



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 06:17 PM GMT

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

This is a 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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

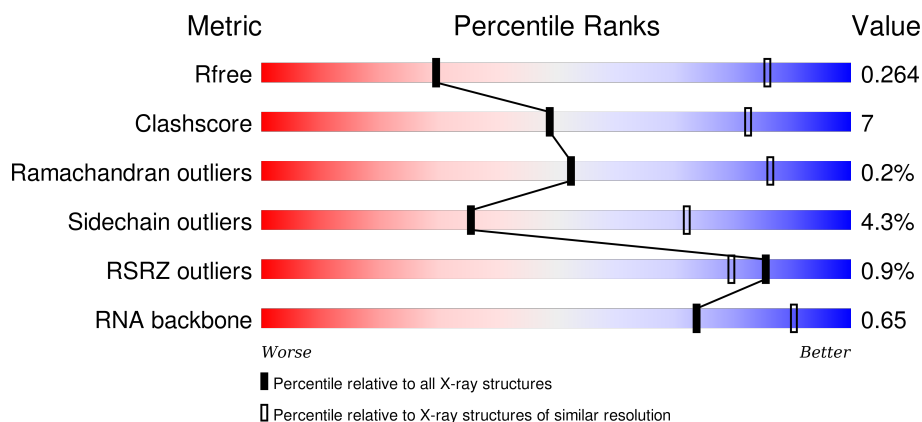
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.20 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1039 (4.80-3.60)
Clashscore	102246	1140 (4.80-3.60)
Ramachandran outliers	100387	1083 (4.80-3.60)
Sidechain outliers	100360	1067 (4.80-3.60)
RSRZ outliers	91569	1042 (4.80-3.60)
RNA backbone	2183	1087 (5.60-2.80)

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. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1522	<div> <div>2%</div> <div>61%</div> <div>31%</div> <div>7%</div> <div>.</div> </div>
2	B	256	<div> <div>64%</div> <div>26%</div> <div>8%</div> <div>.</div> </div>
3	C	239	<div> <div>67%</div> <div>18%</div> <div>14%</div> <div>.</div> </div>
4	D	209	<div> <div>79%</div> <div>19%</div> <div>.</div> </div>

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Mol	Chain	Length	Quality of chain
5	E	162	
6	F	101	
7	G	156	
8	H	138	
9	I	128	
10	J	105	
11	K	129	
12	L	134	
13	M	126	
14	N	61	
15	O	89	
16	P	88	
17	R	88	
18	S	93	
19	T	106	
20	U	27	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
21	MG	A	1621	-	-	-	X
21	MG	A	1631	-	-	-	X
21	MG	A	1632	-	-	-	X
21	MG	A	1653	-	-	-	X
21	MG	A	1654	-	-	-	X
21	MG	A	1661	-	-	-	X
21	MG	A	1666	-	-	-	X
21	MG	A	1678	-	-	-	X
21	MG	A	1700	-	-	-	X
21	MG	A	1702	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
21	MG	A	1713	-	-	-	X
21	MG	A	1721	-	-	-	X
21	MG	A	1725	-	-	-	X
21	MG	A	1727	-	-	-	X
21	MG	A	1732	-	-	-	X
21	MG	A	1735	-	-	-	X
21	MG	A	1742	-	-	-	X
21	MG	A	1745	-	-	-	X
21	MG	A	1747	-	-	-	X
21	MG	A	1787	-	-	-	X
22	K	A	1763	-	-	-	X
22	K	A	1766	-	-	-	X
22	K	A	1774	-	-	-	X

2 Entry composition

There are 23 unique types of molecules in this entry. The entry contains 51128 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1514	Total	C	N	O	P	0	0	0
			32552	14497	6020	10521	1514			

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
9	I	127	Total	C	N	O	0	0	0
			1011	639	198	174			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	J	98	Total	C	N	O	S	0	0	0
			794	499	156	138	1			

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

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

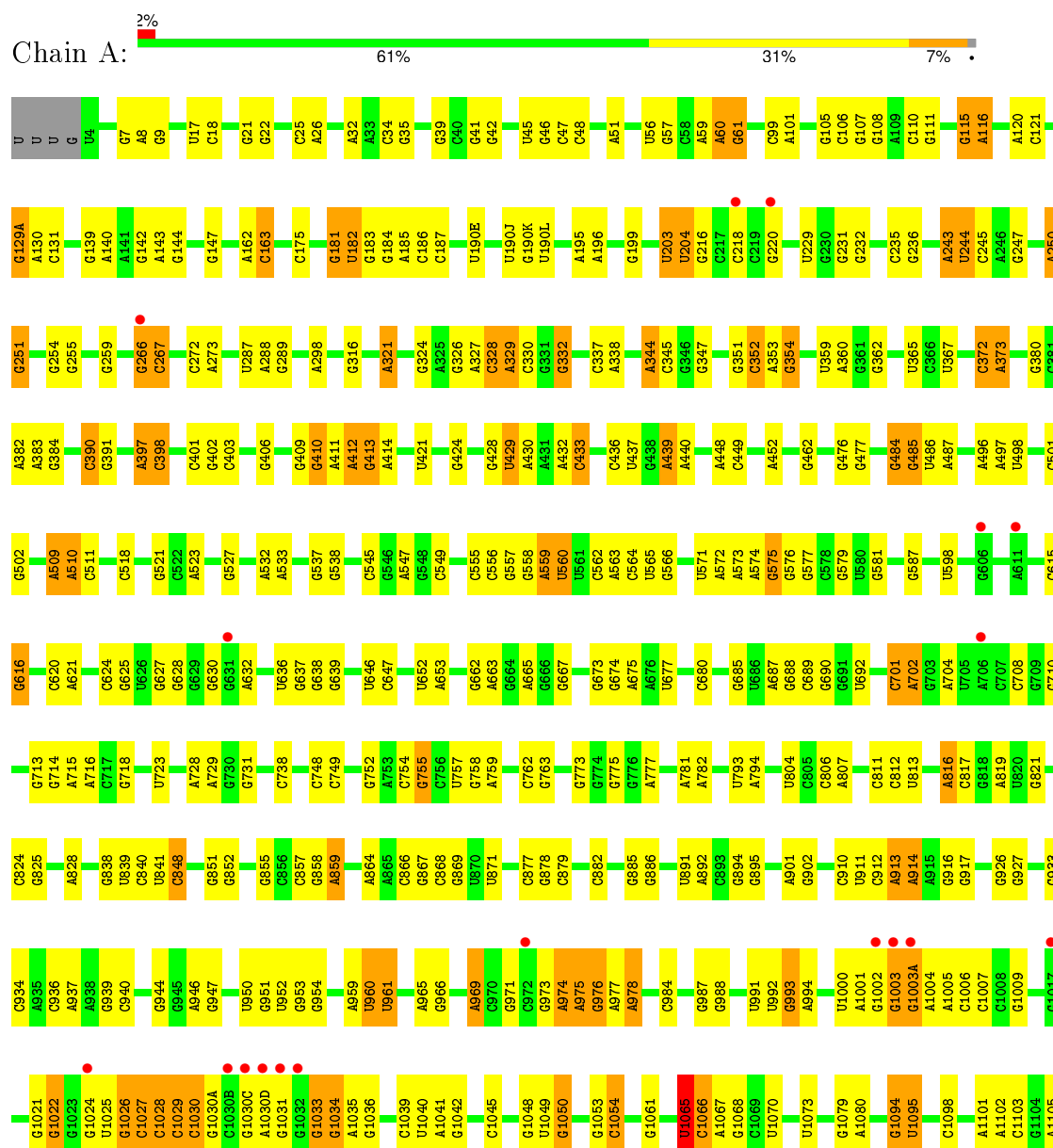
- Molecule 23 is ZINC ION (three-letter code: ZN) (formula: Zn).

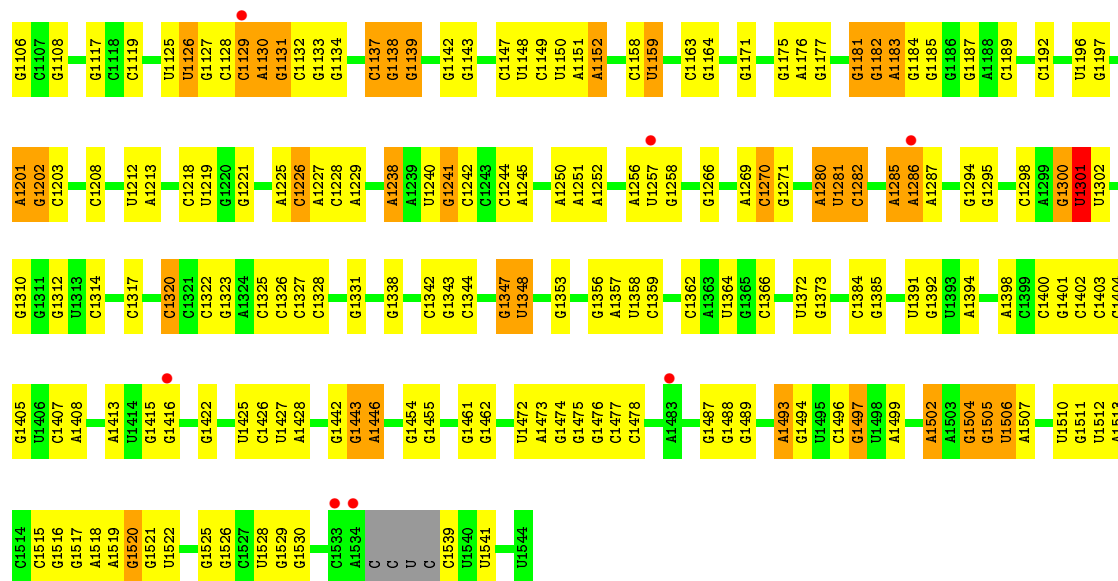
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
23	D	1	Total	Zn	0	0
			1	1		
23	N	1	Total	Zn	0	0
			1	1		

3 Residue-property plots [i](#)

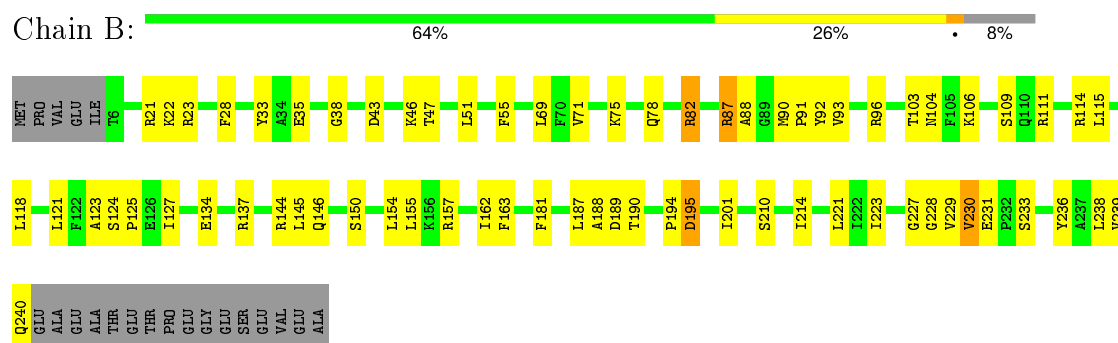
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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 ($\text{RSRZ} > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: 16S rRNA

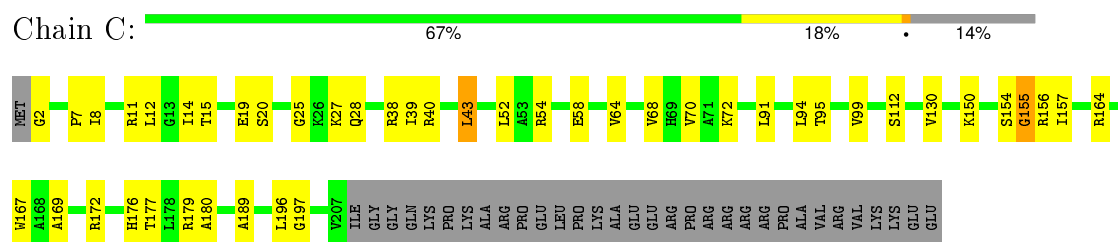




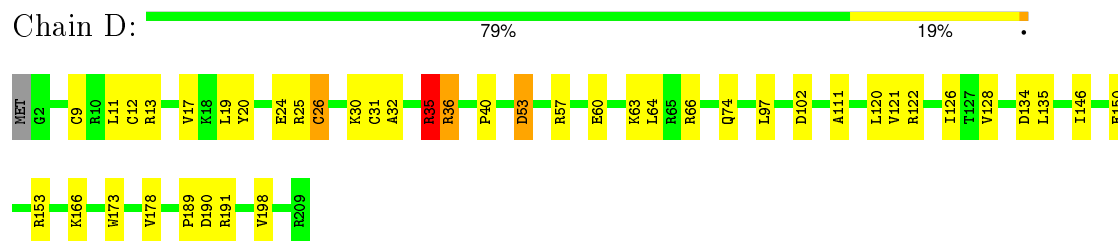
• Molecule 2: 30S ribosomal protein S2



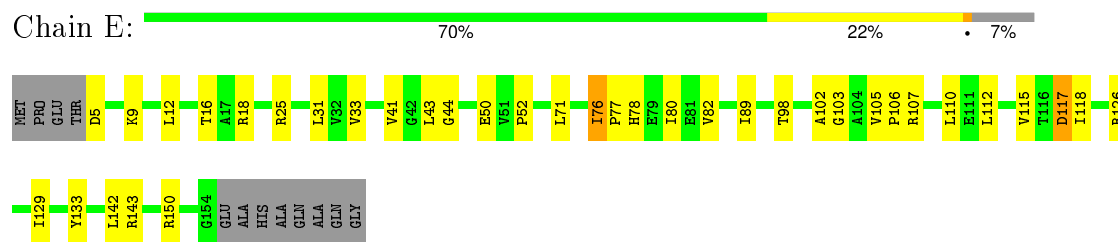
• Molecule 3: 30S ribosomal protein S3



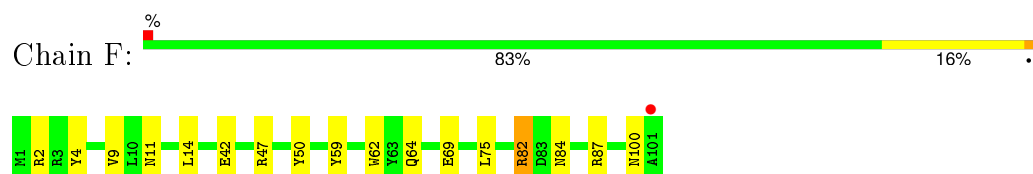
• Molecule 4: 30S ribosomal protein S4



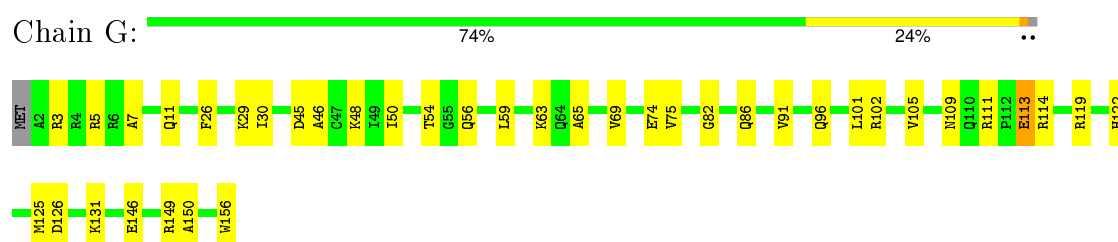
• Molecule 5: 30S ribosomal protein S5



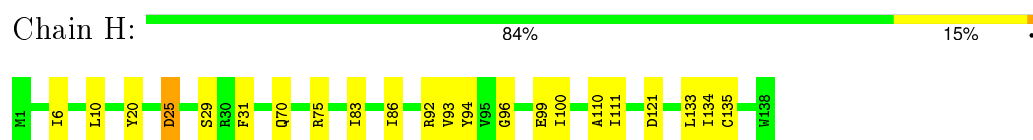
- Molecule 6: 30S ribosomal protein S6



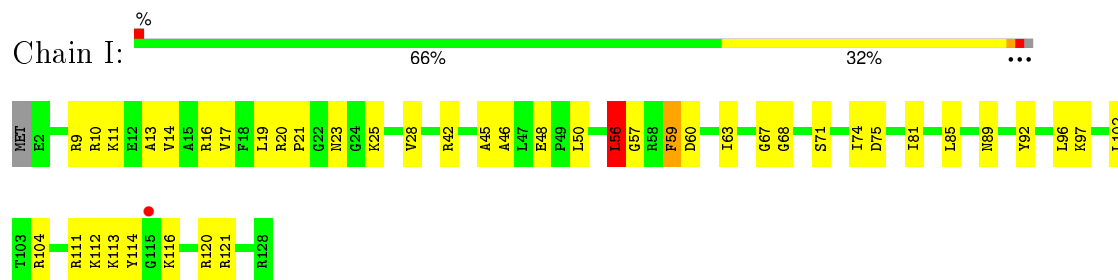
- Molecule 7: 30S ribosomal protein S7



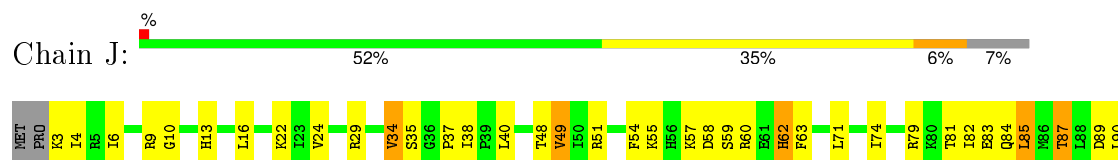
- Molecule 8: 30S ribosomal protein S8

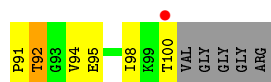


- Molecule 9: 30S ribosomal protein S9

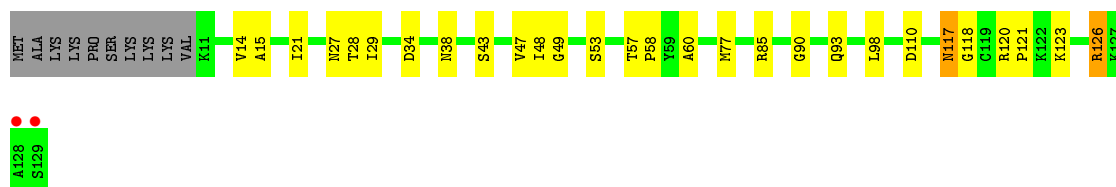


- Molecule 10: 30S ribosomal protein S10

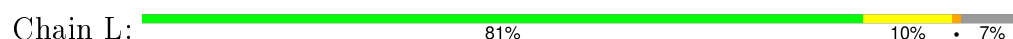




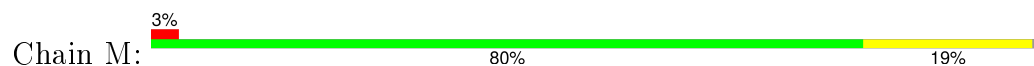
- Molecule 11: 30S ribosomal protein S11



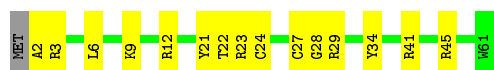
- Molecule 12: 30S ribosomal protein S12



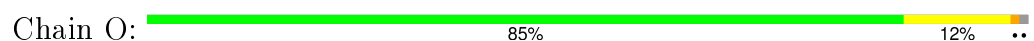
- Molecule 13: 30S ribosomal protein S13



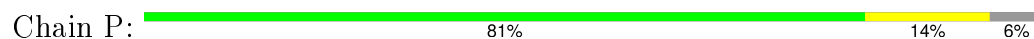
- Molecule 14: 30S ribosomal protein S14 type Z



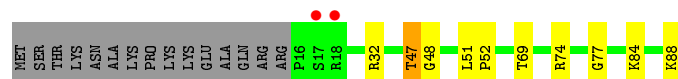
- Molecule 15: 30S ribosomal protein S15



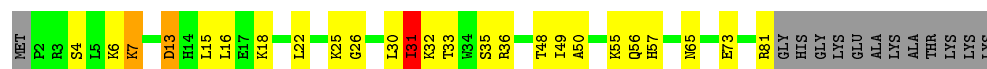
- Molecule 16: 30S ribosomal protein S16



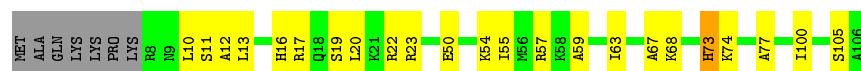
- Molecule 17: 30S ribosomal protein S18



- Molecule 18: 30S ribosomal protein S19



- Molecule 19: 30S ribosomal protein S20



- Molecule 20: 30S ribosomal protein Thx



4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	397.32Å 397.32Å 215.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.91 – 4.20 29.91 – 4.20	Depositor EDS
% Data completeness (in resolution range)	93.0 (29.91-4.20) 93.0 (29.91-4.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.07 (at 4.26Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_1370)	Depositor
R, R_{free}	0.217 , 0.258 0.232 , 0.264	Depositor DCC
R_{free} test set	5806 reflections (5.26%)	DCC
Wilson B-factor (Å ²)	202.1	Xtriage
Anisotropy	0.038	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.21 , 126.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.39$, $\langle L^2 \rangle = 0.22$	Xtriage
Outliers	0 of 116211 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	51128	wwPDB-VP
Average B, all atoms (Å ²)	200.0	wwPDB-VP

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

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: MG, MA6, K, 0TD, ZN, 2MG, 5MC, UR3, 4OC, M2G, 7MG, PSU

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.16	0/36091	0.70	11/56323 (0.0%)
2	B	0.23	0/1940	0.42	0/2616
3	C	0.21	0/1636	0.41	0/2205
4	D	0.21	0/1733	0.38	0/2318
5	E	0.22	0/1162	0.42	0/1564
6	F	0.20	0/856	0.40	0/1154
7	G	0.20	0/1276	0.38	0/1709
8	H	0.20	0/1136	0.39	0/1527
9	I	0.23	0/1029	0.45	0/1378
10	J	0.22	0/807	0.44	0/1085
11	K	0.20	0/900	0.40	0/1213
12	L	0.21	0/977	0.44	0/1306
13	M	0.19	0/1008	0.39	0/1347
14	N	0.22	0/501	0.38	0/664
15	O	0.20	0/745	0.35	0/992
16	P	0.20	0/716	0.37	0/963
17	R	0.21	0/603	0.38	0/799
18	S	0.21	0/661	0.42	0/890
19	T	0.24	0/764	0.45	0/1006
20	U	0.19	0/212	0.42	0/277
All	All	0.18	0/54753	0.63	11/81336 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
3	C	0	1
4	D	0	1
9	I	0	2

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

There are no bond length outliers.

The worst 5 of 11 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1054	C	N1-C2-O2	8.18	123.81	118.90
1	A	1054	C	C2-N1-C1'	8.13	127.74	118.80
1	A	1158	C	N1-C2-O2	7.62	123.47	118.90
1	A	1158	C	C2-N1-C1'	7.25	126.77	118.80
1	A	1054	C	N3-C2-O2	-6.42	117.40	121.90

There are no chirality outliers.

All (4) planarity outliers are listed below:

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

5.2 Too-close contacts [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	32552	0	16453	343	0
2	B	1905	0	1958	41	0
3	C	1612	0	1677	28	0
4	D	1703	0	1763	33	0
5	E	1146	0	1207	24	0
6	F	843	0	857	9	0
7	G	1257	0	1296	23	0
8	H	1116	0	1177	14	0
9	I	1011	0	1043	28	0
10	J	794	0	840	33	1
11	K	885	0	904	17	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
12	L	972	0	1058	11	0
13	M	997	0	1072	19	0
14	N	492	0	529	13	0
15	O	734	0	771	8	0
16	P	700	0	720	8	0
17	R	597	0	666	8	0
18	S	647	0	673	14	0
19	T	762	0	859	13	0
20	U	208	0	221	5	0
21	A	152	0	0	0	0
21	B	1	0	0	0	0
21	D	1	0	0	0	0
21	E	2	0	0	0	0
21	M	1	0	0	0	0
21	U	1	0	0	0	0
22	A	35	0	0	0	0
23	D	1	0	0	0	0
23	N	1	0	0	0	0
All	All	51128	0	35744	608	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

The worst 5 of 608 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:28:VAL:HG22	9:I:63:ILE:HB	1.67	0.76
1:A:1405:G:HO2'	1:A:1518:MA6:HO2'	1.34	0.74
3:C:58:GLU:HB3	10:J:92:THR:HG21	1.69	0.74
6:F:9:VAL:HB	6:F:87:ARG:HB2	1.70	0.74
1:A:959:A:HO2'	1:A:984:C:HO2'	1.33	0.73

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:87:THR:OG1	10:J:87:THR:OG1[8_554]	2.01	0.19

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	233/256 (91%)	204 (88%)	27 (12%)	2 (1%)	21	67
3	C	204/239 (85%)	176 (86%)	28 (14%)	0	100	100
4	D	206/209 (99%)	190 (92%)	16 (8%)	0	100	100
5	E	148/162 (91%)	142 (96%)	6 (4%)	0	100	100
6	F	99/101 (98%)	95 (96%)	4 (4%)	0	100	100
7	G	153/156 (98%)	138 (90%)	15 (10%)	0	100	100
8	H	136/138 (99%)	129 (95%)	7 (5%)	0	100	100
9	I	125/128 (98%)	112 (90%)	13 (10%)	0	100	100
10	J	96/105 (91%)	82 (85%)	13 (14%)	1 (1%)	19	65
11	K	117/129 (91%)	103 (88%)	14 (12%)	0	100	100
12	L	121/134 (90%)	112 (93%)	8 (7%)	1 (1%)	24	69
13	M	123/126 (98%)	112 (91%)	11 (9%)	0	100	100
14	N	58/61 (95%)	53 (91%)	5 (9%)	0	100	100
15	O	86/89 (97%)	79 (92%)	7 (8%)	0	100	100
16	P	81/88 (92%)	78 (96%)	3 (4%)	0	100	100
17	R	71/88 (81%)	66 (93%)	5 (7%)	0	100	100
18	S	78/93 (84%)	71 (91%)	6 (8%)	1 (1%)	15	60
19	T	97/106 (92%)	84 (87%)	13 (13%)	0	100	100
20	U	22/27 (82%)	19 (86%)	3 (14%)	0	100	100
All	All	2254/2435 (93%)	2045 (91%)	204 (9%)	5 (0%)	52	86

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	229	VAL
10	J	34	VAL

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

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	202/220 (92%)	191 (95%)	11 (5%)	27	67
3	C	160/188 (85%)	155 (97%)	5 (3%)	47	78
4	D	180/181 (99%)	171 (95%)	9 (5%)	30	68
5	E	115/123 (94%)	107 (93%)	8 (7%)	19	59
6	F	90/90 (100%)	86 (96%)	4 (4%)	35	71
7	G	126/127 (99%)	123 (98%)	3 (2%)	57	83
8	H	119/119 (100%)	116 (98%)	3 (2%)	55	82
9	I	98/99 (99%)	93 (95%)	5 (5%)	29	68
10	J	88/92 (96%)	80 (91%)	8 (9%)	12	47
11	K	90/99 (91%)	86 (96%)	4 (4%)	35	71
12	L	103/109 (94%)	100 (97%)	3 (3%)	50	79
13	M	100/101 (99%)	98 (98%)	2 (2%)	63	86
14	N	49/50 (98%)	46 (94%)	3 (6%)	23	63
15	O	79/80 (99%)	77 (98%)	2 (2%)	55	82
16	P	72/74 (97%)	71 (99%)	1 (1%)	74	89
17	R	64/77 (83%)	63 (98%)	1 (2%)	70	88
18	S	71/80 (89%)	65 (92%)	6 (8%)	13	51
19	T	76/82 (93%)	73 (96%)	3 (4%)	39	74
20	U	19/22 (86%)	18 (95%)	1 (5%)	28	67
All	All	1901/2013 (94%)	1819 (96%)	82 (4%)	35	72

5 of 82 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
7	G	11	GLN
9	I	85	LEU
18	S	31	ILE
7	G	113	GLU
8	H	29	SER

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

Mol	Chain	Res	Type
2	B	104	ASN
4	D	42	GLN
4	D	201	GLN
16	P	65	GLN

5.3.3 RNA ⓘ

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

5 of 215 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	8	A
1	A	9	G
1	A	32	A
1	A	39	G
1	A	47	C

5 of 40 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	687	A
1	A	913	A
1	A	1347	G
1	A	748	C
1	A	960	U

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
1	2MG	A	1207	1	17,26,27	2.06	3 (17%)	21,38,41	2.12	3 (14%)
1	5MC	A	1400	1	13,22,23	1.01	1 (7%)	15,32,35	0.95	1 (6%)
1	4OC	A	1402	1	13,23,24	0.71	1 (7%)	18,32,35	0.67	0
1	5MC	A	1404	1	13,22,23	0.97	0	15,32,35	0.91	1 (6%)
1	5MC	A	1407	1	13,22,23	0.98	1 (7%)	15,32,35	0.94	1 (6%)
1	UR3	A	1498	1	12,22,23	1.10	2 (16%)	16,32,35	1.09	1 (6%)
1	MA6	A	1518	1	16,26,27	1.11	2 (12%)	18,38,41	1.02	2 (11%)
1	MA6	A	1519	1	16,26,27	1.15	2 (12%)	18,38,41	1.03	2 (11%)
1	PSU	A	1540	1	13,21,22	1.05	1 (7%)	18,30,33	3.60	6 (33%)
1	PSU	A	1541	1	13,21,22	1.09	1 (7%)	18,30,33	3.58	6 (33%)
1	PSU	A	516	1,21	13,21,22	1.08	1 (7%)	18,30,33	3.57	5 (27%)
1	7MG	A	527	1	19,26,27	2.61	5 (26%)	24,39,42	2.03	6 (25%)
1	M2G	A	966	1	17,27,28	2.07	4 (23%)	22,40,43	2.11	3 (13%)
1	5MC	A	967	1	13,22,23	0.99	0	15,32,35	0.90	1 (6%)
12	0TD	L	92	12	4,9,10	0.76	0	4,11,13	1.31	1 (25%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	2MG	A	1207	1	-	0/5/27/28	0/3/3/3
1	5MC	A	1400	1	-	0/3/25/26	0/2/2/2
1	4OC	A	1402	1	-	0/7/29/30	0/2/2/2
1	5MC	A	1404	1	-	0/3/25/26	0/2/2/2
1	5MC	A	1407	1	-	0/3/25/26	0/2/2/2
1	UR3	A	1498	1	-	0/3/25/26	0/2/2/2
1	MA6	A	1518	1	-	0/7/29/30	0/3/3/3
1	MA6	A	1519	1	-	0/7/29/30	0/3/3/3
1	PSU	A	1540	1	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	PSU	A	1541	1	-	0/7/25/26	0/2/2/2
1	PSU	A	516	1,21	-	0/7/25/26	0/2/2/2
1	7MG	A	527	1	-	0/7/37/38	0/3/3/3
1	M2G	A	966	1	-	0/7/29/30	0/3/3/3
1	5MC	A	967	1	-	0/3/25/26	0/2/2/2
12	0TD	L	92	12	-	0/2/12/14	0/0/0/0

The worst 5 of 24 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	527	7MG	C8-N9	-7.21	1.35	1.45
1	A	527	7MG	CM7-N7	-2.08	1.42	1.46
1	A	1407	5MC	C5-C4	2.06	1.44	1.41
1	A	1518	MA6	C2-N1	2.06	1.37	1.33
1	A	1400	5MC	C5-C4	2.15	1.44	1.41

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	516	PSU	N1-C2-N3	-12.89	120.11	128.33
1	A	1540	PSU	N1-C2-N3	-12.83	120.15	128.33
1	A	1541	PSU	N1-C2-N3	-12.81	120.16	128.33
1	A	966	M2G	C5-C6-N1	-8.22	112.35	123.59
1	A	1207	2MG	C5-C6-N1	-7.48	113.37	123.59

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

7 monomers are involved in 11 short contacts:

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 195 ligands modelled in this entry, 195 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

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

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	1500/1522 (98%)	0.15	25 (1%) 73 63	155, 192, 264, 505	0
2	B	235/256 (91%)	-0.44	0 100 100	134, 193, 274, 327	0
3	C	206/239 (86%)	-0.55	0 100 100	134, 182, 248, 311	0
4	D	208/209 (99%)	-0.55	0 100 100	114, 181, 253, 369	0
5	E	150/162 (92%)	-0.59	0 100 100	118, 175, 226, 277	0
6	F	101/101 (100%)	-0.65	1 (0%) 84 77	143, 207, 273, 471	0
7	G	155/156 (99%)	-0.54	0 100 100	153, 204, 257, 309	0
8	H	138/138 (100%)	-0.61	0 100 100	123, 172, 226, 242	0
9	I	127/128 (99%)	-0.28	1 (0%) 87 82	179, 238, 348, 501	0
10	J	98/105 (93%)	-0.42	1 (1%) 84 77	174, 222, 313, 438	0
11	K	119/129 (92%)	-0.33	2 (1%) 73 63	117, 184, 254, 371	0
12	L	123/134 (91%)	-0.52	0 100 100	139, 181, 231, 259	0
13	M	125/126 (99%)	-0.35	4 (3%) 51 39	176, 215, 311, 427	0
14	N	60/61 (98%)	-0.36	0 100 100	140, 200, 285, 315	0
15	O	88/89 (98%)	-0.59	0 100 100	155, 197, 253, 326	0
16	P	83/88 (94%)	-0.59	0 100 100	148, 183, 219, 272	0
17	R	73/88 (82%)	-0.24	2 (2%) 58 47	122, 209, 331, 418	0
18	S	80/93 (86%)	-0.43	0 100 100	189, 220, 289, 312	0
19	T	99/106 (93%)	-0.72	0 100 100	131, 185, 243, 335	0
20	U	24/27 (88%)	0.25	0 100 100	193, 228, 255, 277	0
All	All	3792/3957 (95%)	-0.23	36 (0%) 85 80	114, 193, 274, 505	0

The worst 5 of 36 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1030(D)	A	10.7
11	K	129	SER	7.1
17	R	17	SER	6.0
11	K	128	ALA	6.0
1	A	1003(A)	G	5.0

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
1	M2G	A	966	25/26	0.96	0.14	-	158,179,213,255	0
1	PSU	A	1540	20/21	0.85	0.41	-	194,249,259,261	0
1	UR3	A	1498	21/22	0.94	0.22	-	178,181,221,230	0
1	4OC	A	1402	22/23	0.98	0.19	-	175,177,227,231	0
1	7MG	A	527	24/25	0.96	0.14	-	161,162,170,198	0
1	5MC	A	1407	21/22	0.97	0.14	-	189,192,212,231	0
1	5MC	A	967	21/22	0.96	0.15	-	158,162,188,203	0
1	PSU	A	1541	20/21	0.89	0.23	-	177,179,242,254	0
12	0TD	L	92	10/11	0.95	0.34	-	167,204,309,368	0
1	MA6	A	1518	24/25	0.95	0.19	-	185,186,226,235	0
1	5MC	A	1404	21/22	0.94	0.21	-	178,180,182,204	0
1	5MC	A	1400	21/22	0.92	0.19	-	175,178,193,234	0
1	2MG	A	1207	24/25	0.95	0.16	-	182,186,190,197	0
1	MA6	A	1519	24/25	0.94	0.21	-	180,183,202,229	0
1	PSU	A	516	20/21	0.93	0.14	-	175,181,212,258	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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors

of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
21	MG	A	1653	1/1	0.89	0.60	18.49	111,111,111,111	0
21	MG	A	1702	1/1	0.78	0.95	15.03	197,197,197,197	0
21	MG	A	1747	1/1	0.85	0.40	11.15	173,173,173,173	0
21	MG	A	1745	1/1	0.88	0.47	9.44	214,214,214,214	0
21	MG	A	1700	1/1	0.95	0.71	9.26	102,102,102,102	0
21	MG	A	1632	1/1	0.60	0.71	8.62	103,103,103,103	0
21	MG	A	1713	1/1	0.96	0.55	8.23	113,113,113,113	0
21	MG	A	1721	1/1	0.97	0.43	8.11	121,121,121,121	0
22	K	A	1774	1/1	0.90	0.39	8.05	168,168,168,168	0
21	MG	A	1621	1/1	0.71	0.58	7.78	134,134,134,134	0
21	MG	A	1742	1/1	0.60	0.51	7.72	143,143,143,143	0
21	MG	A	1732	1/1	0.83	0.44	7.22	163,163,163,163	0
21	MG	A	1631	1/1	0.96	0.49	5.97	141,141,141,141	0
21	MG	A	1735	1/1	0.96	0.37	5.51	167,167,167,167	0
21	MG	A	1725	1/1	0.95	0.72	4.72	208,208,208,208	0
21	MG	A	1678	1/1	0.95	0.31	4.70	88,88,88,88	0
21	MG	A	1787	1/1	0.74	0.65	4.27	92,92,92,92	0
22	K	A	1763	1/1	0.97	0.39	4.11	149,149,149,149	0
22	K	A	1766	1/1	0.96	0.32	3.20	168,168,168,168	0
21	MG	A	1727	1/1	0.97	0.25	2.93	177,177,177,177	0
21	MG	A	1654	1/1	0.96	0.28	2.57	114,114,114,114	0
21	MG	A	1666	1/1	0.88	0.32	2.32	138,138,138,138	0
21	MG	A	1741	1/1	0.94	0.18	1.88	193,193,193,193	0
21	MG	A	1661	1/1	0.84	0.41	1.37	75,75,75,75	0
21	MG	E	201	1/1	0.69	0.29	1.18	151,151,151,151	0
21	MG	A	1604	1/1	0.94	0.23	0.82	311,311,311,311	0
23	ZN	D	301	1/1	0.99	0.38	0.80	157,157,157,157	0
21	MG	A	1662	1/1	0.90	0.23	0.72	89,89,89,89	0
21	MG	A	1602	1/1	0.90	0.12	0.45	149,149,149,149	0
21	MG	A	1750	1/1	0.94	0.17	0.32	134,134,134,134	0
21	MG	A	1724	1/1	0.92	0.27	0.29	99,99,99,99	0
21	MG	A	1673	1/1	0.94	0.26	0.25	122,122,122,122	0
21	MG	A	1707	1/1	0.99	0.18	0.15	73,73,73,73	0
21	MG	A	1685	1/1	0.98	0.17	0.09	82,82,82,82	0
21	MG	A	1658	1/1	0.88	0.28	0.03	111,111,111,111	0
21	MG	A	1641	1/1	0.96	0.17	0.02	74,74,74,74	0
21	MG	A	1683	1/1	0.94	0.19	-0.06	133,133,133,133	0
21	MG	A	1636	1/1	0.94	0.18	-0.27	59,59,59,59	0
21	MG	M	201	1/1	0.95	0.21	-0.36	186,186,186,186	0
21	MG	A	1736	1/1	0.97	0.15	-0.40	164,164,164,164	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
21	MG	U	101	1/1	0.94	0.24	-0.42	523,523,523,523	0
21	MG	A	1668	1/1	0.88	0.16	-0.45	159,159,159,159	0
21	MG	A	1743	1/1	0.96	0.15	-0.54	135,135,135,135	0
21	MG	A	1709	1/1	0.97	0.18	-0.82	89,89,89,89	0
21	MG	A	1746	1/1	0.79	0.14	-1.07	114,114,114,114	0
21	MG	D	302	1/1	0.97	0.07	-1.45	100,100,100,100	0
21	MG	A	1699	1/1	0.98	0.14	-1.48	122,122,122,122	0
21	MG	A	1612	1/1	0.93	0.16	-1.71	163,163,163,163	0
23	ZN	N	101	1/1	0.98	0.13	-1.76	124,124,124,124	0
21	MG	A	1720	1/1	0.99	0.12	-1.95	76,76,76,76	0
21	MG	A	1731	1/1	0.97	0.07	-2.29	116,116,116,116	0
21	MG	A	1739	1/1	0.98	0.15	-2.65	126,126,126,126	0
21	MG	A	1628	1/1	0.96	0.23	-	159,159,159,159	0
21	MG	A	1716	1/1	0.90	0.15	-	179,179,179,179	0
22	K	A	1770	1/1	0.93	0.63	-	202,202,202,202	0
21	MG	A	1603	1/1	0.82	1.12	-	98,98,98,98	0
21	MG	A	1728	1/1	0.83	0.39	-	151,151,151,151	0
21	MG	A	1749	1/1	0.90	0.79	-	130,130,130,130	0
21	MG	A	1684	1/1	0.62	0.41	-	150,150,150,150	0
21	MG	A	1711	1/1	0.97	0.31	-	177,177,177,177	0
22	K	A	1753	1/1	0.76	0.25	-	176,176,176,176	0
21	MG	A	1617	1/1	0.94	0.24	-	173,173,173,173	0
21	MG	A	1639	1/1	0.93	0.49	-	157,157,157,157	0
21	MG	A	1649	1/1	0.99	0.17	-	71,71,71,71	0
21	MG	A	1717	1/1	0.98	0.12	-	79,79,79,79	0
21	MG	A	1675	1/1	0.92	0.29	-	94,94,94,94	0
21	MG	A	1633	1/1	0.78	0.47	-	59,59,59,59	0
22	K	A	1756	1/1	0.96	0.73	-	178,178,178,178	0
21	MG	A	1681	1/1	0.97	0.36	-	165,165,165,165	0
21	MG	A	1715	1/1	0.98	0.45	-	105,105,105,105	0
21	MG	A	1695	1/1	0.90	0.21	-	71,71,71,71	0
21	MG	A	1738	1/1	0.98	0.75	-	116,116,116,116	0
21	MG	A	1609	1/1	0.96	0.44	-	51,51,51,51	0
21	MG	A	1615	1/1	0.67	0.26	-	138,138,138,138	0
21	MG	A	1737	1/1	0.93	0.07	-	132,132,132,132	0
21	MG	A	1687	1/1	0.51	0.83	-	143,143,143,143	0
21	MG	A	1689	1/1	0.97	0.42	-	182,182,182,182	0
21	MG	A	1671	1/1	0.96	0.46	-	48,48,48,48	0
21	MG	A	1730	1/1	0.87	0.39	-	188,188,188,188	0
21	MG	A	1729	1/1	0.99	0.18	-	68,68,68,68	0
21	MG	A	1682	1/1	0.88	0.34	-	128,128,128,128	0
21	MG	A	1679	1/1	0.98	0.25	-	116,116,116,116	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
22	K	A	1782	1/1	0.76	0.48	-	162,162,162,162	0
22	K	A	1758	1/1	0.76	0.85	-	199,199,199,199	0
21	MG	A	1710	1/1	0.92	0.31	-	119,119,119,119	0
22	K	A	1754	1/1	0.91	0.34	-	168,168,168,168	0
22	K	A	1765	1/1	0.73	0.86	-	168,168,168,168	0
21	MG	A	1619	1/1	0.91	0.93	-	126,126,126,126	0
21	MG	A	1656	1/1	0.81	1.06	-	65,65,65,65	0
21	MG	A	1694	1/1	0.89	0.33	-	133,133,133,133	0
21	MG	A	1611	1/1	0.77	0.55	-	85,85,85,85	0
22	K	A	1778	1/1	0.97	0.41	-	208,208,208,208	0
21	MG	A	1655	1/1	0.81	0.29	-	65,65,65,65	0
21	MG	A	1703	1/1	0.89	0.93	-	115,115,115,115	0
21	MG	A	1624	1/1	0.92	0.84	-	174,174,174,174	0
21	MG	A	1663	1/1	0.96	0.10	-	147,147,147,147	0
21	MG	A	1613	1/1	0.92	0.25	-	161,161,161,161	0
21	MG	A	1722	1/1	0.98	0.39	-	55,55,55,55	0
22	K	A	1786	1/1	0.77	0.68	-	215,215,215,215	0
21	MG	A	1601	1/1	0.97	0.19	-	187,187,187,187	0
21	MG	A	1622	1/1	0.93	0.33	-	142,142,142,142	0
21	MG	A	1726	1/1	0.97	0.14	-	129,129,129,129	0
21	MG	A	1635	1/1	0.75	0.34	-	61,61,61,61	0
21	MG	A	1674	1/1	0.00	1.81	-	192,192,192,192	0
21	MG	A	1712	1/1	0.88	0.66	-	85,85,85,85	0
22	K	A	1780	1/1	0.78	0.39	-	149,149,149,149	0
21	MG	A	1733	1/1	0.94	0.17	-	170,170,170,170	0
22	K	A	1761	1/1	0.88	0.25	-	181,181,181,181	0
21	MG	A	1676	1/1	0.98	0.22	-	74,74,74,74	0
21	MG	A	1605	1/1	0.86	0.32	-	92,92,92,92	0
22	K	A	1776	1/1	0.15	0.32	-	198,198,198,198	0
21	MG	A	1645	1/1	0.97	0.28	-	55,55,55,55	0
21	MG	A	1626	1/1	0.69	0.24	-	130,130,130,130	0
21	MG	A	1606	1/1	0.95	0.29	-	247,247,247,247	0
21	MG	A	1634	1/1	0.97	0.07	-	118,118,118,118	0
21	MG	A	1701	1/1	0.97	0.45	-	68,68,68,68	0
21	MG	A	1714	1/1	0.95	0.21	-	136,136,136,136	0
21	MG	A	1660	1/1	0.94	0.16	-	121,121,121,121	0
21	MG	A	1748	1/1	0.94	0.17	-	267,267,267,267	0
21	MG	A	1744	1/1	0.87	0.75	-	143,143,143,143	0
21	MG	A	1638	1/1	0.98	0.34	-	116,116,116,116	0
22	K	A	1759	1/1	0.82	0.36	-	186,186,186,186	0
21	MG	A	1705	1/1	0.94	0.45	-	189,189,189,189	0
22	K	A	1760	1/1	0.97	0.16	-	207,207,207,207	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
22	K	A	1772	1/1	0.93	0.10	-	178,178,178,178	0
22	K	A	1781	1/1	0.99	0.13	-	149,149,149,149	0
21	MG	A	1669	1/1	0.97	0.51	-	85,85,85,85	0
21	MG	A	1667	1/1	0.78	0.49	-	236,236,236,236	0
21	MG	A	1657	1/1	0.91	0.53	-	75,75,75,75	0
21	MG	A	1614	1/1	0.97	0.25	-	94,94,94,94	0
22	K	A	1784	1/1	0.93	0.12	-	141,141,141,141	0
21	MG	A	1610	1/1	0.63	1.10	-	130,130,130,130	0
22	K	A	1783	1/1	0.85	0.43	-	187,187,187,187	0
21	MG	A	1719	1/1	0.90	0.72	-	196,196,196,196	0
21	MG	B	301	1/1	0.90	0.46	-	143,143,143,143	0
21	MG	E	202	1/1	0.63	0.34	-	99,99,99,99	0
21	MG	A	1630	1/1	0.93	1.14	-	90,90,90,90	0
21	MG	A	1627	1/1	0.20	1.29	-	177,177,177,177	0
21	MG	A	1688	1/1	0.83	0.51	-	181,181,181,181	0
21	MG	A	1646	1/1	0.99	0.26	-	81,81,81,81	0
22	K	A	1773	1/1	0.95	0.38	-	116,116,116,116	0
21	MG	A	1692	1/1	0.86	0.69	-	101,101,101,101	0
21	MG	A	1706	1/1	0.64	0.89	-	137,137,137,137	0
21	MG	A	1708	1/1	0.95	0.34	-	146,146,146,146	0
21	MG	A	1648	1/1	0.85	0.35	-	112,112,112,112	0
22	K	A	1768	1/1	0.76	0.15	-	229,229,229,229	0
21	MG	A	1608	1/1	0.83	0.48	-	117,117,117,117	0
21	MG	A	1693	1/1	0.94	0.39	-	104,104,104,104	0
21	MG	A	1751	1/1	0.92	0.30	-	113,113,113,113	0
22	K	A	1767	1/1	0.95	0.16	-	149,149,149,149	0
21	MG	A	1690	1/1	0.86	0.30	-	74,74,74,74	0
21	MG	A	1652	1/1	0.98	0.52	-	172,172,172,172	0
22	K	A	1752	1/1	0.78	0.28	-	176,176,176,176	0
21	MG	A	1643	1/1	0.97	0.39	-	170,170,170,170	0
21	MG	A	1697	1/1	0.96	0.15	-	165,165,165,165	0
21	MG	A	1607	1/1	0.79	1.26	-	122,122,122,122	0
21	MG	A	1677	1/1	0.96	0.21	-	120,120,120,120	0
22	K	A	1757	1/1	0.85	0.37	-	204,204,204,204	0
21	MG	A	1650	1/1	0.83	0.95	-	127,127,127,127	0
21	MG	A	1629	1/1	0.85	0.30	-	171,171,171,171	0
22	K	A	1755	1/1	0.28	0.53	-	187,187,187,187	0
21	MG	A	1665	1/1	0.89	0.34	-	205,205,205,205	0
21	MG	A	1623	1/1	0.81	0.55	-	154,154,154,154	0
21	MG	A	1637	1/1	0.93	0.55	-	68,68,68,68	0
21	MG	A	1670	1/1	0.98	0.18	-	74,74,74,74	0
22	K	A	1775	1/1	0.94	0.08	-	273,273,273,273	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
21	MG	A	1672	1/1	0.79	0.41	-	171,171,171,171	0
21	MG	A	1618	1/1	0.79	0.36	-	193,193,193,193	0
21	MG	A	1659	1/1	0.85	0.39	-	81,81,81,81	0
21	MG	A	1616	1/1	0.30	0.90	-	158,158,158,158	0
21	MG	A	1734	1/1	0.98	0.06	-	366,366,366,366	0
21	MG	A	1686	1/1	0.60	0.17	-	97,97,97,97	0
21	MG	A	1723	1/1	0.93	0.64	-	102,102,102,102	0
21	MG	A	1718	1/1	0.99	0.06	-	86,86,86,86	0
21	MG	A	1640	1/1	0.99	0.19	-	90,90,90,90	0
21	MG	A	1704	1/1	0.93	0.22	-	112,112,112,112	0
22	K	A	1779	1/1	0.93	0.40	-	217,217,217,217	0
22	K	A	1777	1/1	0.79	0.11	-	228,228,228,228	0
21	MG	A	1680	1/1	0.80	0.33	-	88,88,88,88	0
21	MG	A	1664	1/1	0.83	0.67	-	166,166,166,166	0
22	K	A	1762	1/1	0.93	0.17	-	181,181,181,181	0
22	K	A	1785	1/1	0.85	0.66	-	158,158,158,158	0
21	MG	A	1647	1/1	0.95	0.61	-	199,199,199,199	0
21	MG	A	1642	1/1	0.88	0.17	-	105,105,105,105	0
21	MG	A	1696	1/1	0.73	0.43	-	156,156,156,156	0
21	MG	A	1698	1/1	0.78	0.28	-	104,104,104,104	0
21	MG	A	1625	1/1	0.91	1.42	-	140,140,140,140	0
21	MG	A	1651	1/1	0.99	0.39	-	70,70,70,70	0
22	K	A	1764	1/1	0.95	0.24	-	206,206,206,206	0
21	MG	A	1620	1/1	0.94	0.20	-	126,126,126,126	0
21	MG	A	1691	1/1	0.77	0.85	-	111,111,111,111	0
22	K	A	1771	1/1	0.82	0.94	-	197,197,197,197	0
21	MG	A	1740	1/1	0.86	0.60	-	114,114,114,114	0
21	MG	A	1644	1/1	0.99	0.05	-	123,123,123,123	0
22	K	A	1769	1/1	0.91	0.27	-	193,193,193,193	0

6.5 Other polymers

There are no such residues in this entry.