



wwPDB X-ray Structure Validation Summary Report

Feb 28, 2014 – 09:30 AM GMT

PDB ID : 3UXR
Title : The structure of thermorubin in complex with the 70S ribosome from *Thermus thermophilus*. This file contains the 50S subunit of one 70S ribosome. The entire crystal structure contains two 70S ribosomes.
Authors : Bulkley, D.; Johnson, F.A.; Steitz, T.A.
Deposited on : 2011-12-05
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>

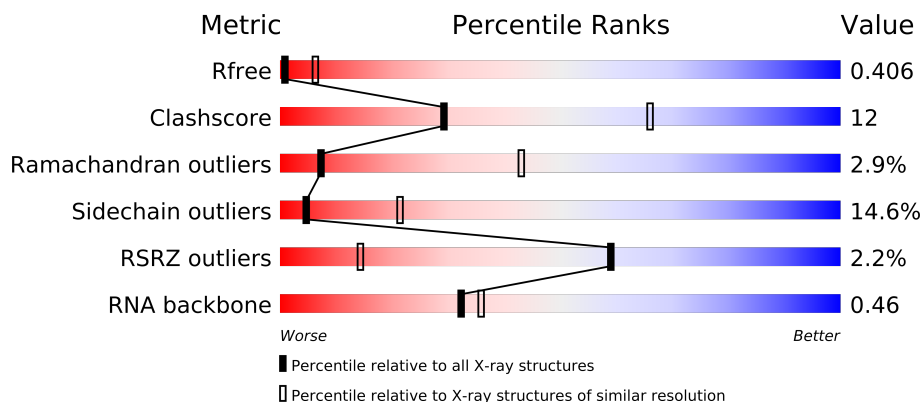
The following versions of software and data (see [references](#)) were used in the production of this report:

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	2915	
2	B	122	
3	D	276	
4	E	206	
5	F	205	
6	G	182	
7	H	180	
8	I	148	
9	N	140	
10	O	122	
11	P	150	
12	Q	141	

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

2 Entry composition

There are 32 unique types of molecules in this entry. The entry contains 89915 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 ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	2827	Total	C	N	O	P	0	0	0
			60900	27102	11403	19569	2826			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	272A	G	U	CONFLICT	GB AP008226.1

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	120	Total	C	N	O	P	0	0	0
			2574	1146	476	833	119			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	120	G	A	CONFLICT	GB AP008226.1

- Molecule 3 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	275	Total	C	N	O	S	0	0	0
			2136	1349	423	361	3			

- Molecule 4 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	E	204	Total	C	N	O	S	0	0	0
			1555	982	297	270	6			

- Molecule 5 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	F	203	Total	C	N	O	S	0	0	1
			1576	1005	297	272	2			

- Molecule 6 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	G	181	Total	C	N	O	S	0	0	0
			1368	879	242	244	3			

- Molecule 7 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	H	174	Total	C	N	O	S	0	0	0
			1317	837	243	236	1			

- Molecule 8 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	I	145	Total	C	N	O	S	0	0	0
			1046	674	180	191	1			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	110	GLU	ASP	CONFLICT	UNP Q5SLQ1

- Molecule 9 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	N	140	Total	C	N	O	S	0	0	0
			1112	717	207	184	4			

- Molecule 10 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	O	122	Total	C	N	O	S	0	0	0
			923	583	168	168	4			

- Molecule 11 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	P	147	Total	C	N	O	S	0	0	0
			1119	695	227	194	3			

- Molecule 12 is a protein called 50S ribosomal protein L16.

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

- Molecule 13 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	R	118	Total	C	N	O	S	0	0	0
			968	604	203	160	1			

- Molecule 14 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	S	110	Total	C	N	O	S	0	0	0
			865	544	172	149				

- Molecule 15 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	T	131	Total	C	N	O	S	0	0	0
			1063	666	213	183	1			

- Molecule 16 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	U	116	Total	C	N	O	S	0	0	0
			959	608	201	149	1			

- Molecule 17 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	V	101	Total	C	N	O	S	0	0	0
			771	495	140	135	1			

- Molecule 18 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	W	112	Total	C	N	O	S	0	0	0
			881	554	172	153	2			

- Molecule 19 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	X	95	Total	C	N	O	S	0	0	0
			742	483	134	124	1			

- Molecule 20 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	Y	107	Total	C	N	O	S	0	0	0
			785	503	145	131	6			

- Molecule 21 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
21	Z	198	Total	C	N	O	S	0	0	0
			1522	972	269	279	2			

- Molecule 22 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	0	76	Total	C	N	O	S	0	0	0
			594	368	125	100	1			

- Molecule 23 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	1	97	Total	C	N	O	S	0	0	0
			745	469	144	131	1			

- Molecule 24 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	2	70	Total	C	N	O	S	0	0	0
			588	365	118	103	2			

- Molecule 25 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
25	3	59	Total	C	N	O	0	0	0
			458	293	87	78			

- Molecule 26 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	4	46	Total	C	N	O	S	0	0	0
			349	223	57	64	5			

- Molecule 27 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	5	59	Total	C	N	O	S	0	0	0
			455	286	90	74	5			

- Molecule 28 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	6	53	Total	C	N	O	S	0	0	0
			449	278	90	77	4			

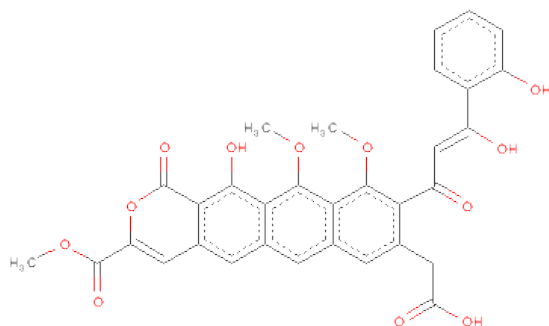
- Molecule 29 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	7	48	Total	C	N	O	S	0	0	0
			418	257	104	55	2			

- Molecule 30 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	8	64	Total	C	N	O	S	0	0	0
			509	326	99	82	2			

- Molecule 31 is THERMORUBIN (three-letter code: T8B) (formula: C₃₂H₂₄O₁₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
31	A	1	Total	C	O	0	0
			44	32	12		

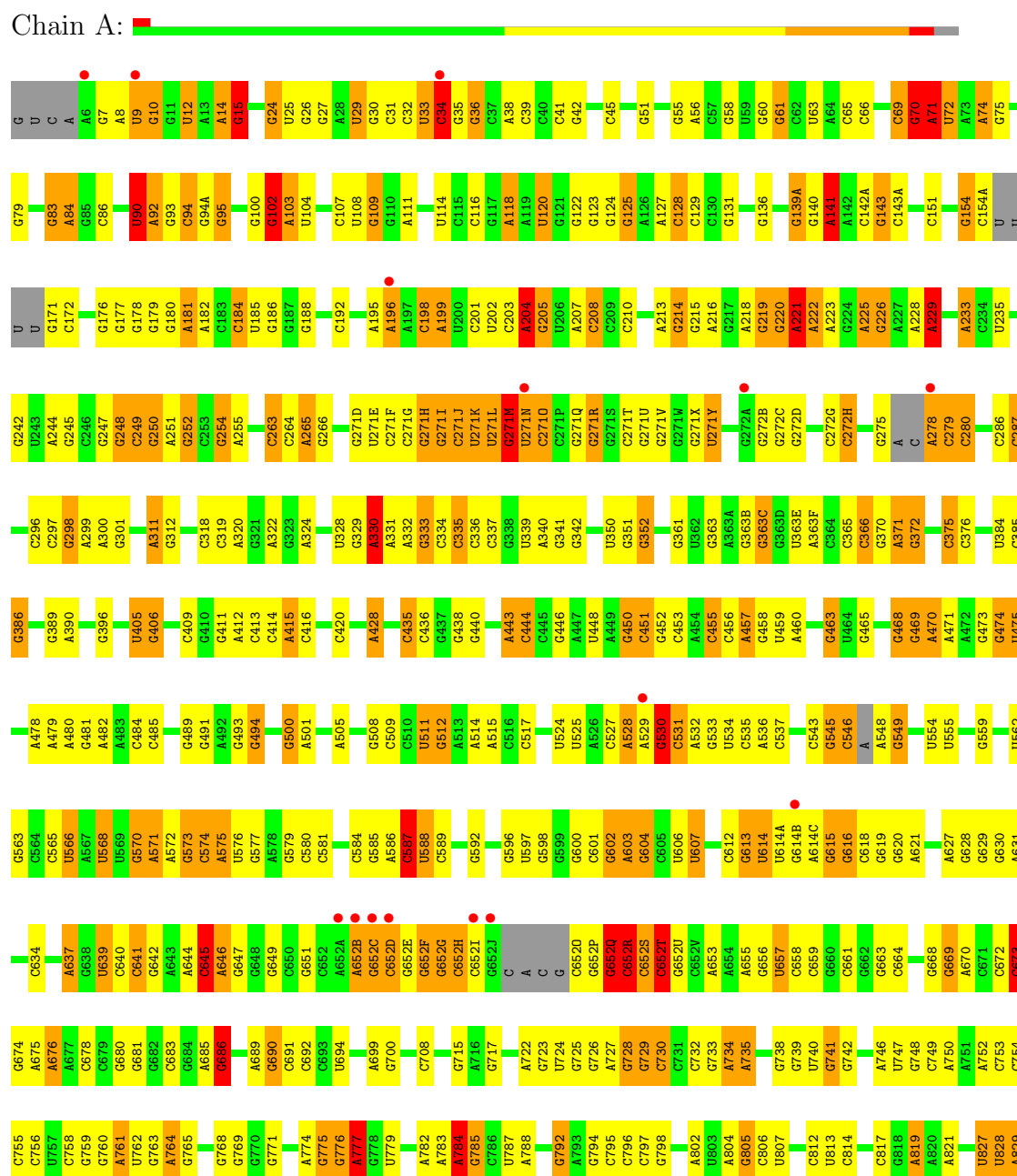
- Molecule 32 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
32	A	2	Total	Mg	0	0
			2	2		

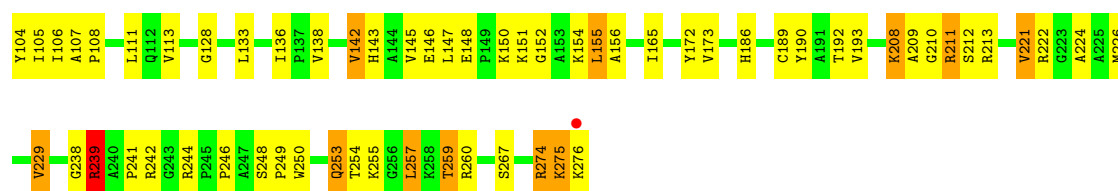
3 Residue-property plots

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 ($\text{RSRZ} > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: 23S ribosomal RNA

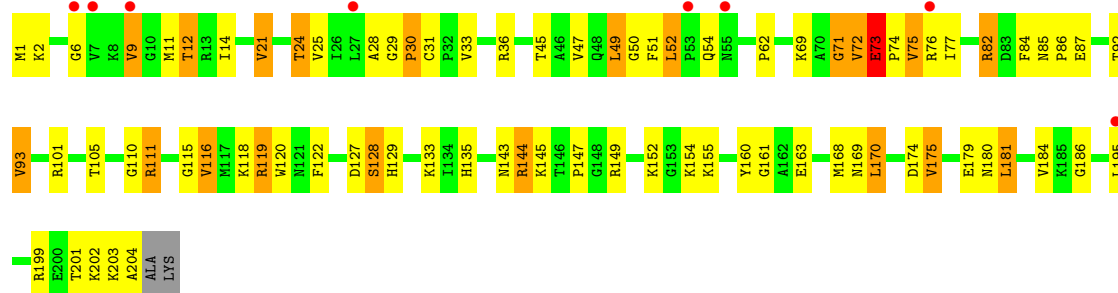


WORLDWIDE
 **PDB**
PROTEIN DATA BANK



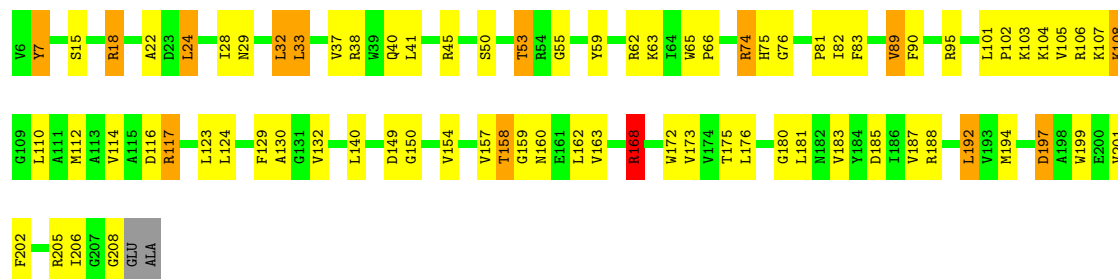
• Molecule 4: 50S ribosomal protein L3

Chain E:



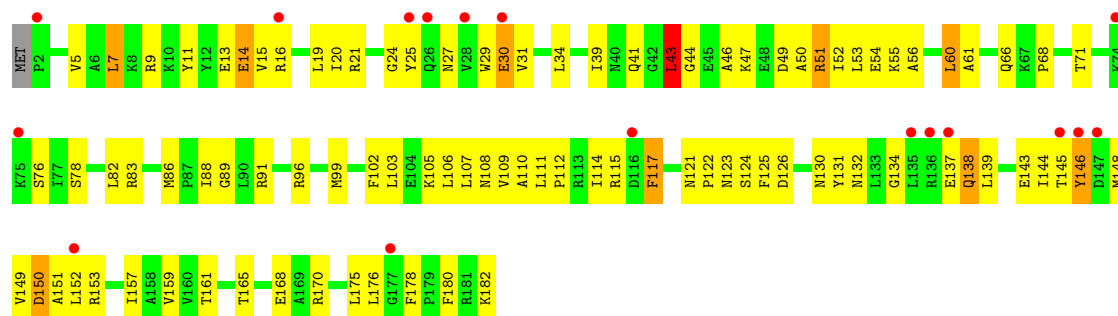
• Molecule 5: 50S ribosomal protein L4

Chain F:



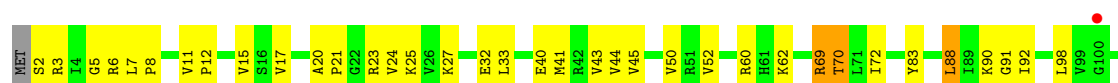
• Molecule 6: 50S ribosomal protein L5

Chain G:



• Molecule 7: 50S ribosomal protein L6

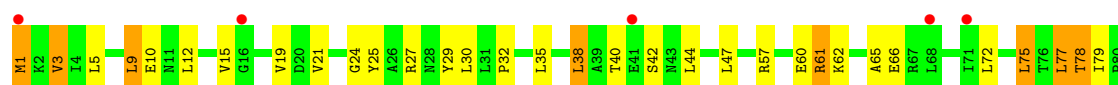
Chain H:





• Molecule 8: 50S ribosomal protein L9

Chain I:



• Molecule 9: 50S ribosomal protein L13

Chain N:



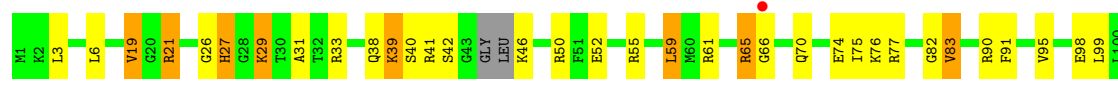
• Molecule 10: 50S ribosomal protein L14

Chain O:



• Molecule 11: 50S ribosomal protein L15

Chain P:



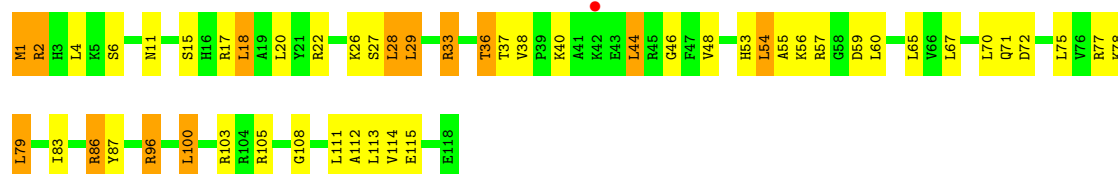
• Molecule 12: 50S ribosomal protein L16

Chain Q:



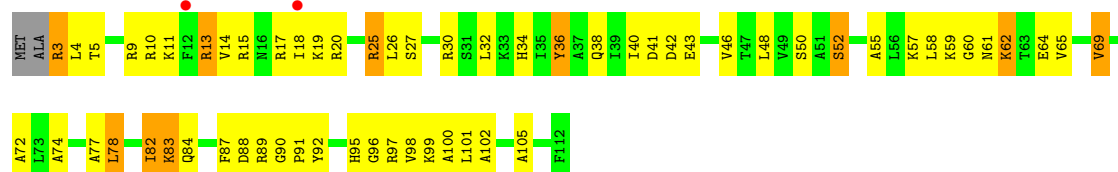
- Molecule 13: 50S ribosomal protein L17

Chain R:



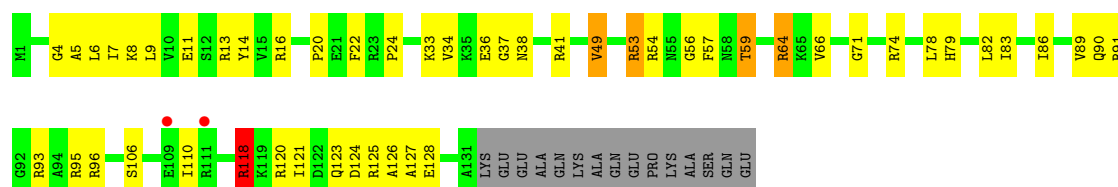
- Molecule 14: 50S ribosomal protein L18

Chain S:



- Molecule 15: 50S ribosomal protein L19

Chain T:



- Molecule 16: 50S ribosomal protein L20

Chain U:



- Molecule 17: 50S ribosomal protein L21

Chain V:



- Molecule 18: 50S ribosomal protein L22

Chain W:



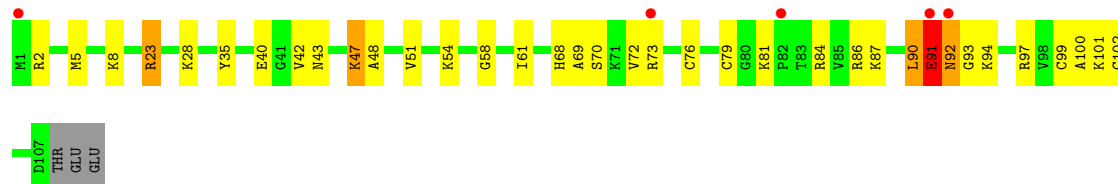
- Molecule 19: 50S ribosomal protein L23

Chain X:



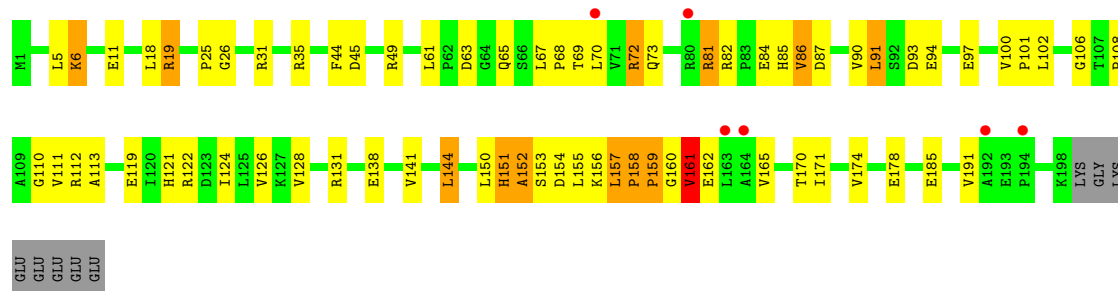
- Molecule 20: 50S ribosomal protein L24

Chain Y:



- Molecule 21: 50S ribosomal protein L25

Chain Z:



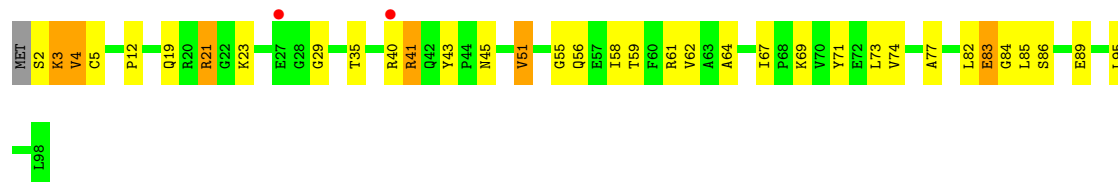
- Molecule 22: 50S ribosomal protein L27

Chain 0:



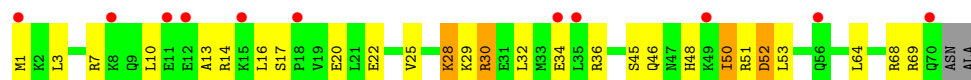
- Molecule 23: 50S ribosomal protein L28

Chain 1:



- Molecule 24: 50S ribosomal protein L29

Chain 2:



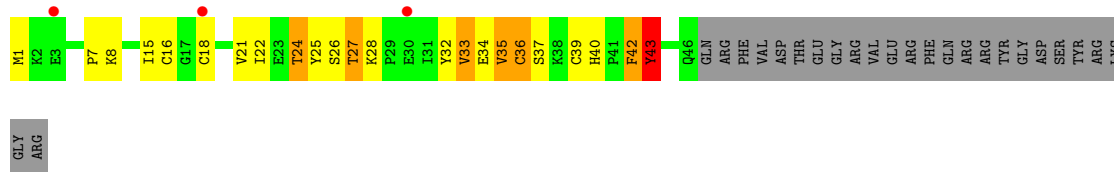
- Molecule 25: 50S ribosomal protein L30

Chain 3:



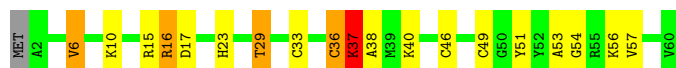
- Molecule 26: 50S ribosomal protein L31

Chain 4:



- Molecule 27: 50S ribosomal protein L32

Chain 5:



- Molecule 28: 50S ribosomal protein L33

Chain 6:



- Molecule 29: 50S ribosomal protein L34

Chain 7:



- Molecule 30: 50S ribosomal protein L35

Chain 8:



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	209.37Å 445.46Å 619.56Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.29 – 3.20 49.43 – 2.90	Depositor EDS
% Data completeness (in resolution range)	100.0 (49.29-3.20) 99.7 (49.43-2.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.13 (at 2.91Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.228 , 0.273 0.403 , 0.406	Depositor DCC
R_{free} test set	63137 reflections (5.27%)	DCC
Wilson B-factor (Å ²)	75.4	Xtriage
Anisotropy	0.180	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 24.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	0 of 1261811 reflections	Xtriage
F_o, F_c correlation	0.72	EDS
Total number of atoms	89915	wwPDB-VP
Average B, all atoms (Å ²)	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.63% 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: MG, T8B

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	1.20	70/68203 (0.1%)	1.37	800/106459 (0.8%)
2	B	0.88	0/2879	1.26	21/4492 (0.5%)
3	D	0.67	0/2186	0.81	4/2944 (0.1%)
4	E	0.72	0/1588	0.83	1/2145 (0.0%)
5	F	0.73	0/1609	0.77	0/2177
6	G	0.46	0/1393	0.64	0/1892
7	H	0.59	0/1343	0.70	0/1820
8	I	0.50	0/1061	0.74	0/1451
9	N	0.74	0/1139	0.78	0/1538
10	O	0.67	0/933	0.74	0/1257
11	P	0.64	0/1135	0.81	2/1510 (0.1%)
12	Q	0.64	0/1143	0.74	0/1527
13	R	0.69	0/982	0.82	1/1312 (0.1%)
14	S	0.53	0/875	0.79	1/1168 (0.1%)
15	T	0.61	0/1077	0.79	1/1444 (0.1%)
16	U	0.88	1/977 (0.1%)	0.81	1/1301 (0.1%)
17	V	0.70	0/782	0.77	0/1049
18	W	0.82	0/891	0.80	0/1197
19	X	0.66	0/756	0.76	1/1016 (0.1%)
20	Y	0.61	0/798	0.80	1/1073 (0.1%)
21	Z	0.49	0/1555	0.71	0/2118
22	0	0.66	0/602	0.77	0/804
23	1	0.62	0/752	0.76	0/1003
24	2	0.60	0/590	0.74	0/781
25	3	0.65	0/463	0.74	0/623
26	4	0.56	0/358	0.74	1/487 (0.2%)
27	5	0.79	0/469	0.88	0/634
28	6	0.68	0/456	0.74	0/609
29	7	0.78	0/426	0.84	0/561
30	8	0.70	0/516	0.82	0/679
All	All	1.07	71/97937 (0.1%)	1.24	835/147071 (0.6%)

The worst 5 of 71 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1142(A)	A	N9-C4	-10.62	1.31	1.37
1	A	1332	G	N9-C4	-9.83	1.30	1.38
1	A	676	A	N9-C4	-8.36	1.32	1.37
1	A	330	A	N9-C4	-8.36	1.32	1.37
1	A	2028	U	C4-O4	8.30	1.30	1.23

The worst 5 of 835 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1332	G	C2-N3-C4	-19.65	102.08	111.90
1	A	1332	G	N3-C4-C5	17.99	137.59	128.60
1	A	1332	G	N3-C4-N9	-16.77	115.94	126.00
1	A	1779	U	C5-C6-N1	-14.96	115.22	122.70
1	A	2249	U	N3-C4-C5	-14.14	106.12	114.60

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	60900	0	30712	1053	0
2	B	2574	0	1306	35	0
3	D	2136	0	2218	81	0
4	E	1555	0	1607	54	0
5	F	1576	0	1616	59	0
6	G	1368	0	1324	61	0
7	H	1317	0	1376	33	0
8	I	1046	0	1067	47	0
9	N	1112	0	1180	34	0
10	O	923	0	981	23	0
11	P	1119	0	1186	40	0
12	Q	1122	0	1179	47	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
13	R	968	0	1033	33	0
14	S	865	0	905	54	0
15	T	1063	0	1103	37	0
16	U	959	0	1019	20	0
17	V	771	0	830	15	0
18	W	881	0	935	24	0
19	X	742	0	799	23	0
20	Y	785	0	832	30	0
21	Z	1522	0	1511	47	0
22	0	594	0	604	21	0
23	1	745	0	804	26	0
24	2	588	0	643	18	0
25	3	458	0	503	6	0
26	4	349	0	340	16	0
27	5	455	0	476	18	0
28	6	449	0	466	17	0
29	7	418	0	467	14	0
30	8	509	0	565	20	0
31	A	44	0	20	19	0
32	A	2	0	0	0	0
All	All	89915	0	59607	1765	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 12.

The worst 5 of 1765 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
31:A:1:T8B:H13	31:A:1:T8B:C22	1.58	1.32
1:A:885:C:H42	1:A:890:A:N6	1.28	1.32
31:A:1:T8B:C19	31:A:1:T8B:H17	1.66	1.25
1:A:1913:A:O2'	31:A:1:T8B:O10	1.59	1.16
1:A:885:C:N4	1:A:890:A:N6	2.02	1.06

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	
3	D	273/276 (99%)	246 (90%)	23 (8%)	4 (2%)	15	64
4	E	202/206 (98%)	174 (86%)	21 (10%)	7 (4%)	6	37
5	F	198/205 (97%)	170 (86%)	21 (11%)	7 (4%)	6	37
6	G	179/182 (98%)	135 (75%)	30 (17%)	14 (8%)	1	11
7	H	172/180 (96%)	144 (84%)	22 (13%)	6 (4%)	6	37
8	I	143/148 (97%)	109 (76%)	24 (17%)	10 (7%)	2	13
9	N	138/140 (99%)	119 (86%)	13 (9%)	6 (4%)	4	30
10	O	120/122 (98%)	109 (91%)	7 (6%)	4 (3%)	6	38
11	P	143/150 (95%)	126 (88%)	12 (8%)	5 (4%)	6	37
12	Q	139/141 (99%)	126 (91%)	9 (6%)	4 (3%)	7	43
13	R	116/118 (98%)	108 (93%)	7 (6%)	1 (1%)	25	76
14	S	108/112 (96%)	93 (86%)	12 (11%)	3 (3%)	8	44
15	T	129/146 (88%)	116 (90%)	12 (9%)	1 (1%)	27	77
16	U	114/118 (97%)	111 (97%)	3 (3%)	0	100	100
17	V	99/101 (98%)	89 (90%)	9 (9%)	1 (1%)	22	74
18	W	110/113 (97%)	104 (94%)	6 (6%)	0	100	100
19	X	93/96 (97%)	82 (88%)	9 (10%)	2 (2%)	10	53
20	Y	105/110 (96%)	88 (84%)	13 (12%)	4 (4%)	5	34
21	Z	196/206 (95%)	158 (81%)	31 (16%)	7 (4%)	5	36
22	0	74/85 (87%)	67 (90%)	6 (8%)	1 (1%)	16	66
23	1	95/98 (97%)	86 (90%)	6 (6%)	3 (3%)	6	39
24	2	68/72 (94%)	63 (93%)	5 (7%)	0	100	100
25	3	57/60 (95%)	54 (95%)	2 (4%)	1 (2%)	13	60
26	4	44/71 (62%)	30 (68%)	10 (23%)	4 (9%)	1	8
27	5	57/60 (95%)	49 (86%)	6 (10%)	2 (4%)	6	37
28	6	51/54 (94%)	47 (92%)	4 (8%)	0	100	100
29	7	46/49 (94%)	42 (91%)	3 (6%)	1 (2%)	10	53
30	8	62/65 (95%)	57 (92%)	5 (8%)	0	100	100
All	All	3331/3484 (96%)	2902 (87%)	331 (10%)	98 (3%)	7	43

5 of 98 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	D	156	ALA
3	D	239	ARG
3	D	275	LYS
6	G	49	ASP
7	H	126	PRO

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	D	215/218 (99%)	189 (88%)	26 (12%)	7	32
4	E	163/166 (98%)	134 (82%)	29 (18%)	2	13
5	F	158/162 (98%)	138 (87%)	20 (13%)	6	29
6	G	128/156 (82%)	114 (89%)	14 (11%)	9	37
7	H	141/148 (95%)	124 (88%)	17 (12%)	7	32
8	I	102/124 (82%)	76 (74%)	26 (26%)	1	3
9	N	117/119 (98%)	91 (78%)	26 (22%)	1	6
10	O	98/100 (98%)	89 (91%)	9 (9%)	13	47
11	P	113/116 (97%)	97 (86%)	16 (14%)	5	22
12	Q	111/111 (100%)	94 (85%)	17 (15%)	4	18
13	R	101/101 (100%)	79 (78%)	22 (22%)	1	7
14	S	84/88 (96%)	72 (86%)	12 (14%)	5	22
15	T	110/127 (87%)	100 (91%)	10 (9%)	14	47
16	U	93/94 (99%)	77 (83%)	16 (17%)	3	14
17	V	80/82 (98%)	63 (79%)	17 (21%)	1	7
18	W	89/92 (97%)	78 (88%)	11 (12%)	7	30
19	X	75/78 (96%)	66 (88%)	9 (12%)	7	32
20	Y	80/91 (88%)	72 (90%)	8 (10%)	11	41
21	Z	159/179 (89%)	137 (86%)	22 (14%)	5	24
22	0	59/67 (88%)	52 (88%)	7 (12%)	8	33
23	1	78/83 (94%)	70 (90%)	8 (10%)	10	40

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
24	2	65/67 (97%)	57 (88%)	8 (12%)	7	31
25	3	49/52 (94%)	43 (88%)	6 (12%)	7	31
26	4	39/63 (62%)	30 (77%)	9 (23%)	1	5
27	5	50/52 (96%)	43 (86%)	7 (14%)	5	23
28	6	50/52 (96%)	41 (82%)	9 (18%)	2	12
29	7	41/42 (98%)	32 (78%)	9 (22%)	1	7
30	8	52/55 (94%)	47 (90%)	5 (10%)	12	44
All	All	2700/2885 (94%)	2305 (85%)	395 (15%)	5	21

5 of 395 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
11	P	106	LEU
13	R	111	LEU
27	5	6	VAL
12	Q	1	MET
13	R	1	MET

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

Mol	Chain	Res	Type
8	I	105	HIS
10	O	5	GLN
19	X	31	HIS
6	G	138	GLN
13	R	13	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	2819/2915 (96%)	586 (20%)	60 (2%)
2	B	119/122 (97%)	21 (17%)	0
All	All	2938/3037 (96%)	607 (20%)	60 (2%)

5 of 607 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	10	G
1	A	15	G
1	A	34	C
1	A	36	G
1	A	45	C

5 of 60 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	1176	G
1	A	1427	A
1	A	2610	C
1	A	1301	A
1	A	1530	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 3 ligands modelled in this entry, 2 are monoatomic - leaving 1 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
31	T8B	A	1	32	48,48,48	1.94	7 (14%)	68,71,71	49.69	9 (13%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means

no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	T8B	A	1	32	-	0/24/26/26	0/1/5/5

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	A	1	T8B	O5-C14	8.16	1.37	1.33
31	A	1	T8B	O5-C11	5.80	1.40	1.35
31	A	1	T8B	C14-C15	5.00	1.48	1.37
31	A	1	T8B	O11-C26	2.81	1.38	1.32
31	A	1	T8B	C11-C12	-2.64	1.46	1.52

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	A	1	T8B	O5-C11-C12	408.48	117.32	112.43
31	A	1	T8B	O5-C14-C15	-28.80	116.59	125.82
31	A	1	T8B	C14-O5-C11	10.11	121.55	118.14
31	A	1	T8B	C16-C15-C9	5.02	120.17	115.82
31	A	1	T8B	O5-C11-C10	3.87	124.04	119.33

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	2827/2915 (96%)	-0.23	47 (1%) 67 19	27, 56, 110, 126	0
2	B	120/122 (98%)	-0.18	1 (0%) 83 35	46, 80, 95, 103	0
3	D	275/276 (99%)	0.21	4 (1%) 70 21	36, 59, 78, 103	0
4	E	204/206 (99%)	0.17	8 (3%) 37 7	33, 60, 81, 96	0
5	F	203/205 (99%)	-0.01	0 100 100	27, 64, 90, 110	0
6	G	181/182 (99%)	0.41	17 (9%) 9 2	81, 101, 110, 118	0
7	H	174/180 (96%)	0.12	3 (1%) 67 19	63, 78, 91, 98	0
8	I	145/148 (97%)	0.55	11 (7%) 14 3	68, 90, 98, 100	0
9	N	140/140 (100%)	0.05	2 (1%) 72 22	38, 57, 82, 85	0
10	O	122/122 (100%)	-0.14	0 100 100	43, 64, 82, 89	0
11	P	147/150 (98%)	0.12	1 (0%) 84 38	28, 68, 91, 100	0
12	Q	141/141 (100%)	0.15	1 (0%) 84 38	44, 65, 78, 88	0
13	R	118/118 (100%)	0.14	1 (0%) 83 35	35, 53, 69, 86	0
14	S	110/112 (98%)	0.24	2 (1%) 65 18	58, 79, 93, 100	0
15	T	131/146 (89%)	0.05	2 (1%) 70 21	55, 68, 91, 102	0
16	U	116/118 (98%)	-0.09	0 100 100	34, 50, 70, 84	0
17	V	101/101 (100%)	-0.02	2 (1%) 62 17	31, 61, 81, 95	0
18	W	112/113 (99%)	-0.10	1 (0%) 81 32	36, 45, 75, 106	0
19	X	95/96 (98%)	-0.02	0 100 100	33, 59, 83, 91	0
20	Y	107/110 (97%)	0.37	5 (4%) 30 6	56, 71, 89, 103	0
21	Z	198/206 (96%)	0.23	6 (3%) 48 10	64, 82, 97, 103	0
22	0	76/85 (89%)	0.42	6 (7%) 13 3	46, 60, 74, 82	0
23	1	97/98 (98%)	0.26	2 (2%) 60 15	42, 65, 91, 95	0
24	2	70/72 (97%)	0.81	11 (15%) 3 1	52, 70, 85, 102	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
25	3	59/60 (98%)	0.44	0 100 100	43, 56, 84, 94	0
26	4	46/71 (64%)	0.38	3 (6%) 18 4	98, 107, 113, 118	0
27	5	59/60 (98%)	-0.13	0 100 100	28, 52, 71, 89	0
28	6	53/54 (98%)	0.07	0 100 100	52, 66, 77, 85	0
29	7	48/49 (97%)	0.60	3 (6%) 19 4	29, 44, 73, 89	0
30	8	64/65 (98%)	0.13	1 (1%) 68 20	45, 56, 65, 79	0
All	All	6339/6521 (97%)	-0.01	140 (2%) 59 14	27, 62, 103, 126	0

The worst 5 of 140 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	652(B)	A	8.0
1	A	1847	A	5.8
1	A	652(A)	A	5.7
22	0	70	GLN	5.0
1	A	2169	A	4.9

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
32	MG	A	2908	1/1	0.08	-	30,30,30,30	0
32	MG	A	2909	1/1	0.19	-	30,30,30,30	0
31	T8B	A	1	44/44	0.21	-	20,20,20,20	0

6.5 Other polymers ⓘ

There are no such residues in this entry.