



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 06:16 PM UTC

PDB ID : 5WNR / pdb_00005wnr
Title : Crystal Structure of 30S ribosomal subunit from *Thermus thermophilus*
Authors : DeMirici, H.
Deposited on : 2017-08-01
Resolution : 3.50 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

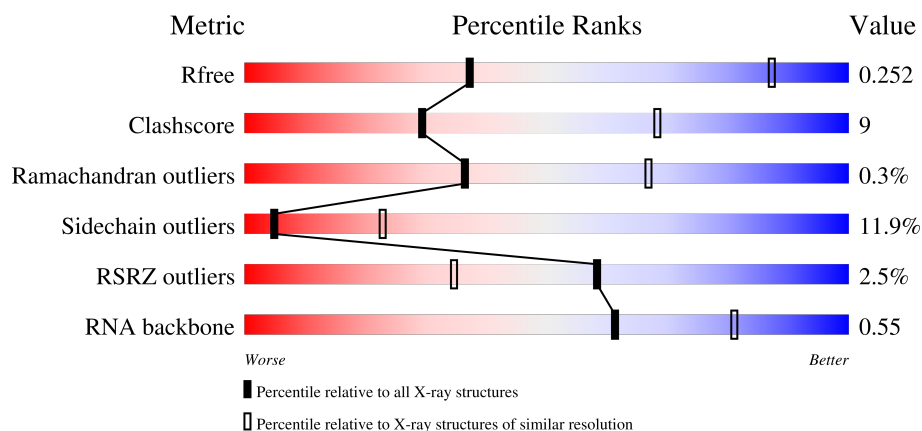
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.50 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.



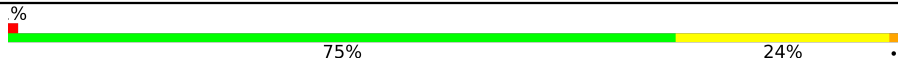
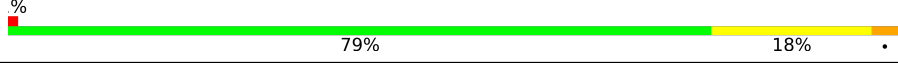
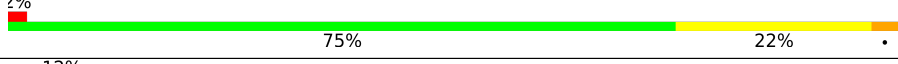
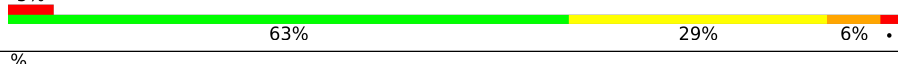
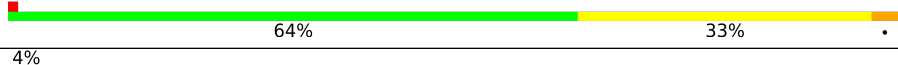
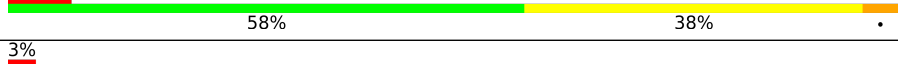
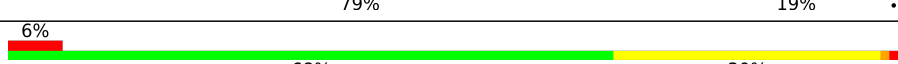
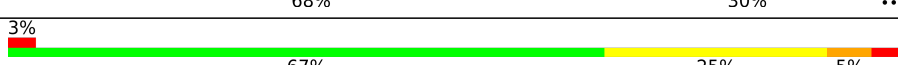
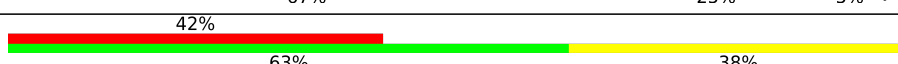
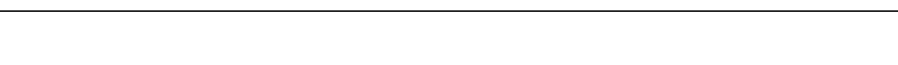
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1085 (3.54-3.46)
Clashscore	190562	1140 (3.54-3.46)
Ramachandran outliers	187476	1113 (3.54-3.46)
Sidechain outliers	187428	1114 (3.54-3.46)
RSRZ outliers	180081	1084 (3.54-3.46)
RNA backbone	3983	1010 (3.98-3.02)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	7% 57% 33% 9%
2	B	234	64% 33%
3	C	206	60% 36%
4	D	208	7% 67% 29%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
5	E	150	
6	F	101	
7	G	155	
8	H	138	
9	I	127	
10	J	98	
11	K	116	
12	L	124	
13	M	118	
14	N	60	
15	O	87	
16	P	83	
17	Q	99	
18	R	70	
19	S	80	
20	T	99	
21	U	24	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
22	MG	A	1625	-	-	-	X
22	MG	A	1632	-	-	-	X
22	MG	A	1666	-	-	-	X
22	MG	A	1684	-	-	-	X
22	MG	A	1697	-	-	-	X
22	MG	A	1728	-	-	-	X
22	MG	A	1734	-	-	-	X
22	MG	A	1738	-	-	-	X

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
22	MG	A	1743	-	-	-	X
22	MG	A	1744	-	-	-	X
22	MG	A	1783	-	-	-	X
22	MG	A	1786	-	-	-	X
22	MG	A	1824	-	-	-	X

2 Entry composition

There are 24 unique types of molecules in this entry. The entry contains 52227 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
1	A	1512	Total	C	N	O	P	0	6	0
			32644	14540	6039	10547	1518			

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
2	B	234	Total	C	N	O	S	0	0	0
			1900	1213	341	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
			1010	639	197	174			

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

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

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

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

- Molecule 12 is a protein called 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			

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 22 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
22	A	234	Total	Mg	0	0
			234	234		
22	B	3	Total	Mg	0	0
			3	3		
22	C	3	Total	Mg	0	0
			3	3		
22	D	4	Total	Mg	0	0
			4	4		
22	E	1	Total	Mg	0	0
			1	1		
22	F	1	Total	Mg	0	0
			1	1		
22	I	1	Total	Mg	0	0
			1	1		
22	P	2	Total	Mg	0	0
			2	2		
22	Q	2	Total	Mg	0	0
			2	2		
22	S	2	Total	Mg	0	0
			2	2		
22	U	1	Total	Mg	0	0
			1	1		

- Molecule 23 is ZINC ION (CCD ID: 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		

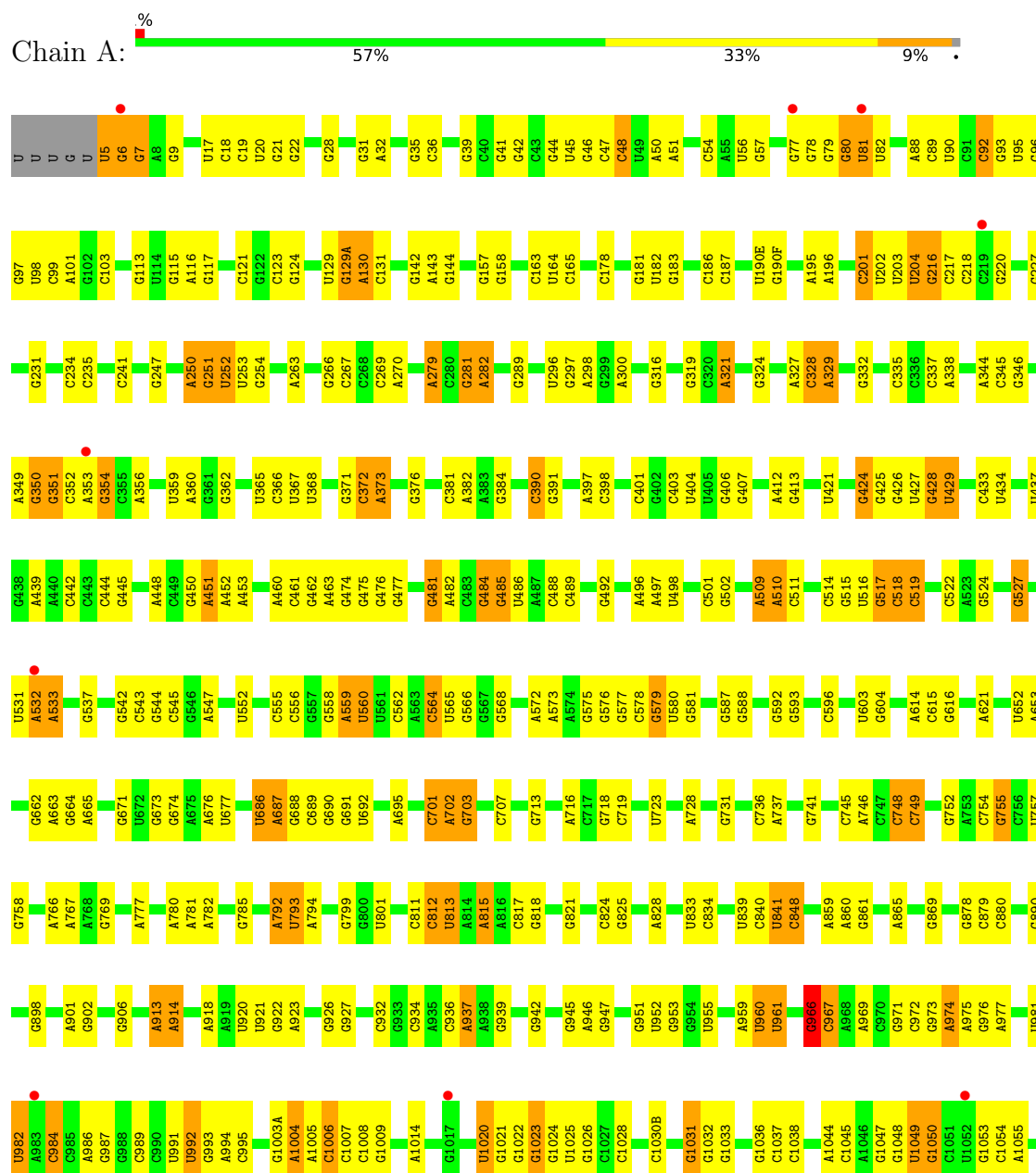
- Molecule 24 is water.

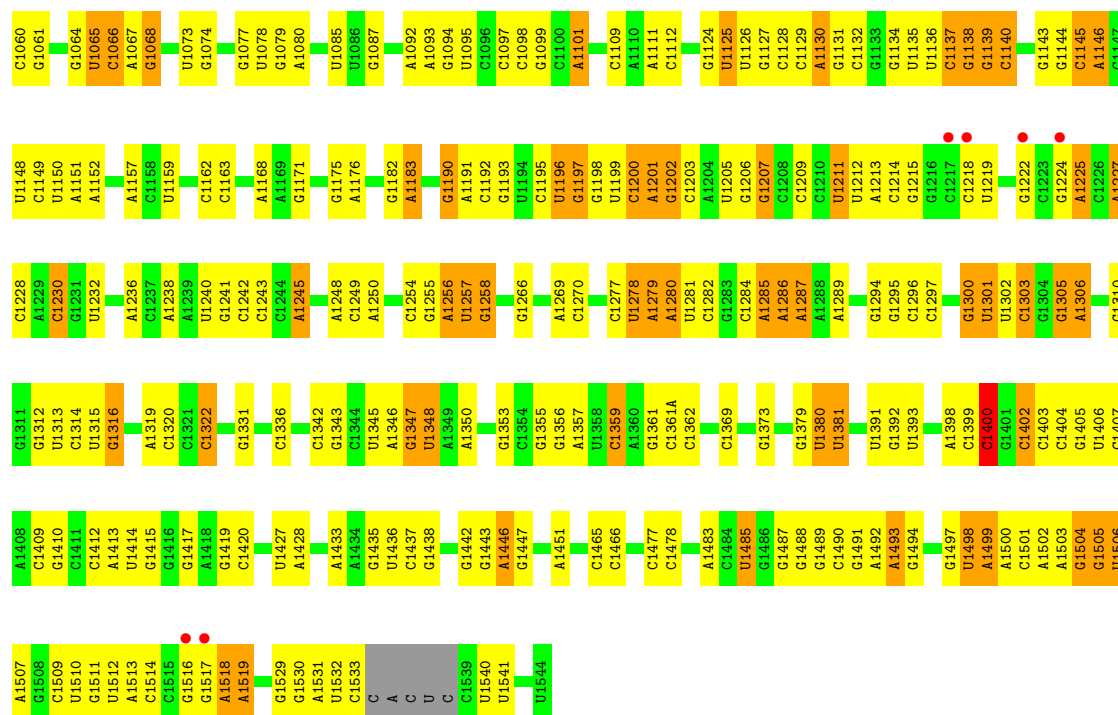
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
24	A	225	Total 225	O 225	0	0
24	D	2	Total 2	O 2	0	0
24	E	5	Total 5	O 5	0	0
24	L	2	Total 2	O 2	0	0
24	N	1	Total 1	O 1	0	0
24	Q	2	Total 2	O 2	0	0
24	T	2	Total 2	O 2	0	0

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.

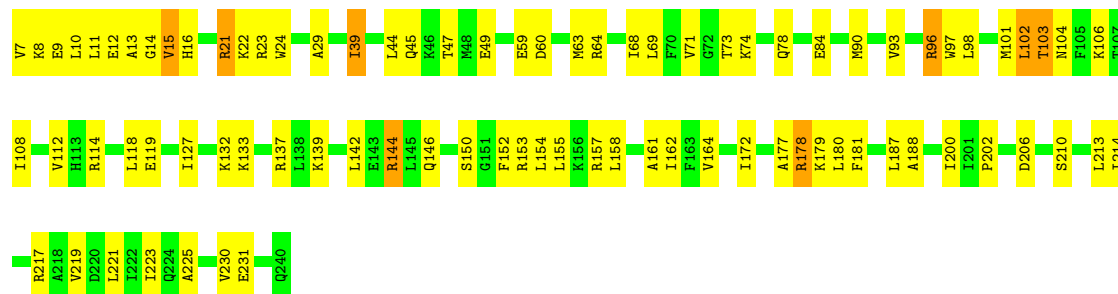
• Molecule 1: 16S Ribosomal RNA rRNA





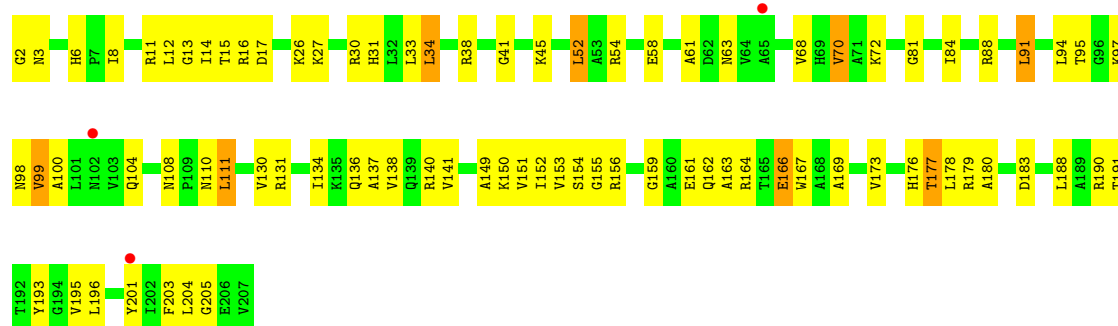
• Molecule 2: 30S ribosomal protein S2

Chain B: 64% 33% .

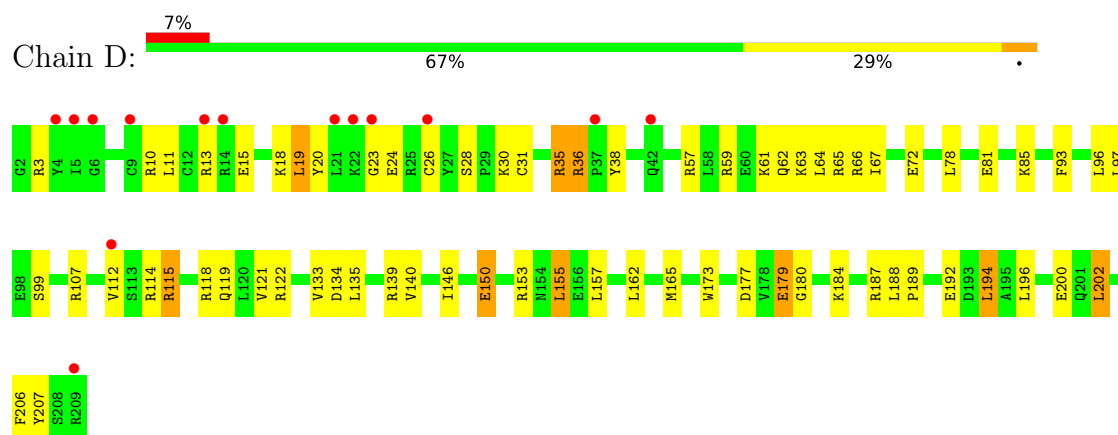


• Molecule 3: 30S ribosomal protein S3

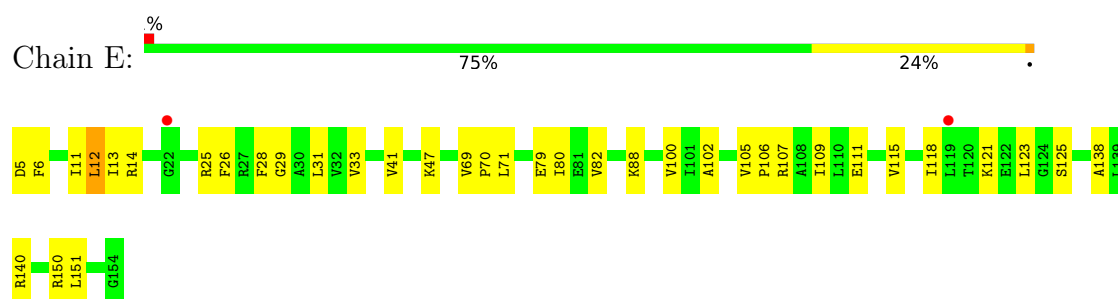
Chain C: 60% 36% .



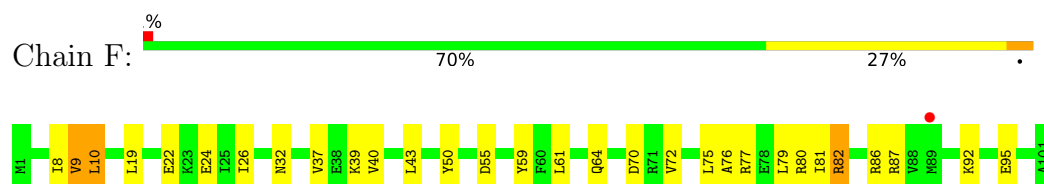
• Molecule 4: 30S ribosomal protein S4



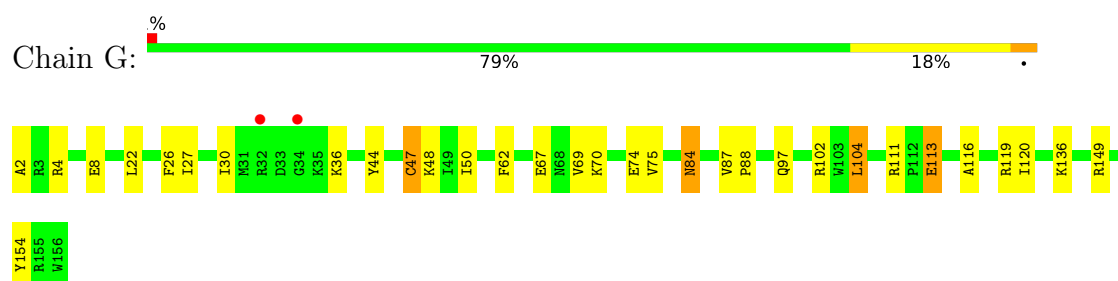
• Molecule 5: 30S ribosomal protein S5



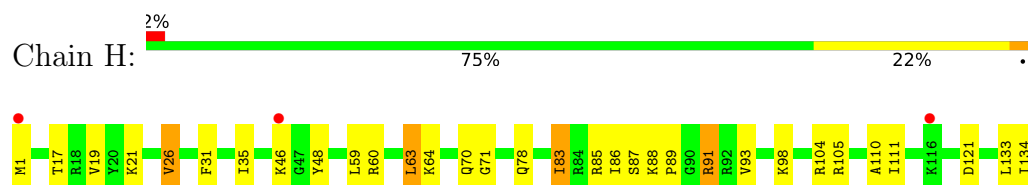
• Molecule 6: 30S ribosomal protein S6



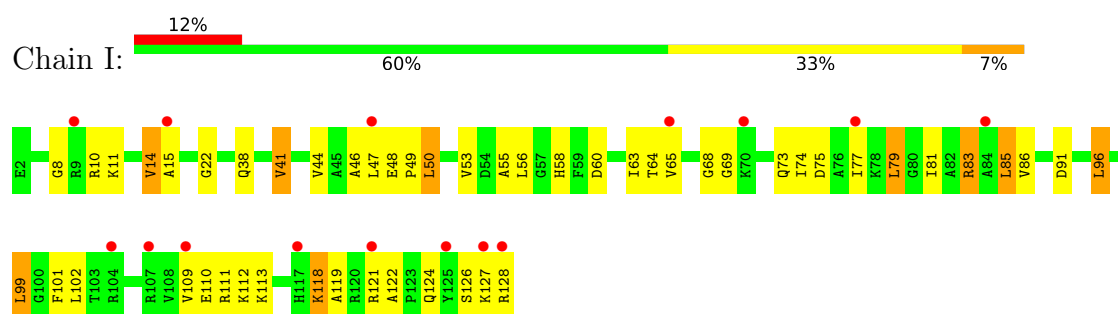
• Molecule 7: 30S ribosomal protein S7



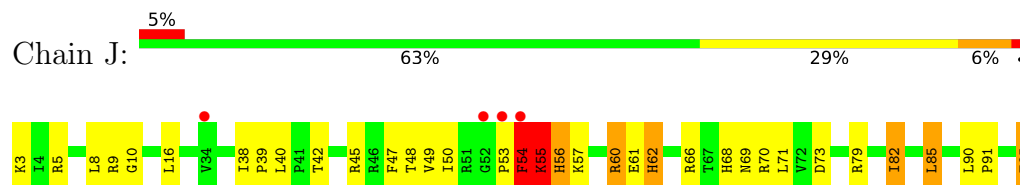
• Molecule 8: 30S ribosomal protein S8



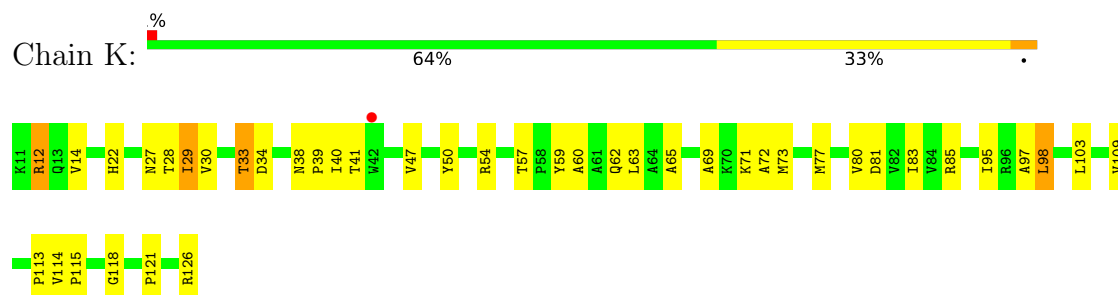
• Molecule 9: 30S ribosomal protein S9



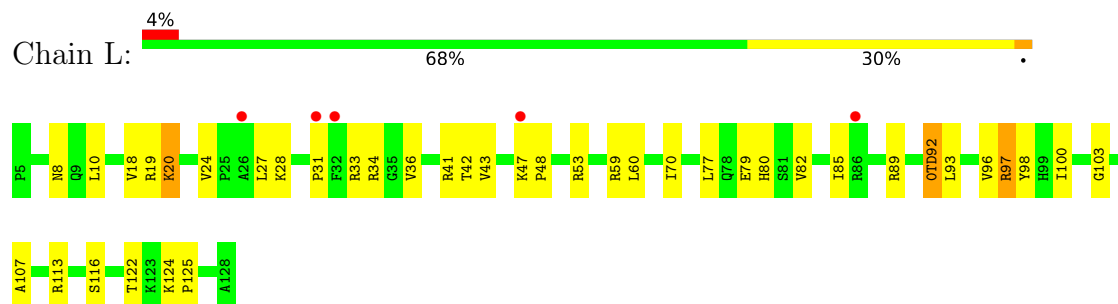
- Molecule 10: 30S ribosomal protein S10



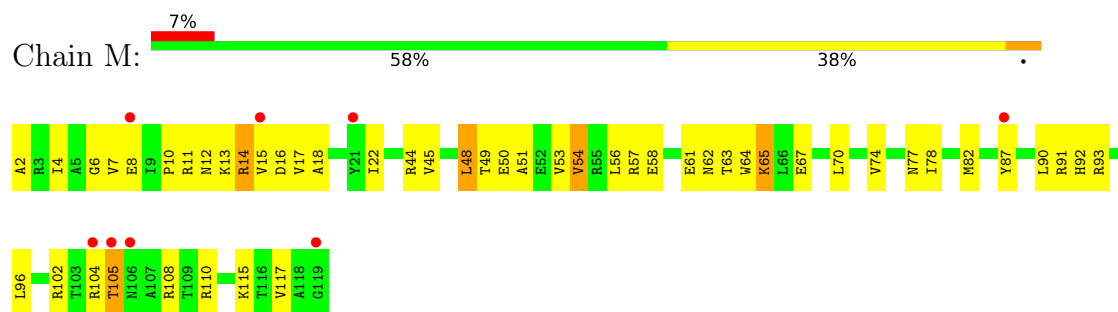
- Molecule 11: 30S ribosomal protein S11



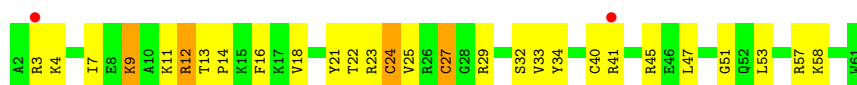
- Molecule 12: 30S ribosomal protein S12



- Molecule 13: 30S ribosomal protein S13



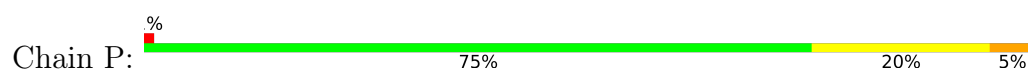
- Molecule 14: 30S ribosomal protein S14 type Z



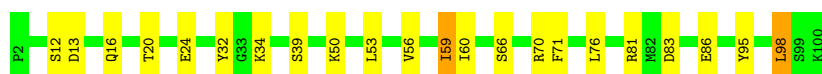
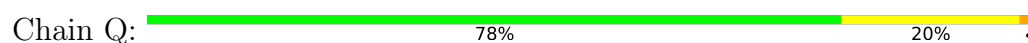
- Molecule 15: 30S ribosomal protein S15



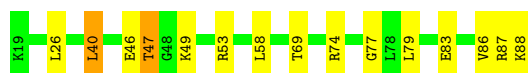
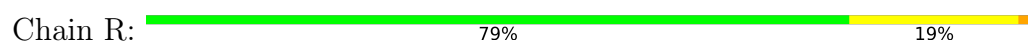
- Molecule 16: 30S ribosomal protein S16



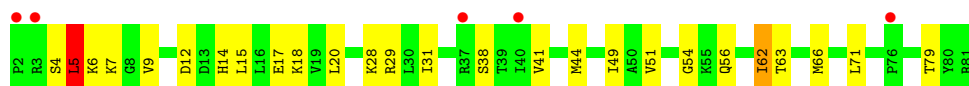
- Molecule 17: 30S ribosomal protein S17



- Molecule 18: 30S ribosomal protein S18



- Molecule 19: 30S ribosomal protein S19

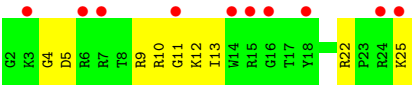


- Molecule 20: 30S ribosomal protein S20



A106

● Molecule 21: 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	400.00Å 400.00Å 173.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.98 – 3.50 29.98 – 3.50	Depositor EDS
% Data completeness (in resolution range)	91.5 (29.98-3.50) 79.9 (29.98-3.50)	Depositor EDS
R_{merge}	1.18	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.46 (at 2.90Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.214 , 0.256 0.216 , 0.252	Depositor DCC
R_{free} test set	2000 reflections (0.67%)	wwPDB-VP
Wilson B-factor (Å ²)	58.0	Xtriage
Anisotropy	0.303	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.25 , 139.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	52227	wwPDB-VP
Average B, all atoms (Å ²)	232.0	wwPDB-VP

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

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: 5MC, 2MG, 7MG, MG, M2G, 0TD, PSU, MA6, ZN, UR3, 4OC

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	0.10	1/36139 (0.0%)	0.28	1/56396 (0.0%)
2	B	0.16	0/1935	0.39	0/2609
3	C	0.14	0/1636	0.41	0/2205
4	D	0.13	0/1733	0.35	0/2318
5	E	0.14	0/1162	0.37	0/1564
6	F	0.11	0/856	0.33	0/1154
7	G	0.13	0/1276	0.35	0/1709
8	H	0.14	0/1136	0.36	0/1527
9	I	0.14	0/1029	0.43	0/1379
10	J	0.16	0/805	0.60	2/1082 (0.2%)
11	K	0.17	0/879	0.41	0/1187
12	L	0.16	0/977	0.47	0/1306
13	M	0.14	0/947	0.42	0/1270
14	N	0.17	0/501	0.51	1/664 (0.2%)
15	O	0.13	0/740	0.32	0/987
16	P	0.12	0/716	0.37	0/963
17	Q	0.13	0/836	0.40	0/1117
18	R	0.12	0/579	0.35	0/768
19	S	0.13	0/661	0.49	2/890 (0.2%)
20	T	0.15	0/765	0.43	0/1007
21	U	0.11	0/212	0.36	0/277
All	All	0.12	1/55520 (0.0%)	0.32	6/82379 (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
3	C	0	1

Continued on next page...

Continued from previous page...

Mol	Chain	#Chirality outliers	#Planarity outliers
10	J	0	2
13	M	0	1
14	N	0	1
20	T	0	1
All	All	0	7

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1498	UR3	O3'-P	5.33	1.61	1.56

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	N	7	ILE	N-CA-C	-6.36	106.25	111.91
10	J	54	PHE	CA-C-N	6.16	133.29	121.54
10	J	54	PHE	C-N-CA	6.16	133.29	121.54
1	A	1139	G	P-O3'-C3'	5.82	128.93	120.20
19	S	5	LEU	CA-C-N	5.06	131.21	121.54
19	S	5	LEU	C-N-CA	5.06	131.21	121.54

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	15	VAL	Peptide
3	C	166	GLU	Peptide
10	J	54	PHE	Peptide
10	J	55	LYS	Peptide
13	M	6	GLY	Peptide
14	N	11	LYS	Peptide
20	T	74	LYS	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	32644	0	16507	386	2
2	B	1900	0	1951	43	0
3	C	1612	0	1677	50	0
4	D	1703	0	1763	45	0
5	E	1146	0	1207	19	0
6	F	843	0	857	13	0
7	G	1257	0	1296	18	0
8	H	1116	0	1177	22	0
9	I	1010	0	1037	32	0
10	J	792	0	835	24	0
11	K	864	0	881	25	0
12	L	972	0	1058	24	0
13	M	937	0	995	32	0
14	N	492	0	529	25	0
15	O	729	0	768	9	0
16	P	700	0	720	14	0
17	Q	823	0	893	11	0
18	R	574	0	644	9	0
19	S	647	0	673	15	0
20	T	763	0	861	20	0
21	U	208	0	221	9	0
22	A	234	0	0	0	0
22	B	3	0	0	0	0
22	C	3	0	0	0	0
22	D	4	0	0	0	0
22	E	1	0	0	0	0
22	F	1	0	0	0	0
22	I	1	0	0	0	0
22	P	2	0	0	0	0
22	Q	2	0	0	0	0
22	S	2	0	0	0	0
22	U	1	0	0	0	0
23	D	1	0	0	0	0
23	N	1	0	0	0	0
24	A	225	0	0	1	0
24	D	2	0	0	0	0
24	E	5	0	0	0	0
24	L	2	0	0	1	0
24	N	1	0	0	0	0
24	Q	2	0	0	0	0
24	T	2	0	0	0	0
All	All	52227	0	36550	736	2

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 9.

All (736) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:664:G:H22	1:A:741:G:H1	1.23	0.86
20:T:100:ILE:HG22	20:T:102:GLY:H	1.41	0.86
1:A:1443:G:H5''	1:A:1446:A:H5'	1.57	0.85
1:A:1125:U:OP2	1:A:1145:C:N4	2.11	0.81
1:A:1347:G:O6	9:I:10:ARG:NH2	2.12	0.81
1:A:1193:G:OP1	3:C:167:TRP:NE1	2.16	0.79
1:A:1417:G:O2'	1:A:1483:A:N6	2.17	0.78
1:A:686:U:HO2'	1:A:687:A:H8	1.34	0.76
4:D:11:LEU:HD13	4:D:66:ARG:HD2	1.68	0.75
1:A:1134:G:H1	1:A:1140:C:H42	1.33	0.74
1:A:1049:U:O2'	14:N:3:ARG:NH1	2.19	0.74
2:B:21:ARG:HA	2:B:39:ILE:HA	1.71	0.73
9:I:50:LEU:HB3	9:I:55:ALA:HB3	1.71	0.73
13:M:10:PRO:HB2	13:M:18:ALA:HB1	1.70	0.73
1:A:1111:A:H61	3:C:177:THR:HB	1.53	0.72
1:A:1373:G:H5''	7:G:36:LYS:HE3	1.72	0.71
16:P:4:ILE:HG12	16:P:21:VAL:HG22	1.73	0.70
20:T:74:LYS:O	20:T:76:ALA:N	2.24	0.70
3:C:33:LEU:HD21	14:N:53:LEU:HD22	1.72	0.70
1:A:1128:C:O2'	1:A:1130:A:N7	2.25	0.70
6:F:10:LEU:HD12	6:F:59:TYR:HB3	1.74	0.70
1:A:974:A:OP2	14:N:29:ARG:NH2	2.25	0.69
17:Q:66:SER:O	17:Q:70:ARG:NH1	2.25	0.69
20:T:75:ASN:OD1	20:T:75:ASN:N	2.25	0.69
1:A:1195:C:H3'	1:A:1196:U:H5''	1.75	0.69
3:C:41:GLY:O	3:C:45:LYS:HG2	1.93	0.69
1:A:1098:C:OP2	2:B:144:ARG:NH2	2.25	0.68
1:A:1073:U:O2	2:B:104:ASN:ND2	2.27	0.68
1:A:1516[B]:G:N2	1:A:1519[B]:MA6:OP2	2.25	0.68
12:L:48:PRO:HD2	12:L:92:OTD:H3	1.74	0.68
1:A:1028:C:H42	1:A:1033:G:H1	1.42	0.68
3:C:52:LEU:HD12	3:C:68:VAL:HG13	1.75	0.67
11:K:85:ARG:HD3	11:K:113:PRO:HD3	1.76	0.67
5:E:71:LEU:HD21	5:E:115:VAL:HG22	1.77	0.67
10:J:82:ILE:HA	10:J:85:LEU:HB2	1.77	0.67
12:L:41:ARG:HE	12:L:43:VAL:HG22	1.58	0.67
9:I:10:ARG:HG2	9:I:75:ASP:HB2	1.77	0.66
1:A:404:U:OP2	4:D:118:ARG:NH1	2.29	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:372:C:H4'	1:A:373:A:O5'	1.94	0.66
12:L:53:ARG:NH1	12:L:92:0TD:OD2	2.27	0.66
1:A:671:G:H5'	6:F:77:ARG:HH21	1.61	0.65
1:A:1399:C:H4'	1:A:1400:5MC:H5''	1.77	0.65
1:A:1004:A:N7	1:A:1036:G:O6	2.30	0.65
1:A:427:U:OP1	4:D:13:ARG:NH2	2.30	0.65
2:B:63:MET:HB3	2:B:225:ALA:HB1	1.79	0.65
1:A:1347:G:H1'	1:A:1348:U:H5	1.61	0.64
1:A:811:C:O2'	1:A:901:A:N1	2.29	0.64
15:O:39:LEU:HD13	15:O:56:LEU:HB2	1.79	0.64
10:J:61:GLU:OE1	14:N:45:ARG:NH1	2.29	0.64
1:A:982:U:OP2	14:N:23:ARG:NH2	2.30	0.64
16:P:28:ARG:NH1	16:P:29:ASP:OD2	2.29	0.64
4:D:107:ARG:HH12	4:D:114:ARG:HH21	1.45	0.64
20:T:46:GLU:OE1	20:T:48:LYS:NZ	2.30	0.64
1:A:462:G:H21	16:P:82:GLN:HE21	1.44	0.64
1:A:297:G:N2	1:A:300:A:OP2	2.26	0.63
13:M:8:GLU:HG3	13:M:22:ILE:HG23	1.81	0.63
1:A:95:U:H2'	1:A:96:G:H8	1.63	0.63
1:A:1266:G:N2	1:A:1269:A:OP2	2.23	0.63
17:Q:12:SER:HB3	17:Q:20:THR:HB	1.80	0.63
1:A:564:C:O2'	8:H:91:ARG:NH2	2.32	0.63
1:A:1242:C:OP1	21:U:10:ARG:NH1	2.21	0.63
3:C:26:LYS:O	3:C:30:ARG:NH1	2.32	0.63
1:A:1243:C:O2	1:A:1295:G:N2	2.32	0.62
1:A:1222:G:OP2	1:A:1322:C:N4	2.29	0.62
1:A:1505:G:O2'	1:A:1506:U:OP2	2.14	0.62
12:L:60:LEU:HD11	12:L:85:ILE:HD12	1.81	0.62
4:D:15:GLU:HB3	4:D:63:LYS:HD3	1.80	0.62
15:O:33:THR:OG1	15:O:63:ARG:NH1	2.32	0.62
1:A:103:C:OP1	20:T:17:ARG:NH1	2.33	0.62
1:A:1009:G:H1	1:A:1020:U:H3	1.48	0.62
1:A:1518[B]:MA6:H102	1:A:1519[B]:MA6:H103	1.81	0.62
13:M:57:ARG:O	13:M:61:GLU:HB2	1.99	0.62
1:A:376:G:H5''	16:P:5:ARG:HB2	1.82	0.62
1:A:1310:G:H5'	13:M:77:ASN:HD21	1.65	0.62
10:J:61:GLU:OE2	14:N:58:LYS:NZ	2.32	0.62
4:D:194:LEU:HB3	4:D:196:LEU:HG	1.81	0.62
10:J:49:VAL:HG13	14:N:41:ARG:HB2	1.82	0.62
16:P:1:MET:HE3	16:P:3:LYS:HD2	1.82	0.62
1:A:1406:U:O2'	1:A:1517[B]:G:N2	2.32	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:107:ARG:HH21	4:D:194:LEU:HD12	1.66	0.61
3:C:156:ARG:H	3:C:163:ALA:HA	1.65	0.61
8:H:111:ILE:HG22	8:H:134:ILE:HD12	1.81	0.61
21:U:9:ARG:HE	21:U:22:ARG:HG3	1.66	0.60
1:A:1150:U:O4	1:A:1151:A:N6	2.34	0.60
1:A:401:C:O2'	1:A:621:A:N3	2.34	0.60
4:D:57:ARG:HB3	4:D:206:PHE:HB2	1.83	0.60
11:K:80:VAL:HG21	11:K:103:LEU:HD13	1.82	0.60
1:A:426:G:OP1	4:D:38:TYR:OH	2.18	0.60
5:E:102:ALA:O	5:E:107:ARG:NH1	2.34	0.60
1:A:321:A:N6	1:A:329:A:OP2	2.34	0.60
13:M:49:THR:HG22	13:M:51:ALA:H	1.67	0.60
1:A:946:A:H2'	1:A:947:G:C8	2.36	0.60
9:I:86:VAL:HG21	9:I:102:LEU:HD11	1.82	0.60
1:A:1245:A:OP2	21:U:9:ARG:NH1	2.34	0.60
11:K:57:THR:HG23	11:K:60:ALA:H	1.66	0.60
1:A:1006:C:H42	1:A:1022:G:H22	1.50	0.59
1:A:1064:G:N2	1:A:1190:G:O2'	2.35	0.59
1:A:1498:UR3:O5'	1:A:1498:UR3:H6	2.02	0.59
1:A:522:C:H41	12:L:53:ARG:HH22	1.48	0.59
1:A:953:G:N7	13:M:104:ARG:NH2	2.49	0.59
13:M:96:LEU:O	13:M:110:ARG:NH1	2.34	0.59
1:A:992:U:H3	1:A:1044:A:H62	1.50	0.59
1:A:981:U:H5'	14:N:21:TYR:CZ	2.38	0.59
1:A:1144:G:H21	1:A:1146:A:H62	1.50	0.59
1:A:1314:C:C5	19:S:6:LYS:HD3	2.38	0.59
1:A:792:A:H4'	1:A:793:U:O5'	2.03	0.59
1:A:951:G:OP2	13:M:102:ARG:NH2	2.36	0.59
20:T:33:ILE:HD13	20:T:62:LEU:HB3	1.85	0.59
2:B:84:GLU:HB3	2:B:219:VAL:HG21	1.85	0.58
16:P:53:VAL:HG12	16:P:79:VAL:HG22	1.85	0.58
1:A:45:U:H2'	1:A:46:G:C8	2.38	0.58
1:A:677:U:H3	1:A:713:G:H22	1.49	0.58
1:A:356:A:N3	1:A:368:U:O2'	2.33	0.58
7:G:69:VAL:HG21	7:G:104:LEU:HD21	1.85	0.58
1:A:403:C:OP2	4:D:3:ARG:NH2	2.36	0.58
1:A:279:A:OP2	17:Q:95:TYR:OH	2.20	0.58
1:A:1532:U:H2'	1:A:1533:C:H3'	1.86	0.57
4:D:62:GLN:OE1	4:D:65:ARG:NH1	2.37	0.57
4:D:57:ARG:HG3	4:D:202:LEU:HD13	1.84	0.57
9:I:46:ALA:HB2	9:I:74:ILE:HG23	1.85	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1405:G:O2'	1:A:1518[A]:MA6:O2'	2.18	0.57
19:S:18:LYS:HD3	19:S:31:ILE:HD11	1.87	0.57
1:A:1305:G:N2	1:A:1331:G:H1'	2.19	0.57
3:C:150:LYS:HB2	3:C:173:VAL:HG21	1.85	0.57
1:A:407:G:OP1	4:D:115:ARG:NH1	2.38	0.57
1:A:1414:U:H2'	1:A:1415:G:C8	2.40	0.57
3:C:156:ARG:NH1	3:C:193:TYR:O	2.38	0.56
11:K:40:ILE:HG22	11:K:41:THR:HG23	1.87	0.56
1:A:898:G:N2	1:A:901:A:OP2	2.33	0.56
1:A:1145:C:O2'	1:A:1146:A:O5'	2.24	0.56
2:B:59:GLU:HB2	2:B:221:LEU:HD11	1.88	0.56
3:C:14:ILE:HG22	3:C:15:THR:HG23	1.87	0.56
3:C:131:ARG:HA	3:C:134:ILE:HD12	1.87	0.56
10:J:79:ARG:HH12	10:J:82:ILE:HD12	1.70	0.56
8:H:83:ILE:HG12	8:H:137:VAL:HG22	1.87	0.56
12:L:41:ARG:HH21	12:L:43:VAL:HG13	1.69	0.56
1:A:17:U:H2'	1:A:18:C:C6	2.40	0.56
1:A:1342:C:H2'	1:A:1343:G:C8	2.41	0.56
6:F:22:GLU:OE1	6:F:82:ARG:NH1	2.39	0.56
2:B:101:MET:HA	2:B:108:ILE:HG13	1.87	0.56
4:D:18:LYS:HE2	4:D:20:TYR:HE2	1.70	0.56
12:L:24:VAL:HG13	12:L:98:TYR:HE2	1.71	0.56
1:A:21:G:H2'	1:A:22:G:C8	2.41	0.56
1:A:250:A:H4'	1:A:251:G:O5'	2.05	0.56
1:A:880:C:OP1	12:L:8:ASN:ND2	2.35	0.56
2:B:21:ARG:HG3	2:B:22:LYS:H	1.71	0.56
12:L:70:ILE:HG12	12:L:100:ILE:HD12	1.87	0.56
1:A:129(A):G:N2	1:A:190(F):G:OP2	2.34	0.56
3:C:91:LEU:HD21	3:C:99:VAL:HG22	1.88	0.56
20:T:39:LYS:HG2	20:T:55:ILE:HD13	1.88	0.56
1:A:1202:G:O2'	14:N:27:CYS:SG	2.65	0.55
1:A:1313:U:O4	19:S:4:SER:OG	2.17	0.55
3:C:137:ALA:HA	3:C:140:ARG:HD2	1.87	0.55
1:A:1491:G:N2	1:A:1492:A:H62	2.03	0.55
9:I:79:LEU:O	9:I:83:ARG:HG2	2.06	0.55
1:A:1391:U:H2'	1:A:1392:G:C8	2.42	0.55
2:B:103:THR:HG23	2:B:180:LEU:HD21	1.88	0.55
1:A:95:U:H2'	1:A:96:G:C8	2.42	0.55
1:A:718:G:O6	18:R:74:ARG:NH1	2.40	0.55
8:H:48:TYR:HA	8:H:60:ARG:O	2.06	0.55
1:A:955:U:H1'	1:A:1227:A:H61	1.72	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:451:A:N6	1:A:481:G:C4	2.75	0.55
1:A:959:A:O2'	1:A:984:C:O2'	2.23	0.55
2:B:162:ILE:HD12	2:B:177:ALA:HB2	1.87	0.55
1:A:1192:C:O2	5:E:25:ARG:NH2	2.40	0.55
1:A:1415:G:H1	1:A:1485:U:H3	1.54	0.55
6:F:39:LYS:HG2	6:F:64:GLN:HB3	1.90	0.54
1:A:1437:C:H2'	1:A:1438:G:H8	1.73	0.54
3:C:68:VAL:HG12	3:C:70:VAL:HG22	1.90	0.54
20:T:50:GLU:HA	20:T:100:ILE:HG13	1.89	0.54
11:K:69:ALA:O	11:K:73:MET:HG2	2.07	0.54
1:A:1048:G:H1	1:A:1209:C:H42	1.56	0.54
1:A:1510:U:H2'	1:A:1511:G:C8	2.42	0.54
1:A:558:G:OP2	1:A:559:A:O2'	2.24	0.54
5:E:102:ALA:HB1	5:E:106:PRO:HB2	1.90	0.54
1:A:923:A:O2'	1:A:1399:C:OP2	2.23	0.54
1:A:1077:G:N2	1:A:1080:A:OP2	2.41	0.54
1:A:7:G:H5'	1:A:298:A:O4'	2.08	0.54
1:A:501:C:H2'	1:A:502:G:C8	2.43	0.54
1:A:1049:U:H4'	1:A:1050:G:O5'	2.08	0.54
3:C:155:GLY:HA2	3:C:164:ARG:H	1.73	0.54
10:J:53:PRO:HA	14:N:41:ARG:NH2	2.23	0.54
11:K:65:ALA:HB1	11:K:98:LEU:HD23	1.89	0.53
1:A:1060:C:OP1	14:N:45:ARG:NH2	2.41	0.53
1:A:1379:G:O6	7:G:2:ALA:N	2.42	0.53
3:C:134:ILE:HG23	3:C:151:VAL:HB	1.90	0.53
4:D:140:VAL:HG11	4:D:146:ILE:HD11	1.91	0.53
12:L:34:ARG:NH2	24:L:201:HOH:O	2.40	0.53
1:A:144:G:H1	1:A:178:C:H42	1.56	0.53
7:G:111:ARG:NH1	7:G:113:GLU:OE2	2.42	0.53
12:L:24:VAL:HG13	12:L:98:TYR:CE2	2.42	0.53
1:A:56:U:H2'	1:A:57:G:H8	1.74	0.53
1:A:19:C:OP1	5:E:125:SER:OG	2.21	0.53
1:A:88:A:H2'	1:A:89:C:O4'	2.09	0.53
1:A:1488:G:H2'	1:A:1489:G:C8	2.43	0.53
20:T:16:HIS:O	20:T:19:SER:HB3	2.09	0.53
1:A:448:A:P	1:A:485:G:H22	2.31	0.53
8:H:86:ILE:HD12	8:H:133:LEU:HD22	1.89	0.53
4:D:99:SER:HB3	4:D:139:ARG:HG3	1.89	0.53
9:I:112:LYS:HA	9:I:119:ALA:HB2	1.90	0.53
1:A:501:C:H2'	1:A:502:G:H8	1.74	0.53
4:D:61:LYS:NZ	4:D:62:GLN:OE1	2.38	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:216:G:H2'	1:A:217:C:C6	2.44	0.52
1:A:1162:C:H2'	1:A:1163:C:C6	2.44	0.52
18:R:47:THR:HA	18:R:83:GLU:HB2	1.91	0.52
1:A:509:A:N3	1:A:543:C:O2'	2.40	0.52
1:A:755:G:H1'	8:H:1:MET:HE3	1.91	0.52
1:A:1195:C:H3'	1:A:1196:U:C5'	2.39	0.52
1:A:1310:G:H5'	13:M:77:ASN:ND2	2.25	0.52
1:A:1498:UR3:O4'	1:A:1519[A]:MA6:H2	2.09	0.52
1:A:77:G:H2'	1:A:78:G:C8	2.44	0.52
1:A:269:C:H2'	1:A:270:A:C8	2.45	0.52
1:A:362:G:N2	1:A:365:U:OP2	2.39	0.52
1:A:390:C:O3'	16:P:28:ARG:NH2	2.43	0.52
1:A:913:A:H4'	1:A:914:A:O5'	2.09	0.52
1:A:1240:U:OP1	7:G:119:ARG:NH2	2.34	0.52
3:C:81:GLY:O	3:C:84:ILE:HG22	2.09	0.52
10:J:5:ARG:HB2	10:J:99:LYS:O	2.09	0.52
10:J:50:ILE:HA	10:J:60:ARG:HB3	1.91	0.52
1:A:56:U:H2'	1:A:57:G:C8	2.44	0.52
1:A:518:C:H4'	1:A:519:C:O5'	2.09	0.52
1:A:937:A:N6	1:A:1345:U:O4	2.42	0.52
1:A:1230:C:N4	13:M:105:THR:HG21	2.25	0.52
14:N:47:LEU:HB3	14:N:53:LEU:HD21	1.92	0.52
1:A:1008:C:N4	1:A:1021:G:H1	2.08	0.52
3:C:150:LYS:HB3	3:C:201:TYR:HB2	1.92	0.52
1:A:92:C:H2'	1:A:93:G:C8	2.44	0.51
1:A:544:G:OP1	4:D:59:ARG:NH1	2.43	0.51
4:D:173:TRP:CD2	4:D:189:PRO:HB3	2.45	0.51
1:A:974:A:OP2	14:N:41:ARG:NH1	2.43	0.51
1:A:1198:G:H2'	1:A:1199:U:C6	2.46	0.51
1:A:1254:C:H2'	1:A:1255:G:C8	2.45	0.51
9:I:99:LEU:HB3	9:I:101:PHE:HD1	1.76	0.51
1:A:41:G:H2'	1:A:42:G:C8	2.45	0.51
1:A:1031:G:H2'	1:A:1032:G:C8	2.46	0.51
20:T:92:LEU:O	20:T:96:GLY:HA2	2.10	0.51
1:A:481:G:O2'	1:A:482:A:H8	1.93	0.51
1:A:227:G:N2	16:P:62:VAL:O	2.38	0.51
1:A:579:G:H5'	1:A:728:A:H1'	1.91	0.51
1:A:1314:C:H2'	1:A:1315:U:C6	2.46	0.51
3:C:88:ARG:HH21	3:C:100:ALA:HB1	1.75	0.51
1:A:537:G:OP1	12:L:113:ARG:NH2	2.44	0.51
1:A:932:C:H5'	7:G:4:ARG:HG3	1.91	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:R:46:GLU:CD	18:R:46:GLU:H	2.17	0.51
1:A:973:G:H3'	1:A:974:A:H5''	1.93	0.51
3:C:108:ASN:HB3	3:C:111:LEU:HB2	1.93	0.51
3:C:180:ALA:HB1	3:C:205:GLY:O	2.11	0.51
4:D:78:LEU:HD21	4:D:96:LEU:HB3	1.93	0.51
8:H:63:LEU:H	8:H:63:LEU:HD22	1.76	0.51
13:M:82:MET:HE3	13:M:92:HIS:HB3	1.93	0.51
1:A:5:U:H4'	1:A:6:G:O5'	2.11	0.51
1:A:281:G:H4'	1:A:282:A:O5'	2.11	0.51
1:A:736:C:H2'	1:A:737:A:C8	2.46	0.51
1:A:662:G:H2'	1:A:663:A:C8	2.46	0.50
1:A:686:U:O2'	1:A:687:A:H8	1.93	0.50
1:A:1305:G:O2'	1:A:1306:A:P	2.70	0.50
3:C:70:VAL:HG12	3:C:72:LYS:H	1.75	0.50
1:A:1148:U:H2'	1:A:1149:C:O4'	2.11	0.50
1:A:1392:G:N2	1:A:1502:A:H8	2.09	0.50
1:A:1435:G:H2'	1:A:1436:U:C6	2.46	0.50
4:D:23:GLY:HA3	4:D:112:VAL:HG12	1.92	0.50
5:E:11:ILE:HG22	5:E:12:LEU:HD12	1.93	0.50
11:K:12:ARG:HB3	11:K:14:VAL:HG13	1.93	0.50
12:L:113:ARG:HH11	12:L:116:SER:H	1.60	0.50
1:A:157:G:H2'	1:A:158:G:H8	1.77	0.50
1:A:514:C:H2'	1:A:515:G:H8	1.76	0.50
1:A:1257:U:O2'	1:A:1258:G:OP2	2.24	0.50
1:A:780:A:N6	1:A:801:U:OP2	2.43	0.50
2:B:60:ASP:CG	2:B:64:ARG:HH12	2.20	0.50
20:T:85:MET:HE2	20:T:104:LEU:HD23	1.93	0.50
1:A:1143:G:H2'	1:A:1144:G:C8	2.46	0.50
1:A:1498:UR3:H1'	1:A:1499:A:OP2	2.12	0.50
1:A:89:C:H2'	1:A:90:U:O4'	2.12	0.50
2:B:45:GLN:O	2:B:49:GLU:HG3	2.12	0.50
1:A:1112:C:O2	3:C:179:ARG:HB2	2.12	0.50
1:A:1504:G:OP1	1:A:1507:A:H4'	2.11	0.50
2:B:119:GLU:OE1	2:B:153:ARG:NH2	2.45	0.50
14:N:9:LYS:HD2	14:N:23:ARG:HB2	1.94	0.49
20:T:70:SER:HA	20:T:73:HIS:CD2	2.47	0.49
1:A:31:G:N2	1:A:48:C:OP1	2.42	0.49
3:C:138:VAL:HG13	3:C:149:ALA:HB3	1.93	0.49
1:A:1301:U:O2'	1:A:1303:C:OP2	2.31	0.49
1:A:1513:A:H2'	1:A:1514:C:C6	2.47	0.49
17:Q:59:ILE:HG23	17:Q:71:PHE:HB3	1.94	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1427:U:H2'	1:A:1428:A:C8	2.47	0.49
1:A:1055:A:O2'	3:C:161:GLU:O	2.28	0.49
8:H:26:VAL:HG13	8:H:59:LEU:HB2	1.94	0.49
9:I:22:GLY:HA3	9:I:60:ASP:HB2	1.94	0.49
1:A:1137:C:H4'	1:A:1138:G:C2	2.48	0.49
1:A:1348:U:OP1	9:I:110:GLU:HB3	2.13	0.49
5:E:13:ILE:HA	5:E:29:GLY:O	2.12	0.49
7:G:22:LEU:HG	7:G:62:PHE:HE2	1.78	0.49
13:M:48:LEU:HB3	13:M:53:VAL:HG23	1.94	0.49
13:M:90:LEU:HD23	13:M:93:ARG:HD2	1.95	0.49
3:C:134:ILE:HG21	3:C:167:TRP:O	2.13	0.49
4:D:81:GLU:O	4:D:85:LYS:HG3	2.13	0.49
8:H:31:PHE:O	8:H:35:ILE:HG12	2.13	0.49
1:A:450:G:H4'	16:P:41:PRO:HB2	1.94	0.49
1:A:1355:G:H2'	1:A:1356:G:C8	2.48	0.49
3:C:130:VAL:HG21	3:C:153:VAL:HG11	1.94	0.49
1:A:328:C:H4'	1:A:329:A:O5'	2.13	0.49
12:L:48:PRO:CD	12:L:92:OTD:H3	2.42	0.49
13:M:63:THR:HG23	13:M:64:TRP:CD2	2.48	0.49
15:O:36:ILE:HD13	15:O:59:MET:HE3	1.95	0.49
20:T:56:MET:HE2	20:T:85:MET:HG2	1.94	0.49
6:F:70:ASP:OD1	6:F:70:ASP:N	2.38	0.48
11:K:121:PRO:HD2	11:K:126:ARG:HD2	1.93	0.48
12:L:27:LEU:HG	12:L:28:LYS:H	1.78	0.48
1:A:1136:U:H5''	1:A:1137:C:OP2	2.13	0.48
1:A:1497:G:H2'	1:A:1498:UR3:H5'	1.95	0.48
12:L:103:GLY:N	12:L:107:ALA:O	2.31	0.48
1:A:442:C:H42	1:A:492:G:H1	1.61	0.48
1:A:1008:C:H42	1:A:1021:G:H1	1.61	0.48
1:A:1256:A:H4'	1:A:1257:U:O5'	2.13	0.48
2:B:98:LEU:O	2:B:101:MET:HG3	2.13	0.48
1:A:235:C:N4	24:A:1904:HOH:O	2.45	0.48
1:A:474:G:H2'	1:A:475:G:C8	2.48	0.48
1:A:859:A:OP2	1:A:869:G:N1	2.30	0.48
1:A:1343:G:H4'	9:I:122:ALA:HB3	1.95	0.48
4:D:93:PHE:CE1	4:D:97:LEU:HD11	2.48	0.48
8:H:110:ALA:N	8:H:121:ASP:OD1	2.47	0.48
1:A:701:C:H4'	1:A:702:A:O5'	2.12	0.48
1:A:1092:A:N3	1:A:1183:A:N6	2.60	0.48
1:A:1196:U:OP1	1:A:1197:G:H5'	2.13	0.48
1:A:1294:G:H2'	1:A:1295:G:C8	2.49	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:12:LEU:HD11	14:N:51:GLY:HA2	1.95	0.48
4:D:19:LEU:HB3	4:D:67:ILE:HG12	1.95	0.48
6:F:77:ARG:O	6:F:81:ILE:HG13	2.13	0.48
11:K:59:TYR:CE2	11:K:63:LEU:HD11	2.49	0.48
11:K:83:ILE:HD13	11:K:109:VAL:HB	1.94	0.48
15:O:56:LEU:HA	15:O:59:MET:HE2	1.95	0.48
18:R:40:LEU:HB3	18:R:79:LEU:HD11	1.94	0.48
19:S:62:ILE:HD12	19:S:66:MET:HG3	1.95	0.48
3:C:16:ARG:NH1	3:C:183:ASP:OD2	2.47	0.48
1:A:517:G:N1	1:A:533:A:OP2	2.46	0.48
5:E:100:VAL:O	5:E:107:ARG:NH2	2.46	0.48
10:J:48:THR:HA	10:J:62:HIS:HB3	1.96	0.48
1:A:337:C:H2'	1:A:338:A:C8	2.49	0.48
1:A:1131:G:H2'	1:A:1132:C:C6	2.49	0.48
1:A:1286:A:H2'	1:A:1287:A:H4'	1.94	0.48
1:A:1300:G:H4'	1:A:1301:U:O5'	2.13	0.48
1:A:652:U:O4	1:A:752:G:O2'	2.26	0.48
1:A:701:C:H5''	1:A:703:G:H5'	1.96	0.48
2:B:68:ILE:O	2:B:90:MET:HB3	2.14	0.48
1:A:474:G:H2'	1:A:475:G:H8	1.79	0.47
1:A:324:G:N1	1:A:327:A:OP2	2.45	0.47
9:I:63:ILE:HG21	9:I:77:ILE:HG12	1.96	0.47
1:A:757:U:H2'	1:A:758:G:O4'	2.13	0.47
5:E:105:VAL:HB	5:E:106:PRO:HD3	1.96	0.47
1:A:1068:G:H8	1:A:1068:G:OP2	1.96	0.47
7:G:26:PHE:O	7:G:30:ILE:HG13	2.14	0.47
11:K:33:THR:OG1	11:K:34:ASP:N	2.47	0.47
11:K:50:TYR:CD2	11:K:54:ARG:HB3	2.49	0.47
1:A:241:C:O3'	12:L:19:ARG:NH2	2.47	0.47
1:A:579:G:H4'	15:O:54:ARG:HH21	1.79	0.47
1:A:673:G:H2'	1:A:674:G:C8	2.49	0.47
1:A:1305:G:H5''	21:U:4:GLY:HA3	1.96	0.47
5:E:33:VAL:HG11	5:E:109:ILE:HA	1.96	0.47
1:A:186:C:H2'	1:A:187:C:C6	2.50	0.47
1:A:316:G:OP2	1:A:351:G:O2'	2.32	0.47
1:A:324:G:OP1	20:T:22:ARG:NH1	2.47	0.47
1:A:437:U:H5'	4:D:155:LEU:HD21	1.96	0.47
1:A:707:C:OP1	11:K:85:ARG:NH1	2.48	0.47
1:A:920:U:H2'	1:A:921:U:C6	2.50	0.47
1:A:974:A:OP1	1:A:974:A:H8	1.97	0.47
4:D:57:ARG:NH2	5:E:111:GLU:OE2	2.48	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:9:ARG:HG3	10:J:95:GLU:HB3	1.96	0.47
19:S:12:ASP:H	19:S:38:SER:HB3	1.80	0.47
1:A:555:C:H2'	1:A:556:C:C6	2.50	0.47
17:Q:50:LYS:HE2	17:Q:50:LYS:HB3	1.79	0.47
1:A:514:C:H2'	1:A:515:G:C8	2.50	0.47
1:A:1301:U:OP2	1:A:1303:C:N4	2.48	0.47
1:A:1319:A:OP1	19:S:5:LEU:HD22	2.15	0.47
3:C:13:GLY:HA3	14:N:57:ARG:HH21	1.79	0.47
3:C:17:ASP:O	3:C:54:ARG:NH2	2.48	0.47
1:A:390:C:H2'	1:A:391:G:C8	2.50	0.47
1:A:1254:C:H2'	1:A:1255:G:H8	1.80	0.47
13:M:74:VAL:O	13:M:78:ILE:HG12	2.15	0.47
14:N:24:CYS:H	14:N:33:VAL:HG21	1.80	0.47
1:A:1359:C:H1'	1:A:1361(A):C:H41	1.79	0.46
1:A:1412:C:H2'	1:A:1413:A:C8	2.50	0.46
4:D:177:ASP:OD1	4:D:179:GLU:HG2	2.14	0.46
9:I:15:ALA:HB2	9:I:65:VAL:HG23	1.98	0.46
9:I:48:GLU:N	9:I:49:PRO:HD2	2.30	0.46
9:I:96:LEU:HD23	9:I:102:LEU:HG	1.97	0.46
1:A:41:G:H2'	1:A:42:G:H8	1.81	0.46
1:A:476:G:H2'	1:A:477:G:H8	1.79	0.46
1:A:532:A:H2'	1:A:533:A:H5''	1.97	0.46
1:A:945:G:O6	1:A:1236:A:N1	2.48	0.46
1:A:1257:U:H4'	1:A:1258:G:O5'	2.15	0.46
1:A:1280:A:H5'	10:J:40:LEU:HD22	1.97	0.46
2:B:142:LEU:HD23	2:B:142:LEU:HA	1.81	0.46
8:H:46:LYS:HG3	8:H:64:LYS:HB3	1.97	0.46
10:J:10:GLY:HA3	10:J:16:LEU:HD21	1.96	0.46
13:M:48:LEU:HD22	13:M:48:LEU:HA	1.79	0.46
20:T:63:ILE:HG21	20:T:81:LYS:HG3	1.97	0.46
1:A:1232:U:H5''	9:I:124:GLN:O	2.14	0.46
2:B:24:TRP:HZ3	2:B:29:ALA:HB2	1.80	0.46
10:J:42:THR:HG21	10:J:66:ARG:HB2	1.97	0.46
1:A:335:C:O2'	1:A:1433:A:N3	2.43	0.46
1:A:1502:A:H2	1:A:1505:G:H1	1.61	0.46
11:K:72:ALA:HB1	11:K:77:MET:HG3	1.97	0.46
13:M:15:VAL:HG21	13:M:48:LEU:HD21	1.97	0.46
1:A:130:A:H1'	1:A:263:A:O2'	2.16	0.46
1:A:1020:U:H2'	1:A:1021:G:H8	1.79	0.46
1:A:1225:A:H2'	1:A:1225:A:N3	2.30	0.46
15:O:26:GLU:HA	15:O:81:LEU:HD11	1.97	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:542:G:OP1	4:D:10:ARG:NH2	2.45	0.46
1:A:1201:A:H4'	1:A:1202:G:O5'	2.15	0.46
1:A:1305:G:O2'	1:A:1306:A:H8	1.98	0.46
1:A:1409:C:H2'	1:A:1410:G:C8	2.51	0.46
2:B:71:VAL:HB	2:B:164:VAL:HG12	1.96	0.46
3:C:6:HIS:CE1	3:C:8:ILE:HB	2.51	0.46
4:D:187:ARG:NH2	4:D:188:LEU:HB2	2.31	0.46
1:A:1305:G:O2'	1:A:1306:A:O5'	2.27	0.46
1:A:1518[A]:MA6:H8	1:A:1518[A]:MA6:O5'	2.16	0.46
4:D:28:SER:O	4:D:30:LYS:N	2.47	0.46
1:A:254:G:O2'	17:Q:16:GLN:O	2.33	0.46
1:A:812:C:H4'	1:A:813:U:O5'	2.14	0.46
1:A:1369:C:OP1	9:I:111:ARG:HB2	2.16	0.46
11:K:33:THR:HG1	11:K:38:ASN:C	2.22	0.46
16:P:68:ASP:OD1	16:P:68:ASP:N	2.49	0.46
1:A:707:C:O2	11:K:39:PRO:HD3	2.16	0.46
1:A:19:C:H2'	1:A:20:U:C6	2.50	0.46
1:A:201:C:H42	1:A:216:G:H1	1.63	0.46
1:A:1157:A:H5'	2:B:132:LYS:HE3	1.97	0.46
1:A:1218:C:H2'	1:A:1219:U:C6	2.50	0.46
2:B:96:ARG:HG3	2:B:97:TRP:N	2.31	0.46
1:A:113:G:H1'	1:A:354:G:H5'	1.98	0.45
5:E:82:VAL:HG21	5:E:138:ALA:HA	1.97	0.45
10:J:8:LEU:O	10:J:69:ASN:HA	2.16	0.45
19:S:5:LEU:HD12	19:S:9:VAL:HG22	1.98	0.45
1:A:129:U:O3'	1:A:129(A):G:H3'	2.15	0.45
1:A:1305:G:O2'	1:A:1306:A:C8	2.70	0.45
19:S:5:LEU:C	19:S:6:LYS:HG3	2.40	0.45
1:A:19:C:H2'	1:A:20:U:H6	1.81	0.45
1:A:766:A:H2'	1:A:767:A:O4'	2.16	0.45
8:H:19:VAL:HG23	8:H:21:LYS:HG3	1.97	0.45
15:O:29:VAL:HG11	15:O:67:LEU:HD21	1.98	0.45
15:O:75:PRO:O	15:O:79:ARG:HG3	2.16	0.45
17:Q:24:GLU:HG2	17:Q:39:SER:HB3	1.97	0.45
1:A:1200:C:H5'	1:A:1201:A:OP1	2.17	0.45
1:A:463:A:OP1	16:P:75:ARG:NH1	2.39	0.45
1:A:1316:G:N2	1:A:1319:A:OP2	2.50	0.45
3:C:180:ALA:HB3	3:C:203:PHE:HE1	1.81	0.45
1:A:142:G:H2'	1:A:143:A:C8	2.52	0.45
1:A:689:C:H2'	1:A:690:G:O4'	2.17	0.45
1:A:1049:U:H5'	1:A:1201:A:OP2	2.16	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1277:C:O2'	1:A:1279:A:H1'	2.16	0.45
1:A:1356:G:H2'	1:A:1357:A:C8	2.52	0.45
3:C:159:GLY:HA2	3:C:193:TYR:CG	2.52	0.45
1:A:300:A:O2'	1:A:564:C:N3	2.45	0.45
1:A:560:U:H5'	1:A:566:G:N2	2.30	0.45
1:A:972:C:H4'	10:J:57:LYS:HD3	1.97	0.45
1:A:1343:G:H1'	9:I:121:ARG:HH12	1.81	0.45
1:A:1347:G:O2'	1:A:1348:U:P	2.75	0.45
1:A:1355:G:H2'	1:A:1356:G:H8	1.82	0.45
2:B:179:LYS:HE3	2:B:179:LYS:HB2	1.72	0.45
9:I:111:ARG:NH1	9:I:112:LYS:O	2.49	0.45
10:J:57:LYS:O	10:J:60:ARG:NH1	2.50	0.45
16:P:21:VAL:HG23	16:P:36:ILE:HG12	1.98	0.45
1:A:1202:G:H2'	1:A:1203:C:O4'	2.17	0.45
1:A:1511:G:H2'	1:A:1512:U:O4'	2.17	0.45
4:D:72:GLU:OE1	4:D:207:TYR:OH	2.33	0.45
20:T:73:HIS:HB3	20:T:74:LYS:H	1.56	0.45
1:A:1098:C:H2'	1:A:1099:G:O4'	2.17	0.45
5:E:88:LYS:HD2	5:E:123:LEU:HD12	1.99	0.45
1:A:966:M2G:HM22	1:A:967:5MC:C2	2.52	0.45
4:D:35:ARG:HD2	4:D:35:ARG:N	2.32	0.45
7:G:84:ASN:OD1	7:G:84:ASN:N	2.29	0.45
14:N:29:ARG:HB3	14:N:33:VAL:HG22	1.99	0.45
1:A:35:G:H2'	1:A:36:C:C6	2.52	0.44
1:A:157:G:H2'	1:A:158:G:C8	2.51	0.44
1:A:1065:U:H1'	1:A:1066:C:OP2	2.16	0.44
1:A:1380:U:H1'	1:A:1381:U:OP2	2.16	0.44
3:C:34:LEU:O	3:C:38:ARG:HG2	2.17	0.44
4:D:177:ASP:OD1	4:D:180:GLY:N	2.38	0.44
1:A:381:C:H2'	1:A:382:A:O4'	2.17	0.44
1:A:452:A:O2'	1:A:453:A:O4'	2.30	0.44
1:A:890:G:O2'	1:A:906:G:O6	2.32	0.44
1:A:1232:U:OP1	9:I:126:SER:HB3	2.16	0.44
2:B:146:GLN:O	2:B:150:SER:HB3	2.16	0.44
4:D:61:LYS:HE3	4:D:61:LYS:HB3	1.87	0.44
4:D:184:LYS:HE3	4:D:184:LYS:HB2	1.80	0.44
20:T:50:GLU:HG3	20:T:100:ILE:HD11	2.00	0.44
1:A:676:A:H1'	11:K:115:PRO:HB3	1.99	0.44
1:A:824:C:H2'	1:A:825:G:C8	2.53	0.44
1:A:952:U:H2'	1:A:953:G:H8	1.83	0.44
1:A:1007:C:H2'	1:A:1008: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:1047:G:H5''	14:N:4:LYS:HD2	1.99	0.44
1:A:1074:G:O2'	1:A:1101:A:N1	2.36	0.44
1:A:1196:U:H3	3:C:162:GLN:HE22	1.65	0.44
8:H:86:ILE:HD11	8:H:136:GLU:HG3	1.99	0.44
14:N:29:ARG:HH22	14:N:41:ARG:HH12	1.65	0.44
18:R:53:ARG:NH1	18:R:58:LEU:O	2.45	0.44
1:A:164:U:H2'	1:A:165:C:C6	2.52	0.44
1:A:1230:C:H41	13:M:105:THR:HG21	1.81	0.44
1:A:1278:U:H5'	1:A:1279:A:O4'	2.17	0.44
2:B:188:ALA:O	2:B:202:PRO:HA	2.17	0.44
3:C:150:LYS:HG3	3:C:169:ALA:HB2	1.99	0.44
8:H:104:ARG:HG3	8:H:138:TRP:CD2	2.52	0.44
1:A:1148:U:H4'	9:I:14:VAL:HG11	2.00	0.44
2:B:187:LEU:HD23	2:B:214:ILE:HG21	1.99	0.44
4:D:133:VAL:HG12	4:D:135:LEU:H	1.82	0.44
11:K:14:VAL:HG21	11:K:40:ILE:HD13	2.00	0.44
21:U:5:ASP:O	21:U:11:GLY:HA3	2.17	0.44
21:U:13:ILE:HG22	21:U:22:ARG:CZ	2.47	0.44
1:A:98:U:H2'	1:A:99:C:C6	2.53	0.44
1:A:615:C:H2'	1:A:616:G:O4'	2.18	0.44
1:A:719:C:O2'	18:R:49:LYS:HB3	2.17	0.44
1:A:824:C:H2'	1:A:825:G:H8	1.81	0.44
1:A:986:A:H2'	1:A:987:G:C8	2.53	0.44
2:B:133:LYS:O	2:B:137:ARG:HG3	2.17	0.44
13:M:16:ASP:OD1	13:M:16:ASP:N	2.50	0.44
1:A:79:G:H2'	1:A:79:G:N3	2.33	0.44
3:C:137:ALA:O	3:C:141:VAL:HG23	2.17	0.44
13:M:54:VAL:O	13:M:58:GLU:HG2	2.17	0.44
10:J:9:ARG:HA	10:J:68:HIS:O	2.18	0.44
1:A:1391:U:H2'	1:A:1392:G:H8	1.82	0.44
1:A:1393:U:O2'	1:A:1501:C:O2'	2.34	0.44
1:A:1399:C:C2	1:A:1502:A:N6	2.86	0.44
1:A:1443:G:C5'	1:A:1446:A:H5'	2.40	0.44
4:D:11:LEU:HD22	4:D:66:ARG:NH1	2.33	0.44
8:H:110:ALA:HB3	8:H:121:ASP:HB3	2.00	0.44
16:P:3:LYS:HE2	16:P:3:LYS:HB3	1.86	0.44
1:A:143:A:O3'	1:A:144:G:H8	2.01	0.43
1:A:986:A:H1'	19:S:54:GLY:O	2.17	0.43
2:B:16:HIS:CE1	2:B:210:SER:HB2	2.52	0.43
2:B:102:LEU:HB3	2:B:180:LEU:HD12	2.00	0.43
2:B:230:VAL:HG12	2:B:231:GLU:O	2.17	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:134:ILE:O	3:C:138:VAL:HG23	2.18	0.43
12:L:10:LEU:HB3	17:Q:32:TYR:CE1	2.52	0.43
13:M:51:ALA:O	13:M:54:VAL:HG12	2.17	0.43
1:A:488:C:H2'	1:A:489:C:C6	2.53	0.43
1:A:580:U:H2'	1:A:581:G:O4'	2.17	0.43
1:A:1112:C:H1'	3:C:179:ARG:HH21	1.83	0.43
6:F:26:ILE:HG23	6:F:79:LEU:HD21	2.00	0.43
9:I:50:LEU:HD11	9:I:81:ILE:HD13	2.00	0.43
1:A:578:C:O2'	1:A:728:A:N3	2.45	0.43
2:B:68:ILE:HG12	2:B:161:ALA:HB3	1.99	0.43
11:K:62:GLN:HG3	11:K:97:ALA:HB2	1.99	0.43
19:S:41:VAL:HG22	19:S:44:MET:HE3	2.00	0.43
1:A:7:G:H21	5:E:121:LYS:HG2	1.84	0.43
4:D:36:ARG:HG2	4:D:38:TYR:CZ	2.54	0.43
11:K:27:ASN:OD1	11:K:28:THR:N	2.52	0.43
17:Q:83:ASP:OD1	17:Q:83:ASP:N	2.50	0.43
1:A:77:G:H2'	1:A:78:G:H8	1.82	0.43
1:A:80:G:H2'	1:A:81:U:H5'	1.99	0.43
1:A:142:G:O2'	1:A:196:A:N1	2.44	0.43
1:A:337:C:H2'	1:A:338:A:H8	1.83	0.43
1:A:371:G:O2'	1:A:372:C:H5'	2.17	0.43
1:A:769:G:H4'	1:A:1513:A:H4'	2.01	0.43
1:A:1211:U:H1'	1:A:1213:A:N3	2.33	0.43
1:A:1437:C:H2'	1:A:1438:G:C8	2.52	0.43
3:C:6:HIS:HE1	3:C:8:ILE:HB	1.83	0.43
5:E:11:ILE:HB	5:E:31:LEU:HB3	2.00	0.43
6:F:50:TYR:CE1	18:R:77:GLY:HA2	2.54	0.43
1:A:28:G:O2'	1:A:296:U:OP1	2.33	0.43
1:A:671:G:H5'	6:F:77:ARG:NH2	2.32	0.43
1:A:1205:U:OP1	3:C:190:ARG:NH2	2.52	0.43
4:D:150:GLU:HA	4:D:153:ARG:HG3	2.00	0.43
11:K:22:HIS:HB3	11:K:29:ILE:HD13	1.99	0.43
11:K:29:ILE:HG12	11:K:30:VAL:N	2.33	0.43
12:L:124:LYS:HD2	12:L:125:PRO:HD2	2.00	0.43
20:T:72:LEU:HD11	20:T:80:ARG:HD2	2.00	0.43
20:T:89:ARG:NH2	20:T:104:LEU:HB3	2.33	0.43
1:A:587:G:N2	1:A:754:C:OP2	2.50	0.43
1:A:1037:C:H2'	1:A:1038:C:C6	2.53	0.43
3:C:110:ASN:O	3:C:141:VAL:HG22	2.19	0.43
1:A:130:A:OP2	1:A:190(E):U:O2'	2.26	0.43
10:J:50:ILE:HD12	10:J:50:ILE:H	1.84	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:20:LYS:H	12:L:20:LYS:HG3	1.53	0.43
1:A:1111:A:N6	3:C:177:THR:HB	2.29	0.43
1:A:1316:G:N1	1:A:1319:A:OP2	2.51	0.43
1:A:234:C:H2'	1:A:235:C:C6	2.53	0.43
1:A:428:G:H1'	1:A:429:U:OP2	2.19	0.43
1:A:1061:G:N7	3:C:2:GLY:HA3	2.34	0.43
1:A:1477:C:H2'	1:A:1478:C:C6	2.54	0.43
1:A:1493:A:H2'	1:A:1494:G:H8	1.83	0.43
3:C:12:LEU:HD23	3:C:12:LEU:HA	1.90	0.43
5:E:28:PHE:O	5:E:47:LYS:HA	2.19	0.43
2:B:223:ILE:HD13	2:B:230:VAL:HG21	2.01	0.42
7:G:26:PHE:CE2	7:G:30:ILE:HD11	2.54	0.42
9:I:8:GLY:H	9:I:83:ARG:HD2	1.83	0.42
10:J:90:LEU:N	10:J:91:PRO:HD2	2.34	0.42
15:O:18:PHE:CZ	15:O:21:ASP:HB2	2.53	0.42
1:A:463:A:H2'	1:A:474:G:O4'	2.19	0.42
1:A:1403:C:H1'	1:A:1500:A:N1	2.34	0.42
6:F:8:ILE:HB	6:F:61:LEU:HB2	2.01	0.42
8:H:87:SER:HB2	8:H:93:VAL:HB	2.02	0.42
13:M:54:VAL:HG23	13:M:57:ARG:NH1	2.35	0.42
1:A:433:C:H2'	1:A:434:U:C6	2.54	0.42
2:B:178:ARG:O	8:H:71:GLY:HA2	2.19	0.42
16:P:58:TYR:O	16:P:61:SER:OG	2.35	0.42
19:S:17:GLU:HA	19:S:20:LEU:HG	2.00	0.42
1:A:279:A:C6	17:Q:98:LEU:HD13	2.54	0.42
1:A:1516[A]:G:H2'	1:A:1518[A]:MA6:OP2	2.19	0.42
2:B:213:LEU:O	2:B:217:ARG:HG2	2.19	0.42
9:I:53:VAL:HG21	9:I:85:LEU:HD21	2.00	0.42
12:L:53:ARG:HG2	12:L:93:LEU:HD11	2.01	0.42
19:S:7:LYS:HE3	19:S:7:LYS:HB3	1.90	0.42
1:A:745:C:H2'	1:A:746:A:C8	2.55	0.42
1:A:967:5MC:H4'	9:I:128:ARG:HG3	2.01	0.42
1:A:1022:G:N2	1:A:1023:G:N7	2.66	0.42
1:A:1213:A:N6	1:A:1215:G:N3	2.67	0.42
13:M:2:ALA:O	13:M:10:PRO:HD2	2.19	0.42
1:A:359:U:H2'	1:A:360:A:C8	2.54	0.42
1:A:716:A:N3	11:K:118:GLY:HA2	2.35	0.42
1:A:860:A:H2'	1:A:861:G:O4'	2.18	0.42
1:A:878:G:H5''	8:H:89:PRO:O	2.20	0.42
4:D:121:VAL:O	4:D:134:ASP:HA	2.19	0.42
7:G:87:VAL:HG11	7:G:154:TYR:O	2.18	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:815:A:N7	1:A:1509:C:O2'	2.49	0.42
1:A:1255:G:C6	1:A:1279:A:N7	2.88	0.42
1:A:1343:G:H1'	9:I:121:ARG:NH1	2.35	0.42
2:B:152:PHE:CE1	2:B:155:LEU:HD12	2.54	0.42
4:D:24:GLU:C	4:D:26:CYS:H	2.28	0.42
20:T:53:LEU:HD22	20:T:53:LEU:HA	1.91	0.42
1:A:46:G:H2'	1:A:366:C:C5	2.55	0.42
1:A:373:A:H1'	1:A:481:G:H1'	2.01	0.42
1:A:691:G:H2'	1:A:692:U:C6	2.54	0.42
1:A:1145:C:HO2'	1:A:1146:A:P	2.41	0.42
1:A:1419:G:H2'	1:A:1420:C:C6	2.55	0.42
6:F:55:ASP:HB3	6:F:86:ARG:HH12	1.85	0.42
12:L:77:LEU:HD23	12:L:77:LEU:HA	1.91	0.42
19:S:28:LYS:HG2	19:S:29:ARG:H	1.85	0.42
21:U:10:ARG:HA	21:U:13:ILE:HG12	2.01	0.42
21:U:12:LYS:HB3	21:U:22:ARG:HD2	2.01	0.42
2:B:71:VAL:HG22	2:B:93:VAL:HB	2.01	0.42
2:B:74:LYS:O	2:B:78:GLN:HG3	2.20	0.42
14:N:32:SER:O	14:N:40:CYS:HB2	2.20	0.42
1:A:484:G:H1'	1:A:485:G:OP2	2.20	0.42
6:F:76:ALA:O	6:F:80:ARG:HG3	2.20	0.42
10:J:39:PRO:HA	10:J:70:ARG:HD3	2.02	0.42
1:A:1093:A:N3	1:A:1109:C:O2'	2.47	0.41
3:C:27:LYS:HA	3:C:30:ARG:HH12	1.85	0.41
3:C:136:GLN:O	3:C:140:ARG:HG3	2.20	0.41
7:G:74:GLU:O	7:G:88:PRO:HA	2.20	0.41
7:G:116:ALA:O	7:G:120:ILE:HG12	2.20	0.41
8:H:104:ARG:HA	8:H:104:ARG:HD3	1.87	0.41
10:J:71:LEU:HD12	10:J:71:LEU:HA	1.83	0.41
1:A:217:C:H2'	1:A:218:C:C6	2.55	0.41
1:A:1248:A:H2'	1:A:1249:C:C6	2.56	0.41
9:I:99:LEU:HB3	9:I:101:PHE:CD1	2.54	0.41
1:A:96:G:H2'	1:A:97:G:C8	2.55	0.41
1:A:1079:G:O3'	5:E:14:ARG:NH2	2.53	0.41
2:B:13:ALA:O	2:B:15:VAL:N	2.53	0.41
2:B:132:LYS:H	2:B:132:LYS:HG3	1.69	0.41
11:K:34:ASP:OD2	11:K:38:ASN:HB2	2.20	0.41
14:N:14:PRO:C	14:N:16:PHE:H	2.28	0.41
1:A:349:A:H2'	1:A:350:G:O4'	2.20	0.41
1:A:841:U:H5'	1:A:848:C:C6	2.55	0.41
1:A:1097:C:H2'	1:A:1098:C:C6	2.56	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:62:ASN:OD1	13:M:62:ASN:N	2.52	0.41
18:R:26:LEU:HA	18:R:26:LEU:HD12	1.79	0.41
1:A:328:C:H1'	1:A:329:A:OP2	2.20	0.41
1:A:865:A:H2	1:A:918:A:H4'	1.85	0.41
1:A:1014:A:H4'	19:S:14:HIS:CD2	2.56	0.41
1:A:1065:U:H4'	1:A:1066:C:O5'	2.20	0.41
2:B:155:LEU:HD23	2:B:155:LEU:HA	1.79	0.41
10:J:47:PHE:HB3	14:N:34:TYR:HE2	1.83	0.41
21:U:12:LYS:HG2	21:U:22:ARG:HB3	2.03	0.41
1:A:252:U:H2'	1:A:253:U:C6	2.55	0.41
1:A:532:A:N6	3:C:159:GLY:O	2.53	0.41
1:A:565:U:OP2	1:A:566:G:O2'	2.35	0.41
1:A:936:C:H2'	1:A:937:A:O4'	2.20	0.41
1:A:1205:U:H2'	1:A:1206:G:H8	1.84	0.41
13:M:4:ILE:O	13:M:57:ARG:HG3	2.21	0.41
13:M:13:LYS:O	13:M:45:VAL:HG23	2.20	0.41
13:M:65:LYS:H	13:M:65:LYS:HG2	1.51	0.41
13:M:87:TYR:CE1	13:M:91:ARG:HD3	2.56	0.41
14:N:12:ARG:H	14:N:12:ARG:HG2	1.61	0.41
17:Q:56:VAL:HG21	17:Q:81:ARG:HD3	2.02	0.41
1:A:1087:G:N2	1:A:1099:G:H1'	2.36	0.41
1:A:1465:C:H2'	1:A:1466:C:O4'	2.21	0.41
5:E:69:VAL:HA	5:E:70:PRO:HD3	1.94	0.41
9:I:10:ARG:HG2	9:I:75:ASP:CB	2.48	0.41
1:A:424:G:H2'	1:A:425:G:H8	1.85	0.41
1:A:757:U:O2'	1:A:879:C:O2	2.37	0.41
1:A:960:U:H4'	1:A:961:U:C5'	2.51	0.41
1:A:1296:C:H5'	13:M:14:ARG:HD2	2.02	0.41
2:B:157:ARG:HG2	2:B:158:LEU:N	2.36	0.41
2:B:158:LEU:HD12	2:B:158:LEU:H	1.84	0.41
3:C:61:ALA:C	3:C:63:ASN:H	2.29	0.41
13:M:57:ARG:HG2	13:M:61:GLU:HG3	2.01	0.41
14:N:12:ARG:O	14:N:13:THR:C	2.63	0.41
1:A:96:G:H2'	1:A:97:G:H8	1.85	0.41
1:A:123:C:H2'	1:A:124:G:H8	1.85	0.41
1:A:552:U:O2	12:L:31:PRO:HB3	2.21	0.41
1:A:1006:C:H2'	1:A:1007:C:C6	2.56	0.41
1:A:1250:A:H4'	9:I:68:GLY:H	1.86	0.41
2:B:108:ILE:O	2:B:112:VAL:HG23	2.21	0.41
4:D:26:CYS:HA	4:D:31:CYS:HB2	2.02	0.41
8:H:17:THR:O	8:H:78:GLN:NE2	2.42	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:R:47:THR:HG22	18:R:83:GLU:H	1.85	0.41
1:A:833:U:H2'	1:A:834:C:C6	2.55	0.41
4:D:187:ARG:HA	4:D:187:ARG:HD2	1.85	0.41
5:E:11:ILE:HG23	5:E:105:VAL:HG22	2.03	0.41
7:G:44:TYR:O	7:G:48:LYS:HG3	2.21	0.41
8:H:105:ARG:HA	8:H:105:ARG:HD3	1.83	0.41
9:I:69:GLY:O	9:I:73:GLN:HG3	2.21	0.41
12:L:89:ARG:HG2	12:L:97:ARG:HA	2.03	0.41
1:A:614:A:H2'	1:A:615:C:C6	2.56	0.40
1:A:748:C:H1'	1:A:749:C:OP2	2.22	0.40
1:A:1359:C:O2'	1:A:1361:G:N7	2.53	0.40
2:B:114:ARG:HH11	2:B:118:LEU:HD21	1.85	0.40
2:B:181:PHE:HD2	8:H:70:GLN:HB3	1.86	0.40
10:J:42:THR:CG2	10:J:66:ARG:HB2	2.51	0.40
1:A:603:U:H2'	1:A:604:G:H8	1.86	0.40
1:A:939:G:H5''	7:G:102:ARG:CZ	2.52	0.40
1:A:1004:A:H5''	1:A:1025:U:C4	2.56	0.40
1:A:1284:C:H3'	1:A:1285:A:H8	1.86	0.40
1:A:1350:A:OP2	9:I:118:LYS:NZ	2.51	0.40
1:A:1488:G:H2'	1:A:1489:G:H8	1.86	0.40
4:D:200:GLU:H	4:D:200:GLU:CD	2.28	0.40
7:G:44:TYR:CD1	9:I:41:VAL:HG11	2.56	0.40
11:K:41:THR:HG21	11:K:71:LYS:HB3	2.02	0.40
13:M:11:ARG:HA	13:M:45:VAL:HG11	2.03	0.40
13:M:56:LEU:HD23	13:M:56:LEU:HA	1.90	0.40
1:A:204:U:H4'	1:A:216:G:O4'	2.22	0.40
1:A:1175:G:H2'	1:A:1176:A:C8	2.56	0.40
1:A:1279:A:H8	1:A:1282:C:N3	2.18	0.40
6:F:9:VAL:HB	6:F:87:ARG:HB2	2.03	0.40
19:S:31:ILE:HG22	19:S:49:ILE:HA	2.03	0.40
1:A:1003(A):G:C5	1:A:1004:A:H1'	2.56	0.40
1:A:1211:U:H1'	1:A:1213:A:C2	2.56	0.40
1:A:1277:C:H1'	1:A:1282:C:H1'	2.02	0.40
4:D:162:LEU:HA	4:D:165:MET:HB2	2.04	0.40
7:G:70:LYS:HE2	7:G:97:GLN:HA	2.03	0.40
1:A:44:G:H2'	1:A:45:U:O4'	2.22	0.40
1:A:444:C:H2'	1:A:445:G:C8	2.56	0.40
1:A:509:A:HO2'	1:A:510:A:P	2.44	0.40
1:A:592:G:H2'	1:A:593:G:H8	1.86	0.40
1:A:1269:A:N1	1:A:1312:G:O2'	2.53	0.40
7:G:47:CYS:HA	7:G:50:ILE:HG22	2.04	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:55:LYS:O	10:J:56:HIS:CG	2.75	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:82:U:O2	1:A:1400:5MC:C2[3_545]	1.99	0.21
1:A:82:U:O2	1:A:1400:5MC:C4[3_545]	2.11	0.09

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	232/234 (99%)	213 (92%)	18 (8%)	1 (0%)	30	62
3	C	204/206 (99%)	188 (92%)	16 (8%)	0	100	100
4	D	206/208 (99%)	202 (98%)	4 (2%)	0	100	100
5	E	148/150 (99%)	143 (97%)	5 (3%)	0	100	100
6	F	99/101 (98%)	98 (99%)	1 (1%)	0	100	100
7	G	153/155 (99%)	149 (97%)	4 (3%)	0	100	100
8	H	136/138 (99%)	134 (98%)	2 (2%)	0	100	100
9	I	125/127 (98%)	115 (92%)	10 (8%)	0	100	100
10	J	96/98 (98%)	80 (83%)	13 (14%)	3 (3%)	3	25
11	K	114/116 (98%)	108 (95%)	6 (5%)	0	100	100
12	L	121/124 (98%)	109 (90%)	12 (10%)	0	100	100
13	M	116/118 (98%)	105 (90%)	11 (10%)	0	100	100
14	N	58/60 (97%)	49 (84%)	9 (16%)	0	100	100
15	O	85/87 (98%)	83 (98%)	2 (2%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
16	P	81/83 (98%)	79 (98%)	2 (2%)	0	100	100
17	Q	97/99 (98%)	94 (97%)	3 (3%)	0	100	100
18	R	68/70 (97%)	68 (100%)	0	0	100	100
19	S	78/80 (98%)	72 (92%)	6 (8%)	0	100	100
20	T	97/99 (98%)	84 (87%)	10 (10%)	3 (3%)	3	25
21	U	22/24 (92%)	21 (96%)	1 (4%)	0	100	100
All	All	2336/2377 (98%)	2194 (94%)	135 (6%)	7 (0%)	36	67

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
10	J	55	LYS
20	T	74	LYS
20	T	75	ASN
10	J	56	HIS
20	T	73	HIS
2	B	14	GLY
10	J	54	PHE

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	202/202 (100%)	177 (88%)	25 (12%)	4	22
3	C	160/160 (100%)	134 (84%)	26 (16%)	2	14
4	D	180/180 (100%)	166 (92%)	14 (8%)	11	36
5	E	115/115 (100%)	104 (90%)	11 (10%)	8	30
6	F	90/90 (100%)	77 (86%)	13 (14%)	3	18
7	G	126/126 (100%)	116 (92%)	10 (8%)	11	36
8	H	119/119 (100%)	112 (94%)	7 (6%)	18	44
9	I	98/98 (100%)	78 (80%)	20 (20%)	1	7

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
10	J	87/88 (99%)	77 (88%)	10 (12%)	5	24
11	K	88/88 (100%)	80 (91%)	8 (9%)	9	32
12	L	103/103 (100%)	90 (87%)	13 (13%)	4	21
13	M	94/94 (100%)	79 (84%)	15 (16%)	2	14
14	N	49/49 (100%)	42 (86%)	7 (14%)	3	18
15	O	79/79 (100%)	64 (81%)	15 (19%)	1	8
16	P	72/72 (100%)	64 (89%)	8 (11%)	6	25
17	Q	94/94 (100%)	86 (92%)	8 (8%)	10	34
18	R	61/61 (100%)	55 (90%)	6 (10%)	7	30
19	S	71/71 (100%)	63 (89%)	8 (11%)	5	25
20	T	76/76 (100%)	65 (86%)	11 (14%)	3	17
21	U	19/19 (100%)	18 (95%)	1 (5%)	20	47
All	All	1983/1984 (100%)	1747 (88%)	236 (12%)	5	23

All (236) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	7	VAL
2	B	8	LYS
2	B	9	GLU
2	B	10	LEU
2	B	11	LEU
2	B	12	GLU
2	B	21	ARG
2	B	23	ARG
2	B	39	ILE
2	B	44	LEU
2	B	47	THR
2	B	69	LEU
2	B	73	THR
2	B	96	ARG
2	B	102	LEU
2	B	103	THR
2	B	106	LYS
2	B	127	ILE
2	B	139	LYS
2	B	144	ARG
2	B	154	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	172	ILE
2	B	178	ARG
2	B	200	ILE
2	B	206	ASP
3	C	3	ASN
3	C	11	ARG
3	C	31	HIS
3	C	34	LEU
3	C	52	LEU
3	C	58	GLU
3	C	70	VAL
3	C	91	LEU
3	C	94	LEU
3	C	95	THR
3	C	97	LYS
3	C	98	ASN
3	C	99	VAL
3	C	104	GLN
3	C	111	LEU
3	C	152	ILE
3	C	154	SER
3	C	166	GLU
3	C	176	HIS
3	C	177	THR
3	C	178	LEU
3	C	188	LEU
3	C	191	THR
3	C	195	VAL
3	C	196	LEU
3	C	204	LEU
4	D	19	LEU
4	D	35	ARG
4	D	36	ARG
4	D	64	LEU
4	D	115	ARG
4	D	119	GLN
4	D	122	ARG
4	D	150	GLU
4	D	155	LEU
4	D	157	LEU
4	D	179	GLU
4	D	192	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	D	194	LEU
4	D	202	LEU
5	E	5	ASP
5	E	6	PHE
5	E	12	LEU
5	E	26	PHE
5	E	41	VAL
5	E	79	GLU
5	E	80	ILE
5	E	118	ILE
5	E	140	ARG
5	E	150	ARG
5	E	151	LEU
6	F	9	VAL
6	F	10	LEU
6	F	19	LEU
6	F	24	GLU
6	F	32	ASN
6	F	37	VAL
6	F	40	VAL
6	F	43	LEU
6	F	72	VAL
6	F	75	LEU
6	F	82	ARG
6	F	92	LYS
6	F	95	GLU
7	G	8	GLU
7	G	27	ILE
7	G	47	CYS
7	G	67	GLU
7	G	75	VAL
7	G	84	ASN
7	G	104	LEU
7	G	113	GLU
7	G	136	LYS
7	G	149	ARG
8	H	26	VAL
8	H	63	LEU
8	H	83	ILE
8	H	85	ARG
8	H	88	LYS
8	H	91	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
8	H	98	LYS
9	I	11	LYS
9	I	14	VAL
9	I	38	GLN
9	I	41	VAL
9	I	44	VAL
9	I	47	LEU
9	I	50	LEU
9	I	56	LEU
9	I	58	HIS
9	I	64	THR
9	I	79	LEU
9	I	83	ARG
9	I	85	LEU
9	I	91	ASP
9	I	96	LEU
9	I	99	LEU
9	I	109	VAL
9	I	113	LYS
9	I	118	LYS
9	I	127	LYS
10	J	3	LYS
10	J	38	ILE
10	J	45	ARG
10	J	55	LYS
10	J	60	ARG
10	J	62	HIS
10	J	73	ASP
10	J	82	ILE
10	J	85	LEU
10	J	95	GLU
11	K	12	ARG
11	K	29	ILE
11	K	33	THR
11	K	47	VAL
11	K	81	ASP
11	K	95	ILE
11	K	98	LEU
11	K	114	VAL
12	L	18	VAL
12	L	20	LYS
12	L	33	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
12	L	36	VAL
12	L	42	THR
12	L	47	LYS
12	L	59	ARG
12	L	79	GLU
12	L	80	HIS
12	L	82	VAL
12	L	96	VAL
12	L	97	ARG
12	L	122	THR
13	M	7	VAL
13	M	12	ASN
13	M	14	ARG
13	M	17	VAL
13	M	44	ARG
13	M	48	LEU
13	M	50	GLU
13	M	54	VAL
13	M	65	LYS
13	M	67	GLU
13	M	70	LEU
13	M	105	THR
13	M	108	ARG
13	M	115	LYS
13	M	117	VAL
14	N	9	LYS
14	N	12	ARG
14	N	18	VAL
14	N	22	THR
14	N	24	CYS
14	N	25	VAL
14	N	27	CYS
15	O	5	LYS
15	O	7	GLU
15	O	8	LYS
15	O	21	ASP
15	O	32	LEU
15	O	33	THR
15	O	39	LEU
15	O	45	VAL
15	O	56	LEU
15	O	70	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
15	O	71	GLN
15	O	81	LEU
15	O	82	ILE
15	O	83	GLU
15	O	87	ILE
16	P	20	VAL
16	P	36	ILE
16	P	42	ARG
16	P	47	ASP
16	P	53	VAL
16	P	54	GLU
16	P	62	VAL
16	P	68	ASP
17	Q	13	ASP
17	Q	34	LYS
17	Q	53	LEU
17	Q	59	ILE
17	Q	60	ILE
17	Q	76	LEU
17	Q	86	GLU
17	Q	98	LEU
18	R	40	LEU
18	R	47	THR
18	R	69	THR
18	R	86	VAL
18	R	87	ARG
18	R	88	LYS
19	S	5	LEU
19	S	15	LEU
19	S	51	VAL
19	S	56	GLN
19	S	62	ILE
19	S	63	THR
19	S	71	LEU
19	S	79	THR
20	T	53	LEU
20	T	56	MET
20	T	57	ARG
20	T	62	LEU
20	T	68	LYS
20	T	72	LEU
20	T	73	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
20	T	75	ASN
20	T	84	LEU
20	T	92	LEU
20	T	93	GLU
21	U	25	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	204	ASN
2	B	212	GLN
3	C	110	ASN
4	D	199	ASN
6	F	13	ASN
7	G	28	ASN
7	G	96	GLN
7	G	97	GLN
7	G	109	ASN
9	I	3	GLN
9	I	23	ASN
9	I	73	GLN
9	I	117	HIS
10	J	69	ASN
13	M	77	ASN
16	P	82	GLN
19	S	65	ASN
20	T	73	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	1505/1522 (98%)	256 (17%)	46 (3%)

All (256) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	6	G
1	A	7	G
1	A	9	G
1	A	32	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	39	G
1	A	47	C
1	A	48	C
1	A	50	A
1	A	51	A
1	A	54	C
1	A	80	G
1	A	81	U
1	A	92	C
1	A	101	A
1	A	116	A
1	A	117	G
1	A	121	C
1	A	129(A)	G
1	A	130	A
1	A	131	C
1	A	163	C
1	A	182	U
1	A	183	G
1	A	195	A
1	A	201	C
1	A	202	U
1	A	203	U
1	A	204	U
1	A	216	G
1	A	220	G
1	A	231	G
1	A	247	G
1	A	251	G
1	A	252	U
1	A	266	G
1	A	267	C
1	A	279	A
1	A	282	A
1	A	289	G
1	A	319	G
1	A	321	A
1	A	328	C
1	A	329	A
1	A	332	G
1	A	344	A
1	A	345	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	346	G
1	A	350	G
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	421	U
1	A	424	G
1	A	429	U
1	A	439	A
1	A	451	A
1	A	460	A
1	A	461	C
1	A	481	G
1	A	485	G
1	A	486	U
1	A	497	A
1	A	498	U
1	A	509	A
1	A	510	A
1	A	511	C
1	A	517	G
1	A	518	C
1	A	519	C
1	A	524	G
1	A	527	7MG
1	A	531	U
1	A	532	A
1	A	533	A
1	A	545	C
1	A	547	A
1	A	559	A
1	A	560	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	562	C
1	A	564	C
1	A	568	G
1	A	572	A
1	A	573	A
1	A	576	G
1	A	577	G
1	A	579	G
1	A	588	G
1	A	596	C
1	A	653	A
1	A	665	A
1	A	686	U
1	A	687	A
1	A	688	G
1	A	695	A
1	A	701	C
1	A	702	A
1	A	703	G
1	A	723	U
1	A	731	G
1	A	749	C
1	A	755	G
1	A	777	A
1	A	781	A
1	A	782	A
1	A	785	G
1	A	792	A
1	A	793	U
1	A	794	A
1	A	799	G
1	A	813	U
1	A	815	A
1	A	817	C
1	A	818	G
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	902	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	914	A
1	A	922	G
1	A	926	G
1	A	927	G
1	A	934	C
1	A	937	A
1	A	942	G
1	A	960	U
1	A	961	U
1	A	966	M2G
1	A	969	A
1	A	971	G
1	A	974	A
1	A	975	A
1	A	976	G
1	A	977	A
1	A	982	U
1	A	984	C
1	A	989	C
1	A	991	U
1	A	992	U
1	A	993	G
1	A	994	A
1	A	995	C
1	A	1004	A
1	A	1005	A
1	A	1006	C
1	A	1020	U
1	A	1023	G
1	A	1024	G
1	A	1026	G
1	A	1030(B)	C
1	A	1031	G
1	A	1045	C
1	A	1050	G
1	A	1053	G
1	A	1054	C
1	A	1065	U
1	A	1066	C
1	A	1068	G
1	A	1078	U
1	A	1085	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	1094	G
1	A	1095	U
1	A	1101	A
1	A	1124	G
1	A	1125	U
1	A	1126	U
1	A	1127	G
1	A	1130	A
1	A	1135	U
1	A	1137	C
1	A	1138	G
1	A	1139	G
1	A	1140	C
1	A	1146	A
1	A	1152	A
1	A	1159	U
1	A	1168	A
1	A	1171	G
1	A	1183	A
1	A	1191	A
1	A	1196	U
1	A	1197	G
1	A	1200	C
1	A	1201	A
1	A	1202	G
1	A	1207	2MG
1	A	1211	U
1	A	1212	U
1	A	1214	C
1	A	1224	G
1	A	1225	A
1	A	1227	A
1	A	1228	C
1	A	1230	C
1	A	1238	A
1	A	1241	G
1	A	1245	A
1	A	1256	A
1	A	1257	U
1	A	1258	G
1	A	1270	C
1	A	1278	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	1279	A
1	A	1280	A
1	A	1281	U
1	A	1286	A
1	A	1287	A
1	A	1289	A
1	A	1297	C
1	A	1300	G
1	A	1301	U
1	A	1302	U
1	A	1303	C
1	A	1305	G
1	A	1306	A
1	A	1316	G
1	A	1320	C
1	A	1322	C
1	A	1336	C
1	A	1346	A
1	A	1347	G
1	A	1348	U
1	A	1353	G
1	A	1359	C
1	A	1362	C
1	A	1381	U
1	A	1398	A
1	A	1400	5MC
1	A	1402	4OC
1	A	1442	G
1	A	1446	A
1	A	1447	G
1	A	1451	A
1	A	1485	U
1	A	1487	G
1	A	1490	C
1	A	1493	A
1	A	1499	A
1	A	1503	A
1	A	1504	G
1	A	1506	U
1	A	1529	G
1	A	1530	G
1	A	1531	A

All (46) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	5	U
1	A	115	G
1	A	129(A)	G
1	A	181	G
1	A	204	U
1	A	250	A
1	A	251	G
1	A	281	G
1	A	328	C
1	A	372	C
1	A	428	G
1	A	484	G
1	A	485	G
1	A	496	A
1	A	509	A
1	A	518	C
1	A	559	A
1	A	575	G
1	A	687	A
1	A	701	C
1	A	748	C
1	A	792	A
1	A	812	C
1	A	913	A
1	A	960	U
1	A	992	U
1	A	1049	U
1	A	1065	U
1	A	1067	A
1	A	1126	U
1	A	1129	C
1	A	1139	G
1	A	1145	C
1	A	1182	G
1	A	1190	G
1	A	1201	A
1	A	1256	A
1	A	1257	U
1	A	1285	A
1	A	1300	G
1	A	1301	U
1	A	1305	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	1346	A
1	A	1347	G
1	A	1380	U
1	A	1505	G

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
1	UR3	A	1498	1	19,22,23	0.72	1 (5%)	26,32,35	1.08	1 (3%)
1	4OC	A	1402	1	20,23,24	0.97	2 (10%)	25,32,35	0.69	0
1	2MG	A	1207	1	23,26,27	1.16	4 (17%)	33,38,41	1.08	3 (9%)
1	M2G	A	966	1	24,27,28	1.04	3 (12%)	33,40,43	0.80	0
1	MA6	A	1518[B]	1	23,26,27	0.80	1 (4%)	33,38,41	0.95	1 (3%)
1	MA6	A	1519[A]	1	23,26,27	0.81	1 (4%)	33,38,41	1.01	1 (3%)
1	5MC	A	1407	1	19,22,23	1.01	2 (10%)	26,32,35	0.96	2 (7%)
1	PSU	A	1540	1	18,21,22	2.02	7 (38%)	21,30,33	1.57	5 (23%)
1	PSU	A	1541	1	18,21,22	2.05	7 (38%)	21,30,33	1.53	4 (19%)
1	5MC	A	967	1	19,22,23	1.03	2 (10%)	26,32,35	0.97	1 (3%)
12	0TD	L	92	12	8,9,10	2.60	1 (12%)	6,11,13	2.24	2 (33%)
1	MA6	A	1518[A]	1	23,26,27	0.80	1 (4%)	33,38,41	0.94	2 (6%)
1	7MG	A	527	1	23,26,27	4.31	4 (17%)	27,39,42	2.23	9 (33%)
1	PSU	A	516	1	18,21,22	2.03	7 (38%)	21,30,33	1.51	4 (19%)
1	5MC	A	1400	1	19,22,23	1.04	2 (10%)	26,32,35	0.95	2 (7%)
1	5MC	A	1404	1	19,22,23	1.02	2 (10%)	26,32,35	0.99	2 (7%)
1	MA6	A	1519[B]	1	23,26,27	0.80	1 (4%)	33,38,41	0.97	1 (3%)

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	UR3	A	1498	1	-	0/7/25/26	0/2/2/2
1	4OC	A	1402	1	-	2/9/29/30	0/2/2/2
1	2MG	A	1207	1	-	2/9/27/28	0/3/3/3
1	M2G	A	966	1	-	3/11/29/30	0/3/3/3
1	MA6	A	1518[B]	1	-	0/11/29/30	0/3/3/3
1	MA6	A	1519[A]	1	-	1/11/29/30	0/3/3/3
1	5MC	A	1407	1	-	0/7/25/26	0/2/2/2
1	PSU	A	1540	1	-	0/7/25/26	0/2/2/2
1	PSU	A	1541	1	-	1/7/25/26	0/2/2/2
1	5MC	A	967	1	-	2/7/25/26	0/2/2/2
12	0TD	L	92	12	-	2/7/12/14	-
1	MA6	A	1518[A]	1	-	1/11/29/30	0/3/3/3
1	7MG	A	527	1	-	2/7/37/38	0/3/3/3
1	PSU	A	516	1	-	0/7/25/26	0/2/2/2
1	5MC	A	1400	1	-	2/7/25/26	0/2/2/2
1	5MC	A	1404	1	-	0/7/25/26	0/2/2/2
1	MA6	A	1519[B]	1	-	0/11/29/30	0/3/3/3

All (48) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	527	7MG	C8-N9	-19.74	1.33	1.45
12	L	92	0TD	CB-CA	-6.75	1.52	1.54
1	A	527	7MG	C2-N2	3.86	1.43	1.34
1	A	1541	PSU	C6-C5	3.79	1.39	1.35
1	A	516	PSU	C6-C5	3.70	1.39	1.35
1	A	1540	PSU	C2-N1	-3.68	1.31	1.36
1	A	1541	PSU	C2-N1	-3.67	1.31	1.36
1	A	516	PSU	C2-N1	-3.64	1.31	1.36
1	A	1540	PSU	C6-C5	3.58	1.39	1.35
1	A	516	PSU	C4-N3	-3.42	1.32	1.38
1	A	1540	PSU	C4-N3	-3.41	1.32	1.38
1	A	1541	PSU	C4-N3	-3.31	1.32	1.38
1	A	1540	PSU	C2-N3	-3.29	1.32	1.37
1	A	1541	PSU	C2-N3	-3.27	1.32	1.37
1	A	516	PSU	C2-N3	-3.25	1.32	1.37
1	A	1207	2MG	C2-N2	2.98	1.39	1.33
1	A	966	M2G	C2-N2	2.86	1.40	1.35
1	A	1541	PSU	O4-C4	-2.70	1.18	1.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1540	PSU	O4-C4	-2.67	1.18	1.23
1	A	516	PSU	O4-C4	-2.64	1.18	1.23
1	A	1400	5MC	C2-N3	2.54	1.41	1.36
1	A	967	5MC	C2-N1	2.53	1.45	1.40
1	A	1400	5MC	C2-N1	2.52	1.45	1.40
1	A	1402	4OC	C2-N3	2.51	1.41	1.36
1	A	966	M2G	C4-N3	2.49	1.39	1.34
1	A	1407	5MC	C2-N1	2.47	1.45	1.40
1	A	1404	5MC	C2-N1	2.44	1.45	1.40
1	A	527	7MG	C5-N7	2.42	1.38	1.35
1	A	1407	5MC	C2-N3	2.36	1.41	1.36
1	A	1498	UR3	C2-N1	2.35	1.41	1.38
1	A	967	5MC	C2-N3	2.35	1.41	1.36
1	A	1404	5MC	C2-N3	2.34	1.41	1.36
1	A	527	7MG	C4-N3	2.32	1.39	1.34
1	A	1207	2MG	C2-N1	2.25	1.40	1.36
1	A	516	PSU	O2-C2	-2.19	1.18	1.23
1	A	1540	PSU	O2-C2	-2.16	1.18	1.23
1	A	1541	PSU	O2-C2	-2.16	1.18	1.23
1	A	516	PSU	C6-N1	-2.11	1.32	1.36
1	A	1402	4OC	O2-C2	-2.10	1.19	1.23
1	A	1519[B]	MA6	C5-C4	2.09	1.42	1.39
1	A	1518[B]	MA6	C5-C4	2.08	1.42	1.39
1	A	1541	PSU	C6-N1	-2.08	1.32	1.36
1	A	1518[A]	MA6	C5-C4	2.07	1.42	1.39
1	A	1540	PSU	C6-N1	-2.07	1.32	1.36
1	A	966	M2G	C6-N1	2.07	1.42	1.38
1	A	1519[A]	MA6	C5-C4	2.06	1.42	1.39
1	A	1207	2MG	C8-N9	2.05	1.42	1.37
1	A	1207	2MG	C4-N3	2.01	1.38	1.34

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	527	7MG	C5-C6-N1	4.96	119.67	110.94
1	A	527	7MG	C2-N3-C4	4.72	120.42	112.30
1	A	527	7MG	N9-C4-N3	4.38	131.88	125.46
1	A	1540	PSU	N1-C2-N3	4.07	119.46	115.17
12	L	92	0TD	CSB-SB-CB	-4.04	95.10	102.36
1	A	527	7MG	C5-C4-N3	-4.01	120.60	128.13
1	A	516	PSU	N1-C2-N3	3.98	119.36	115.17
1	A	1541	PSU	N1-C2-N3	3.96	119.35	115.17

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1498	UR3	C6-N1-C2	-3.76	118.72	121.80
1	A	527	7MG	N9-C8-N7	3.58	108.44	103.37
1	A	1540	PSU	C4-N3-C2	-2.85	122.44	126.37
1	A	527	7MG	C6-C5-C4	-2.84	117.40	122.40
1	A	527	7MG	O6-C6-C5	-2.82	120.70	127.62
12	L	92	0TD	OD1-CG-CB	-2.80	116.58	122.44
1	A	527	7MG	C2-N1-C6	-2.76	120.11	125.11
1	A	1541	PSU	C6-C5-C4	-2.74	116.33	118.17
1	A	1541	PSU	C4-N3-C2	-2.71	122.64	126.37
1	A	516	PSU	C4-N3-C2	-2.64	122.73	126.37
1	A	516	PSU	C6-C5-C4	-2.54	116.46	118.17
1	A	1207	2MG	C5-C4-N3	-2.46	124.47	128.39
1	A	1404	5MC	N4-C4-N3	-2.44	114.09	118.51
1	A	1540	PSU	C6-C5-C4	-2.43	116.53	118.17
1	A	527	7MG	C6-C5-N7	2.42	135.68	131.93
1	A	1407	5MC	N4-C4-N3	-2.42	114.13	118.51
1	A	1518[A]	MA6	C2-N1-C6	2.41	117.71	111.83
1	A	516	PSU	O2-C2-N1	-2.34	120.37	122.79
1	A	1541	PSU	O2-C2-N1	-2.31	120.40	122.79
1	A	1540	PSU	O2-C2-N1	-2.30	120.41	122.79
1	A	967	5MC	N4-C4-N3	-2.30	114.35	118.51
1	A	1207	2MG	N9-C4-N3	2.26	130.48	125.95
1	A	1207	2MG	O6-C6-N1	-2.25	115.88	120.11
1	A	1400	5MC	N4-C4-N3	-2.20	114.53	118.51
1	A	1518[B]	MA6	C2-N1-C6	2.13	117.03	111.83
1	A	1400	5MC	C5-C4-N3	2.07	123.88	121.75
1	A	1519[B]	MA6	C2-N1-C6	2.06	116.87	111.83
1	A	1407	5MC	C5-C4-N3	2.05	123.86	121.75
1	A	1519[A]	MA6	C2-N1-C6	2.04	116.83	111.83
1	A	1404	5MC	C5-C4-N3	2.04	123.84	121.75
1	A	1518[A]	MA6	N1-C6-N6	-2.01	114.40	116.86
1	A	1540	PSU	O4'-C1'-C2'	2.00	107.92	105.15

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	1207	2MG	O4'-C4'-C5'-O5'
1	A	1400	5MC	O4'-C4'-C5'-O5'
1	A	527	7MG	C3'-C4'-C5'-O5'
1	A	1402	4OC	O4'-C4'-C5'-O5'
1	A	967	5MC	O4'-C4'-C5'-O5'

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
1	A	1207	2MG	C3'-C4'-C5'-O5'
1	A	1400	5MC	C3'-C4'-C5'-O5'
1	A	527	7MG	O4'-C4'-C5'-O5'
1	A	966	M2G	C3'-C4'-C5'-O5'
1	A	1402	4OC	C3'-C4'-C5'-O5'
1	A	966	M2G	O4'-C4'-C5'-O5'
1	A	1519[A]	MA6	C5-C6-N6-C9
1	A	967	5MC	C3'-C4'-C5'-O5'
12	L	92	0TD	CG-CB-SB-CSB
12	L	92	0TD	SB-CB-CG-OD1
1	A	1541	PSU	O4'-C1'-C5-C4
1	A	1518[A]	MA6	C5-C6-N6-C10
1	A	966	M2G	C4'-C5'-O5'-P

There are no ring outliers.

9 monomers are involved in 17 short contacts:

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	1498/1522 (98%)	-0.29	15 (1%) 79 56	87, 217, 354, 499	4 (0%)
2	B	234/234 (100%)	-0.43	0 100 100	161, 214, 290, 359	0
3	C	206/206 (100%)	-0.25	3 (1%) 72 47	223, 292, 351, 386	0
4	D	208/208 (100%)	-0.00	14 (6%) 24 15	149, 216, 290, 352	0
5	E	150/150 (100%)	-0.35	2 (1%) 75 50	140, 180, 238, 256	0
6	F	101/101 (100%)	-0.58	1 (0%) 79 56	180, 221, 251, 274	0
7	G	155/155 (100%)	-0.35	2 (1%) 75 50	178, 269, 326, 364	0
8	H	138/138 (100%)	-0.35	3 (2%) 62 37	131, 167, 215, 285	0
9	I	127/127 (100%)	0.61	15 (11%) 9 6	225, 299, 393, 431	0
10	J	98/98 (100%)	0.14	5 (5%) 33 19	227, 303, 376, 442	0
11	K	116/116 (100%)	-0.45	1 (0%) 81 58	148, 195, 244, 267	0
12	L	123/124 (99%)	-0.12	5 (4%) 41 22	125, 208, 253, 300	0
13	M	118/118 (100%)	-0.01	8 (6%) 23 14	202, 263, 344, 382	0
14	N	60/60 (100%)	-0.07	2 (3%) 49 28	209, 283, 320, 375	0
15	O	87/87 (100%)	-0.31	0 100 100	142, 195, 241, 254	0
16	P	83/83 (100%)	-0.07	1 (1%) 76 52	154, 206, 257, 306	0
17	Q	99/99 (100%)	-0.25	0 100 100	139, 180, 220, 251	0
18	R	70/70 (100%)	-0.41	0 100 100	148, 192, 254, 274	0
19	S	80/80 (100%)	-0.01	5 (6%) 26 15	228, 310, 357, 378	0
20	T	99/99 (100%)	0.02	3 (3%) 52 30	148, 212, 253, 306	0
21	U	24/24 (100%)	1.78	10 (41%) 0 1	242, 279, 349, 368	0
All	All	3874/3899 (99%)	-0.21	95 (2%) 58 35	87, 224, 340, 499	4 (0%)

All (95) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1517[A]	G	6.6
19	S	2	PRO	5.5
4	D	4	TYR	5.4
21	U	6	ARG	5.3
16	P	68	ASP	5.2
9	I	9	ARG	5.1
21	U	11	GLY	4.8
4	D	42	GLN	4.7
9	I	65	VAL	4.1
1	A	1217	C	4.0
1	A	353	A	4.0
4	D	22	LYS	3.8
1	A	1218	C	3.5
1	A	1017	G	3.4
9	I	128	ARG	3.2
10	J	96	ILE	3.2
9	I	117	HIS	3.2
21	U	18	TYR	3.2
13	M	106	ASN	3.2
8	H	116	LYS	3.2
20	T	11	SER	3.2
11	K	42	TRP	3.1
9	I	47	LEU	3.1
13	M	105	THR	3.1
4	D	5	ILE	3.1
9	I	125	TYR	3.0
20	T	9	ASN	3.0
21	U	14	TRP	3.0
4	D	21	LEU	2.9
12	L	47	LYS	2.9
4	D	112	VAL	2.9
8	H	46	LYS	2.9
10	J	34	VAL	2.8
13	M	87	TYR	2.8
13	M	104	ARG	2.7
10	J	54	PHE	2.7
13	M	119	GLY	2.7
1	A	532	A	2.7
1	A	6	G	2.6
1	A	77	G	2.6
21	U	25	LYS	2.6
4	D	14	ARG	2.6
21	U	16	GLY	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
9	I	70	LYS	2.6
20	T	106	ALA	2.6
4	D	9	CYS	2.6
1	A	81	U	2.5
10	J	53	PRO	2.5
9	I	104	ARG	2.5
12	L	86	ARG	2.5
12	L	31	PRO	2.5
21	U	3	LYS	2.4
4	D	13	ARG	2.4
9	I	109	VAL	2.4
21	U	15	ARG	2.4
8	H	1	MET	2.4
4	D	6	GLY	2.4
21	U	24	ARG	2.4
9	I	84	ALA	2.4
7	G	34	GLY	2.4
4	D	209	ARG	2.4
13	M	21	TYR	2.4
4	D	26	CYS	2.3
5	E	22	GLY	2.3
7	G	32	ARG	2.3
12	L	32	PHE	2.3
4	D	23	GLY	2.3
9	I	121	ARG	2.3
12	L	26	ALA	2.3
19	S	37	ARG	2.3
1	A	219	C	2.3
9	I	77	ILE	2.2
13	M	8	GLU	2.2
19	S	40	ILE	2.2
1	A	1222	G	2.2
1	A	1224	G	2.2
13	M	15	VAL	2.2
19	S	76	PRO	2.2
9	I	127	LYS	2.2
9	I	15	ALA	2.2
1	A	1516[A]	G	2.2
3	C	102	ASN	2.2
10	J	52	GLY	2.1
9	I	107	ARG	2.1
4	D	37	PRO	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
6	F	89	MET	2.1
14	N	41	ARG	2.1
21	U	7	ARG	2.1
1	A	1052	U	2.1
3	C	201	TYR	2.0
14	N	3	ARG	2.0
1	A	983	A	2.0
19	S	3	ARG	2.0
5	E	119	LEU	2.0
3	C	65	ALA	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
1	PSU	A	1541	20/21	0.84	0.12	341,359,404,493	0
1	PSU	A	1540	20/21	0.89	0.12	339,348,399,414	0
1	PSU	A	516	20/21	0.91	0.07	215,259,275,276	0
1	5MC	A	1407	21/22	0.93	0.06	183,244,266,297	0
1	UR3	A	1498	21/22	0.93	0.13	143,195,236,243	0
1	5MC	A	1400	21/22	0.94	0.10	165,209,227,236	0
1	M2G	A	966	25/26	0.95	0.08	179,209,234,242	0
1	5MC	A	967	21/22	0.95	0.07	194,220,254,264	0
1	2MG	A	1207	24/25	0.95	0.11	271,305,332,336	0
1	7MG	A	527	24/25	0.95	0.08	120,197,233,240	0
1	5MC	A	1404	21/22	0.96	0.11	150,200,229,242	0
12	0TD	L	92	10/11	0.97	0.14	216,285,385,387	0
1	4OC	A	1402	22/23	0.98	0.09	150,184,210,255	0
1	MA6	A	1518[A]	24/25	0.98	0.17	144,178,193,221	24
1	MA6	A	1518[B]	24/25	0.98	0.17	158,184,196,207	24
1	MA6	A	1519[B]	24/25	0.99	0.09	157,177,188,207	24
1	MA6	A	1519[A]	24/25	0.99	0.09	139,162,180,187	24

6.3 Carbohydrates [i](#)

There are no oligosaccharides 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(Å ²)	Q<0.9
22	MG	A	1629	1/1	-0.10	0.32	202,202,202,202	0
22	MG	S	101	1/1	0.07	0.24	177,177,177,177	0
22	MG	A	1714	1/1	0.09	0.26	213,213,213,213	0
22	MG	A	1814	1/1	0.15	0.37	175,175,175,175	0
22	MG	A	1684	1/1	0.22	0.48	173,173,173,173	0
22	MG	A	1734	1/1	0.26	0.46	168,168,168,168	0
22	MG	A	1757	1/1	0.28	0.34	162,162,162,162	0
22	MG	A	1768	1/1	0.33	0.28	177,177,177,177	0
22	MG	A	1827	1/1	0.42	0.15	158,158,158,158	0
22	MG	A	1807	1/1	0.43	0.32	181,181,181,181	0
22	MG	A	1731	1/1	0.44	0.09	252,252,252,252	0
22	MG	A	1707	1/1	0.44	0.11	217,217,217,217	0
22	MG	A	1708	1/1	0.47	0.39	170,170,170,170	0
22	MG	A	1668	1/1	0.48	0.14	167,167,167,167	0
22	MG	A	1674	1/1	0.51	0.17	213,213,213,213	0
22	MG	A	1647	1/1	0.51	0.32	169,169,169,169	0
22	MG	A	1617	1/1	0.51	0.28	260,260,260,260	0
22	MG	D	304	1/1	0.51	0.11	200,200,200,200	0
22	MG	A	1792	1/1	0.51	0.27	151,151,151,151	0
22	MG	Q	202	1/1	0.52	0.25	193,193,193,193	0
22	MG	A	1809	1/1	0.52	0.06	234,234,234,234	0
22	MG	A	1729	1/1	0.53	0.15	191,191,191,191	0
22	MG	A	1753	1/1	0.53	0.30	179,179,179,179	0
22	MG	A	1685	1/1	0.53	0.24	170,170,170,170	0
22	MG	A	1625	1/1	0.54	1.51	161,161,161,161	0
22	MG	S	102	1/1	0.55	0.08	203,203,203,203	0
22	MG	A	1806	1/1	0.56	0.18	198,198,198,198	0
22	MG	A	1774	1/1	0.58	0.23	144,144,144,144	0
22	MG	A	1786	1/1	0.60	0.62	154,154,154,154	0
22	MG	A	1718	1/1	0.60	0.21	216,216,216,216	0
22	MG	A	1803	1/1	0.60	0.15	178,178,178,178	0
22	MG	A	1760	1/1	0.61	0.11	160,160,160,160	0
22	MG	A	1831	1/1	0.61	0.21	164,164,164,164	0
22	MG	A	1697	1/1	0.62	0.62	138,138,138,138	0
22	MG	A	1678	1/1	0.63	0.22	213,213,213,213	0
22	MG	A	1738	1/1	0.63	0.56	128,128,128,128	0
22	MG	A	1744	1/1	0.63	0.96	173,173,173,173	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
22	MG	A	1819	1/1	0.64	0.36	193,193,193,193	0
22	MG	A	1724	1/1	0.65	0.23	352,352,352,352	0
22	MG	A	1813	1/1	0.65	0.14	186,186,186,186	0
22	MG	A	1692	1/1	0.65	0.15	201,201,201,201	0
22	MG	A	1666	1/1	0.65	0.74	170,170,170,170	0
22	MG	A	1687	1/1	0.65	0.08	230,230,230,230	0
22	MG	A	1680	1/1	0.66	0.28	170,170,170,170	0
22	MG	A	1662	1/1	0.66	0.29	167,167,167,167	0
22	MG	A	1823	1/1	0.66	0.12	170,170,170,170	0
22	MG	A	1782	1/1	0.67	0.15	177,177,177,177	0
22	MG	A	1611	1/1	0.68	0.13	155,155,155,155	0
22	MG	A	1825	1/1	0.68	0.38	162,162,162,162	0
22	MG	A	1815	1/1	0.68	0.17	169,169,169,169	0
22	MG	A	1775	1/1	0.68	0.36	131,131,131,131	0
22	MG	A	1723	1/1	0.69	0.40	159,159,159,159	0
22	MG	A	1833	1/1	0.69	0.19	224,224,224,224	0
22	MG	A	1828	1/1	0.69	0.12	178,178,178,178	0
22	MG	A	1605	1/1	0.70	0.39	149,149,149,149	0
22	MG	A	1826	1/1	0.70	0.21	148,148,148,148	0
22	MG	D	305	1/1	0.70	0.38	154,154,154,154	0
22	MG	A	1690	1/1	0.70	0.24	188,188,188,188	0
22	MG	A	1795	1/1	0.70	0.14	186,186,186,186	0
22	MG	A	1783	1/1	0.70	0.52	122,122,122,122	0
22	MG	A	1743	1/1	0.71	0.64	177,177,177,177	0
22	MG	A	1624	1/1	0.72	0.10	183,183,183,183	0
22	MG	A	1614	1/1	0.72	0.18	205,205,205,205	0
22	MG	A	1601	1/1	0.72	0.24	205,205,205,205	0
22	MG	A	1643	1/1	0.72	0.29	153,153,153,153	0
22	MG	A	1830	1/1	0.73	0.06	187,187,187,187	0
22	MG	A	1705	1/1	0.73	0.22	178,178,178,178	0
22	MG	A	1771	1/1	0.73	0.36	173,173,173,173	0
22	MG	A	1805	1/1	0.73	0.11	207,207,207,207	0
22	MG	P	102	1/1	0.74	0.09	190,190,190,190	0
22	MG	A	1767	1/1	0.74	0.19	149,149,149,149	0
22	MG	B	302	1/1	0.75	0.14	186,186,186,186	0
22	MG	A	1632	1/1	0.76	0.45	171,171,171,171	0
22	MG	A	1756	1/1	0.76	0.28	129,129,129,129	0
22	MG	A	1721	1/1	0.77	0.25	198,198,198,198	0
22	MG	A	1800	1/1	0.77	0.07	388,388,388,388	0
22	MG	A	1781	1/1	0.78	0.19	172,172,172,172	0
22	MG	A	1824	1/1	0.78	0.47	162,162,162,162	0
22	MG	A	1728	1/1	0.78	0.62	191,191,191,191	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
22	MG	A	1688	1/1	0.78	0.11	225,225,225,225	0
22	MG	A	1776	1/1	0.78	0.32	119,119,119,119	0
22	MG	B	303	1/1	0.78	0.05	232,232,232,232	0
22	MG	A	1785	1/1	0.79	0.13	192,192,192,192	0
22	MG	A	1834	1/1	0.79	0.15	228,228,228,228	0
22	MG	C	302	1/1	0.79	0.14	226,226,226,226	0
22	MG	C	303	1/1	0.80	0.11	253,253,253,253	0
22	MG	A	1788	1/1	0.80	0.13	168,168,168,168	0
22	MG	A	1791	1/1	0.80	0.06	220,220,220,220	0
22	MG	A	1752	1/1	0.80	0.15	200,200,200,200	0
22	MG	A	1816	1/1	0.80	0.07	171,171,171,171	0
22	MG	A	1726	1/1	0.80	0.45	185,185,185,185	0
22	MG	A	1787	1/1	0.80	0.46	191,191,191,191	0
22	MG	A	1634	1/1	0.81	0.38	141,141,141,141	0
22	MG	A	1636	1/1	0.81	0.11	227,227,227,227	0
22	MG	A	1627	1/1	0.81	1.07	140,140,140,140	0
22	MG	A	1763	1/1	0.81	0.31	155,155,155,155	0
22	MG	A	1780	1/1	0.81	0.44	159,159,159,159	0
22	MG	A	1790	1/1	0.81	0.16	202,202,202,202	0
22	MG	A	1619	1/1	0.81	0.40	162,162,162,162	0
22	MG	A	1620	1/1	0.81	0.32	151,151,151,151	0
22	MG	A	1719	1/1	0.82	0.18	197,197,197,197	0
22	MG	A	1818	1/1	0.82	0.18	162,162,162,162	0
22	MG	A	1609	1/1	0.82	0.23	152,152,152,152	0
22	MG	A	1821	1/1	0.82	0.41	160,160,160,160	0
22	MG	A	1750	1/1	0.82	0.29	169,169,169,169	0
22	MG	A	1638	1/1	0.82	0.08	143,143,143,143	0
22	MG	A	1699	1/1	0.82	0.49	178,178,178,178	0
22	MG	A	1612	1/1	0.82	0.13	197,197,197,197	0
22	MG	A	1755	1/1	0.83	0.07	179,179,179,179	0
22	MG	A	1749	1/1	0.83	0.12	151,151,151,151	0
22	MG	A	1811	1/1	0.83	0.15	241,241,241,241	0
22	MG	A	1740	1/1	0.83	0.13	172,172,172,172	0
22	MG	A	1778	1/1	0.83	0.16	136,136,136,136	0
22	MG	A	1754	1/1	0.83	0.14	171,171,171,171	0
22	MG	A	1712	1/1	0.84	0.13	231,231,231,231	0
22	MG	A	1801	1/1	0.84	0.34	164,164,164,164	0
22	MG	A	1653	1/1	0.84	0.30	207,207,207,207	0
22	MG	A	1730	1/1	0.84	0.36	187,187,187,187	0
22	MG	A	1761	1/1	0.84	0.25	174,174,174,174	0
22	MG	A	1663	1/1	0.84	0.98	220,220,220,220	0
22	MG	A	1661	1/1	0.84	0.10	196,196,196,196	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
22	MG	A	1686	1/1	0.85	0.38	183,183,183,183	0
22	MG	A	1802	1/1	0.85	0.12	188,188,188,188	0
22	MG	A	1628	1/1	0.85	0.44	179,179,179,179	0
22	MG	A	1656	1/1	0.85	0.30	184,184,184,184	0
22	MG	A	1651	1/1	0.85	0.14	166,166,166,166	0
22	MG	A	1798	1/1	0.85	0.13	153,153,153,153	0
22	MG	A	1706	1/1	0.85	0.07	196,196,196,196	0
22	MG	A	1610	1/1	0.86	0.25	165,165,165,165	0
22	MG	A	1720	1/1	0.86	0.12	137,137,137,137	0
22	MG	A	1832	1/1	0.86	0.14	170,170,170,170	0
22	MG	A	1701	1/1	0.86	0.10	218,218,218,218	0
22	MG	A	1658	1/1	0.86	0.15	176,176,176,176	0
22	MG	A	1667	1/1	0.87	0.15	152,152,152,152	0
22	MG	A	1691	1/1	0.87	0.14	171,171,171,171	0
22	MG	A	1641	1/1	0.87	0.10	170,170,170,170	0
22	MG	A	1742	1/1	0.87	0.16	131,131,131,131	0
22	MG	A	1770	1/1	0.87	0.31	142,142,142,142	0
22	MG	B	301	1/1	0.87	0.20	150,150,150,150	0
22	MG	A	1799	1/1	0.87	0.05	166,166,166,166	0
22	MG	A	1694	1/1	0.87	0.11	206,206,206,206	0
22	MG	A	1616	1/1	0.88	0.15	131,131,131,131	0
22	MG	A	1659	1/1	0.88	0.08	175,175,175,175	0
22	MG	A	1660	1/1	0.88	0.07	164,164,164,164	0
22	MG	A	1645	1/1	0.88	0.10	131,131,131,131	0
22	MG	E	201	1/1	0.88	0.05	191,191,191,191	0
22	MG	A	1622	1/1	0.88	0.14	187,187,187,187	0
22	MG	A	1693	1/1	0.88	0.16	186,186,186,186	0
22	MG	A	1789	1/1	0.88	0.22	218,218,218,218	0
22	MG	A	1829	1/1	0.88	0.11	169,169,169,169	0
22	MG	A	1683	1/1	0.89	0.12	215,215,215,215	0
22	MG	A	1759	1/1	0.89	0.07	160,160,160,160	0
22	MG	A	1689	1/1	0.89	0.18	200,200,200,200	0
22	MG	A	1646	1/1	0.89	0.08	192,192,192,192	0
22	MG	A	1700	1/1	0.89	0.16	217,217,217,217	0
22	MG	P	101	1/1	0.89	0.11	111,111,111,111	0
22	MG	A	1635	1/1	0.89	0.09	211,211,211,211	0
22	MG	A	1679	1/1	0.89	0.10	215,215,215,215	0
22	MG	A	1670	1/1	0.89	0.07	194,194,194,194	0
22	MG	A	1804	1/1	0.89	0.30	125,125,125,125	0
22	MG	A	1736	1/1	0.90	0.12	142,142,142,142	0
22	MG	A	1758	1/1	0.90	0.06	179,179,179,179	0
22	MG	A	1784	1/1	0.90	0.07	156,156,156,156	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
22	MG	A	1820	1/1	0.90	0.33	188,188,188,188	0
22	MG	A	1737	1/1	0.90	0.17	157,157,157,157	0
22	MG	A	1621	1/1	0.90	0.12	177,177,177,177	0
22	MG	A	1615	1/1	0.90	0.07	172,172,172,172	0
22	MG	A	1711	1/1	0.90	0.14	234,234,234,234	0
22	MG	A	1722	1/1	0.90	0.17	200,200,200,200	0
22	MG	A	1735	1/1	0.90	0.20	173,173,173,173	0
22	MG	A	1606	1/1	0.91	0.09	160,160,160,160	0
22	MG	A	1644	1/1	0.91	0.26	168,168,168,168	0
22	MG	A	1777	1/1	0.91	0.18	154,154,154,154	0
22	MG	A	1766	1/1	0.91	0.14	187,187,187,187	0
22	MG	A	1717	1/1	0.91	0.14	237,237,237,237	0
22	MG	A	1603	1/1	0.91	0.08	170,170,170,170	0
22	MG	A	1652	1/1	0.91	0.17	139,139,139,139	0
22	MG	A	1709	1/1	0.91	0.08	244,244,244,244	0
22	MG	A	1703	1/1	0.91	0.03	210,210,210,210	0
22	MG	A	1796	1/1	0.92	0.10	188,188,188,188	0
22	MG	A	1765	1/1	0.92	0.21	247,247,247,247	0
22	MG	A	1630	1/1	0.92	0.42	159,159,159,159	0
22	MG	A	1739	1/1	0.92	0.18	181,181,181,181	0
22	MG	A	1608	1/1	0.92	0.04	203,203,203,203	0
22	MG	A	1741	1/1	0.92	0.24	128,128,128,128	0
22	MG	A	1822	1/1	0.92	0.28	136,136,136,136	0
22	MG	A	1673	1/1	0.92	0.93	198,198,198,198	0
22	MG	A	1773	1/1	0.92	0.44	231,231,231,231	0
22	MG	A	1704	1/1	0.92	0.09	207,207,207,207	0
22	MG	A	1681	1/1	0.92	0.19	177,177,177,177	0
22	MG	A	1602	1/1	0.92	0.17	187,187,187,187	0
22	MG	A	1676	1/1	0.92	0.16	148,148,148,148	0
22	MG	A	1727	1/1	0.92	0.06	190,190,190,190	0
22	MG	A	1794	1/1	0.92	0.12	155,155,155,155	0
22	MG	A	1764	1/1	0.92	0.25	116,116,116,116	0
22	MG	D	302	1/1	0.93	0.09	153,153,153,153	0
22	MG	A	1623	1/1	0.93	0.08	128,128,128,128	0
22	MG	A	1817	1/1	0.93	0.36	199,199,199,199	0
22	MG	A	1607	1/1	0.93	0.48	161,161,161,161	0
22	MG	F	201	1/1	0.93	0.05	163,163,163,163	0
22	MG	I	201	1/1	0.93	0.28	198,198,198,198	0
22	MG	A	1710	1/1	0.93	0.16	178,178,178,178	0
22	MG	A	1650	1/1	0.93	0.22	161,161,161,161	0
22	MG	A	1732	1/1	0.93	0.14	126,126,126,126	0
22	MG	A	1747	1/1	0.93	0.19	161,161,161,161	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
22	MG	A	1733	1/1	0.93	0.24	154,154,154,154	0
22	MG	D	303	1/1	0.94	0.12	180,180,180,180	0
22	MG	A	1810	1/1	0.94	0.07	224,224,224,224	0
22	MG	A	1748	1/1	0.94	0.10	188,188,188,188	0
22	MG	A	1665	1/1	0.94	0.23	151,151,151,151	0
22	MG	A	1715	1/1	0.94	0.29	229,229,229,229	0
22	MG	A	1640	1/1	0.94	0.07	211,211,211,211	0
22	MG	A	1633	1/1	0.94	0.10	198,198,198,198	0
22	MG	A	1639	1/1	0.94	0.20	119,119,119,119	0
22	MG	A	1797	1/1	0.94	0.11	158,158,158,158	0
22	MG	A	1677	1/1	0.94	0.10	126,126,126,126	0
22	MG	A	1772	1/1	0.94	0.12	158,158,158,158	0
22	MG	U	101	1/1	0.94	0.17	207,207,207,207	0
22	MG	A	1695	1/1	0.95	0.17	211,211,211,211	0
22	MG	A	1779	1/1	0.95	0.14	154,154,154,154	0
22	MG	Q	201	1/1	0.95	0.12	170,170,170,170	0
22	MG	A	1613	1/1	0.95	0.05	192,192,192,192	0
22	MG	A	1725	1/1	0.95	0.25	195,195,195,195	0
22	MG	A	1648	1/1	0.95	0.07	205,205,205,205	0
22	MG	A	1713	1/1	0.95	0.17	184,184,184,184	0
23	ZN	D	301	1/1	0.95	0.20	196,196,196,196	0
22	MG	A	1698	1/1	0.96	0.10	142,142,142,142	0
22	MG	A	1626	1/1	0.96	0.41	190,190,190,190	0
22	MG	A	1604	1/1	0.96	0.08	158,158,158,158	0
22	MG	A	1642	1/1	0.96	0.18	208,208,208,208	0
22	MG	A	1745	1/1	0.96	0.10	136,136,136,136	0
22	MG	A	1702	1/1	0.96	0.11	124,124,124,124	0
22	MG	C	301	1/1	0.96	0.09	189,189,189,189	0
22	MG	A	1675	1/1	0.96	0.22	211,211,211,211	0
22	MG	A	1793	1/1	0.97	0.11	138,138,138,138	0
22	MG	A	1655	1/1	0.97	0.24	158,158,158,158	0
22	MG	A	1672	1/1	0.97	0.08	218,218,218,218	0
22	MG	A	1808	1/1	0.97	0.13	206,206,206,206	0
22	MG	A	1751	1/1	0.97	0.10	151,151,151,151	0
23	ZN	N	101	1/1	0.97	0.04	308,308,308,308	0
22	MG	A	1649	1/1	0.98	0.09	206,206,206,206	0
22	MG	A	1657	1/1	0.98	0.17	237,237,237,237	0
22	MG	A	1762	1/1	0.98	0.25	153,153,153,153	0
22	MG	A	1669	1/1	0.98	0.25	212,212,212,212	0
22	MG	A	1618	1/1	0.98	0.08	171,171,171,171	0
22	MG	A	1671	1/1	0.98	0.03	185,185,185,185	0
22	MG	A	1664	1/1	0.98	0.08	194,194,194,194	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
22	MG	A	1746	1/1	0.98	0.14	144,144,144,144	0
22	MG	A	1654	1/1	0.98	0.04	167,167,167,167	0
22	MG	A	1769	1/1	0.98	0.12	147,147,147,147	0
22	MG	A	1682	1/1	0.98	0.05	190,190,190,190	0
22	MG	A	1631	1/1	0.98	0.17	180,180,180,180	0
22	MG	A	1716	1/1	0.99	0.18	244,244,244,244	0
22	MG	A	1696	1/1	0.99	0.17	281,281,281,281	0
22	MG	A	1637	1/1	0.99	0.09	133,133,133,133	0
22	MG	A	1812	1/1	0.99	0.09	182,182,182,182	0

6.5 Other polymers [i](#)

There are no such residues in this entry.