



wwPDB X-ray Structure Validation Summary Report

Feb 28, 2014 – 07:39 AM GMT

PDB ID : 4DHB
Title : Crystal structure of YAEJ bound to the 70S ribosome
Authors : Gagnon, M.G.; Seetharaman, S.V.; Bulkley, D.P.; Steitz, T.A.
Deposited on : 2012-01-27
Resolution : 3.20 Å(reported)

This is a wwPDB 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/ValidationPDFNotes.html>

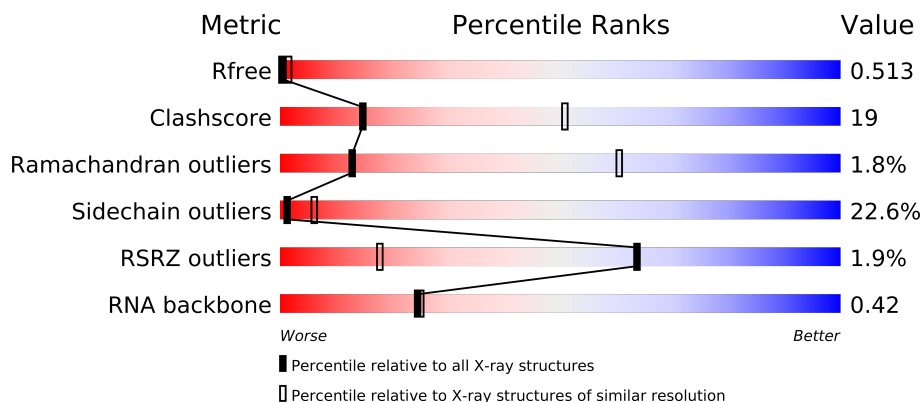
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 3.20 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.



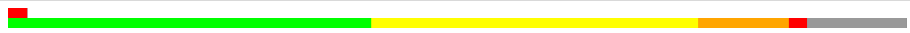
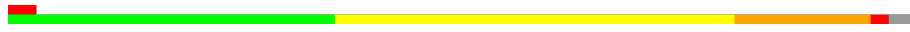


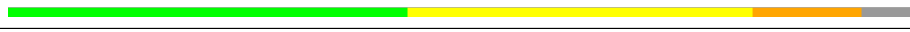

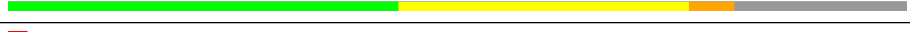


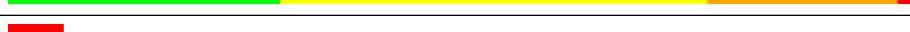
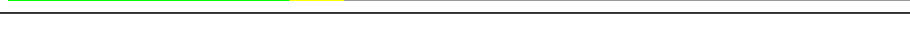
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	66092	1824 (3.30-3.10)
Clashscore	79885	1078 (3.26-3.14)
Ramachandran outliers	78287	1059 (3.26-3.14)
Sidechain outliers	78261	1058 (3.26-3.14)
RSRZ outliers	66119	1825 (3.30-3.10)
RNA backbone	1838	1002 (3.72-2.68)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	1522	
2	B	256	
3	C	239	
4	D	209	
5	E	162	
6	F	101	
7	G	156	
8	H	138	
9	I	128	
10	J	105	
11	K	129	
12	L	132	

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Mol	Chain	Length	Quality of chain
13	M	126	
14	N	61	
15	O	89	
16	P	88	
17	Q	105	
18	R	88	
19	S	93	
20	T	106	
21	U	27	
22	V	77	
23	X	16	

2 Entry composition

There are 26 unique types of molecules in this entry. The entry contains 51411 atoms, of which 0 are hydrogen and 0 are deuterium.

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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1461	Total	C	N	O	P	0	0	0
			31406	13979	5822	10145	1460			

- 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	1
			1817	1160	325	327	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
			1453	908	280	264	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
			1537	968	287	276	6			

- Molecule 5 is a protein called 30S Ribosomal Protein S5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	149	Total	C	N	O	S	0	0	0
			1115	706	206	199	4			

- Molecule 6 is a protein called 30S Ribosomal Protein S6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	100	Total	C	N	O	S	0	0	0
			784	496	137	148	3			

- Molecule 7 is a protein called 30S Ribosomal Protein S7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	G	154	Total	C	N	O	S	0	0	0
			1149	715	222	206	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
			1049	667	188	192	2			

- Molecule 9 is a protein called 30S Ribosomal Protein S9.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
9	I	125	Total	C	N	O	0	0	0
			849	531	161	157			

- Molecule 10 is a protein called 30S Ribosomal Protein S10.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
10	J	96	Total	C	N	O	0	0	0
			657	407	129	121			

- Molecule 11 is a protein called 30S Ribosomal Protein S11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	114	Total	C	N	O	S	0	0	0
			828	516	155	154	3			

- Molecule 12 is a protein called 30S Ribosomal Protein S12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	L	122	Total	C	N	O	S	0	0	0
			905	567	178	159	1			

- Molecule 13 is a protein called 30S Ribosomal Protein S13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	M	112	Total	C	N	O	S	0	0	0
			784	486	159	138	1			

- Molecule 14 is a protein called 30S Ribosomal Protein S14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	N	59	Total	C	N	O	S	0	0	0
			469	297	97	71	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
			724	453	143	126	2			

- Molecule 16 is a protein called 30S Ribosomal Protein S16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	P	82	Total	C	N	O	S	0	0	0
			661	421	126	113	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
			819	525	150	142	2			

- Molecule 18 is a protein called 30S Ribosomal Protein S18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
18	R	68	Total	C	N	O	0	0	0
			514	329	98	87			

- Molecule 19 is a protein called 30S Ribosomal Protein S19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	S	75	Total	C	N	O	S	0	0	0
			529	332	102	93	2			

- Molecule 20 is a protein called 30S Ribosomal Protein S20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	T	104	Total	C	N	O	S	0	0	0
			773	476	162	133	2			

- Molecule 21 is a protein called 30S Ribosomal Protein THX.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
21	U	23	Total	C	N	O	0	0	0
			180	112	41	27			

- Molecule 22 is a RNA chain called P-site fMet-tRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	V	77	Total	C	N	O	P	0	0	0
			1644	732	297	538	77			

- Molecule 23 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	X	6	Total	C	N	O	P	0	0	0
			131	59	27	39	6			

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
24	D	1	Total	Mg	0	0
			1	1		
24	V	13	Total	Mg	0	0
			13	13		
24	A	230	Total	Mg	0	0
			230	230		
24	T	1	Total	Mg	0	0
			1	1		
24	X	1	Total	Mg	0	0
			1	1		
24	O	1	Total	Mg	0	0
			1	1		

- Molecule 25 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 26 is water.

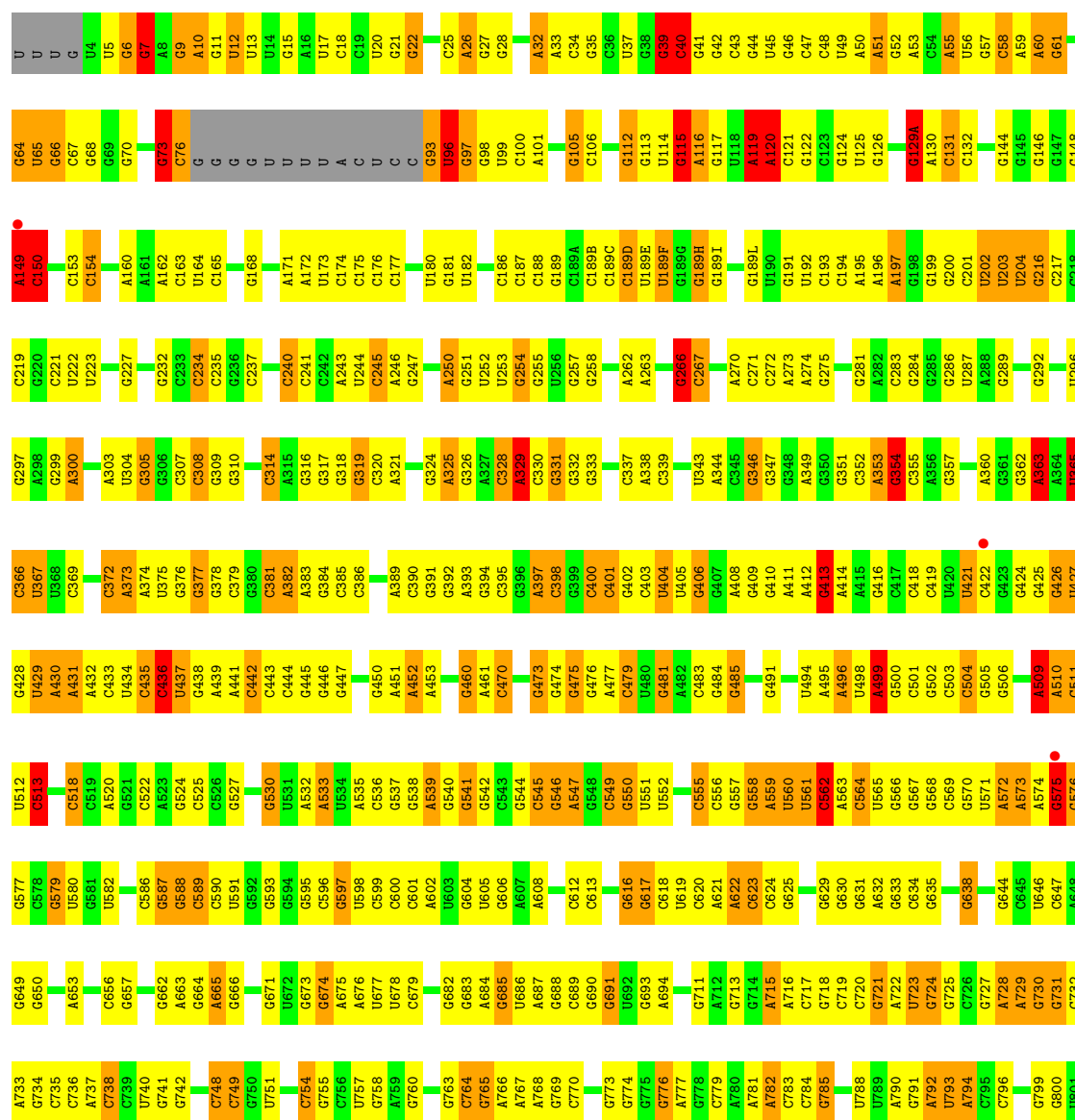
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
26	A	347	Total O 347 347	0	0
26	B	1	Total O 1 1	0	0
26	C	1	Total O 1 1	0	0
26	D	3	Total O 3 3	0	0
26	K	2	Total O 2 2	0	0
26	L	1	Total O 1 1	0	0
26	N	2	Total O 2 2	0	0
26	O	2	Total O 2 2	0	0
26	Q	1	Total O 1 1	0	0
26	T	2	Total O 2 2	0	0
26	V	22	Total O 22 22	0	0
26	X	1	Total O 1 1	0	0

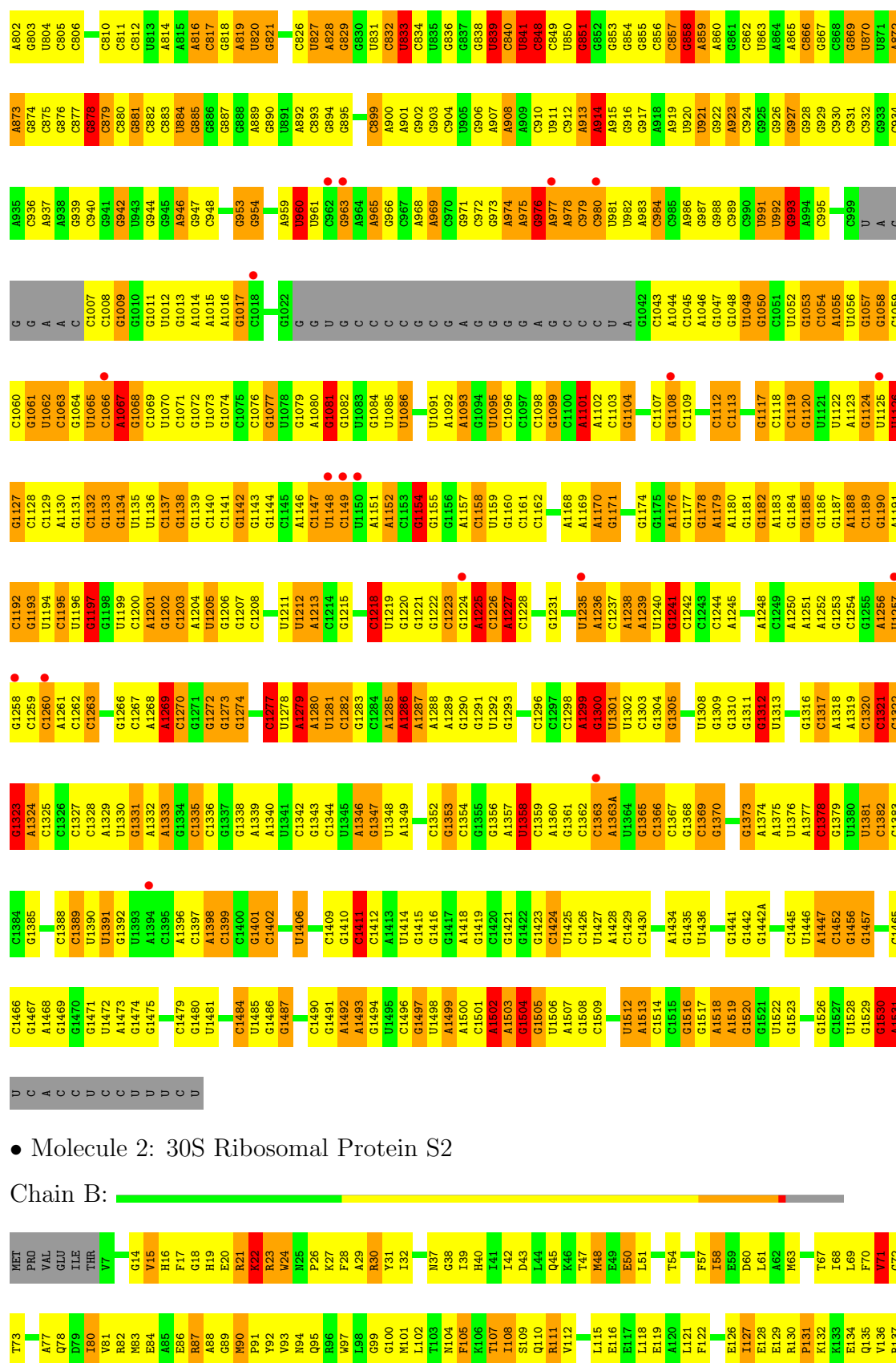
3 Residue-property plots

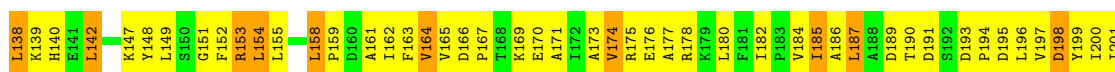
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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 ($RSRZ > 2$). 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

Chain A: 

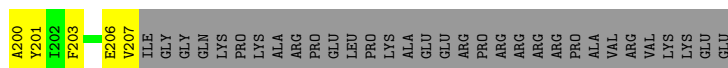
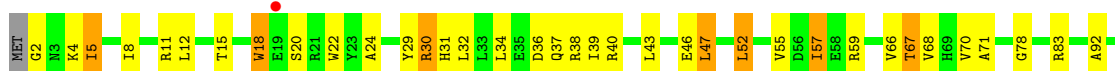






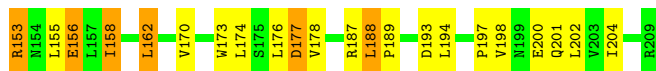
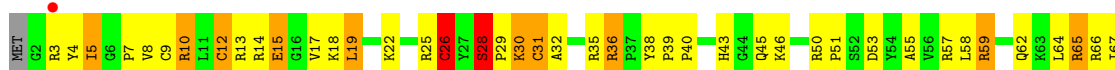
• Molecule 3: 30S Ribosomal Protein S3

Chain C:



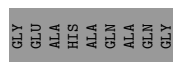
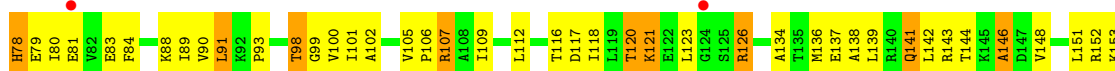
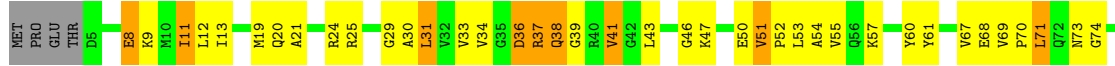
• Molecule 4: 30S Ribosomal Protein S4

Chain D:



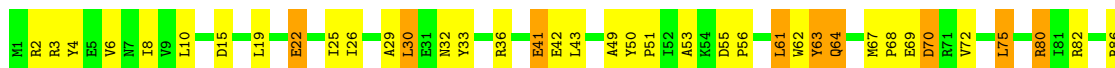
• Molecule 5: 30S Ribosomal Protein S5

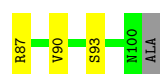
Chain E:



• Molecule 6: 30S Ribosomal Protein S6

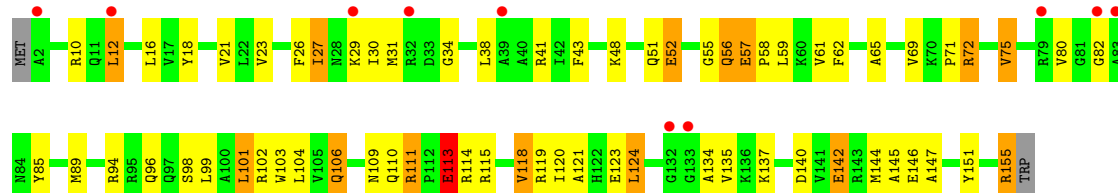
Chain F:





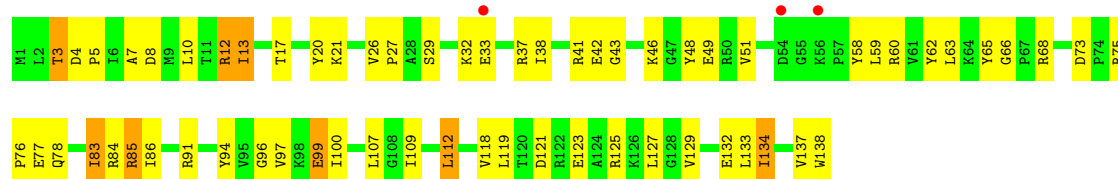
• Molecule 7: 30S Ribosomal Protein S7

Chain G:



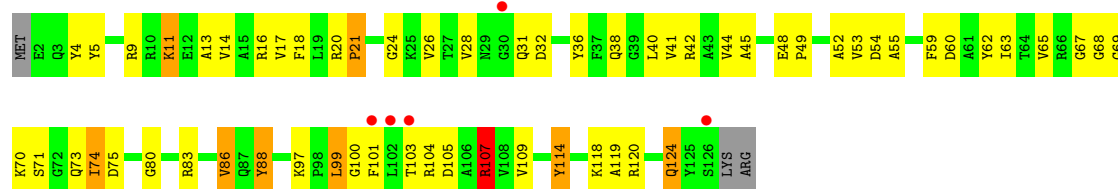
• Molecule 8: 30S Ribosomal Protein S8

Chain H:



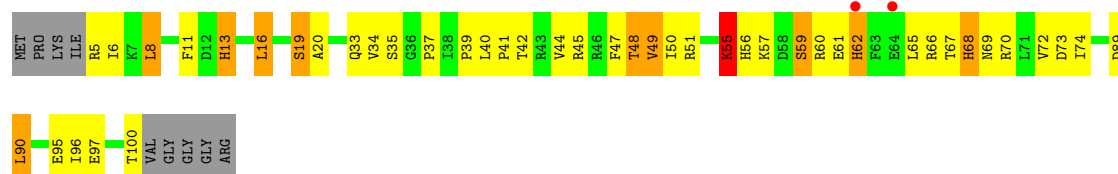
• Molecule 9: 30S Ribosomal Protein S9

Chain I:



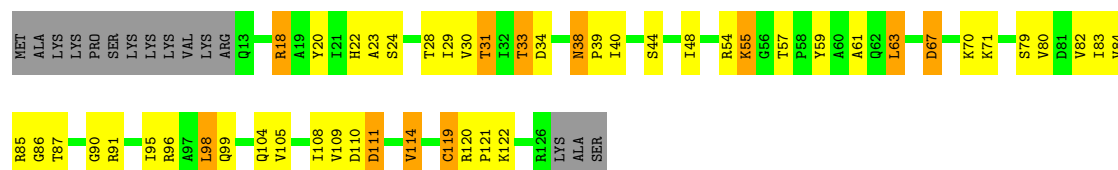
• Molecule 10: 30S Ribosomal Protein S10

Chain J:



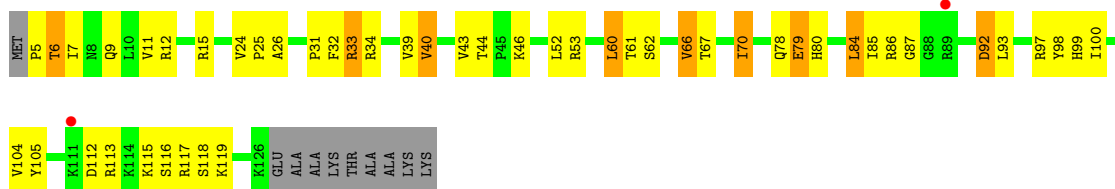
• Molecule 11: 30S Ribosomal Protein S11

Chain K:



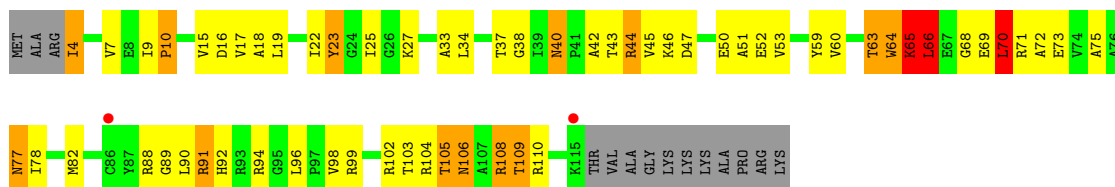
- Molecule 12: 30S Ribosomal Protein S12

Chain L:



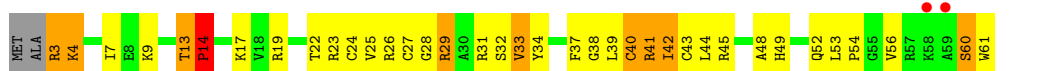
- Molecule 13: 30S Ribosomal Protein S13

Chain M:



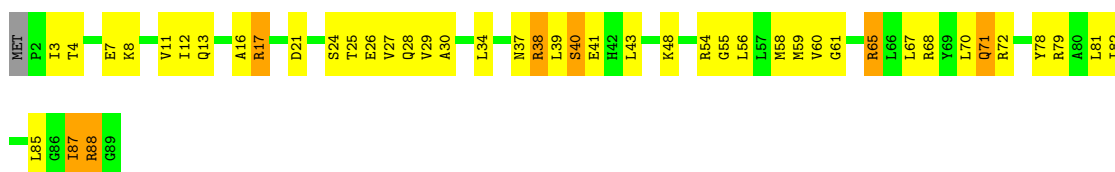
- Molecule 14: 30S Ribosomal Protein S14

Chain N:



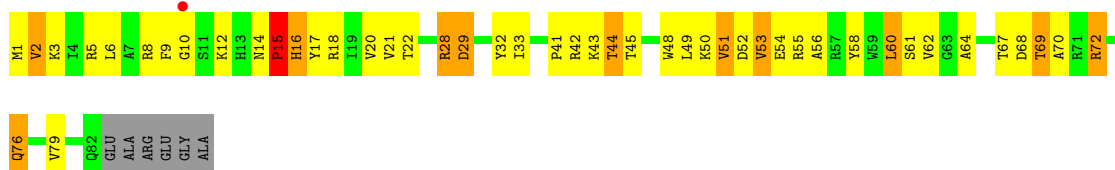
- Molecule 15: 30S Ribosomal Protein S15

Chain O:



- Molecule 16: 30S Ribosomal Protein S16

Chain P:



- Molecule 17: 30S Ribosomal Protein S17

Chain Q:







4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	209.96Å 448.86Å 624.20Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	34.91 – 3.20 34.91 – 3.20	Depositor EDS
% Data completeness (in resolution range)	99.8 (34.91-3.20) 99.8 (34.91-3.20)	Depositor EDS
R_{merge}	0.28	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.32 (at 3.18Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.3_928)	Depositor
R, R_{free}	0.188 , 0.245 0.512 , 0.513	Depositor DCC
R_{free} test set	48022 reflections (5.02%)	DCC
Wilson B-factor (Å ²)	73.8	Xtriage
Anisotropy	0.161	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.25 , 65.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Outliers	0 of 956750 reflections	Xtriage
F_o, F_c correlation	0.45	EDS
Total number of atoms	51411	wwPDB-VP
Average B, all atoms (Å ²)	106.0	wwPDB-VP

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

¹Intensities estimated from amplitudes.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, MG

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	0.89	15/35152 (0.0%)	1.51	525/54858 (1.0%)
2	B	0.55	0/1852	0.79	1/2510 (0.0%)
3	C	0.53	0/1477	0.75	0/2006
4	D	0.70	3/1567 (0.2%)	0.95	4/2125 (0.2%)
5	E	0.68	0/1131	0.92	0/1529
6	F	0.60	0/797	0.81	0/1085
7	G	0.53	0/1166	0.77	0/1576
8	H	0.57	0/1069	0.80	0/1450
9	I	0.53	0/864	0.80	1/1177 (0.1%)
10	J	0.55	0/670	0.84	0/917
11	K	0.58	0/843	0.77	0/1144
12	L	0.64	0/921	0.88	0/1247
13	M	0.55	0/794	0.81	1/1081 (0.1%)
14	N	0.60	0/478	0.86	0/638
15	O	0.59	0/735	0.84	0/981
16	P	0.60	0/677	0.91	0/917
17	Q	0.63	0/832	0.84	1/1113 (0.1%)
18	R	0.59	0/519	0.79	0/699
19	S	0.46	0/543	0.73	1/740 (0.1%)
20	T	0.62	0/776	0.85	0/1026
21	U	0.60	0/184	0.78	0/244
22	V	0.78	1/1836 (0.1%)	1.29	11/2859 (0.4%)
23	X	0.85	0/147	1.11	0/227
All	All	0.80	19/55030 (0.0%)	1.34	545/82149 (0.7%)

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
1	A	0	1
2	B	0	2
4	D	0	5
5	E	0	1
7	G	0	1
10	J	0	2
13	M	0	2
14	N	0	1
16	P	0	1
20	T	0	2
21	U	0	1
All	All	0	19

The worst 5 of 19 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	189(D)	C	N3-C4	-15.70	1.23	1.33
1	A	129(A)	G	N1-C2	-14.59	1.26	1.37
1	A	189(D)	C	C2-N3	-13.63	1.24	1.35
1	A	129(A)	G	C6-N1	-13.61	1.30	1.39
22	V	1	C	OP3-P	-10.44	1.48	1.61

The worst 5 of 545 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	189(D)	C	N1-C2-O2	44.80	145.78	118.90
1	A	189(D)	C	N3-C4-N4	-44.60	86.78	118.00
1	A	129(A)	G	N3-C2-N2	37.08	145.85	119.90
1	A	129(A)	G	C5-C6-O6	36.54	150.53	128.60
1	A	189(D)	C	C5-C4-N4	34.87	144.61	120.20

There are no chirality outliers.

5 of 19 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	129(A)	G	Sidechain
2	B	22	LYS	Peptide
2	B	71	VAL	Peptide
4	D	28	SER	Peptide
4	D	3	ARG	Peptide

5.2 Close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	31406	0	15852	819	0
2	B	1817	0	1785	126	0
3	C	1453	0	1320	64	0
4	D	1537	0	1430	81	0
5	E	1115	0	1145	55	0
6	F	784	0	739	29	0
7	G	1149	0	1096	52	0
8	H	1049	0	1037	52	0
9	I	849	0	735	54	0
10	J	657	0	547	40	0
11	K	828	0	822	31	0
12	L	905	0	916	30	0
13	M	784	0	730	51	0
14	N	469	0	482	37	0
15	O	724	0	749	30	0
16	P	661	0	653	45	0
17	Q	819	0	880	38	0
18	R	514	0	530	21	0
19	S	529	0	443	22	0
20	T	773	0	836	32	0
21	U	180	0	173	4	0
22	V	1644	0	836	36	0
23	X	131	0	66	2	0
24	A	230	0	0	0	0
24	D	1	0	0	0	0
24	O	1	0	0	0	0
24	T	1	0	0	0	0
24	V	13	0	0	0	0
24	X	1	0	0	0	0
25	D	1	0	0	0	0
25	N	1	0	0	0	0
26	A	347	0	0	17	0
26	B	1	0	0	1	0
26	C	1	0	0	0	0
26	D	3	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
26	K	2	0	0	0	0
26	L	1	0	0	1	0
26	N	2	0	0	0	0
26	O	2	0	0	1	0
26	Q	1	0	0	1	0
26	T	2	0	0	0	0
26	V	22	0	0	0	0
26	X	1	0	0	0	0
All	All	51411	0	33802	1587	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 19.

The worst 5 of 1587 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1358:U:H3	1:A:1363(A):A:N6	1.35	1.22
1:A:1162:C:N4	1:A:1174:G:H1	1.58	1.01
1:A:1358:U:O4	1:A:1363(A):A:N1	1.94	0.99
1:A:1502:A:H2	1:A:1505:G:H1	1.16	0.94
1:A:377:G:H1	1:A:386:C:H42	1.12	0.94

There are no symmetry-related clashes.

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%)	182 (78%)	45 (19%)	6 (3%)	8	47
3	C	204/239 (85%)	168 (82%)	36 (18%)	0	100	100
4	D	206/209 (99%)	178 (86%)	23 (11%)	5 (2%)	9	51
5	E	147/162 (91%)	129 (88%)	13 (9%)	5 (3%)	6	38
6	F	98/101 (97%)	89 (91%)	9 (9%)	0	100	100
7	G	152/156 (97%)	131 (86%)	20 (13%)	1 (1%)	30	80

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	H	136/138 (99%)	126 (93%)	10 (7%)	0	100	100
9	I	123/128 (96%)	106 (86%)	13 (11%)	4 (3%)	6	38
10	J	94/105 (90%)	74 (79%)	17 (18%)	3 (3%)	6	39
11	K	112/129 (87%)	98 (88%)	14 (12%)	0	100	100
12	L	120/132 (91%)	111 (92%)	7 (6%)	2 (2%)	14	62
13	M	110/126 (87%)	82 (74%)	21 (19%)	7 (6%)	2	17
14	N	57/61 (93%)	48 (84%)	8 (14%)	1 (2%)	13	60
15	O	86/89 (97%)	75 (87%)	11 (13%)	0	100	100
16	P	80/88 (91%)	66 (82%)	10 (12%)	4 (5%)	3	26
17	Q	97/105 (92%)	83 (86%)	13 (13%)	1 (1%)	22	74
18	R	66/88 (75%)	58 (88%)	8 (12%)	0	100	100
19	S	73/93 (78%)	60 (82%)	13 (18%)	0	100	100
20	T	102/106 (96%)	73 (72%)	26 (26%)	3 (3%)	7	43
21	U	21/27 (78%)	19 (90%)	2 (10%)	0	100	100
All	All	2317/2538 (91%)	1956 (84%)	319 (14%)	42 (2%)	13	60

5 of 42 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	15	VAL
5	E	73	ASN
9	I	54	ASP
13	M	7	VAL
13	M	45	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	181/220 (82%)	132 (73%)	49 (27%)	1	2
3	C	114/188 (61%)	96 (84%)	18 (16%)	4	16
4	D	142/181 (78%)	112 (79%)	30 (21%)	1	8

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	E	109/123 (89%)	84 (77%)	25 (23%)	1	5
6	F	76/90 (84%)	61 (80%)	15 (20%)	2	10
7	G	102/127 (80%)	78 (76%)	24 (24%)	1	5
8	H	104/119 (87%)	89 (86%)	15 (14%)	5	22
9	I	62/99 (63%)	52 (84%)	10 (16%)	3	16
10	J	52/92 (56%)	36 (69%)	16 (31%)	0	1
11	K	81/99 (82%)	61 (75%)	20 (25%)	1	3
12	L	91/109 (84%)	71 (78%)	20 (22%)	1	7
13	M	62/101 (61%)	39 (63%)	23 (37%)	0	0
14	N	45/50 (90%)	30 (67%)	15 (33%)	0	0
15	O	77/80 (96%)	64 (83%)	13 (17%)	3	14
16	P	65/74 (88%)	49 (75%)	16 (25%)	1	3
17	Q	93/97 (96%)	77 (83%)	16 (17%)	3	14
18	R	49/77 (64%)	36 (74%)	13 (26%)	1	2
19	S	42/80 (52%)	28 (67%)	14 (33%)	0	0
20	T	72/82 (88%)	56 (78%)	16 (22%)	1	6
21	U	14/22 (64%)	13 (93%)	1 (7%)	21	63
All	All	1633/2110 (77%)	1264 (77%)	369 (23%)	1	6

5 of 369 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
8	H	84	ARG
11	K	33	THR
19	S	22	LEU
8	H	123	GLU
10	J	13	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 12 such sidechains are listed below:

Mol	Chain	Res	Type
11	K	99	GLN
13	M	40	ASN
18	R	63	GLN
9	I	3	GLN

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Mol	Chain	Res	Type
15	O	28	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	1457/1522 (95%)	367 (25%)	33 (2%)
22	V	76/77 (98%)	21 (27%)	0
23	X	5/16 (31%)	0	0
All	All	1538/1615 (95%)	388 (25%)	33 (2%)

5 of 388 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	13	U

5 of 33 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	793	U
1	A	991	U
1	A	1492	A
1	A	828	A
1	A	840	C

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 249 ligands modelled in this entry, 249 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.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	1461/1522 (95%)	0.07	21 (1%) 72 22	55, 104, 145, 167	0
2	B	235/256 (91%)	-0.03	1 (0%) 90 51	100, 125, 139, 147	0
3	C	206/239 (86%)	-0.07	2 (0%) 79 29	110, 125, 136, 142	0
4	D	208/209 (99%)	-0.04	4 (1%) 64 18	85, 98, 114, 120	0
5	E	149/162 (91%)	-0.14	2 (1%) 74 24	83, 99, 110, 131	0
6	F	100/101 (99%)	-0.25	0 100 100	78, 96, 110, 117	0
7	G	154/156 (98%)	0.10	10 (6%) 18 4	107, 119, 133, 144	0
8	H	138/138 (100%)	-0.07	3 (2%) 59 14	82, 100, 111, 116	0
9	I	125/128 (97%)	0.19	5 (4%) 36 7	101, 130, 138, 142	0
10	J	96/105 (91%)	0.19	2 (2%) 60 15	111, 133, 141, 143	0
11	K	114/129 (88%)	0.01	0 100 100	78, 103, 118, 127	0
12	L	122/132 (92%)	0.04	2 (1%) 68 20	72, 90, 105, 114	0
13	M	112/126 (88%)	0.11	2 (1%) 65 18	102, 127, 135, 139	0
14	N	59/61 (96%)	0.50	2 (3%) 43 9	116, 125, 133, 135	0
15	O	88/89 (98%)	-0.08	0 100 100	74, 96, 114, 118	0
16	P	82/88 (93%)	-0.05	1 (1%) 75 26	84, 94, 112, 122	0
17	Q	99/105 (94%)	-0.09	0 100 100	77, 95, 110, 113	0
18	R	68/88 (77%)	-0.07	1 (1%) 70 21	82, 92, 111, 115	0
19	S	75/93 (80%)	0.10	0 100 100	107, 131, 142, 146	0
20	T	104/106 (98%)	0.01	2 (1%) 64 18	81, 101, 123, 139	0
21	U	23/27 (85%)	1.18	5 (21%) 1 1	115, 126, 132, 134	0
22	V	77/77 (100%)	-0.18	1 (1%) 74 24	73, 109, 133, 156	0
23	X	6/16 (37%)	0.99	1 (16%) 2 1	89, 96, 142, 147	0
All	All	3901/4153 (93%)	0.03	67 (1%) 64 19	55, 108, 139, 167	0

The worst 5 of 67 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1149	C	4.8
1	A	422	C	4.2
23	X	1	A	3.8
21	U	14	TRP	3.8
5	E	124	GLY	3.7

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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	RSR	LLDF	B-factors(Å ²)	Q<0.9
24	MG	A	1794	1/1	0.43	-	118,118,118,118	0
24	MG	A	1694	1/1	0.46	-	84,84,84,84	0
24	MG	A	1688	1/1	0.20	-	70,70,70,70	0
24	MG	A	1732	1/1	0.20	-	70,70,70,70	0
24	MG	A	1672	1/1	0.38	-	78,78,78,78	0
24	MG	A	1635	1/1	0.42	-	81,81,81,81	0
24	MG	A	1713	1/1	1.01	-	91,91,91,91	0
24	MG	A	1612	1/1	0.37	-	84,84,84,84	0
24	MG	A	1636	1/1	0.36	-	63,63,63,63	0
24	MG	A	1601	1/1	0.50	-	79,79,79,79	0
24	MG	A	1763	1/1	0.28	-	94,94,94,94	0
24	MG	A	1761	1/1	0.25	-	93,93,93,93	0
24	MG	D	302	1/1	0.15	-	53,53,53,53	0
24	MG	A	1696	1/1	0.31	-	53,53,53,53	0
24	MG	A	1714	1/1	0.85	-	82,82,82,82	0
24	MG	A	1819	1/1	0.15	-	92,92,92,92	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
24	MG	A	1766	1/1	0.46	-	103,103,103,103	0
24	MG	A	1817	1/1	0.27	-	102,102,102,102	0
24	MG	A	1652	1/1	0.27	-	61,61,61,61	0
24	MG	A	1606	1/1	0.21	-	77,77,77,77	0
24	MG	A	1641	1/1	0.29	-	96,96,96,96	0
24	MG	V	109	1/1	0.28	-	79,79,79,79	0
24	MG	A	1750	1/1	0.26	-	80,80,80,80	0
24	MG	A	1631	1/1	1.02	-	74,74,74,74	0
24	MG	A	1778	1/1	0.15	-	77,77,77,77	0
24	MG	A	1632	1/1	0.32	-	70,70,70,70	0
24	MG	A	1824	1/1	0.17	-	119,119,119,119	0
24	MG	V	101	1/1	0.29	-	59,59,59,59	0
24	MG	A	1827	1/1	0.44	-	87,87,87,87	0
24	MG	A	1657	1/1	0.52	-	66,66,66,66	0
24	MG	A	1825	1/1	0.13	-	110,110,110,110	0
24	MG	A	1756	1/1	0.24	-	56,56,56,56	0
24	MG	A	1602	1/1	0.50	-	72,72,72,72	0
24	MG	A	1802	1/1	0.28	-	102,102,102,102	0
24	MG	A	1700	1/1	0.22	-	94,94,94,94	0
24	MG	A	1818	1/1	0.23	-	101,101,101,101	0
24	MG	A	1755	1/1	0.40	-	92,92,92,92	0
24	MG	A	1643	1/1	0.23	-	80,80,80,80	0
24	MG	A	1796	1/1	0.37	-	64,64,64,64	0
24	MG	A	1651	1/1	0.26	-	78,78,78,78	0
24	MG	A	1624	1/1	0.83	-	68,68,68,68	0
24	MG	A	1753	1/1	0.22	-	96,96,96,96	0
24	MG	A	1620	1/1	0.39	-	71,71,71,71	0
24	MG	A	1667	1/1	1.16	-	76,76,76,76	0
24	MG	O	101	1/1	0.29	-	90,90,90,90	0
24	MG	V	104	1/1	0.25	-	92,92,92,92	0
24	MG	A	1810	1/1	0.21	-	83,83,83,83	0
24	MG	A	1691	1/1	0.33	-	72,72,72,72	0
24	MG	A	1608	1/1	0.27	-	80,80,80,80	0
24	MG	A	1682	1/1	0.22	-	65,65,65,65	0
24	MG	A	1730	1/1	0.15	-	88,88,88,88	0
24	MG	A	1604	1/1	0.83	-	114,114,114,114	0
24	MG	A	1647	1/1	0.81	-	74,74,74,74	0
24	MG	A	1617	1/1	0.28	-	54,54,54,54	0
24	MG	A	1758	1/1	0.18	-	58,58,58,58	0
24	MG	A	1733	1/1	0.44	-	74,74,74,74	0
24	MG	A	1807	1/1	0.10	-	94,94,94,94	0
24	MG	A	1662	1/1	0.45	-	85,85,85,85	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
24	MG	A	1745	1/1	0.20	-	79,79,79,79	0
24	MG	A	1718	1/1	0.52	-	71,71,71,71	0
24	MG	A	1698	1/1	0.37	-	83,83,83,83	0
24	MG	A	1716	1/1	0.26	-	70,70,70,70	0
24	MG	A	1775	1/1	0.36	-	93,93,93,93	0
24	MG	A	1665	1/1	0.20	-	92,92,92,92	0
24	MG	A	1735	1/1	0.13	-	80,80,80,80	0
24	MG	A	1768	1/1	0.13	-	76,76,76,76	0
24	MG	A	1715	1/1	0.09	-	95,95,95,95	0
24	MG	A	1769	1/1	0.14	-	62,62,62,62	0
24	MG	A	1792	1/1	0.57	-	80,80,80,80	0
24	MG	A	1747	1/1	0.07	-	92,92,92,92	0
24	MG	A	1813	1/1	0.58	-	103,103,103,103	0
24	MG	A	1772	1/1	0.17	-	106,106,106,106	0
24	MG	A	1723	1/1	1.15	-	88,88,88,88	0
24	MG	A	1740	1/1	0.14	-	80,80,80,80	0
24	MG	A	1633	1/1	0.71	-	66,66,66,66	0
24	MG	A	1674	1/1	0.62	-	82,82,82,82	0
24	MG	A	1704	1/1	0.85	-	97,97,97,97	0
24	MG	A	1668	1/1	0.49	-	64,64,64,64	0
24	MG	A	1712	1/1	0.98	-	72,72,72,72	0
24	MG	V	110	1/1	0.18	-	102,102,102,102	0
24	MG	A	1695	1/1	0.36	-	74,74,74,74	0
24	MG	A	1613	1/1	0.19	-	58,58,58,58	0
24	MG	A	1780	1/1	0.48	-	111,111,111,111	0
24	MG	A	1655	1/1	0.40	-	78,78,78,78	0
24	MG	A	1711	1/1	0.48	-	75,75,75,75	0
24	MG	A	1685	1/1	0.31	-	73,73,73,73	0
24	MG	A	1720	1/1	0.54	-	66,66,66,66	0
24	MG	A	1603	1/1	0.76	-	72,72,72,72	0
24	MG	A	1671	1/1	0.64	-	59,59,59,59	0
24	MG	V	112	1/1	0.18	-	66,66,66,66	0
24	MG	A	1806	1/1	0.16	-	121,121,121,121	0
24	MG	A	1628	1/1	0.32	-	50,50,50,50	0
24	MG	A	1661	1/1	0.56	-	91,91,91,91	0
24	MG	A	1626	1/1	0.41	-	71,71,71,71	0
24	MG	A	1609	1/1	0.25	-	70,70,70,70	0
24	MG	A	1722	1/1	0.28	-	77,77,77,77	0
24	MG	A	1649	1/1	0.55	-	71,71,71,71	0
24	MG	A	1706	1/1	0.22	-	109,109,109,109	0
24	MG	A	1677	1/1	0.58	-	79,79,79,79	0
24	MG	A	1786	1/1	0.32	-	90,90,90,90	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
24	MG	A	1679	1/1	0.21	-	83,83,83,83	0
24	MG	A	1681	1/1	0.25	-	84,84,84,84	0
24	MG	A	1642	1/1	0.65	-	72,72,72,72	0
24	MG	A	1646	1/1	0.72	-	69,69,69,69	0
24	MG	A	1689	1/1	0.78	-	75,75,75,75	0
24	MG	A	1731	1/1	0.19	-	79,79,79,79	0
24	MG	A	1634	1/1	1.25	-	77,77,77,77	0
24	MG	A	1812	1/1	0.31	-	102,102,102,102	0
24	MG	A	1788	1/1	0.56	-	96,96,96,96	0
25	ZN	N	101	1/1	0.14	-	165,165,165,165	0
24	MG	A	1622	1/1	0.19	-	100,100,100,100	0
24	MG	A	1784	1/1	0.41	-	81,81,81,81	0
24	MG	V	106	1/1	0.20	-	78,78,78,78	0
24	MG	A	1660	1/1	0.24	-	64,64,64,64	0
24	MG	A	1702	1/1	0.32	-	117,117,117,117	0
24	MG	A	1639	1/1	0.40	-	80,80,80,80	0
24	MG	A	1610	1/1	0.14	-	63,63,63,63	0
24	MG	V	102	1/1	0.45	-	85,85,85,85	0
24	MG	A	1719	1/1	0.27	-	74,74,74,74	0
24	MG	A	1697	1/1	0.38	-	84,84,84,84	0
24	MG	A	1767	1/1	0.22	-	68,68,68,68	0
24	MG	A	1658	1/1	0.18	-	80,80,80,80	0
24	MG	A	1738	1/1	0.21	-	81,81,81,81	0
25	ZN	D	301	1/1	0.08	-	90,90,90,90	0
24	MG	V	107	1/1	0.34	-	70,70,70,70	0
24	MG	A	1770	1/1	0.12	-	75,75,75,75	0
24	MG	A	1814	1/1	0.21	-	88,88,88,88	0
24	MG	A	1760	1/1	0.18	-	70,70,70,70	0
24	MG	A	1773	1/1	0.31	-	62,62,62,62	0
24	MG	A	1726	1/1	0.81	-	84,84,84,84	0
24	MG	V	105	1/1	0.23	-	106,106,106,106	0
24	MG	A	1684	1/1	0.25	-	70,70,70,70	0
24	MG	A	1619	1/1	0.28	-	78,78,78,78	0
24	MG	A	1710	1/1	0.57	-	112,112,112,112	0
24	MG	A	1669	1/1	0.16	-	73,73,73,73	0
24	MG	A	1757	1/1	0.06	-	86,86,86,86	0
24	MG	A	1721	1/1	0.21	-	66,66,66,66	0
24	MG	A	1803	1/1	0.25	-	56,56,56,56	0
24	MG	A	1751	1/1	0.11	-	99,99,99,99	0
24	MG	A	1809	1/1	0.26	-	105,105,105,105	0
24	MG	A	1686	1/1	0.48	-	43,43,43,43	0
24	MG	A	1774	1/1	0.14	-	94,94,94,94	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
24	MG	A	1830	1/1	0.15	-	95,95,95,95	0
24	MG	A	1734	1/1	0.27	-	83,83,83,83	0
24	MG	A	1673	1/1	0.20	-	69,69,69,69	0
24	MG	A	1777	1/1	0.32	-	78,78,78,78	0
24	MG	A	1727	1/1	0.40	-	75,75,75,75	0
24	MG	A	1748	1/1	0.35	-	89,89,89,89	0
24	MG	A	1759	1/1	0.18	-	61,61,61,61	0
24	MG	A	1823	1/1	0.18	-	114,114,114,114	0
24	MG	A	1828	1/1	0.14	-	96,96,96,96	0
24	MG	A	1629	1/1	0.36	-	69,69,69,69	0
24	MG	X	101	1/1	0.44	-	99,99,99,99	0
24	MG	A	1752	1/1	0.08	-	65,65,65,65	0
24	MG	A	1762	1/1	0.33	-	84,84,84,84	0
24	MG	A	1653	1/1	0.22	-	54,54,54,54	0
24	MG	A	1725	1/1	0.22	-	85,85,85,85	0
24	MG	A	1764	1/1	0.40	-	56,56,56,56	0
24	MG	A	1640	1/1	0.28	-	99,99,99,99	0
24	MG	A	1623	1/1	0.71	-	80,80,80,80	0
24	MG	A	1650	1/1	0.82	-	73,73,73,73	0
24	MG	A	1821	1/1	0.45	-	114,114,114,114	0
24	MG	A	1801	1/1	0.11	-	100,100,100,100	0
24	MG	A	1616	1/1	0.25	-	74,74,74,74	0
24	MG	A	1754	1/1	0.25	-	75,75,75,75	0
24	MG	A	1693	1/1	0.24	-	68,68,68,68	0
24	MG	A	1707	1/1	0.85	-	114,114,114,114	0
24	MG	A	1785	1/1	0.15	-	95,95,95,95	0
24	MG	A	1656	1/1	0.99	-	74,74,74,74	0
24	MG	A	1703	1/1	0.54	-	114,114,114,114	0
24	MG	T	201	1/1	0.77	-	67,67,67,67	0
24	MG	A	1744	1/1	0.66	-	98,98,98,98	0
24	MG	A	1611	1/1	0.17	-	74,74,74,74	0
24	MG	A	1717	1/1	0.23	-	83,83,83,83	0
24	MG	A	1808	1/1	0.22	-	94,94,94,94	0
24	MG	A	1644	1/1	0.20	-	84,84,84,84	0
24	MG	A	1648	1/1	0.18	-	73,73,73,73	0
24	MG	A	1793	1/1	1.82	-	98,98,98,98	0
24	MG	A	1765	1/1	0.08	-	76,76,76,76	0
24	MG	A	1805	1/1	0.43	-	82,82,82,82	0
24	MG	A	1678	1/1	0.45	-	77,77,77,77	0
24	MG	A	1737	1/1	0.25	-	84,84,84,84	0
24	MG	A	1741	1/1	0.14	-	78,78,78,78	0
24	MG	A	1739	1/1	0.16	-	90,90,90,90	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
24	MG	A	1666	1/1	0.38	-	63,63,63,63	0
24	MG	A	1615	1/1	0.29	-	81,81,81,81	0
24	MG	A	1654	1/1	0.97	-	75,75,75,75	0
24	MG	A	1787	1/1	0.30	-	103,103,103,103	0
24	MG	A	1630	1/1	0.16	-	51,51,51,51	0
24	MG	A	1746	1/1	0.13	-	73,73,73,73	0
24	MG	A	1789	1/1	0.12	-	78,78,78,78	0
24	MG	A	1779	1/1	0.16	-	124,124,124,124	0
24	MG	A	1618	1/1	0.38	-	61,61,61,61	0
24	MG	A	1729	1/1	0.30	-	96,96,96,96	0
24	MG	A	1708	1/1	0.25	-	100,100,100,100	0
24	MG	V	113	1/1	0.13	-	76,76,76,76	0
24	MG	A	1664	1/1	0.12	-	101,101,101,101	0
24	MG	A	1795	1/1	0.54	-	66,66,66,66	0
24	MG	A	1749	1/1	0.13	-	86,86,86,86	0
24	MG	A	1637	1/1	0.52	-	72,72,72,72	0
24	MG	A	1791	1/1	0.11	-	87,87,87,87	0
24	MG	A	1663	1/1	0.21	-	92,92,92,92	0
24	MG	A	1776	1/1	0.19	-	93,93,93,93	0
24	MG	A	1687	1/1	0.15	-	71,71,71,71	0
24	MG	A	1822	1/1	0.23	-	113,113,113,113	0
24	MG	A	1627	1/1	0.50	-	50,50,50,50	0
24	MG	A	1790	1/1	0.14	-	96,96,96,96	0
24	MG	A	1815	1/1	0.26	-	102,102,102,102	0
24	MG	A	1797	1/1	0.18	-	85,85,85,85	0
24	MG	A	1659	1/1	0.59	-	77,77,77,77	0
24	MG	A	1811	1/1	0.16	-	115,115,115,115	0
24	MG	A	1699	1/1	0.76	-	80,80,80,80	0
24	MG	A	1816	1/1	0.23	-	100,100,100,100	0
24	MG	A	1709	1/1	0.75	-	93,93,93,93	0
24	MG	V	103	1/1	0.34	-	88,88,88,88	0
24	MG	A	1607	1/1	0.14	-	73,73,73,73	0
24	MG	A	1724	1/1	0.33	-	73,73,73,73	0
24	MG	A	1680	1/1	0.19	-	88,88,88,88	0
24	MG	A	1798	1/1	0.39	-	82,82,82,82	0
24	MG	A	1683	1/1	0.22	-	70,70,70,70	0
24	MG	A	1675	1/1	0.66	-	76,76,76,76	0
24	MG	A	1826	1/1	0.27	-	111,111,111,111	0
24	MG	A	1742	1/1	0.25	-	97,97,97,97	0
24	MG	A	1705	1/1	1.04	-	90,90,90,90	0
24	MG	A	1645	1/1	0.14	-	53,53,53,53	0
24	MG	A	1676	1/1	0.21	-	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
24	MG	A	1605	1/1	0.25	-	59,59,59,59	0
24	MG	A	1625	1/1	0.14	-	64,64,64,64	0
24	MG	A	1638	1/1	0.28	-	50,50,50,50	0
24	MG	A	1799	1/1	0.15	-	73,73,73,73	0
24	MG	A	1781	1/1	0.16	-	99,99,99,99	0
24	MG	A	1728	1/1	0.71	-	76,76,76,76	0
24	MG	A	1800	1/1	0.14	-	59,59,59,59	0
24	MG	A	1782	1/1	0.23	-	90,90,90,90	0
24	MG	A	1670	1/1	0.20	-	66,66,66,66	0
24	MG	A	1804	1/1	0.29	-	84,84,84,84	0
24	MG	A	1690	1/1	0.23	-	64,64,64,64	0
24	MG	A	1736	1/1	0.19	-	69,69,69,69	0
24	MG	A	1829	1/1	0.30	-	108,108,108,108	0
24	MG	A	1771	1/1	0.21	-	61,61,61,61	0
24	MG	A	1783	1/1	0.45	-	82,82,82,82	0
24	MG	A	1701	1/1	0.19	-	99,99,99,99	0
24	MG	A	1820	1/1	0.10	-	102,102,102,102	0
24	MG	A	1743	1/1	0.31	-	90,90,90,90	0
24	MG	A	1621	1/1	0.26	-	70,70,70,70	0
24	MG	A	1692	1/1	0.24	-	81,81,81,81	0
24	MG	A	1614	1/1	0.43	-	75,75,75,75	0
24	MG	V	108	1/1	0.41	-	78,78,78,78	0
24	MG	V	111	1/1	0.07	-	100,100,100,100	0

6.5 Other polymers ⓘ

There are no such residues in this entry.