



# wwPDB X-ray Structure Validation Summary Report i

Feb 26, 2014 – 05:09 PM GMT

PDB ID : 3V6W  
Title : Crystal structure of the bacterial ribosome ram mutation G347U. this entry contains the 50S ribosomal subunit of the first 70S molecule in the asymmetric unit  
Authors : Fagan, C.E.; Dunkle, J.A.; Maehigashi, T.; Dunham, C.M.  
Deposited on : 2011-12-20  
Resolution : 3.90 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:

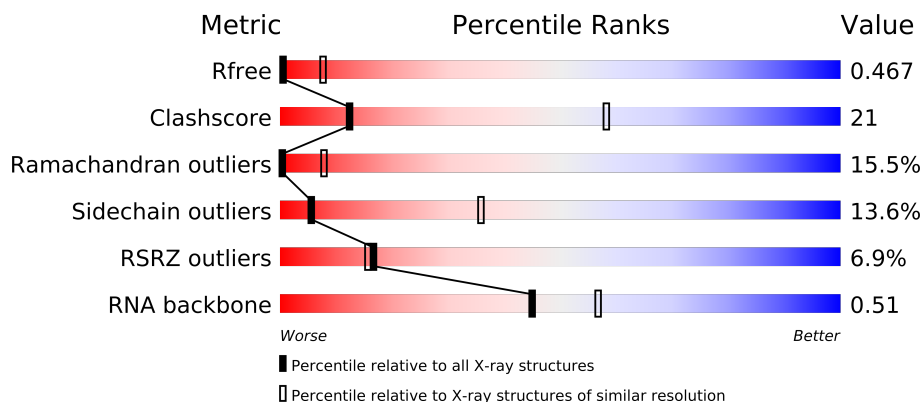
MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP)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



# 1 Overall quality at a glance

The reported resolution of this entry is 3.90 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	1022 (4.38-3.42)
Clashscore	79885	1173 (4.30-3.50)
Ramachandran outliers	78287	1118 (4.30-3.50)
Sidechain outliers	78261	1107 (4.30-3.50)
RSRZ outliers	66119	1000 (4.36-3.44)
RNA backbone	1838	1018 (5.00-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	2916	
2	B	122	
3	C	229	
4	D	276	
5	E	206	
6	F	210	
7	G	182	
8	H	180	
9	I	148	
10	N	140	
11	O	122	
12	P	150	

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Mol	Chain	Length	Quality of chain
13	Q	141	
14	R	118	
15	S	112	
16	T	146	
17	U	118	
18	V	101	
19	W	113	
20	X	96	
21	Y	110	
22	Z	206	
23	0	85	
24	1	98	
25	2	72	
26	3	60	
27	4	71	
28	5	60	
29	6	54	
30	7	49	
31	8	65	
32	9	37	



## 2 Entry composition

There are 32 unique types of molecules in this entry. The entry contains 90631 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 23S rRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	2803	Total	C	N	O	P	0	0	0
			60378	26870	11297	19409	2802			

- Molecule 2 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	119	Total	C	N	O	P	0	0	0
			2551	1136	471	826	118			

- Molecule 3 is a protein called 50S ribosomal protein L1.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	191	Total	C	N	O	0	0	1
			1142	691	221	230			

- Molecule 4 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	272	Total	C	N	O	S	0	0	1
			2105	1329	417	356	3			

- Molecule 5 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	205	Total	C	N	O	S	0	0	1
			1564	988	300	270	6			

- Molecule 6 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	208	Total	C	N	O	S	0	0	1
			1624	1035	304	282	3			



- Molecule 7 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	G	181	Total	C	N	O	S	0	0	0
			1474	942	268	260	4			

- Molecule 8 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	160	Total	C	N	O	S	0	0	1
			1223	773	229	220	1			

- Molecule 9 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	I	146	Total	C	N	O	S	0	0	1
			1132	723	201	207	1			

- Molecule 10 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	N	139	Total	C	N	O	S	0	0	1
			1105	712	207	182	4			

- Molecule 11 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	O	122	Total	C	N	O	S	0	0	0
			933	588	171	170	4			

- Molecule 12 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	P	146	Total	C	N	O	S	0	0	0
			1114	692	227	193	2			

- Molecule 13 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	Q	141	Total	C	N	O	S	0	0	0
			1122	715	212	188	7			

- Molecule 14 is a protein called 50S ribosomal protein L17.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
14	R	117	Total	C	N	O	0	0	0
			960	599	202	159			

- Molecule 15 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
15	S	99	Total	C	N	O	0	0	1
			771	486	155	130			

- Molecule 16 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	T	138	Total	C	N	O	S	0	0	1
			1142	710	235	196	1			

- Molecule 17 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	U	117	Total	C	N	O	S	0	0	0
			958	604	202	151	1			

- Molecule 18 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	V	101	Total	C	N	O	S	0	0	0
			779	501	142	135	1			

- Molecule 19 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	W	113	Total	C	N	O	S	0	0	0
			896	563	176	155	2			

- Molecule 20 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
20	X	93	Total	C	N	O	0	0	1
			726	471	132	123			

- Molecule 21 is a protein called 50S ribosomal protein L24.



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
21	Y	101	Total	C	N	O	S	0	0	1
			776	500	149	123	4			

- Molecule 22 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	Z	177	Total	C	N	O	S	0	0	1
			1404	897	253	252	2			

- Molecule 23 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	0	84	Total	C	N	O	S	0	0	0
			662	410	140	111	1			

- Molecule 24 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	1	94	Total	C	N	O	S	0	0	1
			732	460	146	125	1			

- Molecule 25 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	2	71	Total	C	N	O	S	0	0	0
			598	370	121	106	1			

- Molecule 26 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	3	60	Total	C	N	O	S	0	0	1
			468	298	91	78	1			

- Molecule 27 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	4	31	Total	C	N	O	S	0	0	1
			226	142	37	43	4			

- Molecule 28 is a protein called 50S ribosomal protein L32.



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	5	59	Total	C	N	O	S	0	0	0
			459	288	90	76	5			

- Molecule 29 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	6	45	Total	C	N	O	S	0	0	1
			381	235	78	64	4			

- Molecule 30 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	7	49	Total	C	N	O	S	0	0	1
			419	257	105	55	2			

- Molecule 31 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	8	64	Total	C	N	O	S	0	0	1
			508	326	102	78	2			

- Molecule 32 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	9	36	Total	C	N	O	S	0	0	0
			299	183	67	46	3			

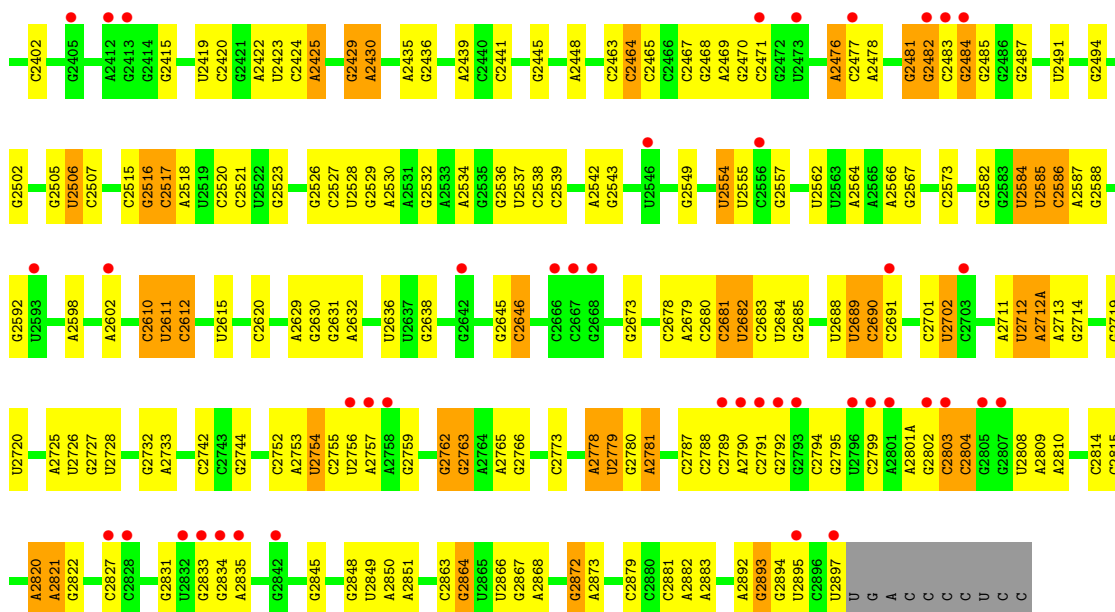






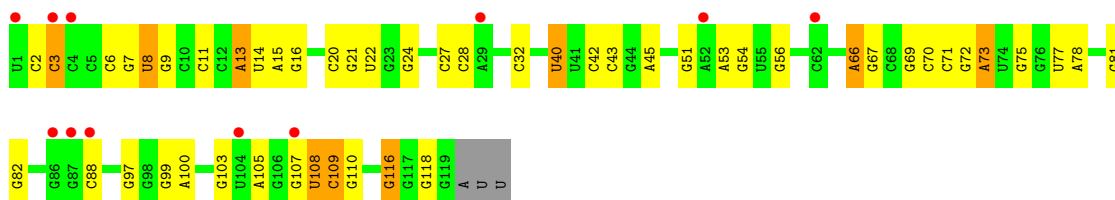






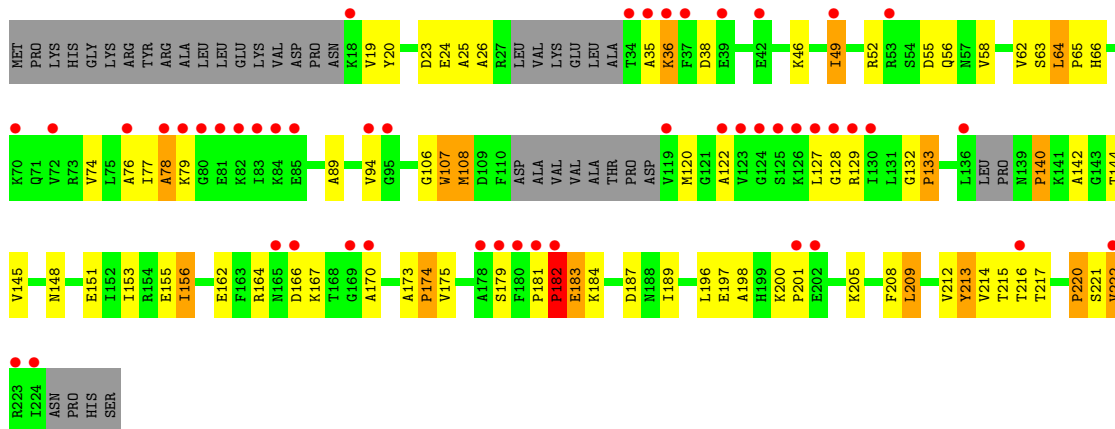
- Molecule 2: 5S rRNA

Chain B: 



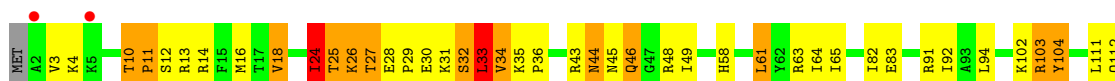
- Molecule 3: 50S ribosomal protein L1

Chain C: 

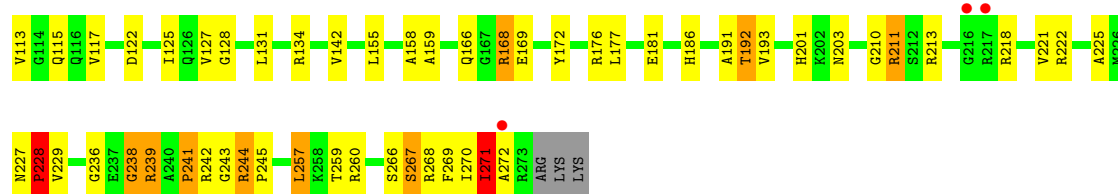


- Molecule 4: 50S ribosomal protein L2

Chain D: 

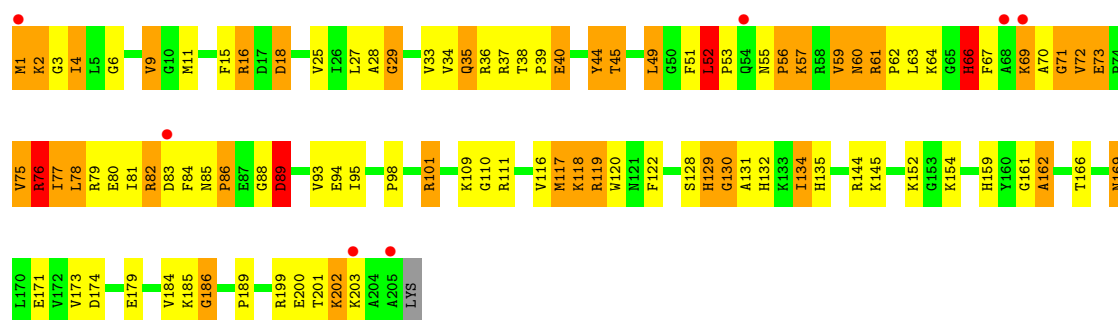






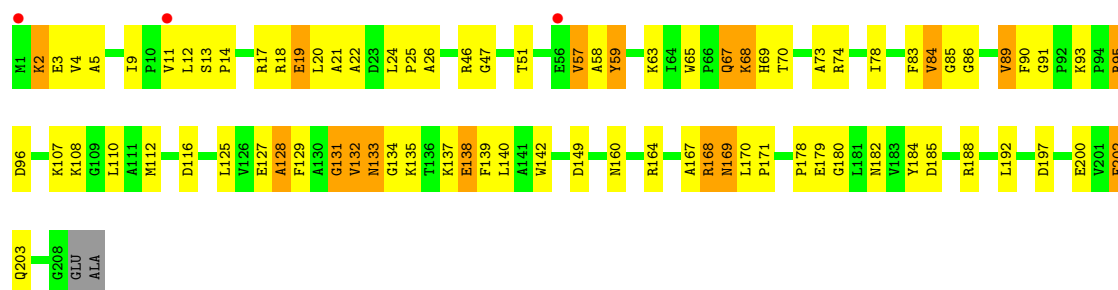
• Molecule 5: 50S ribosomal protein L3

Chain E:



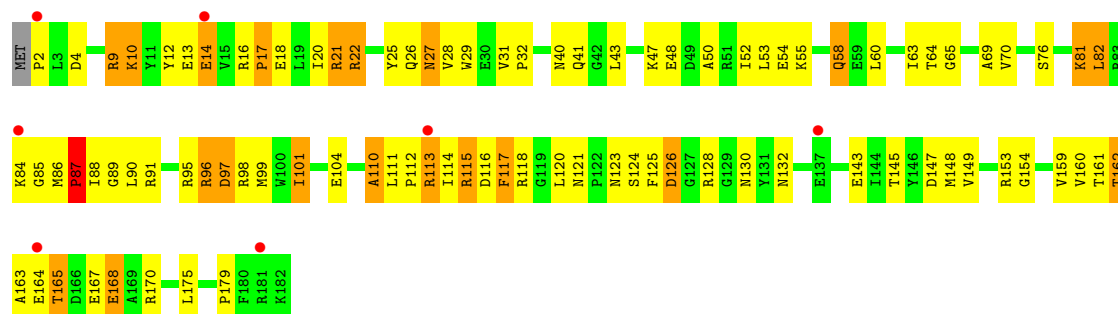
• Molecule 6: 50S ribosomal protein L4

Chain F:



• Molecule 7: 50S ribosomal protein L5

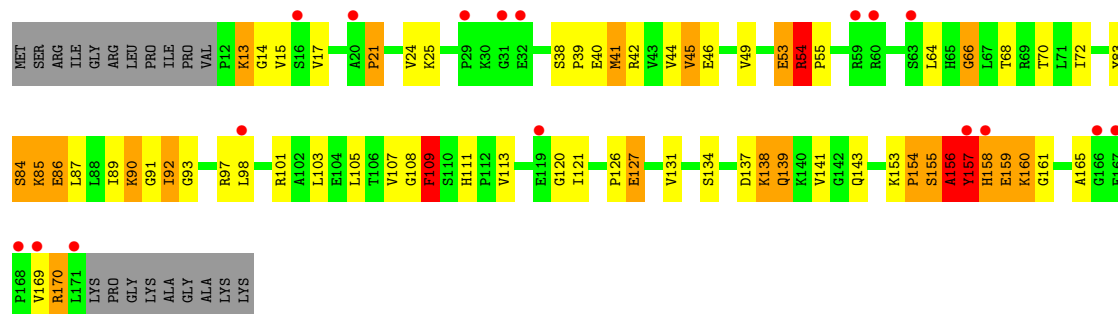
Chain G:



• Molecule 8: 50S ribosomal protein L6

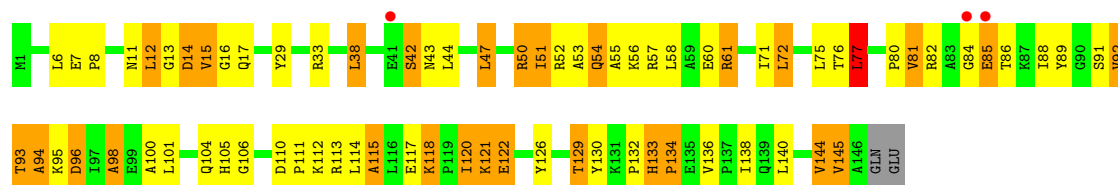
Chain H:





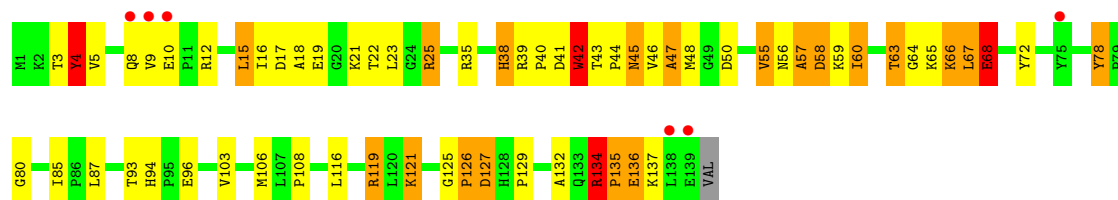
• Molecule 9: 50S ribosomal protein L9

Chain I:



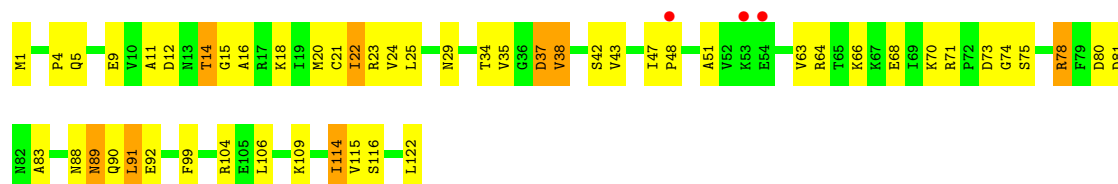
• Molecule 10: 50S ribosomal protein L13

Chain N:



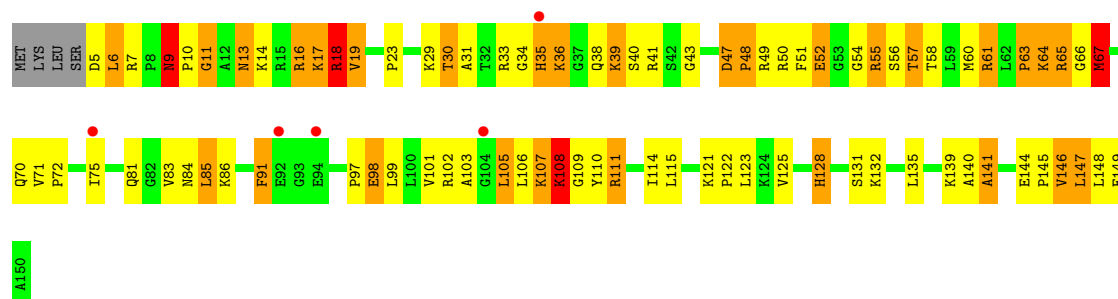
• Molecule 11: 50S ribosomal protein L14

Chain O:



• Molecule 12: 50S ribosomal protein L15

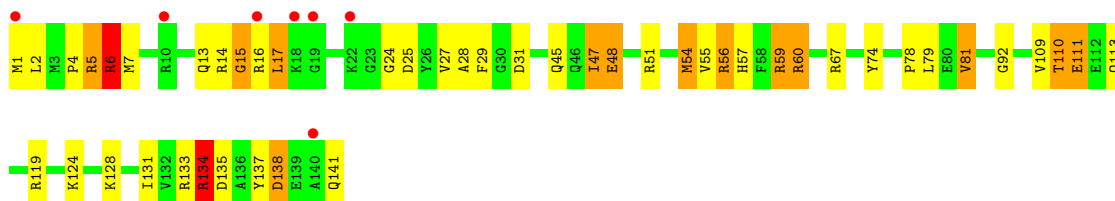
Chain P:





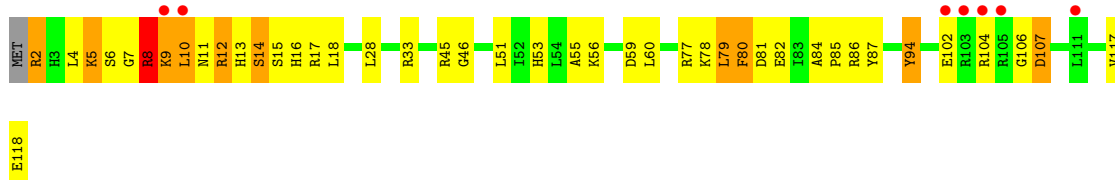
- Molecule 13: 50S ribosomal protein L16

Chain Q:



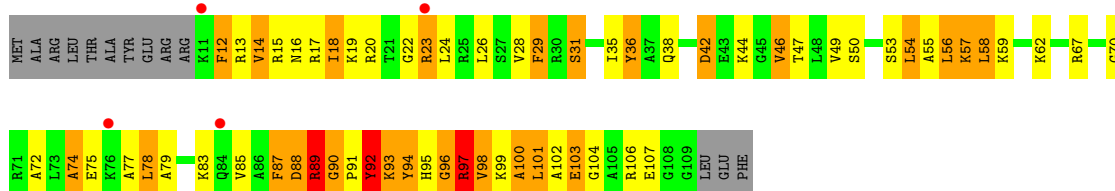
- Molecule 14: 50S ribosomal protein L17

Chain R:



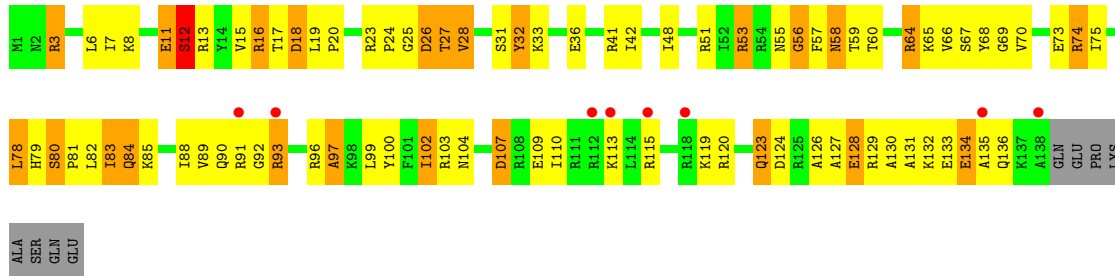
- Molecule 15: 50S ribosomal protein L18

Chain S:



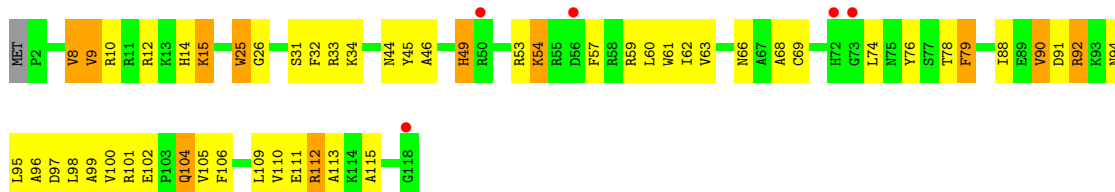
- Molecule 16: 50S ribosomal protein L19

Chain T:



- Molecule 17: 50S ribosomal protein L20

Chain U:









Chain 0:

- Molecule 24: 50S ribosomal protein L28

Chain 1:

- Molecule 25: 50S ribosomal protein L29

Chain 2:

- Molecule 26: 50S ribosomal protein L30

Chain 3:

- Molecule 27: 50S ribosomal protein L31

Chain 4:

- Molecule 28: 50S ribosomal protein L32

Chain 5:

- Molecule 29: 50S ribosomal protein L33

Chain 6:

- Molecule 30: 50S ribosomal protein L34



Chain 7: 



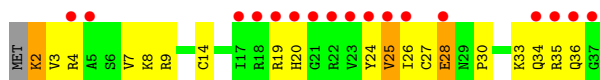
- Molecule 31: 50S ribosomal protein L35

Chain 8: 



- Molecule 32: 50S ribosomal protein L36

Chain 9: 





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	210.20Å 446.16Å 620.95Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 3.90 34.93 – 4.00	Depositor EDS
% Data completeness (in resolution range)	94.3 (50.00-3.90) 95.2 (34.93-4.00)	Depositor EDS
$R_{merge}$	0.35	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.17 (at 3.99Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.1_1168)	Depositor
R, $R_{free}$	0.242 , 0.269 0.466 , 0.467	Depositor DCC
$R_{free}$ test set	20472 reflections (4.41%)	DCC
Wilson B-factor (Å <sup>2</sup> )	115.4	Xtriage
Anisotropy	0.219	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.22 , -9.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.42$ , $\langle L^2 \rangle = 0.25$	Xtriage
Outliers	0 of 464342 reflections	Xtriage
$F_o, F_c$ correlation	0.54	EDS
Total number of atoms	90631	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.56% 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 ⓘ

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	0.52	1/67620 (0.0%)	0.74	24/105555 (0.0%)
2	B	0.41	0/2853	0.71	1/4451 (0.0%)
3	C	0.37	0/1145	0.67	7/1556 (0.4%)
4	D	0.52	0/2155	0.82	0/2907
5	E	0.44	0/1597	0.78	2/2155 (0.1%)
6	F	0.45	0/1659	0.74	0/2246
7	G	0.41	0/1499	0.73	1/2016 (0.0%)
8	H	0.37	0/1246	0.70	2/1684 (0.1%)
9	I	0.35	0/1147	0.71	0/1553
10	N	0.40	0/1132	0.74	1/1527 (0.1%)
11	O	0.66	0/943	0.68	0/1269
12	P	0.47	0/1131	0.84	0/1504
13	Q	0.41	0/1143	0.69	0/1527
14	R	0.40	0/974	0.76	0/1302
15	S	0.41	0/779	0.72	0/1038
16	T	0.58	0/1156	0.68	0/1544
17	U	0.39	0/975	0.70	0/1297
18	V	0.38	0/790	0.70	0/1057
19	W	0.41	0/907	0.69	0/1216
20	X	0.49	0/740	0.72	0/995
21	Y	0.49	0/789	0.77	0/1053
22	Z	0.38	0/1436	0.66	0/1951
23	0	0.39	0/671	0.67	0/892
24	1	0.46	0/739	0.84	1/983 (0.1%)
25	2	0.43	0/600	0.69	0/793
26	3	0.38	0/473	0.67	0/636
27	4	0.44	0/229	0.66	0/311
28	5	0.38	0/473	0.68	0/639
29	6	0.47	0/388	0.65	0/520
30	7	0.56	0/427	0.75	0/563
31	8	0.51	0/516	0.85	0/681
32	9	0.31	0/302	0.58	0/397
All	All	0.49	1/98634 (0.0%)	0.73	39/147818 (0.0%)



All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	271(U)	G	O3'-P	5.17	1.67	1.61

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	52	LEU	C-N-CD	-8.27	102.41	120.60
1	A	1301	A	N9-C1'-C2'	5.81	121.56	114.00
1	A	2225	A	C2'-C3'-O3'	5.77	122.94	113.70
1	A	1786	A	N9-C1'-C2'	5.76	121.49	114.00
1	A	1493	C	N1-C1'-C2'	5.74	121.46	114.00

There are no chirality outliers.

There are no planarity outliers.

## 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	60378	0	44	818	1
2	B	2551	0	0	33	1
3	C	1142	0	0	17	0
4	D	2105	0	0	63	0
5	E	1564	0	0	79	0
6	F	1624	0	0	46	0
7	G	1474	0	0	75	0
8	H	1223	0	0	35	0
9	I	1132	0	0	36	0
10	N	1105	0	0	35	0
11	O	933	0	0	45	0
12	P	1114	0	0	85	0
13	Q	1122	0	0	36	0
14	R	960	0	0	29	0
15	S	771	0	0	50	0
16	T	1142	0	0	60	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
17	U	958	0	0	53	0
18	V	779	0	0	35	0
19	W	896	0	0	29	0
20	X	726	0	0	12	0
21	Y	776	0	0	40	0
22	Z	1404	0	0	38	0
23	0	662	0	0	17	0
24	1	732	0	0	28	0
25	2	598	0	0	21	0
26	3	468	0	0	12	0
27	4	226	0	0	15	0
28	5	459	0	480	56	0
29	6	381	0	391	72	0
30	7	419	0	467	32	0
31	8	508	0	576	99	0
32	9	299	0	326	21	0
All	All	90631	0	2284	1866	1

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 1866 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:272:G:C2	1:A:421:U:C4	2.35	1.14
1:A:2584:U:C2'	1:A:2585:U:C5'	2.30	1.09
29:6:41:PRO:HD2	29:6:46:HIS:H	1.23	1.04
29:6:47:THR:HB	29:6:49:HIS:CE1	1.93	1.03
1:A:2075:U:C4	1:A:2238:G:C6	2.50	0.98

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

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1593:G:N3	2:B:54:G:OP1[1_655]	2.19	0.01

## 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	
3	C	183/229 (80%)	84 (46%)	45 (25%)	54 (30%)	0	1
4	D	270/276 (98%)	212 (78%)	33 (12%)	25 (9%)	1	23
5	E	203/206 (98%)	130 (64%)	35 (17%)	38 (19%)	0	4
6	F	206/210 (98%)	129 (63%)	54 (26%)	23 (11%)	1	16
7	G	179/182 (98%)	115 (64%)	39 (22%)	25 (14%)	0	10
8	H	158/180 (88%)	93 (59%)	31 (20%)	34 (22%)	0	3
9	I	144/148 (97%)	89 (62%)	28 (19%)	27 (19%)	0	4
10	N	137/140 (98%)	84 (61%)	33 (24%)	20 (15%)	0	9
11	O	120/122 (98%)	88 (73%)	25 (21%)	7 (6%)	3	39
12	P	144/150 (96%)	83 (58%)	32 (22%)	29 (20%)	0	4
13	Q	139/141 (99%)	104 (75%)	19 (14%)	16 (12%)	1	15
14	R	115/118 (98%)	83 (72%)	22 (19%)	10 (9%)	1	25
15	S	97/112 (87%)	38 (39%)	27 (28%)	32 (33%)	0	0
16	T	136/146 (93%)	82 (60%)	31 (23%)	23 (17%)	0	6
17	U	115/118 (98%)	70 (61%)	34 (30%)	11 (10%)	1	21
18	V	99/101 (98%)	63 (64%)	19 (19%)	17 (17%)	0	6
19	W	111/113 (98%)	75 (68%)	24 (22%)	12 (11%)	1	17
20	X	91/96 (95%)	66 (72%)	20 (22%)	5 (6%)	3	41
21	Y	99/110 (90%)	54 (54%)	18 (18%)	27 (27%)	0	1
22	Z	175/206 (85%)	103 (59%)	35 (20%)	37 (21%)	0	3
23	0	82/85 (96%)	63 (77%)	12 (15%)	7 (8%)	1	26
24	1	92/98 (94%)	64 (70%)	19 (21%)	9 (10%)	1	21
25	2	69/72 (96%)	47 (68%)	13 (19%)	9 (13%)	0	12
26	3	58/60 (97%)	41 (71%)	7 (12%)	10 (17%)	0	6
27	4	29/71 (41%)	15 (52%)	7 (24%)	7 (24%)	0	2
28	5	57/60 (95%)	42 (74%)	8 (14%)	7 (12%)	1	14
29	6	43/54 (80%)	20 (46%)	12 (28%)	11 (26%)	0	2
30	7	47/49 (96%)	44 (94%)	2 (4%)	1 (2%)	11	66
31	8	62/65 (95%)	40 (64%)	13 (21%)	9 (14%)	0	9
32	9	34/37 (92%)	27 (79%)	6 (18%)	1 (3%)	7	59

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	3494/3755 (93%)	2248 (64%)	703 (20%)	543 (16%)	<b>0</b> <b>8</b>

5 of 543 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	20	TYR
3	C	35	ALA
3	C	38	ASP
3	C	46	LYS
3	C	58	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
3	C	61/181 (34%)	56 (92%)	5 (8%)	<b>17</b> 62
4	D	213/218 (98%)	179 (84%)	34 (16%)	<b>3</b> <b>27</b>
5	E	165/166 (99%)	140 (85%)	25 (15%)	<b>4</b> <b>30</b>
6	F	165/166 (99%)	146 (88%)	19 (12%)	<b>8</b> 44
7	G	155/156 (99%)	138 (89%)	17 (11%)	<b>9</b> 47
8	H	132/148 (89%)	119 (90%)	13 (10%)	<b>12</b> 53
9	I	122/124 (98%)	102 (84%)	20 (16%)	<b>3</b> <b>25</b>
10	N	117/119 (98%)	96 (82%)	21 (18%)	<b>2</b> <b>20</b>
11	O	100/100 (100%)	92 (92%)	8 (8%)	<b>17</b> 64
12	P	112/116 (97%)	86 (77%)	26 (23%)	<b>1</b> <b>9</b>
13	Q	111/111 (100%)	96 (86%)	15 (14%)	<b>6</b> 36
14	R	100/101 (99%)	87 (87%)	13 (13%)	<b>6</b> 38
15	S	77/88 (88%)	66 (86%)	11 (14%)	<b>5</b> 33
16	T	120/127 (94%)	90 (75%)	30 (25%)	<b>1</b> <b>8</b>
17	U	92/94 (98%)	85 (92%)	7 (8%)	<b>19</b> 66
18	V	82/82 (100%)	72 (88%)	10 (12%)	<b>7</b> 41
19	W	91/92 (99%)	82 (90%)	9 (10%)	<b>11</b> 52

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
20	X	74/78 (95%)	67 (90%)	7 (10%)	12	54
21	Y	84/91 (92%)	72 (86%)	12 (14%)	5	33
22	Z	155/179 (87%)	138 (89%)	17 (11%)	9	47
23	0	66/67 (98%)	58 (88%)	8 (12%)	7	41
24	1	78/83 (94%)	67 (86%)	11 (14%)	5	34
25	2	66/67 (98%)	55 (83%)	11 (17%)	3	24
26	3	51/52 (98%)	49 (96%)	2 (4%)	43	85
27	4	27/63 (43%)	24 (89%)	3 (11%)	9	46
28	5	51/52 (98%)	45 (88%)	6 (12%)	8	43
29	6	43/52 (83%)	32 (74%)	11 (26%)	1	8
30	7	41/42 (98%)	37 (90%)	4 (10%)	12	53
31	8	53/55 (96%)	44 (83%)	9 (17%)	3	23
32	9	33/34 (97%)	30 (91%)	3 (9%)	14	57
All	All	2837/3104 (91%)	2450 (86%)	387 (14%)	5	36

5 of 387 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
12	P	61	ARG
15	S	12	PHE
28	5	40	LYS
12	P	91	PHE
13	Q	56	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
29	6	20	ASN
29	6	26	ASN
29	6	32	ASN
29	6	46	HIS
32	9	34	GLN

### 5.3.3 RNA ⓘ



Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	2796/2916 (95%)	557 (19%)	53 (1%)
2	B	118/122 (96%)	18 (15%)	1 (0%)
All	All	2914/3038 (95%)	575 (19%)	54 (1%)

5 of 575 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	10	G
1	A	35	G
1	A	45	C
1	A	48	G
1	A	49	A

5 of 54 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	1378	A
1	A	1819	A
1	A	2756	U
1	A	1395	A
1	A	1558	A

## 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 ⓘ

There are no ligands in this entry.

## 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	2803/2916 (96%)	0.60	222 (7%) 13 13	6, 38, 143, 240	0
2	B	119/122 (97%)	0.58	11 (9%) 9 11	32, 70, 127, 179	0
3	C	191/229 (83%)	1.32	48 (25%) 1 2	44, 115, 155, 180	0
4	D	272/276 (98%)	0.19	5 (1%) 65 50	6, 23, 70, 121	0
5	E	205/206 (99%)	0.22	7 (3%) 43 33	13, 50, 111, 161	0
6	F	208/210 (99%)	0.13	3 (1%) 72 56	10, 43, 115, 172	0
7	G	181/182 (99%)	0.30	7 (3%) 37 29	9, 63, 118, 169	0
8	H	160/180 (88%)	0.71	17 (10%) 7 9	37, 115, 166, 197	0
9	I	146/148 (98%)	0.20	3 (2%) 60 45	19, 68, 125, 152	0
10	N	139/140 (99%)	0.39	6 (4%) 34 27	23, 58, 106, 176	0
11	O	122/122 (100%)	0.13	3 (2%) 54 41	17, 42, 82, 99	0
12	P	146/150 (97%)	0.41	5 (3%) 43 33	8, 49, 108, 157	0
13	Q	141/141 (100%)	0.29	7 (4%) 28 23	7, 50, 102, 180	0
14	R	117/118 (99%)	0.30	7 (5%) 21 19	18, 39, 91, 120	0
15	S	99/112 (88%)	0.48	4 (4%) 36 29	15, 67, 116, 158	0
16	T	138/146 (94%)	0.32	8 (5%) 22 19	24, 57, 109, 142	0
17	U	117/118 (99%)	0.30	5 (4%) 34 27	14, 48, 114, 142	0
18	V	101/101 (100%)	0.32	6 (5%) 22 19	15, 72, 122, 175	0
19	W	113/113 (100%)	0.15	2 (1%) 65 50	11, 32, 89, 159	0
20	X	93/96 (96%)	0.16	2 (2%) 59 44	15, 35, 72, 98	0
21	Y	101/110 (91%)	0.61	8 (7%) 13 13	20, 63, 128, 197	0
22	Z	177/206 (85%)	0.60	17 (9%) 8 10	0, 83, 131, 156	0
23	0	84/85 (98%)	0.40	7 (8%) 11 12	11, 44, 92, 147	0
24	1	94/98 (95%)	0.18	3 (3%) 45 35	6, 33, 89, 106	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
25	2	71/72 (98%)	0.02	1 (1%) 72 56	18, 49, 104, 122	0
26	3	60/60 (100%)	0.32	3 (5%) 28 23	20, 59, 111, 177	0
27	4	31/71 (43%)	0.16	0 100 100	33, 76, 100, 107	0
28	5	59/60 (98%)	0.43	4 (6%) 17 16	1, 43, 128, 147	0
29	6	45/54 (83%)	0.94	6 (13%) 4 5	26, 85, 131, 153	0
30	7	49/49 (100%)	0.35	2 (4%) 35 28	0, 18, 70, 86	0
31	8	64/65 (98%)	0.30	0 100 100	0, 39, 92, 121	0
32	9	36/37 (97%)	2.23	17 (47%) 1 1	79, 117, 145, 155	0
All	All	6482/6793 (95%)	0.49	446 (6%) 17 16	0, 47, 133, 240	0

The worst 5 of 446 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	362	U	12.8
1	A	2116	G	12.7
1	A	2758	A	10.2
3	C	95	GLY	9.3
1	A	2125	G	9.2

## 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 ⓘ

There are no ligands in this entry.

## 6.5 Other polymers ⓘ

There are no such residues in this entry.