



wwPDB X-ray Structure Validation Summary Report i

Jul 11, 2014 – 11:45 PM EDT

PDB ID : 4L6J
Title : Crystal Structure of Blastcidin S Bound to Thermus Thermophilus 70S Ribosome. This file contains the 50S subunit and blastcidin S molecule from the first 70S ribosome.
Authors : Svidritskiy, E.; Ling, C.; Ermolenko, D.N.; Korostelev, A.A.
Deposited on : 2013-06-12
Resolution : 3.40 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>

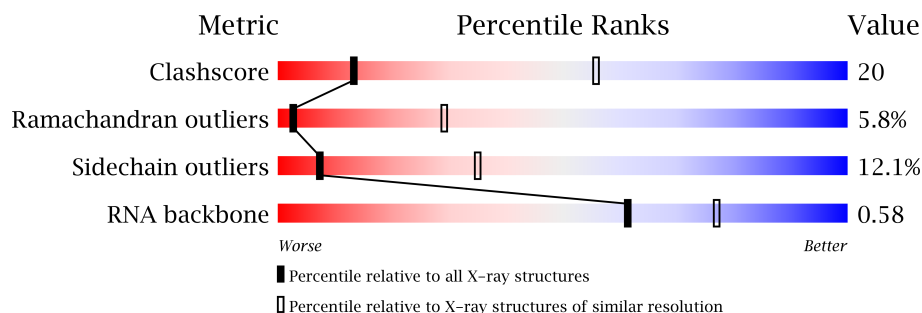
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.16 November 2013
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	21963
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	stable23161

1 Overall quality at a glance

The reported resolution of this entry is 3.40 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))
Clashscore	79885	1214 (3.50-3.30)
Ramachandran outliers	78287	1177 (3.50-3.30)
Sidechain outliers	78261	1177 (3.50-3.30)
RNA backbone	1838	1002 (4.02-2.76)





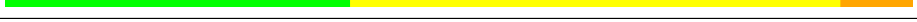

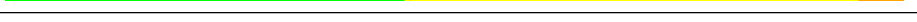

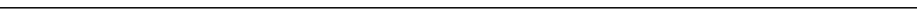





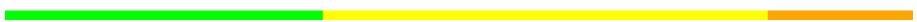

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	2879	
2	B	119	
3	D	271	
4	E	204	
5	F	202	
6	G	181	
7	H	159	
8	I	145	
9	J	137	
10	K	122	
11	L	146	
12	M	134	
13	N	117	
14	O	98	

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Mol	Chain	Length	Quality of chain
15	P	137	
16	Q	117	
17	R	101	
18	S	112	
19	T	92	
20	U	100	
21	V	187	
22	W	76	
23	X	88	
24	Y	62	
25	Z	59	
26	1	30	
27	2	52	
28	3	44	
29	4	48	
30	5	63	

2 Entry composition

There are 32 unique types of molecules in this entry. The entry contains 93956 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	2832	Total	C	N	O	P	0	0	0
			60991	27143	11396	19620	2832			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	276	C	A	CONFLICT	GB AE017221.1
A	277	A	C	CONFLICT	GB AE017221.1
A	1142	U	C	CONFLICT	GB AE017221.1
A	2825	U	G	CONFLICT	GB AE017221.1

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	119	Total	C	N	O	P	0	0	0
			2555	1136	471	829	119			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	271	Total	C	N	O	S	0	0	0
			2105	1329	416	357	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
			1564	988	299	271	6			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	F	202	Total	C	N	O	S	0	0	0
			1587	1011	297	276	3			

- 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
			1475	943	268	260	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	H	159	Total	C	N	O	S	0	0	0
			1223	773	228	221	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
			1133	724	200	208	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	J	137	Total	C	N	O	S	0	0	0
			1097	707	205	182	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	K	122	Total	C	N	O	S	0	0	0
			932	587	171	170	4			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	M	134	Total	C	N	O	S	0	0	0
			1065	680	201	179	5			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	O	98	Total	C	N	O		0	0	0
			771	486	154	131				

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	P	137	Total	C	N	O	S	0	0	0
			1144	713	234	196	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	Q	117	Total	C	N	O	S	0	0	0
			964	610	202	151	1			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	S	112	Total	C	N	O	S	0	0	0
			891	560	175	154	2			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
19	T	92	Total	C	N	O			
			726	471	131	124	0	0	0

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
20	U	100	Total	C	N	O	S		
			776	500	148	124	4	0	0

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
21	V	187	Total	C	N	O	S		
			1483	945	264	272	2	0	0

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
22	W	76	Total	C	N	O	S		
			605	376	126	102	1	0	0

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
23	X	88	Total	C	N	O			
			695	435	141	119		0	0

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
24	Y	62	Total	C	N	O	S		
			521	325	102	92	2	0	0

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
25	Z	59	Total	C	N	O	S		
			468	298	90	79	1	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	1	30	Total	C	N	O	S	0	0	0
			226	142	36	44	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	2	52	Total	C	N	O	S	0	0	0
			405	255	79	66	5			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	3	44	Total	C	N	O	S	0	0	0
			381	235	77	65	4			

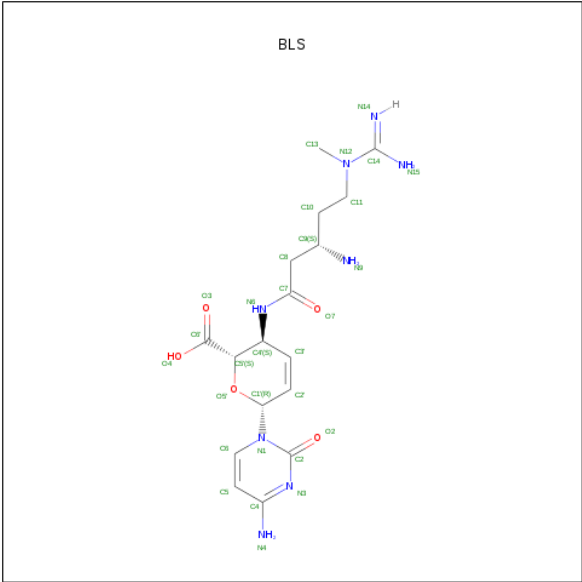
- Molecule 29 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	4	48	Total	C	N	O	S	0	0	0
			419	257	104	56	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	5	63	Total	C	N	O	S	0	0	0
			508	326	101	79	2			

- Molecule 31 is BLASTICIDIN S (three-letter code: BLS) (formula: C₁₇H₂₆N₈O₅).



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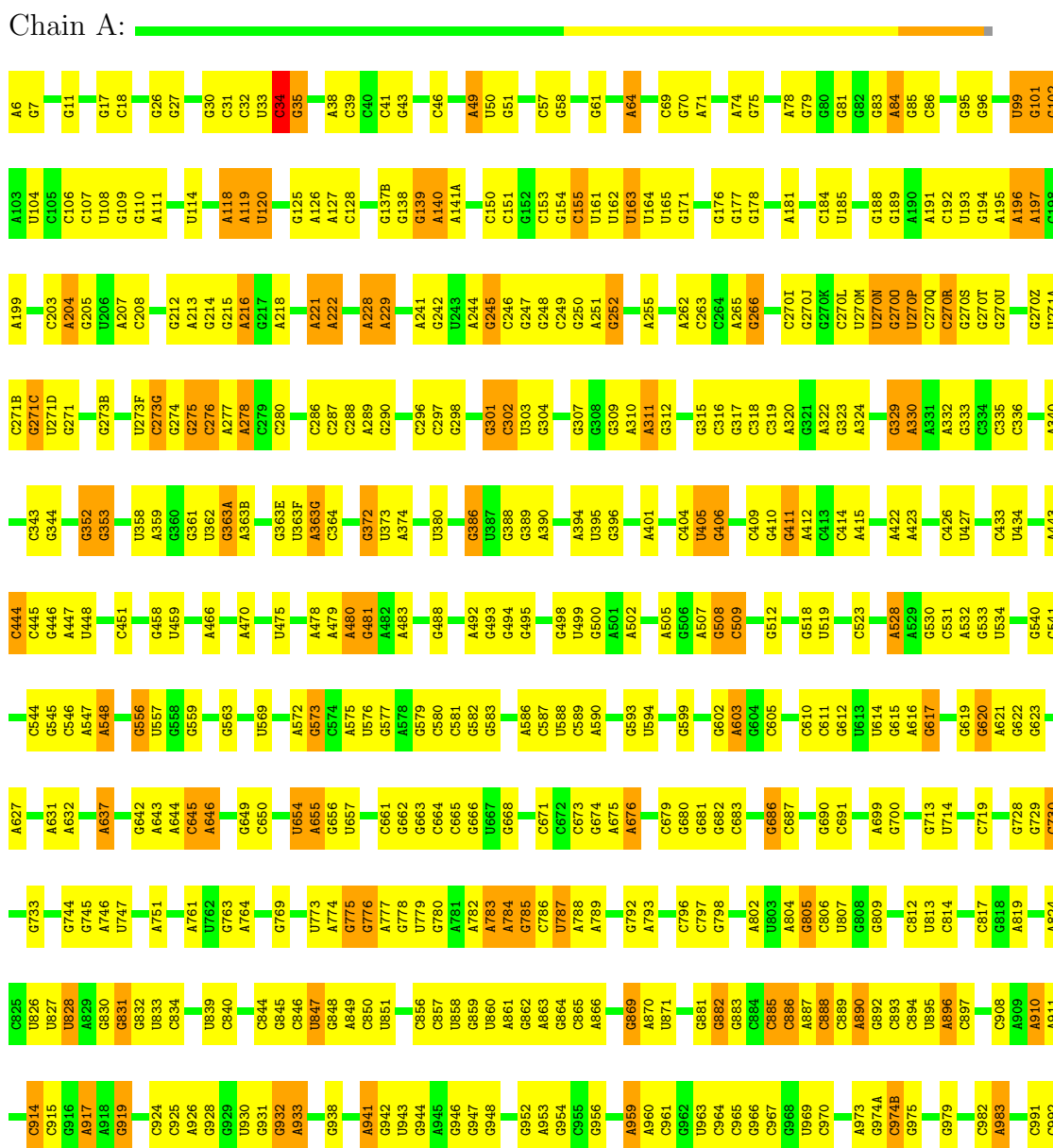
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
32	N	4	Total 4	Mg 4	0	0
32	X	7	Total 7	Mg 7	0	0
32	O	1	Total 1	Mg 1	0	0
32	R	5	Total 5	Mg 5	0	0
32	Y	1	Total 1	Mg 1	0	0
32	L	2	Total 2	Mg 2	0	0
32	S	6	Total 6	Mg 6	0	0
32	F	6	Total 6	Mg 6	0	0
32	M	4	Total 4	Mg 4	0	0

3 Residue-property plots

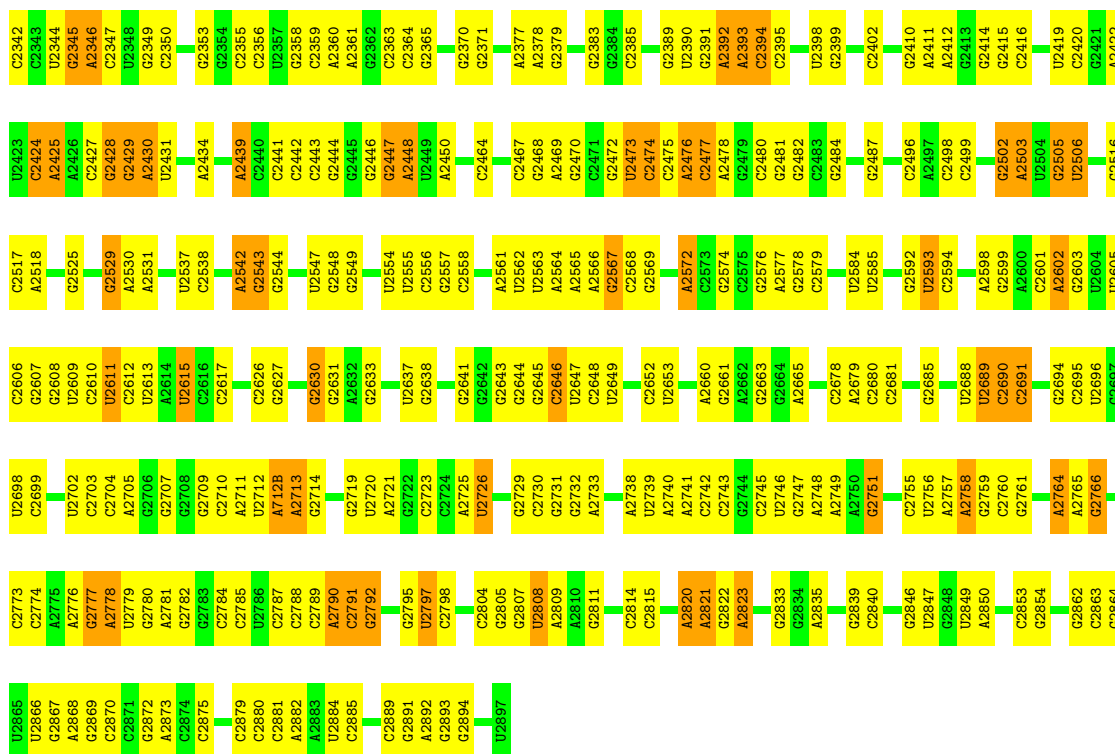
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

Note EDS was not executed.

• Molecule 1: 23S ribosomal RNA

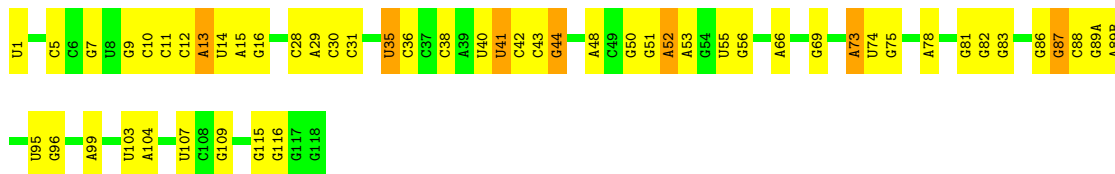






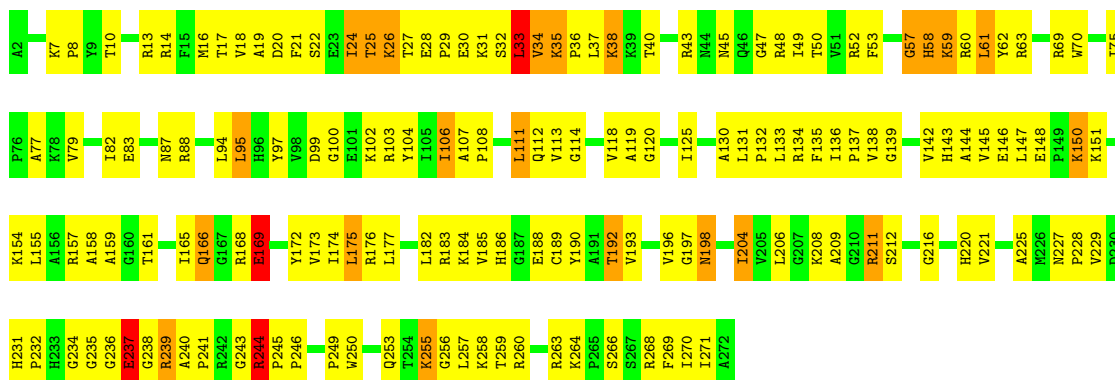
• Molecule 2: 5S ribosomal RNA

Chain B:



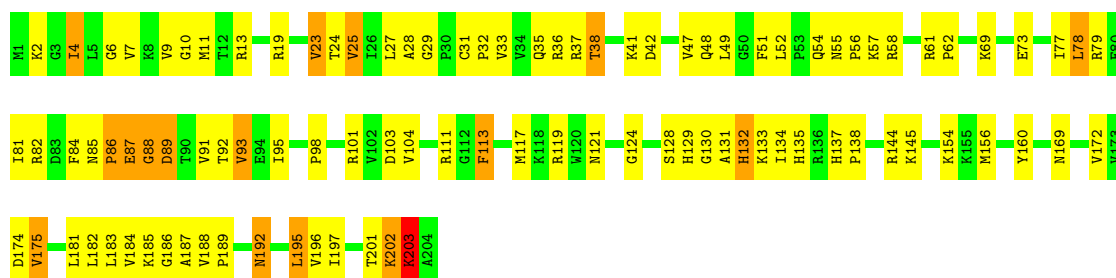
• Molecule 3: 50S ribosomal protein L2

Chain D:



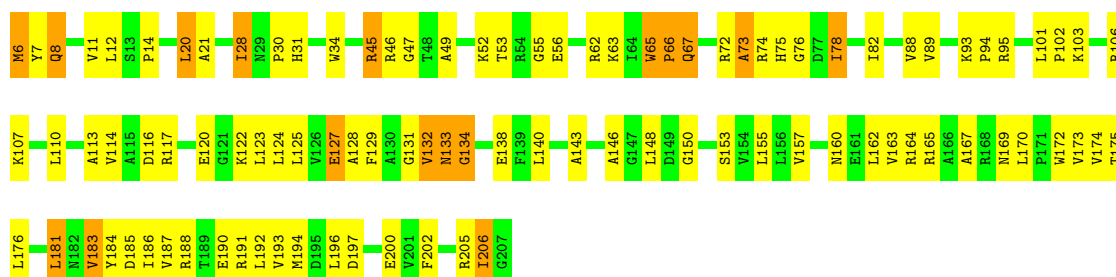
• Molecule 4: 50S ribosomal protein L3

Chain E:



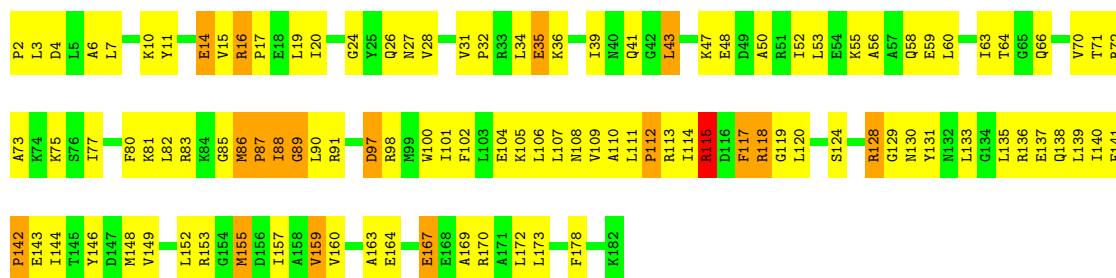
• Molecule 5: 50S ribosomal protein L4

Chain F:



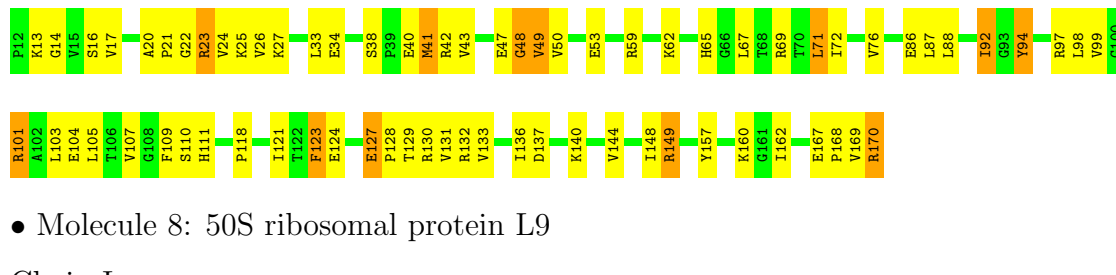
• Molecule 6: 50S ribosomal protein L5

Chain G:



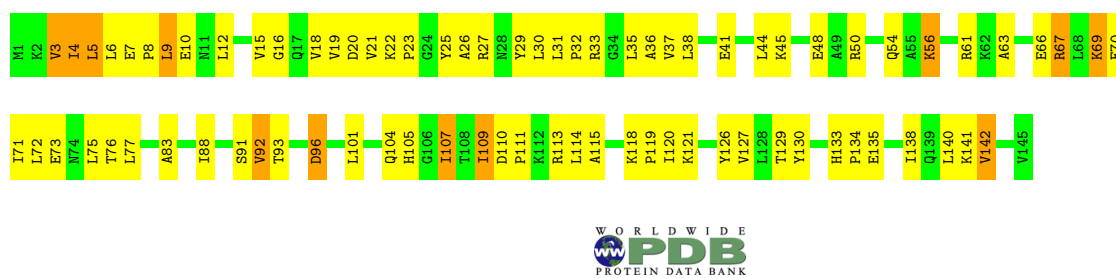
• Molecule 7: 50S ribosomal protein L6

Chain H:



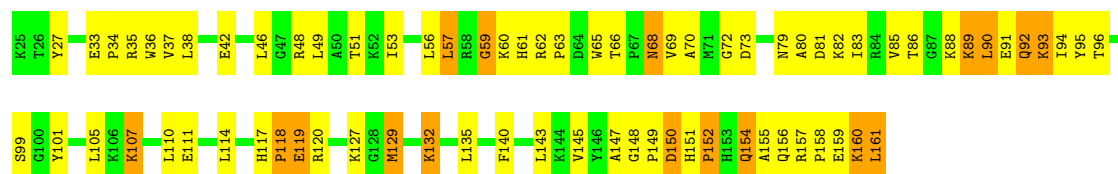
• Molecule 8: 50S ribosomal protein L9

Chain I:



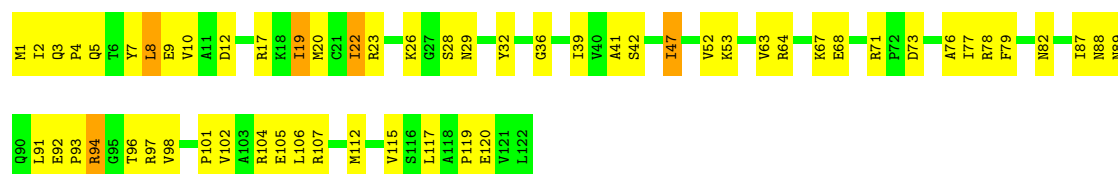
- Molecule 9: 50S ribosomal protein L13

Chain J:



- Molecule 10: 50S ribosomal protein L14

Chain K:



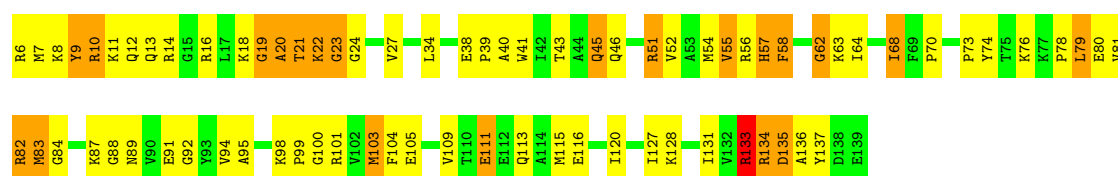
- Molecule 11: 50S ribosomal protein L15

Chain L:



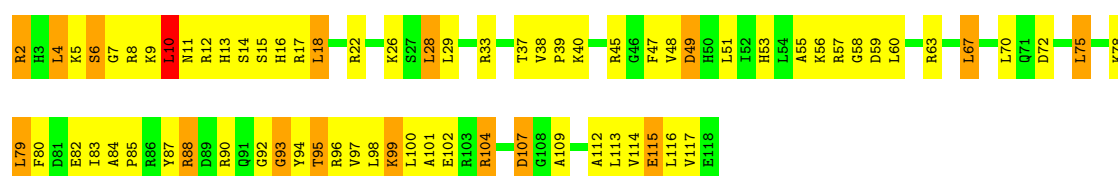
- Molecule 12: 50S ribosomal protein L16

Chain M:



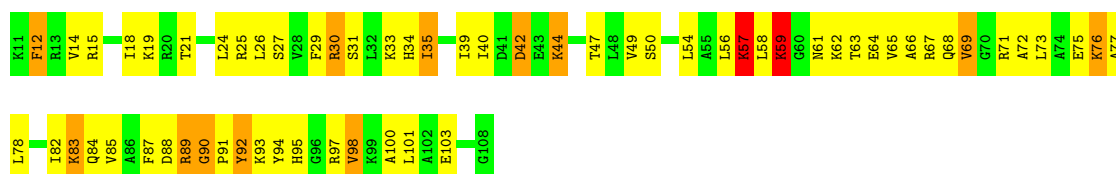
- Molecule 13: 50S ribosomal protein L17

Chain N:



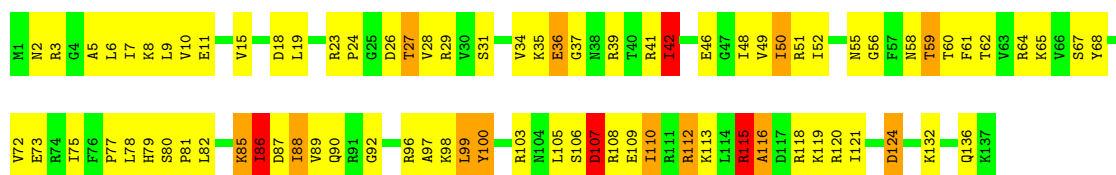
- Molecule 14: 50S ribosomal protein L18

Chain O:



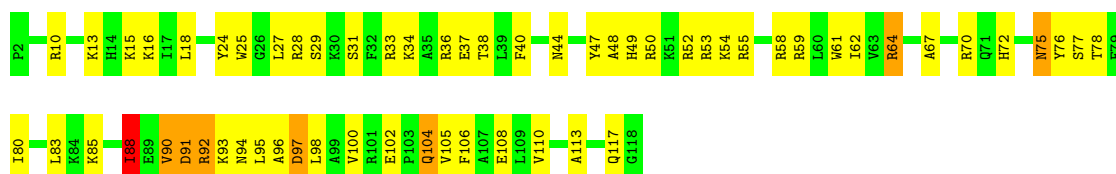
• Molecule 15: 50S ribosomal protein L19

Chain P:



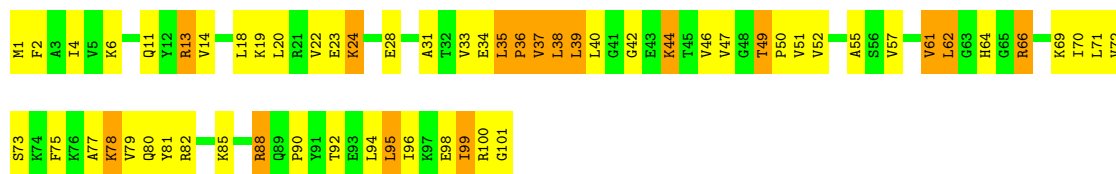
• Molecule 16: 50S ribosomal protein L20

Chain Q:



• Molecule 17: 50S ribosomal protein L21

Chain R:



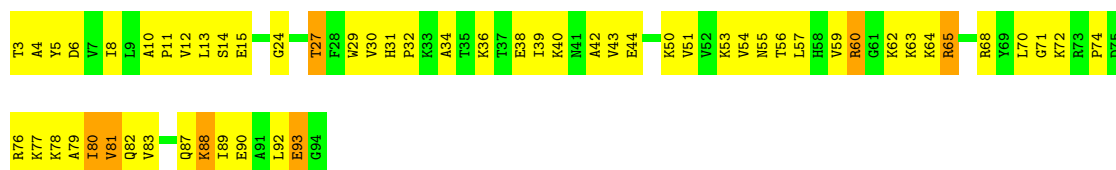
• Molecule 18: 50S ribosomal protein L22

Chain S:



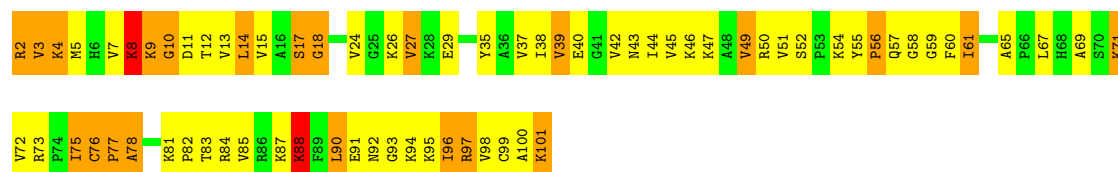
• Molecule 19: 50S ribosomal protein L23

Chain T:



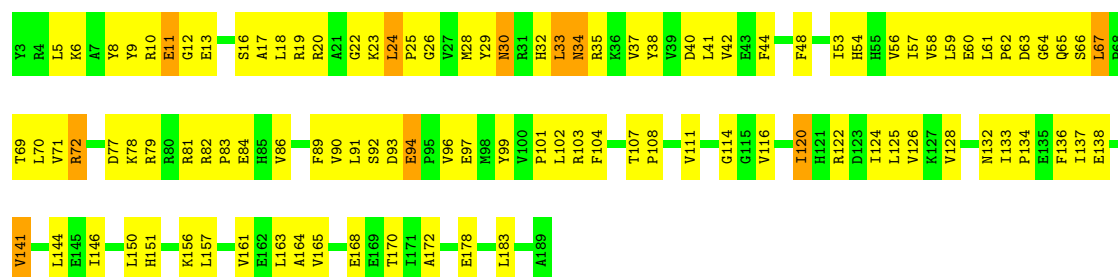
- Molecule 20: 50S ribosomal protein L24

Chain U: 



- Molecule 21: 50S ribosomal protein L25

Chain V: 



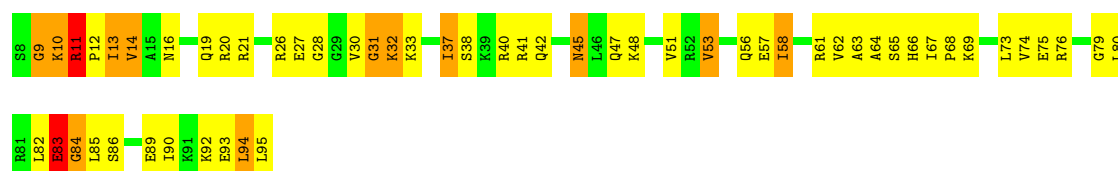
- Molecule 22: 50S ribosomal protein L27

Chain W: 



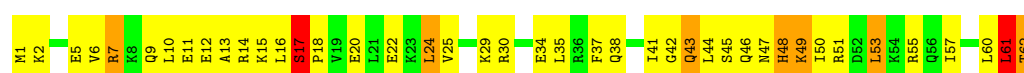
- Molecule 23: 50S ribosomal protein L28

Chain X: 



- Molecule 24: 50S ribosomal protein L29

Chain Y: 



- Molecule 25: 50S ribosomal protein L30

Chain Z: 



- Molecule 26: 50S ribosomal protein L31

Chain 1: 



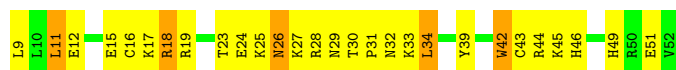
- Molecule 27: 50S ribosomal protein L32

Chain 2: 



- Molecule 28: 50S ribosomal protein L33

Chain 3: 



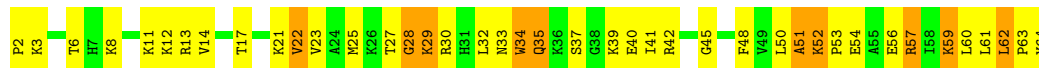
- Molecule 29: 50S ribosomal protein L34

Chain 4: 



- Molecule 30: 50S ribosomal protein L35

Chain 5: 



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	211.53Å 454.44Å 620.87Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.98 – 3.40	Depositor
% Data completeness (in resolution range)	99.8 (49.98-3.40)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PHENIX (phenix.refine: 1.6.4_486)	Depositor
R, R_{free}	0.231 , 0.268	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	93956	wwPDB-VP
Average B, all atoms (Å ²)	89.0	wwPDB-VP

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	0.34	1/68308 (0.0%)	0.64	11/106635 (0.0%)
2	B	0.31	1/2857 (0.0%)	0.52	0/4455
3	D	0.31	0/2155	0.52	0/2905
4	E	0.27	0/1597	0.49	0/2153
5	F	0.27	0/1622	0.47	0/2194
6	G	0.22	0/1500	0.41	0/2017
7	H	0.22	0/1246	0.43	0/1682
8	I	0.22	0/1148	0.42	0/1552
9	J	0.26	0/1124	0.49	0/1515
10	K	0.28	0/942	0.46	0/1268
11	L	0.31	0/1131	0.61	0/1504
12	M	0.28	0/1085	0.49	0/1449
13	N	0.28	0/974	0.47	0/1302
14	O	0.24	0/779	0.43	0/1036
15	P	0.27	0/1158	0.45	0/1544
16	Q	0.28	0/982	0.44	0/1306
17	R	0.29	0/790	0.51	0/1057
18	S	0.28	0/902	0.46	0/1209
19	T	0.29	0/740	0.46	0/993
20	U	0.30	0/789	0.46	0/1051
21	V	0.22	0/1515	0.42	0/2056
22	W	0.28	0/613	0.47	0/816
23	X	0.32	0/702	0.56	0/932
24	Y	0.27	0/523	0.49	0/690
25	Z	0.24	0/473	0.46	0/634
26	1	0.20	0/229	0.42	0/309
27	2	0.28	0/419	0.52	0/567
28	3	0.21	0/388	0.44	0/518
29	4	0.31	0/427	0.50	0/561
30	5	0.32	0/516	0.52	0/679
All	All	0.32	2/97634 (0.0%)	0.60	11/146589 (0.0%)

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
13	N	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1	U	OP3-P	-10.65	1.48	1.61
1	A	6	A	OP3-P	-10.59	1.48	1.61

The worst 5 of 11 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1420	U	C2-N1-C1'	6.88	125.96	117.70
1	A	1420	U	C6-N1-C1'	-6.57	112.00	121.20
1	A	34	C	C6-N1-C1'	-5.98	113.63	120.80
1	A	2593	U	N3-C4-C5	-5.67	111.20	114.60
1	A	34	C	N3-C4-C5	5.57	124.13	121.90

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
13	N	10	LEU	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	60991	0	30744	1326	0
2	B	2555	0	1294	52	0
3	D	2105	0	2182	184	0
4	E	1564	0	1629	103	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	F	1587	0	1632	102	0
6	G	1475	0	1537	124	0
7	H	1223	0	1282	65	0
8	I	1133	0	1220	75	0
9	J	1097	0	1168	80	0
10	K	932	0	994	50	0
11	L	1114	0	1187	196	0
12	M	1065	0	1114	93	0
13	N	960	0	1021	81	0
14	O	771	0	832	62	0
15	P	1144	0	1211	75	0
16	Q	964	0	1022	77	0
17	R	779	0	852	79	0
18	S	891	0	951	50	0
19	T	726	0	778	60	0
20	U	776	0	870	94	0
21	V	1483	0	1507	88	0
22	W	605	0	628	28	0
23	X	695	0	764	85	0
24	Y	521	0	575	62	0
25	Z	468	0	523	23	0
26	1	226	0	225	21	0
27	2	405	0	420	43	0
28	3	381	0	391	33	0
29	4	419	0	467	29	0
30	5	508	0	576	64	0
31	A	30	0	24	4	0
32	3	2	0	0	0	0
32	4	4	0	0	0	0
32	A	4209	0	0	0	0
32	B	50	0	0	0	0
32	D	20	0	0	0	0
32	E	4	0	0	0	0
32	F	6	0	0	0	0
32	G	7	0	0	0	0
32	J	1	0	0	0	0
32	K	15	0	0	0	0
32	L	2	0	0	0	0
32	M	4	0	0	0	0
32	N	4	0	0	0	0
32	O	1	0	0	0	0
32	P	13	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
32	R	5	0	0	0	0
32	S	6	0	0	0	0
32	V	2	0	0	0	0
32	X	7	0	0	0	0
32	Y	1	0	0	0	0
All	All	93956	0	59620	3121	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 20.

The worst 5 of 3121 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1541:U:H3'	1:A:1542:G:H3'	1.16	1.16
1:A:2502:G:H5'	1:A:2503:A:H5''	1.28	1.14
1:A:2303:G:H2'	1:A:2304:G:H5''	1.33	1.10
1:A:1899:G:N2	1:A:1902:C:H41	1.48	1.09
23:X:11:ARG:HB3	23:X:12:PRO:HD2	1.34	1.05

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	269/271 (99%)	220 (82%)	35 (13%)	14 (5%)	3	32
4	E	202/204 (99%)	164 (81%)	27 (13%)	11 (5%)	3	31
5	F	200/202 (99%)	168 (84%)	24 (12%)	8 (4%)	5	43
6	G	179/181 (99%)	128 (72%)	38 (21%)	13 (7%)	2	22
7	H	157/159 (99%)	122 (78%)	29 (18%)	6 (4%)	5	45
8	I	143/145 (99%)	120 (84%)	22 (15%)	1 (1%)	30	83
9	J	135/137 (98%)	104 (77%)	21 (16%)	10 (7%)	2	22
10	K	120/122 (98%)	107 (89%)	10 (8%)	3 (2%)	9	57

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
11	L	144/146 (99%)	89 (62%)	35 (24%)	20 (14%)	0	6
12	M	132/134 (98%)	96 (73%)	21 (16%)	15 (11%)	1	9
13	N	115/117 (98%)	92 (80%)	15 (13%)	8 (7%)	2	23
14	O	96/98 (98%)	65 (68%)	23 (24%)	8 (8%)	1	18
15	P	135/137 (98%)	105 (78%)	22 (16%)	8 (6%)	2	29
16	Q	115/117 (98%)	102 (89%)	10 (9%)	3 (3%)	8	56
17	R	99/101 (98%)	79 (80%)	16 (16%)	4 (4%)	5	43
18	S	110/112 (98%)	102 (93%)	8 (7%)	0	100	100
19	T	90/92 (98%)	76 (84%)	12 (13%)	2 (2%)	10	60
20	U	98/100 (98%)	63 (64%)	23 (24%)	12 (12%)	1	8
21	V	185/187 (99%)	159 (86%)	19 (10%)	7 (4%)	5	45
22	W	74/76 (97%)	59 (80%)	13 (18%)	2 (3%)	8	55
23	X	86/88 (98%)	56 (65%)	19 (22%)	11 (13%)	0	7
24	Y	60/62 (97%)	47 (78%)	8 (13%)	5 (8%)	1	18
25	Z	57/59 (97%)	52 (91%)	4 (7%)	1 (2%)	13	65
26	1	28/30 (93%)	13 (46%)	13 (46%)	2 (7%)	2	23
27	2	50/52 (96%)	45 (90%)	3 (6%)	2 (4%)	5	43
28	3	42/44 (96%)	26 (62%)	12 (29%)	4 (10%)	1	14
29	4	46/48 (96%)	44 (96%)	1 (2%)	1 (2%)	10	60
30	5	61/63 (97%)	46 (75%)	9 (15%)	6 (10%)	1	13
All	All	3228/3284 (98%)	2549 (79%)	492 (15%)	187 (6%)	3	29

5 of 187 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	D	33	LEU
3	D	40	THR
3	D	59	LYS
3	D	239	ARG
4	E	86	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	213/213 (100%)	187 (88%)	26 (12%)	7	34
4	E	165/165 (100%)	147 (89%)	18 (11%)	9	42
5	F	161/161 (100%)	143 (89%)	18 (11%)	9	39
6	G	155/155 (100%)	138 (89%)	17 (11%)	9	41
7	H	132/132 (100%)	119 (90%)	13 (10%)	12	48
8	I	122/122 (100%)	107 (88%)	15 (12%)	7	34
9	J	116/116 (100%)	103 (89%)	13 (11%)	9	39
10	K	100/100 (100%)	91 (91%)	9 (9%)	14	54
11	L	112/112 (100%)	86 (77%)	26 (23%)	1	6
12	M	105/105 (100%)	92 (88%)	13 (12%)	7	34
13	N	100/100 (100%)	86 (86%)	14 (14%)	5	28
14	O	77/77 (100%)	64 (83%)	13 (17%)	3	18
15	P	121/121 (100%)	102 (84%)	19 (16%)	4	23
16	Q	93/93 (100%)	84 (90%)	9 (10%)	12	49
17	R	82/82 (100%)	67 (82%)	15 (18%)	2	13
18	S	91/91 (100%)	82 (90%)	9 (10%)	11	47
19	T	74/74 (100%)	66 (89%)	8 (11%)	9	42
20	U	84/84 (100%)	70 (83%)	14 (17%)	3	19
21	V	162/162 (100%)	152 (94%)	10 (6%)	26	72
22	W	61/61 (100%)	55 (90%)	6 (10%)	12	48
23	X	73/73 (100%)	65 (89%)	8 (11%)	9	41
24	Y	58/58 (100%)	51 (88%)	7 (12%)	7	35
25	Z	51/51 (100%)	45 (88%)	6 (12%)	8	36
26	1	27/27 (100%)	24 (89%)	3 (11%)	9	40
27	2	45/45 (100%)	40 (89%)	5 (11%)	9	40
28	3	43/43 (100%)	40 (93%)	3 (7%)	21	68
29	4	41/41 (100%)	33 (80%)	8 (20%)	2	10
30	5	53/53 (100%)	49 (92%)	4 (8%)	19	64
All	All	2717/2717 (100%)	2388 (88%)	329 (12%)	7	35

5 of 329 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
11	L	115	LEU
14	O	35	ILE
25	Z	53	LEU
11	L	146	VAL
12	M	133	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 68 such sidechains are listed below:

Mol	Chain	Res	Type
13	N	16	HIS
16	Q	75	ASN
26	1	46	ASN
13	N	53	HIS
15	P	79	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	2830/2879 (98%)	442 (15%)	0
2	B	118/119 (99%)	9 (7%)	0
All	All	2948/2998 (98%)	451 (15%)	0

5 of 451 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	11	G
1	A	34	C
1	A	35	G
1	A	46	C
1	A	49	A

There are no RNA pucker outliers to report.

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 4364 ligands modelled in this entry, 4363 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	BLS	A	4001	-	31,31,31	2.86	11 (35%)	40,43,43	2.42	14 (35%)

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	BLS	A	4001	-	-	0/22/38/38	0/2/2/2

The worst 5 of 11 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	A	4001	BLS	C7-N6	7.46	1.49	1.34
31	A	4001	BLS	C14-N12	7.35	1.54	1.35
31	A	4001	BLS	O5'-C5'	4.61	1.51	1.43
31	A	4001	BLS	C11-N12	4.53	1.56	1.47
31	A	4001	BLS	C3'-C2'	4.42	1.47	1.33

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	A	4001	BLS	C1'-C2'-C3'	-8.07	111.48	122.69
31	A	4001	BLS	O5'-C1'-C2'	-4.70	110.48	113.13
31	A	4001	BLS	C10-C11-N12	4.36	116.19	112.58
31	A	4001	BLS	C6-C5-C4	4.24	119.53	117.51
31	A	4001	BLS	O3-C6'-C5'	-3.32	109.32	121.10

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 ⓘ

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.