



# wwPDB X-ray Structure Validation Summary Report i

Feb 27, 2014 – 01:35 PM GMT

PDB ID : 4GD2  
Title : Structures of the bacterial ribosome in classical and hybrid states of tRNA binding  
Authors : Dunkle, J.A.; Wang, L.; Feldman, M.B.; Pulk, A.; Chen, V.B.; Kapral, G.J.; Noeske, J.; Richardson, J.S.; Blanchard, S.C.; Cate, J.H.D.  
Deposited on : 2012-07-31  
Resolution : 3.00 Å(reported)

This is a wwPDB validation summary report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

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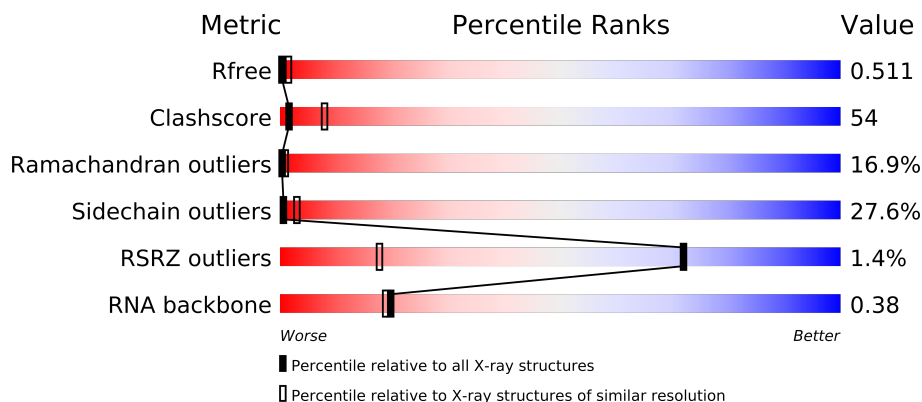
The following versions of software and data (see [references](#)) were used in the production of this report:

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 3.00 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	1216 (3.00-3.00)
Clashscore	79885	1594 (3.00-3.00)
Ramachandran outliers	78287	1537 (3.00-3.00)
Sidechain outliers	78261	1540 (3.00-3.00)
RSRZ outliers	66119	1217 (3.00-3.00)
RNA backbone	1838	1070 (3.50-2.50)

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  $\geq 3$ , 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	1539	
2	B	218	
3	C	206	
4	D	205	
5	E	150	
6	F	100	
7	G	151	
8	H	129	
9	I	127	
10	J	98	
11	K	117	
12	L	123	

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Mol	Chain	Length	Quality of chain
13	M	114	
14	N	100	
15	O	88	
16	P	82	
17	Q	80	
18	R	55	
19	S	79	
20	T	85	
21	U	51	
22	V	76	
23	X	16	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
24	MG	A	1615	-	X
24	MG	A	1627	-	X
24	MG	A	1633	-	X
24	MG	A	1637	-	X
24	MG	A	1638	-	X
24	MG	A	1646	-	X
24	MG	A	1647	-	X
24	MG	A	1650	-	X
24	MG	A	1651	-	X
24	MG	A	1654	-	X
24	MG	A	1655	-	X

## 2 Entry composition

There are 25 unique types of molecules in this entry. The entry contains 53792 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 rRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1539	Total	C	N	O	P	0	0	0
			33015	14725	6052	10699	1539			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	218	Total	C	N	O	S	0	0	0
			1705	1081	305	312	7			

- 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
			1625	1028	305	289	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	205	Total	C	N	O	S	0	0	0
			1643	1026	315	298	4			

- 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
			1106	687	211	202	6			

- 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
			818	515	148	149	6			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	G	151	Total	C	N	O	S	0	0	0
			1182	735	227	216	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	129	Total	C	N	O	S	0	0	0
			979	616	173	184	6			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	I	127	Total	C	N	O	S	0	0	0
			1022	634	206	179	3			

- 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
			787	493	150	143	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	117	Total	C	N	O	S	0	0	0
			877	540	174	160	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	L	123	Total	C	N	O	S	0	0	0
			955	590	196	165	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	M	114	Total	C	N	O	S	0	0	0
			884	546	178	157	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	N	96	Total	C	N	O	S	0	0	0
			774	483	160	128	3			

- 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
			714	439	144	130	1			

- 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
			649	406	128	114	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	Q	80	Total	C	N	O	S	0	0	0
			649	411	121	114	3			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
18	R	55	Total	C	N	O	0	0	0
			456	288	86	82			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	S	79	Total	C	N	O	S	0	0	0
			638	408	120	108	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	T	85	Total	C	N	O	S	0	0	0
			665	411	137	114	3			

- Molecule 21 is a protein called 30S ribosomal protein S21.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
21	U	51	Total	C	N	O	S	0	0	0
			426	265	86	74	1			

- Molecule 22 is a RNA chain called phenylalanine specific transfer RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	V	76	Total	C	N	O	P	0	0	0
			1623	723	290	534	76			

- Molecule 23 is a RNA chain called messenger RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	X	16	Total	C	N	O	P	0	0	0
			346	155	66	109	16			

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
24	A	56	Total	Mg	0	0
			56	56		

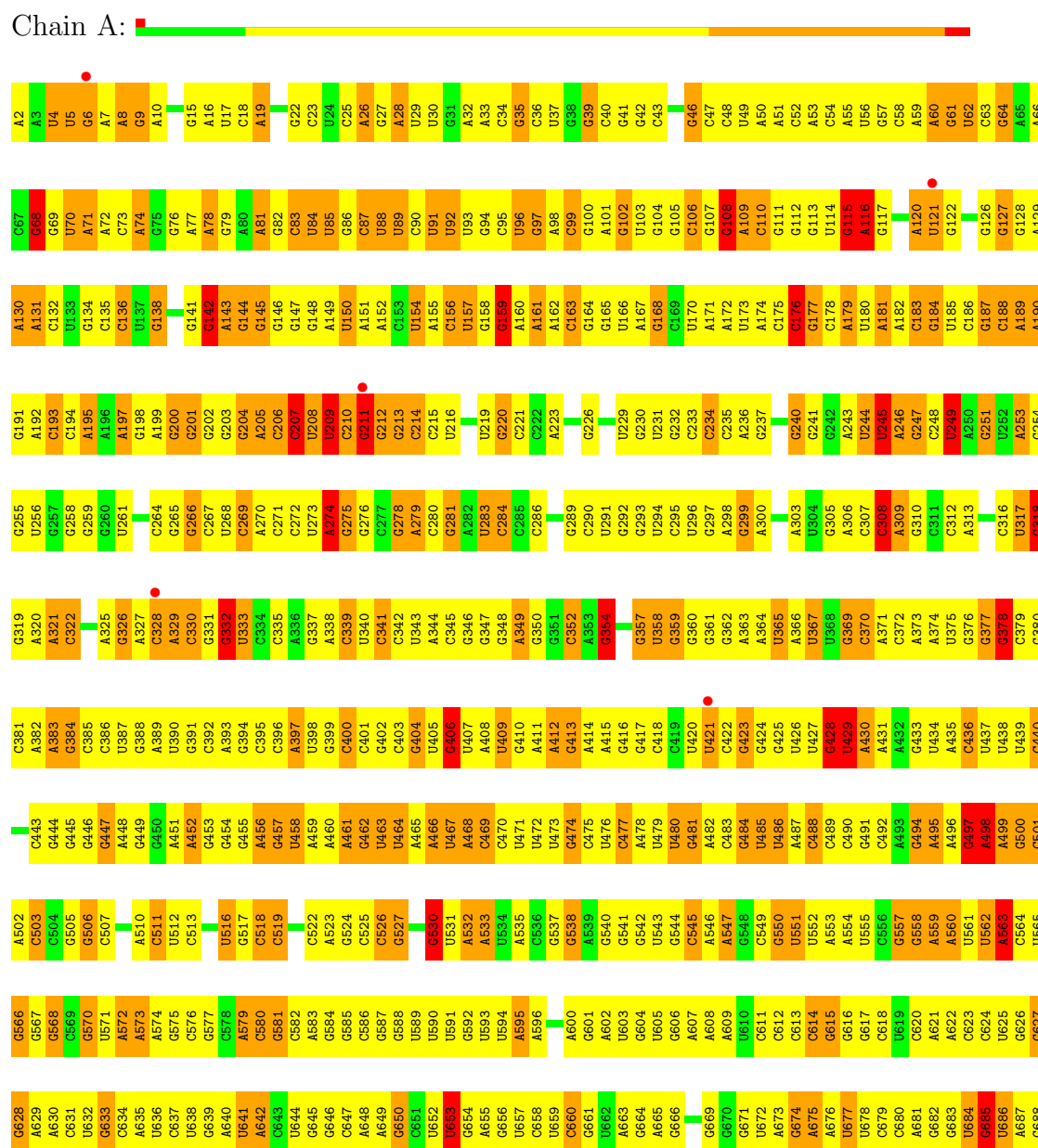
- Molecule 25 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
25	A	190	Total	O	0	0
			190	190		
25	L	1	Total	O	0	0
			1	1		
25	N	5	Total	O	0	0
			5	5		
25	U	2	Total	O	0	0
			2	2		

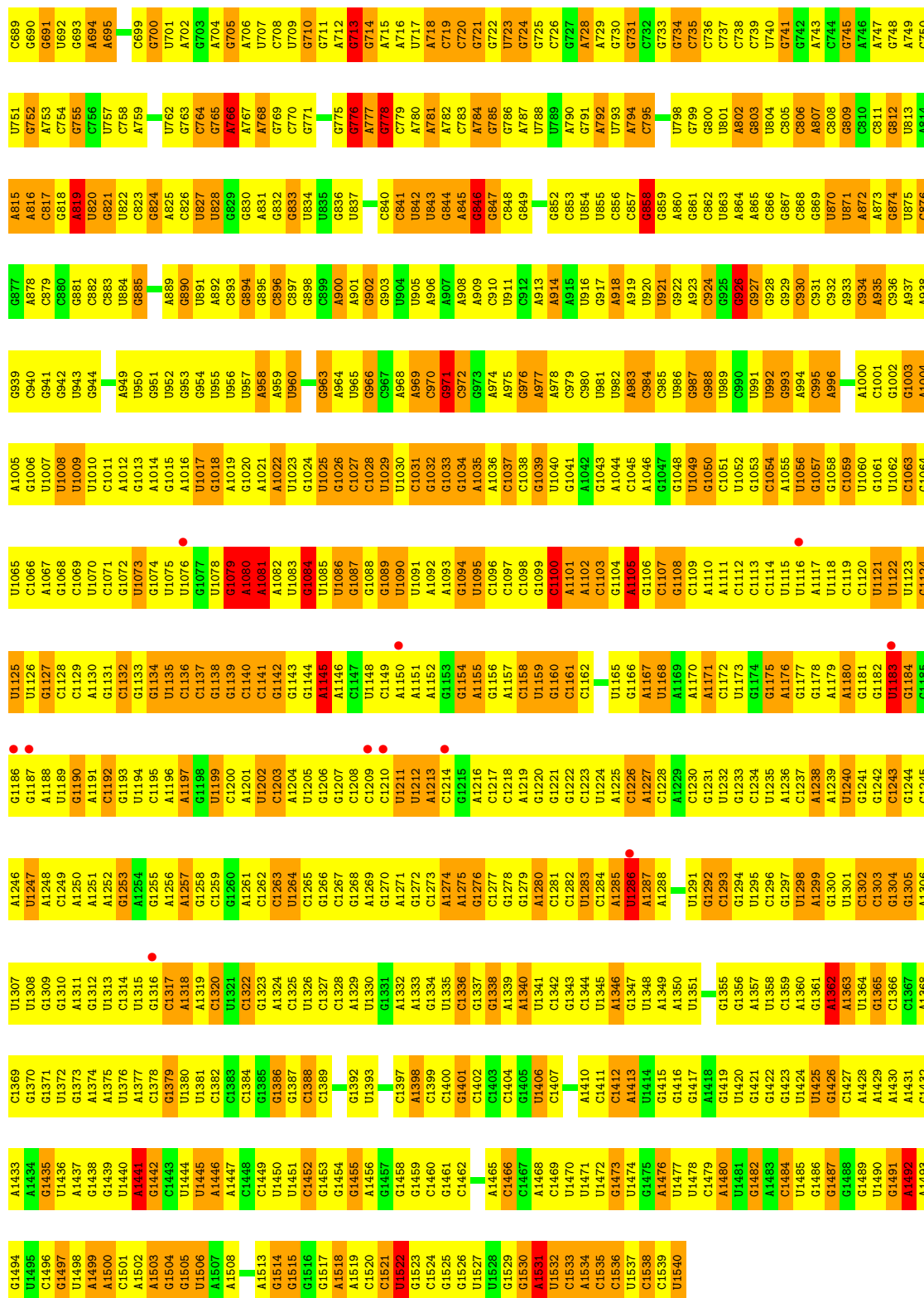
### 3 Residue-property plots

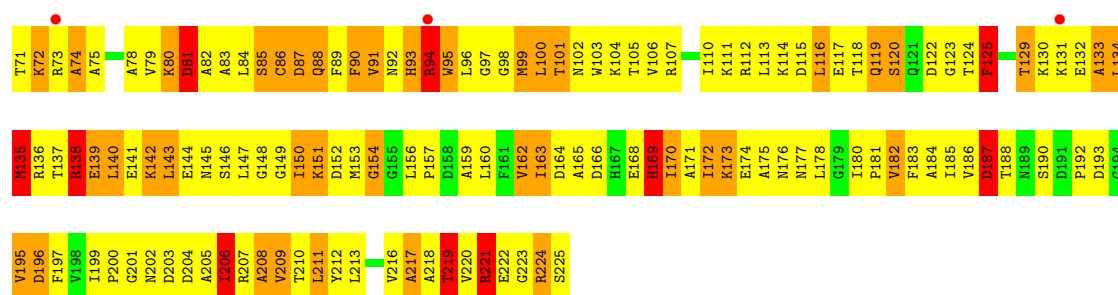
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according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



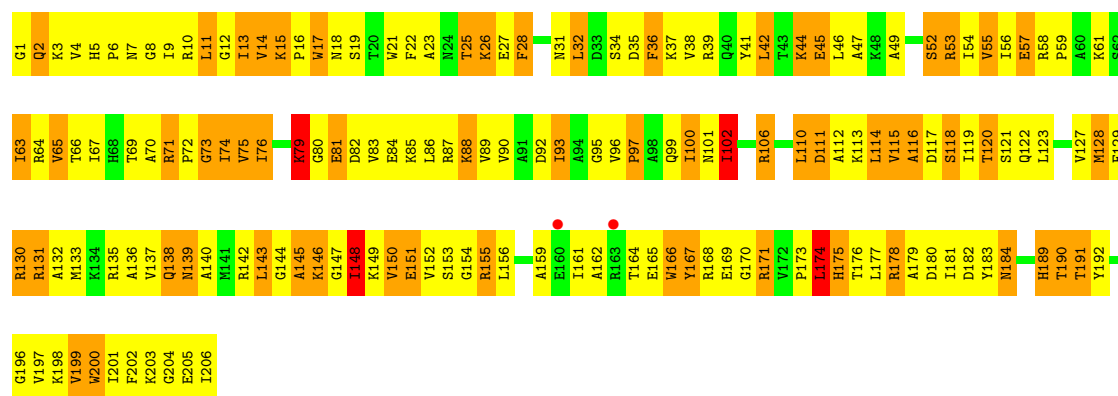






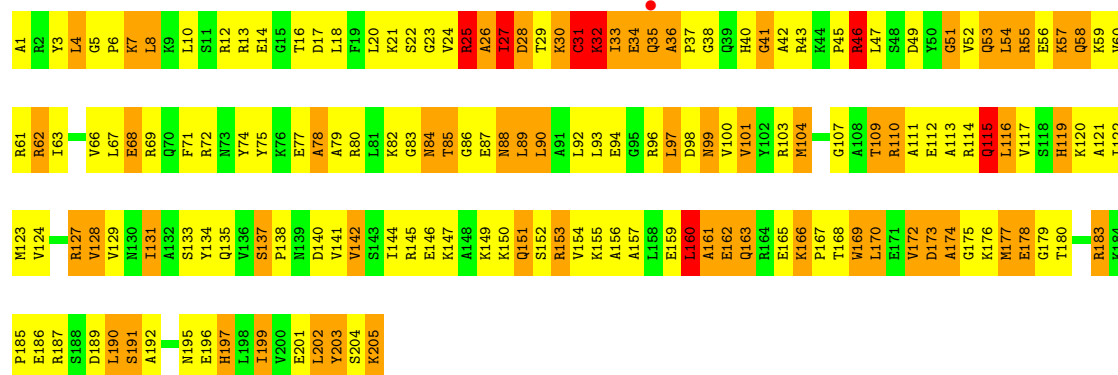
• Molecule 3: 30S ribosomal protein S3

Chain C:



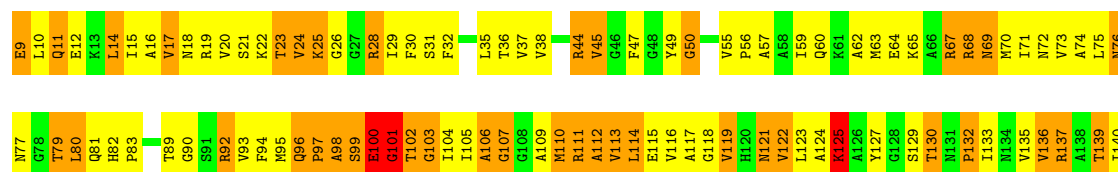
• Molecule 4: 30S ribosomal protein S4

Chain D:



• Molecule 5: 30S ribosomal protein S5

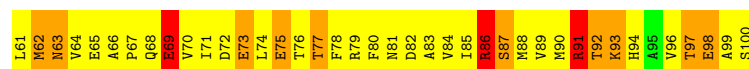
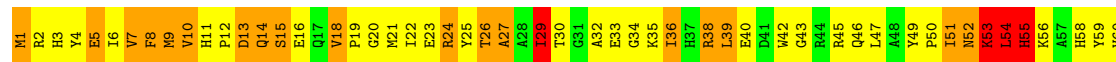
Chain E:





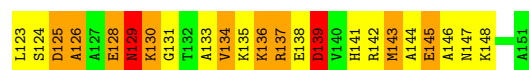
• Molecule 6: 30S ribosomal protein S6

Chain F:



• Molecule 7: 30S ribosomal protein S7

Chain G:



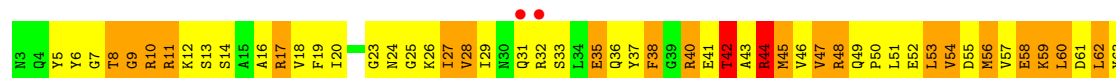
• Molecule 8: 30S ribosomal protein S8

Chain H:



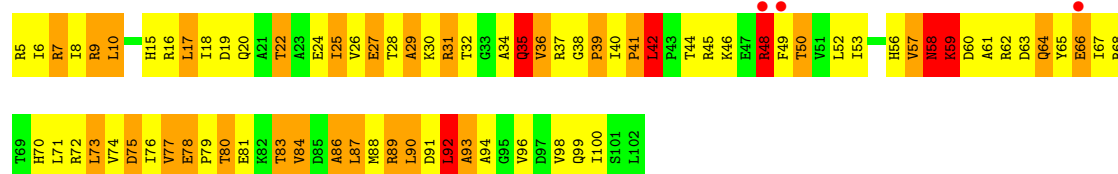
• Molecule 9: 30S ribosomal protein S9

Chain I:



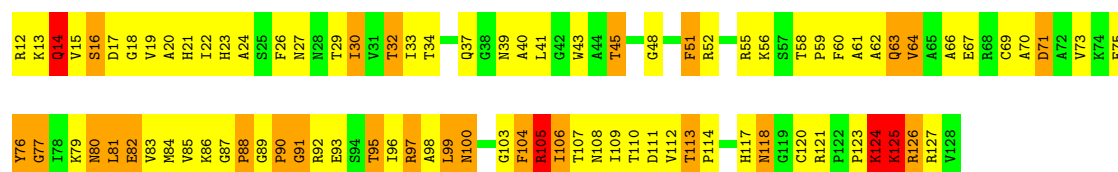
• Molecule 10: 30S ribosomal protein S10

Chain J:



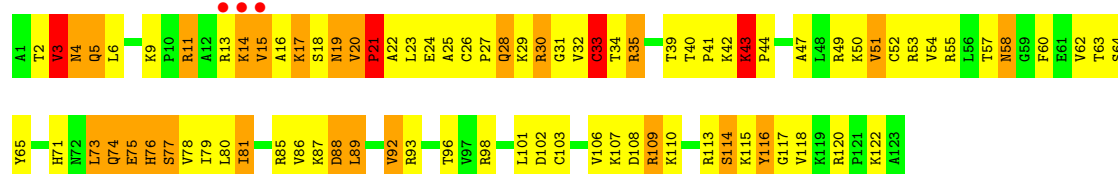
• Molecule 11: 30S ribosomal protein S11

Chain K:



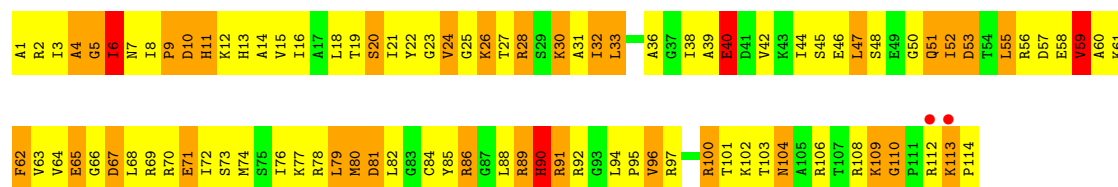
• Molecule 12: 30S ribosomal protein S12

Chain L:



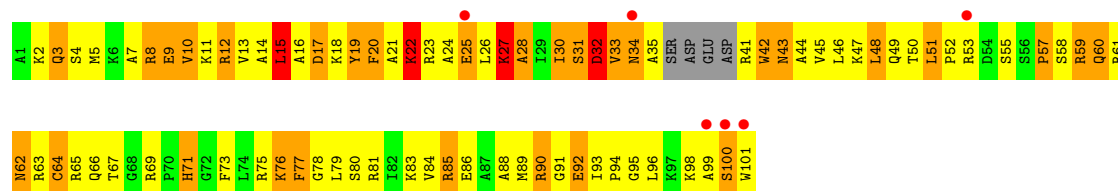
• Molecule 13: 30S ribosomal protein S13

Chain M:



• Molecule 14: 30S ribosomal protein S14

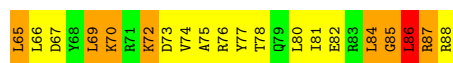
Chain N:



• Molecule 15: 30S ribosomal protein S15

Chain O:





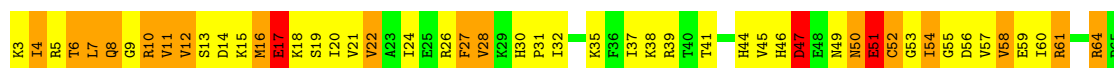
- Molecule 16: 30S ribosomal protein S16

Chain P:



- Molecule 17: 30S ribosomal protein S17

Chain Q:



- Molecule 18: 30S ribosomal protein S18

Chain R:



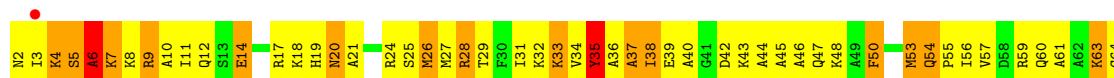
- Molecule 19: 30S ribosomal protein S19

Chain S:



- Molecule 20: 30S ribosomal protein S20

Chain T:



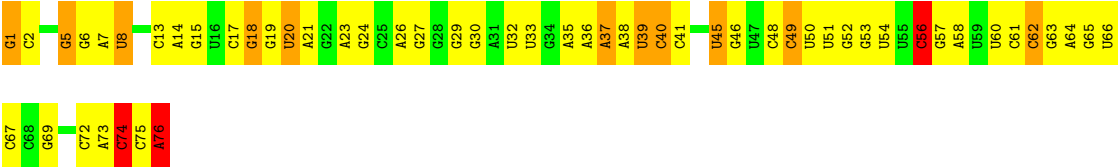
- Molecule 21: 30S ribosomal protein S21

Chain U:



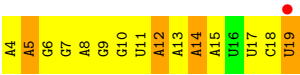
● Molecule 22: phenylalanine specific transfer RNA

Chain V:



● Molecule 23: messenger RNA

Chain X:



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	211.67Å 438.07Å 613.42Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 3.00 69.21 – 3.00	Depositor EDS
% Data completeness (in resolution range)	(Not available) (40.00-3.00) 83.5 (69.21-3.00)	Depositor EDS
$R_{merge}$	0.19	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.58 (at 3.01Å)	Xtriage
Refinement program	PHENIX	Depositor
R, $R_{free}$	0.202 , 0.260 0.503 , 0.511	Depositor DCC
$R_{free}$ test set	19047 reflections (2.03%)	DCC
Wilson B-factor (Å <sup>2</sup> )	44.7	Xtriage
Anisotropy	0.180	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.21 , 36.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.28$	Xtriage
Outliers	0 of 938380 reflections	Xtriage
$F_o, F_c$ correlation	0.37	EDS
Total number of atoms	53792	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.44% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities 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: 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	0.86	8/36966 (0.0%)	1.30	335/57666 (0.6%)
2	B	0.54	0/1736	0.72	0/2338
3	C	0.51	0/1652	0.72	1/2225 (0.0%)
4	D	0.65	0/1665	0.80	1/2227 (0.0%)
5	E	0.62	0/1119	0.85	0/1504
6	F	0.55	0/836	0.80	1/1128 (0.1%)
7	G	0.48	0/1196	0.67	0/1602
8	H	0.58	0/989	0.74	0/1326
9	I	0.53	0/1034	0.75	0/1375
10	J	0.52	0/797	0.76	1/1077 (0.1%)
11	K	0.59	0/893	0.75	0/1205
12	L	0.72	0/969	0.92	0/1300
13	M	0.50	0/893	0.71	0/1193
14	N	0.51	0/785	0.65	0/1043
15	O	0.53	0/722	0.73	0/964
16	P	0.61	0/659	0.79	1/884 (0.1%)
17	Q	0.62	0/658	0.76	0/881
18	R	0.54	0/463	0.68	0/621
19	S	0.55	0/653	0.67	0/877
20	T	0.57	0/671	0.73	0/888
21	U	0.78	0/431	0.85	0/570
22	V	0.74	1/1813 (0.1%)	1.22	10/2823 (0.4%)
23	X	0.73	0/388	1.09	0/603
All	All	0.77	9/57988 (0.0%)	1.17	350/86320 (0.4%)

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
4	D	0	1
5	E	0	2
6	F	0	1
11	K	0	2
12	L	0	2
20	T	0	1
21	U	0	1
All	All	0	10

The worst 5 of 9 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	V	1	G	OP3-P	-9.45	1.49	1.61
1	A	283	U	C2-N3	5.96	1.42	1.37
1	A	816	A	N9-C4	-5.93	1.34	1.37
1	A	397	A	N3-C4	-5.75	1.31	1.34
1	A	1514	G	C5-C4	-5.71	1.34	1.38

The worst 5 of 350 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	245	U	C2-N1-C1'	-13.58	101.40	117.70
1	A	283	U	C2-N1-C1'	10.34	130.10	117.70
1	A	245	U	C6-N1-C1'	10.30	135.62	121.20
1	A	677	U	N3-C2-O2	-10.19	115.07	122.20
1	A	713	G	N1-C6-O6	-10.01	113.89	119.90

There are no chirality outliers.

5 of 10 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	D	25	ARG	Peptide
5	E	101	GLY	Peptide
5	E	103	GLY	Peptide
6	F	54	LEU	Peptide
11	K	124	LYS	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	33015	0	16617	2186	0
2	B	1705	0	1732	298	0
3	C	1625	0	1699	237	0
4	D	1643	0	1710	224	0
5	E	1106	0	1148	211	0
6	F	818	0	808	156	0
7	G	1182	0	1240	166	0
8	H	979	0	1034	119	0
9	I	1022	0	1070	186	0
10	J	787	0	828	140	0
11	K	877	0	887	136	0
12	L	955	0	1019	118	0
13	M	884	0	944	140	0
14	N	774	0	827	131	0
15	O	714	0	737	87	0
16	P	649	0	666	87	0
17	Q	649	0	691	103	0
18	R	456	0	478	57	0
19	S	638	0	665	96	0
20	T	665	0	714	129	0
21	U	426	0	449	119	0
22	V	1623	0	821	46	0
23	X	346	0	173	24	0
24	A	56	0	0	0	0
25	A	190	0	0	12	0
25	L	1	0	0	0	0
25	N	5	0	0	1	0
25	U	2	0	0	0	0
All	All	53792	0	36957	4869	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 54.

The worst 5 of 4869 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1053:G:H4'	1:A:1054:C:H5'	1.29	1.11
12:L:33:CYS:HA	12:L:54:VAL:HA	1.44	0.99
1:A:1362:A:H4'	1:A:1362:A:OP1	1.61	0.98
1:A:1053:G:C4'	1:A:1054:C:H5'	1.94	0.96

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
4:D:25:ARG:HG3	4:D:26:ALA:N	1.80	0.95

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	216/218 (99%)	112 (52%)	49 (23%)	55 (26%)	0	0
3	C	204/206 (99%)	126 (62%)	47 (23%)	31 (15%)	0	1
4	D	203/205 (99%)	136 (67%)	36 (18%)	31 (15%)	0	1
5	E	148/150 (99%)	90 (61%)	31 (21%)	27 (18%)	0	1
6	F	98/100 (98%)	54 (55%)	23 (24%)	21 (21%)	0	0
7	G	149/151 (99%)	79 (53%)	46 (31%)	24 (16%)	0	1
8	H	127/129 (98%)	82 (65%)	32 (25%)	13 (10%)	1	4
9	I	125/127 (98%)	77 (62%)	33 (26%)	15 (12%)	1	2
10	J	96/98 (98%)	64 (67%)	14 (15%)	18 (19%)	0	1
11	K	115/117 (98%)	81 (70%)	19 (16%)	15 (13%)	0	2
12	L	121/123 (98%)	91 (75%)	16 (13%)	14 (12%)	1	3
13	M	112/114 (98%)	65 (58%)	24 (21%)	23 (20%)	0	0
14	N	92/100 (92%)	39 (42%)	30 (33%)	23 (25%)	0	0
15	O	86/88 (98%)	52 (60%)	17 (20%)	17 (20%)	0	0
16	P	80/82 (98%)	47 (59%)	22 (28%)	11 (14%)	0	2
17	Q	78/80 (98%)	48 (62%)	18 (23%)	12 (15%)	0	1
18	R	53/55 (96%)	31 (58%)	19 (36%)	3 (6%)	3	16
19	S	77/79 (98%)	56 (73%)	14 (18%)	7 (9%)	1	5
20	T	83/85 (98%)	46 (55%)	23 (28%)	14 (17%)	0	1
21	U	49/51 (96%)	22 (45%)	10 (20%)	17 (35%)	0	0

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	2312/2358 (98%)	1398 (60%)	523 (23%)	391 (17%)	<b>0</b> <b>1</b>

5 of 391 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	9	LEU
2	B	15	PHE
2	B	21	TYR
2	B	35	ASN
2	B	56	LEU

### 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	180/180 (100%)	131 (73%)	49 (27%)	<b>0</b> <b>3</b>
3	C	170/170 (100%)	123 (72%)	47 (28%)	<b>0</b> <b>3</b>
4	D	172/172 (100%)	123 (72%)	49 (28%)	<b>0</b> <b>3</b>
5	E	113/113 (100%)	87 (77%)	26 (23%)	<b>1</b> <b>6</b>
6	F	87/87 (100%)	61 (70%)	26 (30%)	<b>0</b> <b>2</b>
7	G	124/124 (100%)	85 (68%)	39 (32%)	<b>0</b> <b>2</b>
8	H	104/104 (100%)	78 (75%)	26 (25%)	<b>1</b> <b>4</b>
9	I	105/105 (100%)	67 (64%)	38 (36%)	<b>0</b> <b>1</b>
10	J	86/86 (100%)	61 (71%)	25 (29%)	<b>0</b> <b>2</b>
11	K	90/90 (100%)	67 (74%)	23 (26%)	<b>1</b> <b>4</b>
12	L	103/103 (100%)	75 (73%)	28 (27%)	<b>0</b> <b>3</b>
13	M	92/92 (100%)	71 (77%)	21 (23%)	<b>1</b> <b>6</b>
14	N	79/83 (95%)	60 (76%)	19 (24%)	<b>1</b> <b>5</b>
15	O	76/76 (100%)	60 (79%)	16 (21%)	<b>1</b> <b>8</b>
16	P	65/65 (100%)	48 (74%)	17 (26%)	<b>1</b> <b>4</b>
17	Q	74/74 (100%)	47 (64%)	27 (36%)	<b>0</b> <b>1</b>
18	R	48/48 (100%)	40 (83%)	8 (17%)	<b>3</b> <b>16</b>

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
19	S	70/70 (100%)	53 (76%)	17 (24%)	1	5
20	T	65/65 (100%)	47 (72%)	18 (28%)	0	3
21	U	44/44 (100%)	26 (59%)	18 (41%)	0	0
All	All	1947/1951 (100%)	1410 (72%)	537 (28%)	0	3

5 of 537 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
8	H	41	GLU
10	J	9	ARG
19	S	38	THR
8	H	66	GLN
9	I	44	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 52 such sidechains are listed below:

Mol	Chain	Res	Type
10	J	20	GLN
11	K	27	ASN
20	T	19	HIS
10	J	64	GLN
10	J	99	GLN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	1538/1539 (99%)	445 (28%)	20 (1%)
22	V	75/76 (98%)	15 (20%)	1 (1%)
23	X	15/16 (93%)	4 (26%)	0
All	All	1628/1631 (99%)	464 (28%)	21 (1%)

5 of 464 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	4	U
1	A	5	U
1	A	6	G
1	A	7	A
1	A	8	A

5 of 21 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	733	G
1	A	1049	U
1	A	1317	C
1	A	653	U
1	A	1491	G

## 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 56 ligands modelled in this entry, 56 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	1539/1539 (100%)	-0.03	16 (1%) 79 22	0, 33, 101, 147	0
2	B	218/218 (100%)	-0.25	3 (1%) 72 18	19, 59, 88, 113	0
3	C	206/206 (100%)	-0.06	2 (0%) 79 22	9, 46, 75, 92	0
4	D	205/205 (100%)	-0.26	1 (0%) 88 36	0, 24, 64, 82	0
5	E	150/150 (100%)	-0.24	0 100 100	0, 31, 68, 98	0
6	F	100/100 (100%)	-0.16	0 100 100	17, 54, 80, 93	0
7	G	151/151 (100%)	-0.04	7 (4%) 31 7	20, 54, 81, 94	0
8	H	129/129 (100%)	-0.15	0 100 100	4, 34, 58, 82	0
9	I	127/127 (100%)	0.09	3 (2%) 56 11	20, 55, 85, 117	0
10	J	98/98 (100%)	0.14	3 (3%) 47 9	25, 58, 82, 113	0
11	K	117/117 (100%)	-0.12	0 100 100	0, 32, 66, 79	0
12	L	123/123 (100%)	-0.18	3 (2%) 56 11	0, 17, 58, 93	0
13	M	114/114 (100%)	-0.03	2 (1%) 65 14	26, 63, 87, 97	0
14	N	96/100 (96%)	0.48	6 (6%) 19 5	10, 56, 84, 98	0
15	O	88/88 (100%)	-0.23	0 100 100	1, 33, 66, 89	0
16	P	82/82 (100%)	-0.26	1 (1%) 75 20	0, 24, 67, 91	0
17	Q	80/80 (100%)	-0.03	0 100 100	7, 44, 79, 94	0
18	R	55/55 (100%)	-0.14	0 100 100	5, 38, 80, 101	0
19	S	79/79 (100%)	-0.07	0 100 100	37, 65, 83, 95	0
20	T	85/85 (100%)	-0.02	2 (2%) 56 11	8, 38, 69, 96	0
21	U	51/51 (100%)	0.14	5 (9%) 8 2	8, 47, 74, 80	0
22	V	76/76 (100%)	-0.39	0 100 100	22, 43, 72, 119	0
23	X	16/16 (100%)	0.57	1 (6%) 19 5	16, 77, 102, 124	0
All	All	3985/3989 (99%)	-0.07	55 (1%) 72 18	0, 41, 85, 147	0

The worst 5 of 55 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1209	C	5.9
1	A	1210	C	5.4
23	X	19	U	5.1
7	G	10	LYS	4.7
1	A	421	U	4.6

## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
24	MG	A	1647	1/1	0.36	24.83	0,0,0,0	0
24	MG	A	1615	1/1	0.35	20.27	9,9,9,9	0
24	MG	A	1633	1/1	0.41	13.35	11,11,11,11	0
24	MG	A	1654	1/1	0.46	9.92	22,22,22,22	0
24	MG	A	1655	1/1	0.30	6.60	9,9,9,9	0
24	MG	A	1651	1/1	0.19	5.07	7,7,7,7	0
24	MG	A	1627	1/1	0.41	4.46	35,35,35,35	0
24	MG	A	1638	1/1	0.19	4.46	27,27,27,27	0
24	MG	A	1637	1/1	0.26	3.21	19,19,19,19	0
24	MG	A	1646	1/1	0.28	3.20	10,10,10,10	0
24	MG	A	1650	1/1	0.26	2.08	5,5,5,5	0
24	MG	A	1639	1/1	0.18	1.99	0,0,0,0	0
24	MG	A	1656	1/1	0.17	1.26	9,9,9,9	0
24	MG	A	1618	1/1	0.18	0.66	4,4,4,4	0
24	MG	A	1648	1/1	0.18	0.57	0,0,0,0	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
24	MG	A	1649	1/1	0.16	-0.53	11,11,11,11	0
24	MG	A	1642	1/1	0.13	-0.61	6,6,6,6	0
24	MG	A	1609	1/1	0.20	-0.88	26,26,26,26	0
24	MG	A	1626	1/1	0.12	-1.09	14,14,14,14	0
24	MG	A	1634	1/1	0.17	-1.14	10,10,10,10	0
24	MG	A	1603	1/1	0.14	-1.27	13,13,13,13	0
24	MG	A	1614	1/1	0.12	-1.41	19,19,19,19	0
24	MG	A	1652	1/1	0.15	-1.50	1,1,1,1	0
24	MG	A	1640	1/1	0.14	-1.65	0,0,0,0	0
24	MG	A	1619	1/1	0.15	-1.73	0,0,0,0	0
24	MG	A	1607	1/1	0.13	-1.80	1,1,1,1	0
24	MG	A	1617	1/1	0.13	-1.85	13,13,13,13	0
24	MG	A	1610	1/1	0.12	-1.88	0,0,0,0	0
24	MG	A	1630	1/1	0.16	-1.94	41,41,41,41	0
24	MG	A	1612	1/1	0.10	-1.95	18,18,18,18	0
24	MG	A	1611	1/1	0.06	-2.40	13,13,13,13	0
24	MG	A	1604	1/1	0.05	-2.48	13,13,13,13	0
24	MG	A	1623	1/1	0.07	-2.71	3,3,3,3	0
24	MG	A	1606	1/1	0.11	-2.80	24,24,24,24	0
24	MG	A	1631	1/1	0.08	-2.82	35,35,35,35	0
24	MG	A	1653	1/1	0.09	-2.93	7,7,7,7	0
24	MG	A	1644	1/1	0.16	-3.00	0,0,0,0	0
24	MG	A	1624	1/1	0.10	-3.02	1,1,1,1	0
24	MG	A	1643	1/1	0.11	-3.12	3,3,3,3	0
24	MG	A	1636	1/1	0.15	-3.59	42,42,42,42	0
24	MG	A	1620	1/1	0.07	-3.66	19,19,19,19	0
24	MG	A	1641	1/1	0.11	-3.73	20,20,20,20	0
24	MG	A	1608	1/1	0.09	-3.74	18,18,18,18	0
24	MG	A	1602	1/1	0.06	-3.76	21,21,21,21	0
24	MG	A	1629	1/1	0.14	-4.02	17,17,17,17	0
24	MG	A	1613	1/1	0.07	-4.57	0,0,0,0	0
24	MG	A	1616	1/1	0.10	-4.94	0,0,0,0	0
24	MG	A	1635	1/1	0.07	-5.11	21,21,21,21	0
24	MG	A	1605	1/1	0.06	-5.21	21,21,21,21	0
24	MG	A	1645	1/1	0.09	-5.34	8,8,8,8	0
24	MG	A	1628	1/1	0.05	-5.67	25,25,25,25	0
24	MG	A	1632	1/1	0.04	-6.04	18,18,18,18	0
24	MG	A	1621	1/1	0.07	-7.29	12,12,12,12	0
24	MG	A	1601	1/1	0.07	-8.56	2,2,2,2	0
24	MG	A	1625	1/1	0.06	-9.05	0,0,0,0	0
24	MG	A	1622	1/1	0.07	-10.55	4,4,4,4	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.