



# wwPDB X-ray Structure Validation Summary Report

Feb 27, 2014 – 04:00 PM GMT

PDB ID : 3V24  
Title : Crystal structure of RMF bound to the 70S ribosome. This PDB entry contains coordinates for the 30S subunit with bound RMF of the 2nd ribosome in the ASU  
Authors : Polikanov, Y.S.; Blaha, G.M.; Steitz, T.A.  
Deposited on : 2011-12-11  
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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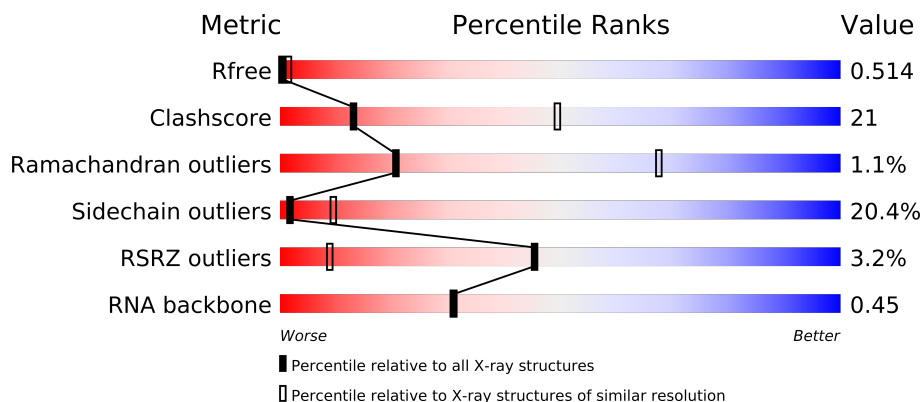
The following versions of software and data (see [references](#)) were used in the production of this report:

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	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	<div><div></div></div>
14	N	61	<div><div></div></div>
15	O	89	<div><div></div></div>
16	P	88	<div><div></div></div>
17	Q	105	<div><div></div></div>
18	R	88	<div><div></div></div>
19	S	93	<div><div></div></div>
20	T	106	<div><div></div></div>
21	U	27	<div><div></div></div>
22	V	61	<div><div></div></div>

## 2 Entry composition

There are 25 unique types of molecules in this entry. The entry contains 50378 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	1501	Total	C	N	O	P	0	0	0
			32270	14362	5983	10424	1501			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	229	Total	C	N	O	S	0	0	0
			1775	1132	318	320	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
			1450	906	279	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
			1526	963	283	274	6			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	148	Total	C	N	O	S	0	0	0
			1105	699	204	198	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
			777	493	137	144	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
			1164	726	224	208	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
			1045	665	188	190	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
			852	533	163	156			

- 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
			663	410	132	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	114	Total	C	N	O	S	0	0	0
			804	497	164	142	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	N	60	Total	C	N	O	S	0	0	0
			478	303	99	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
			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
			651	416	123	111	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	Q	99	Total	C	N	O	S	0	0	0
			823	528	151	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	81	Total	C	N	O	S	0	0	0
			560	351	108	99	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	T	97	Total	C	N	O	S	0	0	0
			713	438	152	121	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
			199	122	48	29			

- Molecule 22 is a protein called Ribosome modulation factor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	V	53	Total	C	N	O	S	0	0	0
			353	218	67	66	2			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
V	56	HIS	-	EXPRESSION TAG	UNP P0AFW2
V	57	HIS	-	EXPRESSION TAG	UNP P0AFW2
V	58	HIS	-	EXPRESSION TAG	UNP P0AFW2
V	59	HIS	-	EXPRESSION TAG	UNP P0AFW2
V	60	HIS	-	EXPRESSION TAG	UNP P0AFW2
V	61	HIS	-	EXPRESSION TAG	UNP P0AFW2

- Molecule 23 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
23	A	71	Total	Mg	0	0
			71	71		

- Molecule 24 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 25 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
25	A	120	Total	O	0	0
			120	120		
25	D	1	Total	O	0	0
			1	1		
25	K	2	Total	O	0	0
			2	2		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
25	P	1	Total	O	0	0
			1	1		
25	T	2	Total	O	0	0
			2	2		

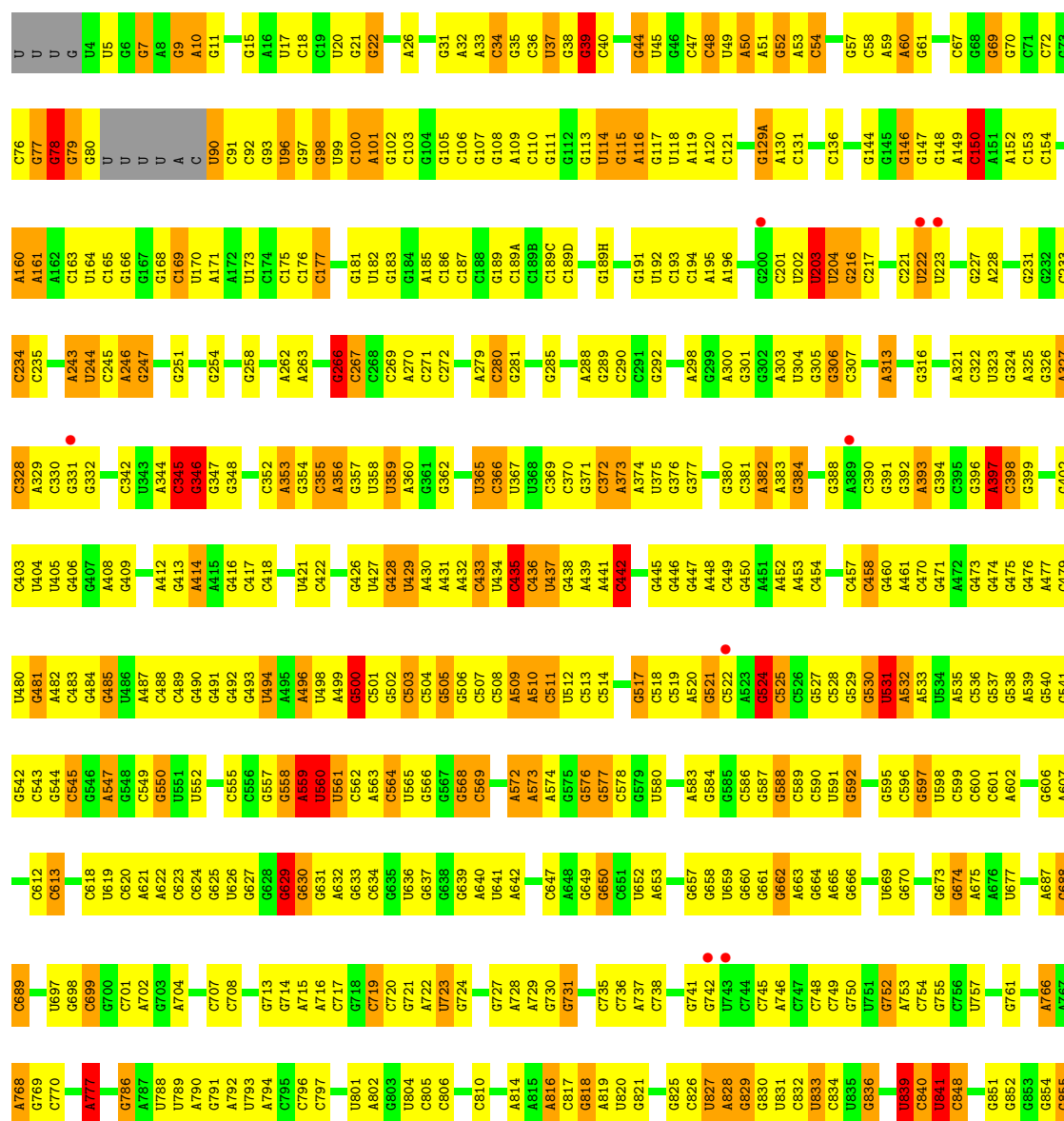


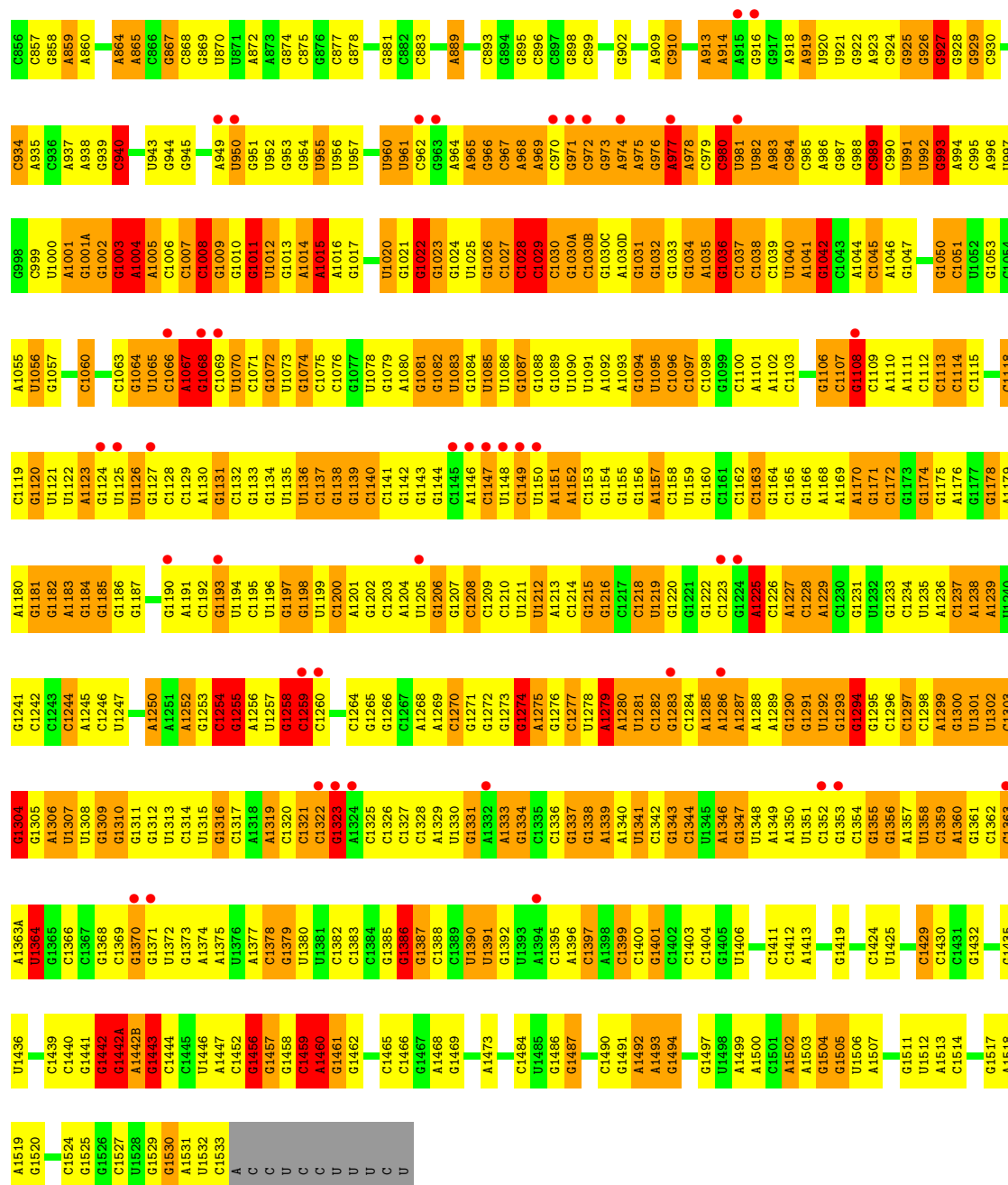
### 3 Residue-property plots

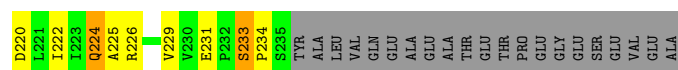
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according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

Chain A: 

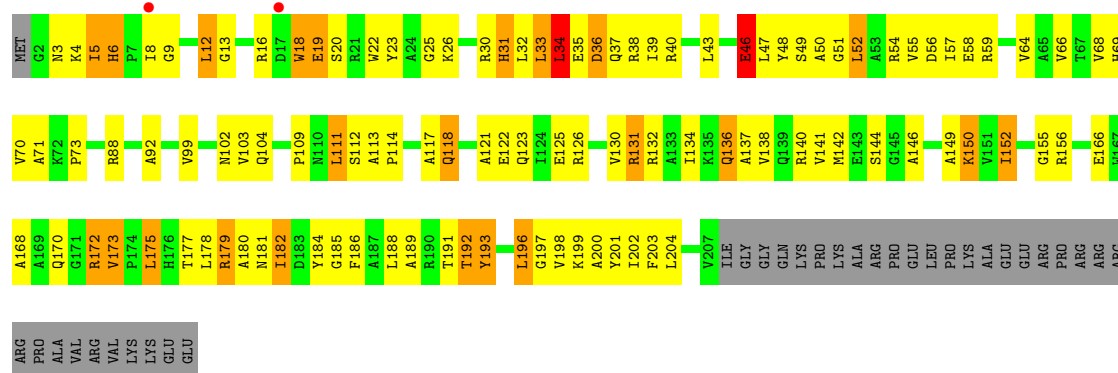






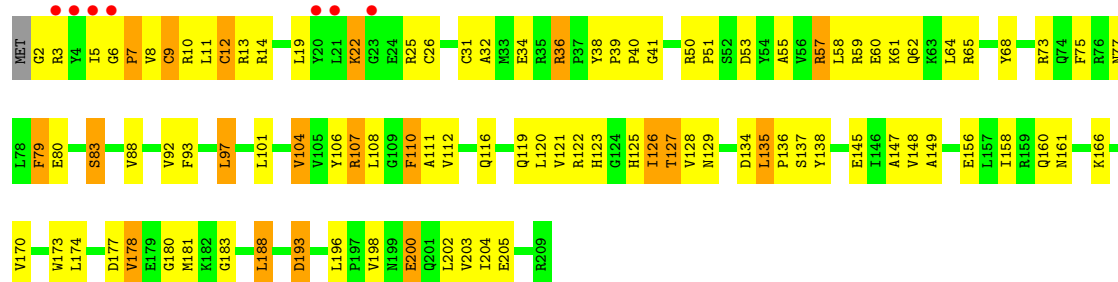
• Molecule 3: 30S ribosomal protein S3

Chain C:



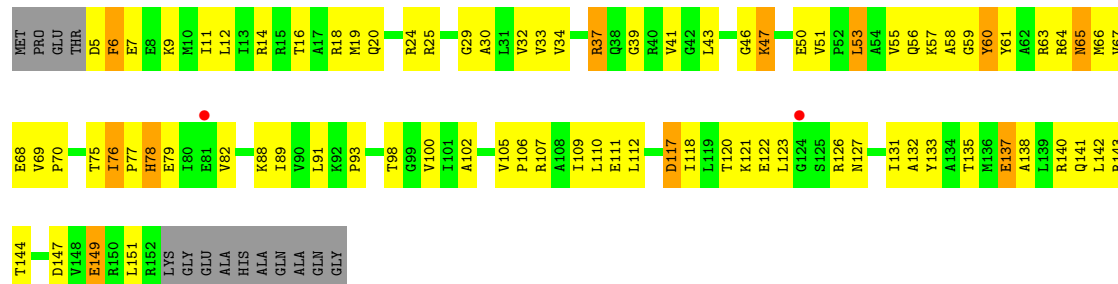
• Molecule 4: 30S ribosomal protein S4

Chain D:



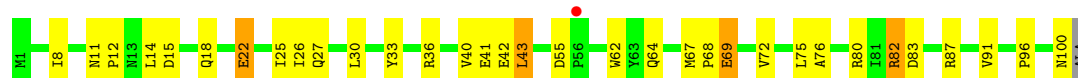
• Molecule 5: 30S ribosomal protein S5

Chain E:



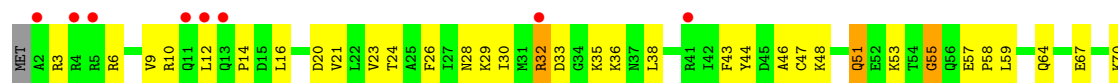
• Molecule 6: 30S ribosomal protein S6

Chain F:



• Molecule 7: 30S ribosomal protein S7

Chain G:



- Molecule 8: 30S ribosomal protein S8

Chain H:



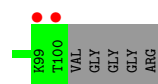
- Molecule 9: 30S ribosomal protein S9

Chain I:



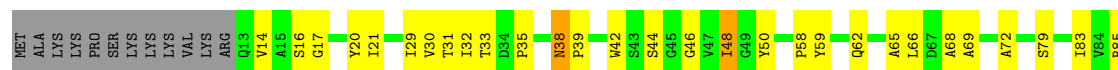
- Molecule 10: 30S ribosomal protein S10

Chain J:



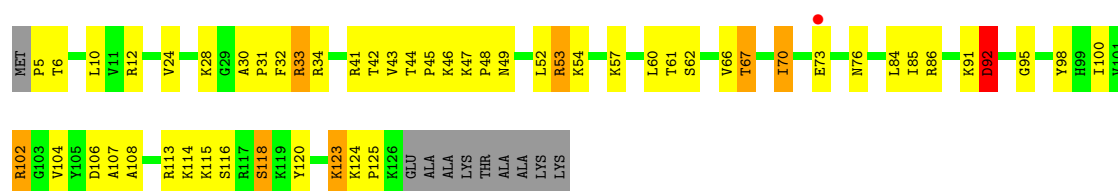
- Molecule 11: 30S ribosomal protein S11

Chain K:



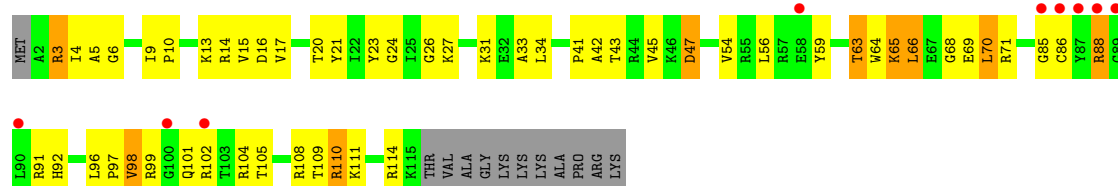
- Molecule 12: 30S ribosomal protein S12

Chain L:



- Molecule 13: 30S ribosomal protein S13

Chain M:



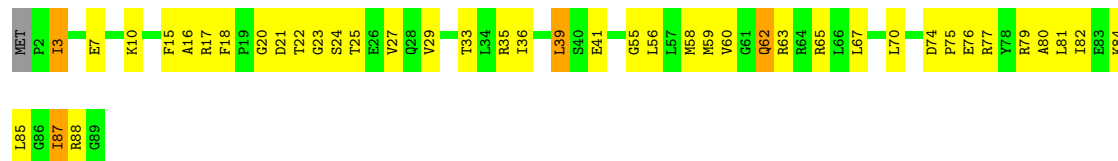
- Molecule 14: 30S ribosomal protein S14

Chain N:



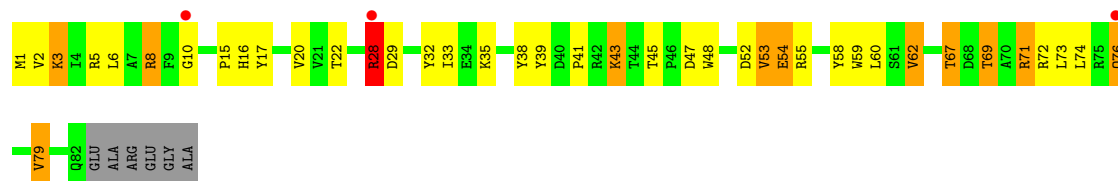
- Molecule 15: 30S ribosomal protein S15

Chain O:



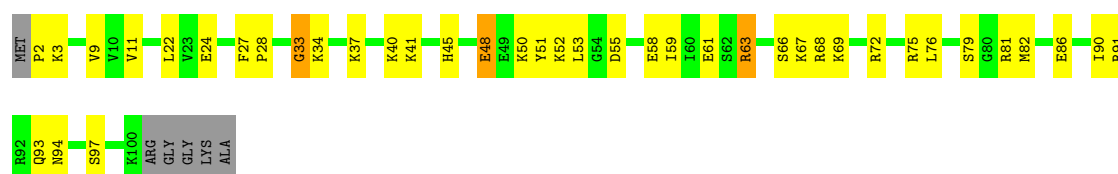
- Molecule 16: 30S ribosomal protein S16

Chain P:



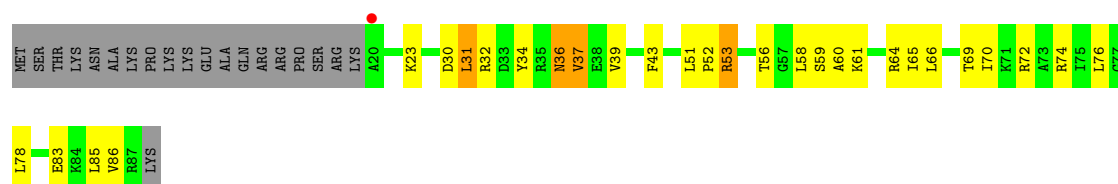
- Molecule 17: 30S ribosomal protein S17

Chain Q:



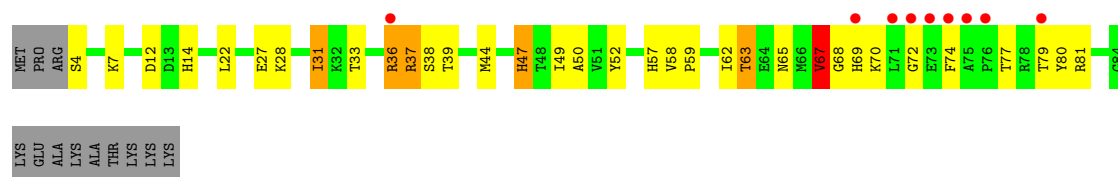
- Molecule 18: 30S ribosomal protein S18

Chain R:



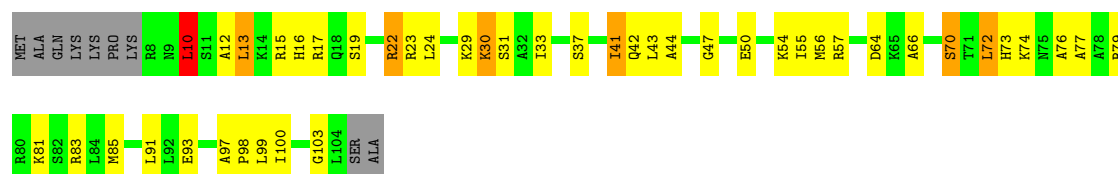
- Molecule 19: 30S ribosomal protein S19

Chain S:



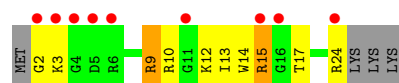
- Molecule 20: 30S ribosomal protein S20

Chain T:



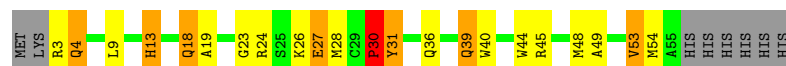
- Molecule 21: 30S ribosomal protein THX

Chain U:



- Molecule 22: Ribosome modulation factor

Chain V:



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	210.24Å 451.44Å 621.64Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.75 – 3.00 49.75 – 3.00	Depositor EDS
% Data completeness (in resolution range)	97.9 (49.75-3.00) 98.0 (49.75-3.00)	Depositor EDS
$R_{merge}$	0.27	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.34 (at 3.01Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.2_869)	Depositor
R, $R_{free}$	0.218 , 0.254 0.512 , 0.514	Depositor DCC
$R_{free}$ test set	57194 reflections (5.27%)	DCC
Wilson B-factor (Å <sup>2</sup> )	68.3	Xtriage
Anisotropy	0.254	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.27 , 74.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.27$	Xtriage
Outliers	0 of 1142037 reflections	Xtriage
$F_o, F_c$ correlation	0.49	EDS
Total number of atoms	50378	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	118.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.58% 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: 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	0.91	21/36123 (0.1%)	1.38	452/56379 (0.8%)
2	B	0.61	0/1809	0.73	1/2450 (0.0%)
3	C	0.68	0/1474	0.79	2/2003 (0.1%)
4	D	0.64	2/1556 (0.1%)	0.74	2/2113 (0.1%)
5	E	0.58	0/1121	0.78	1/1517 (0.1%)
6	F	0.54	0/790	0.70	0/1077
7	G	0.72	0/1183	0.77	0/1599
8	H	0.50	0/1065	0.67	0/1445
9	I	0.74	0/867	0.84	1/1180 (0.1%)
10	J	0.75	0/676	0.88	2/924 (0.2%)
11	K	0.53	0/843	0.69	0/1144
12	L	0.54	0/921	0.73	0/1247
13	M	0.72	0/814	0.83	0/1107
14	N	0.66	0/487	0.71	1/649 (0.2%)
15	O	0.52	0/735	0.72	0/981
16	P	0.54	0/667	0.84	1/905 (0.1%)
17	Q	0.57	0/836	0.72	0/1117
18	R	0.56	0/519	0.79	0/699
19	S	0.69	0/574	0.81	0/781
20	T	0.52	0/715	0.77	0/947
21	U	0.73	0/203	0.68	0/266
22	V	0.65	0/360	0.85	1/492 (0.2%)
All	All	0.82	23/54338 (0.0%)	1.22	464/81022 (0.6%)

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

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

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Mol	Chain	#Chirality outliers	#Planarity outliers
3	C	0	2
5	E	0	1
7	G	0	1
9	I	0	1
12	L	0	1
13	M	0	1
17	Q	0	1
20	T	0	1
22	V	0	3
All	All	0	15

The worst 5 of 23 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1459	C	N1-C2	17.17	1.57	1.40
1	A	1442(A)	G	N9-C4	15.91	1.50	1.38
1	A	90	U	C4-O4	13.40	1.34	1.23
1	A	1442(A)	G	C2-N3	11.63	1.42	1.32
1	A	1459	C	C1'-N1	10.41	1.64	1.48

The worst 5 of 464 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1442(A)	G	N3-C4-C5	-27.29	114.95	128.60
1	A	1459	C	N3-C2-O2	-27.00	103.00	121.90
1	A	1459	C	C6-N1-C2	-26.34	109.77	120.30
1	A	1442(A)	G	N3-C4-N9	23.46	140.08	126.00
1	A	1459	C	N1-C2-O2	21.61	131.87	118.90

There are no chirality outliers.

5 of 15 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	128	GLU	Peptide
2	B	14	GLY	Peptide
2	B	71	VAL	Peptide
3	C	19	GLU	Peptide
3	C	46	GLU	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	32270	0	16287	982	0
2	B	1775	0	1743	93	0
3	C	1450	0	1314	99	0
4	D	1526	0	1415	91	0
5	E	1105	0	1130	60	0
6	F	777	0	737	23	0
7	G	1164	0	1106	54	0
8	H	1045	0	1033	52	0
9	I	852	0	742	62	0
10	J	663	0	558	30	0
11	K	828	0	822	31	0
12	L	905	0	916	44	0
13	M	804	0	752	47	0
14	N	478	0	497	35	0
15	O	724	0	749	29	0
16	P	651	0	638	35	0
17	Q	823	0	891	18	0
18	R	514	0	530	24	0
19	S	560	0	466	23	0
20	T	713	0	766	30	0
21	U	199	0	208	9	0
22	V	353	0	266	13	0
23	A	71	0	0	0	0
24	D	1	0	0	0	0
24	N	1	0	0	0	0
25	A	120	0	0	13	0
25	D	1	0	0	0	0
25	K	2	0	0	0	0
25	P	1	0	0	0	0
25	T	2	0	0	0	0
All	All	50378	0	33566	1672	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 21.

The worst 5 of 1672 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:559:A:H4'	1:A:560:U:H3'	1.36	1.07
1:A:1003:G:H1	1:A:1037:C:N4	1.56	1.02
1:A:1010:G:H2'	1:A:1011:G:H8	1.28	0.98
1:A:1010:G:H2'	1:A:1011:G:C8	2.00	0.96
1:A:346:G:N2	1:A:347:G:N3	2.15	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	227/256 (89%)	192 (85%)	33 (14%)	2 (1%)	25	73
3	C	204/239 (85%)	177 (87%)	27 (13%)	0	100	100
4	D	206/209 (99%)	180 (87%)	24 (12%)	2 (1%)	22	70
5	E	146/162 (90%)	126 (86%)	20 (14%)	0	100	100
6	F	98/101 (97%)	88 (90%)	10 (10%)	0	100	100
7	G	153/156 (98%)	128 (84%)	23 (15%)	2 (1%)	18	62
8	H	136/138 (99%)	125 (92%)	11 (8%)	0	100	100
9	I	123/128 (96%)	109 (89%)	12 (10%)	2 (2%)	14	56
10	J	94/105 (90%)	74 (79%)	18 (19%)	2 (2%)	11	47
11	K	112/129 (87%)	100 (89%)	12 (11%)	0	100	100
12	L	120/132 (91%)	107 (89%)	11 (9%)	2 (2%)	14	54
13	M	112/126 (89%)	84 (75%)	27 (24%)	1 (1%)	25	73
14	N	58/61 (95%)	51 (88%)	6 (10%)	1 (2%)	14	54
15	O	86/89 (97%)	72 (84%)	14 (16%)	0	100	100
16	P	80/88 (91%)	71 (89%)	7 (9%)	2 (2%)	9	40
17	Q	97/105 (92%)	86 (89%)	11 (11%)	0	100	100
18	R	66/88 (75%)	60 (91%)	6 (9%)	0	100	100
19	S	79/93 (85%)	60 (76%)	16 (20%)	3 (4%)	5	27

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
20	T	95/106 (90%)	81 (85%)	11 (12%)	3 (3%)	6	33
21	U	21/27 (78%)	19 (90%)	2 (10%)	0	100	100
22	V	51/61 (84%)	34 (67%)	14 (28%)	3 (6%)	2	14
All	All	2364/2599 (91%)	2024 (86%)	315 (13%)	25 (1%)	21	67

5 of 25 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
12	L	92	ASP
2	B	129	GLU
16	P	53	VAL
19	S	47	HIS
20	T	100	ILE

### 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	177/220 (80%)	135 (76%)	42 (24%)	1	5
3	C	114/188 (61%)	78 (68%)	36 (32%)	0	2
4	D	141/181 (78%)	114 (81%)	27 (19%)	2	12
5	E	108/123 (88%)	84 (78%)	24 (22%)	1	7
6	F	76/90 (84%)	69 (91%)	7 (9%)	13	46
7	G	103/127 (81%)	77 (75%)	26 (25%)	1	4
8	H	103/119 (87%)	84 (82%)	19 (18%)	2	13
9	I	62/99 (63%)	48 (77%)	14 (23%)	1	6
10	J	53/92 (58%)	39 (74%)	14 (26%)	1	4
11	K	81/99 (82%)	70 (86%)	11 (14%)	5	24
12	L	91/109 (84%)	79 (87%)	12 (13%)	6	25
13	M	64/101 (63%)	49 (77%)	15 (23%)	1	5
14	N	46/50 (92%)	33 (72%)	13 (28%)	0	3
15	O	77/80 (96%)	71 (92%)	6 (8%)	18	55

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
16	P	63/74 (85%)	47 (75%)	16 (25%)	1	4
17	Q	94/97 (97%)	80 (85%)	14 (15%)	4	20
18	R	49/77 (64%)	42 (86%)	7 (14%)	5	22
19	S	43/80 (54%)	32 (74%)	11 (26%)	1	4
20	T	65/82 (79%)	55 (85%)	10 (15%)	4	19
21	U	18/22 (82%)	13 (72%)	5 (28%)	0	3
22	V	21/50 (42%)	14 (67%)	7 (33%)	0	2
All	All	1649/2160 (76%)	1313 (80%)	336 (20%)	2	9

5 of 336 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
7	G	104	LEU
9	I	60	ASP
19	S	63	THR
7	G	143	ARG
8	H	49	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 28 such sidechains are listed below:

Mol	Chain	Res	Type
9	I	73	GLN
10	J	33	GLN
22	V	4	GLN
9	I	87	GLN
9	I	117	HIS

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	1499/1522 (98%)	383 (25%)	29 (1%)

5 of 383 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	5	U
1	A	9	G

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Mol	Chain	Res	Type
1	A	10	A
1	A	22	G
1	A	26	A

5 of 29 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	687	A
1	A	913	A
1	A	1442	G
1	A	748	C
1	A	991	U

## 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 73 ligands modelled in this entry, 73 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	1501/1522 (98%)	0.06	52 (3%) 42 8	53, 112, 168, 181	0
2	B	229/256 (89%)	-0.17	4 (1%) 67 15	113, 135, 150, 160	0
3	C	206/239 (86%)	-0.09	2 (0%) 79 22	119, 140, 153, 162	0
4	D	208/209 (99%)	-0.05	7 (3%) 43 8	95, 111, 129, 142	0
5	E	148/162 (91%)	-0.18	2 (1%) 72 18	87, 108, 124, 132	0
6	F	100/101 (99%)	-0.27	1 (1%) 79 22	93, 107, 123, 135	0
7	G	155/156 (99%)	0.11	9 (5%) 22 5	118, 144, 151, 158	0
8	H	138/138 (100%)	-0.08	0 100 100	89, 110, 120, 133	0
9	I	125/128 (97%)	0.22	6 (4%) 29 6	129, 151, 161, 173	0
10	J	96/105 (91%)	0.08	3 (3%) 47 9	130, 149, 161, 169	0
11	K	114/129 (88%)	-0.17	0 100 100	79, 109, 122, 124	0
12	L	122/132 (92%)	-0.05	1 (0%) 83 26	72, 92, 106, 116	0
13	M	114/126 (90%)	0.25	9 (7%) 13 3	124, 145, 155, 158	0
14	N	60/61 (98%)	0.76	7 (11%) 5 2	136, 146, 152, 155	0
15	O	88/89 (98%)	-0.18	0 100 100	79, 102, 122, 129	0
16	P	82/88 (93%)	0.09	3 (3%) 39 8	89, 105, 123, 132	0
17	Q	99/105 (94%)	-0.15	0 100 100	84, 98, 113, 117	0
18	R	68/88 (77%)	-0.17	1 (1%) 70 16	95, 107, 138, 143	0
19	S	81/93 (87%)	0.33	9 (11%) 6 2	125, 146, 153, 155	0
20	T	97/106 (91%)	-0.02	0 100 100	84, 103, 125, 132	0
21	U	23/27 (85%)	1.85	9 (39%) 1 0	130, 145, 153, 154	0
22	V	53/61 (86%)	-0.46	0 100 100	90, 115, 141, 151	0
All	All	3907/4121 (94%)	0.02	125 (3%) 45 9	53, 118, 159, 181	0

The worst 5 of 125 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1149	C	9.5
1	A	1148	U	7.6
13	M	86	CYS	6.5
1	A	1224	G	6.3
13	M	87	TYR	6.1

## 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
23	MG	A	1655	1/1	0.09	-	83,83,83,83	0
23	MG	A	1601	1/1	0.39	-	62,62,62,62	0
23	MG	A	1620	1/1	0.51	-	69,69,69,69	0
23	MG	A	1639	1/1	0.19	-	71,71,71,71	0
23	MG	A	1638	1/1	0.49	-	67,67,67,67	0
23	MG	A	1628	1/1	0.14	-	79,79,79,79	0
23	MG	A	1618	1/1	0.12	-	70,70,70,70	0
23	MG	A	1614	1/1	0.28	-	71,71,71,71	0
23	MG	A	1642	1/1	0.39	-	67,67,67,67	0
23	MG	A	1635	1/1	0.09	-	101,101,101,101	0
23	MG	A	1607	1/1	0.22	-	81,81,81,81	0
23	MG	A	1622	1/1	0.14	-	64,64,64,64	0
23	MG	A	1643	1/1	0.29	-	74,74,74,74	0
23	MG	A	1646	1/1	0.32	-	74,74,74,74	0
23	MG	A	1604	1/1	0.22	-	73,73,73,73	0
23	MG	A	1669	1/1	0.07	-	64,64,64,64	0
23	MG	A	1648	1/1	0.32	-	92,92,92,92	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
23	MG	A	1650	1/1	0.10	-	100,100,100,100	0
23	MG	A	1654	1/1	0.20	-	65,65,65,65	0
23	MG	A	1605	1/1	0.24	-	110,110,110,110	0
23	MG	A	1666	1/1	0.14	-	94,94,94,94	0
23	MG	A	1621	1/1	0.21	-	57,57,57,57	0
23	MG	A	1624	1/1	0.48	-	73,73,73,73	0
23	MG	A	1657	1/1	0.28	-	74,74,74,74	0
23	MG	A	1602	1/1	0.18	-	50,50,50,50	0
24	ZN	D	301	1/1	0.06	-	96,96,96,96	0
23	MG	A	1608	1/1	0.20	-	72,72,72,72	0
23	MG	A	1611	1/1	0.30	-	80,80,80,80	0
23	MG	A	1656	1/1	0.15	-	95,95,95,95	0
23	MG	A	1658	1/1	0.39	-	97,97,97,97	0
23	MG	A	1668	1/1	0.19	-	131,131,131,131	0
23	MG	A	1609	1/1	0.36	-	67,67,67,67	0
23	MG	A	1665	1/1	0.62	-	91,91,91,91	0
23	MG	A	1651	1/1	0.17	-	92,92,92,92	0
23	MG	A	1627	1/1	0.35	-	86,86,86,86	0
23	MG	A	1663	1/1	0.26	-	100,100,100,100	0
23	MG	A	1660	1/1	0.14	-	83,83,83,83	0
23	MG	A	1616	1/1	0.19	-	76,76,76,76	0
23	MG	A	1636	1/1	0.14	-	68,68,68,68	0
23	MG	A	1633	1/1	0.35	-	65,65,65,65	0
23	MG	A	1625	1/1	0.39	-	82,82,82,82	0
23	MG	A	1603	1/1	0.17	-	82,82,82,82	0
23	MG	A	1667	1/1	0.13	-	76,76,76,76	0
23	MG	A	1626	1/1	0.99	-	88,88,88,88	0
23	MG	A	1610	1/1	0.28	-	70,70,70,70	0
23	MG	A	1659	1/1	0.22	-	86,86,86,86	0
23	MG	A	1617	1/1	0.32	-	72,72,72,72	0
23	MG	A	1623	1/1	0.14	-	74,74,74,74	0
24	ZN	N	101	1/1	0.07	-	188,188,188,188	0
23	MG	A	1613	1/1	0.16	-	84,84,84,84	0
23	MG	A	1629	1/1	0.16	-	55,55,55,55	0
23	MG	A	1649	1/1	0.12	-	78,78,78,78	0
23	MG	A	1661	1/1	0.09	-	60,60,60,60	0
23	MG	A	1652	1/1	0.41	-	100,100,100,100	0
23	MG	A	1612	1/1	0.19	-	64,64,64,64	0
23	MG	A	1653	1/1	0.26	-	61,61,61,61	0
23	MG	A	1632	1/1	0.41	-	88,88,88,88	0
23	MG	A	1619	1/1	0.20	-	75,75,75,75	0
23	MG	A	1662	1/1	0.23	-	106,106,106,106	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
23	MG	A	1647	1/1	0.22	-	63,63,63,63	0
23	MG	A	1615	1/1	0.35	-	69,69,69,69	0
23	MG	A	1640	1/1	0.67	-	61,61,61,61	0
23	MG	A	1631	1/1	0.43	-	72,72,72,72	0
23	MG	A	1641	1/1	0.16	-	62,62,62,62	0
23	MG	A	1606	1/1	0.14	-	74,74,74,74	0
23	MG	A	1637	1/1	0.09	-	77,77,77,77	0
23	MG	A	1671	1/1	0.70	-	117,117,117,117	0
23	MG	A	1645	1/1	0.10	-	109,109,109,109	0
23	MG	A	1670	1/1	0.20	-	105,105,105,105	0
23	MG	A	1630	1/1	0.16	-	72,72,72,72	0
23	MG	A	1664	1/1	0.16	-	95,95,95,95	0
23	MG	A	1634	1/1	0.20	-	71,71,71,71	0
23	MG	A	1644	1/1	0.11	-	87,87,87,87	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.