wwPDB EM Validation Summary Report

Apr 16, 2024 – 01:19 am BST

PDB ID	:	7PWF
EMDB ID	:	EMD-13680
Title	:	Cryo-EM structure of small subunit of Giardia lamblia ribosome at 2.9 A resolution
Authors	:	Hiregange, D.G.; Rivalta, A.; Bose, T.; Breiner-Goldstein, E.; Samiya, S.; Cimicata, G.; Kulakova, L.; Zimmerman, E.; Bashan, A.; Herzberg, O.; Yonath, A.
Deposited on	:	2021-10-06
Resolution	:	2.85 Å(reported)

This is a wwPDB EM Validation Summary Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

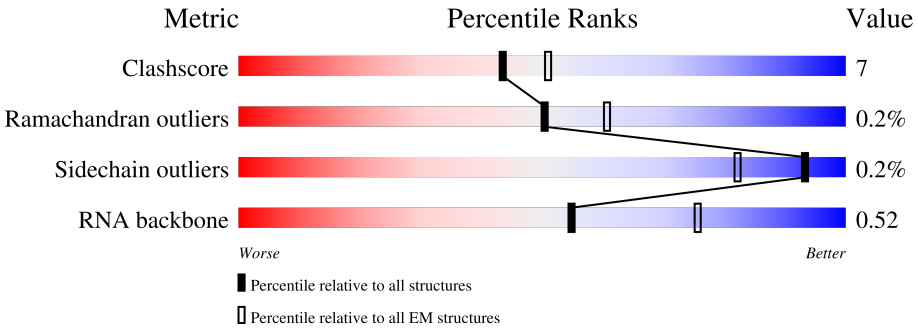
EMDB validation analysis	:	0.0.1.dev92
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	FAILED
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 2.85 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)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5%

Mol	Chain	Length	Quality of chain
1	d	137	35% 65%
2	T	139	81% 11% • 6%
3	N	154	87% 10% ••
4	J	189	75% 13% 12%
5	D	217	63% 21% 16%
6	X	143	84% 15% •
7	S	154	54% 32% 14%

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Mol	Chain	Length	Quality of chain
8	Q	158	57% 22% 21%
9	C	242	70% 17% 12%
10	A	245	67% 13% 21%
11	B	248	74% 14% 12%
12	Y	132	55% 14% 32%
13	b	124	64% 36%
14	a	109	89% 11%
15	Z	88	43% 24% 33%
16	V	89	82% 10% 8%
17	P	145	43% 28% 28%
18	R	137	56% 18% 26%
19	K	134	37% 25% 38%
20	I	174	75% 18% 6%
21	e	69	54% 46%
22	H	190	72% 14% 15%
23	n	41	59% 41%
24	c	64	84% 14%
25	O	145	77% 10% 13%
26	W	130	84% 15%
27	E	268	74% 22%
28	2	1452	53% 30% 10% 7%
29	L	199	84% 7% 9%
30	U	126	48% 10% 41%
31	G	248	58% 20% 21%
32	F	190	67% 18% 15%

2 Entry composition (i)

There are 34 unique types of molecules in this entry. The entry contains 60466 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 protein called Ribosomal protein S29A.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	d	48	Total	C	N	O	S	0	0
			398	253	75	65	5		

- Molecule 2 is a protein called Ribosomal protein S19e.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	T	130	Total	C	N	O	S	0	0
			934	592	176	164	2		

- Molecule 3 is a protein called Ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	N	152	Total	C	N	O	S	0	0
			1198	762	230	201	5		

- Molecule 4 is a protein called Ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	J	166	Total	C	N	O	S	0	0
			1322	827	257	232	6		

- Molecule 5 is a protein called Ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	D	182	Total	C	N	O	S	0	0
			1402	890	254	244	14		

- Molecule 6 is a protein called Ribosomal protein S23.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	X	142	Total	C	N	O	S	0	0
			1104	697	219	184	4		

- Molecule 7 is a protein called Ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	S	133	Total	C	N	O	S	0	0
			1055	651	210	188	6		

- Molecule 8 is a protein called Ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	Q	125	Total	C	N	O	S	0	0
			960	603	190	164	3		

- Molecule 9 is a protein called Ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	C	212	Total	C	N	O	S	0	0
			1641	1043	298	296	4		

- Molecule 10 is a protein called 40S ribosomal protein SA.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	A	194	Total	C	N	O	S	0	0
			1546	998	269	271	8		

- Molecule 11 is a protein called 40S ribosomal protein S3a.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	B	218	Total	C	N	O	S	0	0
			1758	1113	323	309	13		

- Molecule 12 is a protein called Ribosomal protein S24.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	Y	90	Total	C	N	O	S	0	0
			708	451	125	126	6		

- Molecule 13 is a protein called Ribosomal protein S27.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	b	79	Total	C	N	O	S	0	0
			614	389	105	114	6		

- Molecule 14 is a protein called 40S ribosomal protein S26.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	a	97	Total 785	C 484	N 162	O 131	S 8	0	0

- Molecule 15 is a protein called 40S ribosomal protein S25.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	Z	59	Total 419	C 266	N 73	O 75	S 5	0	0

- Molecule 16 is a protein called 40S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	V	82	Total 605	C 377	N 112	O 110	S 6	0	0

- Molecule 17 is a protein called Ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	P	105	Total 836	C 531	N 166	O 133	S 6	0	0

- Molecule 18 is a protein called Ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	R	101	Total 780	C 485	N 145	O 147	S 3	0	0

- Molecule 19 is a protein called Ribosomal protein S10B.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	K	83	Total 689	C 446	N 116	O 123	S 4	0	0

- Molecule 20 is a protein called 40S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	I	163	Total 1282	C 804	N 246	O 229	S 3	0	0

- Molecule 21 is a protein called 40S ribosomal protein S30.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	e	37	Total	C	N	O	S	0	0
			291	185	59	46	1		

- Molecule 22 is a protein called Ribosomal protein eS7.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	H	162	Total	C	N	O	S	0	0
			1194	772	210	207	5		

- Molecule 23 is a protein called Ribosomal protein eL41.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	n	24	Total	C	N	O	S	0	0
			217	134	55	25	3		

- Molecule 24 is a protein called Ribosomal protein S28.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	c	55	Total	C	N	O	S	0	0
			439	269	89	80	1		

- Molecule 25 is a protein called Ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	O	126	Total	C	N	O	S	0	0
			935	572	189	170	4		

- Molecule 26 is a protein called Ribosomal protein S15A.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	W	129	Total	C	N	O	S	0	0
			1031	659	192	177	3		

- Molecule 27 is a protein called 40S ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	E	258	Total	C	N	O	S	0	0
			2058	1317	377	352	12		

- Molecule 28 is a RNA chain called rRNA 18S.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	2	1355	Total	C	N	O	P	0	0
			29096	12946	5388	9407	1355		

- Molecule 29 is a protein called SSU ribosomal protein S17P.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	L	181	Total	C	N	O	S	0	0
			1481	933	293	248	7		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	12	SER	GLY	variant	UNP V6TVJ7

- Molecule 30 is a protein called Ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	U	74	Total	C	N	O	S	0	0
			609	394	111	102	2		

- Molecule 31 is a protein called 40S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	G	197	Total	C	N	O	S	0	0
			1530	961	296	263	10		

- Molecule 32 is a protein called Ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	F	161	Total	C	N	O	S	0	0
			1246	771	240	227	8		

- Molecule 33 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		AltConf
33	d	1	Total	K	0
			1	1	
33	N	7	Total	K	0
			7	7	
33	S	2	Total	K	0
			2	2	

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Mol	Chain	Residues	Atoms	AltConf
33	A	1	Total K 1 1	0
33	b	1	Total K 1 1	0
33	R	1	Total K 1 1	0
33	O	6	Total K 6 6	0
33	W	1	Total K 1 1	0
33	E	3	Total K 3 3	0
33	2	239	Total K 239 239	0
33	L	3	Total K 3 3	0
33	G	1	Total K 1 1	0

- Molecule 34 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

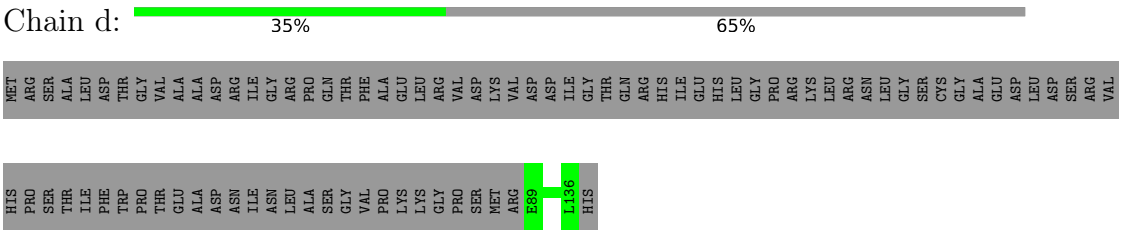
Mol	Chain	Residues	Atoms	AltConf
34	N	1	Total Mg 1 1	0
34	I	1	Total Mg 1 1	0
34	2	35	Total Mg 35 35	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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. 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.

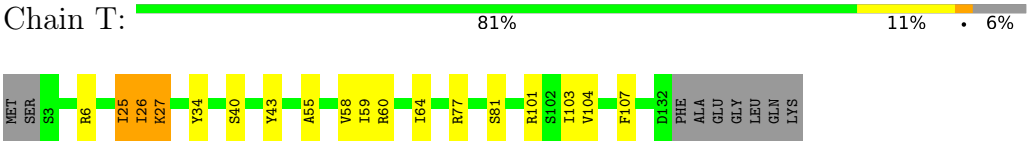
- Molecule 1: Ribosomal protein S29A

Chain d:



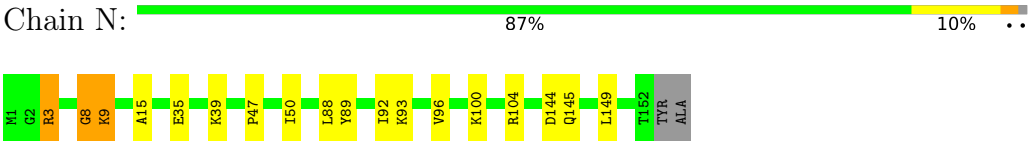
- Molecule 2: Ribosomal protein S19e

Chain T:



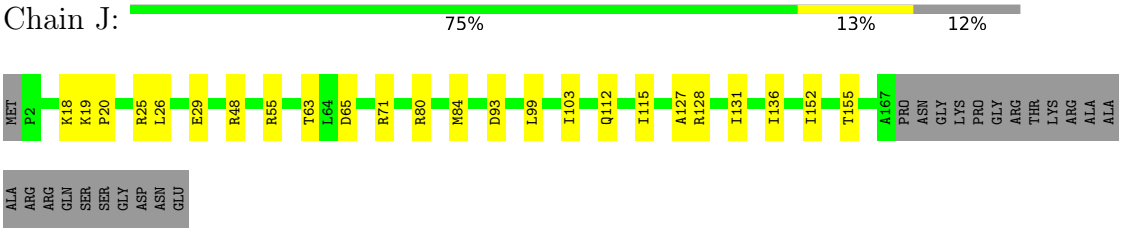
- Molecule 3: Ribosomal protein S13

Chain N:



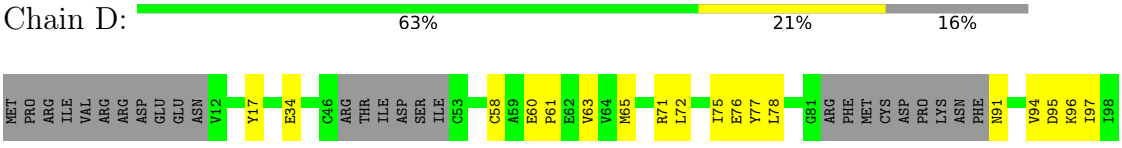
- Molecule 4: Ribosomal protein S9

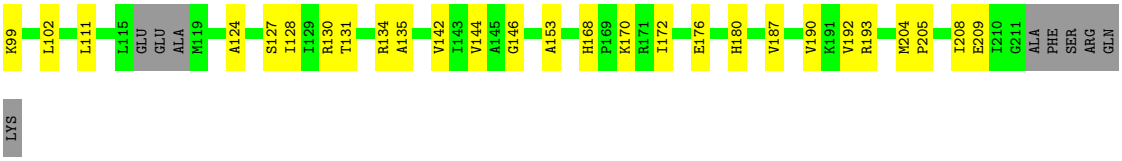
Chain J:



- Molecule 5: Ribosomal protein S3

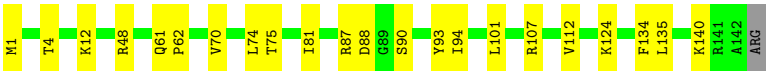
Chain D:





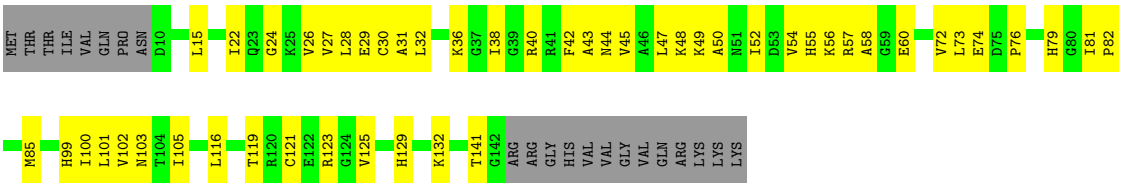
• Molecule 6: Ribosomal protein S23

Chain X:



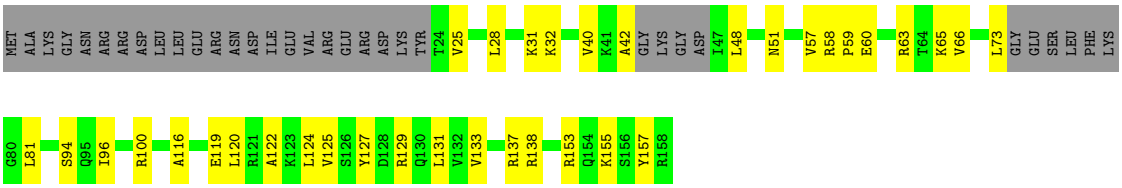
• Molecule 7: Ribosomal protein S18

Chain S:



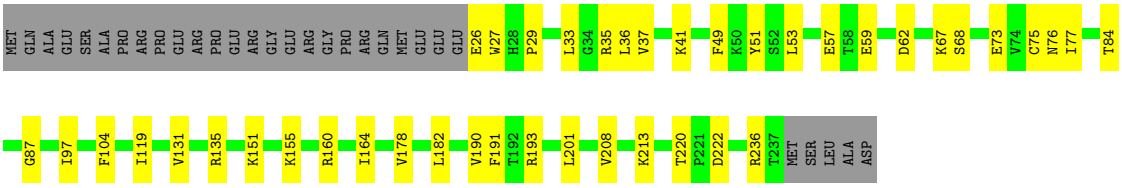
• Molecule 8: Ribosomal protein S16

Chain Q:



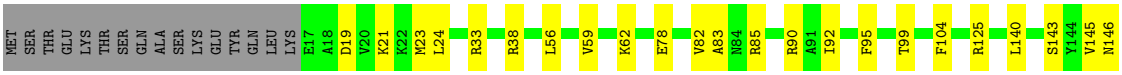
• Molecule 9: Ribosomal protein S2

Chain C:



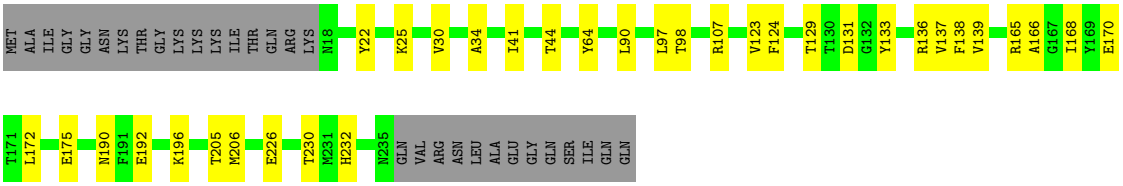
• Molecule 10: 40S ribosomal protein SA

Chain A:



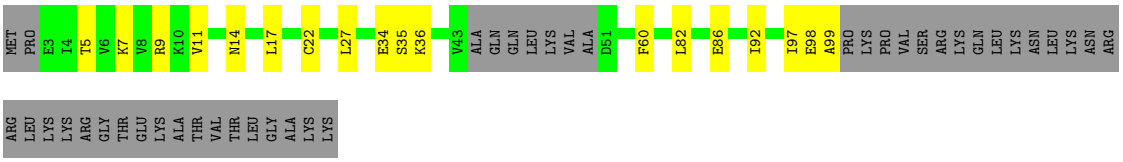
• Molecule 11: 40S ribosomal protein S3a

Chain B:



• Molecule 12: Ribosomal protein S24

Chain Y:



• Molecule 13: Ribosomal protein S27

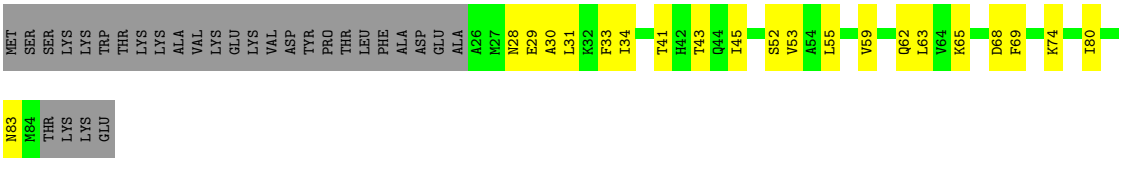
Chain b:

• Molecule 14: 40S ribosomal protein S26

Chain a:

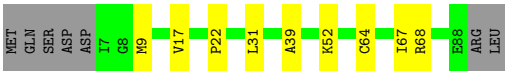
• Molecule 15: 40S ribosomal protein S25

Chain Z:



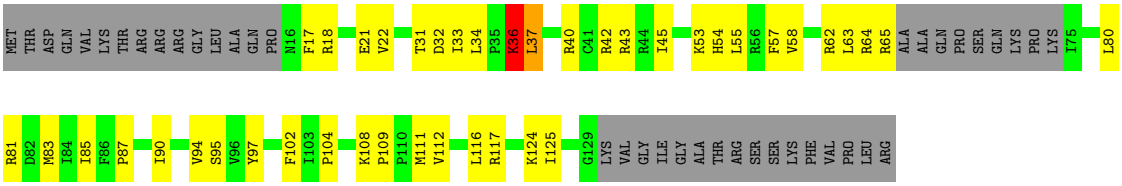
• Molecule 16: 40S ribosomal protein S21

Chain V:



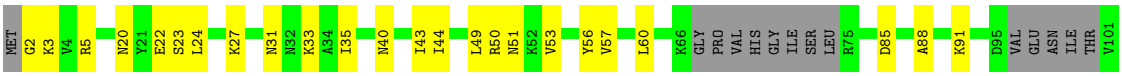
• Molecule 17: Ribosomal protein S15

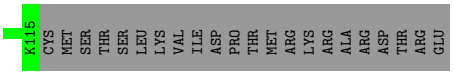
Chain P:



• Molecule 18: Ribosomal protein S17

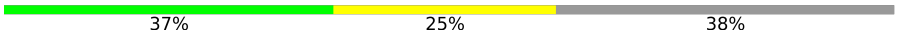
Chain R:





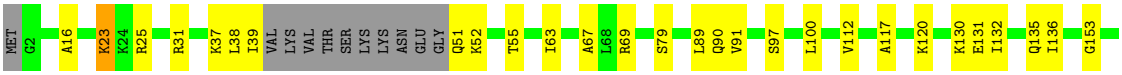
• Molecule 19: Ribosomal protein S10B

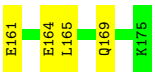
Chain K:



• Molecule 20: 40S ribosomal protein S8

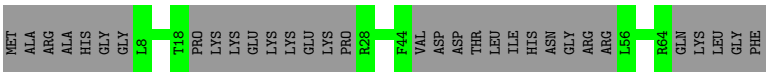
Chain I:





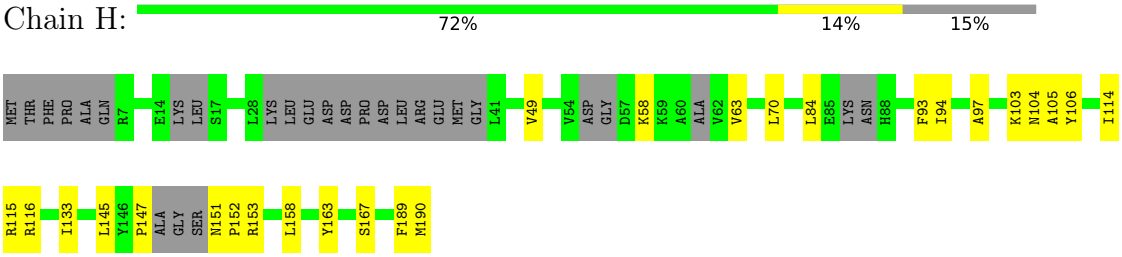
• Molecule 21: 40S ribosomal protein S30

Chain e:



• Molecule 22: Ribosomal protein eS7

Chain H:

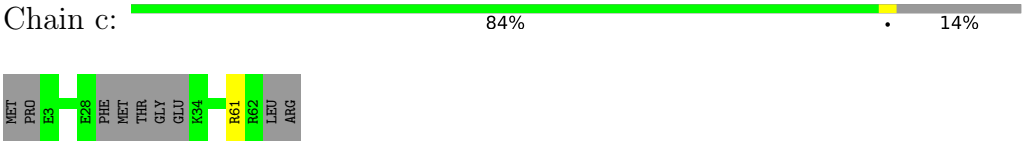


• Molecule 23: Ribosomal protein eL41

Chain n:

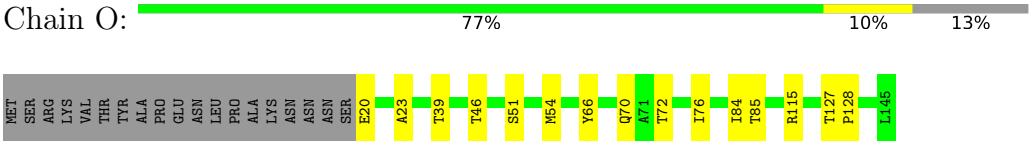
• Molecule 24: Ribosomal protein S28

Chain c:



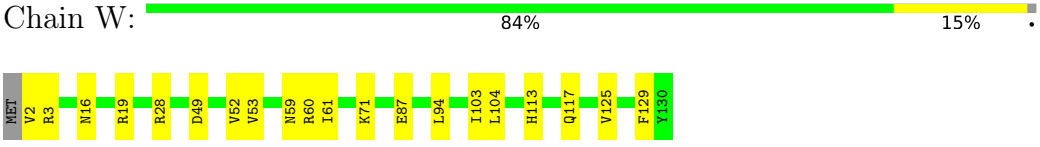
• Molecule 25: Ribosomal protein S14

Chain O:



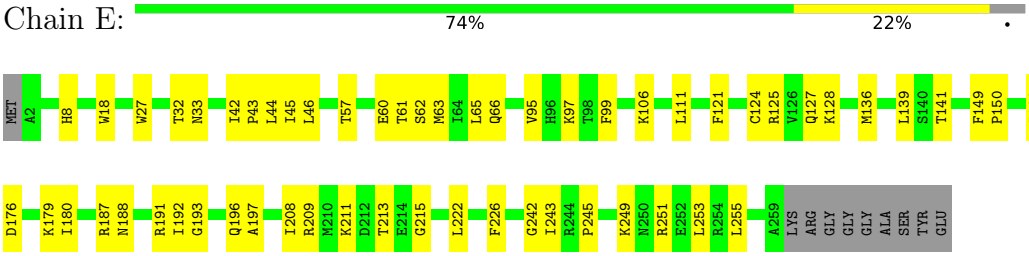
• Molecule 26: Ribosomal protein S15A

Chain W:



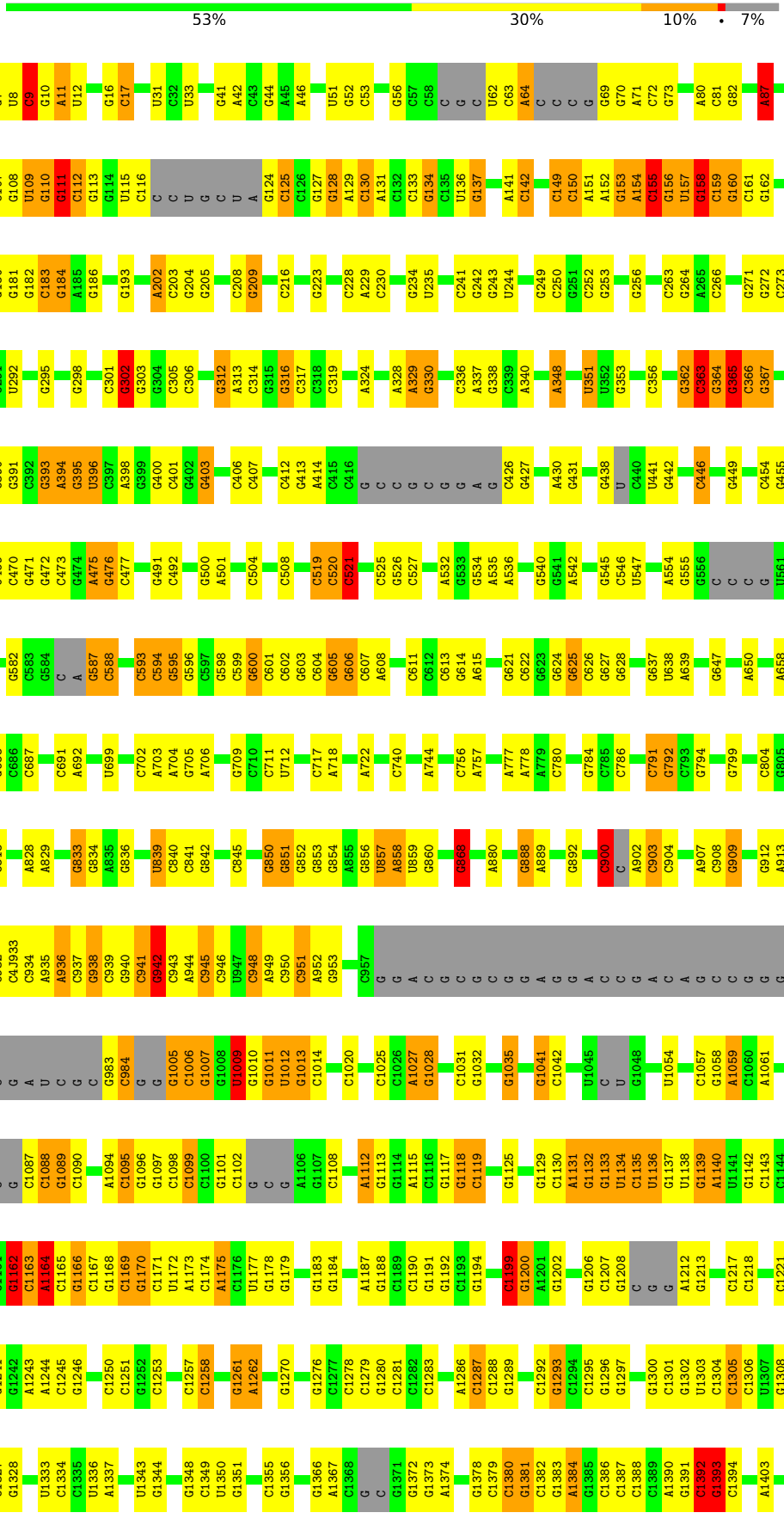
• Molecule 27: 40S ribosomal protein S4

Chain E:



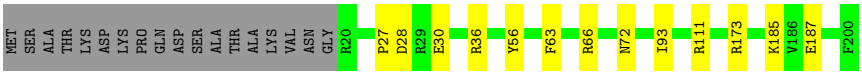
• Molecule 28: rRNA 18S

Chain 2:



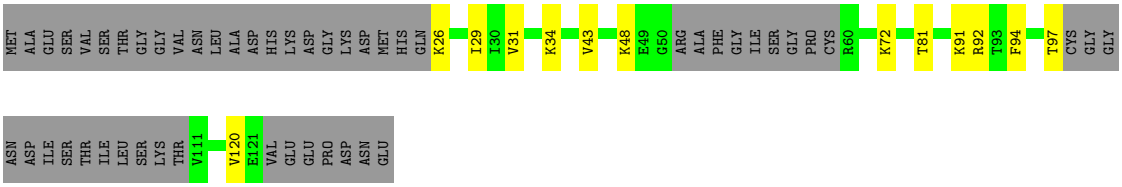
• Molecule 29: SSU ribosomal protein S17P

Chain L:



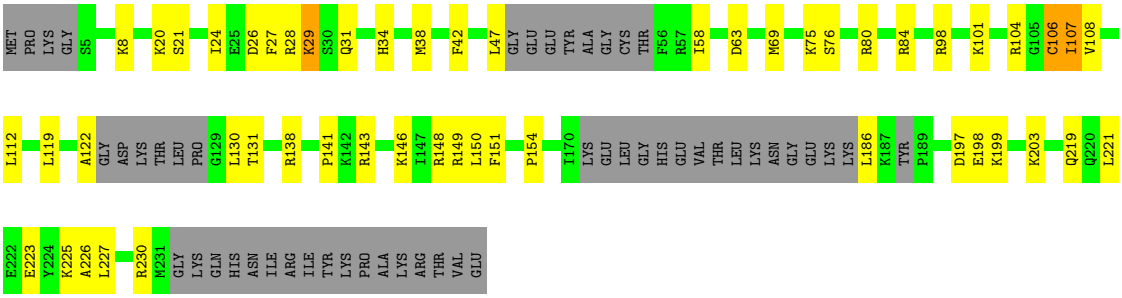
• Molecule 30: Ribosomal protein S20

Chain U:



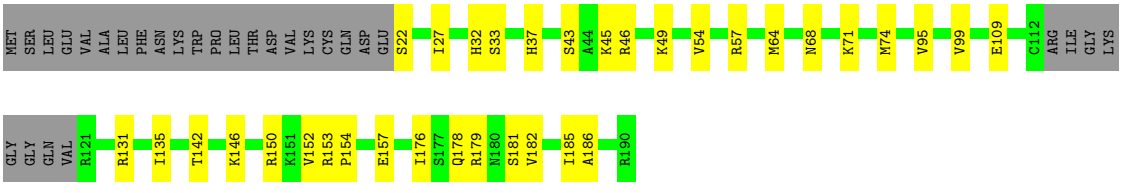
• Molecule 31: 40S ribosomal protein S6

Chain G:



• Molecule 32: Ribosomal protein S5

Chain F:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	91058	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	1.0	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	1500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: MA6, OMU, A2M, 4OC, OMG, 7MG, MG, M7A, OMC, 4AC, K, C4J

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	d	0.30	0/406	0.53	0/539
2	T	0.29	0/955	0.52	1/1297 (0.1%)
3	N	0.33	0/1221	0.50	0/1641
4	J	0.28	0/1340	0.48	0/1796
5	D	0.31	0/1422	0.53	0/1909
6	X	0.30	0/1119	0.56	0/1498
7	S	0.28	0/1070	0.55	0/1435
8	Q	0.27	0/968	0.52	0/1295
9	C	0.31	0/1674	0.50	0/2259
10	A	0.31	0/1580	0.50	0/2149
11	B	0.29	0/1793	0.50	0/2419
12	Y	0.30	0/719	0.51	0/964
13	b	0.33	0/628	0.57	0/852
14	a	0.31	0/797	0.49	0/1072
15	Z	0.30	0/422	0.56	0/565
16	V	0.30	0/613	0.53	0/823
17	P	0.30	0/850	0.60	1/1138 (0.1%)
18	R	0.30	0/786	0.52	0/1052
19	K	0.32	0/707	0.60	0/957
20	I	0.31	0/1302	0.54	0/1746
21	e	0.27	0/294	0.53	0/392
22	H	0.29	0/1210	0.49	0/1638
23	n	0.30	0/219	0.45	0/280
24	c	0.27	0/439	0.53	0/585
25	O	0.29	0/947	0.56	0/1273
26	W	0.31	0/1048	0.49	0/1412
27	E	0.29	0/2104	0.54	0/2841
28	2	0.56	0/32117	1.01	149/50066 (0.3%)
29	L	0.31	0/1514	0.52	0/2030
30	U	0.29	0/619	0.49	0/833
31	G	0.29	0/1545	0.56	0/2061
32	F	0.29	0/1264	0.46	0/1697

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
All	All	0.45	0/63692	0.83	151/92514 (0.2%)

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
17	P	0	1
18	R	0	1
31	G	0	3
All	All	0	5

There are no bond length outliers.

The worst 5 of 151 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	2	175	C	P-O3'-C3'	-15.08	101.60	119.70
28	2	1132	G	P-O3'-C3'	-11.54	105.85	119.70
28	2	363	C	P-O3'-C3'	-10.32	107.32	119.70
28	2	1410	G	P-O3'-C3'	-10.24	107.42	119.70
28	2	366	C	P-O3'-C3'	-10.17	107.49	119.70

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
31	G	106	CYS	Peptide
31	G	107	ILE	Peptide
31	G	29	LYS	Peptide
17	P	36	LYS	Peptide
18	R	40	ASN	Peptide

5.2 Too-close contacts (i)

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 hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	d	398	0	398	0	0
2	T	934	0	882	17	0
3	N	1198	0	1266	11	0
4	J	1322	0	1378	18	0
5	D	1402	0	1424	30	0
6	X	1104	0	1194	12	0
7	S	1055	0	1076	38	0
8	Q	960	0	1037	23	0
9	C	1641	0	1687	26	0
10	A	1546	0	1575	22	0
11	B	1758	0	1797	20	0
12	Y	708	0	724	11	0
13	b	614	0	604	0	0
14	a	785	0	818	0	0
15	Z	419	0	413	13	0
16	V	605	0	606	6	0
17	P	836	0	866	31	0
18	R	780	0	782	18	0
19	K	689	0	671	26	0
20	I	1282	0	1336	23	0
21	e	291	0	306	0	0
22	H	1194	0	1169	21	0
23	n	217	0	259	0	0
24	c	439	0	473	0	0
25	O	935	0	935	11	0
26	W	1031	0	1082	14	0
27	E	2058	0	2135	36	0
28	2	29096	0	14778	262	0
29	L	1481	0	1496	10	0
30	U	609	0	649	9	0
31	G	1530	0	1613	42	0
32	F	1246	0	1268	25	0
33	2	239	0	0	0	0
33	A	1	0	0	0	0
33	E	3	0	0	0	0
33	G	1	0	0	0	0
33	L	3	0	0	0	0
33	N	7	0	0	0	0
33	O	6	0	0	0	0
33	R	1	0	0	0	0
33	S	2	0	0	0	0
33	W	1	0	0	0	0
33	b	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
33	d	1	0	0	0	0
34	2	35	0	0	0	0
34	I	1	0	0	0	0
34	N	1	0	0	0	0
All	All	60466	0	46697	700	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

The worst 5 of 700 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:G:27:PHE:HD1	31:G:28:ARG:H	1.23	0.85
2:T:25:ILE:HG22	2:T:26:ILE:H	1.41	0.84
28:2:593:C:H4'	28:2:594:C:H5'	1.58	0.84
28:2:124:G:H1	31:G:203:LYS:HE2	1.49	0.78
31:G:143:ARG:HB3	31:G:146:LYS:HD3	1.65	0.78

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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
1	d	46/137 (34%)	43 (94%)	3 (6%)	0	100 100
2	T	128/139 (92%)	116 (91%)	10 (8%)	2 (2%)	9 28
3	N	150/154 (97%)	145 (97%)	3 (2%)	2 (1%)	12 33
4	J	164/189 (87%)	162 (99%)	2 (1%)	0	100 100
5	D	174/217 (80%)	160 (92%)	14 (8%)	0	100 100
6	X	140/143 (98%)	133 (95%)	6 (4%)	1 (1%)	22 50

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	S	131/154 (85%)	116 (88%)	15 (12%)	0	100	100
8	Q	119/158 (75%)	110 (92%)	9 (8%)	0	100	100
9	C	210/242 (87%)	201 (96%)	9 (4%)	0	100	100
10	A	192/245 (78%)	185 (96%)	7 (4%)	0	100	100
11	B	216/248 (87%)	210 (97%)	6 (3%)	0	100	100
12	Y	86/132 (65%)	82 (95%)	4 (5%)	0	100	100
13	b	77/124 (62%)	74 (96%)	3 (4%)	0	100	100
14	a	95/109 (87%)	91 (96%)	4 (4%)	0	100	100
15	Z	57/88 (65%)	52 (91%)	5 (9%)	0	100	100
16	V	80/89 (90%)	73 (91%)	7 (9%)	0	100	100
17	P	101/145 (70%)	88 (87%)	11 (11%)	2 (2%)	7	23
18	R	95/137 (69%)	91 (96%)	4 (4%)	0	100	100
19	K	79/134 (59%)	69 (87%)	10 (13%)	0	100	100
20	I	159/174 (91%)	155 (98%)	4 (2%)	0	100	100
21	e	31/69 (45%)	31 (100%)	0	0	100	100
22	H	148/190 (78%)	137 (93%)	11 (7%)	0	100	100
23	n	22/41 (54%)	22 (100%)	0	0	100	100
24	c	51/64 (80%)	48 (94%)	3 (6%)	0	100	100
25	O	124/145 (86%)	121 (98%)	3 (2%)	0	100	100
26	W	127/130 (98%)	118 (93%)	9 (7%)	0	100	100
27	E	256/268 (96%)	246 (96%)	10 (4%)	0	100	100
29	L	179/199 (90%)	169 (94%)	10 (6%)	0	100	100
30	U	68/126 (54%)	66 (97%)	2 (3%)	0	100	100
31	G	187/248 (75%)	170 (91%)	17 (9%)	0	100	100
32	F	157/190 (83%)	154 (98%)	3 (2%)	0	100	100
All	All	3849/4828 (80%)	3638 (94%)	204 (5%)	7 (0%)	50	75

5 of 7 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	T	26	ILE
17	P	37	LEU
2	T	27	LYS

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Mol	Chain	Res	Type
3	N	8	GLY
17	P	36	LYS

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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
1	d	42/116 (36%)	42 (100%)	0	100 100
2	T	86/115 (75%)	86 (100%)	0	100 100
3	N	124/130 (95%)	123 (99%)	1 (1%)	81 93
4	J	141/164 (86%)	141 (100%)	0	100 100
5	D	142/182 (78%)	142 (100%)	0	100 100
6	X	113/114 (99%)	113 (100%)	0	100 100
7	S	112/131 (86%)	112 (100%)	0	100 100
8	Q	101/130 (78%)	101 (100%)	0	100 100
9	C	176/201 (88%)	175 (99%)	1 (1%)	86 95
10	A	168/217 (77%)	167 (99%)	1 (1%)	86 95
11	B	196/220 (89%)	196 (100%)	0	100 100
12	Y	77/113 (68%)	77 (100%)	0	100 100
13	b	70/112 (62%)	70 (100%)	0	100 100
14	a	90/103 (87%)	90 (100%)	0	100 100
15	Z	41/79 (52%)	40 (98%)	1 (2%)	49 77
16	V	62/72 (86%)	62 (100%)	0	100 100
17	P	87/128 (68%)	87 (100%)	0	100 100
18	R	82/123 (67%)	81 (99%)	1 (1%)	71 89
19	K	73/119 (61%)	73 (100%)	0	100 100
20	I	138/148 (93%)	137 (99%)	1 (1%)	84 94
21	e	30/58 (52%)	30 (100%)	0	100 100
22	H	116/170 (68%)	116 (100%)	0	100 100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
23	n	21/38 (55%)	21 (100%)	0	100 100
24	c	49/57 (86%)	48 (98%)	1 (2%)	55 80
25	O	91/113 (80%)	91 (100%)	0	100 100
26	W	114/115 (99%)	114 (100%)	0	100 100
27	E	224/232 (97%)	224 (100%)	0	100 100
29	L	154/173 (89%)	153 (99%)	1 (1%)	86 95
30	U	68/110 (62%)	68 (100%)	0	100 100
31	G	162/213 (76%)	162 (100%)	0	100 100
32	F	132/157 (84%)	132 (100%)	0	100 100
All	All	3282/4153 (79%)	3274 (100%)	8 (0%)	93 98

5 of 8 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
29	L	111	ARG
24	c	61	ARG
18	R	5	ARG
15	Z	74	LYS
20	I	23	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
4	J	112	GLN
27	E	163	ASN
29	L	136	HIS
31	G	31	GLN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
28	2	1329/1452 (91%)	283 (21%)	15 (1%)

5 of 283 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
28	2	4	C

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Mol	Chain	Res	Type
28	2	9	C
28	2	17	C
28	2	33	U
28	2	41	G

5 of 15 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
28	2	850	G
28	2	1380	C
28	2	941	C
28	2	1421	G
28	2	1135	C

5.4 Non-standard residues in protein, DNA, RNA chains (i)

15 non-standard protein/DNA/RNA residues are modelled in this entry.

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	$\#\|Z\| > 2$
28	C4J	2	933	28	24,29,30	3.28	9 (37%)	29,42,45	1.38	5 (17%)
28	OMG	2	1011	28	18,26,27	1.00	1 (5%)	19,38,41	1.19	2 (10%)
28	7MG	2	1261	28	22,26,27	3.73	10 (45%)	29,39,42	2.07	9 (31%)
28	4AC	2	1426	28,33	21,24,25	4.43	16 (76%)	29,34,37	1.30	2 (6%)
28	MA6	2	1435	28	18,26,27	1.03	2 (11%)	19,38,41	3.64	2 (10%)
28	OMG	2	1035	28,33	18,26,27	1.00	1 (5%)	19,38,41	1.14	2 (10%)
28	OMG	2	868	28	18,26,27	2.36	8 (44%)	19,38,41	1.43	3 (15%)
28	A2M	2	348	34,28	18,25,26	3.64	8 (44%)	18,36,39	3.40	4 (22%)
28	OMU	2	1314	28	19,22,23	2.94	8 (42%)	26,31,34	1.69	4 (15%)
28	OMC	2	104	28	19,22,23	0.85	0	26,31,34	0.89	2 (7%)
28	A2M	2	87	28,33	18,25,26	3.60	7 (38%)	18,36,39	3.26	4 (22%)
28	OMG	2	371	28,33	18,26,27	2.47	8 (44%)	19,38,41	1.60	4 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
28	M7A	2	1390	28	20,25,26	0.41	0	28,37,40	0.69	1 (3%)
28	MA6	2	1434	28	18,26,27	1.05	2 (11%)	19,38,41	3.45	2 (10%)
28	4OC	2	1325	28	20,23,24	3.12	8 (40%)	26,32,35	1.00	1 (3%)

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
28	C4J	2	933	28	-	4/16/34/35	0/2/2/2
28	OMG	2	1011	28	-	3/5/27/28	0/3/3/3
28	7MG	2	1261	28	-	0/7/37/38	0/3/3/3
28	4AC	2	1426	28,33	-	2/11/29/30	0/2/2/2
28	MA6	2	1435	28	-	2/7/29/30	0/3/3/3
28	OMG	2	1035	28,33	-	1/5/27/28	0/3/3/3
28	OMG	2	868	28	-	3/5/27/28	0/3/3/3
28	A2M	2	348	34,28	-	0/5/27/28	0/3/3/3
28	OMU	2	1314	28	-	0/9/27/28	0/2/2/2
28	OMC	2	104	28	-	0/9/27/28	0/2/2/2
28	A2M	2	87	28,33	-	3/5/27/28	0/3/3/3
28	OMG	2	371	28,33	-	1/5/27/28	0/3/3/3
28	M7A	2	1390	28	-	0/7/37/38	0/3/3/3
28	MA6	2	1434	28	-	0/7/29/30	0/3/3/3
28	4OC	2	1325	28	-	0/9/29/30	0/2/2/2

The worst 5 of 88 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	2	933	C4J	C6-C5	11.76	1.51	1.34
28	2	1261	7MG	C8-N9	9.39	1.51	1.46
28	2	1426	4AC	O4'-C1'	8.76	1.62	1.42
28	2	87	A2M	C3'-C4'	-8.74	1.30	1.53
28	2	348	A2M	C3'-C4'	-8.63	1.30	1.53

The worst 5 of 47 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	2	1435	MA6	N1-C6-N6	-14.40	101.90	117.06
28	2	1434	MA6	N1-C6-N6	-13.76	102.57	117.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	2	348	A2M	C5-C6-N6	10.45	136.24	120.35
28	2	87	A2M	C5-C6-N6	10.16	135.79	120.35
28	2	348	A2M	N6-C6-N1	-7.21	103.60	118.57

There are no chirality outliers.

5 of 19 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
28	2	87	A2M	C1'-C2'-O2'-CM'
28	2	371	OMG	C1'-C2'-O2'-CM2
28	2	868	OMG	C1'-C2'-O2'-CM2
28	2	933	C4J	C3'-C4'-C5'-O5'
28	2	933	C4J	C4'-C5'-O5'-P

There are no ring outliers.

9 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
28	2	1011	OMG	1	0
28	2	1261	7MG	1	0
28	2	1035	OMG	1	0
28	2	868	OMG	1	0
28	2	348	A2M	1	0
28	2	1314	OMU	1	0
28	2	87	A2M	1	0
28	2	371	OMG	1	0
28	2	1434	MA6	1	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 303 ligands modelled in this entry, 303 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.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Map visualisation

This section contains visualisations of the EMDB entry EMD-13680. These allow visual inspection of the internal detail of the map and identification of artifacts.

No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

This section was not generated.

6.2 Central slices

This section was not generated.

6.3 Largest variance slices

This section was not generated.

6.4 Orthogonal standard-deviation projections (False-color)

This section was not generated.

6.5 Orthogonal surface views

This section was not generated.

6.6 Mask visualisation

This section was not generated. No masks/segmentation were deposited.

7 Map analysis

This section contains the results of statistical analysis of the map.

7.1 Map-value distribution

This section was not generated.

7.2 Volume estimate versus contour level

This section was not generated.

7.3 Rotationally averaged power spectrum

This section was not generated. The rotationally averaged power spectrum had issues being displayed.

8 Fourier-Shell correlation (i)

This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit

This section was not generated.