	76/76 (100%)	66 (87%)	10 (13%)	4	17
21	U	19/20 (95%)	18 (95%)	1 (5%)	22	53
All	All	1980/1995 (99%)	1864 (94%)	116 (6%)	19	49

All (116) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	24	TRP
2	B	46	LYS
2	B	69	LEU
2	B	82	ARG
2	B	114	ARG
2	B	139	LYS
2	B	142	LEU
2	B	144	ARG
2	B	190	THR
2	B	221	LEU
2	B	236	TYR
3	C	27	LYS
3	C	28	GLN
3	C	34	LEU
3	C	91	LEU
3	C	95	THR
3	C	126	ARG
3	C	167	TRP
3	C	204	LEU
4	D	3	ARG
4	D	15	GLU
4	D	122	ARG
4	D	127	THR
5	E	6	PHE
5	E	10	MET
5	E	12	LEU
5	E	41	VAL
5	E	64	ARG
5	E	76	ILE
5	E	79	GLU
5	E	80	ILE
5	E	89	ILE
5	E	120	THR
5	E	150	ARG

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
6	F	10	LEU
6	F	24	GLU
6	F	69	GLU
6	F	100	ASN
7	G	8	GLU
7	G	11	GLN
7	G	48	LYS
7	G	52	GLU
7	G	114	ARG
7	G	156	TRP
8	H	39	LEU
8	H	54	ASP
8	H	85	ARG
8	H	91	ARG
8	H	92	ARG
8	H	102	ARG
8	H	133	LEU
9	I	12	GLU
9	I	79	LEU
9	I	102	LEU
9	I	111	ARG
9	I	118	LYS
9	I	121	ARG
10	J	15	THR
10	J	49	VAL
10	J	61	GLU
10	J	71	LEU
10	J	80	LYS
10	J	83	GLU
10	J	86	MET
11	K	11	LYS
11	K	29	ILE
11	K	91	ARG
11	K	92	GLU
12	L	20	LYS
12	L	27	LEU
12	L	33	ARG
12	L	53	ARG
12	L	111	LYS
12	L	127	GLU
13	M	37	THR
13	M	44	ARG

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
13	M	58	GLU
13	M	64	TRP
13	M	70	LEU
13	M	105	THR
13	M	106	ASN
13	M	109	THR
14	N	9	LYS
14	N	33	VAL
15	O	5	LYS
15	O	6	GLU
15	O	39	LEU
15	O	70	LEU
15	O	81	LEU
16	P	1	MET
16	P	20	VAL
16	P	53	VAL
16	P	67	THR
17	Q	38	ARG
17	Q	52	LYS
17	Q	74	LEU
17	Q	98	LEU
18	R	25	THR
18	R	47	THR
19	S	5	LEU
19	S	7	LYS
19	S	12	ASP
19	S	15	LEU
19	S	27	GLU
19	S	31	ILE
20	T	8	ARG
20	T	9	ASN
20	T	10	LEU
20	T	48	LYS
20	T	57	ARG
20	T	72	LEU
20	T	73	HIS
20	T	74	LYS
20	T	75	ASN
20	T	84	LEU
21	U	9	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
3	C	6	HIS
4	D	119	GLN
9	I	124	GLN

### 5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	1507/1522 (99%)	210 (13%)	36 (2%)
22	a	5/6 (83%)	1 (20%)	0
23	b	11/15 (73%)	2 (18%)	0
All	All	1523/1543 (98%)	213 (13%)	36 (2%)

All (213) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	7	G
1	A	9	G
1	A	32	A
1	A	39	G
1	A	47	C
1	A	48	C
1	A	51	A
1	A	61	G
1	A	63	C
1	A	101	A
1	A	116	A
1	A	117	G
1	A	120	A
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	190(E)	U
1	A	195	A
1	A	197	A
1	A	201	C
1	A	202	U
1	A	204	U
1	A	216	G
1	A	220	G

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	244	U
1	A	247	G
1	A	251	G
1	A	267	C
1	A	270	A
1	A	289	G
1	A	298	A
1	A	321	A
1	A	328	C
1	A	329	A
1	A	332	G
1	A	344	A
1	A	351	G
1	A	352	C
1	A	353	A
1	A	354	G
1	A	367	U
1	A	373	A
1	A	384	G
1	A	390	C
1	A	397	A
1	A	398	C
1	A	406	G
1	A	412	A
1	A	413	G
1	A	414	A
1	A	421	U
1	A	429	U
1	A	433	C
1	A	439	A
1	A	442	C
1	A	452	A
1	A	460	A
1	A	461	C
1	A	485	G
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	527	7MG

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	532	A
1	A	533	A
1	A	545	C
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	596	C
1	A	630	G
1	A	631	G
1	A	653	A
1	A	665	A
1	A	666	G
1	A	687	A
1	A	688	G
1	A	702	A
1	A	703	G
1	A	721	G
1	A	723	U
1	A	731	G
1	A	734	G
1	A	749	C
1	A	755	G
1	A	777	A
1	A	781	A
1	A	782	A
1	A	793	U
1	A	794	A
1	A	813	U
1	A	817	C
1	A	819	A
1	A	821	G
1	A	828	A
1	A	836	G
1	A	839	U
1	A	840	C
1	A	841	U

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
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	960	U
1	A	961	U
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	994	A
1	A	1004	A
1	A	1005	A
1	A	1025	U
1	A	1026	G
1	A	1027	C
1	A	1050	G
1	A	1054	C
1	A	1064	G
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	1108	G
1	A	1117	G
1	A	1125	U
1	A	1126	U
1	A	1129	C
1	A	1130	A
1	A	1131	G

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	1137	C
1	A	1138	G
1	A	1139	G
1	A	1159	U
1	A	1171	G
1	A	1180	A
1	A	1181	G
1	A	1182	G
1	A	1183	A
1	A	1190	G
1	A	1196	U
1	A	1197	G
1	A	1201	A
1	A	1202	G
1	A	1212	U
1	A	1213	A
1	A	1227	A
1	A	1238	A
1	A	1257	U
1	A	1258	G
1	A	1270	C
1	A	1280	A
1	A	1281	U
1	A	1282	C
1	A	1286	A
1	A	1287	A
1	A	1290	G
1	A	1300	G
1	A	1301	U
1	A	1302	U
1	A	1320	C
1	A	1331	G
1	A	1332	A
1	A	1348	U
1	A	1353	G
1	A	1359	C
1	A	1362	C
1	A	1363	A
1	A	1364	U
1	A	1397	C
1	A	1398	A
1	A	1421	G

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Mol	Chain	Res	Type
1	A	1442	G
1	A	1443	G
1	A	1446	A
1	A	1487	G
1	A	1492	A
1	A	1497	G
1	A	1499	A
1	A	1502	A
1	A	1504	G
1	A	1505	G
1	A	1506	U
1	A	1517	G
1	A	1520	G
1	A	1529	G
1	A	1530	G
22	a	6	U
23	b	32	C
23	b	33	U

All (36) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	60	A
1	A	115	G
1	A	129(A)	G
1	A	181	G
1	A	250	A
1	A	266	G
1	A	328	C
1	A	372	C
1	A	428	G
1	A	484	G
1	A	496	A
1	A	509	A
1	A	559	A
1	A	687	A
1	A	701	C
1	A	748	C
1	A	812	C
1	A	913	A
1	A	960	U
1	A	1049	U

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Mol	Chain	Res	Type
1	A	1065	U
1	A	1067	A
1	A	1129	C
1	A	1179	A
1	A	1182	G
1	A	1201	A
1	A	1256	A
1	A	1281	U
1	A	1285	A
1	A	1300	G
1	A	1301	U
1	A	1331	G
1	A	1347	G
1	A	1443	G
1	A	1505	G
1	A	1528	U

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

18 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	MA6	A	1518	1	19,26,27	0.70	0	18,38,41	0.85	1 (5%)
1	PSU	A	1540	1	17,21,22	1.43	3 (17%)	20,30,33	3.62	5 (25%)
1	PSU	A	516	1	17,21,22	1.46	4 (23%)	20,30,33	3.68	5 (25%)
12	0TD	L	92	12	4,9,10	0.97	0	3,11,13	1.74	1 (33%)
1	MA6	A	1519	1	19,26,27	0.69	0	18,38,41	0.89	1 (5%)
1	2MG	A	1207	1	19,26,27	1.99	2 (10%)	21,38,41	2.02	3 (14%)
1	UR3	A	1498	1	14,22,23	0.69	0	15,32,35	0.95	0
23	PSU	b	39	23	17,21,22	1.41	3 (17%)	20,30,33	3.60	5 (25%)
1	5MC	A	1400	1	15,22,23	0.88	0	19,32,35	1.02	1 (5%)
1	M2G	A	966	1	20,27,28	1.80	4 (20%)	22,40,43	2.51	5 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
23	70U	b	34	22,23	19,26,27	2.77	7 (36%)	21,37,40	2.05	3 (14%)
1	5MC	A	1404	1	15,22,23	0.88	0	19,32,35	1.00	1 (5%)
1	5MC	A	967	1	15,22,23	0.85	0	19,32,35	1.03	1 (5%)
1	5MC	A	1407	1	15,22,23	0.87	0	19,32,35	1.03	2 (10%)
1	4OC	A	1402	1	16,23,24	0.76	0	17,32,35	0.71	0
1	PSU	A	1541	1,24	17,21,22	1.44	3 (17%)	20,30,33	3.65	5 (25%)
23	12A	b	37	23	26,36,37	5.32	13 (50%)	29,52,55	2.80	10 (34%)
1	7MG	A	527	1	22,26,27	2.06	6 (27%)	28,39,42	1.63	7 (25%)

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	MA6	A	1518	1	-	2/7/29/30	0/3/3/3
1	PSU	A	1540	1	-	0/7/25/26	0/2/2/2
1	PSU	A	516	1	-	0/7/25/26	0/2/2/2
12	0TD	L	92	12	-	2/3/12/14	-
1	MA6	A	1519	1	-	1/7/29/30	0/3/3/3
1	2MG	A	1207	1	-	0/5/27/28	0/3/3/3
1	UR3	A	1498	1	-	0/5/25/26	0/2/2/2
23	PSU	b	39	23	-	2/7/25/26	0/2/2/2
1	5MC	A	1400	1	-	2/5/25/26	0/2/2/2
1	M2G	A	966	1	-	2/7/29/30	0/3/3/3
23	70U	b	34	22,23	-	4/11/31/32	0/2/2/2
1	5MC	A	1404	1	-	0/5/25/26	0/2/2/2
1	5MC	A	967	1	-	2/5/25/26	0/2/2/2
1	5MC	A	1407	1	-	0/5/25/26	0/2/2/2
1	4OC	A	1402	1	-	2/9/29/30	0/2/2/2
1	PSU	A	1541	1,24	-	0/7/25/26	0/2/2/2
23	12A	b	37	23	1/1/9/11	5/17/43/44	0/3/3/3
1	7MG	A	527	1	-	2/7/37/38	0/3/3/3

All (45) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	37	12A	C2'-C1'	-15.26	1.30	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	37	12A	O4'-C1'	14.75	1.61	1.41
23	b	37	12A	C6-N6	9.16	1.52	1.36
23	b	37	12A	C2-S2	7.18	1.81	1.75
23	b	34	70U	C2-S2	7.05	1.81	1.66
1	A	1207	2MG	C2-N2	6.27	1.39	1.34
23	b	34	70U	O4-C4	6.17	1.40	1.24
23	b	37	12A	O4'-C4'	-6.05	1.31	1.45
1	A	966	M2G	C6-N1	5.58	1.42	1.33
1	A	527	7MG	C8-N9	-5.34	1.33	1.45
23	b	37	12A	CC-N	5.19	1.46	1.35
1	A	1207	2MG	C6-N1	5.07	1.41	1.33
1	A	527	7MG	C2-N2	4.65	1.43	1.33
23	b	37	12A	O2'-C2'	4.15	1.52	1.43
23	b	34	70U	C5M-C5	4.13	1.57	1.51
1	A	527	7MG	C4-N3	3.98	1.39	1.34
23	b	34	70U	O9-C8	3.59	1.44	1.33
23	b	37	12A	CC-N6	3.56	1.44	1.37
1	A	966	M2G	C2-N2	3.44	1.40	1.34
23	b	34	70U	O9-C9	-3.29	1.37	1.45
1	A	966	M2G	C2-N1	3.27	1.40	1.34
23	b	37	12A	O3'-C3'	-3.20	1.35	1.43
23	b	37	12A	OO-CC	-3.20	1.16	1.23
1	A	1540	PSU	C2-N1	-3.19	1.31	1.38
1	A	516	PSU	C2-N1	-3.17	1.31	1.38
23	b	39	PSU	C2-N1	-3.17	1.31	1.38
1	A	1541	PSU	C2-N1	-3.16	1.31	1.38
23	b	39	PSU	C2-N3	-3.11	1.32	1.38
1	A	516	PSU	C2-N3	-3.10	1.32	1.38
1	A	1540	PSU	C2-N3	-3.09	1.32	1.38
1	A	1541	PSU	C2-N3	-3.09	1.32	1.38
23	b	37	12A	O5'-C5'	-3.09	1.37	1.44
23	b	37	12A	CA-N	-3.03	1.40	1.46
1	A	966	M2G	C4-N3	2.81	1.40	1.35
23	b	34	70U	C6-C5	2.75	1.43	1.37
1	A	527	7MG	CM7-N7	-2.48	1.41	1.46
1	A	516	PSU	O4-C4	-2.45	1.18	1.24
1	A	1541	PSU	O4-C4	-2.45	1.18	1.24
1	A	527	7MG	C6-N1	2.43	1.37	1.33
1	A	1540	PSU	O4-C4	-2.42	1.18	1.24
23	b	39	PSU	O4-C4	-2.41	1.18	1.24
23	b	34	70U	C4-N3	-2.11	1.29	1.33
1	A	516	PSU	O4'-C1'	-2.08	1.41	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	527	7MG	C2-N3	-2.06	1.31	1.35
23	b	37	12A	CB-CA	2.01	1.59	1.53

All (56) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	516	PSU	N1-C2-N3	-11.43	119.34	128.43
1	A	1541	PSU	N1-C2-N3	-11.39	119.37	128.43
1	A	1540	PSU	N1-C2-N3	-11.30	119.44	128.43
23	b	39	PSU	N1-C2-N3	-11.19	119.54	128.43
23	b	37	12A	C2M-S2-C2	9.92	109.67	102.27
1	A	516	PSU	C4-N3-C2	8.93	122.69	115.14
1	A	1541	PSU	C4-N3-C2	8.82	122.59	115.14
1	A	1540	PSU	C4-N3-C2	8.77	122.54	115.14
23	b	39	PSU	C4-N3-C2	8.65	122.45	115.14
1	A	966	M2G	C5-C6-N1	-8.51	111.80	123.43
1	A	1207	2MG	C5-C6-N1	-7.53	113.13	123.43
1	A	966	M2G	C6-N1-C2	6.08	123.42	116.18
23	b	34	70U	O9-C8-C5M	5.81	119.51	111.45
23	b	37	12A	N6-CC-N	5.28	121.14	113.76
23	b	34	70U	C2-N3-C4	5.28	121.33	115.93
1	A	1541	PSU	C5-C4-N3	-4.50	119.56	125.36
1	A	516	PSU	C5-C4-N3	-4.48	119.59	125.36
23	b	39	PSU	C5-C4-N3	-4.47	119.60	125.36
1	A	1540	PSU	C5-C4-N3	-4.47	119.60	125.36
23	b	37	12A	C2-N3-C4	4.16	121.06	115.32
23	b	37	12A	O4'-C1'-C2'	-4.00	101.09	106.93
23	b	34	70U	C5-C4-N3	-3.98	119.42	125.25
23	b	39	PSU	C6-N1-C2	3.97	121.91	115.36
1	A	1541	PSU	C6-N1-C2	3.97	121.90	115.36
1	A	1540	PSU	C6-N1-C2	3.94	121.86	115.36
1	A	516	PSU	C6-N1-C2	3.90	121.79	115.36
23	b	37	12A	OO-CC-N6	-3.85	117.10	123.62
1	A	1207	2MG	C6-N1-C2	3.83	122.05	115.18
23	b	37	12A	C3'-C2'-C1'	-3.72	95.37	100.98
23	b	39	PSU	C5-C6-N1	-3.65	119.95	124.44
1	A	1540	PSU	C5-C6-N1	-3.56	120.06	124.44
1	A	1541	PSU	C5-C6-N1	-3.54	120.08	124.44
1	A	527	7MG	C5-C4-N3	-3.54	120.71	126.49
1	A	527	7MG	N3-C4-N9	3.52	131.43	126.91
1	A	527	7MG	N7-C8-N9	3.44	108.30	103.38
1	A	516	PSU	C5-C6-N1	-3.39	120.27	124.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	966	M2G	N3-C2-N2	3.02	120.24	117.18
1	A	527	7MG	C6-N1-C2	2.53	119.95	115.93
1	A	966	M2G	N1-C2-N2	-2.52	114.64	117.19
1	A	1519	MA6	N1-C6-N6	-2.51	114.41	117.06
23	b	37	12A	CA-N-CC	2.49	125.41	122.75
12	L	92	0TD	CSB-SB-CB	-2.49	96.96	101.85
23	b	37	12A	N3-C2-N1	-2.45	122.47	126.98
1	A	527	7MG	C2-N3-C4	2.39	120.48	113.89
1	A	1207	2MG	C4-C5-N7	2.29	111.79	109.40
1	A	966	M2G	C2-N3-C4	-2.29	112.67	115.28
1	A	527	7MG	N1-C2-N3	-2.28	121.84	125.42
1	A	1518	MA6	N1-C6-N6	-2.26	114.67	117.06
23	b	37	12A	N6-C6-N1	2.21	122.80	118.84
23	b	37	12A	C1'-N9-C4	2.18	130.47	126.64
1	A	1404	5MC	N4-C4-N3	-2.07	114.11	117.03
1	A	967	5MC	C2-N3-C4	2.04	118.48	116.02
1	A	1407	5MC	C2-N3-C4	2.03	118.47	116.02
1	A	1400	5MC	C2-N3-C4	2.03	118.46	116.02
1	A	527	7MG	C4-N9-C1'	-2.02	121.79	126.60
1	A	1407	5MC	N4-C4-N3	-2.01	114.19	117.03

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
23	b	37	12A	C1'

All (26) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
12	L	92	0TD	CA-CB-SB-CSB
12	L	92	0TD	CG-CB-SB-CSB
1	A	527	7MG	O4'-C4'-C5'-O5'
1	A	527	7MG	C3'-C4'-C5'-O5'
23	b	37	12A	N1-C2-S2-C2M
23	b	37	12A	N3-C2-S2-C2M
1	A	1402	4OC	O4'-C4'-C5'-O5'
23	b	34	70U	O8-C8-O9-C9
1	A	1402	4OC	C3'-C4'-C5'-O5'
23	b	34	70U	C5M-C8-O9-C9
1	A	1518	MA6	C3'-C4'-C5'-O5'
1	A	1400	5MC	O4'-C4'-C5'-O5'
1	A	1400	5MC	C3'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
1	A	1518	MA6	O4'-C4'-C5'-O5'
1	A	967	5MC	O4'-C4'-C5'-O5'
23	b	37	12A	C-CA-CB-OG1
23	b	39	PSU	O4'-C4'-C5'-O5'
23	b	37	12A	CB-CA-N-CC
23	b	34	70U	O4'-C4'-C5'-O5'
23	b	37	12A	N-CA-CB-CG2
23	b	34	70U	C3'-C4'-C5'-O5'
1	A	967	5MC	C3'-C4'-C5'-O5'
1	A	966	M2G	N3-C2-N2-CM2
1	A	966	M2G	N1-C2-N2-CM2
1	A	1519	MA6	C3'-C4'-C5'-O5'
23	b	39	PSU	C3'-C4'-C5'-O5'

There are no ring outliers.

8 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	1518	MA6	4	0
12	L	92	0TD	1	0
1	A	1519	MA6	1	0
1	A	1207	2MG	1	0
1	A	1498	UR3	1	0
1	A	1400	5MC	1	0
1	A	967	5MC	1	0
1	A	1402	4OC	2	0

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 277 ligands modelled in this entry, 277 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.



There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
23	b	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	b	40:C	O3'	41:U	P	3.24

## 6 Fit of model and data i

### 6.1 Protein, DNA and RNA chains i

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	1498/1522 (98%)	-0.43	18 (1%) 79 78	103, 147, 228, 340	0
2	B	236/236 (100%)	0.07	14 (5%) 22 22	121, 180, 260, 310	0
3	C	207/207 (100%)	-0.03	6 (2%) 51 50	110, 184, 236, 264	0
4	D	208/208 (100%)	0.44	24 (11%) 4 4	117, 167, 222, 268	0
5	E	151/151 (100%)	0.04	3 (1%) 65 64	102, 141, 186, 259	0
6	F	101/101 (100%)	0.30	10 (9%) 7 7	130, 171, 200, 256	0
7	G	155/155 (100%)	-0.06	5 (3%) 47 46	123, 166, 230, 276	0
8	H	138/138 (100%)	-0.35	2 (1%) 75 75	94, 133, 174, 238	0
9	I	127/127 (100%)	0.28	11 (8%) 10 10	139, 190, 236, 303	0
10	J	99/99 (100%)	0.67	15 (15%) 2 2	125, 214, 311, 340	0
11	K	119/119 (100%)	0.13	9 (7%) 13 13	109, 144, 190, 267	0
12	L	124/125 (99%)	0.23	6 (4%) 30 28	100, 155, 201, 300	0
13	M	118/118 (100%)	0.54	15 (12%) 3 3	124, 165, 214, 291	0
14	N	60/60 (100%)	0.18	2 (3%) 46 44	142, 169, 232, 301	0
15	O	88/88 (100%)	-0.09	3 (3%) 45 43	106, 151, 204, 260	0
16	P	84/84 (100%)	-0.20	1 (1%) 79 78	106, 147, 180, 251	0
17	Q	99/99 (100%)	-0.02	2 (2%) 65 64	106, 135, 188, 224	0
18	R	73/73 (100%)	0.54	9 (12%) 4 3	118, 153, 244, 293	0
19	S	81/81 (100%)	0.40	8 (9%) 7 7	113, 189, 247, 311	0
20	T	99/99 (100%)	0.04	1 (1%) 82 82	105, 145, 199, 264	0
21	U	25/25 (100%)	2.08	10 (40%) 0 0	99, 171, 229, 273	0
22	a	6/6 (100%)	-0.49	0 100 100	178, 181, 205, 237	0
23	b	12/15 (80%)	0.29	0 100 100	187, 249, 305, 306	0
All	All	3908/3936 (99%)	-0.06	174 (4%) 33 32	94, 158, 237, 340	0

All (174) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
13	M	7	VAL	11.6
11	K	128	ALA	9.0
12	L	129	ALA	8.6
4	D	32	ALA	8.3
10	J	34	VAL	7.9
21	U	18	TYR	7.6
13	M	119	GLY	7.3
13	M	2	ALA	7.3
18	R	17	SER	6.8
13	M	8	GLU	6.6
2	B	132	LYS	6.4
14	N	12	ARG	6.3
18	R	16	PRO	6.3
4	D	42	GLN	6.2
10	J	33	GLN	5.5
21	U	17	THR	5.5
2	B	131	PRO	5.1
14	N	13	THR	5.1
6	F	88	VAL	4.9
4	D	13	ARG	4.9
13	M	9	ILE	4.8
13	M	5	ALA	4.7
4	D	37	PRO	4.7
1	A	990	C	4.6
11	K	129	SER	4.5
9	I	124	GLN	4.5
7	G	2	ALA	4.5
21	U	22	ARG	4.4
9	I	15	ALA	4.3
13	M	3	ARG	4.3
1	A	1443	G	4.3
4	D	41	GLY	4.3
19	S	74	PHE	4.1
10	J	72	VAL	4.1
4	D	38	TYR	4.1
6	F	89	MET	3.9
10	J	74	ILE	3.9
2	B	229	VAL	3.9
9	I	8	GLY	3.9
19	S	4	SER	3.8
2	B	228	GLY	3.8
9	I	128	ARG	3.8

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	A	991	U	3.7
4	D	35	ARG	3.7
1	A	1017	G	3.7
13	M	4	ILE	3.7
9	I	126	SER	3.6
10	J	70	ARG	3.6
3	C	196	LEU	3.6
9	I	65	VAL	3.6
4	D	36	ARG	3.5
15	O	89	GLY	3.5
10	J	39	PRO	3.5
1	A	1018	C	3.5
18	R	18	ARG	3.5
1	A	1129	C	3.5
4	D	7	PRO	3.5
9	I	125	TYR	3.4
9	I	121	ARG	3.4
1	A	1539	C	3.4
4	D	40	PRO	3.3
21	U	12	LYS	3.3
4	D	181	MET	3.3
12	L	128	ALA	3.3
13	M	118	ALA	3.3
12	L	49	ASN	3.2
3	C	189	ALA	3.2
18	R	58	LEU	3.2
12	L	19	ARG	3.2
20	T	9	ASN	3.1
10	J	73	ASP	3.1
19	S	3	ARG	3.1
4	D	2	GLY	3.1
4	D	33	MET	3.1
21	U	25	LYS	3.0
2	B	230	VAL	3.0
7	G	103	TRP	3.0
13	M	117	VAL	3.0
13	M	116	THR	3.0
10	J	36	GLY	2.9
2	B	152	PHE	2.9
2	B	133	LYS	2.9
1	A	1019	C	2.9
1	A	1031	G	2.9

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
13	M	11	ARG	2.9
11	K	31	THR	2.9
4	D	30	LYS	2.9
3	C	193	TYR	2.8
21	U	24	ARG	2.8
19	S	6	LYS	2.8
19	S	40	ILE	2.8
6	F	6	VAL	2.8
4	D	34	GLU	2.8
7	G	33	ASP	2.8
12	L	50	SER	2.8
19	S	69	HIS	2.8
21	U	2	GLY	2.7
4	D	9	CYS	2.7
11	K	127	LYS	2.7
6	F	7	ASN	2.7
13	M	104	ARG	2.7
7	G	156	TRP	2.7
2	B	238	LEU	2.6
9	I	33	PHE	2.6
12	L	53	ARG	2.6
1	A	412	A	2.6
1	A	1212	U	2.6
6	F	8	ILE	2.6
4	D	8	VAL	2.6
11	K	126	ARG	2.5
2	B	231	GLU	2.5
5	E	119	LEU	2.5
10	J	90	LEU	2.5
13	M	6	GLY	2.5
6	F	101	ALA	2.5
10	J	5	ARG	2.5
4	D	6	GLY	2.4
10	J	71	LEU	2.4
5	E	71	LEU	2.4
19	S	41	VAL	2.4
3	C	201	TYR	2.4
3	C	190	ARG	2.4
6	F	63	TYR	2.4
18	R	88	LYS	2.4
10	J	75	ILE	2.4
2	B	135	GLN	2.4

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	A	994	A	2.3
8	H	1	MET	2.3
11	K	43	SER	2.3
2	B	90	MET	2.3
4	D	10	ARG	2.3
4	D	179	GLU	2.3
1	A	1030(D)	A	2.3
2	B	237	ALA	2.3
13	M	60	VAL	2.3
1	A	1030(B)	C	2.3
21	U	9	ARG	2.3
1	A	1286	A	2.3
3	C	52	LEU	2.3
6	F	79	LEU	2.3
18	R	54	ARG	2.3
1	A	630	G	2.2
17	Q	100	LYS	2.2
1	A	1260	C	2.2
15	O	26	GLU	2.2
8	H	2	LEU	2.2
2	B	136	VAL	2.2
9	I	9	ARG	2.2
15	O	22	THR	2.2
4	D	4	TYR	2.2
9	I	14	VAL	2.2
1	A	1446	A	2.2
4	D	25	ARG	2.1
11	K	30	VAL	2.1
4	D	45	GLN	2.1
10	J	40	LEU	2.1
21	U	23	PRO	2.1
6	F	97	PHE	2.1
19	S	60	VAL	2.1
18	R	43	PHE	2.1
10	J	35	SER	2.1
16	P	83	GLU	2.1
11	K	32	ILE	2.1
21	U	11	GLY	2.1
7	G	82	GLY	2.1
10	J	28	ARG	2.1
18	R	34	TYR	2.1
11	K	42	TRP	2.0

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Mol	Chain	Res	Type	RSRZ
17	Q	45	HIS	2.0
2	B	134	GLU	2.0
5	E	120	THR	2.0
4	D	74	GLN	2.0
18	R	19	LYS	2.0
6	F	9	VAL	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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
23	PSU	b	39	20/21	0.81	0.26	206,245,268,270	0
1	PSU	A	1540	20/21	0.87	0.59	224,248,282,289	0
1	PSU	A	1541	20/21	0.87	0.34	208,239,260,291	0
1	7MG	A	527	24/25	0.90	0.22	116,133,148,157	0
1	PSU	A	516	20/21	0.91	0.11	161,182,190,198	0
23	12A	b	37	34/35	0.91	0.24	182,203,239,249	0
12	0TD	L	92	10/11	0.93	0.80	136,224,278,290	0
23	70U	b	34	25/26	0.93	0.14	178,189,202,225	0
1	MA6	A	1519	24/25	0.94	0.25	122,129,142,155	0
1	5MC	A	1404	21/22	0.94	0.16	124,129,137,139	0
1	MA6	A	1518	24/25	0.95	0.16	132,141,147,157	0
1	2MG	A	1207	24/25	0.95	0.14	151,160,173,182	0
1	UR3	A	1498	21/22	0.95	0.22	126,131,155,159	0
1	4OC	A	1402	22/23	0.95	0.21	132,138,153,164	0
1	M2G	A	966	25/26	0.96	0.16	128,153,181,186	0
1	5MC	A	1407	21/22	0.97	0.09	132,145,166,182	0
1	5MC	A	1400	21/22	0.97	0.14	107,139,149,153	0
1	5MC	A	967	21/22	0.97	0.11	129,145,165,171	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
24	MG	A	1802	1/1	0.07	1.31	142,142,142,142	0
26	ZN	D	301	1/1	0.31	0.56	453,453,453,453	0
24	MG	A	1636	1/1	0.31	0.15	121,121,121,121	0
24	MG	A	1769	1/1	0.42	0.56	136,136,136,136	0
24	MG	A	1803	1/1	0.45	0.69	133,133,133,133	0
25	K	A	1847	1/1	0.45	0.24	203,203,203,203	0
24	MG	A	1627	1/1	0.46	1.04	162,162,162,162	0
24	MG	A	1692	1/1	0.48	0.89	130,130,130,130	0
24	MG	A	1782	1/1	0.48	0.58	156,156,156,156	0
25	K	A	1854	1/1	0.48	0.22	177,177,177,177	0
24	MG	A	1770	1/1	0.50	0.51	130,130,130,130	0
24	MG	L	201	1/1	0.53	0.15	118,118,118,118	0
24	MG	A	1629	1/1	0.55	1.16	117,117,117,117	0
24	MG	A	1826	1/1	0.60	0.09	122,122,122,122	0
24	MG	A	1795	1/1	0.60	0.72	123,123,123,123	0
24	MG	A	1807	1/1	0.61	0.18	150,150,150,150	0
24	MG	A	1690	1/1	0.61	0.94	136,136,136,136	0
24	MG	Q	202	1/1	0.62	0.49	116,116,116,116	0
24	MG	A	1805	1/1	0.63	0.49	140,140,140,140	0
24	MG	A	1817	1/1	0.64	0.51	134,134,134,134	0
24	MG	A	1781	1/1	0.64	0.22	136,136,136,136	0
24	MG	P	101	1/1	0.65	0.88	104,104,104,104	0
24	MG	A	1778	1/1	0.65	0.16	188,188,188,188	0
24	MG	A	1827	1/1	0.65	0.39	112,112,112,112	0
24	MG	A	1818	1/1	0.65	0.72	119,119,119,119	0
24	MG	A	1757	1/1	0.66	1.32	136,136,136,136	0
24	MG	A	1824	1/1	0.67	0.40	129,129,129,129	0
24	MG	A	1704	1/1	0.67	0.55	115,115,115,115	0
24	MG	N	101	1/1	0.68	0.21	169,169,169,169	0
24	MG	A	1678	1/1	0.68	0.27	134,134,134,134	0
25	K	A	1834	1/1	0.68	0.79	181,181,181,181	0
24	MG	A	1699	1/1	0.70	0.55	156,156,156,156	0
24	MG	A	1687	1/1	0.70	1.00	105,105,105,105	0
24	MG	A	1701	1/1	0.71	0.40	134,134,134,134	0
24	MG	A	1683	1/1	0.71	0.63	115,115,115,115	0
24	MG	A	1750	1/1	0.72	0.29	116,116,116,116	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
25	K	A	1845	1/1	0.72	0.26	229,229,229,229	0
24	MG	A	1619	1/1	0.73	0.20	127,127,127,127	0
24	MG	H	201	1/1	0.73	0.54	115,115,115,115	0
24	MG	A	1666	1/1	0.73	0.58	121,121,121,121	0
24	MG	A	1705	1/1	0.74	0.16	144,144,144,144	0
24	MG	Q	201	1/1	0.74	0.05	133,133,133,133	0
24	MG	A	1784	1/1	0.74	0.50	144,144,144,144	0
25	K	A	1839	1/1	0.74	0.66	186,186,186,186	0
24	MG	A	1830	1/1	0.75	0.30	126,126,126,126	0
25	K	A	1841	1/1	0.75	0.60	189,189,189,189	0
24	MG	A	1641	1/1	0.75	0.08	121,121,121,121	0
24	MG	A	1730	1/1	0.75	0.71	142,142,142,142	0
25	K	A	1844	1/1	0.76	0.72	193,193,193,193	0
24	MG	A	1634	1/1	0.76	0.28	112,112,112,112	0
24	MG	A	1610	1/1	0.76	0.19	122,122,122,122	0
24	MG	A	1677	1/1	0.76	0.47	123,123,123,123	0
24	MG	A	1766	1/1	0.77	0.27	160,160,160,160	0
24	MG	A	1780	1/1	0.77	0.57	131,131,131,131	0
24	MG	A	1664	1/1	0.78	0.10	131,131,131,131	0
24	MG	A	1613	1/1	0.78	0.20	128,128,128,128	0
24	MG	P	103	1/1	0.78	0.16	124,124,124,124	0
24	MG	A	1609	1/1	0.78	0.28	140,140,140,140	0
24	MG	A	1791	1/1	0.78	0.41	155,155,155,155	0
24	MG	A	1759	1/1	0.78	0.17	125,125,125,125	0
25	K	A	1852	1/1	0.78	0.25	195,195,195,195	0
24	MG	A	1630	1/1	0.78	0.22	147,147,147,147	0
24	MG	A	1794	1/1	0.79	1.50	138,138,138,138	0
24	MG	A	1779	1/1	0.79	0.07	208,208,208,208	0
24	MG	A	1698	1/1	0.80	0.10	176,176,176,176	0
25	K	A	1843	1/1	0.80	0.50	189,189,189,189	0
24	MG	A	1693	1/1	0.80	0.29	120,120,120,120	0
24	MG	A	1709	1/1	0.80	0.33	135,135,135,135	0
24	MG	A	1749	1/1	0.80	0.65	99,99,99,99	0
24	MG	A	1714	1/1	0.80	0.26	118,118,118,118	0
24	MG	A	1787	1/1	0.80	0.41	155,155,155,155	0
24	MG	A	1711	1/1	0.81	0.31	161,161,161,161	0
24	MG	A	1661	1/1	0.81	0.28	132,132,132,132	0
25	K	A	1838	1/1	0.81	1.37	199,199,199,199	0
25	K	A	1853	1/1	0.81	0.79	208,208,208,208	0
24	MG	A	1738	1/1	0.81	0.71	112,112,112,112	0
24	MG	A	1753	1/1	0.81	0.20	144,144,144,144	0
24	MG	A	1700	1/1	0.81	1.21	155,155,155,155	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
24	MG	A	1708	1/1	0.81	0.24	130,130,130,130	0
24	MG	A	1798	1/1	0.82	0.20	102,102,102,102	0
24	MG	A	1746	1/1	0.82	0.49	133,133,133,133	0
24	MG	A	1732	1/1	0.82	0.42	108,108,108,108	0
24	MG	A	1720	1/1	0.82	0.46	110,110,110,110	0
24	MG	A	1806	1/1	0.82	0.89	94,94,94,94	0
24	MG	A	1825	1/1	0.82	0.07	149,149,149,149	0
24	MG	A	1831	1/1	0.82	0.16	181,181,181,181	0
25	K	A	1836	1/1	0.82	0.54	208,208,208,208	0
24	MG	A	1715	1/1	0.82	0.85	129,129,129,129	0
24	MG	A	1819	1/1	0.83	0.37	141,141,141,141	0
25	K	A	1851	1/1	0.83	0.76	170,170,170,170	0
24	MG	A	1659	1/1	0.83	0.20	99,99,99,99	0
24	MG	H	202	1/1	0.83	0.52	123,123,123,123	0
24	MG	A	1741	1/1	0.83	0.45	117,117,117,117	0
24	MG	A	1762	1/1	0.83	0.46	99,99,99,99	0
24	MG	A	1856	1/1	0.83	0.11	151,151,151,151	0
24	MG	D	302	1/1	0.84	0.06	121,121,121,121	0
24	MG	E	201	1/1	0.84	0.07	154,154,154,154	0
24	MG	A	1649	1/1	0.84	0.14	135,135,135,135	0
24	MG	A	1614	1/1	0.84	0.42	119,119,119,119	0
24	MG	A	1638	1/1	0.84	0.10	125,125,125,125	0
24	MG	A	1823	1/1	0.84	0.85	145,145,145,145	0
24	MG	A	1653	1/1	0.85	0.29	155,155,155,155	0
24	MG	A	1620	1/1	0.85	0.34	121,121,121,121	0
24	MG	A	1674	1/1	0.85	0.04	146,146,146,146	0
24	MG	A	1768	1/1	0.85	0.36	152,152,152,152	0
24	MG	A	1813	1/1	0.85	0.53	150,150,150,150	0
24	MG	A	1765	1/1	0.85	0.04	163,163,163,163	0
24	MG	A	1601	1/1	0.85	0.16	164,164,164,164	0
24	MG	A	1822	1/1	0.85	0.10	153,153,153,153	0
24	MG	A	1675	1/1	0.85	0.18	167,167,167,167	0
24	MG	A	1688	1/1	0.85	0.14	181,181,181,181	0
24	MG	A	1771	1/1	0.86	0.24	128,128,128,128	0
24	MG	A	1786	1/1	0.86	0.85	119,119,119,119	0
25	K	A	1840	1/1	0.86	0.17	205,205,205,205	0
24	MG	A	1624	1/1	0.86	1.76	135,135,135,135	0
24	MG	A	1832	1/1	0.86	0.42	172,172,172,172	0
24	MG	A	1631	1/1	0.86	0.27	117,117,117,117	0
24	MG	A	1716	1/1	0.86	0.81	152,152,152,152	0
24	MG	A	1671	1/1	0.86	0.38	124,124,124,124	0
24	MG	A	1812	1/1	0.87	0.21	105,105,105,105	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
24	MG	A	1744	1/1	0.87	0.34	112,112,112,112	0
24	MG	A	1737	1/1	0.87	0.47	126,126,126,126	0
24	MG	A	1814	1/1	0.87	0.47	153,153,153,153	0
24	MG	A	1760	1/1	0.87	0.28	114,114,114,114	0
24	MG	A	1855	1/1	0.87	0.05	144,144,144,144	0
24	MG	A	1673	1/1	0.87	0.31	147,147,147,147	0
24	MG	A	1761	1/1	0.87	0.62	98,98,98,98	0
24	MG	A	1793	1/1	0.87	0.21	113,113,113,113	0
24	MG	A	1743	1/1	0.87	0.37	116,116,116,116	0
24	MG	A	1858	1/1	0.88	0.14	203,203,203,203	0
24	MG	A	1607	1/1	0.88	0.10	161,161,161,161	0
24	MG	A	1707	1/1	0.88	0.38	103,103,103,103	0
24	MG	A	1637	1/1	0.88	0.22	124,124,124,124	0
24	MG	A	1644	1/1	0.88	0.28	146,146,146,146	0
24	MG	S	102	1/1	0.88	0.27	133,133,133,133	0
24	MG	A	1606	1/1	0.88	0.74	137,137,137,137	0
24	MG	A	1623	1/1	0.88	0.86	100,100,100,100	0
24	MG	A	1668	1/1	0.88	0.43	125,125,125,125	0
24	MG	G	201	1/1	0.88	1.21	136,136,136,136	0
24	MG	A	1628	1/1	0.89	0.08	129,129,129,129	0
24	MG	A	1776	1/1	0.89	0.06	107,107,107,107	0
24	MG	A	1710	1/1	0.89	1.58	140,140,140,140	0
24	MG	A	1657	1/1	0.89	0.21	104,104,104,104	0
24	MG	A	1808	1/1	0.89	0.92	132,132,132,132	0
24	MG	A	1821	1/1	0.89	0.32	143,143,143,143	0
24	MG	A	1706	1/1	0.89	0.41	96,96,96,96	0
24	MG	A	1667	1/1	0.89	0.48	191,191,191,191	0
24	MG	A	1747	1/1	0.89	0.15	124,124,124,124	0
24	MG	A	1756	1/1	0.89	0.09	103,103,103,103	0
24	MG	A	1616	1/1	0.89	0.36	120,120,120,120	0
24	MG	A	1686	1/1	0.89	0.41	106,106,106,106	0
24	MG	A	1640	1/1	0.89	0.45	103,103,103,103	0
24	MG	A	1829	1/1	0.89	0.66	120,120,120,120	0
24	MG	A	1748	1/1	0.89	0.92	129,129,129,129	0
24	MG	A	1774	1/1	0.89	0.30	121,121,121,121	0
24	MG	A	1804	1/1	0.90	0.57	146,146,146,146	0
24	MG	A	1681	1/1	0.90	0.95	133,133,133,133	0
24	MG	A	1719	1/1	0.90	0.30	129,129,129,129	0
24	MG	A	1820	1/1	0.90	0.12	105,105,105,105	0
24	MG	P	102	1/1	0.90	0.15	119,119,119,119	0
24	MG	A	1764	1/1	0.90	0.21	149,149,149,149	0
24	MG	A	1660	1/1	0.90	0.55	105,105,105,105	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
24	MG	A	1717	1/1	0.90	0.40	97,97,97,97	0
24	MG	A	1663	1/1	0.90	0.28	143,143,143,143	0
24	MG	A	1815	1/1	0.90	1.39	109,109,109,109	0
24	MG	A	1801	1/1	0.90	0.29	128,128,128,128	0
24	MG	A	1783	1/1	0.90	0.90	122,122,122,122	0
24	MG	A	1785	1/1	0.90	0.25	130,130,130,130	0
24	MG	S	103	1/1	0.90	0.04	122,122,122,122	0
24	MG	A	1680	1/1	0.91	0.20	133,133,133,133	0
24	MG	A	1773	1/1	0.91	0.12	116,116,116,116	0
24	MG	A	1603	1/1	0.91	0.21	158,158,158,158	0
24	MG	A	1718	1/1	0.91	0.15	131,131,131,131	0
25	K	A	1846	1/1	0.91	0.19	201,201,201,201	0
24	MG	A	1724	1/1	0.91	0.20	131,131,131,131	0
24	MG	A	1654	1/1	0.91	0.36	117,117,117,117	0
24	MG	A	1739	1/1	0.91	0.31	113,113,113,113	0
24	MG	A	1767	1/1	0.92	0.42	207,207,207,207	0
24	MG	A	1684	1/1	0.92	0.26	132,132,132,132	0
24	MG	A	1679	1/1	0.92	0.49	130,130,130,130	0
24	MG	A	1656	1/1	0.92	0.15	154,154,154,154	0
24	MG	A	1792	1/1	0.92	0.79	136,136,136,136	0
24	MG	A	1617	1/1	0.92	0.24	108,108,108,108	0
24	MG	A	1625	1/1	0.92	0.07	150,150,150,150	0
24	MG	A	1796	1/1	0.92	0.20	121,121,121,121	0
24	MG	A	1648	1/1	0.92	0.16	112,112,112,112	0
24	MG	A	1775	1/1	0.92	0.56	97,97,97,97	0
24	MG	A	1702	1/1	0.92	0.60	92,92,92,92	0
25	K	A	1848	1/1	0.92	0.41	186,186,186,186	0
24	MG	A	1670	1/1	0.92	0.15	144,144,144,144	0
24	MG	A	1755	1/1	0.92	0.25	120,120,120,120	0
24	MG	A	1612	1/1	0.93	0.24	163,163,163,163	0
24	MG	A	1731	1/1	0.93	0.46	93,93,93,93	0
24	MG	A	1622	1/1	0.93	0.22	123,123,123,123	0
24	MG	A	1790	1/1	0.93	1.12	127,127,127,127	0
24	MG	A	1696	1/1	0.93	0.29	137,137,137,137	0
24	MG	A	1694	1/1	0.93	0.68	198,198,198,198	0
24	MG	A	1655	1/1	0.93	0.13	133,133,133,133	0
24	MG	A	1682	1/1	0.93	0.74	424,424,424,424	0
24	MG	A	1799	1/1	0.93	0.23	120,120,120,120	0
25	K	A	1833	1/1	0.93	0.63	200,200,200,200	0
24	MG	A	1828	1/1	0.93	0.73	127,127,127,127	0
25	K	A	1842	1/1	0.93	0.12	190,190,190,190	0
24	MG	A	1646	1/1	0.93	0.34	124,124,124,124	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
24	MG	A	1676	1/1	0.93	0.08	132,132,132,132	0
24	MG	A	1645	1/1	0.93	0.18	113,113,113,113	0
24	MG	A	1650	1/1	0.93	0.14	84,84,84,84	0
24	MG	A	1811	1/1	0.93	0.05	121,121,121,121	0
24	MG	A	1662	1/1	0.93	0.15	123,123,123,123	0
24	MG	A	1789	1/1	0.93	0.47	135,135,135,135	0
24	MG	A	1665	1/1	0.93	0.26	117,117,117,117	0
24	MG	A	1810	1/1	0.94	0.93	159,159,159,159	0
24	MG	A	1643	1/1	0.94	0.32	169,169,169,169	0
24	MG	A	1721	1/1	0.94	0.75	136,136,136,136	0
25	K	A	1837	1/1	0.94	0.40	200,200,200,200	0
24	MG	A	1615	1/1	0.95	0.11	127,127,127,127	0
24	MG	A	1633	1/1	0.95	0.29	138,138,138,138	0
24	MG	A	1658	1/1	0.95	0.23	110,110,110,110	0
24	MG	A	1758	1/1	0.95	0.42	107,107,107,107	0
24	MG	A	1685	1/1	0.95	0.28	79,79,79,79	0
24	MG	A	1777	1/1	0.95	0.16	91,91,91,91	0
24	MG	A	1725	1/1	0.95	0.44	124,124,124,124	0
24	MG	A	1697	1/1	0.95	0.20	97,97,97,97	0
24	MG	A	1742	1/1	0.95	0.08	126,126,126,126	0
24	MG	A	1605	1/1	0.95	0.17	137,137,137,137	0
24	MG	S	101	1/1	0.96	0.14	95,95,95,95	0
24	MG	T	201	1/1	0.96	0.16	108,108,108,108	0
24	MG	A	1754	1/1	0.96	0.30	94,94,94,94	0
24	MG	A	1809	1/1	0.96	0.11	102,102,102,102	0
24	MG	A	1728	1/1	0.96	0.19	108,108,108,108	0
24	MG	A	1857	1/1	0.96	0.17	108,108,108,108	0
24	MG	A	1745	1/1	0.96	0.13	138,138,138,138	0
24	MG	A	1635	1/1	0.96	0.19	156,156,156,156	0
24	MG	A	1713	1/1	0.96	0.22	130,130,130,130	0
24	MG	A	1788	1/1	0.96	0.14	100,100,100,100	0
24	MG	F	201	1/1	0.96	0.05	130,130,130,130	0
24	MG	A	1816	1/1	0.96	0.33	99,99,99,99	0
24	MG	A	1727	1/1	0.96	0.24	131,131,131,131	0
24	MG	A	1800	1/1	0.96	0.29	101,101,101,101	0
24	MG	A	1797	1/1	0.96	0.30	140,140,140,140	0
24	MG	A	1647	1/1	0.96	0.17	99,99,99,99	0
24	MG	A	1712	1/1	0.96	0.25	108,108,108,108	0
24	MG	A	1642	1/1	0.96	0.69	127,127,127,127	0
25	K	A	1835	1/1	0.96	0.35	142,142,142,142	0
24	MG	A	1602	1/1	0.96	0.40	123,123,123,123	0
24	MG	A	1611	1/1	0.96	0.04	135,135,135,135	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
24	MG	A	1763	1/1	0.96	0.06	115,115,115,115	0
24	MG	A	1722	1/1	0.96	0.15	86,86,86,86	0
24	MG	A	1736	1/1	0.96	0.11	102,102,102,102	0
24	MG	A	1703	1/1	0.96	0.07	98,98,98,98	0
24	MG	A	1723	1/1	0.96	0.35	117,117,117,117	0
24	MG	A	1689	1/1	0.96	0.25	132,132,132,132	0
24	MG	A	1626	1/1	0.97	0.14	94,94,94,94	0
24	MG	A	1672	1/1	0.97	0.66	101,101,101,101	0
24	MG	A	1751	1/1	0.97	0.43	159,159,159,159	0
24	MG	A	1752	1/1	0.97	0.44	113,113,113,113	0
24	MG	A	1691	1/1	0.97	0.04	132,132,132,132	0
25	K	A	1849	1/1	0.97	0.50	174,174,174,174	0
24	MG	A	1695	1/1	0.97	0.21	129,129,129,129	0
24	MG	A	1621	1/1	0.97	0.17	78,78,78,78	0
24	MG	A	1772	1/1	0.97	0.18	137,137,137,137	0
26	ZN	N	102	1/1	0.97	0.22	161,161,161,161	0
24	MG	A	1651	1/1	0.97	0.17	124,124,124,124	0
25	K	A	1850	1/1	0.97	0.43	187,187,187,187	0
24	MG	A	1726	1/1	0.97	0.21	126,126,126,126	0
24	MG	A	1652	1/1	0.98	0.33	162,162,162,162	0
24	MG	A	1669	1/1	0.98	0.21	137,137,137,137	0
24	MG	A	1639	1/1	0.98	0.06	108,108,108,108	0
24	MG	A	1632	1/1	0.98	0.16	100,100,100,100	0
24	MG	A	1604	1/1	0.98	0.20	145,145,145,145	0
24	MG	A	1740	1/1	0.98	0.18	94,94,94,94	0
24	MG	A	1733	1/1	0.98	0.18	120,120,120,120	0
24	MG	A	1618	1/1	0.98	0.27	136,136,136,136	0
24	MG	A	1729	1/1	0.99	0.16	115,115,115,115	0
24	MG	A	1735	1/1	0.99	0.07	104,104,104,104	0
24	MG	A	1608	1/1	0.99	0.16	108,108,108,108	0
24	MG	A	1734	1/1	0.99	0.43	128,128,128,128	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.