Full wwPDB X-ray Structure Validation Report (i)

May 17, 2020 – 03:07 am BST

PDB ID	:	6CAQ
Title	:	Crystal Structure of 30S ribosomal subunit from Thermus thermophilus
Authors	:	DeMirci, H.
Deposited on	:	2018-01-31
Resolution	:	3.40 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 (i) symbol.

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

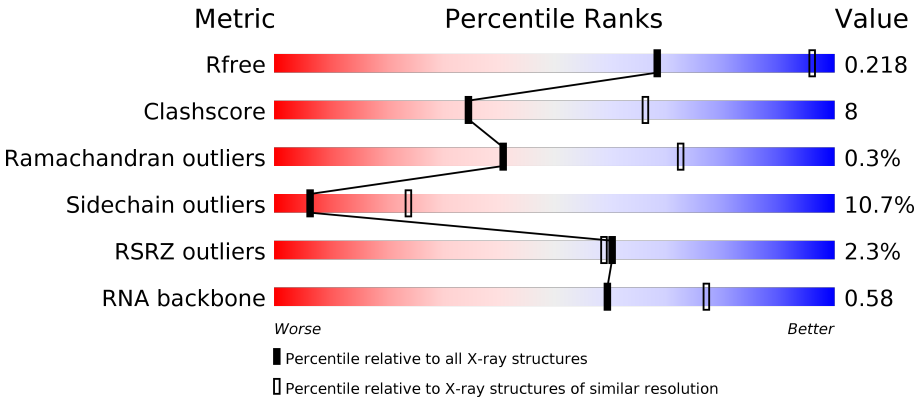
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.40 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	1026 (3.48-3.32)
Clashscore	141614	1055 (3.48-3.32)
Ramachandran outliers	138981	1038 (3.48-3.32)
Sidechain outliers	138945	1038 (3.48-3.32)
RSRZ outliers	127900	2173 (3.50-3.30)
RNA backbone	3102	1006 (3.84-2.96)

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

Mol	Chain	Length	Quality of chain
1	A	1522	2% 61% 31% 7%
2	B	234	% 63% 32%
3	C	206	8% 67% 29%
4	D	208	2% 69% 28%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
5	E	150	73% 21% 5%
6	F	101	84% 15%
7	G	155	2% 74% 25%
8	H	138	70% 25% 5%
9	I	127	2% 67% 30%
10	J	98	5% 57% 36% 6%
11	K	116	73% 26%
12	L	124	2% 62% 31% 6%
13	M	118	3% 58% 37%
14	N	60	57% 40%
15	O	87	62% 31% 7%
16	P	83	69% 28%
17	Q	99	80% 14% 6%
18	R	70	71% 24%
19	S	80	10% 60% 33% 8%
20	T	99	3% 75% 20% 5%
21	U	24	67% 33%
22	Y	6	17% 33% 67%
23	W	15	67% 33%

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
24	MG	A	1601	-	-	-	X
24	MG	A	1602	-	-	-	X
24	MG	A	1629	-	-	-	X
24	MG	A	1630	-	-	-	X
24	MG	A	1655	-	-	-	X

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
24	MG	A	1690	-	-	-	X
24	MG	A	1693	-	-	-	X
24	MG	A	1710	-	-	-	X
24	MG	A	1713	-	-	-	X
24	MG	A	1717	-	-	-	X
24	MG	A	1736	-	-	-	X
24	MG	A	1745	-	-	-	X
24	MG	A	1766	-	-	-	X
24	MG	A	1773	-	-	-	X
24	MG	A	1785	-	-	-	X
24	MG	A	1805	-	-	-	X
24	MG	A	1807	-	-	-	X
24	MG	A	1811	-	-	-	X
24	MG	A	1824	-	-	-	X
24	MG	A	1832	-	-	-	X
24	MG	A	1842	-	-	-	X
24	MG	A	1844	-	-	-	X
24	MG	A	1846	-	-	-	X
24	MG	A	1857	-	-	-	X
24	MG	A	1862	-	-	-	X
24	MG	A	1868	-	-	-	X
24	MG	A	1872	-	-	-	X
24	MG	A	1873	-	-	-	X
24	MG	A	1874	-	-	-	X
24	MG	A	1877	-	-	-	X
24	MG	A	1878	-	-	-	X
24	MG	A	1883	-	-	-	X
24	MG	A	1884	-	-	-	X
24	MG	A	1885	-	-	-	X
24	MG	A	1886	-	-	-	X
24	MG	A	1888	-	-	-	X
24	MG	A	1893	-	-	-	X
24	MG	A	1894	-	-	-	X
24	MG	A	1895	-	-	-	X
24	MG	A	1896	-	-	-	X
24	MG	A	1897	-	-	-	X
24	MG	A	1898	-	-	-	X
24	MG	A	1902	-	-	-	X
24	MG	A	1903	-	-	-	X
24	MG	A	1904	-	-	-	X
24	MG	A	1907	-	-	-	X
24	MG	A	1908	-	-	-	X

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
24	MG	A	1914	-	-	-	X
24	MG	A	1920	-	-	-	X
24	MG	A	1922	-	-	-	X
24	MG	A	1926	-	-	-	X
24	MG	A	1927	-	-	-	X
24	MG	A	1928	-	-	-	X
24	MG	A	1933	-	-	-	X
24	MG	A	1939	-	-	-	X
24	MG	H	204	-	-	-	X
24	MG	H	208	-	-	-	X
24	MG	K	207	-	-	-	X
24	MG	N	102	-	-	-	X
24	MG	Q	208	-	-	-	X
24	MG	T	201	-	-	-	X

2 Entry composition

There are 27 unique types of molecules in this entry. The entry contains 52861 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a RNA chain called 16S Ribosomal RNA rRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
1	A	1512	32644	14540	6040	10546	1518	0	6	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	13	C	U	conflict	GB 55771382

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	234	1900	1213	341	341	5	0	0	0

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
5	E	150	1146	724	217	201	4	0	0	0

- 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			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Q	96	GLN	GLU	conflict	UNP P0DOY7

- 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 a RNA chain called RNA (5'-R(*UP*UP*UP*UP*UP*U)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	Y	6	Total	C	N	O	P	0	0	0
			117	54	12	46	5			

- Molecule 23 is a RNA chain called RNA (5'-R(*GP*GP*GP*AP*UP*UP*GP*AP*AP*AP *AP*UP*CP*CP*C)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	W	15	Total	C	N	O	P	0	0	0
			319	144	60	101	14			

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

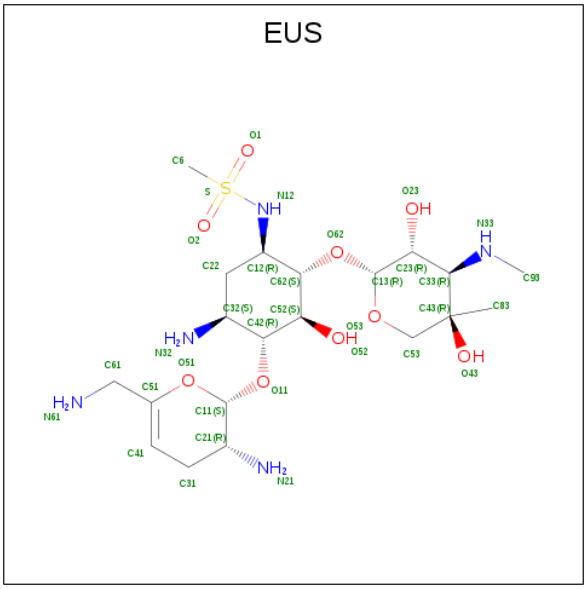
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
24	P	6	Total	Mg	0	0
			6	6		
24	G	4	Total	Mg	0	0
			4	4		
24	J	1	Total	Mg	0	0
			1	1		
24	Q	8	Total	Mg	0	0
			8	8		
24	D	5	Total	Mg	0	0
			5	5		
24	K	10	Total	Mg	0	0
			10	10		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
24	E	4	Total Mg 4 4	0	0
24	H	8	Total Mg 8 8	0	0
24	B	2	Total Mg 2 2	0	0
24	C	5	Total Mg 5 5	0	0
24	A	338	Total Mg 338 338	0	0
24	T	1	Total Mg 1 1	0	0
24	N	1	Total Mg 1 1	0	0
24	Y	2	Total Mg 2 2	0	0
24	L	4	Total Mg 4 4	0	0
24	F	1	Total Mg 1 1	0	0

- Molecule 25 is N-[(1R,2S,3S,4R,5S)-5-amino-4-{[(2S,3R)-3-amino-6-(aminomethyl)-3,4-dihydro-2H-pyran-2-yl]oxy}-2-{[3-deoxy-4-C-methyl-3-(methylamino)-beta-L-arabinopyranosyl]oxy}-3-hydroxycyclohexyl]methanesulfonamide (three-letter code: EUS) (formula: $C_{20}H_{39}N_5O_9S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
25	A	1	Total	C	N	O	S	0	0
			35	20	5	9	1		

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

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

- Molecule 27 is water.

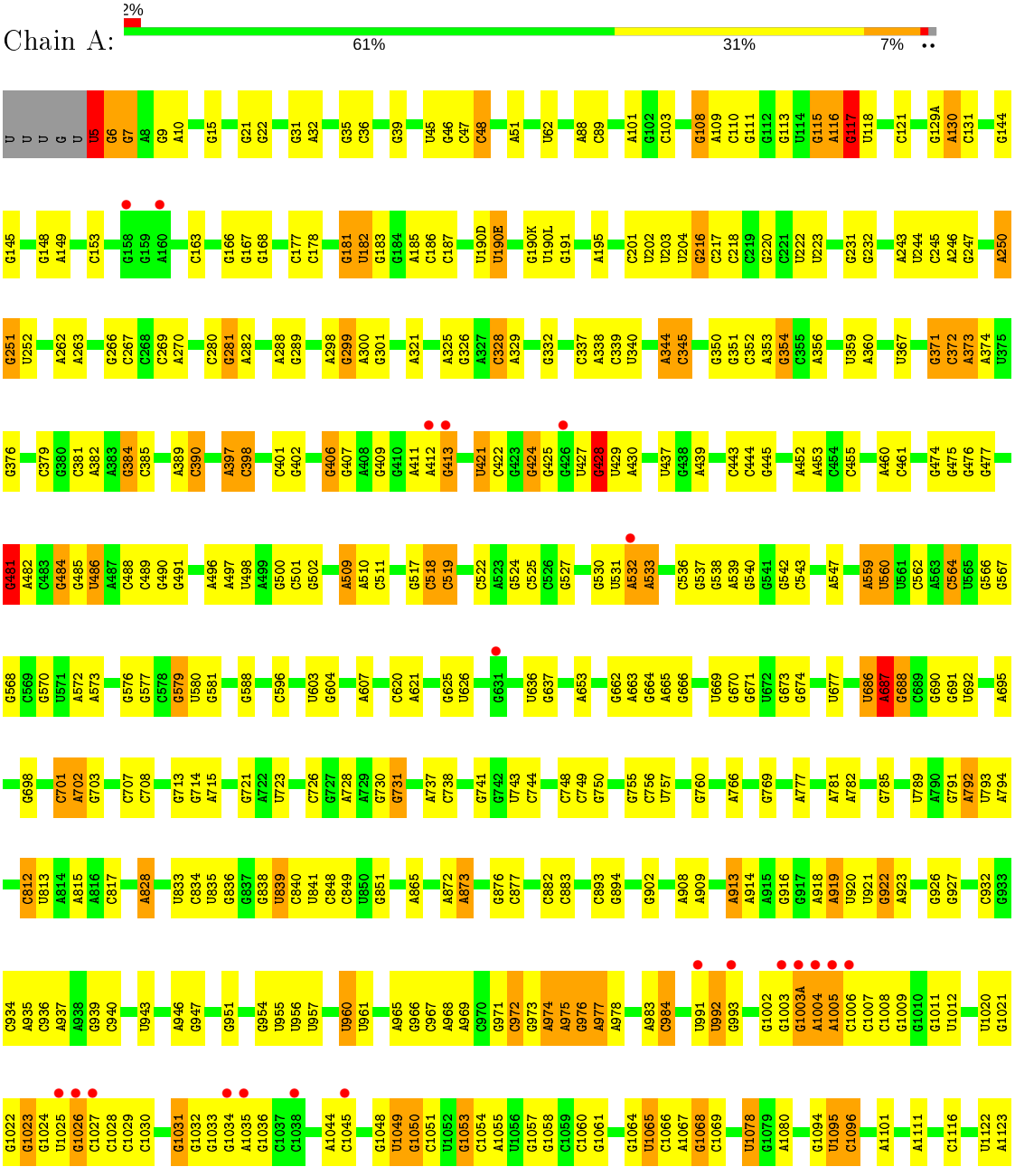
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
27	A	225	Total	O	0	0
			225	225		
27	C	1	Total	O	0	0
			1	1		
27	D	1	Total	O	0	0
			1	1		
27	E	6	Total	O	0	0
			6	6		
27	H	4	Total	O	0	0
			4	4		
27	L	1	Total	O	0	0
			1	1		
27	N	2	Total	O	0	0
			2	2		
27	P	6	Total	O	0	0
			6	6		
27	Q	8	Total	O	0	0
			8	8		
27	T	2	Total	O	0	0
			2	2		

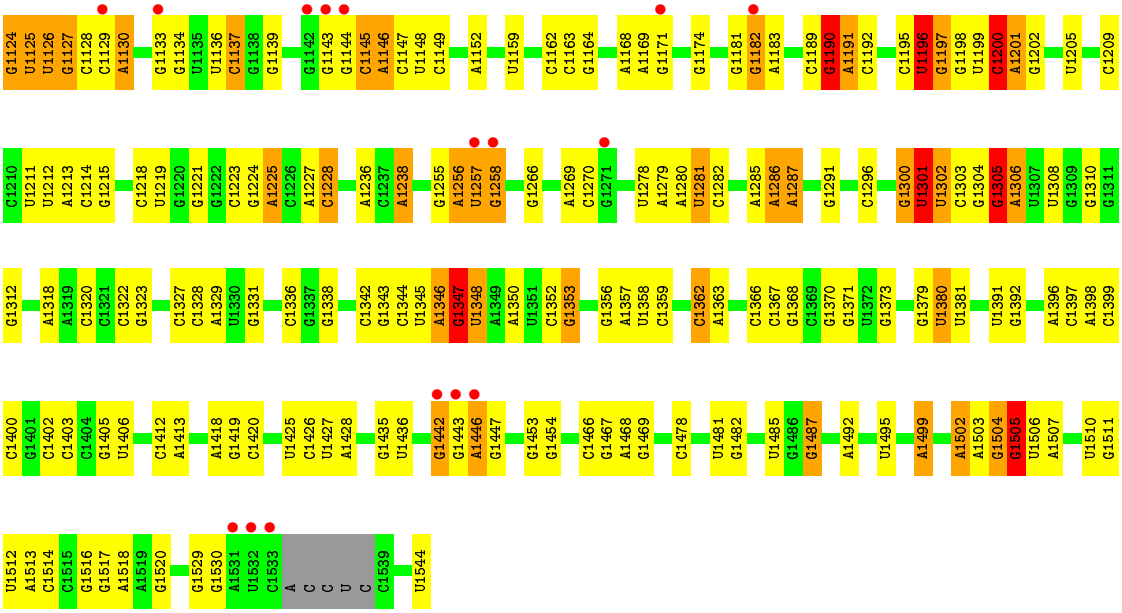
3 Residue-property plots (i)

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

- Molecule 1: 16S Ribosomal RNA rRNA

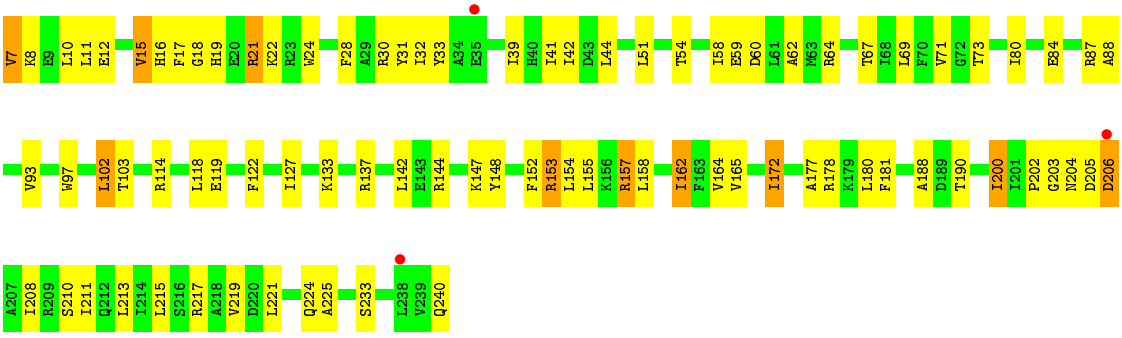
Chain A:





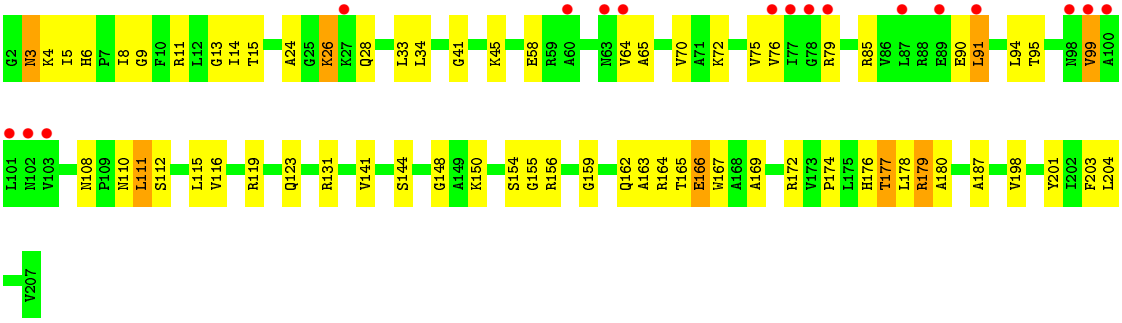
• Molecule 2: 30S ribosomal protein S2

Chain B:



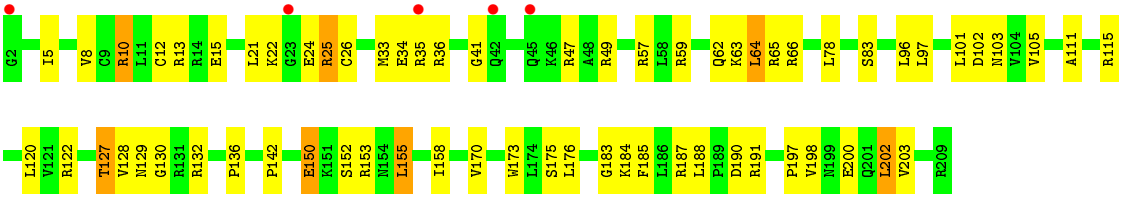
• Molecule 3: 30S ribosomal protein S3

Chain C:



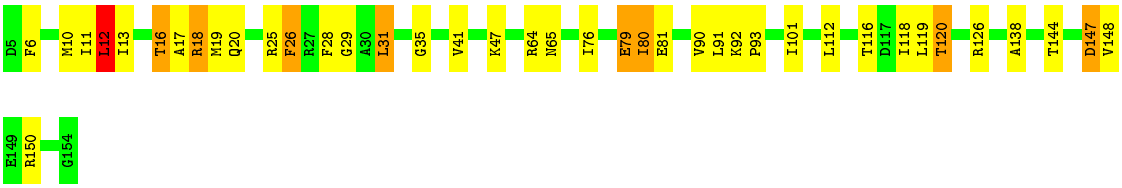
• Molecule 4: 30S ribosomal protein S4

Chain D:



• Molecule 5: 30S ribosomal protein S5

Chain E:

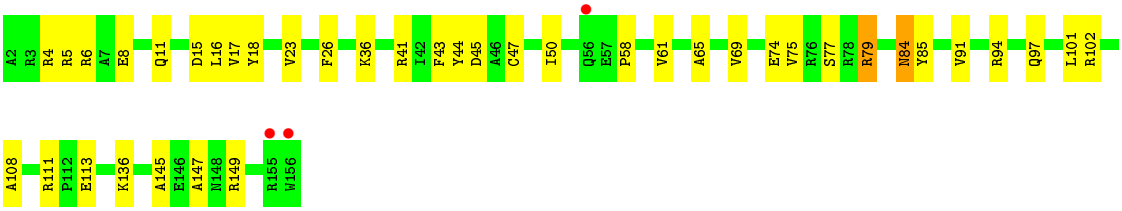


• Molecule 6: 30S ribosomal protein S6

Chain F:

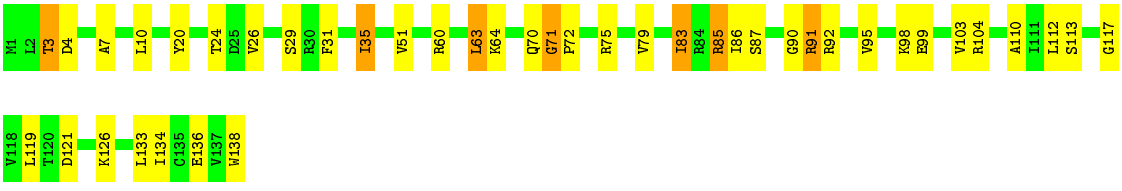
• Molecule 7: 30S ribosomal protein S7

Chain G:



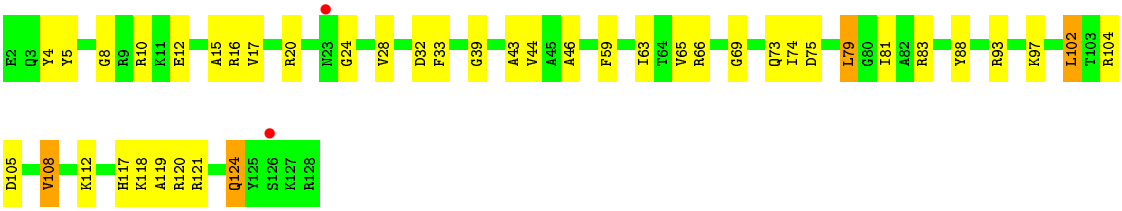
• Molecule 8: 30S ribosomal protein S8

Chain H:



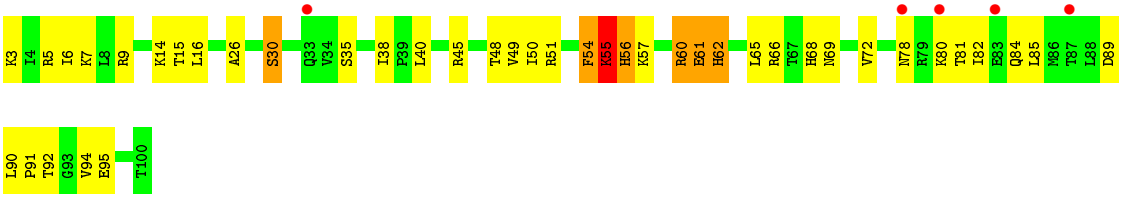
• Molecule 9: 30S ribosomal protein S9

Chain I:



• Molecule 10: 30S ribosomal protein S10

Chain J:

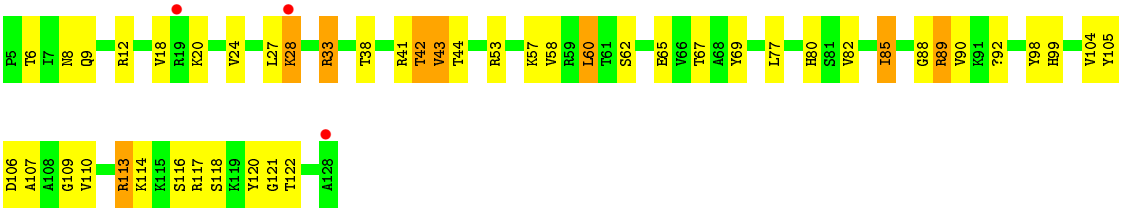


• Molecule 11: 30S ribosomal protein S11

Chain K:

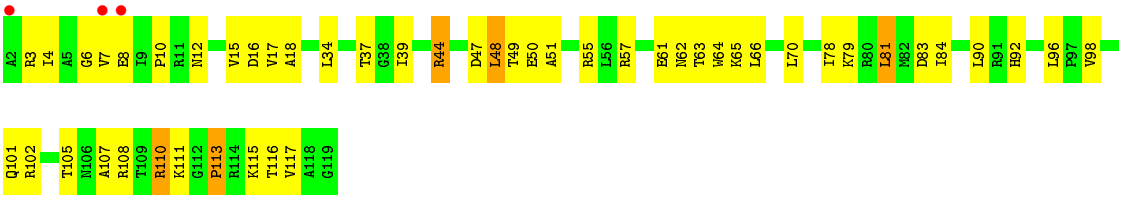
• Molecule 12: 30S ribosomal protein S12

Chain L:



• Molecule 13: 30S ribosomal protein S13

Chain M:



• Molecule 14: 30S ribosomal protein S14 type Z

Chain N:

- Molecule 15: 30S ribosomal protein S15

Chain O:

- Molecule 16: 30S ribosomal protein S16

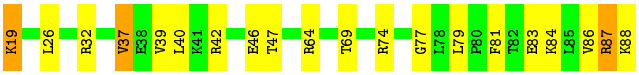
Chain P:

- Molecule 17: 30S ribosomal protein S17

Chain Q:

- Molecule 18: 30S ribosomal protein S18

Chain R:

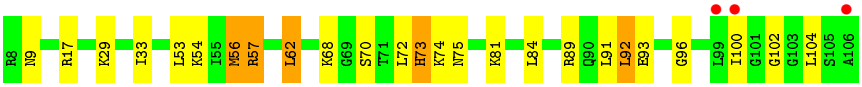


- Molecule 19: 30S ribosomal protein S19

Chain S:

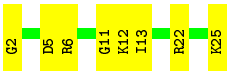
- Molecule 20: 30S ribosomal protein S20

Chain T:



- Molecule 21: 30S ribosomal protein Thx

Chain U:

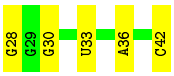


• Molecule 22: RNA (5'-R(*UP*UP*UP*UP*UP*U)-3')

Chain Y:

• Molecule 23: RNA (5'-R(*GP*GP*GP*AP*UP*UP*GP*AP*AP*AP*AP*UP*CP*CP*C)-3')

Chain W:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α, β, γ	400.97Å 400.97Å 175.05Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.91 – 3.40 39.91 – 3.13	Depositor EDS
% Data completeness (in resolution range)	99.7 (39.91-3.40) 84.9 (39.91-3.13)	Depositor EDS
R_{merge}	2.44	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.11 (at 3.12Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.190 , 0.220 0.190 , 0.218	Depositor DCC
R_{free} test set	2000 reflections (0.82%)	wwPDB-VP
Wilson B-factor (Å^2)	35.5	Xtriage
Anisotropy	0.430	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.25 , 62.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.44$, $< L^2 > = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.83	EDS
Total number of atoms	52861	wwPDB-VP
Average B, all atoms (Å^2)	78.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.46% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, MA6, G7M, 0TD, MG, 2MG, 5MC, UR3, 4OC, M2G, EUS, 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	0.41	0/36139	0.93	34/56396 (0.1%)
2	B	0.30	0/1935	0.47	0/2609
3	C	0.30	0/1636	0.48	0/2205
4	D	0.32	0/1733	0.47	0/2318
5	E	0.34	0/1162	0.54	1/1564 (0.1%)
6	F	0.27	0/856	0.45	0/1154
7	G	0.30	0/1276	0.44	0/1709
8	H	0.35	0/1136	0.53	0/1527
9	I	0.30	0/1029	0.51	1/1379 (0.1%)
10	J	0.29	0/805	0.54	0/1082
11	K	0.33	0/879	0.51	0/1187
12	L	0.33	0/977	0.57	0/1306
13	M	0.28	0/947	0.52	0/1270
14	N	0.31	0/501	0.51	0/664
15	O	0.29	0/740	0.44	0/987
16	P	0.33	0/716	0.54	0/963
17	Q	0.33	0/836	0.55	1/1117 (0.1%)
18	R	0.30	0/579	0.49	0/768
19	S	0.28	0/661	0.51	0/890
20	T	0.29	0/765	0.49	0/1007
21	U	0.28	0/212	0.45	0/277
22	Y	0.34	0/128	0.95	0/196
23	W	0.31	0/357	0.80	0/555
All	All	0.37	0/56005	0.82	37/83130 (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	2
8	H	0	1
10	J	0	2
13	M	0	2
14	N	0	1
All	All	0	9

There are no bond length outliers.

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	299	G	C5-C6-N1	-8.61	107.20	111.50
1	A	328	C	C2-N1-C1'	8.49	128.14	118.80
1	A	839	U	C2-N1-C1'	6.93	126.02	117.70
1	A	117	G	C6-C5-N7	-6.79	126.33	130.40
1	A	1305	G	P-O3'-C3'	6.58	127.60	119.70
1	A	1346	A	P-O3'-C3'	6.34	127.31	119.70
1	A	328	C	N1-C2-O2	6.31	122.68	118.90
1	A	1200	C	N1-C2-O2	6.26	122.66	118.90
1	A	913	A	P-O3'-C3'	6.21	127.15	119.70
1	A	117	G	N1-C6-O6	6.19	123.61	119.90
1	A	1301	U	P-O3'-C3'	6.18	127.12	119.70
1	A	1347	G	P-O3'-C3'	6.06	126.98	119.70
1	A	481	G	N3-C4-N9	6.06	129.63	126.00
1	A	1190	G	P-O3'-C3'	6.02	126.92	119.70
1	A	792	A	P-O3'-C3'	6.00	126.90	119.70
1	A	839	U	N1-C2-O2	5.96	126.97	122.80
1	A	1505	G	C8-N9-C4	-5.94	104.02	106.40
1	A	328	C	C6-N1-C1'	-5.92	113.70	120.80
17	Q	98	LEU	CA-CB-CG	5.78	128.60	115.30
9	I	39	GLY	N-CA-C	-5.76	98.69	113.10
1	A	1300	G	P-O3'-C3'	5.74	126.59	119.70
1	A	328	C	N3-C2-O2	-5.67	117.94	121.90
1	A	1065	U	P-O3'-C3'	5.57	126.39	119.70
1	A	328	C	P-O3'-C3'	5.54	126.35	119.70
1	A	1181	G	C8-N9-C4	5.49	108.59	106.40
1	A	5	U	P-O3'-C3'	5.44	126.23	119.70
1	A	328	C	C6-N1-C2	-5.38	118.15	120.30
1	A	687	A	P-O3'-C3'	5.29	126.05	119.70
1	A	428	G	P-O3'-C3'	5.26	126.01	119.70
1	A	1201	A	P-O3'-C3'	5.23	125.97	119.70
1	A	1196	U	O4'-C1'-N1	5.18	112.35	108.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	481	G	N3-C4-C5	-5.17	126.01	128.60
1	A	1502	A	C6-C5-N7	-5.14	128.70	132.30
1	A	299	G	C6-N1-C2	5.10	128.16	125.10
1	A	281	G	C4-N9-C1'	5.08	133.10	126.50
5	E	12	LEU	CA-CB-CG	5.05	126.92	115.30
1	A	1380	U	P-O3'-C3'	5.01	125.71	119.70

There are no chirality outliers.

All (9) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	15	VAL	Peptide
3	C	166	GLU	Peptide
3	C	179	ARG	Peptide
8	H	71	GLY	Peptide
10	J	54	PHE	Peptide
10	J	55	LYS	Peptide
13	M	113	PRO	Peptide
13	M	6	GLY	Peptide
14	N	11	LYS	Peptide

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	32644	0	16507	342	0
2	B	1900	0	1951	54	0
3	C	1612	0	1677	39	0
4	D	1703	0	1763	36	0
5	E	1146	0	1207	24	0
6	F	843	0	857	10	0
7	G	1257	0	1296	21	0
8	H	1116	0	1177	25	0
9	I	1010	0	1037	27	0
10	J	792	0	835	28	0
11	K	864	0	881	17	0
12	L	972	0	1058	29	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
13	M	937	0	995	30	0
14	N	492	0	529	23	0
15	O	729	0	768	19	0
16	P	700	0	720	17	0
17	Q	823	0	893	11	0
18	R	574	0	644	14	0
19	S	647	0	673	20	0
20	T	763	0	861	15	0
21	U	208	0	221	5	0
22	Y	117	0	62	1	0
23	W	319	0	164	1	0
24	A	338	0	0	0	0
24	B	2	0	0	0	0
24	C	5	0	0	0	0
24	D	5	0	0	0	0
24	E	4	0	0	0	0
24	F	1	0	0	0	0
24	G	4	0	0	0	0
24	H	8	0	0	0	0
24	J	1	0	0	0	0
24	K	10	0	0	0	0
24	L	4	0	0	0	0
24	N	1	0	0	0	0
24	P	6	0	0	0	0
24	Q	8	0	0	0	0
24	T	1	0	0	0	0
24	Y	2	0	0	0	0
25	A	35	0	0	2	0
26	D	1	0	0	0	0
26	N	1	0	0	0	0
27	A	225	0	0	2	0
27	C	1	0	0	0	0
27	D	1	0	0	0	0
27	E	6	0	0	0	0
27	H	4	0	0	0	0
27	L	1	0	0	0	0
27	N	2	0	0	0	0
27	P	6	0	0	0	0
27	Q	8	0	0	0	0
27	T	2	0	0	0	0
All	All	52861	0	36776	724	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including

hydrogen atoms). The all-atom clashscore for this structure is 8.

All (724) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:481:G:HO2'	1:A:482:A:H8	1.00	0.93
1:A:1022:G:N2	1:A:1023:G:N7	2.23	0.87
1:A:677:U:H3	1:A:713:G:H22	1.26	0.83
20:T:100:ILE:HG22	20:T:102:GLY:H	1.42	0.83
1:A:664:G:H22	1:A:741:G:H1	1.21	0.82
13:M:10:PRO:HB2	13:M:18:ALA:HB1	1.61	0.82
17:Q:66:SER:O	17:Q:70:ARG:NH1	2.12	0.82
1:A:1502:A:H2	1:A:1505:G:H1	1.29	0.80
1:A:1111:A:N1	3:C:177:THR:HB	1.98	0.78
15:O:39:LEU:HD13	15:O:56:LEU:HB2	1.65	0.77
1:A:1005:A:N3	1:A:1026:G:N2	2.33	0.77
11:K:48:ILE:HD12	11:K:63:LEU:HB2	1.65	0.75
1:A:955:U:H1'	1:A:1227:A:H61	1.51	0.74
1:A:525:C:OP1	12:L:89:ARG:NH1	2.20	0.74
1:A:407:G:OP1	4:D:115:ARG:NH1	2.20	0.74
1:A:686:U:HO2'	1:A:687:A:H8	1.34	0.73
13:M:107:ALA:HB3	13:M:111:LYS:HE3	1.71	0.72
8:H:4:ASP:OD2	8:H:85:ARG:NH1	2.23	0.72
7:G:74:GLU:HG2	7:G:91:VAL:HG22	1.72	0.71
9:I:97:LYS:HA	9:I:102:LEU:HD11	1.71	0.71
1:A:542:G:OP1	4:D:10:ARG:NH2	2.23	0.71
1:A:537:G:OP1	12:L:113:ARG:NH2	2.23	0.71
3:C:156:ARG:H	3:C:163:ALA:HA	1.55	0.71
1:A:1057:G:H5"	3:C:154:SER:HB2	1.73	0.70
3:C:14:ILE:HG22	3:C:15:THR:HG23	1.71	0.70
1:A:1504:G:OP1	1:A:1507:A:H4'	1.92	0.70
1:A:1291:G:OP1	7:G:41:ARG:NH2	2.23	0.70
2:B:84:GLU:OE2	2:B:233:SER:OG	2.06	0.69
1:A:1419:G:H1	1:A:1481:U:H3	1.40	0.69
1:A:1126:U:O4	1:A:1127:G:N2	2.25	0.69
1:A:1064:G:N2	1:A:1190:G:O2'	2.25	0.69
5:E:81:GLU:HG2	5:E:90:VAL:HG22	1.75	0.69
19:S:12:ASP:H	19:S:38:SER:HB3	1.58	0.68
16:P:15:PRO:HD2	16:P:42:ARG:HD3	1.76	0.68
1:A:976:G:OP2	1:A:1358:U:O2'	2.11	0.68
1:A:1499:A:H1'	1:A:1520[A]:G:H5'	1.76	0.67
2:B:71:VAL:HB	2:B:164:VAL:HG12	1.76	0.67
14:N:8:GLU:HB2	14:N:11:LYS:HE3	1.75	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:P:28:ARG:NH1	16:P:29:ASP:OD1	2.27	0.67
9:I:112:LYS:HA	9:I:119:ALA:HB2	1.77	0.67
1:A:975:A:H5'	1:A:975:A:H8	1.59	0.66
12:L:41:ARG:HH21	12:L:43:VAL:HG13	1.59	0.66
1:A:113:G:H1'	1:A:354:G:H5'	1.77	0.66
1:A:1128:C:OP1	9:I:66:ARG:NH1	2.29	0.66
5:E:11:ILE:HB	5:E:31:LEU:HB3	1.76	0.66
1:A:1053:G:HO2'	1:A:1199:U:H5	1.42	0.66
1:A:951:G:OP2	13:M:102:ARG:NH2	2.29	0.66
4:D:63:LYS:NZ	4:D:197:PRO:O	2.29	0.65
1:A:1145:C:O2'	1:A:1146:A:O5'	2.14	0.65
10:J:61:GLU:OE1	14:N:45:ARG:NH1	2.29	0.64
9:I:15:ALA:HB2	9:I:65:VAL:HG13	1.80	0.64
1:A:1391:U:H2'	1:A:1392:G:C8	2.32	0.64
2:B:80:ILE:HD11	2:B:208:ILE:HG23	1.80	0.64
8:H:86:ILE:HD12	8:H:133:LEU:HD22	1.79	0.64
14:N:27:CYS:SG	14:N:29:ARG:HB2	2.38	0.64
2:B:16:HIS:HD2	2:B:204:ASN:HD22	1.45	0.64
1:A:527:G7M:H8	1:A:527:G7M:H5"	1.80	0.63
4:D:22:LYS:HB2	4:D:26:CYS:SG	2.38	0.63
1:A:1228:C:H4'	13:M:116:THR:HA	1.79	0.63
13:M:49:THR:HG22	13:M:51:ALA:H	1.63	0.63
1:A:250:A:H4'	1:A:251:G:O5'	1.98	0.63
1:A:835:U:OP1	18:R:64:ARG:NH2	2.29	0.63
7:G:84:ASN:N	7:G:84:ASN:OD1	2.29	0.63
1:A:1031:G:H2'	1:A:1032:G:H8	1.64	0.63
1:A:673:G:H2'	1:A:674:G:C8	2.33	0.63
1:A:1060:C:OP1	14:N:45:ARG:NH2	2.32	0.62
10:J:55:LYS:HD2	10:J:56:HIS:H	1.63	0.62
1:A:509:A:N3	1:A:543:C:O2'	2.28	0.62
1:A:972:C:H4'	10:J:57:LYS:HD3	1.81	0.62
1:A:538:G:H5"	12:L:114:LYS:HB2	1.80	0.62
11:K:90:GLY:HA2	11:K:93:GLN:HB2	1.82	0.62
17:Q:6:LEU:HB2	17:Q:59:ILE:HG22	1.82	0.62
15:O:56:LEU:HA	15:O:59:MET:HE2	1.82	0.62
1:A:1255:G:OP2	3:C:26:LYS:NZ	2.33	0.61
20:T:92:LEU:O	20:T:96:GLY:HA2	2.00	0.61
1:A:967:5MC:H2'	1:A:968:A:C8	2.36	0.61
8:H:113:SER:HB2	8:H:134:ILE:HD11	1.82	0.61
1:A:1266:G:N2	1:A:1269:A:OP2	2.31	0.61
12:L:24:VAL:HG13	12:L:98:TYR:HE2	1.65	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:532:A:N6	3:C:159:GLY:O	2.32	0.61
13:M:96:LEU:O	13:M:110:ARG:NH1	2.33	0.61
18:R:46:GLU:CD	18:R:46:GLU:H	2.05	0.60
1:A:31:G:N2	1:A:48:C:OP1	2.25	0.60
14:N:47:LEU:HD12	14:N:52:GLN:HB2	1.83	0.60
11:K:84:VAL:HG11	11:K:91:ARG:HD3	1.83	0.60
15:O:62:GLN:OE1	15:O:65:ARG:NH2	2.34	0.60
15:O:64:ARG:HH21	15:O:68:ARG:HH21	1.48	0.60
1:A:1281:U:H5'	1:A:1282:C:H5	1.66	0.60
11:K:15:ALA:HA	11:K:77:MET:HA	1.83	0.60
10:J:48:THR:HA	10:J:62:HIS:HB3	1.84	0.60
1:A:21:G:H2'	1:A:22:G:C8	2.36	0.60
4:D:187:ARG:NH1	4:D:188:LEU:H	1.99	0.60
11:K:57:THR:HG23	11:K:60:ALA:H	1.66	0.60
17:Q:6:LEU:HB3	17:Q:23:VAL:HG11	1.84	0.60
19:S:28:LYS:HG2	19:S:29:ARG:H	1.67	0.60
1:A:372:C:H4'	1:A:373:A:O5'	2.00	0.59
3:C:70:VAL:HG21	3:C:76:VAL:HG21	1.84	0.59
1:A:45:U:H2'	1:A:46:G:C8	2.37	0.59
2:B:162:ILE:HD12	2:B:177:ALA:HB2	1.83	0.59
17:Q:45:HIS:CD2	17:Q:47:PRO:HG3	2.37	0.59
19:S:45:VAL:HA	19:S:62:ILE:HG13	1.84	0.59
1:A:1128:C:O2'	1:A:1130:A:N7	2.35	0.59
1:A:1412:C:H2'	1:A:1413:A:C8	2.38	0.59
1:A:299:G:H2'	1:A:300:A:C8	2.37	0.59
10:J:61:GLU:OE2	14:N:58:LYS:NZ	2.29	0.59
1:A:427:U:OP1	4:D:13:ARG:NH2	2.36	0.59
1:A:397:A:H5'	1:A:398:C:OP1	2.03	0.59
19:S:36:ARG:NH1	19:S:52:TYR:O	2.35	0.59
3:C:91:LEU:HD21	3:C:99:VAL:HG22	1.85	0.58
13:M:3:ARG:HE	13:M:7:VAL:HG12	1.67	0.58
2:B:32:ILE:HD11	2:B:190:THR:HG23	1.85	0.58
14:N:24:CYS:HB3	14:N:29:ARG:HB3	1.85	0.58
16:P:53:VAL:HG12	16:P:79:VAL:HG22	1.86	0.58
4:D:15:GLU:OE1	4:D:59:ARG:NH2	2.30	0.58
1:A:1002:G:H2'	1:A:1003:G:C8	2.39	0.58
1:A:1007:C:H1'	1:A:1023:G:H1	1.69	0.57
1:A:411:A:N3	1:A:413:G:O2'	2.28	0.57
15:O:29:VAL:HG11	15:O:67:LEU:HD21	1.84	0.57
1:A:603:U:H2'	1:A:604:G:C8	2.39	0.57
9:I:43:ALA:HA	9:I:74:ILE:HD13	1.85	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:119:GLU:OE1	2:B:153:ARG:NH2	2.38	0.57
10:J:50:ILE:H	10:J:50:ILE:HD12	1.70	0.57
12:L:24:VAL:HG13	12:L:98:TYR:CE2	2.40	0.57
1:A:1200:C:O2'	1:A:1205:U:O4	2.17	0.57
1:A:877:C:O2	8:H:3:THR:HG21	2.04	0.57
4:D:150:GLU:HA	4:D:153:ARG:HG3	1.87	0.57
7:G:26:PHE:HD1	7:G:101:LEU:HD22	1.69	0.57
15:O:87:ILE:HG22	15:O:88:ARG:HG2	1.87	0.57
17:Q:59:ILE:HD12	17:Q:73:VAL:HA	1.86	0.56
1:A:1125:U:OP2	1:A:1145:C:N4	2.39	0.56
2:B:15:VAL:HG12	2:B:210:SER:HB3	1.87	0.56
3:C:6:HIS:CE1	3:C:8:ILE:HB	2.40	0.56
1:A:452:A:O2'	1:A:453:A:O4'	2.12	0.56
1:A:144:G:H1	1:A:178:C:H42	1.52	0.56
1:A:501:C:H2'	1:A:502:G:C8	2.40	0.56
3:C:24:ALA:HB1	3:C:28:GLN:HB2	1.88	0.56
1:A:579:G:H5'	1:A:728:A:H1'	1.88	0.56
4:D:78:LEU:HD13	4:D:97:LEU:HD23	1.88	0.56
1:A:280:C:O2	17:Q:38:ARG:HD3	2.06	0.56
1:A:1196:U:OP1	1:A:1197:G:H5'	2.06	0.55
1:A:522:C:H41	12:L:53:ARG:HH22	1.53	0.55
1:A:406:G:H5'	4:D:5:ILE:HG21	1.89	0.55
2:B:102:LEU:HD21	2:B:162:ILE:HD11	1.89	0.55
4:D:102:ASP:OD1	4:D:103:ASN:N	2.38	0.55
1:A:932:C:H5'	7:G:4:ARG:HG2	1.88	0.55
8:H:86:ILE:HD11	8:H:136:GLU:HG3	1.87	0.55
1:A:1162:C:H42	1:A:1174:G:H1	1.53	0.55
1:A:1195:C:H3'	1:A:1196:U:H5"	1.88	0.55
1:A:707:C:H2'	1:A:708:C:C6	2.42	0.55
4:D:102:ASP:HB3	4:D:136:PRO:HB3	1.89	0.55
8:H:10:LEU:HD22	8:H:83:ILE:HD13	1.87	0.55
1:A:974:A:OP2	14:N:41:ARG:NH1	2.39	0.55
1:A:376:G:H5"	16:P:5:ARG:HD2	1.87	0.55
1:A:1031:G:H2'	1:A:1032:G:C8	2.41	0.55
10:J:30:SER:HB3	10:J:80:LYS:HB2	1.89	0.55
1:A:413:G:H2'	1:A:428:G:N2	2.21	0.55
1:A:390:C:O3'	16:P:28:ARG:NH2	2.40	0.55
1:A:1221:G:O3'	19:S:77:THR:HG21	2.06	0.55
1:A:103:C:OP1	20:T:17:ARG:NH1	2.40	0.54
1:A:1006:C:H2'	1:A:1007:C:H6	1.72	0.54
1:A:789:U:O2'	1:A:791:G:N7	2.35	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:112:SER:HB3	3:C:115:LEU:HD12	1.89	0.54
1:A:1443:G:H5"	1:A:1446:A:H5'	1.90	0.54
1:A:216:G:H2'	1:A:217:C:C6	2.43	0.54
1:A:833:U:H2'	1:A:834:C:C6	2.43	0.54
1:A:1392:G:H21	1:A:1502:A:H8	1.55	0.54
1:A:1419:G:N2	1:A:1481:U:O2	2.37	0.54
9:I:17:VAL:HG11	9:I:81:ILE:HA	1.89	0.54
1:A:344:A:H5'	1:A:345:C:C5	2.42	0.54
9:I:8:GLY:HA2	9:I:79:LEU:HB3	1.89	0.54
1:A:973:G:H3'	1:A:974:A:H5"	1.90	0.54
1:A:1405:G:N7	25:A:1809:EUS:N33	2.56	0.54
1:A:560:U:H5'	1:A:566:G:C2	2.43	0.54
4:D:57:ARG:HG3	4:D:202:LEU:HD13	1.90	0.54
1:A:1345:U:OP1	9:I:120:ARG:NH1	2.41	0.54
1:A:501:C:H2'	1:A:502:G:H8	1.73	0.53
10:J:80:LYS:H	10:J:80:LYS:HD2	1.73	0.53
2:B:21:ARG:HA	2:B:39:ILE:HA	1.89	0.53
1:A:692:U:OP1	11:K:124:LYS:NZ	2.29	0.53
6:F:11:ASN:HD22	6:F:86:ARG:NH2	2.05	0.53
13:M:3:ARG:NE	13:M:7:VAL:HG12	2.23	0.53
15:O:64:ARG:HH21	15:O:68:ARG:NH2	2.07	0.53
11:K:57:THR:CG2	11:K:60:ALA:H	2.22	0.53
2:B:158:LEU:H	2:B:158:LEU:HD12	1.73	0.53
18:R:32:ARG:HA	18:R:69:THR:HG21	1.91	0.53
2:B:59:GLU:HB2	2:B:221:LEU:HD11	1.91	0.53
12:L:77:LEU:HD21	12:L:107:ALA:HB2	1.90	0.52
18:R:47:THR:HA	18:R:83:GLU:HB2	1.91	0.52
20:T:72:LEU:O	20:T:74:LYS:N	2.42	0.52
1:A:1305:G:N2	1:A:1331:G:H1'	2.25	0.52
5:E:80:ILE:HD13	5:E:138:ALA:HB1	1.91	0.52
14:N:8:GLU:O	14:N:11:LYS:HG3	2.10	0.52
1:A:1435:G:H2'	1:A:1436:U:C6	2.44	0.52
1:A:475:G:H2'	1:A:476:G:H8	1.74	0.52
1:A:662:G:H2'	1:A:663:A:C8	2.45	0.52
15:O:5:LYS:HA	15:O:8:LYS:HB2	1.92	0.52
16:P:10:GLY:HA3	16:P:14:ASN:O	2.10	0.52
1:A:1020:U:H2'	1:A:1021:G:H8	1.75	0.52
2:B:60:ASP:CG	2:B:64:ARG:HH12	2.12	0.52
15:O:55:GLY:HA2	15:O:58:MET:HE2	1.92	0.52
6:F:50:TYR:CE1	18:R:77:GLY:HA2	2.45	0.52
1:A:474:G:H2'	1:A:475:G:H8	1.75	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:114:ARG:HH11	2:B:118:LEU:HD21	1.75	0.52
1:A:489:C:H2'	1:A:490:G:H8	1.74	0.51
4:D:62:GLN:OE1	4:D:65:ARG:NH1	2.44	0.51
1:A:1510:U:H2'	1:A:1511:G:C8	2.45	0.51
1:A:5:U:H4'	1:A:6:G:O5'	2.10	0.51
3:C:15:THR:HG21	3:C:179:ARG:O	2.10	0.51
12:L:53:ARG:HH12	12:L:92:0TD:CG	2.18	0.51
21:U:13:ILE:HG22	21:U:22:ARG:CZ	2.41	0.51
2:B:97:TRP:HZ2	2:B:102:LEU:HD22	1.76	0.51
4:D:24:GLU:HG2	4:D:25:ARG:H	1.75	0.51
9:I:112:LYS:HE3	9:I:117:HIS:O	2.10	0.51
1:A:1004:A:H5"	1:A:1025:U:C4	2.46	0.51
1:A:1009:G:H1	1:A:1020:U:H3	1.57	0.51
5:E:65:ASN:ND2	5:E:65:ASN:O	2.43	0.51
1:A:1008:C:N4	1:A:1021:G:H1	2.09	0.50
1:A:413:G:H2'	1:A:428:G:H22	1.75	0.50
2:B:84:GLU:HB3	2:B:219:VAL:HG21	1.93	0.50
18:R:40:LEU:HB3	18:R:79:LEU:HD11	1.94	0.50
5:E:147:ASP:OD1	5:E:147:ASP:N	2.44	0.50
1:A:1413:A:H2	1:A:1487:G:H22	1.58	0.50
1:A:975:A:H5'	1:A:975:A:C8	2.43	0.50
8:H:63:LEU:HD22	8:H:63:LEU:H	1.76	0.50
9:I:10:ARG:HG2	9:I:75:ASP:HB2	1.92	0.50
10:J:57:LYS:O	10:J:60:ARG:NH1	2.44	0.50
6:F:46:ARG:HH22	18:R:37:VAL:HG21	1.76	0.50
3:C:58:GLU:HB3	10:J:92:THR:HG21	1.92	0.50
13:M:34:LEU:HD13	13:M:39:ILE:HB	1.93	0.50
1:A:1003(A):G:C5	1:A:1004:A:H1'	2.47	0.50
1:A:939:G:H2'	1:A:940:C:C6	2.47	0.50
2:B:16:HIS:CD2	2:B:204:ASN:H	2.30	0.50
1:A:1342:C:O2'	9:I:124:GLN:HB2	2.12	0.50
1:A:1027:C:H42	1:A:1034:G:H1	1.59	0.50
1:A:1218:C:H2'	1:A:1219:U:C6	2.47	0.50
1:A:564:C:O2'	8:H:91:ARG:NH2	2.44	0.50
11:K:33:THR:HA	11:K:39:PRO:HA	1.93	0.50
1:A:686:U:O2'	1:A:687:A:H8	1.92	0.50
1:A:972:C:OP1	10:J:57:LYS:NZ	2.34	0.50
1:A:1189:C:H5"	3:C:5:ILE:HG12	1.92	0.50
1:A:1048:G:H1	1:A:1209:C:H42	1.59	0.50
1:A:1366:C:H2'	1:A:1367:C:C6	2.46	0.50
5:E:35:GLY:HA3	5:E:112:LEU:HB3	1.92	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:6:ILE:HB	10:J:72:VAL:HB	1.94	0.50
10:J:49:VAL:HG22	14:N:41:ARG:HB2	1.94	0.50
11:K:80:VAL:HG21	11:K:103:LEU:HD13	1.93	0.50
19:S:13:ASP:OD1	19:S:13:ASP:N	2.45	0.50
1:A:153:C:H42	1:A:168:G:H1	1.59	0.49
1:A:444:C:H2'	1:A:445:G:C8	2.47	0.49
2:B:147:LYS:HE3	2:B:148:TYR:CE1	2.47	0.49
3:C:58:GLU:HB2	3:C:65:ALA:HB3	1.93	0.49
7:G:108:ALA:O	7:G:111:ARG:HB2	2.11	0.49
9:I:10:ARG:HD3	9:I:105:ASP:HB3	1.93	0.49
1:A:191:G:O2'	20:T:102:GLY:O	2.27	0.49
1:A:437:U:H5'	4:D:155:LEU:HD21	1.93	0.49
2:B:19:HIS:CE1	2:B:206:ASP:HB2	2.47	0.49
2:B:16:HIS:CE1	2:B:210:SER:HB2	2.48	0.49
15:O:45:VAL:HG23	15:O:46:HIS:HD2	1.78	0.49
19:S:50:ALA:HB1	19:S:57:HIS:HB3	1.94	0.49
1:A:1373:G:H5"	7:G:36:LYS:HE3	1.94	0.49
1:A:190(K):G:H2'	1:A:190(L):U:C6	2.48	0.49
2:B:240:GLN:OE1	2:B:240:GLN:N	2.45	0.49
12:L:6:THR:OG1	12:L:9:GLN:HG3	2.13	0.49
1:A:1190:G:O2'	1:A:1191:A:OP2	2.30	0.49
1:A:452:A:O2'	1:A:453:A:O5'	2.30	0.49
2:B:59:GLU:HG3	2:B:225:ALA:HB2	1.95	0.49
7:G:5:ARG:HG2	7:G:6:ARG:H	1.78	0.49
8:H:7:ALA:HB2	8:H:85:ARG:HG3	1.94	0.49
9:I:28:VAL:HG22	9:I:63:ILE:HB	1.94	0.49
19:S:5:LEU:HD12	19:S:9:VAL:HG13	1.93	0.49
1:A:1049:U:H4'	1:A:1050:G:O5'	2.11	0.49
1:A:1197:G:H5"	27:A:2018:HOH:O	2.12	0.49
1:A:636:U:H2'	1:A:637:G:C8	2.48	0.49
1:A:1356:G:H2'	1:A:1357:A:C8	2.46	0.49
1:A:371:G:O2'	1:A:372:C:H5'	2.13	0.49
1:A:983:A:O2'	1:A:1050:G:OP2	2.30	0.49
18:R:87:ARG:O	18:R:88:LYS:HB2	2.13	0.49
1:A:269:C:H2'	1:A:270:A:C8	2.48	0.49
3:C:187:ALA:HB3	3:C:198:VAL:HB	1.95	0.49
9:I:65:VAL:HG11	9:I:73:GLN:HB3	1.95	0.49
1:A:6:G:O2'	1:A:7:G:H5'	2.13	0.49
18:R:26:LEU:HD21	18:R:39:VAL:HG23	1.95	0.49
1:A:1003(A):G:C6	1:A:1004:A:H1'	2.48	0.48
1:A:217:C:H2'	1:A:218:C:C6	2.48	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:170:VAL:HG11	4:D:175:SER:HA	1.95	0.48
1:A:411:A:OP2	4:D:25:ARG:NH2	2.46	0.48
10:J:55:LYS:HD2	10:J:56:HIS:N	2.28	0.48
1:A:62:U:O2'	1:A:379:C:O2	2.29	0.48
2:B:181:PHE:CD2	8:H:70:GLN:HB3	2.48	0.48
3:C:108:ASN:HB3	3:C:111:LEU:HB2	1.94	0.48
1:A:444:C:H2'	1:A:445:G:H8	1.77	0.48
2:B:16:HIS:HD2	2:B:204:ASN:ND2	2.10	0.48
7:G:50:ILE:HD11	7:G:61:VAL:HG11	1.96	0.48
1:A:1544:U:H4'	22:Y:1:U:H5'	1.96	0.48
4:D:12:CYS:HB3	4:D:33:MET:HG2	1.95	0.48
1:A:1143:G:H2'	1:A:1144:G:C8	2.49	0.48
10:J:14:LYS:HB3	10:J:14:LYS:HE2	1.58	0.48
13:M:49:THR:HG22	13:M:51:ALA:N	2.29	0.48
4:D:190:ASP:OD1	4:D:191:ARG:N	2.46	0.48
5:E:12:LEU:HD13	5:E:31:LEU:HB2	1.96	0.48
8:H:85:ARG:NE	8:H:87:SER:O	2.47	0.48
1:A:337:C:H2'	1:A:338:A:C8	2.49	0.48
1:A:337:C:H2'	1:A:338:A:H8	1.79	0.48
1:A:475:G:H2'	1:A:476:G:C8	2.48	0.48
1:A:570:G:C6	1:A:873:A:C2	3.02	0.48
5:E:144:THR:O	5:E:147:ASP:N	2.47	0.48
9:I:5:TYR:HE1	9:I:16:ARG:HB3	1.79	0.48
11:K:14:VAL:HG21	11:K:40:ILE:HD13	1.95	0.48
17:Q:63:ARG:HG2	17:Q:64:PRO:HD2	1.94	0.48
20:T:33:ILE:HD13	20:T:62:LEU:HB3	1.96	0.48
1:A:1256:A:H4'	1:A:1257:U:O5'	2.13	0.48
1:A:603:U:H2'	1:A:604:G:H8	1.78	0.48
2:B:16:HIS:CD2	2:B:204:ASN:HD22	2.30	0.48
3:C:155:GLY:HA2	3:C:164:ARG:H	1.79	0.48
4:D:176:LEU:HA	4:D:183:GLY:HA2	1.95	0.48
1:A:1028:C:H42	1:A:1033:G:H1	1.60	0.48
1:A:1405:G:O2'	1:A:1518[B]:MA6:O2'	2.31	0.48
1:A:421:U:H5'	1:A:422:C:C5	2.49	0.48
2:B:155:LEU:HD22	2:B:157:ARG:O	2.14	0.48
7:G:17:VAL:HG12	7:G:18:TYR:CD1	2.49	0.48
1:A:1286:A:H2'	1:A:1287:A:H4'	1.95	0.47
1:A:474:G:H2'	1:A:475:G:C8	2.49	0.47
1:A:1060:C:H2'	1:A:1061:G:H8	1.78	0.47
1:A:401:C:O2'	1:A:621:A:N3	2.38	0.47
1:A:967:5MC:H2'	1:A:968:A:N7	2.29	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:939:G:H5"	7:G:102:ARG:NH2	2.28	0.47
1:A:1425:U:H2'	1:A:1426:C:C6	2.49	0.47
3:C:174:PRO:HB2	3:C:177:THR:CG2	2.44	0.47
8:H:3:THR:HG23	8:H:4:ASP:H	1.79	0.47
20:T:54:LYS:HA	20:T:57:ARG:NH1	2.30	0.47
1:A:976:G:N2	1:A:1362:C:OP2	2.41	0.47
2:B:205:ASP:OD1	2:B:206:ASP:N	2.47	0.47
2:B:16:HIS:NE2	2:B:204:ASN:N	2.62	0.47
2:B:28:PHE:CD2	2:B:190:THR:HA	2.49	0.47
2:B:17:PHE:HD1	2:B:41:ILE:HD12	1.78	0.47
12:L:38:THR:HB	12:L:57:LYS:HB2	1.97	0.47
1:A:1399:C:H4'	1:A:1400:5MC:H5"	1.95	0.47
1:A:1466:C:H2'	1:A:1467:G:O4'	2.14	0.47
2:B:7:VAL:HG11	2:B:221:LEU:HD23	1.96	0.47
7:G:79:ARG:HA	7:G:84:ASN:HB3	1.97	0.47
17:Q:59:ILE:HG23	17:Q:71:PHE:CD2	2.50	0.47
11:K:85:ARG:HD3	11:K:113:PRO:HD3	1.97	0.47
1:A:1350:A:H8	1:A:1350:A:O5'	1.98	0.47
16:P:22:THR:HA	16:P:33:ILE:HG13	1.96	0.47
3:C:3:ASN:N	3:C:3:ASN:OD1	2.48	0.47
16:P:9:PHE:CE2	16:P:18:ARG:HD2	2.50	0.47
18:R:86:VAL:O	18:R:87:ARG:HD3	2.15	0.47
21:U:12:LYS:HG2	21:U:22:ARG:HB3	1.97	0.47
1:A:339:C:H2'	1:A:340:U:C6	2.50	0.47
1:A:1427:U:H2'	1:A:1428:A:C8	2.51	0.46
1:A:381:C:H2'	1:A:382:A:O4'	2.15	0.46
3:C:41:GLY:O	3:C:45:LYS:HG2	2.14	0.46
4:D:184:LYS:HB2	4:D:184:LYS:HE3	1.77	0.46
1:A:1080:A:O3'	5:E:16:THR:OG1	2.32	0.46
1:A:501:C:OP1	12:L:117:ARG:NH2	2.47	0.46
1:A:108:G:H5'	1:A:109:A:H5"	1.97	0.46
1:A:833:U:H2'	1:A:834:C:H6	1.79	0.46
1:A:908:A:H2'	1:A:909:A:C8	2.50	0.46
1:A:918:A:H2'	1:A:919:A:C8	2.50	0.46
1:A:110:C:H2'	1:A:111:G:O4'	2.16	0.46
1:A:280:C:O2'	27:A:2001:HOH:O	2.21	0.46
1:A:243:A:C2	1:A:246:A:C8	3.03	0.46
4:D:8:VAL:HG11	4:D:21:LEU:HB2	1.97	0.46
7:G:47:CYS:HA	7:G:50:ILE:HG22	1.98	0.46
10:J:40:LEU:HB2	10:J:69:ASN:HB2	1.98	0.46
1:A:1125:U:H3	10:J:5:ARG:HH21	1.61	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:80:ILE:HD12	5:E:91:LEU:HB2	1.96	0.46
6:F:2:ARG:NE	6:F:69:GLU:HG2	2.31	0.46
8:H:51:VAL:HG11	8:H:60:ARG:HG2	1.96	0.46
10:J:26:ALA:HB1	10:J:84:GLN:HB2	1.98	0.46
12:L:69:TYR:CD1	12:L:90:VAL:HG21	2.50	0.46
13:M:16:ASP:OD1	13:M:16:ASP:N	2.49	0.46
14:N:27:CYS:HB3	14:N:43:CYS:SG	2.56	0.46
16:P:34:GLU:OE2	16:P:55:ARG:HD2	2.15	0.46
2:B:102:LEU:HB3	2:B:180:LEU:HD12	1.96	0.46
5:E:101:ILE:O	5:E:120:THR:HB	2.16	0.46
1:A:1124:G:H5'	10:J:35:SER:O	2.15	0.46
12:L:104:VAL:HG22	12:L:105:TYR:H	1.81	0.46
1:A:518:C:H4'	1:A:519:C:O5'	2.15	0.46
8:H:35:ILE:HG12	8:H:35:ILE:H	1.56	0.46
12:L:33:ARG:HD3	12:L:62:SER:HB3	1.96	0.46
12:L:77:LEU:HD23	12:L:77:LEU:HA	1.77	0.46
1:A:666:G:H5'	1:A:726:C:H1'	1.98	0.46
7:G:145:ALA:C	7:G:147:ALA:H	2.19	0.46
15:O:3:ILE:HD11	15:O:38:ARG:HG3	1.98	0.46
20:T:56:MET:HE1	20:T:104:LEU:HD21	1.98	0.46
1:A:1130:A:OP1	1:A:1130:A:H3'	2.15	0.46
1:A:1257:U:O2'	1:A:1258:G:OP2	2.26	0.46
2:B:7:VAL:HG22	2:B:224:GLN:HE22	1.81	0.46
2:B:21:ARG:HG3	2:B:22:LYS:H	1.81	0.46
15:O:2:PRO:O	15:O:38:ARG:NH1	2.48	0.46
1:A:190(D):U:O2'	1:A:190(E):U:H5'	2.16	0.45
1:A:500:G:H2'	1:A:501:C:C6	2.51	0.45
1:A:502:G:P	12:L:118:SER:HG	2.39	0.45
1:A:992:U:H3	1:A:1044:A:H62	1.64	0.45
3:C:155:GLY:HA3	3:C:163:ALA:HB1	1.98	0.45
4:D:111:ALA:HB2	4:D:120:LEU:HD12	1.98	0.45
1:A:1035:A:H2'	1:A:1036:G:C8	2.51	0.45
1:A:1511:G:H2'	1:A:1512:U:O4'	2.16	0.45
1:A:559:A:OP1	5:E:126:ARG:NH1	2.41	0.45
12:L:8:ASN:O	12:L:12:ARG:HG3	2.15	0.45
19:S:29:ARG:N	19:S:29:ARG:HD2	2.32	0.45
1:A:1057:G:H5"	3:C:154:SER:CB	2.44	0.45
1:A:116:A:H2'	1:A:117:G:H8	1.82	0.45
1:A:35:G:H2'	1:A:36:C:C6	2.51	0.45
1:A:714:G:H2'	1:A:715:A:C8	2.52	0.45
1:A:1148:U:H2'	1:A:1149:C:O4'	2.16	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1238:A:N7	1:A:1303:C:H1'	2.31	0.45
1:A:1516[A]:G:H2'	1:A:1518[A]:MA6:OP2	2.16	0.45
1:A:730:G:C5	1:A:731:G:H1'	2.52	0.45
9:I:24:GLY:HA2	9:I:59:PHE:O	2.17	0.45
16:P:26:ARG:HD2	16:P:31:LYS:O	2.17	0.45
1:A:1122:U:O4	1:A:1123:A:N6	2.49	0.45
1:A:109:A:H2'	1:A:326:G:N2	2.31	0.45
2:B:12:GLU:HG3	2:B:213:LEU:HD11	1.99	0.45
2:B:152:PHE:CE1	2:B:155:LEU:HD12	2.52	0.45
2:B:208:ILE:HA	2:B:211:ILE:HD12	1.98	0.45
2:B:93:VAL:HG11	2:B:97:TRP:HD1	1.80	0.45
13:M:96:LEU:C	13:M:110:ARG:HG2	2.37	0.45
18:R:19:LYS:HB2	18:R:19:LYS:HE3	1.72	0.45
1:A:1029:C:H2'	1:A:1030:C:C6	2.52	0.45
1:A:443:C:H42	1:A:491:G:H1	1.65	0.45
1:A:424:G:H2'	1:A:425:G:H8	1.81	0.45
16:P:40:ASP:HB3	16:P:48:TRP:HB2	1.97	0.45
19:S:62:ILE:HD12	19:S:66:MET:HG3	1.97	0.45
10:J:16:LEU:HD22	10:J:94:VAL:HG23	1.99	0.45
17:Q:13:ASP:HB2	17:Q:53:LEU:HD12	1.99	0.45
13:M:51:ALA:O	13:M:55:ARG:HG3	2.17	0.45
1:A:1213:A:N6	1:A:1215:G:N3	2.65	0.44
1:A:1305:G:OP2	21:U:2:GLY:N	2.50	0.44
1:A:489:C:H2'	1:A:490:G:C8	2.51	0.44
6:F:10:LEU:HD12	6:F:59:TYR:HB3	1.99	0.44
7:G:50:ILE:CG2	7:G:58:PRO:HB3	2.47	0.44
13:M:90:LEU:HD23	13:M:90:LEU:HA	1.86	0.44
20:T:89:ARG:HH21	20:T:104:LEU:HB3	1.82	0.44
1:A:1392:G:N2	1:A:1502:A:H8	2.14	0.44
1:A:518:C:H2'	1:A:530:G:N3	2.33	0.44
5:E:80:ILE:CD1	5:E:91:LEU:HB2	2.47	0.44
1:A:1371:G:O3'	9:I:69:GLY:HA3	2.17	0.44
9:I:93:ARG:HB3	9:I:93:ARG:NH1	2.33	0.44
1:A:974:A:OP1	14:N:31:ARG:HG2	2.16	0.44
1:A:1305:G:O2'	1:A:1306:A:OP2	2.24	0.44
3:C:150:LYS:HG3	3:C:169:ALA:HB2	2.00	0.44
3:C:33:LEU:HD21	14:N:53:LEU:HD22	2.00	0.44
12:L:82:VAL:O	12:L:106:ASP:HB2	2.17	0.44
1:A:750:G:N3	15:O:23:GLY:HA3	2.33	0.44
1:A:1366:C:H2'	1:A:1367:C:H6	1.82	0.44
1:A:580:U:H2'	1:A:581:G:O4'	2.18	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:180:ALA:HB3	3:C:203:PHE:HE1	1.83	0.44
4:D:142:PRO:HA	4:D:185:PHE:HD1	1.82	0.44
8:H:112:LEU:HD23	8:H:133:LEU:HA	1.99	0.44
1:A:1310:G:N7	19:S:2:PRO:HD3	2.32	0.44
1:A:1225:A:N3	1:A:1225:A:H2'	2.33	0.44
9:I:79:LEU:HD22	9:I:83:ARG:HG3	1.99	0.44
12:L:109:GLY:HA3	12:L:121:GLY:O	2.18	0.44
1:A:1128:C:H42	1:A:1143:G:H1	1.65	0.44
1:A:1069:C:O2'	1:A:1192:C:H1'	2.18	0.44
1:A:222:U:H2'	1:A:223:U:C6	2.53	0.44
1:A:669:U:H2'	1:A:670:G:C8	2.53	0.44
9:I:8:GLY:HA2	9:I:79:LEU:HD13	2.00	0.44
10:J:7:LYS:HE3	10:J:9:ARG:NH2	2.32	0.44
19:S:40:ILE:HB	19:S:67:VAL:O	2.18	0.44
1:A:1027:C:N4	1:A:1034:G:H1	2.15	0.44
3:C:110:ASN:O	3:C:141:VAL:HG22	2.17	0.44
6:F:39:LYS:HB2	6:F:39:LYS:HE3	1.73	0.44
15:O:64:ARG:NH2	15:O:68:ARG:HH21	2.15	0.44
19:S:41:VAL:HG23	19:S:43:GLU:HG2	1.99	0.44
1:A:1347:G:N2	1:A:1373:G:H2'	2.33	0.44
1:A:359:U:H2'	1:A:360:A:C8	2.52	0.44
2:B:18:GLY:HA3	2:B:41:ILE:HA	2.00	0.44
13:M:44:ARG:N	13:M:44:ARG:HD2	2.33	0.44
4:D:127:THR:HG23	4:D:130:GLY:H	1.82	0.44
8:H:121:ASP:OD1	8:H:121:ASP:N	2.51	0.44
1:A:1348:U:OP2	1:A:1373:G:N1	2.45	0.43
2:B:213:LEU:O	2:B:217:ARG:HG2	2.18	0.43
2:B:215:LEU:O	2:B:219:VAL:HG23	2.18	0.43
9:I:46:ALA:HB2	9:I:74:ILE:HG23	2.00	0.43
15:O:2:PRO:HB2	15:O:3:ILE:H	1.64	0.43
1:A:148:G:H2'	1:A:149:A:H8	1.83	0.43
1:A:1513:A:H2'	1:A:1514:C:C6	2.53	0.43
1:A:401:C:H2'	1:A:402:G:C8	2.52	0.43
1:A:936:C:H2'	1:A:937:A:O4'	2.17	0.43
1:A:946:A:H2'	1:A:947:G:C8	2.53	0.43
2:B:188:ALA:O	2:B:202:PRO:HA	2.18	0.43
13:M:70:LEU:HD23	13:M:70:LEU:HA	1.84	0.43
14:N:12:ARG:HG3	14:N:13:THR:H	1.83	0.43
14:N:26:ARG:NH1	14:N:43:CYS:SG	2.92	0.43
18:R:26:LEU:HA	18:R:26:LEU:HD12	1.79	0.43
1:A:1068:G:H8	1:A:1068:G:OP2	2.01	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1236:A:O2'	1:A:1304:G:H4'	2.17	0.43
1:A:298:A:H2'	1:A:299:G:O4'	2.18	0.43
1:A:687:A:H4'	1:A:688:G:O5'	2.18	0.43
2:B:93:VAL:HG11	2:B:97:TRP:CD1	2.54	0.43
1:A:1190:G:H5'	3:C:176:HIS:NE2	2.33	0.43
13:M:78:ILE:HD12	13:M:92:HIS:CE1	2.54	0.43
20:T:89:ARG:NH2	20:T:104:LEU:HB3	2.33	0.43
1:A:731:G:OP1	1:A:766:A:H1'	2.17	0.43
1:A:838:G:N2	1:A:849:C:C2	2.86	0.43
2:B:200:ILE:HG12	2:B:202:PRO:HD3	2.00	0.43
3:C:72:LYS:HE2	3:C:75:VAL:HG21	1.99	0.43
1:A:921:U:O2'	5:E:19:MET:O	2.20	0.43
5:E:28:PHE:O	5:E:47:LYS:HA	2.18	0.43
8:H:90:GLY:O	17:Q:34:LYS:HE2	2.17	0.43
1:A:1308:U:OP1	13:M:98:VAL:N	2.50	0.43
19:S:10:PHE:O	19:S:39:THR:OG1	2.36	0.43
1:A:15:G:H21	5:E:18:ARG:HA	1.84	0.43
1:A:983:A:H5'	1:A:984:C:OP2	2.18	0.43
6:F:76:ALA:O	6:F:80:ARG:HG3	2.18	0.43
13:M:101:GLN:OE1	13:M:101:GLN:N	2.51	0.43
15:O:18:PHE:CZ	15:O:21:ASP:HB2	2.54	0.43
1:A:115:G:H4'	1:A:116:A:O5'	2.18	0.43
1:A:1406:U:O2'	1:A:1517[B]:G:N2	2.51	0.43
1:A:488:C:H2'	1:A:489:C:C6	2.53	0.43
1:A:756:C:H2'	1:A:757:U:O4'	2.19	0.43
1:A:882:C:O2'	1:A:883:C:H5'	2.19	0.43
2:B:54:THR:O	2:B:58:ILE:HG13	2.19	0.43
4:D:200:GLU:O	4:D:203:VAL:N	2.51	0.43
7:G:65:ALA:O	7:G:69:VAL:HG23	2.19	0.43
8:H:95:VAL:HB	8:H:99:GLU:HB2	2.01	0.43
9:I:69:GLY:O	9:I:73:GLN:HG3	2.19	0.43
1:A:1301:U:O2'	1:A:1302:U:H3'	2.19	0.43
1:A:1343:G:H2'	1:A:1344:C:C6	2.54	0.43
1:A:148:G:H2'	1:A:149:A:C8	2.54	0.43
11:K:69:ALA:O	11:K:73:MET:HG2	2.19	0.43
13:M:15:VAL:HG21	13:M:48:LEU:HD21	2.01	0.43
13:M:57:ARG:HG2	13:M:61:GLU:HG3	2.01	0.43
14:N:24:CYS:H	14:N:33:VAL:HG21	1.83	0.43
16:P:4:ILE:HG12	16:P:21:VAL:HG22	2.01	0.43
16:P:70:ALA:O	16:P:74:LEU:HG	2.19	0.43
18:R:74:ARG:HB3	18:R:81:PHE:CE1	2.54	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1512:U:H2'	1:A:1513:A:C8	2.53	0.43
1:A:701:C:H4'	1:A:702:A:O5'	2.19	0.43
10:J:15:THR:HG22	10:J:94:VAL:HB	2.01	0.43
12:L:110:VAL:CG2	12:L:120:TYR:HB3	2.49	0.43
13:M:63:THR:HG23	13:M:64:TRP:CD2	2.54	0.43
18:R:87:ARG:HD2	18:R:87:ARG:HA	1.83	0.43
1:A:620:C:H2'	1:A:621:A:O4'	2.19	0.43
1:A:872:A:H4'	1:A:873:A:OP1	2.19	0.43
5:E:17:ALA:HB2	5:E:26:PHE:HD2	1.83	0.43
8:H:103:VAL:HG21	8:H:110:ALA:HB2	2.01	0.43
12:L:88:GLY:O	12:L:99:HIS:ND1	2.43	0.43
15:O:29:VAL:HG13	15:O:63:ARG:HG3	2.00	0.43
1:A:954:G:H2'	1:A:955:U:O4'	2.18	0.42
3:C:150:LYS:HB3	3:C:201:TYR:HB2	2.01	0.42
1:A:1116:C:O2'	9:I:108:VAL:HG21	2.19	0.42
16:P:45:THR:O	16:P:48:TRP:HD1	2.01	0.42
1:A:1020:U:H2'	1:A:1021:G:C8	2.52	0.42
1:A:1125:U:H3	10:J:5:ARG:NH2	2.17	0.42
1:A:1255:G:C6	1:A:1279:A:N7	2.87	0.42
2:B:172:ILE:H	2:B:172:ILE:HG13	1.44	0.42
3:C:119:ARG:HH21	3:C:123:GLN:HE21	1.66	0.42
10:J:82:ILE:HA	10:J:85:LEU:HB2	2.00	0.42
15:O:17:ARG:HD3	15:O:26:GLU:OE2	2.20	0.42
1:A:116:A:H2'	1:A:117:G:C8	2.54	0.42
1:A:1419:G:H2'	1:A:1420:C:C6	2.54	0.42
1:A:522:C:H41	12:L:53:ARG:NH2	2.16	0.42
1:A:812:C:H6	1:A:812:C:H2'	1.67	0.42
1:A:922:G:H2'	1:A:923:A:C8	2.54	0.42
4:D:101:LEU:O	4:D:105:VAL:HG23	2.19	0.42
4:D:64:LEU:HD23	4:D:198:VAL:HG21	2.00	0.42
1:A:542:G:H5'	4:D:41:GLY:HA3	2.01	0.42
1:A:1327:C:OP2	21:U:12:LYS:NZ	2.52	0.42
1:A:1402:4OC:HM22	1:A:1403:C:H5'	2.01	0.42
1:A:1495:U:O4	25:A:1809:EUS:N12	2.52	0.42
1:A:384:G:H2'	1:A:385:C:C6	2.54	0.42
10:J:66:ARG:HD3	10:J:68:HIS:CE1	2.55	0.42
11:K:84:VAL:CG1	11:K:91:ARG:HD3	2.48	0.42
12:L:58:VAL:HG12	12:L:60:LEU:HD22	2.01	0.42
1:A:1095:U:H2'	1:A:1096:C:O4'	2.19	0.42
1:A:1182:G:H8	1:A:1182:G:H2'	1.77	0.42
1:A:185:A:N3	20:T:81:LYS:NZ	2.63	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:455:C:H42	1:A:477:G:H1	1.66	0.42
3:C:64:VAL:HB	3:C:99:VAL:HB	2.01	0.42
13:M:62:ASN:OD1	13:M:62:ASN:N	2.51	0.42
3:C:9:GLY:HA3	14:N:49:HIS:HA	2.01	0.42
19:S:31:ILE:HG22	19:S:49:ILE:HG23	2.01	0.42
1:A:1163:C:H2'	1:A:1164:G:C8	2.54	0.42
2:B:30:ARG:HD2	2:B:31:TYR:CZ	2.55	0.42
3:C:112:SER:O	3:C:116:VAL:HG23	2.20	0.42
3:C:148:GLY:HA3	3:C:172:ARG:O	2.19	0.42
9:I:32:ASP:OD1	9:I:33:PHE:N	2.52	0.42
9:I:4:TYR:CE2	9:I:88:TYR:HD1	2.37	0.42
12:L:42:THR:HA	12:L:53:ARG:O	2.19	0.42
1:A:1136:U:H5"	1:A:1137:C:OP2	2.19	0.42
1:A:1328:C:H2'	1:A:1329:A:H8	1.85	0.42
1:A:166:G:H2'	1:A:167:G:H8	1.84	0.42
1:A:113:G:C1'	1:A:354:G:H5'	2.46	0.42
1:A:397:A:N3	1:A:397:A:H3'	2.33	0.42
1:A:533:A:N6	1:A:536:C:C2	2.87	0.42
8:H:104:ARG:HG3	8:H:138:TRP:CG	2.54	0.42
1:A:232:G:H1'	1:A:262:A:N1	2.35	0.42
3:C:11:ARG:HG2	3:C:178:LEU:CD2	2.50	0.42
7:G:94:ARG:O	7:G:97:GLN:HB3	2.20	0.42
12:L:58:VAL:O	12:L:65:GLU:HA	2.19	0.42
1:A:118:U:H3'	1:A:288:A:H61	1.85	0.42
1:A:1453:G:H2'	1:A:1454:G:O4'	2.20	0.42
12:L:113:ARG:HH11	12:L:116:SER:H	1.66	0.42
1:A:1145:C:HO2'	1:A:1146:A:P	2.41	0.42
1:A:1213:A:N1	1:A:1215:G:H1'	2.35	0.42
1:A:130:A:OP2	1:A:190(E):U:O2'	2.25	0.42
1:A:186:C:H2'	1:A:187:C:C6	2.55	0.42
1:A:560:U:H5'	1:A:566:G:N2	2.34	0.42
1:A:737:A:H2'	1:A:738:C:C6	2.55	0.42
7:G:15:ASP:OD1	7:G:44:TYR:OH	2.38	0.42
10:J:81:THR:O	10:J:85:LEU:HD23	2.20	0.42
11:K:61:ALA:HB1	11:K:94:ALA:HB2	2.02	0.42
19:S:63:THR:HG22	19:S:64:GLU:H	1.85	0.42
1:A:1057:G:H2'	1:A:1058:G:O4'	2.20	0.41
1:A:1468:A:H2'	1:A:1469:G:O4'	2.20	0.41
1:A:181:G:H4'	1:A:182:U:H5'	2.02	0.41
1:A:109:A:C6	1:A:326:G:C6	3.08	0.41
1:A:836:G:C6	1:A:851:G:C6	3.08	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:671:G:H5'	6:F:77:ARG:HH21	1.85	0.41
20:T:29:LYS:O	20:T:33:ILE:HG12	2.19	0.41
1:A:1296:C:H4'	1:A:1302:U:C5	2.56	0.41
1:A:1418:A:N6	1:A:1482:G:H1'	2.35	0.41
1:A:244:U:H4'	1:A:245:C:H5"	2.02	0.41
1:A:262:A:C6	1:A:263:A:C6	3.08	0.41
2:B:58:ILE:O	2:B:62:ALA:N	2.45	0.41
1:A:490:G:P	4:D:132:ARG:HH22	2.42	0.41
4:D:78:LEU:HD22	4:D:96:LEU:HB3	2.01	0.41
7:G:77:SER:HA	7:G:85:TYR:O	2.20	0.41
12:L:60:LEU:HD21	12:L:85:ILE:HD12	2.02	0.41
17:Q:55:ASP:HB3	17:Q:76:LEU:HD21	2.02	0.41
19:S:36:ARG:H	19:S:36:ARG:HG2	1.62	0.41
1:A:484:G:H5'	1:A:486:U:O4'	2.21	0.41
10:J:48:THR:O	14:N:34:TYR:OH	2.38	0.41
16:P:9:PHE:CD2	16:P:18:ARG:HD2	2.55	0.41
1:A:1007:C:C2	1:A:1023:G:N1	2.88	0.41
1:A:1396:A:H2	5:E:19:MET:HG2	1.85	0.41
1:A:769:G:H4'	1:A:1513:A:H4'	2.02	0.41
2:B:133:LYS:O	2:B:137:ARG:HG3	2.20	0.41
2:B:215:LEU:HD23	2:B:215:LEU:HA	1.75	0.41
6:F:70:ASP:N	6:F:70:ASP:OD1	2.53	0.41
8:H:31:PHE:O	8:H:35:ILE:HG12	2.21	0.41
12:L:27:LEU:HG	12:L:28:LYS:H	1.85	0.41
1:A:1007:C:O2	1:A:1023:G:N1	2.54	0.41
1:A:1163:C:H2'	1:A:1164:G:H8	1.86	0.41
1:A:1352:C:H2'	1:A:1353:G:C8	2.56	0.41
1:A:153:C:N4	1:A:168:G:H1	2.19	0.41
1:A:567:G:H2'	1:A:568:G:O4'	2.20	0.41
1:A:960:U:H1'	1:A:1223:C:H5'	2.01	0.41
10:J:90:LEU:N	10:J:91:PRO:HD2	2.35	0.41
1:A:376:G:H5"	16:P:5:ARG:HB2	2.02	0.41
1:A:421:U:OP2	1:A:422:C:N4	2.54	0.41
4:D:21:LEU:HD21	4:D:66:ARG:O	2.20	0.41
13:M:44:ARG:HB2	13:M:47:ASP:OD2	2.21	0.41
1:A:690:G:C6	1:A:691:G:C6	3.09	0.41
3:C:11:ARG:NH1	3:C:178:LEU:HA	2.36	0.41
13:M:79:LYS:O	13:M:83:ASP:N	2.46	0.41
1:A:1168:A:C6	1:A:1169:A:C6	3.09	0.41
1:A:923:A:O2'	1:A:1399:C:OP2	2.29	0.41
1:A:539:A:N6	1:A:540:G:O6	2.53	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:625:G:H2'	1:A:626:U:C6	2.56	0.41
1:A:707:C:H2'	1:A:708:C:H6	1.84	0.41
8:H:64:LYS:HG3	8:H:79:VAL:HG21	2.03	0.41
1:A:1147:C:O2	9:I:16:ARG:NH1	2.54	0.41
21:U:5:ASP:O	21:U:11:GLY:HA3	2.21	0.41
1:A:1425:U:H2'	1:A:1426:C:H6	1.85	0.41
1:A:956:U:H2'	1:A:957:U:O4'	2.20	0.41
2:B:42:ILE:HD12	2:B:203:GLY:HA2	2.03	0.41
4:D:173:TRP:HB2	4:D:187:ARG:O	2.20	0.41
11:K:29:ILE:HB	11:K:44:SER:HB2	2.03	0.41
13:M:66:LEU:O	13:M:70:LEU:HB2	2.21	0.41
15:O:3:ILE:HG12	15:O:34:LEU:HD21	2.01	0.41
1:A:1318:A:O2'	19:S:37:ARG:HB3	2.21	0.41
1:A:828:A:H4'	1:A:828:A:OP1	2.21	0.41
8:H:20:TYR:HE2	8:H:75:ARG:HD2	1.86	0.41
11:K:122:LYS:HE3	11:K:122:LYS:HB2	1.90	0.41
11:K:40:ILE:HG22	11:K:41:THR:HG23	2.02	0.41
1:A:1133:G:H2'	1:A:1134:G:H8	1.85	0.41
1:A:1499:A:C1'	1:A:1520[A]:G:H5'	2.49	0.41
1:A:145:G:H1	1:A:177:C:H42	1.69	0.41
1:A:88:A:H2'	1:A:89:C:O4'	2.21	0.41
5:E:79:GLU:O	8:H:104:ARG:NH1	2.54	0.41
8:H:117:GLY:O	8:H:119:LEU:HG	2.21	0.41
13:M:81:LEU:HA	13:M:84:ILE:HG12	2.02	0.41
14:N:9:LYS:HE2	14:N:21:TYR:O	2.21	0.41
14:N:9:LYS:HD2	14:N:23:ARG:HB2	2.02	0.41
3:C:13:GLY:HA3	14:N:57:ARG:HH21	1.85	0.41
20:T:54:LYS:HA	20:T:57:ARG:HH11	1.86	0.41
23:W:28:G:H2'	23:W:28:G:N3	2.35	0.41
1:A:1198:G:H2'	1:A:1199:U:C6	2.56	0.40
1:A:1257:U:O2'	1:A:1258:G:P	2.80	0.40
1:A:1391:U:H2'	1:A:1392:G:H8	1.82	0.40
1:A:1442:G:N1	1:A:1446:A:N7	2.69	0.40
1:A:389:A:C6	1:A:390:C:H1'	2.56	0.40
1:A:920:U:H2'	1:A:921:U:C6	2.56	0.40
2:B:21:ARG:NH1	2:B:22:LYS:HB3	2.37	0.40
5:E:13:ILE:HA	5:E:29:GLY:O	2.21	0.40
14:N:37:PHE:CE2	14:N:53:LEU:HD13	2.56	0.40
19:S:25:LYS:N	19:S:25:LYS:HD2	2.36	0.40
1:A:299:G:C6	1:A:300:A:C6	3.10	0.40
1:A:743:U:H2'	1:A:744:C:C6	2.57	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:943:U:H1'	9:I:124:GLN:HE22	1.87	0.40
4:D:128:VAL:HG12	4:D:129:ASN:HD22	1.86	0.40
4:D:152:SER:O	4:D:158:ILE:HD12	2.21	0.40
5:E:118:ILE:HG12	5:E:119:LEU:N	2.36	0.40
7:G:16:LEU:H	7:G:16:LEU:HD22	1.85	0.40
1:A:865:A:H5'	1:A:1078:U:O4	2.21	0.40
1:A:181:G:H4'	1:A:182:U:C5'	2.52	0.40
1:A:977:A:H2'	1:A:978:A:H5"	2.03	0.40
5:E:76:ILE:HG21	5:E:76:ILE:HD13	1.82	0.40
5:E:92:LYS:HA	5:E:93:PRO:HD3	1.92	0.40
20:T:81:LYS:HE2	20:T:81:LYS:HB3	1.90	0.40
1:A:1011:G:H2'	1:A:1012:U:O4'	2.21	0.40
1:A:1328:C:H2'	1:A:1329:A:C8	2.56	0.40
1:A:1342:C:H2'	1:A:1343:G:C8	2.57	0.40
1:A:893:C:H2'	1:A:894:G:C8	2.56	0.40
2:B:88:ALA:HB2	2:B:219:VAL:HG13	2.02	0.40
1:A:1191:A:OP1	3:C:4:LYS:HE3	2.22	0.40
5:E:76:ILE:HD11	5:E:118:ILE:HD11	2.03	0.40
6:F:9:VAL:HA	6:F:59:TYR:O	2.21	0.40
7:G:23:VAL:HG13	7:G:43:PHE:CE2	2.56	0.40
13:M:3:ARG:HA	13:M:8:GLU:O	2.21	0.40
1:A:1060:C:H2'	1:A:1061:G:C8	2.56	0.40
1:A:1358:U:H5"	14:N:35:ARG:HG3	2.03	0.40
1:A:1399:C:C2	1:A:1502:A:N6	2.90	0.40
2:B:142:LEU:HD23	2:B:142:LEU:HA	1.91	0.40
13:M:4:ILE:O	13:M:57:ARG:HG3	2.21	0.40
13:M:65:LYS:H	13:M:65:LYS:HG2	1.68	0.40
16:P:21:VAL:HG12	16:P:33:ILE:HD12	2.04	0.40
19:S:7:LYS:HE3	19:S:7:LYS:HB3	1.75	0.40
1:A:325:A:OP2	20:T:70:SER:HB2	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	232/234 (99%)	217 (94%)	15 (6%)	0	100	100
3	C	204/206 (99%)	185 (91%)	19 (9%)	0	100	100
4	D	206/208 (99%)	199 (97%)	7 (3%)	0	100	100
5	E	148/150 (99%)	143 (97%)	5 (3%)	0	100	100
6	F	99/101 (98%)	96 (97%)	3 (3%)	0	100	100
7	G	153/155 (99%)	145 (95%)	8 (5%)	0	100	100
8	H	136/138 (99%)	128 (94%)	6 (4%)	2 (2%)	10	36
9	I	125/127 (98%)	113 (90%)	12 (10%)	0	100	100
10	J	96/98 (98%)	81 (84%)	12 (12%)	3 (3%)	4	23
11	K	114/116 (98%)	108 (95%)	6 (5%)	0	100	100
12	L	121/124 (98%)	112 (93%)	9 (7%)	0	100	100
13	M	116/118 (98%)	99 (85%)	16 (14%)	1 (1%)	17	49
14	N	58/60 (97%)	50 (86%)	8 (14%)	0	100	100
15	O	85/87 (98%)	83 (98%)	2 (2%)	0	100	100
16	P	81/83 (98%)	77 (95%)	4 (5%)	0	100	100
17	Q	97/99 (98%)	94 (97%)	3 (3%)	0	100	100
18	R	68/70 (97%)	64 (94%)	4 (6%)	0	100	100
19	S	78/80 (98%)	74 (95%)	4 (5%)	0	100	100
20	T	97/99 (98%)	86 (89%)	10 (10%)	1 (1%)	15	46
21	U	22/24 (92%)	21 (96%)	1 (4%)	0	100	100
All	All	2336/2377 (98%)	2175 (93%)	154 (7%)	7 (0%)	41	72

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
10	J	55	LYS
10	J	56	HIS
8	H	71	GLY
10	J	54	PHE
13	M	113	PRO
8	H	72	PRO
20	T	73	HIS

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	B	202/202 (100%)	175 (87%)	27 (13%)	4 15
3	C	160/160 (100%)	141 (88%)	19 (12%)	5 19
4	D	180/180 (100%)	166 (92%)	14 (8%)	12 39
5	E	115/115 (100%)	97 (84%)	18 (16%)	2 10
6	F	90/90 (100%)	87 (97%)	3 (3%)	38 66
7	G	126/126 (100%)	117 (93%)	9 (7%)	14 44
8	H	119/119 (100%)	107 (90%)	12 (10%)	7 27
9	I	98/98 (100%)	88 (90%)	10 (10%)	7 26
10	J	87/88 (99%)	74 (85%)	13 (15%)	3 12
11	K	88/88 (100%)	83 (94%)	5 (6%)	20 50
12	L	103/103 (100%)	89 (86%)	14 (14%)	3 14
13	M	94/94 (100%)	82 (87%)	12 (13%)	4 16
14	N	49/49 (100%)	46 (94%)	3 (6%)	18 48
15	O	79/79 (100%)	67 (85%)	12 (15%)	3 11
16	P	72/72 (100%)	67 (93%)	5 (7%)	15 45
17	Q	94/94 (100%)	86 (92%)	8 (8%)	10 35
18	R	61/61 (100%)	56 (92%)	5 (8%)	11 37
19	S	71/71 (100%)	62 (87%)	9 (13%)	4 16
20	T	76/76 (100%)	64 (84%)	12 (16%)	2 10
21	U	19/19 (100%)	17 (90%)	2 (10%)	7 25
All	All	1983/1984 (100%)	1771 (89%)	212 (11%)	6 24

All (212) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	7	VAL
2	B	8	LYS
2	B	10	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	11	LEU
2	B	21	ARG
2	B	24	TRP
2	B	33	TYR
2	B	44	LEU
2	B	51	LEU
2	B	67	THR
2	B	69	LEU
2	B	73	THR
2	B	87	ARG
2	B	102	LEU
2	B	103	THR
2	B	122	PHE
2	B	127	ILE
2	B	144	ARG
2	B	153	ARG
2	B	154	LEU
2	B	157	ARG
2	B	162	ILE
2	B	165	VAL
2	B	172	ILE
2	B	178	ARG
2	B	200	ILE
2	B	206	ASP
3	C	3	ASN
3	C	26	LYS
3	C	34	LEU
3	C	79	ARG
3	C	85	ARG
3	C	90	GLU
3	C	91	LEU
3	C	94	LEU
3	C	95	THR
3	C	99	VAL
3	C	111	LEU
3	C	131	ARG
3	C	144	SER
3	C	162	GLN
3	C	165	THR
3	C	166	GLU
3	C	167	TRP
3	C	177	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	C	204	LEU
4	D	10	ARG
4	D	25	ARG
4	D	34	GLU
4	D	35	ARG
4	D	36	ARG
4	D	47	ARG
4	D	49	ARG
4	D	64	LEU
4	D	83	SER
4	D	122	ARG
4	D	127	THR
4	D	150	GLU
4	D	155	LEU
4	D	202	LEU
5	E	6	PHE
5	E	10	MET
5	E	12	LEU
5	E	16	THR
5	E	18	ARG
5	E	20	GLN
5	E	25	ARG
5	E	26	PHE
5	E	31	LEU
5	E	41	VAL
5	E	64	ARG
5	E	79	GLU
5	E	80	ILE
5	E	116	THR
5	E	120	THR
5	E	147	ASP
5	E	148	VAL
5	E	150	ARG
6	F	10	LEU
6	F	24	GLU
6	F	82	ARG
7	G	8	GLU
7	G	11	GLN
7	G	45	ASP
7	G	75	VAL
7	G	79	ARG
7	G	84	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
7	G	113	GLU
7	G	136	LYS
7	G	149	ARG
8	H	3	THR
8	H	24	THR
8	H	26	VAL
8	H	29	SER
8	H	35	ILE
8	H	63	LEU
8	H	83	ILE
8	H	85	ARG
8	H	91	ARG
8	H	92	ARG
8	H	98	LYS
8	H	126	LYS
9	I	12	GLU
9	I	20	ARG
9	I	44	VAL
9	I	79	LEU
9	I	102	LEU
9	I	104	ARG
9	I	108	VAL
9	I	118	LYS
9	I	121	ARG
9	I	124	GLN
10	J	3	LYS
10	J	30	SER
10	J	38	ILE
10	J	45	ARG
10	J	51	ARG
10	J	55	LYS
10	J	60	ARG
10	J	61	GLU
10	J	62	HIS
10	J	65	LEU
10	J	78	ASN
10	J	89	ASP
10	J	95	GLU
11	K	12	ARG
11	K	29	ILE
11	K	92	GLU
11	K	114	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
11	K	119	CYS
12	L	18	VAL
12	L	20	LYS
12	L	28	LYS
12	L	33	ARG
12	L	42	THR
12	L	43	VAL
12	L	44	THR
12	L	60	LEU
12	L	67	THR
12	L	80	HIS
12	L	85	ILE
12	L	89	ARG
12	L	113	ARG
12	L	122	THR
13	M	12	ASN
13	M	17	VAL
13	M	37	THR
13	M	44	ARG
13	M	48	LEU
13	M	50	GLU
13	M	81	LEU
13	M	105	THR
13	M	108	ARG
13	M	110	ARG
13	M	115	LYS
13	M	117	VAL
14	N	11	LYS
14	N	22	THR
14	N	24	CYS
15	O	5	LYS
15	O	8	LYS
15	O	21	ASP
15	O	32	LEU
15	O	36	ILE
15	O	39	LEU
15	O	56	LEU
15	O	65	ARG
15	O	70	LEU
15	O	71	GLN
15	O	81	LEU
15	O	83	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
16	P	2	VAL
16	P	29	ASP
16	P	53	VAL
16	P	55	ARG
16	P	62	VAL
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	91	ARG
17	Q	98	LEU
18	R	19	LYS
18	R	37	VAL
18	R	42	ARG
18	R	84	LYS
18	R	87	ARG
19	S	6	LYS
19	S	13	ASP
19	S	15	LEU
19	S	29	ARG
19	S	31	ILE
19	S	39	THR
19	S	56	GLN
19	S	62	ILE
19	S	63	THR
20	T	9	ASN
20	T	53	LEU
20	T	56	MET
20	T	57	ARG
20	T	62	LEU
20	T	68	LYS
20	T	73	HIS
20	T	75	ASN
20	T	84	LEU
20	T	91	LEU
20	T	92	LEU
20	T	93	GLU
21	U	6	ARG
21	U	25	LYS

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	16	HIS
2	B	204	ASN
3	C	123	GLN
13	M	12	ASN

5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	1504/1522 (98%)	246 (16%)	45 (2%)
22	Y	5/6 (83%)	3 (60%)	0
23	W	14/15 (93%)	4 (28%)	0
All	All	1523/1543 (98%)	253 (16%)	45 (2%)

All (253) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	6	G
1	A	7	G
1	A	9	G
1	A	10	A
1	A	32	A
1	A	39	G
1	A	47	C
1	A	48	C
1	A	51	A
1	A	101	A
1	A	108	G
1	A	116	A
1	A	117	G
1	A	121	C
1	A	129(A)	G
1	A	130	A
1	A	131	C
1	A	163	C
1	A	182	U
1	A	183	G
1	A	190(E)	U
1	A	195	A
1	A	201	C
1	A	202	U
1	A	203	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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	281	G
1	A	282	A
1	A	289	G
1	A	301	G
1	A	321	A
1	A	328	C
1	A	329	A
1	A	332	G
1	A	344	A
1	A	345	C
1	A	350	G
1	A	351	G
1	A	352	C
1	A	353	A
1	A	354	G
1	A	356	A
1	A	367	U
1	A	371	G
1	A	373	A
1	A	374	A
1	A	384	G
1	A	390	C
1	A	397	A
1	A	398	C
1	A	406	G
1	A	409	G
1	A	412	A
1	A	413	G
1	A	421	U
1	A	424	G
1	A	429	U
1	A	430	A
1	A	439	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	460	A
1	A	461	C
1	A	481	G
1	A	484	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	531	U
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
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	607	A
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	698	G
1	A	701	C
1	A	702	A
1	A	703	G
1	A	721	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	723	U
1	A	731	G
1	A	749	C
1	A	755	G
1	A	760	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	813	U
1	A	815	A
1	A	817	C
1	A	828	A
1	A	839	U
1	A	840	C
1	A	841	U
1	A	848	C
1	A	873	A
1	A	876	G
1	A	902	G
1	A	914	A
1	A	916	G
1	A	919	A
1	A	922	G
1	A	926	G
1	A	927	G
1	A	934	C
1	A	935	A
1	A	960	U
1	A	961	U
1	A	966	M2G
1	A	969	A
1	A	971	G
1	A	972	C
1	A	974	A
1	A	975	A
1	A	976	G
1	A	977	A
1	A	984	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	991	U
1	A	992	U
1	A	993	G
1	A	1003(A)	G
1	A	1004	A
1	A	1005	A
1	A	1023	G
1	A	1024	G
1	A	1026	G
1	A	1031	G
1	A	1045	C
1	A	1050	G
1	A	1051	C
1	A	1053	G
1	A	1054	C
1	A	1055	A
1	A	1065	U
1	A	1066	C
1	A	1068	G
1	A	1078	U
1	A	1094	G
1	A	1095	U
1	A	1096	C
1	A	1101	A
1	A	1124	G
1	A	1125	U
1	A	1126	U
1	A	1127	G
1	A	1129	C
1	A	1130	A
1	A	1137	C
1	A	1139	G
1	A	1146	A
1	A	1152	A
1	A	1159	U
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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	1202	G
1	A	1211	U
1	A	1212	U
1	A	1214	C
1	A	1224	G
1	A	1225	A
1	A	1228	C
1	A	1238	A
1	A	1256	A
1	A	1257	U
1	A	1258	G
1	A	1270	C
1	A	1278	U
1	A	1280	A
1	A	1281	U
1	A	1286	A
1	A	1287	A
1	A	1300	G
1	A	1301	U
1	A	1302	U
1	A	1306	A
1	A	1312	G
1	A	1320	C
1	A	1322	C
1	A	1323	G
1	A	1336	C
1	A	1338	G
1	A	1346	A
1	A	1347	G
1	A	1348	U
1	A	1353	G
1	A	1359	C
1	A	1362	C
1	A	1363	A
1	A	1368	G
1	A	1370	G
1	A	1379	G
1	A	1381	U
1	A	1397	C
1	A	1398	A
1	A	1442	G
1	A	1446	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	1447	G
1	A	1478	C
1	A	1485	U
1	A	1487	G
1	A	1492	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
22	Y	3	U
22	Y	5	U
22	Y	6	U
23	W	30	G
23	W	33	U
23	W	36	A
23	W	42	C

All (45) 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	429	U
1	A	484	G
1	A	485	G
1	A	496	A
1	A	509	A
1	A	518	C
1	A	559	A
1	A	687	A
1	A	701	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	748	C
1	A	792	A
1	A	812	C
1	A	913	A
1	A	960	U
1	A	965	A
1	A	991	U
1	A	992	U
1	A	1049	U
1	A	1065	U
1	A	1067	A
1	A	1145	C
1	A	1182	G
1	A	1190	G
1	A	1201	A
1	A	1256	A
1	A	1257	U
1	A	1285	A
1	A	1300	G
1	A	1301	U
1	A	1305	G
1	A	1346	A
1	A	1347	G
1	A	1380	U
1	A	1505	G

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
1	5MC	A	1404	1	15,22,23	0.84	0	19,32,35	1.11	3 (15%)
1	5MC	A	1407	1	15,22,23	0.95	0	19,32,35	1.01	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
1	G7M	A	527	1,24	20,26,27	1.69	4 (20%)	20,39,42	1.94	7 (35%)
1	5MC	A	967	1	15,22,23	1.09	2 (13%)	19,32,35	1.06	2 (10%)
1	4OC	A	1402	1,24	16,23,24	0.83	0	17,32,35	0.72	0
1	2MG	A	1207	1	19,26,27	2.18	4 (21%)	21,38,41	2.08	3 (14%)
1	UR3	A	1498	1	14,22,23	0.72	0	15,32,35	1.21	1 (6%)
1	MA6	A	1518[A]	1	19,26,27	0.77	0	18,38,41	0.67	0
1	PSU	A	516	1,24	17,21,22	1.01	2 (11%)	20,30,33	3.17	6 (30%)
1	M2G	A	966	1	20,27,28	1.96	4 (20%)	22,40,43	2.53	5 (22%)
1	MA6	A	1518[B]	1	19,26,27	1.26	2 (10%)	18,38,41	0.73	0
1	MA6	A	1519[B]	1	19,26,27	1.24	3 (15%)	18,38,41	0.59	0
12	0TD	L	92	12	4,9,10	0.89	0	3,11,13	1.64	1 (33%)
1	PSU	A	1540	1	17,21,22	0.99	1 (5%)	20,30,33	3.19	6 (30%)
1	PSU	A	1541	1,24	17,21,22	1.02	2 (11%)	20,30,33	3.16	6 (30%)
1	5MC	A	1400	1	15,22,23	0.76	0	19,32,35	1.17	3 (15%)
1	MA6	A	1519[A]	1	19,26,27	0.75	0	18,38,41	0.82	0

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	5MC	A	1404	1	-	0/5/25/26	0/2/2/2
1	5MC	A	1407	1	-	0/5/25/26	0/2/2/2
1	G7M	A	527	1,24	-	1/3/25/26	0/3/3/3
1	5MC	A	967	1	-	0/5/25/26	0/2/2/2
1	4OC	A	1402	1,24	-	2/9/29/30	0/2/2/2
1	2MG	A	1207	1	-	0/5/27/28	0/3/3/3
1	UR3	A	1498	1	-	0/5/25/26	0/2/2/2
1	MA6	A	1518[A]	1	-	2/7/29/30	0/3/3/3
1	PSU	A	516	1,24	-	0/7/25/26	0/2/2/2
1	M2G	A	966	1	-	2/7/29/30	0/3/3/3
1	MA6	A	1518[B]	1	-	2/7/29/30	0/3/3/3
1	MA6	A	1519[B]	1	-	3/7/29/30	0/3/3/3
12	0TD	L	92	12	-	1/3/12/14	-
1	PSU	A	1540	1	-	0/7/25/26	0/2/2/2
1	PSU	A	1541	1,24	-	0/7/25/26	0/2/2/2
1	5MC	A	1400	1	-	2/5/25/26	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	MA6	A	1519[A]	1	-	3/7/29/30	0/3/3/3

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1207	2MG	C2-N2	6.68	1.39	1.34
1	A	966	M2G	C6-N1	6.17	1.43	1.33
1	A	1207	2MG	C6-N1	5.68	1.42	1.33
1	A	527	G7M	C2-N2	5.01	1.43	1.33
1	A	966	M2G	C2-N1	3.95	1.41	1.34
1	A	1518[B]	MA6	C6-N1	3.62	1.38	1.33
1	A	1519[B]	MA6	C6-N1	3.43	1.38	1.33
1	A	1541	PSU	C4-N3	3.18	1.38	1.33
1	A	966	M2G	C2-N2	3.14	1.40	1.34
1	A	1540	PSU	C4-N3	3.12	1.38	1.33
1	A	527	G7M	C6-N1	3.02	1.38	1.33
1	A	516	PSU	C4-N3	2.98	1.38	1.33
1	A	966	M2G	C4-N3	2.92	1.40	1.35
1	A	527	G7M	C4-N3	2.68	1.39	1.35
1	A	967	5MC	C5-C4	2.43	1.45	1.41
1	A	1519[B]	MA6	C2-N1	2.33	1.38	1.33
1	A	1518[B]	MA6	C2-N1	2.18	1.38	1.33
1	A	1207	2MG	C4-N3	2.17	1.39	1.35
1	A	1207	2MG	C2-N1	2.16	1.41	1.34
1	A	967	5MC	C4-N4	2.16	1.39	1.34
1	A	1541	PSU	O4'-C1'	-2.15	1.41	1.44
1	A	1519[B]	MA6	C2-N3	2.11	1.35	1.32
1	A	516	PSU	O4'-C1'	-2.11	1.41	1.44
1	A	527	G7M	C6-C5	2.11	1.45	1.41

All (44) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	516	PSU	N1-C2-N3	-11.09	119.61	128.43
1	A	1541	PSU	N1-C2-N3	-11.05	119.64	128.43
1	A	1540	PSU	N1-C2-N3	-10.94	119.74	128.43
1	A	966	M2G	C5-C6-N1	-8.73	111.49	123.43
1	A	1207	2MG	C5-C6-N1	-7.73	112.86	123.43
1	A	966	M2G	C6-N1-C2	6.05	123.39	116.18
1	A	1540	PSU	C4-N3-C2	6.00	120.20	115.14
1	A	516	PSU	C4-N3-C2	5.85	120.08	115.14
1	A	1541	PSU	C4-N3-C2	5.75	119.99	115.14

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	527	G7M	C2-N3-C4	4.30	120.27	115.36
1	A	1540	PSU	C5-C4-N3	-4.15	120.01	125.36
1	A	527	G7M	C6-C5-C4	-3.99	116.99	120.80
1	A	1541	PSU	C5-C4-N3	-3.97	120.25	125.36
1	A	516	PSU	C5-C4-N3	-3.95	120.27	125.36
1	A	1207	2MG	C6-N1-C2	3.89	122.14	115.18
1	A	527	G7M	N3-C2-N1	-3.71	122.28	127.22
1	A	1541	PSU	C6-N1-C2	3.22	120.67	115.36
1	A	516	PSU	C6-N1-C2	3.21	120.66	115.36
1	A	516	PSU	C5-C6-N1	-3.13	120.59	124.44
1	A	1540	PSU	C6-N1-C2	3.10	120.47	115.36
1	A	527	G7M	C5-C6-N1	-3.01	119.31	123.43
1	A	1541	PSU	C5-C6-N1	-2.81	120.99	124.44
1	A	1540	PSU	C5-C6-N1	-2.77	121.03	124.44
1	A	527	G7M	C6-N1-C2	2.64	120.13	115.93
1	A	966	M2G	C2-N3-C4	-2.38	112.57	115.28
1	A	966	M2G	N3-C2-N2	2.36	119.58	117.18
1	A	1207	2MG	C4-C5-N7	2.29	111.78	109.40
1	A	1400	5MC	C2-N3-C4	2.28	118.77	116.02
1	A	1498	UR3	C3'-C2'-C1'	2.27	104.39	100.98
1	A	1400	5MC	CM5-C5-C6	2.27	123.47	118.68
1	A	1540	PSU	C5-C1'-C2'	-2.26	111.29	115.32
1	A	1407	5MC	C2-N3-C4	2.25	118.74	116.02
1	A	527	G7M	C1'-N9-C4	-2.24	122.70	126.64
1	A	1400	5MC	CM5-C5-C4	-2.23	119.47	121.72
1	A	966	M2G	N1-C2-N2	-2.22	114.95	117.19
1	A	516	PSU	O4'-C1'-C2'	2.19	108.20	104.66
12	L	92	0TD	CSB-SB-CB	-2.16	97.60	101.85
1	A	527	G7M	N2-C2-N1	2.14	120.57	117.25
1	A	967	5MC	N4-C4-N3	-2.13	114.02	117.03
1	A	1404	5MC	N4-C4-N3	-2.12	114.03	117.03
1	A	1541	PSU	O4'-C1'-C2'	2.11	108.09	104.66
1	A	1404	5MC	C2-N3-C4	2.10	118.55	116.02
1	A	967	5MC	C2-N3-C4	2.05	118.49	116.02
1	A	1404	5MC	CM5-C5-C6	2.02	122.94	118.68

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	1519[B]	MA6	C5-C6-N6-C9
1	A	1519[B]	MA6	N1-C6-N6-C9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
12	L	92	0TD	CG-CB-SB-CSB
1	A	1519[A]	MA6	O4'-C4'-C5'-O5'
1	A	1519[A]	MA6	C3'-C4'-C5'-O5'
1	A	1518[B]	MA6	O4'-C4'-C5'-O5'
1	A	1402	4OC	O4'-C4'-C5'-O5'
1	A	1518[B]	MA6	C3'-C4'-C5'-O5'
1	A	1400	5MC	O4'-C4'-C5'-O5'
1	A	966	M2G	C4'-C5'-O5'-P
1	A	1400	5MC	C3'-C4'-C5'-O5'
1	A	1518[A]	MA6	O4'-C4'-C5'-O5'
1	A	1519[A]	MA6	C5-C6-N6-C9
1	A	1518[A]	MA6	C3'-C4'-C5'-O5'
1	A	527	G7M	C3'-C4'-C5'-O5'
1	A	1519[B]	MA6	C5-C6-N6-C10
1	A	1402	4OC	C3'-C4'-C5'-O5'
1	A	966	M2G	O4'-C4'-C5'-O5'

There are no ring outliers.

7 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	527	G7M	1	0
1	A	967	5MC	2	0
1	A	1402	4OC	1	0
1	A	1518[A]	MA6	1	0
1	A	1518[B]	MA6	1	0
12	L	92	0TD	1	0
1	A	1400	5MC	1	0

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 403 ligands modelled in this entry, 402 are monoatomic - leaving 1 for Mogul analysis.

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	$\#\|Z\| > 2$
25	EUS	A	1809	-	32,37,37	2.03	5 (15%)	34,56,56	1.58	4 (11%)

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
25	EUS	A	1809	-	-	4/14/70/70	0/3/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	A	1809	EUS	O1-S	6.15	1.54	1.43
25	A	1809	EUS	O2-S	5.74	1.53	1.43
25	A	1809	EUS	C31-C41	-4.92	1.39	1.50
25	A	1809	EUS	C61-C51	-4.03	1.39	1.48
25	A	1809	EUS	C62-C12	-2.70	1.48	1.52

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	A	1809	EUS	O2-S-O1	-5.87	110.41	118.85
25	A	1809	EUS	C93-N33-C33	-4.23	108.22	114.38
25	A	1809	EUS	C13-O62-C62	-2.15	112.65	117.96
25	A	1809	EUS	O11-C42-C32	-2.11	104.15	109.18

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
25	A	1809	EUS	C23-C33-N33-C93
25	A	1809	EUS	C12-N12-S-C6
25	A	1809	EUS	C12-N12-S-O1
25	A	1809	EUS	C52-C42-O11-C11

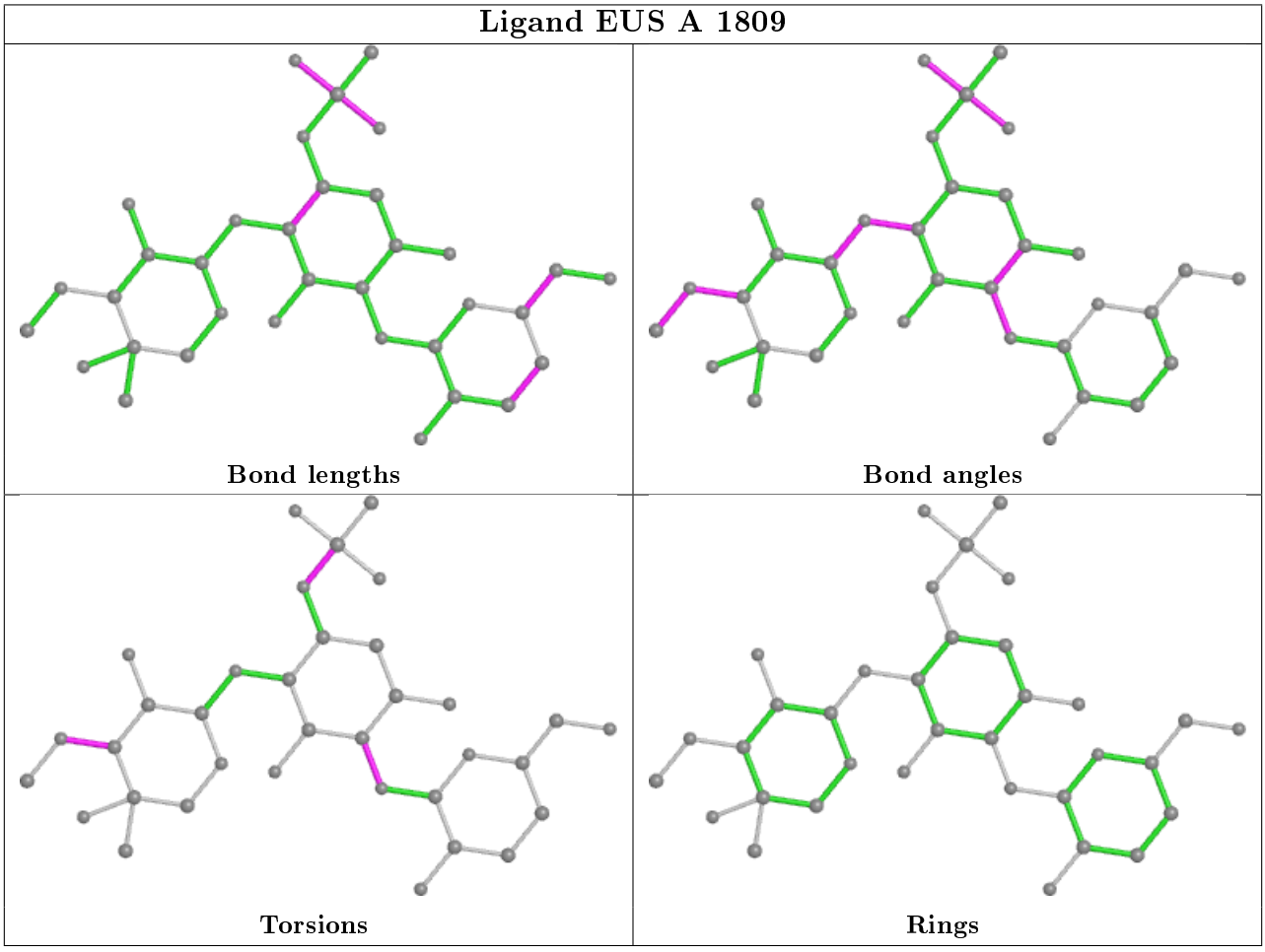
There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	A	1809	EUS	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand EUS A 1809



5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	1498/1522 (98%)	0.12	37 (2%) 57 55	36, 65, 142, 270	0
2	B	234/234 (100%)	0.03	3 (1%) 77 76	59, 94, 172, 208	0
3	C	206/206 (100%)	0.33	17 (8%) 11 13	70, 98, 138, 177	0
4	D	208/208 (100%)	0.00	5 (2%) 59 57	47, 77, 127, 165	0
5	E	150/150 (100%)	-0.25	0 100 100	33, 57, 95, 153	0
6	F	101/101 (100%)	0.01	0 100 100	53, 95, 123, 149	0
7	G	155/155 (100%)	0.03	3 (1%) 66 65	51, 81, 132, 184	0
8	H	138/138 (100%)	-0.48	0 100 100	26, 51, 76, 121	0
9	I	127/127 (100%)	0.07	2 (1%) 72 70	53, 97, 135, 162	0
10	J	98/98 (100%)	0.50	5 (5%) 28 28	69, 134, 210, 282	0
11	K	116/116 (100%)	-0.08	0 100 100	35, 62, 108, 138	0
12	L	123/124 (99%)	-0.12	3 (2%) 59 57	30, 66, 117, 169	0
13	M	118/118 (100%)	0.07	3 (2%) 57 55	55, 86, 133, 203	0
14	N	60/60 (100%)	-0.07	0 100 100	66, 87, 135, 192	0
15	O	87/87 (100%)	-0.20	0 100 100	35, 64, 108, 156	0
16	P	83/83 (100%)	-0.27	0 100 100	46, 61, 83, 153	0
17	Q	99/99 (100%)	-0.25	0 100 100	34, 54, 90, 125	0
18	R	70/70 (100%)	-0.09	0 100 100	40, 74, 140, 167	0
19	S	80/80 (100%)	0.67	8 (10%) 7 8	75, 115, 181, 216	0
20	T	99/99 (100%)	-0.07	3 (3%) 50 49	45, 65, 124, 153	0
21	U	24/24 (100%)	0.09	0 100 100	60, 82, 110, 119	0
22	Y	6/6 (100%)	1.00	1 (16%) 1 2	88, 100, 156, 203	0
23	W	15/15 (100%)	0.57	0 100 100	81, 103, 179, 190	0
All	All	3895/3920 (99%)	0.05	90 (2%) 60 59	26, 74, 145, 282	0

All (90) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1129	C	9.2
7	G	156	TRP	6.1
1	A	1003(A)	G	5.0
3	C	99	VAL	4.6
1	A	532	A	4.5
1	A	1257	U	4.3
19	S	3	ARG	4.3
19	S	27	GLU	4.2
1	A	1446	A	4.2
1	A	1533	C	4.0
13	M	7	VAL	3.9
10	J	83	GLU	3.8
1	A	1005	A	3.8
10	J	33	GLN	3.8
1	A	993	G	3.7
19	S	2	PRO	3.7
20	T	99	LEU	3.6
1	A	1006	C	3.5
4	D	35	ARG	3.5
19	S	28	LYS	3.5
1	A	1026	G	3.3
12	L	19	ARG	3.3
3	C	63	ASN	3.3
3	C	64	VAL	3.2
2	B	206	ASP	3.2
22	Y	6	U	3.2
1	A	1027	C	3.1
3	C	77	ILE	3.1
1	A	631	G	3.1
3	C	102	ASN	3.1
1	A	1443	G	3.0
1	A	1144	G	3.0
1	A	1004	A	2.9
1	A	1143	G	2.9
3	C	87	LEU	2.9
3	C	100	ALA	2.9
3	C	101	LEU	2.9
4	D	2	GLY	2.8
19	S	81	ARG	2.8
1	A	412	A	2.8
1	A	1025	U	2.8
7	G	56	GLN	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
4	D	45	GLN	2.7
1	A	1003	G	2.6
3	C	76	VAL	2.6
19	S	14	HIS	2.6
10	J	80	LYS	2.5
4	D	23	GLY	2.5
1	A	991	U	2.5
10	J	78	ASN	2.5
3	C	91	LEU	2.5
1	A	1045	C	2.5
3	C	60	ALA	2.5
3	C	78	GLY	2.5
1	A	1034	G	2.5
1	A	1133	G	2.5
3	C	27	LYS	2.5
3	C	89	GLU	2.5
9	I	126	SER	2.5
12	L	28	LYS	2.4
20	T	106	ALA	2.4
10	J	87	THR	2.4
1	A	1271	G	2.4
1	A	1038	C	2.4
1	A	1182	G	2.4
1	A	1035	A	2.4
1	A	1142	G	2.4
2	B	238	LEU	2.4
4	D	42	GLN	2.3
19	S	35	SER	2.3
3	C	103	VAL	2.3
1	A	426	G	2.3
1	A	1258	G	2.3
9	I	23	ASN	2.3
1	A	1171	G	2.2
1	A	1532	U	2.2
7	G	155	ARG	2.2
13	M	8	GLU	2.2
3	C	98	ASN	2.2
3	C	79	ARG	2.1
13	M	2	ALA	2.1
1	A	160	A	2.1
1	A	158	G	2.1
20	T	100	ILE	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	1442	G	2.1
19	S	4	SER	2.1
2	B	35	GLU	2.1
1	A	1531	A	2.1
1	A	413	G	2.0
12	L	128	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, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
1	PSU	A	1540	20/21	0.77	0.36	142,144,150,151	0
1	PSU	A	1541	20/21	0.84	0.27	131,143,156,189	0
1	PSU	A	516	20/21	0.90	0.18	74,91,98,100	0
12	0TD	L	92	10/11	0.93	0.20	58,79,102,106	0
1	2MG	A	1207	24/25	0.93	0.17	75,81,87,95	0
1	MA6	A	1518[A]	24/25	0.94	0.23	42,43,44,44	24
1	MA6	A	1518[B]	24/25	0.94	0.23	42,43,44,44	24
1	G7M	A	527	24/25	0.94	0.17	45,51,59,74	0
1	MA6	A	1519[B]	24/25	0.94	0.22	41,42,42,42	24
1	MA6	A	1519[A]	24/25	0.94	0.22	41,42,43,63	0
1	M2G	A	966	25/26	0.95	0.16	53,72,82,83	0
1	5MC	A	1400	21/22	0.95	0.16	46,57,75,78	0
1	4OC	A	1402	22/23	0.95	0.18	47,50,55,61	0
1	5MC	A	1407	21/22	0.95	0.20	48,50,59,69	0
1	UR3	A	1498	21/22	0.96	0.20	42,43,47,76	0
1	5MC	A	967	21/22	0.96	0.15	51,59,68,70	0
1	5MC	A	1404	21/22	0.96	0.17	43,45,47,47	0

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
24	MG	A	1846	1/1	0.06	0.93	74,74,74,74	0
24	MG	A	1939	1/1	0.10	0.49	161,161,161,161	0
24	MG	N	102	1/1	0.10	0.84	69,69,69,69	0
24	MG	A	1883	1/1	0.11	0.87	59,59,59,59	0
24	MG	A	1885	1/1	0.13	0.95	72,72,72,72	0
24	MG	A	1791	1/1	0.17	0.29	82,82,82,82	0
24	MG	C	303	1/1	0.20	0.38	71,71,71,71	0
24	MG	A	1908	1/1	0.23	0.91	87,87,87,87	0
24	MG	A	1724	1/1	0.23	0.33	125,125,125,125	0
24	MG	H	206	1/1	0.23	0.28	69,69,69,69	0
24	MG	A	1921	1/1	0.25	0.34	81,81,81,81	0
24	MG	A	1904	1/1	0.26	0.80	78,78,78,78	0
24	MG	A	1601	1/1	0.28	2.43	194,194,194,194	0
24	MG	A	1860	1/1	0.30	0.33	102,102,102,102	0
24	MG	A	1862	1/1	0.31	0.46	73,73,73,73	0
24	MG	A	1893	1/1	0.34	0.56	80,80,80,80	0
24	MG	G	204	1/1	0.35	0.32	84,84,84,84	0
24	MG	G	203	1/1	0.37	0.38	102,102,102,102	0
24	MG	K	207	1/1	0.38	0.62	67,67,67,67	0
24	MG	A	1805	1/1	0.39	0.66	541,541,541,541	0
24	MG	A	1727	1/1	0.39	0.39	54,54,54,54	0
24	MG	A	1868	1/1	0.39	0.89	70,70,70,70	0
24	MG	A	1723	1/1	0.40	0.40	60,60,60,60	0
24	MG	A	1914	1/1	0.40	0.43	62,62,62,62	0
24	MG	A	1736	1/1	0.41	0.70	63,63,63,63	0
24	MG	A	1629	1/1	0.43	0.50	59,59,59,59	0
24	MG	A	1826	1/1	0.45	0.27	73,73,73,73	0
24	MG	A	1928	1/1	0.45	0.64	82,82,82,82	0
24	MG	A	1857	1/1	0.45	0.55	75,75,75,75	0
24	MG	A	1929	1/1	0.45	0.28	72,72,72,72	0
24	MG	A	1832	1/1	0.46	0.80	66,66,66,66	0
24	MG	A	1602	1/1	0.50	0.85	543,543,543,543	0
24	MG	A	1888	1/1	0.50	0.55	64,64,64,64	0
24	MG	A	1911	1/1	0.50	0.23	63,63,63,63	0
24	MG	A	1902	1/1	0.50	0.55	70,70,70,70	0
24	MG	A	1807	1/1	0.52	0.50	74,74,74,74	0
24	MG	B	302	1/1	0.52	0.33	78,78,78,78	0
24	MG	A	1878	1/1	0.52	0.49	67,67,67,67	0
24	MG	A	1645	1/1	0.52	0.17	77,77,77,77	0
24	MG	A	1703	1/1	0.54	0.36	151,151,151,151	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
24	MG	A	1895	1/1	0.55	0.43	49,49,49,49	0
24	MG	A	1873	1/1	0.55	0.52	58,58,58,58	0
24	MG	A	1811	1/1	0.55	0.54	55,55,55,55	0
24	MG	A	1894	1/1	0.56	0.40	74,74,74,74	0
24	MG	A	1713	1/1	0.56	0.40	70,70,70,70	0
24	MG	A	1930	1/1	0.57	0.30	57,57,57,57	0
24	MG	A	1903	1/1	0.57	0.54	73,73,73,73	0
24	MG	A	1886	1/1	0.58	0.50	70,70,70,70	0
24	MG	A	1897	1/1	0.58	0.77	56,56,56,56	0
24	MG	A	1745	1/1	0.59	0.54	58,58,58,58	0
24	MG	Q	204	1/1	0.59	0.26	63,63,63,63	0
24	MG	A	1688	1/1	0.59	0.34	47,47,47,47	0
24	MG	A	1933	1/1	0.60	0.86	72,72,72,72	0
24	MG	A	1931	1/1	0.60	0.20	54,54,54,54	0
24	MG	A	1785	1/1	0.61	0.42	64,64,64,64	0
24	MG	A	1858	1/1	0.61	0.35	64,64,64,64	0
24	MG	A	1920	1/1	0.61	0.45	61,61,61,61	0
24	MG	C	301	1/1	0.61	0.17	73,73,73,73	0
24	MG	A	1877	1/1	0.62	0.41	62,62,62,62	0
24	MG	D	304	1/1	0.62	0.30	66,66,66,66	0
24	MG	A	1839	1/1	0.62	0.39	84,84,84,84	0
24	MG	A	1836	1/1	0.62	0.40	50,50,50,50	0
24	MG	A	1927	1/1	0.63	0.45	76,76,76,76	0
24	MG	A	1834	1/1	0.64	0.40	62,62,62,62	0
24	MG	A	1833	1/1	0.64	0.35	78,78,78,78	0
24	MG	L	203	1/1	0.64	0.40	59,59,59,59	0
24	MG	A	1892	1/1	0.64	0.34	56,56,56,56	0
24	MG	C	305	1/1	0.64	0.21	71,71,71,71	0
24	MG	A	1766	1/1	0.65	0.40	67,67,67,67	0
24	MG	A	1630	1/1	0.65	0.49	48,48,48,48	0
24	MG	K	208	1/1	0.66	0.36	74,74,74,74	0
24	MG	A	1898	1/1	0.66	0.42	66,66,66,66	0
24	MG	A	1820	1/1	0.66	0.37	48,48,48,48	0
24	MG	A	1606	1/1	0.66	0.17	55,55,55,55	0
24	MG	Y	101	1/1	0.66	0.28	65,65,65,65	0
24	MG	A	1899	1/1	0.66	0.25	65,65,65,65	0
24	MG	A	1770	1/1	0.67	0.31	81,81,81,81	0
24	MG	A	1887	1/1	0.67	0.34	73,73,73,73	0
24	MG	Q	201	1/1	0.67	0.13	75,75,75,75	0
24	MG	A	1797	1/1	0.68	0.17	59,59,59,59	0
24	MG	Q	203	1/1	0.68	0.31	54,54,54,54	0
24	MG	K	202	1/1	0.68	0.19	56,56,56,56	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
24	MG	A	1827	1/1	0.68	0.36	53,53,53,53	0
24	MG	A	1793	1/1	0.69	0.28	43,43,43,43	0
24	MG	A	1773	1/1	0.69	0.43	61,61,61,61	0
24	MG	A	1901	1/1	0.69	0.30	54,54,54,54	0
24	MG	A	1896	1/1	0.70	0.46	64,64,64,64	0
24	MG	A	1701	1/1	0.70	0.28	54,54,54,54	0
24	MG	A	1851	1/1	0.70	0.40	54,54,54,54	0
24	MG	K	201	1/1	0.70	0.27	65,65,65,65	0
24	MG	H	203	1/1	0.70	0.28	38,38,38,38	0
24	MG	A	1938	1/1	0.70	0.28	138,138,138,138	0
24	MG	A	1792	1/1	0.70	0.23	68,68,68,68	0
24	MG	H	208	1/1	0.70	0.40	66,66,66,66	0
24	MG	A	1937	1/1	0.70	0.30	132,132,132,132	0
24	MG	A	1844	1/1	0.71	0.79	66,66,66,66	0
24	MG	A	1810	1/1	0.71	0.30	79,79,79,79	0
24	MG	A	1872	1/1	0.71	0.53	69,69,69,69	0
24	MG	A	1852	1/1	0.71	0.29	61,61,61,61	0
24	MG	A	1917	1/1	0.72	0.33	60,60,60,60	0
24	MG	A	1936	1/1	0.72	0.19	198,198,198,198	0
24	MG	A	1711	1/1	0.72	0.17	133,133,133,133	0
24	MG	A	1925	1/1	0.73	0.36	48,48,48,48	0
24	MG	A	1690	1/1	0.73	0.45	69,69,69,69	0
24	MG	P	102	1/1	0.73	0.26	51,51,51,51	0
24	MG	A	1683	1/1	0.73	0.29	35,35,35,35	0
24	MG	A	1865	1/1	0.73	0.30	62,62,62,62	0
24	MG	A	1919	1/1	0.73	0.27	46,46,46,46	0
24	MG	A	1884	1/1	0.73	0.49	57,57,57,57	0
24	MG	A	1781	1/1	0.73	0.20	65,65,65,65	0
24	MG	A	1675	1/1	0.73	0.31	59,59,59,59	0
24	MG	A	1789	1/1	0.74	0.10	86,86,86,86	0
24	MG	A	1847	1/1	0.74	0.39	86,86,86,86	0
24	MG	L	202	1/1	0.74	0.36	70,70,70,70	0
24	MG	E	202	1/1	0.74	0.21	44,44,44,44	0
24	MG	Q	208	1/1	0.74	0.47	221,221,221,221	0
24	MG	A	1710	1/1	0.75	0.63	54,54,54,54	0
24	MG	A	1798	1/1	0.75	0.20	54,54,54,54	0
24	MG	A	1741	1/1	0.75	0.19	42,42,42,42	0
24	MG	A	1824	1/1	0.75	0.62	108,108,108,108	0
24	MG	A	1835	1/1	0.75	0.30	58,58,58,58	0
24	MG	A	1668	1/1	0.75	0.22	85,85,85,85	0
24	MG	H	204	1/1	0.75	0.44	60,60,60,60	0
24	MG	A	1815	1/1	0.75	0.38	42,42,42,42	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
24	MG	A	1874	1/1	0.75	0.51	47,47,47,47	0
24	MG	A	1837	1/1	0.76	0.34	78,78,78,78	0
24	MG	A	1728	1/1	0.76	0.31	59,59,59,59	0
24	MG	A	1749	1/1	0.76	0.20	46,46,46,46	0
24	MG	H	207	1/1	0.76	0.12	80,80,80,80	0
24	MG	H	202	1/1	0.76	0.32	63,63,63,63	0
24	MG	E	203	1/1	0.76	0.24	44,44,44,44	0
24	MG	A	1867	1/1	0.76	0.29	57,57,57,57	0
24	MG	A	1794	1/1	0.77	0.33	56,56,56,56	0
24	MG	A	1926	1/1	0.77	0.56	73,73,73,73	0
24	MG	G	201	1/1	0.77	0.29	71,71,71,71	0
24	MG	A	1632	1/1	0.77	0.14	65,65,65,65	0
24	MG	A	1722	1/1	0.77	0.13	53,53,53,53	0
24	MG	A	1831	1/1	0.77	0.36	75,75,75,75	0
24	MG	A	1922	1/1	0.77	0.53	56,56,56,56	0
24	MG	A	1866	1/1	0.77	0.29	59,59,59,59	0
24	MG	A	1640	1/1	0.77	0.34	116,116,116,116	0
24	MG	A	1840	1/1	0.77	0.18	85,85,85,85	0
24	MG	A	1678	1/1	0.78	0.25	68,68,68,68	0
24	MG	A	1655	1/1	0.78	0.42	99,99,99,99	0
24	MG	C	304	1/1	0.78	0.17	83,83,83,83	0
24	MG	A	1882	1/1	0.78	0.37	62,62,62,62	0
24	MG	A	1755	1/1	0.78	0.20	53,53,53,53	0
24	MG	A	1907	1/1	0.78	0.41	96,96,96,96	0
24	MG	A	1672	1/1	0.78	0.13	60,60,60,60	0
24	MG	A	1841	1/1	0.78	0.37	66,66,66,66	0
24	MG	A	1693	1/1	0.79	0.60	167,167,167,167	0
24	MG	A	1612	1/1	0.79	0.14	73,73,73,73	0
24	MG	D	303	1/1	0.79	0.12	63,63,63,63	0
24	MG	T	201	1/1	0.79	0.41	67,67,67,67	0
24	MG	A	1717	1/1	0.79	0.46	91,91,91,91	0
24	MG	A	1818	1/1	0.79	0.26	69,69,69,69	0
24	MG	P	104	1/1	0.79	0.25	68,68,68,68	0
24	MG	A	1776	1/1	0.79	0.24	39,39,39,39	0
24	MG	A	1747	1/1	0.80	0.27	71,71,71,71	0
24	MG	A	1631	1/1	0.80	0.24	48,48,48,48	0
24	MG	A	1699	1/1	0.80	0.33	44,44,44,44	0
24	MG	A	1647	1/1	0.80	0.25	112,112,112,112	0
24	MG	A	1676	1/1	0.80	0.23	73,73,73,73	0
24	MG	A	1918	1/1	0.80	0.36	43,43,43,43	0
24	MG	A	1720	1/1	0.80	0.17	7,7,7,7	0
24	MG	A	1870	1/1	0.80	0.28	41,41,41,41	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
24	MG	A	1705	1/1	0.80	0.29	85,85,85,85	0
24	MG	K	209	1/1	0.80	0.40	64,64,64,64	0
24	MG	A	1842	1/1	0.80	0.51	58,58,58,58	0
24	MG	A	1788	1/1	0.80	0.20	48,48,48,48	0
24	MG	Y	102	1/1	0.80	0.27	72,72,72,72	0
24	MG	A	1817	1/1	0.81	0.36	46,46,46,46	0
24	MG	A	1763	1/1	0.81	0.33	50,50,50,50	0
24	MG	G	202	1/1	0.81	0.16	118,118,118,118	0
24	MG	A	1790	1/1	0.81	0.23	115,115,115,115	0
24	MG	A	1838	1/1	0.81	0.27	67,67,67,67	0
24	MG	A	1775	1/1	0.81	0.30	51,51,51,51	0
24	MG	A	1700	1/1	0.81	0.17	68,68,68,68	0
24	MG	A	1875	1/1	0.81	0.26	52,52,52,52	0
24	MG	A	1850	1/1	0.81	0.49	69,69,69,69	0
24	MG	A	1859	1/1	0.81	0.36	91,91,91,91	0
24	MG	A	1823	1/1	0.81	0.31	41,41,41,41	0
24	MG	A	1734	1/1	0.81	0.23	49,49,49,49	0
24	MG	A	1694	1/1	0.81	0.28	40,40,40,40	0
24	MG	A	1682	1/1	0.82	0.14	28,28,28,28	0
24	MG	A	1808	1/1	0.82	0.21	67,67,67,67	0
24	MG	A	1677	1/1	0.82	0.19	43,43,43,43	0
24	MG	A	1702	1/1	0.82	0.12	64,64,64,64	0
24	MG	A	1726	1/1	0.82	0.24	46,46,46,46	0
24	MG	A	1806	1/1	0.82	0.23	54,54,54,54	0
24	MG	A	1698	1/1	0.82	0.18	72,72,72,72	0
24	MG	A	1771	1/1	0.82	0.58	50,50,50,50	0
24	MG	A	1906	1/1	0.82	0.32	63,63,63,63	0
24	MG	A	1607	1/1	0.82	0.20	43,43,43,43	0
24	MG	A	1782	1/1	0.83	0.23	64,64,64,64	0
24	MG	A	1796	1/1	0.83	0.24	43,43,43,43	0
24	MG	A	1801	1/1	0.83	0.27	75,75,75,75	0
24	MG	A	1696	1/1	0.83	0.49	51,51,51,51	0
24	MG	A	1915	1/1	0.83	0.28	61,61,61,61	0
24	MG	A	1689	1/1	0.83	0.22	71,71,71,71	0
24	MG	A	1633	1/1	0.83	0.34	42,42,42,42	0
24	MG	A	1861	1/1	0.83	0.20	53,53,53,53	0
24	MG	A	1669	1/1	0.83	0.13	78,78,78,78	0
24	MG	A	1687	1/1	0.83	0.27	39,39,39,39	0
24	MG	A	1819	1/1	0.83	0.18	24,24,24,24	0
24	MG	A	1730	1/1	0.83	0.20	55,55,55,55	0
24	MG	A	1784	1/1	0.83	0.25	27,27,27,27	0
24	MG	K	205	1/1	0.83	0.20	68,68,68,68	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
24	MG	A	1670	1/1	0.83	0.30	133,133,133,133	0
24	MG	A	1780	1/1	0.83	0.20	34,34,34,34	0
24	MG	A	1742	1/1	0.84	0.25	42,42,42,42	0
24	MG	A	1759	1/1	0.84	0.35	57,57,57,57	0
24	MG	D	306	1/1	0.84	0.30	58,58,58,58	0
24	MG	A	1880	1/1	0.84	0.25	69,69,69,69	0
24	MG	A	1628	1/1	0.84	0.18	64,64,64,64	0
24	MG	A	1617	1/1	0.84	0.42	56,56,56,56	0
24	MG	A	1889	1/1	0.84	0.25	57,57,57,57	0
24	MG	F	201	1/1	0.84	0.09	67,67,67,67	0
24	MG	A	1799	1/1	0.84	0.24	66,66,66,66	0
24	MG	A	1830	1/1	0.84	0.30	26,26,26,26	0
24	MG	A	1729	1/1	0.84	0.22	47,47,47,47	0
24	MG	A	1900	1/1	0.84	0.32	51,51,51,51	0
24	MG	A	1905	1/1	0.84	0.36	38,38,38,38	0
24	MG	A	1814	1/1	0.84	0.20	46,46,46,46	0
24	MG	H	205	1/1	0.85	0.18	47,47,47,47	0
24	MG	A	1619	1/1	0.85	0.24	57,57,57,57	0
24	MG	A	1624	1/1	0.85	0.22	46,46,46,46	0
24	MG	A	1935	1/1	0.85	0.37	181,181,181,181	0
24	MG	K	210	1/1	0.85	0.25	34,34,34,34	0
24	MG	A	1879	1/1	0.85	0.21	56,56,56,56	0
24	MG	A	1637	1/1	0.85	0.17	53,53,53,53	0
24	MG	A	1662	1/1	0.85	0.37	35,35,35,35	0
24	MG	H	201	1/1	0.85	0.18	55,55,55,55	0
24	MG	A	1638	1/1	0.85	0.35	36,36,36,36	0
24	MG	A	1876	1/1	0.85	0.29	58,58,58,58	0
24	MG	Q	207	1/1	0.85	0.25	53,53,53,53	0
24	MG	A	1768	1/1	0.85	0.18	48,48,48,48	0
24	MG	A	1714	1/1	0.85	0.16	36,36,36,36	0
24	MG	A	1804	1/1	0.85	0.26	39,39,39,39	0
24	MG	A	1881	1/1	0.86	0.35	71,71,71,71	0
24	MG	A	1685	1/1	0.86	0.29	119,119,119,119	0
24	MG	A	1864	1/1	0.86	0.38	43,43,43,43	0
24	MG	A	1654	1/1	0.86	0.12	7,7,7,7	0
24	MG	A	1740	1/1	0.86	0.13	41,41,41,41	0
24	MG	P	106	1/1	0.86	0.19	162,162,162,162	0
24	MG	A	1671	1/1	0.86	0.49	66,66,66,66	0
24	MG	P	103	1/1	0.86	0.12	60,60,60,60	0
24	MG	L	204	1/1	0.86	0.21	62,62,62,62	0
24	MG	A	1849	1/1	0.86	0.41	82,82,82,82	0
24	MG	A	1924	1/1	0.86	0.32	49,49,49,49	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
24	MG	A	1657	1/1	0.86	0.15	36,36,36,36	0
24	MG	A	1725	1/1	0.86	0.16	19,19,19,19	0
24	MG	A	1783	1/1	0.86	0.23	45,45,45,45	0
24	MG	A	1828	1/1	0.86	0.26	40,40,40,40	0
24	MG	A	1891	1/1	0.86	0.41	72,72,72,72	0
24	MG	A	1800	1/1	0.87	0.12	29,29,29,29	0
24	MG	A	1615	1/1	0.87	0.11	66,66,66,66	0
24	MG	A	1761	1/1	0.87	0.27	27,27,27,27	0
24	MG	A	1738	1/1	0.87	0.30	35,35,35,35	0
24	MG	L	201	1/1	0.87	0.22	53,53,53,53	0
24	MG	A	1762	1/1	0.87	0.27	42,42,42,42	0
24	MG	A	1854	1/1	0.87	0.23	48,48,48,48	0
24	MG	A	1764	1/1	0.87	0.23	36,36,36,36	0
24	MG	A	1856	1/1	0.87	0.27	50,50,50,50	0
24	MG	A	1642	1/1	0.87	0.23	54,54,54,54	0
24	MG	A	1916	1/1	0.87	0.30	47,47,47,47	0
24	MG	D	305	1/1	0.87	0.24	55,55,55,55	0
24	MG	A	1663	1/1	0.87	0.34	70,70,70,70	0
24	MG	A	1821	1/1	0.87	0.35	40,40,40,40	0
24	MG	A	1709	1/1	0.87	0.26	75,75,75,75	0
24	MG	B	301	1/1	0.87	0.16	80,80,80,80	0
24	MG	A	1621	1/1	0.87	0.19	45,45,45,45	0
24	MG	A	1758	1/1	0.87	0.12	28,28,28,28	0
24	MG	E	201	1/1	0.88	0.11	87,87,87,87	0
24	MG	A	1825	1/1	0.88	0.25	63,63,63,63	0
24	MG	Q	206	1/1	0.88	0.19	40,40,40,40	0
24	MG	A	1913	1/1	0.88	0.22	59,59,59,59	0
24	MG	A	1863	1/1	0.88	0.40	53,53,53,53	0
24	MG	A	1845	1/1	0.88	0.49	62,62,62,62	0
24	MG	A	1719	1/1	0.88	0.18	58,58,58,58	0
24	MG	A	1816	1/1	0.88	0.28	34,34,34,34	0
24	MG	A	1829	1/1	0.88	0.17	30,30,30,30	0
24	MG	K	204	1/1	0.88	0.27	46,46,46,46	0
24	MG	A	1623	1/1	0.88	0.29	68,68,68,68	0
24	MG	A	1732	1/1	0.88	0.24	55,55,55,55	0
24	MG	A	1756	1/1	0.88	0.27	49,49,49,49	0
24	MG	A	1934	1/1	0.88	0.35	44,44,44,44	0
24	MG	A	1909	1/1	0.88	0.65	111,111,111,111	0
24	MG	A	1634	1/1	0.89	0.15	54,54,54,54	0
24	MG	J	201	1/1	0.89	0.22	29,29,29,29	0
24	MG	A	1708	1/1	0.89	0.16	44,44,44,44	0
24	MG	Q	202	1/1	0.89	0.24	65,65,65,65	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
24	MG	A	1616	1/1	0.89	0.33	67,67,67,67	0
24	MG	A	1848	1/1	0.89	0.27	61,61,61,61	0
24	MG	A	1735	1/1	0.89	0.33	52,52,52,52	0
24	MG	E	204	1/1	0.89	0.19	48,48,48,48	0
24	MG	A	1748	1/1	0.89	0.14	26,26,26,26	0
24	MG	A	1753	1/1	0.89	0.46	43,43,43,43	0
24	MG	A	1691	1/1	0.89	0.15	62,62,62,62	0
24	MG	A	1812	1/1	0.89	0.23	41,41,41,41	0
24	MG	A	1604	1/1	0.89	0.17	80,80,80,80	0
24	MG	A	1697	1/1	0.90	0.38	43,43,43,43	0
24	MG	A	1635	1/1	0.90	0.20	73,73,73,73	0
24	MG	A	1787	1/1	0.90	0.10	20,20,20,20	0
24	MG	Q	205	1/1	0.90	0.29	41,41,41,41	0
24	MG	A	1653	1/1	0.90	0.37	149,149,149,149	0
24	MG	A	1739	1/1	0.90	0.17	30,30,30,30	0
24	MG	A	1752	1/1	0.90	0.17	61,61,61,61	0
24	MG	A	1673	1/1	0.90	0.17	33,33,33,33	0
24	MG	P	105	1/1	0.90	0.27	52,52,52,52	0
24	MG	A	1651	1/1	0.90	0.16	23,23,23,23	0
24	MG	A	1890	1/1	0.90	0.15	38,38,38,38	0
24	MG	A	1910	1/1	0.90	0.12	49,49,49,49	0
24	MG	A	1684	1/1	0.90	0.12	88,88,88,88	0
24	MG	A	1912	1/1	0.90	0.23	51,51,51,51	0
24	MG	A	1605	1/1	0.90	0.20	50,50,50,50	0
24	MG	A	1666	1/1	0.91	0.23	32,32,32,32	0
24	MG	A	1786	1/1	0.91	0.36	39,39,39,39	0
24	MG	A	1627	1/1	0.91	0.17	20,20,20,20	0
24	MG	A	1695	1/1	0.91	0.12	51,51,51,51	0
24	MG	A	1610	1/1	0.91	0.13	32,32,32,32	0
24	MG	A	1744	1/1	0.91	0.09	44,44,44,44	0
24	MG	A	1803	1/1	0.91	0.21	42,42,42,42	0
24	MG	K	206	1/1	0.91	0.17	53,53,53,53	0
24	MG	A	1733	1/1	0.91	0.37	36,36,36,36	0
24	MG	A	1659	1/1	0.91	0.29	72,72,72,72	0
24	MG	A	1681	1/1	0.91	0.16	43,43,43,43	0
24	MG	A	1769	1/1	0.91	0.17	36,36,36,36	0
24	MG	A	1754	1/1	0.91	0.17	23,23,23,23	0
24	MG	A	1641	1/1	0.91	0.13	54,54,54,54	0
24	MG	A	1871	1/1	0.92	0.19	54,54,54,54	0
24	MG	A	1757	1/1	0.92	0.14	42,42,42,42	0
24	MG	A	1869	1/1	0.92	0.20	41,41,41,41	0
24	MG	A	1644	1/1	0.92	0.21	35,35,35,35	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
24	MG	A	1795	1/1	0.92	0.21	69,69,69,69	0
24	MG	A	1765	1/1	0.92	0.14	34,34,34,34	0
24	MG	A	1772	1/1	0.92	0.17	14,14,14,14	0
24	MG	A	1779	1/1	0.92	0.12	36,36,36,36	0
24	MG	A	1751	1/1	0.92	0.16	45,45,45,45	0
24	MG	A	1746	1/1	0.92	0.12	42,42,42,42	0
24	MG	A	1620	1/1	0.92	0.29	67,67,67,67	0
24	MG	A	1813	1/1	0.92	0.13	35,35,35,35	0
24	MG	A	1855	1/1	0.92	0.24	30,30,30,30	0
24	MG	A	1664	1/1	0.92	0.10	39,39,39,39	0
24	MG	A	1646	1/1	0.92	0.18	31,31,31,31	0
24	MG	A	1932	1/1	0.92	0.16	62,62,62,62	0
24	MG	A	1923	1/1	0.92	0.17	46,46,46,46	0
24	MG	A	1750	1/1	0.93	0.18	64,64,64,64	0
24	MG	A	1704	1/1	0.93	0.33	70,70,70,70	0
24	MG	A	1822	1/1	0.93	0.21	57,57,57,57	0
24	MG	A	1853	1/1	0.93	0.15	40,40,40,40	0
25	EUS	A	1809	35/35	0.93	0.30	24,45,106,109	0
24	MG	A	1680	1/1	0.93	0.19	63,63,63,63	0
24	MG	A	1656	1/1	0.93	0.21	70,70,70,70	0
24	MG	A	1649	1/1	0.94	0.08	41,41,41,41	0
24	MG	A	1706	1/1	0.94	0.18	46,46,46,46	0
24	MG	A	1731	1/1	0.94	0.14	20,20,20,20	0
24	MG	A	1674	1/1	0.94	0.15	47,47,47,47	0
24	MG	A	1716	1/1	0.94	0.18	48,48,48,48	0
24	MG	A	1712	1/1	0.94	0.16	70,70,70,70	0
24	MG	A	1721	1/1	0.94	0.19	44,44,44,44	0
24	MG	C	302	1/1	0.94	0.20	81,81,81,81	0
24	MG	D	302	1/1	0.94	0.15	37,37,37,37	0
24	MG	K	203	1/1	0.94	0.21	56,56,56,56	0
24	MG	A	1652	1/1	0.94	0.18	37,37,37,37	0
24	MG	A	1802	1/1	0.94	0.20	24,24,24,24	0
24	MG	A	1613	1/1	0.94	0.17	78,78,78,78	0
24	MG	A	1692	1/1	0.94	0.19	79,79,79,79	0
24	MG	A	1648	1/1	0.94	0.12	53,53,53,53	0
24	MG	A	1614	1/1	0.94	0.12	43,43,43,43	0
24	MG	A	1665	1/1	0.94	0.27	30,30,30,30	0
24	MG	A	1715	1/1	0.95	0.14	30,30,30,30	0
24	MG	A	1679	1/1	0.95	0.10	78,78,78,78	0
24	MG	A	1843	1/1	0.95	0.16	31,31,31,31	0
24	MG	A	1707	1/1	0.95	0.18	39,39,39,39	0
24	MG	A	1667	1/1	0.95	0.28	37,37,37,37	0

Continued on next page...

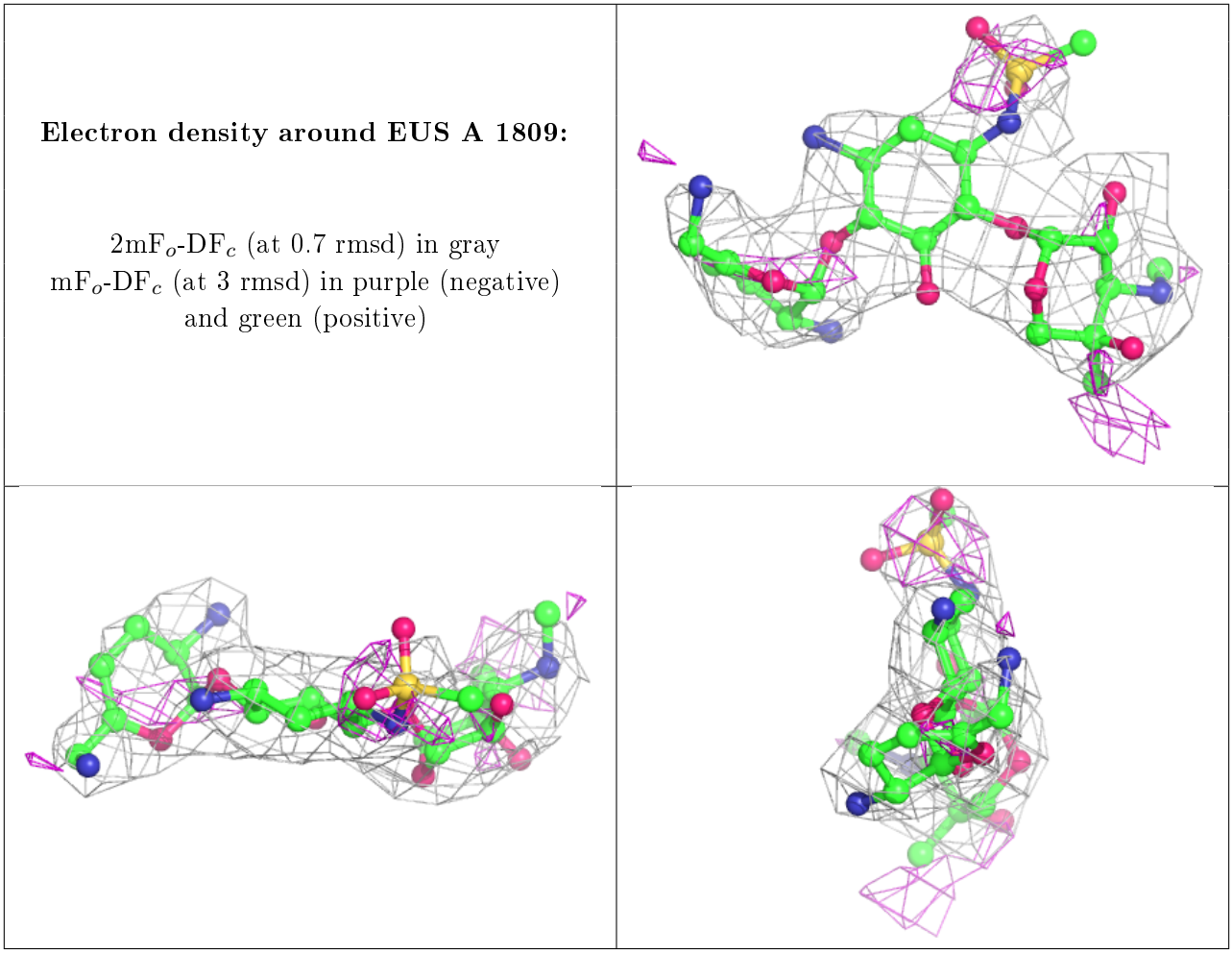
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
24	MG	A	1658	1/1	0.95	0.20	21,21,21,21	0
24	MG	A	1778	1/1	0.95	0.10	9,9,9,9	0
24	MG	A	1777	1/1	0.95	0.13	37,37,37,37	0
24	MG	A	1609	1/1	0.95	0.13	25,25,25,25	0
24	MG	A	1718	1/1	0.96	0.12	39,39,39,39	0
24	MG	A	1661	1/1	0.96	0.10	53,53,53,53	0
24	MG	A	1622	1/1	0.96	0.11	50,50,50,50	0
24	MG	A	1760	1/1	0.96	0.08	10,10,10,10	0
24	MG	A	1774	1/1	0.96	0.26	37,37,37,37	0
24	MG	A	1636	1/1	0.96	0.13	36,36,36,36	0
26	ZN	D	301	1/1	0.97	0.26	46,46,46,46	0
24	MG	A	1626	1/1	0.97	0.15	20,20,20,20	0
24	MG	A	1639	1/1	0.97	0.10	119,119,119,119	0
24	MG	A	1686	1/1	0.97	0.08	51,51,51,51	0
24	MG	A	1737	1/1	0.97	0.13	8,8,8,8	0
24	MG	A	1650	1/1	0.97	0.16	43,43,43,43	0
26	ZN	N	101	1/1	0.97	0.10	64,64,64,64	0
24	MG	A	1743	1/1	0.97	0.09	54,54,54,54	0
24	MG	A	1603	1/1	0.97	0.15	42,42,42,42	0
24	MG	A	1767	1/1	0.97	0.12	31,31,31,31	0
24	MG	A	1660	1/1	0.97	0.07	64,64,64,64	0
24	MG	A	1625	1/1	0.98	0.09	0,0,0,0	0
24	MG	P	101	1/1	0.98	0.14	24,24,24,24	0
24	MG	A	1608	1/1	0.98	0.07	61,61,61,61	0
24	MG	A	1618	1/1	0.98	0.09	57,57,57,57	0
24	MG	A	1643	1/1	0.98	0.09	26,26,26,26	0
24	MG	A	1611	1/1	0.99	0.22	68,68,68,68	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around EUS A 1809:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



6.5 Other polymers

There are no such residues in this entry.