wwPDB X-ray Structure Validation Summary Report (i)

Oct 12, 2020 – 11:03 AM EDT

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

This is a wwPDB X-ray Structure Validation Summary 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 (1)) were used in the production of this report:

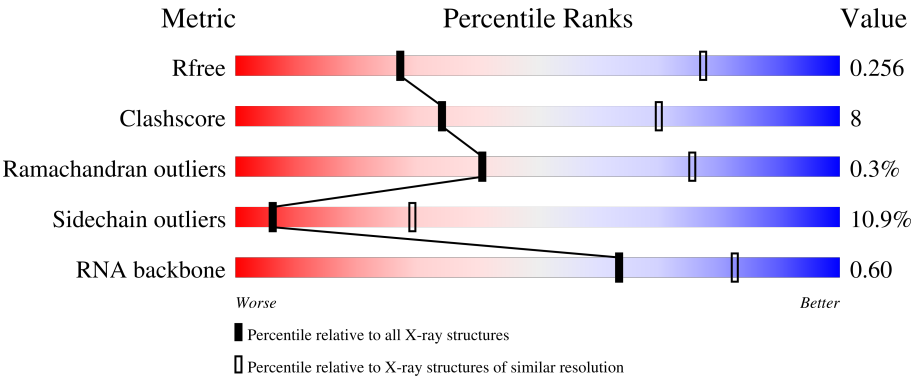
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.14.6
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.50 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1659 (3.60-3.40)
Clashscore	141614	1036 (3.58-3.42)
Ramachandran outliers	138981	1005 (3.58-3.42)
Sidechain outliers	138945	1006 (3.58-3.42)
RNA backbone	3102	1002 (4.00-3.00)

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

Mol	Chain	Length	Quality of chain
1	A	1522	57% 33% 9% ·
2	B	234	65% 30% 5%
3	C	206	62% 34% ·
4	D	208	68% 29% ·
5	E	150	76% 23% ·
6	F	101	74% 24% ·

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Mol	Chain	Length	Quality of chain
7	G	155	80% 17%
8	H	138	73% 24%
9	I	127	61% 33% 6%
10	J	98	62% 31% 6%
11	K	116	66% 30%
12	L	124	68% 28%
13	M	118	59% 35% 6%
14	N	60	60% 35% 5%
15	O	87	72% 22% 6%
16	P	83	78% 18%
17	Q	99	79% 21%
18	R	70	81% 16%
19	S	80	70% 30%
20	T	99	68% 25% 5%
21	U	24	63% 38%

2 Entry composition (i)

There are 24 unique types of molecules in this entry. The entry contains 52227 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
1	A	1512	32644	14540	6039	10547	1518	0	6	0

There are 2 discrepancies between the modelled and reference sequences:

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	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			

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

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

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

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

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

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

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

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

- Molecule 22 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

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

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

- Molecule 24 is water.

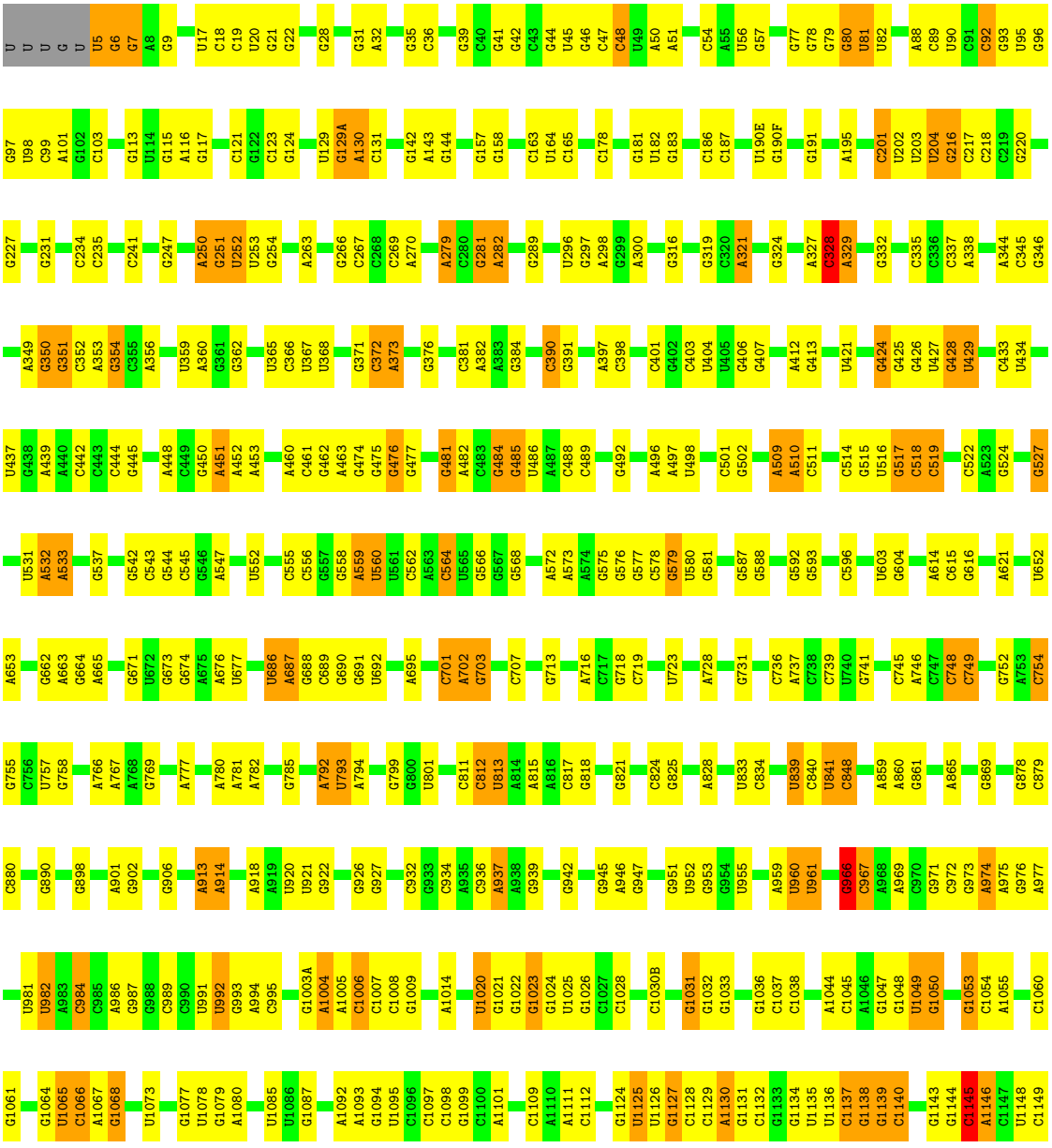
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
24	A	225	Total O 225 225	0	0
24	D	2	Total O 2 2	0	0
24	E	5	Total O 5 5	0	0
24	L	2	Total O 2 2	0	0
24	N	1	Total O 1 1	0	0
24	Q	2	Total O 2 2	0	0
24	T	2	Total O 2 2	0	0

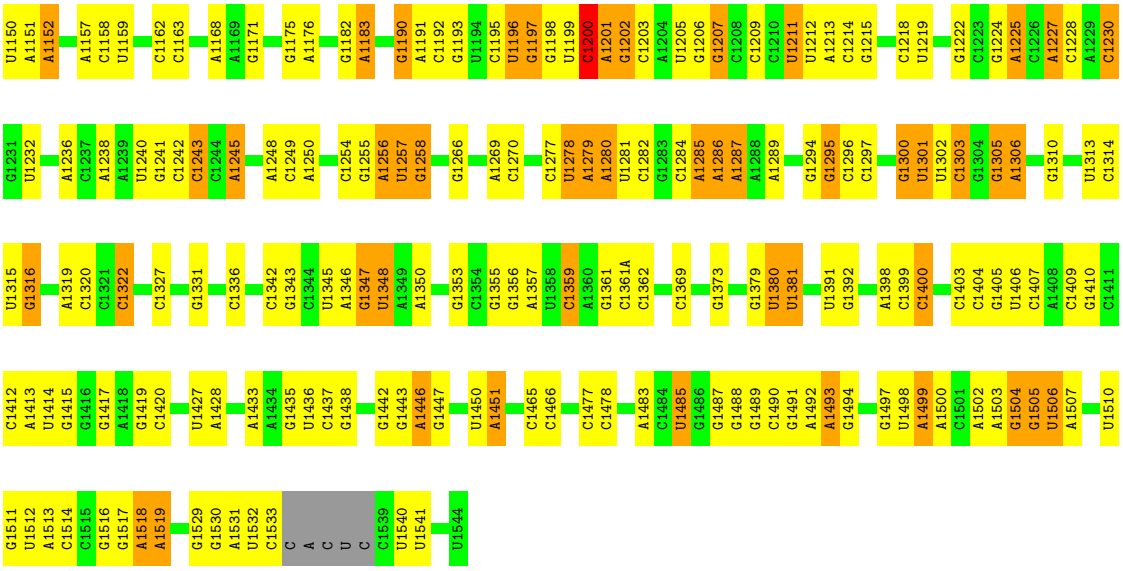
3 Residue-property plots (i)

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

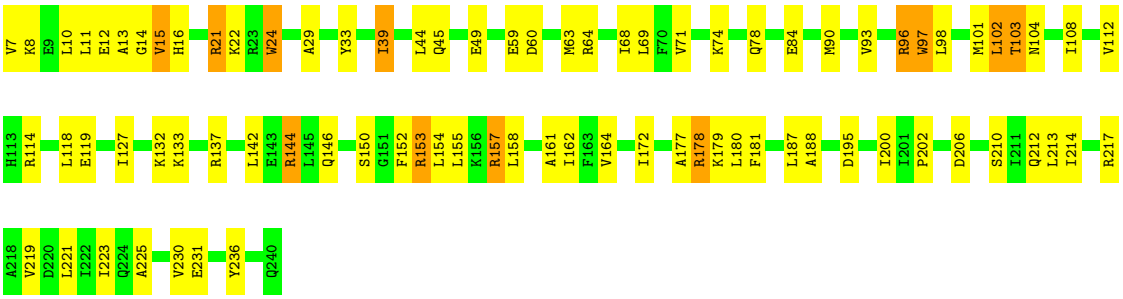
Chain A:





• Molecule 2: 30S ribosomal protein S2

Chain B:



• Molecule 3: 30S ribosomal protein S3

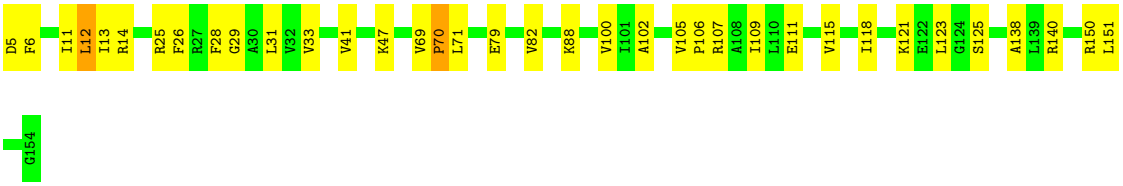
Chain C:

• Molecule 4: 30S ribosomal protein S4

Chain D:

• Molecule 5: 30S ribosomal protein S5

Chain E:



• Molecule 6: 30S ribosomal protein S6

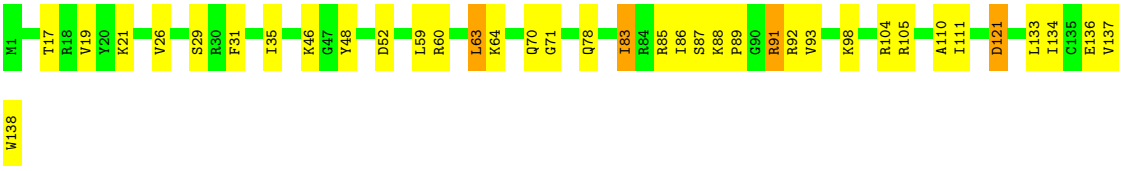
Chain F:

• Molecule 7: 30S ribosomal protein S7

Chain G:

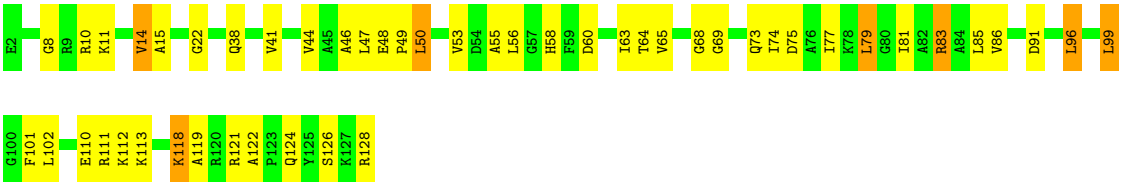
• Molecule 8: 30S ribosomal protein S8

Chain H:



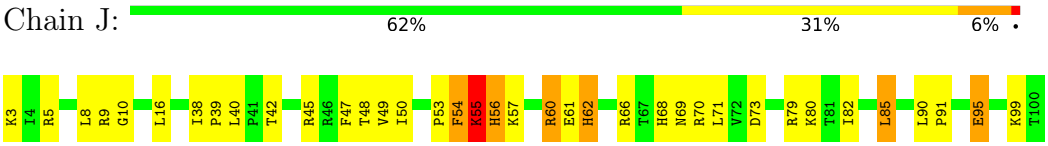
• Molecule 9: 30S ribosomal protein S9

Chain I:



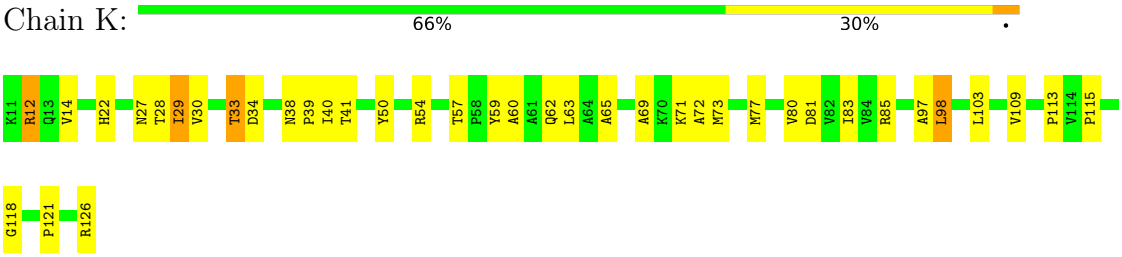
• Molecule 10: 30S ribosomal protein S10

Chain J:



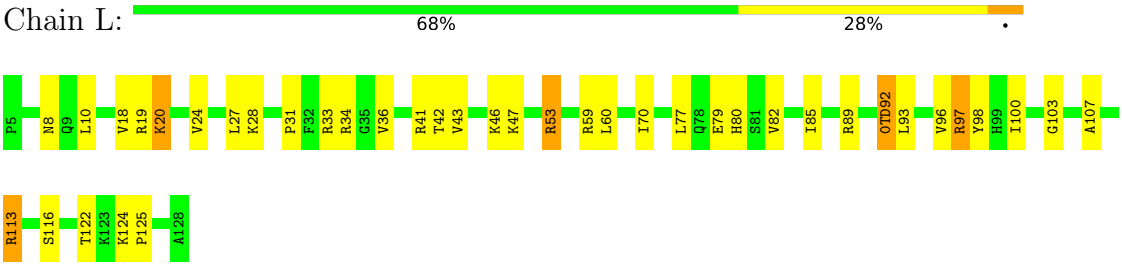
• Molecule 11: 30S ribosomal protein S11

Chain K:



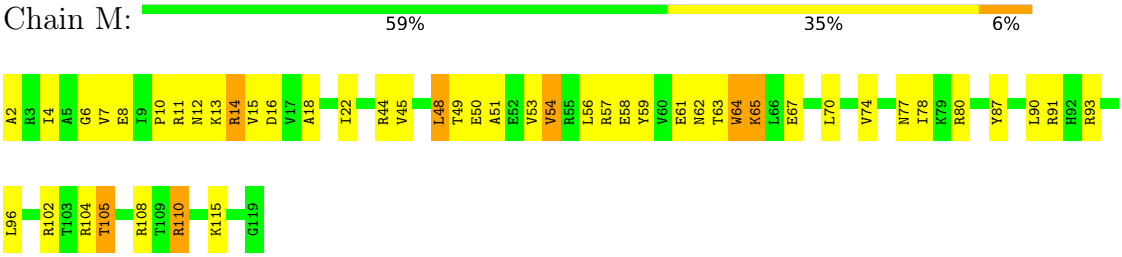
• Molecule 12: 30S ribosomal protein S12

Chain L:



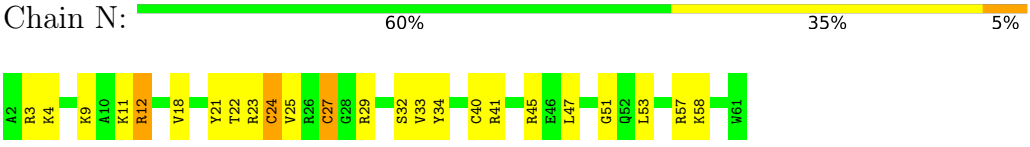
• Molecule 13: 30S ribosomal protein S13

Chain M:



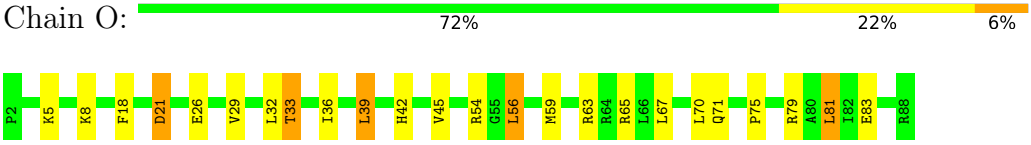
• Molecule 14: 30S ribosomal protein S14 type Z

Chain N:



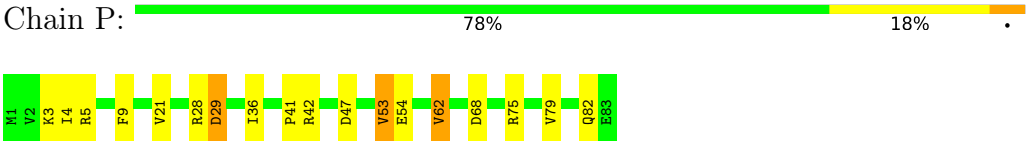
• Molecule 15: 30S ribosomal protein S15

Chain O:



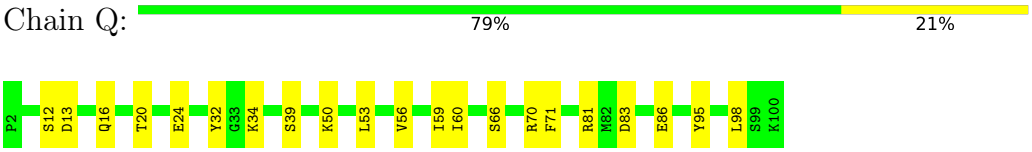
• Molecule 16: 30S ribosomal protein S16

Chain P:



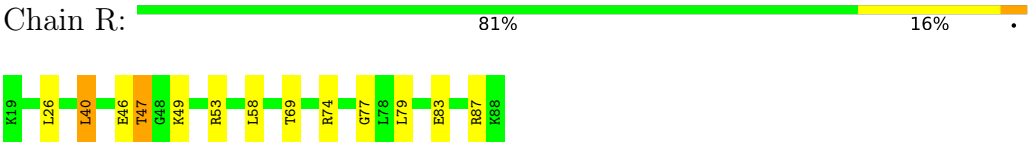
• Molecule 17: 30S ribosomal protein S17

Chain Q:



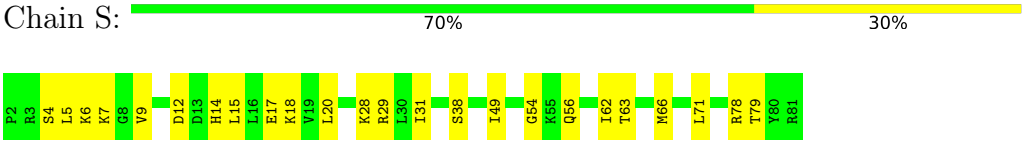
• Molecule 18: 30S ribosomal protein S18

Chain R:



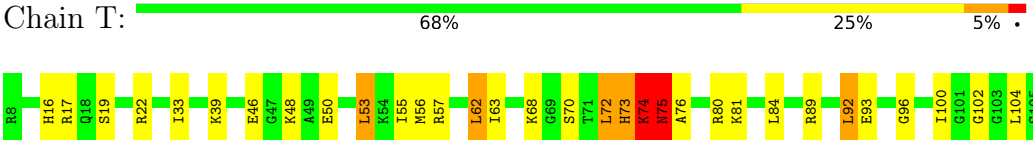
• Molecule 19: 30S ribosomal protein S19

Chain S:



• Molecule 20: 30S ribosomal protein S20

Chain T:



• Molecule 21: 30S ribosomal protein Thx

Chain U:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α, β, γ	400.00Å 400.00Å 173.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.98 – 3.50 39.78 – 2.92	Depositor EDS
% Data completeness (in resolution range)	91.5 (29.98-3.50) 71.0 (39.78-2.92)	Depositor EDS
R_{merge}	1.18	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.46 (at 2.90Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.214 , 0.256 0.217 , 0.256	Depositor DCC
R_{free} test set	2000 reflections (0.67%)	wwPDB-VP
Wilson B-factor (Å^2)	58.0	Xtriage
Anisotropy	0.303	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.07 , -10.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	52227	wwPDB-VP
Average B, all atoms (Å^2)	232.0	wwPDB-VP

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

[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 (i)

5.1 Standard geometry (i)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.19	0/36139	0.80	22/56396 (0.0%)
2	B	0.25	0/1935	0.43	0/2609
3	C	0.25	0/1636	0.47	0/2205
4	D	0.24	0/1733	0.40	0/2318
5	E	0.25	0/1162	0.45	0/1564
6	F	0.23	0/856	0.43	0/1154
7	G	0.24	0/1276	0.40	0/1709
8	H	0.24	0/1136	0.46	0/1527
9	I	0.26	0/1029	0.45	0/1379
10	J	0.25	0/805	0.52	0/1082
11	K	0.26	0/879	0.47	0/1187
12	L	0.25	0/977	0.51	0/1306
13	M	0.23	0/947	0.45	0/1270
14	N	0.25	0/501	0.46	0/664
15	O	0.24	0/740	0.39	0/987
16	P	0.24	0/716	0.44	0/963
17	Q	0.24	0/836	0.46	0/1117
18	R	0.24	0/579	0.44	0/768
19	S	0.24	0/661	0.51	0/890
20	T	0.25	0/765	0.43	0/1007
21	U	0.22	0/212	0.42	0/277
All	All	0.21	0/55520	0.71	22/82379 (0.0%)

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

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

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

There are no bond length outliers.

The worst 5 of 22 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	328	C	C2-N1-C1'	7.91	127.50	118.80
1	A	1139	G	P-O3'-C3'	7.69	128.93	119.70
1	A	1127	G	N1-C6-O6	-7.66	115.30	119.90
1	A	328	C	N1-C2-O2	7.39	123.33	118.90
1	A	1127	G	C5-C6-O6	7.22	132.93	128.60

There are no chirality outliers.

5 of 7 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	15	VAL	Peptide
3	C	166	GLU	Peptide
10	J	54	PHE	Peptide
10	J	55	LYS	Peptide
13	M	6	GLY	Peptide

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	384	2
2	B	1900	0	1951	43	0
3	C	1612	0	1677	49	0
4	D	1703	0	1763	43	0
5	E	1146	0	1207	19	0
6	F	843	0	857	13	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	G	1257	0	1296	18	0
8	H	1116	0	1177	21	0
9	I	1010	0	1037	32	0
10	J	792	0	835	24	0
11	K	864	0	881	25	0
12	L	972	0	1058	23	0
13	M	937	0	995	31	0
14	N	492	0	529	23	0
15	O	729	0	768	10	0
16	P	700	0	720	12	0
17	Q	823	0	893	11	0
18	R	574	0	644	9	0
19	S	647	0	673	14	0
20	T	763	0	861	19	0
21	U	208	0	221	10	0
22	A	234	0	0	0	0
22	B	3	0	0	0	0
22	C	3	0	0	0	0
22	D	4	0	0	0	0
22	E	1	0	0	0	0
22	F	1	0	0	0	0
22	I	1	0	0	0	0
22	P	2	0	0	0	0
22	Q	2	0	0	0	0
22	S	2	0	0	0	0
22	U	1	0	0	0	0
23	D	1	0	0	0	0
23	N	1	0	0	0	0
24	A	225	0	0	1	0
24	D	2	0	0	0	0
24	E	5	0	0	0	0
24	L	2	0	0	1	0
24	N	1	0	0	0	0
24	Q	2	0	0	0	0
24	T	2	0	0	0	0
All	All	52227	0	36550	722	2

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

The worst 5 of 722 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:664:G:H22	1:A:741:G:H1	1.23	0.86
20:T:100:ILE:HG22	20:T:102:GLY:H	1.41	0.86
1:A:1443:G:H5"	1:A:1446:A:H5'	1.57	0.85
1:A:1125:U:OP2	1:A:1145:C:N4	2.11	0.81
1:A:1347:G:O6	9:I:10:ARG:NH2	2.12	0.81

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

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

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
2	B	232/234 (99%)	213 (92%)	18 (8%)	1 (0%)	34 72
3	C	204/206 (99%)	188 (92%)	16 (8%)	0	100 100
4	D	206/208 (99%)	202 (98%)	4 (2%)	0	100 100
5	E	148/150 (99%)	143 (97%)	5 (3%)	0	100 100
6	F	99/101 (98%)	98 (99%)	1 (1%)	0	100 100
7	G	153/155 (99%)	149 (97%)	4 (3%)	0	100 100
8	H	136/138 (99%)	134 (98%)	2 (2%)	0	100 100
9	I	125/127 (98%)	115 (92%)	10 (8%)	0	100 100
10	J	96/98 (98%)	80 (83%)	13 (14%)	3 (3%)	4 30
11	K	114/116 (98%)	108 (95%)	6 (5%)	0	100 100
12	L	121/124 (98%)	109 (90%)	12 (10%)	0	100 100
13	M	116/118 (98%)	105 (90%)	11 (10%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
14	N	58/60 (97%)	49 (84%)	9 (16%)	0	100 100
15	O	85/87 (98%)	83 (98%)	2 (2%)	0	100 100
16	P	81/83 (98%)	79 (98%)	2 (2%)	0	100 100
17	Q	97/99 (98%)	94 (97%)	3 (3%)	0	100 100
18	R	68/70 (97%)	68 (100%)	0	0	100 100
19	S	78/80 (98%)	72 (92%)	6 (8%)	0	100 100
20	T	97/99 (98%)	84 (87%)	10 (10%)	3 (3%)	4 30
21	U	22/24 (92%)	21 (96%)	1 (4%)	0	100 100
All	All	2336/2377 (98%)	2194 (94%)	135 (6%)	7 (0%)	41 75

5 of 7 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
10	J	55	LYS
20	T	74	LYS
20	T	75	ASN
10	J	56	HIS
20	T	73	HIS

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 21
3	C	160/160 (100%)	136 (85%)	24 (15%)	3 17
4	D	180/180 (100%)	169 (94%)	11 (6%)	18 51
5	E	115/115 (100%)	104 (90%)	11 (10%)	8 34
6	F	90/90 (100%)	82 (91%)	8 (9%)	9 37
7	G	126/126 (100%)	116 (92%)	10 (8%)	12 41
8	H	119/119 (100%)	109 (92%)	10 (8%)	11 40
9	I	98/98 (100%)	82 (84%)	16 (16%)	2 13

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
10	J	87/88 (99%)	77 (88%)	10 (12%)	5 26
11	K	88/88 (100%)	83 (94%)	5 (6%)	20 53
12	L	103/103 (100%)	88 (85%)	15 (15%)	3 18
13	M	94/94 (100%)	77 (82%)	17 (18%)	1 9
14	N	49/49 (100%)	43 (88%)	6 (12%)	5 23
15	O	79/79 (100%)	66 (84%)	13 (16%)	2 13
16	P	72/72 (100%)	65 (90%)	7 (10%)	8 33
17	Q	94/94 (100%)	89 (95%)	5 (5%)	22 55
18	R	61/61 (100%)	57 (93%)	4 (7%)	16 49
19	S	71/71 (100%)	65 (92%)	6 (8%)	10 39
20	T	76/76 (100%)	65 (86%)	11 (14%)	3 18
21	U	19/19 (100%)	18 (95%)	1 (5%)	22 55
All	All	1983/1984 (100%)	1766 (89%)	217 (11%)	6 29

5 of 217 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
8	H	92	ARG
10	J	60	ARG
19	S	56	GLN
9	I	11	LYS
9	I	79	LEU

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	204	ASN
2	B	212	GLN
9	I	3	GLN
16	P	82	GLN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	1504/1522 (98%)	255 (16%)	46 (3%)

5 of 255 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	6	G
1	A	7	G
1	A	9	G
1	A	32	A
1	A	39	G

5 of 46 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	748	C
1	A	992	U
1	A	1346	A
1	A	792	A
1	A	913	A

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
1	M2G	A	966	1	20,27,28	1.78	4 (20%)	22,40,43	2.46	5 (22%)
1	PSU	A	1541	1	17,21,22	1.47	4 (23%)	20,30,33	3.67	5 (25%)
1	2MG	A	1207	1	19,26,27	2.03	3 (15%)	21,38,41	2.10	3 (14%)
1	5MC	A	1404	1	15,22,23	0.86	0	19,32,35	1.00	1 (5%)
1	MA6	A	1519[A]	1	19,26,27	0.68	0	18,38,41	0.96	1 (5%)
1	UR3	A	1498	1	14,22,23	0.70	0	15,32,35	1.00	0
1	7MG	A	527	1	22,26,27	2.06	5 (22%)	28,39,42	1.65	7 (25%)
1	5MC	A	1400	1	15,22,23	0.89	0	19,32,35	1.00	0
1	5MC	A	1407	1	15,22,23	0.87	0	19,32,35	1.02	1 (5%)
1	MA6	A	1519[B]	1	19,26,27	0.67	0	18,38,41	0.91	1 (5%)
1	MA6	A	1518[B]	1	19,26,27	0.67	0	18,38,41	0.92	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
12	0TD	L	92	12	4,9,10	1.02	0	3,11,13	2.31	1 (33%)
1	PSU	A	1540	1	17,21,22	1.44	3 (17%)	20,30,33	3.65	6 (30%)
1	PSU	A	516	1	17,21,22	1.43	3 (17%)	20,30,33	3.67	5 (25%)
1	5MC	A	967	1	15,22,23	0.85	0	19,32,35	1.05	1 (5%)
1	4OC	A	1402	1	16,23,24	0.77	0	17,32,35	0.74	0
1	MA6	A	1518[A]	1	19,26,27	0.66	0	18,38,41	0.89	1 (5%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

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

The worst 5 of 22 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1207	2MG	C2-N2	6.49	1.39	1.34
1	A	966	M2G	C6-N1	5.56	1.42	1.33
1	A	527	7MG	C8-N9	-5.38	1.33	1.45
1	A	1207	2MG	C6-N1	5.07	1.41	1.33
1	A	527	7MG	C2-N2	4.65	1.43	1.33

The worst 5 of 39 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1541	PSU	N1-C2-N3	-11.42	119.35	128.43
1	A	516	PSU	N1-C2-N3	-11.41	119.36	128.43
1	A	1540	PSU	N1-C2-N3	-11.28	119.46	128.43
1	A	516	PSU	C4-N3-C2	8.99	122.73	115.14
1	A	1541	PSU	C4-N3-C2	8.88	122.64	115.14

There are no chirality outliers.

5 of 21 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	1207	2MG	O4'-C4'-C5'-O5'
1	A	1498	UR3	O4'-C1'-N1-C6
1	A	527	7MG	C3'-C4'-C5'-O5'
1	A	1400	5MC	O4'-C4'-C5'-O5'
1	A	1400	5MC	O4'-C1'-N1-C6

There are no ring outliers.

9 monomers are involved in 16 short contacts:

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates

Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands

Unable to reproduce the depositors R factor - this section is therefore empty.

6.5 Other polymers

Unable to reproduce the depositors R factor - this section is therefore empty.