



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 20, 2020 – 01:40 PM BST

PDB ID : 4KVB
Title : Thermus thermophilus HB27 30S ribosomal subunit lacking ribosomal protein S17
Authors : Murphy, E.L.; Jogl, G.
Deposited on : 2013-05-22
Resolution : 4.20 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.13.1
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.13.1

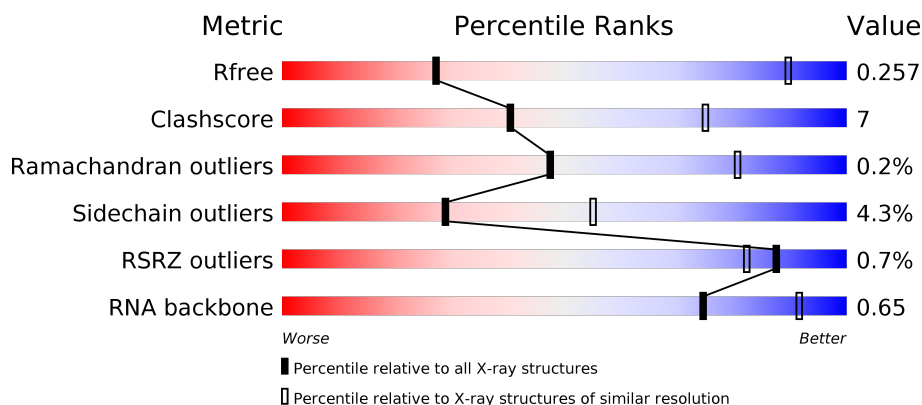
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.20 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	1005 (4.62-3.78)
Clashscore	141614	1044 (4.60-3.80)
Ramachandran outliers	138981	1000 (4.60-3.80)
Sidechain outliers	138945	1007 (4.62-3.78)
RSRZ outliers	127900	1063 (4.70-3.70)
RNA backbone	3102	1049 (5.04-3.00)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	<div> <div></div> <div>61% 30% 8% .</div> </div>
2	B	256	<div> <div>64% 26% . 8%</div> </div>
3	C	239	<div> <div>67% 18% . 14%</div> </div>
4	D	209	<div> <div>79% 19% .</div> </div>

Continued on next page...

Continued from previous page...

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	134	
13	M	126	
14	N	61	
15	O	89	
16	P	88	
17	R	88	
18	S	93	
19	T	106	
20	U	27	

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
21	MG	A	1607	-	-	-	X
21	MG	A	1610	-	-	-	X
21	MG	A	1611	-	-	-	X
21	MG	A	1616	-	-	-	X
21	MG	A	1621	-	-	-	X
21	MG	A	1623	-	-	-	X
21	MG	A	1627	-	-	-	X
21	MG	A	1632	-	-	-	X
21	MG	A	1633	-	-	-	X
21	MG	A	1667	-	-	-	X

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
21	MG	A	1672	-	-	-	X
21	MG	A	1674	-	-	-	X
21	MG	A	1684	-	-	-	X
21	MG	A	1687	-	-	-	X
21	MG	A	1691	-	-	-	X
21	MG	A	1696	-	-	-	X
21	MG	A	1702	-	-	-	X
21	MG	A	1706	-	-	-	X
21	MG	A	1742	-	-	-	X
21	MG	A	1787	-	-	-	X
22	K	A	1755	-	-	-	X
22	K	A	1758	-	-	-	X
22	K	A	1765	-	-	-	X
22	K	A	1780	-	-	-	X
22	K	A	1782	-	-	-	X
22	K	A	1786	-	-	-	X

2 Entry composition

There are 23 unique types of molecules in this entry. The entry contains 51128 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
1	A	1514	Total	C	N	O	P	0	0	0
			32552	14497	6020	10521	1514			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	235	Total	C	N	O	S	0	0	0
			1905	1217	342	341	5			

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

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

- 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
			1011	639	198	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
			794	499	156	138	1			

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

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	3	ALA	-	EXPRESSION TAG	UNP P61941
L	4	LEU	-	EXPRESSION TAG	UNP P61941

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	M	125	Total	C	N	O	S	0	0	0
			997	617	207	171	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	88	Total	C	N	O	S	0	0	0
			734	459	147	126	2			

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

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

- Molecule 17 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
17	R	73	Total	C	N	O	0	0	0
			597	380	118	99			

- Molecule 18 is a protein called 30S ribosomal protein S19.

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

- Molecule 19 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	T	99	Total	C	N	O	S	0	0	0
			762	469	162	129	2			

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

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

- Molecule 21 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
21	D	1	Total	Mg	0	0
			1	1		
21	E	2	Total	Mg	0	0
			2	2		
21	B	1	Total	Mg	0	0
			1	1		
21	A	152	Total	Mg	0	0
			152	152		
21	U	1	Total	Mg	0	0
			1	1		
21	M	1	Total	Mg	0	0
			1	1		

- Molecule 22 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
22	A	35	Total	K	0	0
			35	35		

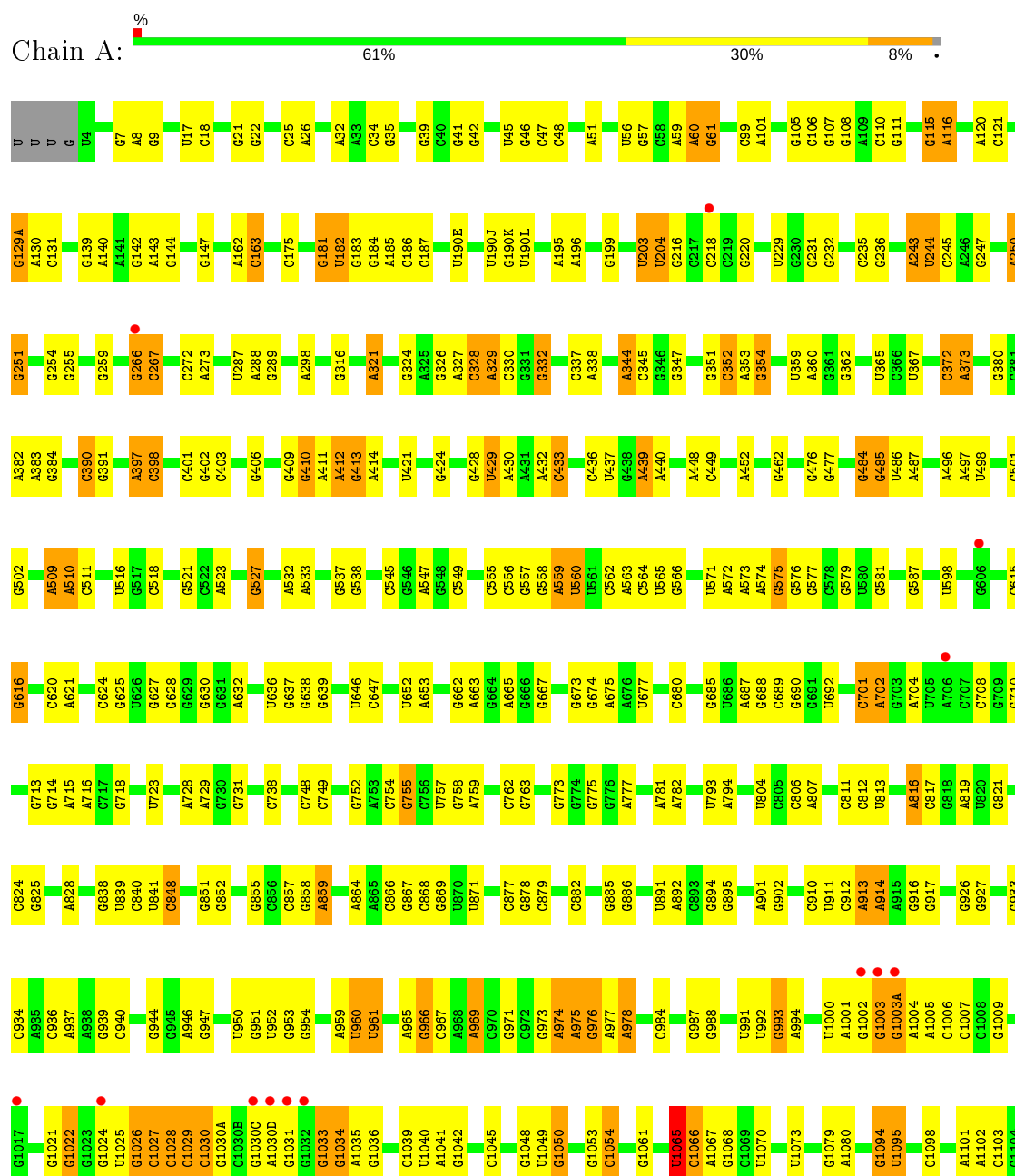
- Molecule 23 is ZINC ION (three-letter code: ZN) (formula: Zn).

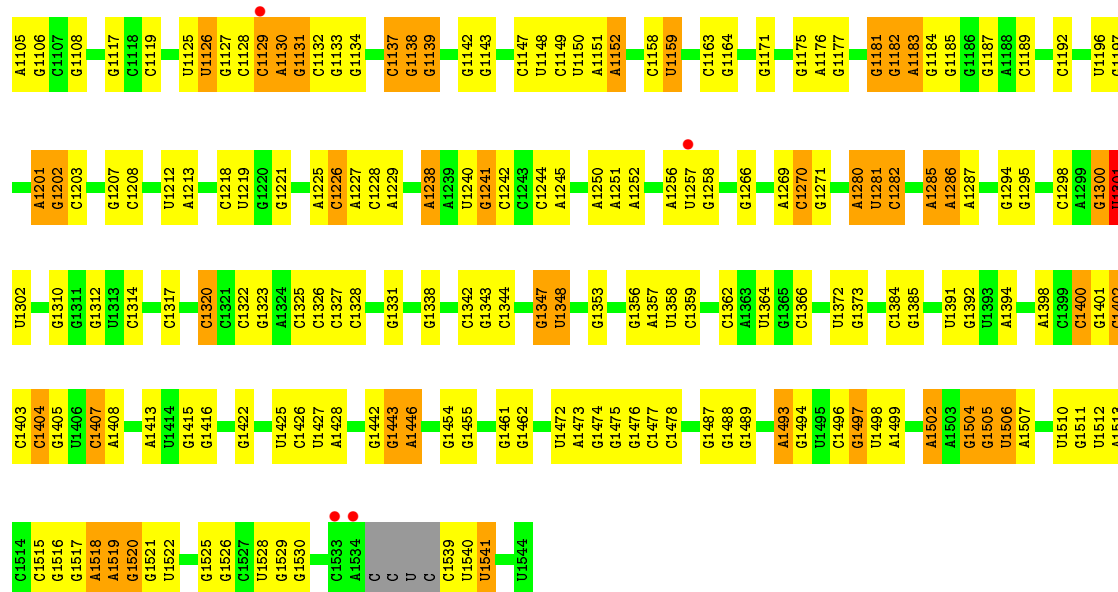
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
23	D	1	Total	Zn	0	0
			1	1		
23	N	1	Total	Zn	0	0
			1	1		

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.

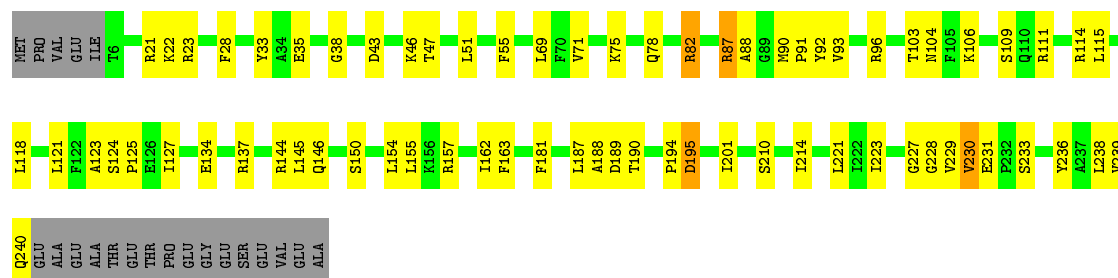
• Molecule 1: 16S rRNA





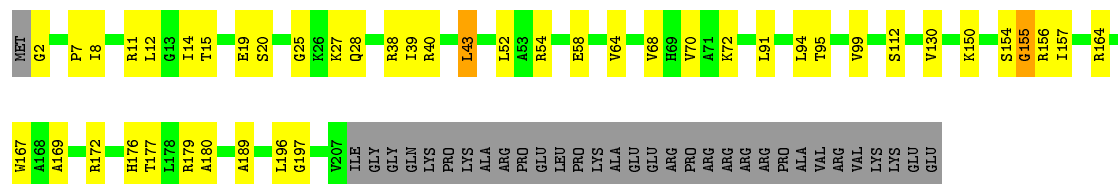
• Molecule 2: 30S ribosomal protein S2

Chain B: 64% 26% 8%



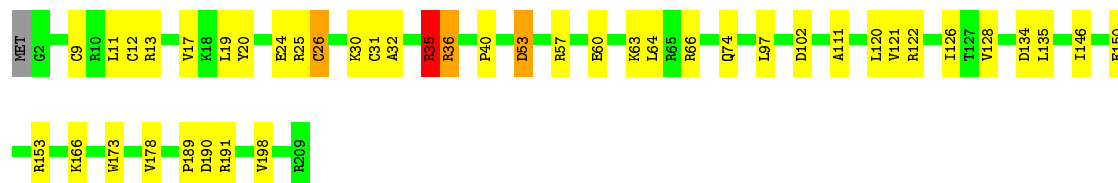
• Molecule 3: 30S ribosomal protein S3

Chain C: 67% 18% 14%

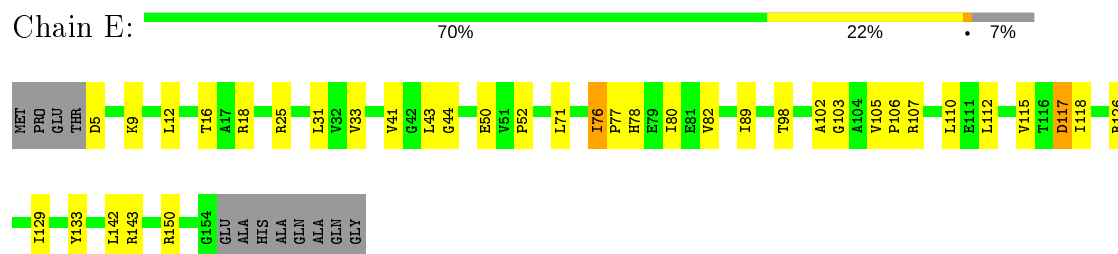


• Molecule 4: 30S ribosomal protein S4

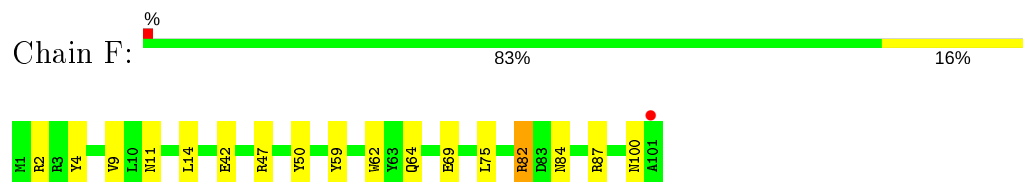
Chain D: 79% 19% 2%



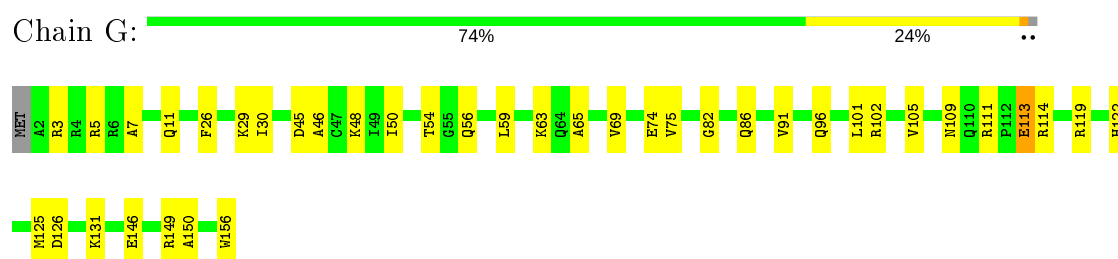
- Molecule 5: 30S ribosomal protein S5



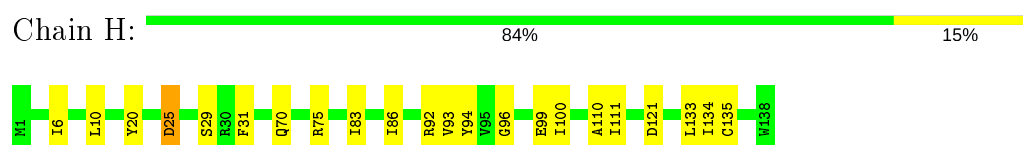
- Molecule 6: 30S ribosomal protein S6



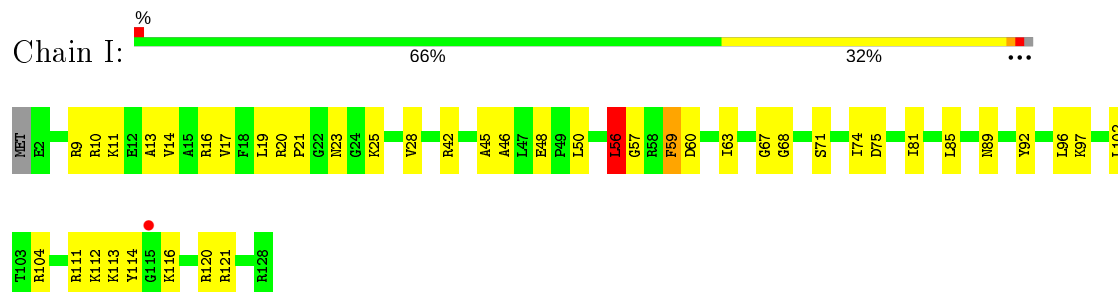
- Molecule 7: 30S ribosomal protein S7



- Molecule 8: 30S ribosomal protein S8

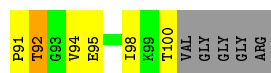
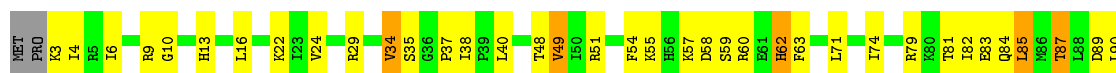


- Molecule 9: 30S ribosomal protein S9

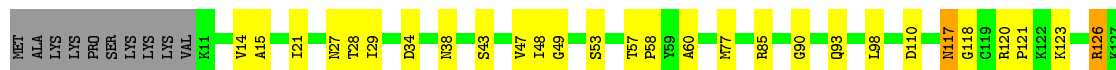


- Molecule 10: 30S ribosomal protein S10

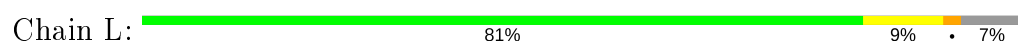




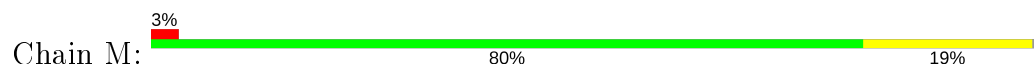
- Molecule 11: 30S ribosomal protein S11



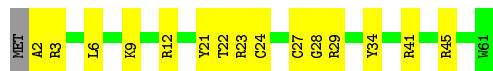
- Molecule 12: 30S ribosomal protein S12



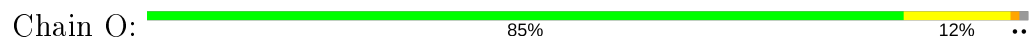
- Molecule 13: 30S ribosomal protein S13



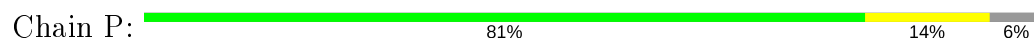
- Molecule 14: 30S ribosomal protein S14 type Z

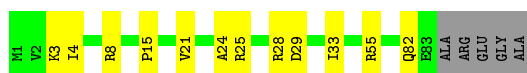


- Molecule 15: 30S ribosomal protein S15

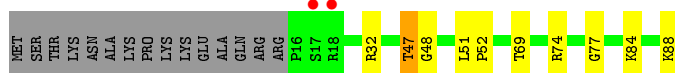
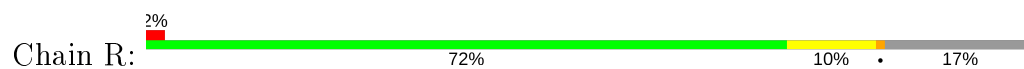


- Molecule 16: 30S ribosomal protein S16

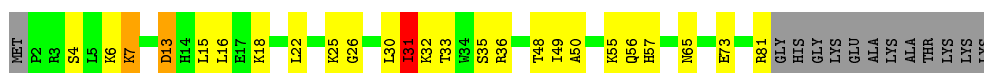




- Molecule 17: 30S ribosomal protein S18



- Molecule 18: 30S ribosomal protein S19



- Molecule 19: 30S ribosomal protein S20



- Molecule 20: 30S ribosomal protein Thx



4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	397.32Å 397.32Å 215.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.91 – 4.20 29.91 – 4.20	Depositor EDS
% Data completeness (in resolution range)	93.0 (29.91-4.20) 93.0 (29.91-4.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.07 (at 4.26Å)	Xtriage
Refinement program	PHENIX dev_1370	Depositor
R, R_{free}	0.217 , 0.258 0.218 , 0.257	Depositor DCC
R_{free} test set	5806 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	202.1	Xtriage
Anisotropy	0.038	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.21 , 126.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.39$, $\langle L^2 \rangle = 0.22$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	51128	wwPDB-VP
Average B, all atoms (Å ²)	200.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.24% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, MA6, K, 0TD, ZN, 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	0.16	0/36091	0.70	11/56323 (0.0%)
2	B	0.23	0/1940	0.42	0/2616
3	C	0.21	0/1636	0.41	0/2205
4	D	0.21	0/1733	0.38	0/2318
5	E	0.22	0/1162	0.42	0/1564
6	F	0.20	0/856	0.40	0/1154
7	G	0.20	0/1276	0.38	0/1709
8	H	0.20	0/1136	0.39	0/1527
9	I	0.23	0/1029	0.45	0/1378
10	J	0.22	0/807	0.44	0/1085
11	K	0.20	0/900	0.40	0/1213
12	L	0.21	0/977	0.44	0/1306
13	M	0.19	0/1008	0.39	0/1347
14	N	0.22	0/501	0.38	0/664
15	O	0.20	0/745	0.35	0/992
16	P	0.20	0/716	0.37	0/963
17	R	0.21	0/603	0.38	0/799
18	S	0.21	0/661	0.42	0/890
19	T	0.24	0/764	0.45	0/1006
20	U	0.19	0/212	0.42	0/277
All	All	0.18	0/54753	0.63	11/81336 (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
4	D	0	1
9	I	0	2

Continued on next page...

Continued from previous page...

Mol	Chain	#Chirality outliers	#Planarity outliers
All	All	0	4

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1054	C	N1-C2-O2	8.18	123.81	118.90
1	A	1054	C	C2-N1-C1'	8.13	127.74	118.80
1	A	1158	C	N1-C2-O2	7.62	123.47	118.90
1	A	1158	C	C2-N1-C1'	7.25	126.77	118.80
1	A	1054	C	N3-C2-O2	-6.42	117.40	121.90
1	A	1158	C	N3-C2-O2	-6.25	117.53	121.90
1	A	1054	C	C6-N1-C1'	-5.73	113.93	120.80
1	A	1301	U	P-O3'-C3'	5.19	125.92	119.70
1	A	1158	C	C6-N1-C2	-5.16	118.23	120.30
1	A	575	G	P-O3'-C3'	5.07	125.78	119.70
1	A	1065	U	P-O3'-C3'	5.02	125.72	119.70

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	C	155	GLY	Peptide
4	D	35	ARG	Peptide
9	I	56	LEU	Peptide
9	I	57	GLY	Peptide

5.2 Too-close contacts

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	32552	0	16453	343	0
2	B	1905	0	1958	41	0
3	C	1612	0	1677	28	0
4	D	1703	0	1763	33	0
5	E	1146	0	1207	24	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	F	843	0	857	9	0
7	G	1257	0	1296	23	0
8	H	1116	0	1177	14	0
9	I	1011	0	1043	28	0
10	J	794	0	840	33	1
11	K	885	0	904	17	0
12	L	972	0	1058	11	0
13	M	997	0	1072	19	0
14	N	492	0	529	13	0
15	O	734	0	771	8	0
16	P	700	0	720	8	0
17	R	597	0	666	8	0
18	S	647	0	673	14	0
19	T	762	0	859	13	0
20	U	208	0	221	5	0
21	A	152	0	0	0	0
21	B	1	0	0	0	0
21	D	1	0	0	0	0
21	E	2	0	0	0	0
21	M	1	0	0	0	0
21	U	1	0	0	0	0
22	A	35	0	0	0	0
23	D	1	0	0	0	0
23	N	1	0	0	0	0
All	All	51128	0	35744	608	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 7.

All (608) 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)
9:I:28:VAL:HG22	9:I:63:ILE:HB	1.67	0.76
1:A:1405:G:HO2'	1:A:1518:MA6:HO2'	1.34	0.74
3:C:58:GLU:HB3	10:J:92:THR:HG21	1.69	0.74
6:F:9:VAL:HB	6:F:87:ARG:HB2	1.70	0.74
1:A:1026:G:O6	1:A:1036:G:N2	2.21	0.73
1:A:959:A:HO2'	1:A:984:C:HO2'	1.33	0.73
2:B:75:LYS:HA	2:B:78:GLN:HB2	1.73	0.71
3:C:155:GLY:HA3	3:C:164:ARG:H	1.54	0.71
1:A:993:G:H1	1:A:1045:C:H42	1.39	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:38:ILE:HB	10:J:71:LEU:HB3	1.71	0.70
1:A:110:C:O2'	16:P:25:ARG:O	2.10	0.69
1:A:587:G:N2	1:A:754:C:OP2	2.24	0.69
3:C:64:VAL:HG23	3:C:99:VAL:HG11	1.74	0.69
3:C:7:PRO:HB3	3:C:11:ARG:HH21	1.57	0.69
3:C:70:VAL:HG12	3:C:72:LYS:H	1.58	0.69
1:A:1366:C:O2'	10:J:60:ARG:NH2	2.26	0.69
2:B:43:ASP:O	2:B:47:THR:OG1	2.10	0.68
1:A:501:C:OP1	12:L:117:ARG:NH2	2.28	0.67
1:A:1266:G:N2	1:A:1269:A:OP2	2.24	0.67
1:A:1539:C:H5'	7:G:82:GLY:HA3	1.77	0.67
2:B:134:GLU:HG2	2:B:137:ARG:HH21	1.61	0.66
1:A:816:A:OP2	1:A:1526:G:O2'	2.14	0.66
17:R:48:GLY:O	17:R:74:ARG:NH2	2.28	0.65
4:D:57:ARG:HH22	5:E:107:ARG:HD3	1.60	0.65
1:A:1505:G:O2'	1:A:1506:U:OP2	2.14	0.65
1:A:410:G:H5''	4:D:25:ARG:HE	1.62	0.65
1:A:953:G:N7	13:M:104:ARG:NH2	2.45	0.64
5:E:33:VAL:HG22	5:E:43:LEU:HD23	1.79	0.64
18:S:33:THR:HG22	18:S:35:SER:H	1.62	0.64
1:A:362:G:N2	1:A:365:U:OP2	2.30	0.64
3:C:155:GLY:HA2	3:C:157:ILE:HG13	1.78	0.64
18:S:22:LEU:O	18:S:26:GLY:N	2.31	0.63
1:A:1226:C:OP2	13:M:103:THR:OG1	2.12	0.63
3:C:20:SER:OG	3:C:40:ARG:NH2	2.31	0.63
9:I:50:LEU:HB3	9:I:56:LEU:HA	1.81	0.63
1:A:380:G:N2	1:A:383:A:OP2	2.29	0.63
14:N:9:LYS:HE2	14:N:23:ARG:HB2	1.81	0.63
1:A:448:A:OP2	1:A:485:G:N2	2.26	0.62
1:A:587:G:OP1	8:H:92:ARG:NH2	2.31	0.62
3:C:11:ARG:NH1	3:C:177:THR:O	2.32	0.62
1:A:718:G:O6	17:R:74:ARG:NH1	2.32	0.62
1:A:951:G:OP2	13:M:102:ARG:NH2	2.32	0.62
1:A:1192:C:O2	5:E:25:ARG:NH2	2.33	0.62
1:A:521:G:OP2	12:L:54:LYS:NZ	2.30	0.62
5:E:9:LYS:HB3	5:E:112:LEU:HD11	1.80	0.62
2:B:223:ILE:O	2:B:227:GLY:N	2.32	0.62
19:T:10:LEU:HG	19:T:12:ALA:H	1.64	0.62
1:A:1035:A:H2'	1:A:1036:G:C8	2.35	0.61
1:A:969:A:H61	13:M:126:LYS:HB2	1.64	0.61
1:A:1006:C:N4	1:A:1022:G:O6	2.32	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:976:G:OP2	1:A:1358:U:O2'	2.19	0.61
1:A:196:A:OP1	19:T:68:LYS:NZ	2.32	0.61
5:E:71:LEU:HD21	5:E:115:VAL:HG22	1.83	0.61
1:A:738:C:H5''	6:F:69:GLU:HB2	1.83	0.61
1:A:1310:G:OP2	13:M:88:ARG:NH2	2.34	0.61
1:A:1392:G:H21	1:A:1502:A:H8	1.49	0.61
1:A:954:G:O6	1:A:1225:A:N6	2.33	0.61
1:A:1314:C:N4	18:S:4:SER:OG	2.32	0.61
4:D:13:ARG:HD3	4:D:36:ARG:HG2	1.81	0.61
11:K:15:ALA:HA	11:K:77:MET:HA	1.83	0.61
14:N:23:ARG:NH1	14:N:28:GLY:O	2.33	0.61
1:A:975:A:H4'	1:A:976:G:H5''	1.82	0.61
13:M:88:ARG:HG3	13:M:98:VAL:HG11	1.81	0.61
1:A:1147:C:O2	9:I:16:ARG:NH1	2.34	0.60
18:S:15:LEU:HD23	18:S:33:THR:HG21	1.82	0.60
7:G:122:HIS:HA	7:G:125:MET:HE2	1.83	0.60
15:O:87:ILE:HG13	15:O:88:ARG:HG2	1.83	0.60
2:B:82:ARG:NH2	2:B:92:TYR:OH	2.34	0.60
1:A:401:C:O2'	1:A:621:A:N3	2.34	0.60
13:M:4:ILE:HG12	13:M:5:ALA:H	1.65	0.60
1:A:1106:G:H5''	3:C:172:ARG:HG2	1.84	0.60
9:I:13:ALA:HB2	9:I:68:GLY:HA3	1.84	0.59
1:A:708:C:OP1	11:K:85:ARG:NH2	2.36	0.59
1:A:558:G:OP2	1:A:559:A:O2'	2.19	0.59
1:A:1002:G:N2	1:A:1039:C:O2	2.36	0.59
1:A:1029:C:OP1	1:A:1033:G:N2	2.35	0.59
2:B:22:LYS:HG3	2:B:23:ARG:HG3	1.84	0.59
18:S:55:LYS:HG2	18:S:56:GLN:HG3	1.85	0.59
1:A:1003:G:O2'	1:A:1003(A):G:N7	2.36	0.58
4:D:128:VAL:HG22	4:D:146:ILE:HG13	1.85	0.58
1:A:1405:G:H1	1:A:1496:C:H42	1.51	0.58
10:J:24:VAL:HG21	10:J:37:PRO:HD3	1.84	0.58
1:A:259:G:H1	1:A:267:C:H42	1.51	0.58
5:E:102:ALA:HB1	5:E:106:PRO:HG2	1.85	0.58
2:B:123:ALA:H	2:B:127:ILE:HD11	1.67	0.58
3:C:14:ILE:HG22	3:C:15:THR:HG23	1.84	0.58
5:E:76:ILE:HG13	5:E:77:PRO:HD2	1.84	0.58
1:A:563:A:HO2'	1:A:566:G:HO2'	1.51	0.58
15:O:26:GLU:OE1	15:O:77:ARG:NH1	2.35	0.58
1:A:1203:C:OP1	14:N:2:ALA:N	2.36	0.58
13:M:16:ASP:OD1	13:M:16:ASP:N	2.36	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1132:C:H2'	1:A:1133:G:H8	1.69	0.58
9:I:25:LYS:N	9:I:60:ASP:OD1	2.37	0.58
1:A:1422:G:H1	1:A:1478:C:H42	1.52	0.58
1:A:115:G:H4'	1:A:116:A:O5'	2.03	0.58
1:A:243:A:H4'	1:A:244:U:O5'	2.02	0.58
11:K:123:LYS:HA	11:K:126:ARG:HG3	1.86	0.58
1:A:1326:C:OP1	20:U:12:LYS:NZ	2.37	0.58
1:A:1413:A:H2	1:A:1487:G:H22	1.51	0.57
18:S:13:ASP:HA	18:S:16:LEU:HB3	1.86	0.57
19:T:54:LYS:HA	19:T:57:ARG:HD2	1.86	0.57
1:A:18:C:H1'	1:A:1079:G:H21	1.69	0.57
1:A:1128:C:H42	1:A:1143:G:H1	1.50	0.57
9:I:17:VAL:HG11	9:I:81:ILE:HG12	1.87	0.57
1:A:882:C:OP2	12:L:13:LYS:NZ	2.37	0.57
1:A:574:A:O2'	1:A:882:C:O2'	2.19	0.57
12:L:46:LYS:HG3	12:L:48:PRO:HD2	1.87	0.57
2:B:69:LEU:HB3	2:B:162:ILE:HG22	1.86	0.57
4:D:26:CYS:HA	4:D:31:CYS:HB2	1.87	0.57
1:A:1119:C:OP2	9:I:9:ARG:NH2	2.38	0.57
1:A:775:G:N2	1:A:804:U:O4	2.37	0.57
6:F:14:LEU:HD11	6:F:84:ASN:HB3	1.86	0.56
10:J:48:THR:O	14:N:34:TYR:OH	2.23	0.56
10:J:6:ILE:HG12	10:J:98:ILE:HG23	1.86	0.56
1:A:574:A:HO2'	1:A:882:C:HO2'	1.54	0.56
1:A:581:G:N2	1:A:759:A:OP2	2.36	0.56
10:J:29:ARG:NH1	10:J:84:GLN:OE1	2.35	0.56
1:A:372:C:H4'	1:A:373:A:O5'	2.05	0.56
3:C:52:LEU:HA	3:C:70:VAL:HG22	1.87	0.56
1:A:652:U:O4	1:A:752:G:O2'	2.20	0.56
2:B:187:LEU:HA	2:B:201:ILE:HB	1.88	0.56
7:G:105:VAL:O	7:G:109:ASN:ND2	2.39	0.56
9:I:45:ALA:O	9:I:48:GLU:HB2	2.06	0.56
1:A:235:C:H2'	1:A:236:G:H8	1.70	0.55
10:J:3:LYS:N	10:J:74:ILE:O	2.39	0.55
11:K:110:ASP:OD2	17:R:88:LYS:NZ	2.39	0.55
18:S:31:ILE:HG22	18:S:49:ILE:HA	1.88	0.55
1:A:1515:C:H2'	1:A:1516:G:H8	1.71	0.55
5:E:5:ASP:OD1	5:E:5:ASP:N	2.40	0.55
3:C:91:LEU:HD21	3:C:99:VAL:HG22	1.87	0.55
14:N:3:ARG:HB3	14:N:6:LEU:HD23	1.89	0.55
1:A:1150:U:O4	1:A:1151:A:N6	2.40	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:484:G:H4'	1:A:485:G:O5'	2.05	0.55
1:A:944:G:N1	1:A:1338:G:OP2	2.38	0.55
10:J:79:ARG:HD2	10:J:82:ILE:HD12	1.89	0.55
1:A:1238:A:H62	1:A:1301:U:H3	1.56	0.54
9:I:46:ALA:HB2	9:I:74:ILE:HG23	1.89	0.54
1:A:987:G:H2'	1:A:988:G:H8	1.72	0.54
3:C:130:VAL:HG21	3:C:157:ILE:HG23	1.90	0.54
19:T:10:LEU:HD12	19:T:11:SER:H	1.72	0.54
1:A:523:A:H61	12:L:92:0TD:CG	2.21	0.54
10:J:48:THR:HA	10:J:62:HIS:HB3	1.89	0.54
5:E:102:ALA:O	5:E:107:ARG:NH1	2.40	0.54
1:A:1252:A:H61	1:A:1285:A:H61	1.55	0.54
7:G:29:LYS:HG3	7:G:101:LEU:HB3	1.89	0.54
19:T:67:ALA:O	19:T:73:HIS:ND1	2.41	0.54
19:T:50:GLU:HA	19:T:100:ILE:HG22	1.89	0.53
1:A:1187:G:O2'	9:I:111:ARG:NH1	2.41	0.53
1:A:231:G:H2'	1:A:232:G:H8	1.73	0.53
1:A:1137:C:H4'	1:A:1138:G:C2	2.44	0.53
7:G:150:ALA:HA	11:K:57:THR:HG21	1.91	0.53
1:A:1080:A:H5''	5:E:16:THR:HG21	1.90	0.53
1:A:1098:C:OP2	2:B:144:ARG:NH2	2.41	0.53
1:A:21:G:H2'	1:A:22:G:C8	2.43	0.53
4:D:63:LYS:HD2	4:D:198:VAL:HG22	1.91	0.53
1:A:147:G:H1	1:A:175:C:H42	1.57	0.53
1:A:545:C:O2'	1:A:549:C:OP1	2.26	0.53
2:B:51:LEU:HD21	2:B:201:ILE:HG23	1.91	0.53
1:A:662:G:H2'	1:A:663:A:C8	2.44	0.53
10:J:49:VAL:HG23	14:N:41:ARG:HB2	1.91	0.53
5:E:76:ILE:HG23	5:E:78:HIS:H	1.73	0.53
8:H:10:LEU:HD22	8:H:83:ILE:HD11	1.90	0.52
1:A:1342:C:H2'	1:A:1343:G:C8	2.44	0.52
1:A:139:G:H2'	1:A:140:A:H8	1.73	0.52
1:A:1493:A:HO2'	1:A:1494:G:H8	1.57	0.52
1:A:673:G:H2'	1:A:674:G:C8	2.44	0.52
1:A:757:U:H2'	1:A:758:G:O4'	2.09	0.52
2:B:121:LEU:O	2:B:124:SER:OG	2.21	0.52
4:D:53:ASP:O	4:D:57:ARG:HG2	2.09	0.52
10:J:16:LEU:HD23	10:J:94:VAL:HG22	1.91	0.52
1:A:410:G:H5'	4:D:30:LYS:HD3	1.92	0.52
5:E:31:LEU:HD11	5:E:129:ILE:HA	1.91	0.52
13:M:33:ALA:O	13:M:37:THR:OG1	2.20	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1094:G:O2'	1:A:1108:G:N2	2.43	0.52
1:A:773:G:H1	1:A:806:C:H42	1.57	0.52
13:M:87:TYR:CZ	13:M:91:ARG:HD3	2.44	0.52
1:A:344:A:H5''	1:A:345:C:H5	1.74	0.52
1:A:324:G:N2	1:A:327:A:OP2	2.43	0.51
1:A:579:G:H5'	1:A:728:A:H1'	1.92	0.51
1:A:143:A:H2	1:A:220:G:H22	1.58	0.51
1:A:811:C:O2'	1:A:901:A:N1	2.43	0.51
3:C:177:THR:HB	3:C:180:ALA:HB2	1.90	0.51
16:P:21:VAL:HG12	16:P:33:ILE:HD12	1.91	0.51
1:A:1427:U:H2'	1:A:1428:A:H8	1.76	0.51
1:A:715:A:H2'	1:A:716:A:C8	2.46	0.51
9:I:42:ARG:NH2	9:I:71:SER:OG	2.36	0.51
7:G:146:GLU:HA	7:G:149:ARG:HG2	1.93	0.51
1:A:891:U:H2'	1:A:892:A:H8	1.76	0.51
10:J:4:ILE:HG22	10:J:100:THR:HG22	1.93	0.51
1:A:56:U:H2'	1:A:57:G:C8	2.45	0.51
3:C:8:ILE:O	3:C:12:LEU:N	2.44	0.51
1:A:624:C:H2'	1:A:625:G:H8	1.76	0.51
1:A:806:C:H2'	1:A:807:A:H8	1.76	0.51
2:B:188:ALA:N	2:B:201:ILE:O	2.40	0.51
1:A:462:G:N2	16:P:82:GLN:OE1	2.33	0.50
1:A:1454:G:H2'	1:A:1455:G:H8	1.77	0.50
1:A:501:C:H2'	1:A:502:G:C8	2.47	0.50
1:A:855:G:OP2	1:A:871:U:N3	2.45	0.50
1:A:973:G:H3'	1:A:974:A:H5''	1.94	0.50
2:B:28:PHE:HD1	2:B:194:PRO:HG3	1.77	0.50
1:A:1516:G:N2	1:A:1519:MA6:OP2	2.33	0.50
1:A:559:A:OP2	5:E:126:ARG:NH2	2.44	0.50
1:A:859:A:OP2	1:A:869:G:N2	2.38	0.50
8:H:86:ILE:HG22	8:H:93:VAL:HG21	1.93	0.50
11:K:21:ILE:HD11	11:K:98:LEU:HD12	1.94	0.50
2:B:91:PRO:HG2	2:B:155:LEU:HG	1.93	0.50
1:A:1270:C:H2'	1:A:1271:G:H8	1.76	0.50
1:A:1218:C:H2'	1:A:1219:U:C6	2.47	0.49
1:A:244:U:O4'	1:A:894:G:N2	2.45	0.49
7:G:54:THR:HG22	7:G:56:GLN:H	1.76	0.49
1:A:272:C:H2'	1:A:273:A:H8	1.77	0.49
1:A:987:G:H2'	1:A:988:G:C8	2.47	0.49
4:D:64:LEU:HB2	4:D:198:VAL:HG11	1.93	0.49
15:O:26:GLU:HA	15:O:81:LEU:HD11	1.93	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1159:U:O4'	1:A:1182:G:N2	2.45	0.49
1:A:913:A:H4'	1:A:914:A:O5'	2.13	0.49
10:J:9:ARG:HG3	10:J:95:GLU:HB3	1.93	0.49
1:A:523:A:N6	12:L:92:OTD:OD2	2.44	0.49
1:A:1373:G:O6	9:I:11:LYS:NZ	2.29	0.49
10:J:40:LEU:HD11	10:J:71:LEU:HB2	1.93	0.49
11:K:58:PRO:HB2	11:K:93:GLN:HG3	1.93	0.49
1:A:1001:A:H2	1:A:1040:U:H3	1.59	0.49
1:A:1152:A:H5''	10:J:13:HIS:HB2	1.94	0.49
1:A:1294:G:H2'	1:A:1295:G:H8	1.76	0.49
15:O:39:LEU:HD11	15:O:52:SER:HB3	1.94	0.49
3:C:64:VAL:H	3:C:99:VAL:HB	1.77	0.49
1:A:1108:G:H5''	3:C:176:HIS:CE1	2.47	0.49
2:B:51:LEU:HD22	2:B:55:PHE:HE2	1.78	0.49
1:A:974:A:P	14:N:41:ARG:HH12	2.36	0.49
1:A:266:G:H4'	1:A:267:C:O5'	2.12	0.49
4:D:11:LEU:HD13	4:D:66:ARG:HD3	1.94	0.49
4:D:102:ASP:N	4:D:102:ASP:OD1	2.45	0.49
1:A:1294:G:H2'	1:A:1295:G:C8	2.48	0.49
1:A:838:G:N2	1:A:848:C:O2	2.44	0.49
4:D:111:ALA:HB2	4:D:120:LEU:HD12	1.95	0.49
1:A:565:U:OP2	1:A:566:G:O2'	2.30	0.48
1:A:946:A:H2'	1:A:947:G:C8	2.47	0.48
4:D:35:ARG:O	4:D:35:ARG:HD2	2.12	0.48
1:A:1281:U:H5'	1:A:1282:C:H5	1.78	0.48
1:A:410:G:H3'	4:D:25:ARG:HH21	1.77	0.48
1:A:636:U:H2'	1:A:637:G:C8	2.48	0.48
1:A:250:A:H4'	1:A:251:G:O5'	2.13	0.48
1:A:974:A:OP2	14:N:29:ARG:NH2	2.45	0.48
4:D:190:ASP:OD1	4:D:191:ARG:N	2.45	0.48
7:G:111:ARG:HB3	7:G:113:GLU:HG2	1.94	0.48
1:A:1427:U:H2'	1:A:1428:A:C8	2.48	0.48
1:A:1028:C:H3'	1:A:1033:G:H22	1.77	0.48
1:A:316:G:OP2	1:A:351:G:O2'	2.31	0.48
1:A:337:C:H2'	1:A:338:A:C8	2.48	0.48
2:B:189:ASP:OD1	2:B:190:THR:N	2.39	0.48
4:D:13:ARG:HB3	4:D:40:PRO:HD3	1.96	0.48
14:N:24:CYS:O	14:N:28:GLY:N	2.42	0.48
7:G:75:VAL:HG21	7:G:86:GLN:HB3	1.96	0.48
11:K:27:ASN:OD1	11:K:28:THR:N	2.46	0.48
13:M:22:ILE:HB	13:M:25:ILE:HB	1.95	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:P:8:ARG:HE	16:P:15:PRO:HB3	1.78	0.48
5:E:98:THR:N	5:E:117:ASP:OD2	2.47	0.48
7:G:91:VAL:O	7:G:96:GLN:NE2	2.46	0.48
1:A:910:C:OP1	12:L:97:ARG:NH1	2.42	0.48
1:A:1048:G:H5''	14:N:3:ARG:HG3	1.95	0.48
1:A:1250:A:H2'	1:A:1251:A:C8	2.48	0.48
2:B:21:ARG:NE	2:B:38:GLY:HA2	2.28	0.48
1:A:1139:G:N2	1:A:1142:G:O6	2.41	0.47
1:A:1519:MA6:O5'	1:A:1519:MA6:H8	2.14	0.47
1:A:106:C:H2'	1:A:107:G:H8	1.78	0.47
1:A:620:C:C2	4:D:135:LEU:HD13	2.49	0.47
16:P:4:ILE:HG12	16:P:21:VAL:HG22	1.96	0.47
1:A:105:G:OP1	19:T:22:ARG:NH2	2.47	0.47
1:A:328:C:H4'	1:A:329:A:C5'	2.45	0.47
1:A:439:A:C5	1:A:440:A:H1'	2.49	0.47
1:A:950:U:H2'	1:A:951:G:H8	1.78	0.47
1:A:1095:U:OP1	1:A:1108:G:N2	2.45	0.47
1:A:638:G:H2'	1:A:639:G:H8	1.78	0.47
1:A:41:G:H2'	1:A:42:G:H8	1.79	0.47
5:E:110:LEU:HD13	5:E:118:ILE:HG21	1.94	0.47
7:G:74:GLU:HG2	7:G:91:VAL:HG22	1.96	0.47
1:A:272:C:H2'	1:A:273:A:C8	2.49	0.47
1:A:824:C:H2'	1:A:825:G:C8	2.49	0.47
12:L:117:ARG:HB3	12:L:122:THR:O	2.15	0.47
1:A:1151:A:HO2'	1:A:1152:A:H8	1.62	0.47
1:A:1347:G:O6	9:I:10:ARG:NH2	2.35	0.47
10:J:63:PHE:HE2	14:N:45:ARG:HA	1.80	0.47
1:A:1026:G:H2'	1:A:1027:C:H5''	1.97	0.47
1:A:1175:G:H2'	1:A:1176:A:H8	1.79	0.47
1:A:571:U:O4	1:A:864:A:N6	2.47	0.47
1:A:627:G:H2'	1:A:628:G:H8	1.80	0.47
3:C:25:GLY:H	3:C:28:GLN:HB2	1.78	0.47
11:K:48:ILE:HG22	11:K:49:GLY:H	1.80	0.47
4:D:24:GLU:HG2	4:D:25:ARG:H	1.79	0.47
9:I:23:ASN:N	9:I:60:ASP:OD2	2.47	0.47
1:A:885:G:H2'	1:A:886:G:H8	1.79	0.47
2:B:118:LEU:HD23	2:B:121:LEU:HD12	1.96	0.47
1:A:560:U:H5'	1:A:566:G:N2	2.29	0.47
1:A:939:G:O3'	7:G:102:ARG:NH2	2.48	0.47
1:A:1151:A:H5'	10:J:40:LEU:O	2.15	0.47
1:A:401:C:H2'	1:A:402:G:H8	1.79	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:41:G:H2'	1:A:42:G:C8	2.50	0.46
1:A:559:A:H4'	1:A:560:U:O5'	2.15	0.46
18:S:31:ILE:HG12	18:S:32:LYS:H	1.80	0.46
10:J:6:ILE:HG23	10:J:98:ILE:HG12	1.96	0.46
1:A:689:C:H2'	1:A:690:G:O4'	2.15	0.46
7:G:65:ALA:O	7:G:69:VAL:HG23	2.16	0.46
10:J:54:PHE:CD2	10:J:55:LYS:HG2	2.50	0.46
11:K:57:THR:HG22	11:K:60:ALA:H	1.80	0.46
1:A:1391:U:H2'	1:A:1392:G:C8	2.51	0.46
1:A:911:U:H2'	1:A:912:C:C6	2.51	0.46
3:C:19:GLU:HG2	3:C:54:ARG:HH21	1.80	0.46
9:I:21:PRO:HA	9:I:59:PHE:HB3	1.96	0.46
18:S:50:ALA:HB1	18:S:57:HIS:HB3	1.98	0.46
1:A:1415:G:H2'	1:A:1416:G:C8	2.50	0.46
1:A:99:C:H2'	1:A:101:A:C8	2.49	0.46
10:J:82:ILE:HA	10:J:85:LEU:HB2	1.97	0.46
2:B:239:VAL:HG12	2:B:240:GLN:HG2	1.98	0.46
1:A:1269:A:HO2'	1:A:1325:C:HO2'	1.64	0.46
2:B:114:ARG:HH21	2:B:118:LEU:HD21	1.80	0.46
1:A:1443:G:H4'	1:A:1446:A:O5'	2.16	0.46
1:A:254:G:H2'	1:A:255:G:H8	1.80	0.46
1:A:674:G:H2'	1:A:675:A:H8	1.80	0.46
5:E:142:LEU:O	5:E:143:ARG:NE	2.46	0.46
1:A:674:G:H2'	1:A:675:A:C8	2.51	0.46
2:B:195:ASP:OD1	2:B:195:ASP:N	2.49	0.46
2:B:87:ARG:NH2	2:B:233:SER:HB2	2.31	0.46
2:B:103:THR:OG1	2:B:104:ASN:N	2.49	0.46
7:G:46:ALA:O	7:G:50:ILE:HG12	2.15	0.46
1:A:1300:G:O2'	1:A:1301:U:O5'	2.29	0.45
1:A:129(A):G:H21	1:A:190(E):U:H3'	1.80	0.45
1:A:1177:G:OP2	9:I:97:LYS:NZ	2.37	0.45
1:A:1344:C:H4'	9:I:120:ARG:HB3	1.98	0.45
1:A:1356:G:H2'	1:A:1357:A:C8	2.51	0.45
1:A:1506:U:N3	1:A:1522:U:OP1	2.41	0.45
1:A:1505:G:O2'	1:A:1541:PSU:OP2	2.31	0.45
2:B:88:ALA:HB1	2:B:90:MET:HG2	1.96	0.45
6:F:11:ASN:HB3	6:F:14:LEU:HG	1.97	0.45
1:A:328:C:H4'	1:A:329:A:O5'	2.16	0.45
8:H:6:ILE:HD12	8:H:6:ILE:H	1.81	0.45
1:A:1281:U:H4'	1:A:1282:C:OP2	2.17	0.45
1:A:476:G:H2'	1:A:477:G:C8	2.52	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:559:A:H1'	1:A:560:U:OP2	2.16	0.45
1:A:701:C:H4'	1:A:702:A:O5'	2.16	0.45
5:E:50:GLU:HG3	5:E:52:PRO:HD2	1.97	0.45
1:A:1105:A:H2'	1:A:1106:G:H8	1.81	0.45
1:A:1515:C:H2'	1:A:1516:G:C8	2.50	0.45
1:A:556:C:H2'	1:A:557:G:O4'	2.16	0.45
2:B:21:ARG:NE	2:B:35:GLU:OE2	2.42	0.45
9:I:96:LEU:HB3	9:I:102:LEU:HD21	1.97	0.45
1:A:1510:U:H2'	1:A:1511:G:C8	2.51	0.45
1:A:692:U:H3	11:K:53:SER:HB3	1.82	0.45
1:A:409:G:H1	1:A:433:C:H42	1.65	0.45
8:H:111:ILE:HG22	8:H:134:ILE:HD12	1.99	0.45
12:L:38:THR:N	12:L:57:LYS:O	2.38	0.45
13:M:4:ILE:HA	13:M:57:ARG:HD3	1.98	0.45
1:A:203:U:O2'	1:A:204:U:O5'	2.26	0.45
1:A:685:G:N1	1:A:704:A:OP2	2.46	0.45
1:A:868:C:H2'	1:A:869:G:O4'	2.15	0.45
1:A:403:C:OP2	4:D:74:GLN:NE2	2.47	0.45
5:E:43:LEU:HD22	5:E:44:GLY:H	1.82	0.45
1:A:1250:A:O3'	9:I:67:GLY:HA2	2.17	0.45
1:A:1129:C:N4	1:A:1134:G:N7	2.65	0.45
1:A:390:C:H2'	1:A:391:G:C8	2.52	0.45
1:A:728:A:H2'	1:A:729:A:H8	1.81	0.45
3:C:189:ALA:HB3	3:C:196:LEU:HB2	1.98	0.45
8:H:110:ALA:HB3	8:H:121:ASP:HB3	1.98	0.45
1:A:1065:U:H1'	1:A:1066:C:OP2	2.17	0.45
1:A:1461:G:H2'	1:A:1462:G:H8	1.81	0.45
1:A:162:A:C5	1:A:163:C:H1'	2.51	0.45
1:A:190(L):U:O2	19:T:105:SER:OG	2.29	0.45
1:A:337:C:H2'	1:A:338:A:H8	1.81	0.45
1:A:969:A:N6	13:M:126:LYS:HE3	2.32	0.45
13:M:10:PRO:HB2	13:M:18:ALA:HB1	1.99	0.45
1:A:142:G:H2'	1:A:143:A:H8	1.82	0.44
9:I:89:ASN:HB3	9:I:92:TYR:CD2	2.52	0.44
1:A:190(J):U:H2'	1:A:190(K):G:C8	2.52	0.44
19:T:20:LEU:O	19:T:23:ARG:HB3	2.17	0.44
1:A:1488:G:H2'	1:A:1489:G:C8	2.52	0.44
1:A:410:G:OP1	4:D:30:LYS:NZ	2.40	0.44
1:A:950:U:H2'	1:A:951:G:C8	2.51	0.44
4:D:32:ALA:O	4:D:36:ARG:HB2	2.18	0.44
1:A:186:C:H2'	1:A:187:C:C6	2.53	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:509:A:O2'	1:A:510:A:OP1	2.34	0.44
7:G:111:ARG:NH2	7:G:126:ASP:OD2	2.48	0.44
10:J:57:LYS:O	10:J:58:ASP:HB2	2.18	0.44
1:A:1320:C:O2	18:S:36:ARG:NH1	2.50	0.44
1:A:1030:C:N4	1:A:1031:G:N7	2.58	0.44
1:A:254:G:H2'	1:A:255:G:C8	2.52	0.44
1:A:45:U:H2'	1:A:46:G:C8	2.52	0.44
1:A:1298:C:P	7:G:114:ARG:HH22	2.40	0.44
18:S:6:LYS:HG2	18:S:7:LYS:HD3	1.98	0.44
1:A:448:A:H2'	1:A:449:C:C6	2.52	0.44
1:A:555:C:H2'	1:A:556:C:C6	2.53	0.44
1:A:713:G:H2'	1:A:714:G:C8	2.53	0.44
2:B:123:ALA:N	2:B:127:ILE:HD11	2.31	0.44
1:A:1372:U:H2'	1:A:1373:G:O4'	2.17	0.44
1:A:34:C:H2'	1:A:35:G:C8	2.53	0.44
6:F:62:TRP:CH2	6:F:64:GLN:HB2	2.52	0.44
1:A:1130:A:H4'	9:I:20:ARG:HH22	1.82	0.44
1:A:1242:C:H42	1:A:1295:G:H1	1.66	0.44
12:L:33:ARG:HA	12:L:33:ARG:HD2	1.76	0.44
1:A:1007:C:H42	1:A:1022:G:H1	1.64	0.44
4:D:57:ARG:HH12	5:E:107:ARG:HE	1.65	0.44
5:E:129:ILE:H	5:E:129:ILE:HD12	1.82	0.44
10:J:10:GLY:N	10:J:16:LEU:HD11	2.33	0.44
1:A:1103:C:OP1	2:B:96:ARG:NH1	2.51	0.43
1:A:1131:G:H2'	1:A:1132:C:C6	2.53	0.43
1:A:321:A:H61	1:A:332:G:H1	1.66	0.43
1:A:59:A:H1'	1:A:354:G:N2	2.33	0.43
1:A:936:C:H2'	1:A:937:A:O4'	2.17	0.43
9:I:10:ARG:HG2	9:I:75:ASP:HB2	2.00	0.43
1:A:1240:U:OP1	7:G:119:ARG:NH1	2.41	0.43
1:A:1244:C:H2'	1:A:1245:A:C8	2.53	0.43
2:B:146:GLN:O	2:B:150:SER:HB2	2.17	0.43
8:H:96:GLY:O	8:H:100:ILE:HG13	2.17	0.43
16:P:3:LYS:HD3	16:P:24:ALA:HB2	2.00	0.43
1:A:1461:G:H2'	1:A:1462:G:C8	2.53	0.43
1:A:1520:G:H2'	1:A:1521:G:C8	2.53	0.43
1:A:762:C:H2'	1:A:763:G:C8	2.53	0.43
1:A:851:G:H2'	1:A:852:G:C8	2.53	0.43
10:J:34:VAL:HG12	10:J:35:SER:H	1.83	0.43
11:K:43:SER:HA	11:K:47:VAL:HG21	2.00	0.43
1:A:106:C:H2'	1:A:107:G:C8	2.53	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1384:C:H2'	1:A:1385:G:H8	1.83	0.43
1:A:486:U:H2'	1:A:487:A:H8	1.83	0.43
1:A:716:A:N3	11:K:118:GLY:HA2	2.33	0.43
4:D:60:GLU:HG3	4:D:198:VAL:HG13	2.00	0.43
4:D:57:ARG:HH12	5:E:107:ARG:NE	2.15	0.43
10:J:79:ARG:HA	10:J:82:ILE:HG13	2.00	0.43
19:T:16:HIS:O	19:T:19:SER:OG	2.18	0.43
1:A:110:C:H2'	1:A:111:G:O4'	2.19	0.43
1:A:1201:A:H1'	1:A:1202:G:OP2	2.18	0.43
1:A:1472:U:H2'	1:A:1473:A:C8	2.53	0.43
1:A:7:G:H5''	1:A:298:A:O4'	2.18	0.43
13:M:37:THR:HG22	13:M:55:ARG:HD2	2.00	0.43
1:A:667:G:O2'	15:O:49:ASP:OD1	2.31	0.43
1:A:1035:A:H2'	1:A:1036:G:H8	1.82	0.43
1:A:1270:C:H2'	1:A:1271:G:C8	2.54	0.43
1:A:1425:U:H3	1:A:1475:G:H1	1.67	0.43
1:A:229:U:H5''	16:P:33:ILE:HD13	2.01	0.43
9:I:71:SER:O	9:I:74:ILE:HB	2.19	0.43
11:K:117:ASN:N	11:K:117:ASN:OD1	2.52	0.43
1:A:1454:G:H2'	1:A:1455:G:C8	2.54	0.43
1:A:1392:G:N2	1:A:1502:A:H8	2.14	0.43
1:A:677:U:H3	1:A:713:G:H22	1.65	0.43
1:A:939:G:H2'	1:A:940:C:C6	2.54	0.43
1:A:952:U:H2'	1:A:953:G:C8	2.54	0.43
3:C:15:THR:HG21	3:C:179:ARG:HA	2.00	0.43
11:K:34:ASP:OD1	11:K:38:ASN:N	2.52	0.43
16:P:28:ARG:NH1	16:P:29:ASP:OD1	2.51	0.43
1:A:1426:C:H2'	1:A:1427:U:C6	2.54	0.43
1:A:757:U:O2'	1:A:879:C:O2	2.32	0.43
1:A:1244:C:H2'	1:A:1245:A:H8	1.84	0.43
1:A:537:G:H2'	1:A:538:G:C8	2.54	0.43
1:A:728:A:H2'	1:A:729:A:C8	2.53	0.43
20:U:5:ASP:O	20:U:11:GLY:HA3	2.19	0.43
1:A:1181:G:O2'	1:A:1184:G:H5'	2.19	0.43
2:B:90:MET:HA	2:B:91:PRO:HD3	1.87	0.43
4:D:25:ARG:NH1	4:D:30:LYS:O	2.52	0.43
1:A:1132:C:H2'	1:A:1133:G:C8	2.52	0.42
1:A:1504:G:OP1	1:A:1507:A:H4'	2.18	0.42
1:A:1512:U:H2'	1:A:1513:A:C8	2.54	0.42
1:A:25:C:H2'	1:A:26:A:C8	2.54	0.42
1:A:287:U:H2'	1:A:288:A:H8	1.82	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:59:LEU:HD11	7:G:63:LYS:HE3	2.01	0.42
1:A:108:G:OP2	1:A:326:G:N1	2.47	0.42
1:A:1175:G:H2'	1:A:1176:A:C8	2.54	0.42
1:A:1050:G:N2	1:A:1208:C:O2	2.52	0.42
1:A:978:A:O2'	1:A:1322:C:N3	2.50	0.42
1:A:1415:G:H2'	1:A:1416:G:H8	1.84	0.42
1:A:615:C:H2'	1:A:616:G:O4'	2.18	0.42
1:A:680:C:H42	1:A:710:G:H1	1.67	0.42
2:B:124:SER:HB2	2:B:125:PRO:HD2	2.02	0.42
2:B:91:PRO:HA	2:B:154:LEU:HD12	2.00	0.42
14:N:9:LYS:HD3	14:N:21:TYR:O	2.19	0.42
1:A:1327:C:H2'	1:A:1328:C:C6	2.54	0.42
1:A:1404:5MC:HN41	1:A:1497:G:H1	1.65	0.42
1:A:824:C:H2'	1:A:825:G:H8	1.83	0.42
8:H:86:ILE:HD12	8:H:133:LEU:HG	2.01	0.42
9:I:19:LEU:HD13	9:I:59:PHE:CE1	2.53	0.42
13:M:87:TYR:O	13:M:91:ARG:HG2	2.20	0.42
1:A:1228:C:H2'	1:A:1229:A:H8	1.84	0.42
1:A:1126:U:H1'	1:A:1280:A:C5	2.54	0.42
1:A:1347:G:HO2'	1:A:1348:U:H6	1.65	0.42
1:A:1516:G:H2'	1:A:1518:MA6:OP2	2.19	0.42
1:A:181:G:H4'	1:A:182:U:C5'	2.49	0.42
2:B:33:TYR:HB2	2:B:43:ASP:HA	2.00	0.42
3:C:154:SER:OG	3:C:197:GLY:N	2.50	0.42
6:F:2:ARG:HB2	6:F:4:TYR:CE1	2.54	0.42
7:G:5:ARG:HG3	7:G:7:ALA:H	1.84	0.42
10:J:22:LYS:HD3	10:J:89:ASP:HB3	2.01	0.42
1:A:1475:G:H2'	1:A:1476:G:C8	2.54	0.42
1:A:199:G:H1	1:A:218:C:H42	1.68	0.42
1:A:412:A:H5'	1:A:413:G:OP1	2.19	0.42
1:A:960:U:H4'	1:A:961:U:O5'	2.18	0.42
2:B:51:LEU:HD22	2:B:55:PHE:CE2	2.53	0.42
6:F:82:ARG:HE	6:F:82:ARG:HA	1.84	0.42
9:I:9:ARG:HG2	9:I:14:VAL:HG12	2.02	0.42
11:K:58:PRO:HA	11:K:90:GLY:HA2	2.02	0.42
13:M:86:CYS:SG	18:S:73:GLU:HB3	2.59	0.42
1:A:1183:A:O2'	1:A:1185:G:OP2	2.38	0.42
1:A:60:A:H4'	1:A:61:G:O5'	2.19	0.42
1:A:627:G:H2'	1:A:628:G:C8	2.54	0.42
1:A:851:G:H2'	1:A:852:G:H8	1.85	0.42
3:C:150:LYS:HG3	3:C:169:ALA:HB2	2.00	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:166:LYS:HG2	4:D:178:VAL:HG11	2.01	0.42
5:E:80:ILE:HG22	5:E:82:VAL:HG23	2.01	0.42
8:H:20:TYR:CZ	8:H:75:ARG:HB3	2.55	0.42
17:R:47:THR:HG22	17:R:48:GLY:H	1.85	0.42
19:T:59:ALA:O	19:T:63:ILE:HG13	2.19	0.42
1:A:563:A:O4'	1:A:566:G:N2	2.51	0.42
2:B:106:LYS:O	2:B:109:SER:OG	2.26	0.42
2:B:91:PRO:HG3	2:B:154:LEU:HB2	2.02	0.42
8:H:96:GLY:H	8:H:99:GLU:HB2	1.85	0.42
12:L:70:ILE:HD13	12:L:77:LEU:HD12	2.02	0.42
1:A:1347:G:O2'	1:A:1348:U:O5'	2.38	0.42
1:A:250:A:H1'	1:A:251:G:OP2	2.19	0.42
1:A:397:A:H5'	1:A:398:C:OP1	2.20	0.42
1:A:413:G:N2	1:A:429:U:OP2	2.53	0.42
10:J:82:ILE:HA	10:J:85:LEU:CB	2.50	0.42
1:A:1342:C:H2'	1:A:1343:G:H8	1.85	0.42
1:A:952:U:H2'	1:A:953:G:H8	1.85	0.42
4:D:121:VAL:O	4:D:134:ASP:HA	2.20	0.42
4:D:173:TRP:CD2	4:D:189:PRO:HB3	2.55	0.42
18:S:30:LEU:HD23	18:S:48:THR:HB	2.02	0.42
1:A:1241:G:H2'	1:A:1242:C:C6	2.54	0.42
1:A:1353:G:OP2	20:U:3:LYS:NZ	2.47	0.42
1:A:1404:5MC:N4	1:A:1497:G:H1	2.18	0.42
1:A:646:U:H2'	1:A:647:C:C6	2.55	0.42
2:B:228:GLY:O	2:B:230:VAL:HG23	2.20	0.42
1:A:1061:G:N7	3:C:2:GLY:HA3	2.34	0.42
8:H:25:ASP:OD1	8:H:25:ASP:N	2.52	0.42
2:B:181:PHE:HD2	8:H:70:GLN:HB3	1.84	0.42
1:A:1049:U:O2'	14:N:3:ARG:NH1	2.53	0.41
1:A:598:U:H4'	8:H:94:TYR:CD2	2.55	0.41
1:A:857:C:H2'	1:A:858:G:O4'	2.20	0.41
1:A:877:C:H2'	1:A:878:G:C8	2.54	0.41
4:D:9:CYS:O	4:D:12:CYS:HB2	2.19	0.41
10:J:4:ILE:HD11	10:J:74:ILE:HD12	2.02	0.41
17:R:84:LYS:HE2	17:R:84:LYS:HB3	1.90	0.41
1:A:184:G:H2'	1:A:185:A:H8	1.83	0.41
1:A:352:C:O2'	1:A:354:G:OP1	2.25	0.41
1:A:34:C:H2'	1:A:35:G:H8	1.85	0.41
4:D:150:GLU:HA	4:D:153:ARG:HG3	2.00	0.41
13:M:92:HIS:HA	13:M:110:ARG:NH2	2.35	0.41
1:A:1041:A:H2'	1:A:1042:G:C8	2.55	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1285:A:H1'	1:A:1286:A:OP2	2.20	0.41
3:C:27:LYS:HB3	3:C:27:LYS:HE2	1.89	0.41
6:F:42:GLU:OE1	6:F:59:TYR:OH	2.35	0.41
2:B:115:LEU:HD13	2:B:145:LEU:HB3	2.03	0.41
13:M:110:ARG:HD2	13:M:110:ARG:HA	1.82	0.41
1:A:21:G:H2'	1:A:22:G:H8	1.84	0.41
1:A:916:G:H2'	1:A:917:G:H8	1.85	0.41
7:G:126:ASP:HB3	7:G:131:LYS:HG3	2.03	0.41
11:K:120:ARG:HA	11:K:121:PRO:HD3	1.85	0.41
7:G:26:PHE:CE2	7:G:30:ILE:HD11	2.55	0.41
1:A:412:A:H4'	1:A:413:G:O5'	2.21	0.41
1:A:436:C:H2'	1:A:437:U:C6	2.56	0.41
1:A:762:C:H2'	1:A:763:G:H8	1.85	0.41
10:J:89:ASP:OD1	10:J:91:PRO:HD2	2.21	0.41
1:A:754:C:P	15:O:72:ARG:HH12	2.44	0.41
1:A:1347:G:O2'	1:A:1348:U:P	2.79	0.41
1:A:1402:4OC:H2'	1:A:1403:C:O4'	2.20	0.41
1:A:1525:G:H2'	1:A:1526:G:C8	2.56	0.41
1:A:382:A:H2'	1:A:383:A:C8	2.56	0.41
1:A:638:G:H2'	1:A:639:G:C8	2.56	0.41
1:A:894:G:H2'	1:A:895:G:C8	2.56	0.41
1:A:933:G:O6	7:G:3:ARG:NH2	2.53	0.41
4:D:53:ASP:OD1	4:D:53:ASP:N	2.54	0.41
9:I:9:ARG:HB3	9:I:104:ARG:HH21	1.86	0.41
1:A:755:G:OP2	15:O:65:ARG:HD2	2.21	0.41
17:R:51:LEU:HA	17:R:52:PRO:HD3	1.81	0.41
6:F:50:TYR:CE1	17:R:77:GLY:HA2	2.55	0.41
1:A:17:U:H2'	1:A:18:C:C6	2.56	0.41
3:C:39:ILE:O	3:C:43:LEU:HB2	2.20	0.41
9:I:114:TYR:HB2	10:J:60:ARG:HG3	2.03	0.41
10:J:81:THR:HG22	10:J:85:LEU:HD23	2.02	0.41
15:O:47:LYS:HG2	15:O:47:LYS:H	1.72	0.41
1:A:1070:U:OP1	5:E:18:ARG:NH1	2.38	0.41
1:A:984:C:H42	1:A:1221:G:H1	1.69	0.41
2:B:210:SER:O	2:B:214:ILE:HG12	2.20	0.41
3:C:38:ARG:HB3	3:C:94:LEU:HD21	2.03	0.41
3:C:68:VAL:HG12	3:C:70:VAL:HG23	2.02	0.41
8:H:86:ILE:HG13	8:H:135:CYS:HA	2.02	0.41
1:A:1148:U:H2'	1:A:1149:C:O4'	2.21	0.41
1:A:1520:G:H2'	1:A:1521:G:H8	1.86	0.41
4:D:24:GLU:C	4:D:26:CYS:H	2.25	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:U:17:THR:O	20:U:22:ARG:NH1	2.54	0.41
1:A:1033:G:H3'	1:A:1034:G:H5'	2.02	0.40
1:A:1407:5MC:H2'	1:A:1408:A:H8	1.86	0.40
1:A:359:U:H2'	1:A:360:A:C8	2.56	0.40
5:E:103:GLY:O	5:E:107:ARG:HB3	2.21	0.40
9:I:116:LYS:HB3	9:I:121:ARG:O	2.20	0.40
1:A:624:C:H2'	1:A:625:G:C8	2.54	0.40
1:A:1163:C:H2'	1:A:1164:G:C8	2.56	0.40
1:A:1201:A:H4'	1:A:1202:G:O5'	2.21	0.40
4:D:97:LEU:HD23	4:D:97:LEU:HA	1.91	0.40
17:R:32:ARG:HA	17:R:69:THR:HG21	2.03	0.40
1:A:1073:U:H3	1:A:1102:A:H61	1.70	0.40
1:A:1347:G:H1'	1:A:1348:U:H5	1.87	0.40
1:A:1476:G:H2'	1:A:1477:C:C6	2.57	0.40
19:T:13:LEU:O	19:T:17:ARG:HG3	2.21	0.40
19:T:67:ALA:HB2	19:T:77:ALA:HB2	2.04	0.40
1:A:1269:A:H5'	20:U:19:GLY:HA2	2.03	0.40
1:A:1129:C:H4'	1:A:1130:A:H5'	2.04	0.40
1:A:1189:C:OP1	10:J:51:ARG:NH2	2.52	0.40
1:A:1473:A:H2'	1:A:1474:G:C8	2.57	0.40
1:A:866:C:C4	1:A:867:G:H1'	2.56	0.40
2:B:71:VAL:HG22	2:B:93:VAL:HB	2.04	0.40
7:G:45:ASP:O	7:G:48:LYS:HG2	2.21	0.40
10:J:38:ILE:N	10:J:71:LEU:O	2.45	0.40
18:S:18:LYS:O	18:S:22:LEU:HG	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)
10:J:87:THR:OG1	10:J:87:THR:OG1[8_554]	2.01	0.19

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	233/256 (91%)	204 (88%)	27 (12%)	2 (1%)	17	56
3	C	204/239 (85%)	176 (86%)	28 (14%)	0	100	100
4	D	206/209 (99%)	190 (92%)	16 (8%)	0	100	100
5	E	148/162 (91%)	142 (96%)	6 (4%)	0	100	100
6	F	99/101 (98%)	95 (96%)	4 (4%)	0	100	100
7	G	153/156 (98%)	138 (90%)	15 (10%)	0	100	100
8	H	136/138 (99%)	129 (95%)	7 (5%)	0	100	100
9	I	125/128 (98%)	112 (90%)	13 (10%)	0	100	100
10	J	96/105 (91%)	82 (85%)	13 (14%)	1 (1%)	15	54
11	K	117/129 (91%)	103 (88%)	14 (12%)	0	100	100
12	L	121/134 (90%)	112 (93%)	8 (7%)	1 (1%)	19	60
13	M	123/126 (98%)	112 (91%)	11 (9%)	0	100	100
14	N	58/61 (95%)	53 (91%)	5 (9%)	0	100	100
15	O	86/89 (97%)	79 (92%)	7 (8%)	0	100	100
16	P	81/88 (92%)	78 (96%)	3 (4%)	0	100	100
17	R	71/88 (81%)	66 (93%)	5 (7%)	0	100	100
18	S	78/93 (84%)	71 (91%)	6 (8%)	1 (1%)	12	48
19	T	97/106 (92%)	84 (87%)	13 (13%)	0	100	100
20	U	22/27 (82%)	19 (86%)	3 (14%)	0	100	100
All	All	2254/2435 (93%)	2045 (91%)	204 (9%)	5 (0%)	47	81

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	229	VAL
10	J	34	VAL
12	L	28	LYS
18	S	31	ILE
2	B	230	VAL

5.3.2 Protein sidechains ⓘ

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%)	191 (95%)	11 (5%)	22	50
3	C	160/188 (85%)	155 (97%)	5 (3%)	40	62
4	D	180/181 (99%)	171 (95%)	9 (5%)	24	51
5	E	115/123 (94%)	107 (93%)	8 (7%)	15	42
6	F	90/90 (100%)	86 (96%)	4 (4%)	28	54
7	G	126/127 (99%)	123 (98%)	3 (2%)	49	69
8	H	119/119 (100%)	116 (98%)	3 (2%)	47	68
9	I	98/99 (99%)	93 (95%)	5 (5%)	24	51
10	J	88/92 (96%)	80 (91%)	8 (9%)	9	32
11	K	90/99 (91%)	86 (96%)	4 (4%)	28	54
12	L	103/109 (94%)	100 (97%)	3 (3%)	42	64
13	M	100/101 (99%)	98 (98%)	2 (2%)	55	73
14	N	49/50 (98%)	46 (94%)	3 (6%)	18	46
15	O	79/80 (99%)	77 (98%)	2 (2%)	47	68
16	P	72/74 (97%)	71 (99%)	1 (1%)	67	80
17	R	64/77 (83%)	63 (98%)	1 (2%)	62	79
18	S	71/80 (89%)	65 (92%)	6 (8%)	10	36
19	T	76/82 (93%)	73 (96%)	3 (4%)	32	57
20	U	19/22 (86%)	18 (95%)	1 (5%)	22	50
All	All	1901/2013 (94%)	1819 (96%)	82 (4%)	29	55

All (82) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	46	LYS
2	B	82	ARG
2	B	87	ARG
2	B	111	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	157	ARG
2	B	163	PHE
2	B	195	ASP
2	B	221	LEU
2	B	231	GLU
2	B	236	TYR
2	B	238	LEU
3	C	43	LEU
3	C	95	THR
3	C	112	SER
3	C	156	ARG
3	C	167	TRP
4	D	17	VAL
4	D	19	LEU
4	D	20	TYR
4	D	26	CYS
4	D	35	ARG
4	D	36	ARG
4	D	53	ASP
4	D	122	ARG
4	D	126	ILE
5	E	12	LEU
5	E	41	VAL
5	E	76	ILE
5	E	89	ILE
5	E	105	VAL
5	E	117	ASP
5	E	133	TYR
5	E	150	ARG
6	F	47	ARG
6	F	75	LEU
6	F	82	ARG
6	F	100	ASN
7	G	11	GLN
7	G	113	GLU
7	G	156	TRP
8	H	25	ASP
8	H	29	SER
8	H	31	PHE
9	I	56	LEU
9	I	59	PHE
9	I	85	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
9	I	112	LYS
9	I	113	LYS
10	J	49	VAL
10	J	59	SER
10	J	62	HIS
10	J	83	GLU
10	J	85	LEU
10	J	87	THR
10	J	90	LEU
10	J	92	THR
11	K	14	VAL
11	K	29	ILE
11	K	117	ASN
11	K	126	ARG
12	L	33	ARG
12	L	39	VAL
12	L	54	LYS
13	M	12	ASN
13	M	125	ARG
14	N	12	ARG
14	N	22	THR
14	N	27	CYS
15	O	6	GLU
15	O	81	LEU
16	P	55	ARG
17	R	47	THR
18	S	7	LYS
18	S	13	ASP
18	S	25	LYS
18	S	31	ILE
18	S	65	ASN
18	S	81	ARG
19	T	55	ILE
19	T	73	HIS
19	T	74	LYS
20	U	9	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	104	ASN
4	D	42	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	D	201	GLN
16	P	65	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	1509/1522 (99%)	215 (14%)	40 (2%)

All (215) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	8	A
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	116	A
1	A	120	A
1	A	121	C
1	A	129(A)	G
1	A	130	A
1	A	131	C
1	A	144	G
1	A	163	C
1	A	182	U
1	A	183	G
1	A	195	A
1	A	204	U
1	A	216	G
1	A	244	U
1	A	245	C
1	A	247	G
1	A	251	G
1	A	267	C
1	A	289	G
1	A	321	A
1	A	328	C
1	A	329	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	330	C
1	A	332	G
1	A	344	A
1	A	347	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	411	A
1	A	412	A
1	A	413	G
1	A	414	A
1	A	421	U
1	A	424	G
1	A	429	U
1	A	430	A
1	A	432	A
1	A	433	C
1	A	439	A
1	A	452	A
1	A	485	G
1	A	496	A
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
1	A	532	A
1	A	533	A
1	A	547	A
1	A	559	A
1	A	560	U
1	A	562	C
1	A	564	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	572	A
1	A	573	A
1	A	576	G
1	A	577	G
1	A	616	G
1	A	630	G
1	A	632	A
1	A	653	A
1	A	665	A
1	A	687	A
1	A	688	G
1	A	702	A
1	A	723	U
1	A	731	G
1	A	749	C
1	A	755	G
1	A	777	A
1	A	781	A
1	A	782	A
1	A	793	U
1	A	794	A
1	A	813	U
1	A	816	A
1	A	817	C
1	A	819	A
1	A	821	G
1	A	828	A
1	A	839	U
1	A	840	C
1	A	841	U
1	A	848	C
1	A	859	A
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	966	M2G
1	A	969	A
1	A	971	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	974	A
1	A	975	A
1	A	976	G
1	A	977	A
1	A	978	A
1	A	991	U
1	A	992	U
1	A	993	G
1	A	994	A
1	A	1000	U
1	A	1003	G
1	A	1003(A)	G
1	A	1004	A
1	A	1005	A
1	A	1009	G
1	A	1021	G
1	A	1022	G
1	A	1024	G
1	A	1025	U
1	A	1026	G
1	A	1027	C
1	A	1028	C
1	A	1029	C
1	A	1030	C
1	A	1030(A)	G
1	A	1030(C)	G
1	A	1030(D)	A
1	A	1033	G
1	A	1034	G
1	A	1050	G
1	A	1053	G
1	A	1054	C
1	A	1065	U
1	A	1066	C
1	A	1068	G
1	A	1094	G
1	A	1095	U
1	A	1101	A
1	A	1117	G
1	A	1125	U
1	A	1126	U
1	A	1127	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	1129	C
1	A	1130	A
1	A	1131	G
1	A	1137	C
1	A	1138	G
1	A	1139	G
1	A	1152	A
1	A	1159	U
1	A	1171	G
1	A	1181	G
1	A	1183	A
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	1226	C
1	A	1227	A
1	A	1238	A
1	A	1241	G
1	A	1256	A
1	A	1257	U
1	A	1258	G
1	A	1270	C
1	A	1280	A
1	A	1281	U
1	A	1282	C
1	A	1286	A
1	A	1287	A
1	A	1300	G
1	A	1301	U
1	A	1302	U
1	A	1312	G
1	A	1317	C
1	A	1320	C
1	A	1323	G
1	A	1331	G
1	A	1348	U
1	A	1359	C
1	A	1362	C
1	A	1364	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	1394	A
1	A	1398	A
1	A	1400	5MC
1	A	1401	G
1	A	1442	G
1	A	1446	A
1	A	1493	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

All (40) 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	203	U
1	A	243	A
1	A	250	A
1	A	266	G
1	A	328	C
1	A	372	C
1	A	410	G
1	A	412	A
1	A	428	G
1	A	429	U
1	A	484	G
1	A	509	A
1	A	559	A
1	A	575	G
1	A	687	A
1	A	701	C
1	A	748	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	812	C
1	A	913	A
1	A	960	U
1	A	965	A
1	A	992	U
1	A	993	G
1	A	1065	U
1	A	1067	A
1	A	1129	C
1	A	1182	G
1	A	1201	A
1	A	1281	U
1	A	1285	A
1	A	1300	G
1	A	1301	U
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](#)

15 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	2.02	4 (20%)	22,40,43	2.49	5 (22%)
1	PSU	A	1540	1	17,21,22	1.03	1 (5%)	20,30,33	3.14	6 (30%)
1	UR3	A	1498	1	14,22,23	1.10	2 (14%)	15,32,35	0.95	0
1	4OC	A	1402	1	16,23,24	0.91	1 (6%)	17,32,35	0.78	0
1	7MG	A	527	1	22,26,27	2.19	6 (27%)	28,39,42	1.73	7 (25%)
1	5MC	A	1407	1	15,22,23	0.92	1 (6%)	19,32,35	1.08	2 (10%)
1	5MC	A	967	1	15,22,23	0.90	0	19,32,35	1.08	2 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	PSU	A	1541	1	17,21,22	1.07	2 (11%)	20,30,33	3.11	6 (30%)
12	0TD	L	92	12	4,9,10	0.80	0	3,11,13	1.34	1 (33%)
1	MA6	A	1518	1	19,26,27	1.14	2 (10%)	18,38,41	0.64	0
1	5MC	A	1404	1	15,22,23	0.90	0	19,32,35	1.06	1 (5%)
1	5MC	A	1400	1	15,22,23	0.96	1 (6%)	19,32,35	1.08	2 (10%)
1	2MG	A	1207	1	19,26,27	2.35	4 (21%)	21,38,41	2.02	4 (19%)
1	MA6	A	1519	1	19,26,27	1.18	2 (10%)	18,38,41	0.57	0
1	PSU	A	516	1,21	17,21,22	1.06	2 (11%)	20,30,33	3.10	6 (30%)

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	-	1/7/29/30	0/3/3/3
1	PSU	A	1540	1	-	1/7/25/26	0/2/2/2
1	UR3	A	1498	1	-	0/5/25/26	0/2/2/2
1	4OC	A	1402	1	-	2/9/29/30	0/2/2/2
1	7MG	A	527	1	-	0/7/37/38	0/3/3/3
1	5MC	A	1407	1	-	0/5/25/26	0/2/2/2
1	5MC	A	967	1	-	0/5/25/26	0/2/2/2
1	PSU	A	1541	1	-	0/7/25/26	0/2/2/2
12	0TD	L	92	12	-	1/3/12/14	-
1	MA6	A	1518	1	-	2/7/29/30	0/3/3/3
1	5MC	A	1404	1	-	1/5/25/26	0/2/2/2
1	5MC	A	1400	1	-	2/5/25/26	0/2/2/2
1	2MG	A	1207	1	-	0/5/27/28	0/3/3/3
1	MA6	A	1519	1	-	3/7/29/30	0/3/3/3
1	PSU	A	516	1,21	-	0/7/25/26	0/2/2/2

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1207	2MG	C2-N2	7.49	1.40	1.34
1	A	527	7MG	C4-N3	5.98	1.41	1.34
1	A	966	M2G	C6-N1	5.77	1.43	1.33
1	A	1207	2MG	C6-N1	5.74	1.43	1.33
1	A	527	7MG	C2-N2	4.94	1.43	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	527	7MG	C8-N9	-4.56	1.35	1.45
1	A	966	M2G	C2-N2	4.19	1.41	1.34
1	A	966	M2G	C2-N1	3.54	1.40	1.34
1	A	966	M2G	C4-N3	3.52	1.41	1.35
1	A	527	7MG	C6-N1	3.28	1.38	1.33
1	A	1518	MA6	C6-N1	3.18	1.37	1.33
1	A	1519	MA6	C6-N1	3.13	1.37	1.33
1	A	516	PSU	C4-N3	3.11	1.38	1.33
1	A	1540	PSU	C4-N3	3.07	1.38	1.33
1	A	1541	PSU	C4-N3	3.04	1.38	1.33
1	A	1498	UR3	C6-N1	2.83	1.39	1.35
1	A	1207	2MG	C4-N3	2.81	1.40	1.35
1	A	527	7MG	C6-C5	2.47	1.44	1.41
1	A	1498	UR3	C4-N3	2.44	1.41	1.38
1	A	1519	MA6	C2-N1	2.26	1.38	1.33
1	A	1402	4OC	C5-C4	2.18	1.44	1.39
1	A	1207	2MG	C2-N1	2.16	1.41	1.34
1	A	1400	5MC	C5-C4	2.11	1.44	1.41
1	A	527	7MG	CM7-N7	-2.11	1.42	1.46
1	A	1518	MA6	C2-N1	2.11	1.37	1.33
1	A	516	PSU	O4'-C1'	-2.04	1.41	1.44
1	A	1407	5MC	C5-C4	2.03	1.44	1.41
1	A	1541	PSU	O4'-C1'	-2.02	1.41	1.44

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	516	PSU	N1-C2-N3	-10.47	120.11	128.43
1	A	1540	PSU	N1-C2-N3	-10.42	120.15	128.43
1	A	1541	PSU	N1-C2-N3	-10.40	120.16	128.43
1	A	966	M2G	C5-C6-N1	-8.10	112.35	123.43
1	A	1207	2MG	C5-C6-N1	-7.36	113.37	123.43
1	A	966	M2G	C6-N1-C2	6.07	123.40	116.18
1	A	516	PSU	C4-N3-C2	5.60	119.87	115.14
1	A	1540	PSU	C4-N3-C2	5.43	119.72	115.14
1	A	1541	PSU	C4-N3-C2	5.35	119.66	115.14
1	A	527	7MG	N3-C4-N9	4.58	132.79	126.91
1	A	516	PSU	C5-C4-N3	-4.43	119.65	125.36
1	A	1540	PSU	C5-C4-N3	-4.34	119.78	125.36
1	A	1541	PSU	C5-C4-N3	-4.30	119.83	125.36
1	A	527	7MG	C5-C4-N3	-4.03	119.91	126.49
1	A	527	7MG	N7-C8-N9	3.85	108.88	103.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1207	2MG	C6-N1-C2	3.77	121.92	115.18
1	A	1540	PSU	C5-C6-N1	-3.54	120.09	124.44
1	A	1541	PSU	C5-C6-N1	-3.53	120.10	124.44
1	A	516	PSU	C5-C6-N1	-3.27	120.42	124.44
1	A	966	M2G	N3-C2-N2	3.25	120.48	117.18
1	A	1540	PSU	C6-N1-C2	3.21	120.66	115.36
1	A	1541	PSU	C6-N1-C2	3.21	120.66	115.36
1	A	516	PSU	C6-N1-C2	3.09	120.46	115.36
1	A	1540	PSU	C5-C1'-C2'	-2.85	110.24	115.32
1	A	966	M2G	N1-C2-N2	-2.72	114.44	117.19
1	A	527	7MG	C6-N1-C2	2.57	120.00	115.93
1	A	1541	PSU	C5-C1'-C2'	-2.51	110.84	115.32
1	A	527	7MG	C2-N3-C4	2.39	120.50	113.89
1	A	1207	2MG	C4-C5-N7	2.39	111.89	109.40
1	A	527	7MG	C6-C5-C4	2.36	117.73	115.20
1	A	967	5MC	C2-N3-C4	2.30	118.79	116.02
1	A	1407	5MC	C2-N3-C4	2.26	118.75	116.02
1	A	1404	5MC	C2-N3-C4	2.24	118.72	116.02
1	A	527	7MG	N1-C2-N3	-2.19	121.98	125.42
12	L	92	0TD	O-C-CA	-2.16	119.13	124.78
1	A	1400	5MC	C2-N3-C4	2.14	118.60	116.02
1	A	966	M2G	C2-N3-C4	-2.14	112.85	115.28
1	A	1407	5MC	N4-C4-N3	-2.08	114.09	117.03
1	A	1400	5MC	N4-C4-N3	-2.08	114.10	117.03
1	A	1207	2MG	N2-C2-N3	2.04	118.92	116.96
1	A	967	5MC	N4-C4-N3	-2.01	114.20	117.03
1	A	516	PSU	O4'-C1'-C2'	2.00	107.91	104.66

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	966	M2G	C4'-C5'-O5'-P
1	A	1402	4OC	O4'-C4'-C5'-O5'
1	A	1402	4OC	C3'-C4'-C5'-O5'
12	L	92	0TD	CG-CB-SB-CSB
1	A	1404	5MC	C2'-C1'-N1-C6
1	A	1400	5MC	O4'-C4'-C5'-O5'
1	A	1519	MA6	C5-C6-N6-C9
1	A	1519	MA6	C5-C6-N6-C10
1	A	1400	5MC	C3'-C4'-C5'-O5'
1	A	1519	MA6	N1-C6-N6-C9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
1	A	1518	MA6	C5-C6-N6-C9
1	A	1518	MA6	C5-C6-N6-C10
1	A	1540	PSU	O4'-C4'-C5'-O5'

There are no ring outliers.

7 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	1402	4OC	1	0
1	A	1407	5MC	1	0
1	A	1541	PSU	1	0
12	L	92	0TD	2	0
1	A	1518	MA6	2	0
1	A	1404	5MC	2	0
1	A	1519	MA6	2	0

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 195 ligands modelled in this entry, 195 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

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	1500/1522 (98%)	0.06	17 (1%) 80 72	155, 192, 264, 505	0
2	B	235/256 (91%)	-0.46	0 100 100	134, 193, 274, 327	0
3	C	206/239 (86%)	-0.57	0 100 100	134, 182, 248, 311	0
4	D	208/209 (99%)	-0.57	0 100 100	114, 181, 253, 369	0
5	E	150/162 (92%)	-0.60	0 100 100	118, 175, 226, 277	0
6	F	101/101 (100%)	-0.66	1 (0%) 82 74	143, 207, 273, 471	0
7	G	155/156 (99%)	-0.56	0 100 100	153, 204, 257, 309	0
8	H	138/138 (100%)	-0.62	0 100 100	123, 172, 226, 242	0
9	I	127/128 (99%)	-0.32	1 (0%) 86 79	179, 238, 348, 501	0
10	J	98/105 (93%)	-0.44	0 100 100	174, 222, 313, 438	0
11	K	119/129 (92%)	-0.36	2 (1%) 70 61	117, 184, 254, 371	0
12	L	123/134 (91%)	-0.53	0 100 100	139, 181, 231, 259	0
13	M	125/126 (99%)	-0.37	4 (3%) 47 37	176, 215, 311, 427	0
14	N	60/61 (98%)	-0.39	0 100 100	140, 200, 285, 315	0
15	O	88/89 (98%)	-0.61	0 100 100	155, 197, 253, 326	0
16	P	83/88 (94%)	-0.62	0 100 100	148, 183, 219, 272	0
17	R	73/88 (82%)	-0.28	2 (2%) 54 44	122, 209, 331, 418	0
18	S	80/93 (86%)	-0.45	0 100 100	189, 220, 289, 312	0
19	T	99/106 (93%)	-0.74	0 100 100	131, 185, 243, 335	0
20	U	24/27 (88%)	0.20	0 100 100	193, 228, 255, 277	0
All	All	3792/3957 (95%)	-0.28	27 (0%) 87 82	114, 193, 274, 505	0

All (27) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1030(D)	A	9.8
11	K	129	SER	6.9
17	R	17	SER	5.8
11	K	128	ALA	5.5
1	A	1003(A)	G	4.5
1	A	1031	G	4.4
13	M	122	LYS	4.3
13	M	123	ALA	4.1
1	A	1533	C	4.0
6	F	101	ALA	3.5
1	A	1030(C)	G	3.4
1	A	1129	C	3.3
1	A	1257	U	3.3
1	A	1003	G	3.2
17	R	18	ARG	3.1
1	A	1534	A	3.0
1	A	266	G	2.8
1	A	1032	G	2.8
9	I	115	GLY	2.7
1	A	1024	G	2.6
1	A	706	A	2.3
1	A	606	G	2.3
1	A	1002	G	2.2
13	M	3	ARG	2.2
1	A	1017	G	2.1
13	M	120	LYS	2.1
1	A	218	C	2.1

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
1	PSU	A	1540	20/21	0.85	0.42	194,249,259,261	0
1	PSU	A	1541	20/21	0.88	0.24	177,179,242,254	0
1	5MC	A	1400	21/22	0.92	0.19	175,178,193,234	0
1	PSU	A	516	20/21	0.93	0.14	175,181,212,258	0
1	UR3	A	1498	21/22	0.94	0.22	178,181,221,230	0
1	5MC	A	1404	21/22	0.94	0.21	178,180,182,204	0
1	MA6	A	1518	24/25	0.95	0.18	185,186,226,235	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
1	2MG	A	1207	24/25	0.95	0.16	182,186,190,197	0
1	MA6	A	1519	24/25	0.95	0.20	180,183,202,229	0
12	0TD	L	92	10/11	0.95	0.34	167,204,309,368	0
1	5MC	A	967	21/22	0.96	0.15	158,162,188,203	0
1	M2G	A	966	25/26	0.96	0.15	158,179,213,255	0
1	7MG	A	527	24/25	0.96	0.14	161,162,170,198	0
1	5MC	A	1407	21/22	0.97	0.14	189,192,212,231	0
1	4OC	A	1402	22/23	0.98	0.19	175,177,227,231	0

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

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(\AA^2)	Q<0.9
21	MG	A	1674	1/1	0.01	1.79	192,192,192,192	0
22	K	A	1776	1/1	0.14	0.32	198,198,198,198	0
21	MG	A	1627	1/1	0.18	1.21	177,177,177,177	0
22	K	A	1755	1/1	0.28	0.52	187,187,187,187	0
21	MG	A	1616	1/1	0.28	0.90	158,158,158,158	0
21	MG	A	1687	1/1	0.50	0.81	143,143,143,143	0
21	MG	A	1686	1/1	0.59	0.16	97,97,97,97	0
21	MG	A	1632	1/1	0.60	0.72	103,103,103,103	0
21	MG	A	1742	1/1	0.60	0.52	143,143,143,143	0
21	MG	E	202	1/1	0.61	0.34	99,99,99,99	0
21	MG	A	1684	1/1	0.61	0.42	150,150,150,150	0
21	MG	A	1610	1/1	0.64	1.09	130,130,130,130	0
21	MG	A	1706	1/1	0.65	0.89	137,137,137,137	0
21	MG	A	1615	1/1	0.67	0.26	138,138,138,138	0
21	MG	E	201	1/1	0.67	0.29	151,151,151,151	0
21	MG	A	1626	1/1	0.71	0.23	130,130,130,130	0
21	MG	A	1621	1/1	0.72	0.58	134,134,134,134	0
22	K	A	1765	1/1	0.72	0.85	168,168,168,168	0
21	MG	A	1696	1/1	0.73	0.42	156,156,156,156	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
21	MG	A	1787	1/1	0.74	0.66	92,92,92,92	0
22	K	A	1782	1/1	0.75	0.49	162,162,162,162	0
21	MG	A	1635	1/1	0.75	0.34	61,61,61,61	0
22	K	A	1786	1/1	0.76	0.67	215,215,215,215	0
21	MG	A	1672	1/1	0.76	0.43	171,171,171,171	0
22	K	A	1768	1/1	0.76	0.15	229,229,229,229	0
22	K	A	1753	1/1	0.76	0.26	176,176,176,176	0
22	K	A	1758	1/1	0.76	0.83	199,199,199,199	0
21	MG	A	1691	1/1	0.76	0.88	111,111,111,111	0
21	MG	A	1611	1/1	0.76	0.57	85,85,85,85	0
22	K	A	1780	1/1	0.77	0.40	149,149,149,149	0
21	MG	A	1618	1/1	0.78	0.36	193,193,193,193	0
22	K	A	1777	1/1	0.78	0.11	228,228,228,228	0
21	MG	A	1702	1/1	0.78	0.93	197,197,197,197	0
21	MG	A	1698	1/1	0.78	0.29	104,104,104,104	0
21	MG	A	1633	1/1	0.78	0.46	59,59,59,59	0
22	K	A	1752	1/1	0.79	0.27	176,176,176,176	0
21	MG	A	1607	1/1	0.79	1.29	122,122,122,122	0
21	MG	A	1680	1/1	0.79	0.35	88,88,88,88	0
21	MG	A	1746	1/1	0.79	0.14	114,114,114,114	0
21	MG	A	1667	1/1	0.79	0.48	236,236,236,236	0
21	MG	A	1623	1/1	0.80	0.58	154,154,154,154	0
21	MG	A	1603	1/1	0.81	1.12	98,98,98,98	0
21	MG	A	1608	1/1	0.82	0.48	117,117,117,117	0
22	K	A	1759	1/1	0.82	0.37	186,186,186,186	0
21	MG	A	1656	1/1	0.82	1.05	65,65,65,65	0
21	MG	A	1650	1/1	0.82	0.94	127,127,127,127	0
22	K	A	1771	1/1	0.82	0.94	197,197,197,197	0
21	MG	A	1655	1/1	0.82	0.28	65,65,65,65	0
21	MG	A	1659	1/1	0.83	0.39	81,81,81,81	0
21	MG	A	1664	1/1	0.83	0.68	166,166,166,166	0
21	MG	A	1688	1/1	0.83	0.49	181,181,181,181	0
21	MG	A	1661	1/1	0.83	0.42	75,75,75,75	0
21	MG	A	1732	1/1	0.84	0.44	163,163,163,163	0
21	MG	A	1728	1/1	0.84	0.40	151,151,151,151	0
21	MG	A	1648	1/1	0.84	0.35	112,112,112,112	0
22	K	A	1757	1/1	0.85	0.38	204,204,204,204	0
21	MG	A	1747	1/1	0.85	0.40	173,173,173,173	0
21	MG	A	1629	1/1	0.85	0.31	171,171,171,171	0
21	MG	A	1692	1/1	0.85	0.67	101,101,101,101	0
22	K	A	1783	1/1	0.86	0.43	187,187,187,187	0
21	MG	A	1690	1/1	0.86	0.31	74,74,74,74	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
22	K	A	1785	1/1	0.86	0.62	158,158,158,158	0
21	MG	A	1730	1/1	0.86	0.39	188,188,188,188	0
21	MG	A	1605	1/1	0.86	0.32	92,92,92,92	0
21	MG	A	1740	1/1	0.86	0.61	114,114,114,114	0
21	MG	A	1745	1/1	0.87	0.48	214,214,214,214	0
21	MG	A	1668	1/1	0.87	0.17	159,159,159,159	0
22	K	A	1761	1/1	0.87	0.25	181,181,181,181	0
21	MG	A	1642	1/1	0.87	0.17	105,105,105,105	0
21	MG	A	1744	1/1	0.87	0.76	143,143,143,143	0
21	MG	A	1712	1/1	0.88	0.65	85,85,85,85	0
21	MG	A	1658	1/1	0.88	0.28	111,111,111,111	0
21	MG	A	1682	1/1	0.89	0.33	128,128,128,128	0
21	MG	A	1666	1/1	0.89	0.32	138,138,138,138	0
21	MG	A	1694	1/1	0.89	0.33	133,133,133,133	0
21	MG	A	1703	1/1	0.89	0.93	115,115,115,115	0
21	MG	A	1719	1/1	0.90	0.72	196,196,196,196	0
22	K	A	1754	1/1	0.90	0.35	168,168,168,168	0
21	MG	A	1695	1/1	0.90	0.22	71,71,71,71	0
21	MG	A	1716	1/1	0.90	0.15	179,179,179,179	0
21	MG	A	1749	1/1	0.90	0.78	130,130,130,130	0
22	K	A	1774	1/1	0.90	0.38	168,168,168,168	0
21	MG	B	301	1/1	0.90	0.46	143,143,143,143	0
21	MG	A	1653	1/1	0.90	0.59	111,111,111,111	0
21	MG	A	1665	1/1	0.90	0.33	205,205,205,205	0
21	MG	A	1602	1/1	0.90	0.12	149,149,149,149	0
21	MG	A	1625	1/1	0.91	1.43	140,140,140,140	0
21	MG	A	1619	1/1	0.91	0.93	126,126,126,126	0
21	MG	A	1662	1/1	0.91	0.23	89,89,89,89	0
21	MG	A	1710	1/1	0.91	0.32	119,119,119,119	0
21	MG	A	1675	1/1	0.92	0.30	94,94,94,94	0
21	MG	A	1612	1/1	0.92	0.16	163,163,163,163	0
21	MG	A	1624	1/1	0.92	0.84	174,174,174,174	0
21	MG	A	1751	1/1	0.92	0.30	113,113,113,113	0
21	MG	A	1657	1/1	0.92	0.54	75,75,75,75	0
21	MG	A	1613	1/1	0.92	0.26	161,161,161,161	0
21	MG	A	1637	1/1	0.92	0.55	68,68,68,68	0
22	K	A	1769	1/1	0.92	0.26	193,193,193,193	0
21	MG	A	1630	1/1	0.93	1.14	90,90,90,90	0
22	K	A	1762	1/1	0.93	0.17	181,181,181,181	0
21	MG	A	1723	1/1	0.93	0.64	102,102,102,102	0
22	K	A	1784	1/1	0.93	0.12	141,141,141,141	0
21	MG	A	1704	1/1	0.93	0.22	112,112,112,112	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
21	MG	A	1724	1/1	0.93	0.27	99,99,99,99	0
21	MG	A	1639	1/1	0.93	0.49	157,157,157,157	0
22	K	A	1772	1/1	0.93	0.09	178,178,178,178	0
22	K	A	1779	1/1	0.93	0.41	217,217,217,217	0
22	K	A	1770	1/1	0.93	0.65	202,202,202,202	0
21	MG	A	1741	1/1	0.94	0.17	193,193,193,193	0
21	MG	A	1693	1/1	0.94	0.39	104,104,104,104	0
21	MG	A	1750	1/1	0.94	0.17	134,134,134,134	0
21	MG	U	101	1/1	0.94	0.24	523,523,523,523	0
21	MG	A	1604	1/1	0.94	0.22	311,311,311,311	0
22	K	A	1775	1/1	0.94	0.08	273,273,273,273	0
21	MG	A	1733	1/1	0.94	0.17	170,170,170,170	0
21	MG	A	1622	1/1	0.94	0.30	142,142,142,142	0
21	MG	A	1683	1/1	0.94	0.19	133,133,133,133	0
21	MG	A	1737	1/1	0.94	0.07	132,132,132,132	0
21	MG	A	1748	1/1	0.94	0.16	267,267,267,267	0
21	MG	A	1636	1/1	0.94	0.18	59,59,59,59	0
21	MG	A	1617	1/1	0.94	0.24	173,173,173,173	0
21	MG	A	1620	1/1	0.94	0.21	126,126,126,126	0
21	MG	A	1705	1/1	0.94	0.44	189,189,189,189	0
21	MG	A	1673	1/1	0.94	0.24	122,122,122,122	0
21	MG	A	1660	1/1	0.94	0.16	121,121,121,121	0
21	MG	A	1725	1/1	0.95	0.71	208,208,208,208	0
22	K	A	1767	1/1	0.95	0.17	149,149,149,149	0
21	MG	A	1647	1/1	0.95	0.62	199,199,199,199	0
22	K	A	1773	1/1	0.95	0.39	116,116,116,116	0
21	MG	A	1700	1/1	0.95	0.71	102,102,102,102	0
21	MG	M	201	1/1	0.95	0.22	186,186,186,186	0
21	MG	A	1708	1/1	0.95	0.34	146,146,146,146	0
22	K	A	1764	1/1	0.95	0.25	206,206,206,206	0
21	MG	A	1714	1/1	0.95	0.21	136,136,136,136	0
21	MG	A	1735	1/1	0.95	0.38	167,167,167,167	0
21	MG	A	1678	1/1	0.95	0.30	88,88,88,88	0
22	K	A	1756	1/1	0.95	0.73	178,178,178,178	0
21	MG	A	1641	1/1	0.96	0.16	74,74,74,74	0
21	MG	A	1609	1/1	0.96	0.44	51,51,51,51	0
21	MG	A	1628	1/1	0.96	0.23	159,159,159,159	0
21	MG	A	1654	1/1	0.96	0.27	114,114,114,114	0
22	K	A	1766	1/1	0.96	0.33	168,168,168,168	0
21	MG	A	1663	1/1	0.96	0.11	147,147,147,147	0
21	MG	A	1743	1/1	0.96	0.17	135,135,135,135	0
22	K	A	1760	1/1	0.96	0.16	207,207,207,207	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
21	MG	A	1713	1/1	0.96	0.57	113,113,113,113	0
21	MG	A	1631	1/1	0.96	0.47	141,141,141,141	0
21	MG	A	1671	1/1	0.96	0.46	48,48,48,48	0
21	MG	A	1697	1/1	0.96	0.15	165,165,165,165	0
21	MG	A	1606	1/1	0.96	0.28	247,247,247,247	0
21	MG	A	1677	1/1	0.96	0.21	120,120,120,120	0
21	MG	A	1736	1/1	0.97	0.15	164,164,164,164	0
21	MG	A	1726	1/1	0.97	0.14	129,129,129,129	0
21	MG	A	1669	1/1	0.97	0.51	85,85,85,85	0
21	MG	A	1645	1/1	0.97	0.28	55,55,55,55	0
21	MG	A	1689	1/1	0.97	0.41	182,182,182,182	0
21	MG	A	1731	1/1	0.97	0.07	116,116,116,116	0
21	MG	A	1614	1/1	0.97	0.25	94,94,94,94	0
21	MG	A	1643	1/1	0.97	0.39	170,170,170,170	0
21	MG	A	1634	1/1	0.97	0.07	118,118,118,118	0
22	K	A	1778	1/1	0.97	0.40	208,208,208,208	0
21	MG	A	1721	1/1	0.97	0.42	121,121,121,121	0
21	MG	A	1711	1/1	0.97	0.29	177,177,177,177	0
21	MG	D	302	1/1	0.97	0.07	100,100,100,100	0
21	MG	A	1727	1/1	0.97	0.25	177,177,177,177	0
21	MG	A	1701	1/1	0.97	0.44	68,68,68,68	0
22	K	A	1763	1/1	0.97	0.39	149,149,149,149	0
21	MG	A	1709	1/1	0.97	0.18	89,89,89,89	0
21	MG	A	1738	1/1	0.98	0.75	116,116,116,116	0
21	MG	A	1739	1/1	0.98	0.14	126,126,126,126	0
21	MG	A	1722	1/1	0.98	0.39	55,55,55,55	0
21	MG	A	1681	1/1	0.98	0.37	165,165,165,165	0
21	MG	A	1670	1/1	0.98	0.18	74,74,74,74	0
21	MG	A	1652	1/1	0.98	0.51	172,172,172,172	0
21	MG	A	1685	1/1	0.98	0.16	82,82,82,82	0
21	MG	A	1601	1/1	0.98	0.18	187,187,187,187	0
21	MG	A	1699	1/1	0.98	0.13	122,122,122,122	0
21	MG	A	1676	1/1	0.98	0.22	74,74,74,74	0
21	MG	A	1734	1/1	0.98	0.06	366,366,366,366	0
21	MG	A	1715	1/1	0.98	0.45	105,105,105,105	0
23	ZN	N	101	1/1	0.98	0.13	124,124,124,124	0
21	MG	A	1638	1/1	0.98	0.35	116,116,116,116	0
21	MG	A	1679	1/1	0.98	0.25	116,116,116,116	0
21	MG	A	1717	1/1	0.98	0.12	79,79,79,79	0
21	MG	A	1640	1/1	0.99	0.19	90,90,90,90	0
21	MG	A	1729	1/1	0.99	0.18	68,68,68,68	0
22	K	A	1781	1/1	0.99	0.13	149,149,149,149	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
21	MG	A	1651	1/1	0.99	0.41	70,70,70,70	0
21	MG	A	1646	1/1	0.99	0.26	81,81,81,81	0
23	ZN	D	301	1/1	0.99	0.38	157,157,157,157	0
21	MG	A	1649	1/1	0.99	0.17	71,71,71,71	0
21	MG	A	1707	1/1	0.99	0.18	73,73,73,73	0
21	MG	A	1720	1/1	0.99	0.12	76,76,76,76	0
21	MG	A	1644	1/1	0.99	0.05	123,123,123,123	0
21	MG	A	1718	1/1	0.99	0.06	86,86,86,86	0

6.5 Other polymers [i](#)

There are no such residues in this entry.