wwPDB EM Validation Summary Report (i)

Apr 16, 2024 – 03:56 am BST

PDB ID	:	5ME1
EMDB ID	:	EMD-3495
Title	:	Structure of the 30S Pre-Initiation Complex 2 (30S IC-2) Stalled by GE81112
Authors	:	Lopez-Alonso, J.P.; Fabbretti, A.; Kaminishi, T.; Iturrioz, I.; Brandi, L.; Gil Carton, D.; Gualerzi, C.; Fucini, P.; Connell, S.
Deposited on	:	2016-11-14
Resolution	:	13.50 Å(reported)
Based on initial models	:	1TIF, 1HR0, 2IFE, 4YBB, 3JCN

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:

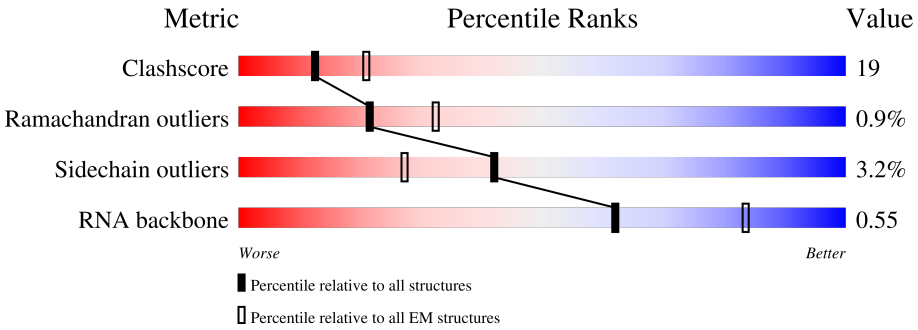
EMDB validation analysis	:	0.0.1.dev92
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	FAILED
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)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

1 Overall quality at a glance

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

The reported resolution of this entry is 13.50 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	A	1534	69% 24% 6%
2	B	241	71% 20% • 7%
3	C	233	73% 15% • 12%
4	D	206	87% 12%
5	E	167	66% 25% • 7%
6	F	131	69% 11% 19%
7	G	156	73% 22% • •

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Mol	Chain	Length	Quality of chain
8	H	130	78% 20%
9	I	130	72% 26%
10	J	103	53% 39%
11	K	129	71% 20% 9%
12	L	123	85% 15%
13	M	118	65% 31%
14	N	101	71% 27%
15	O	89	88% 10%
16	P	102	75% 20%
17	Q	84	76% 19% 5%
18	R	75	63% 11% 27%
19	S	92	67% 16% 14%
20	T	87	80% 18%
21	U	71	61% 17% 21%
22	V	72	17% 67% 15%
23	W	890	36% 19% 44%
24	Y	171	32% 11% 56%
25	Z	144	31% 25% 7% 37%
26	X	77	13% 57% 21% 9%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
1	2MG	A	966	-	-	X	-
26	4SU	X	8	-	-	X	-
27	FME	X	101	-	-	X	-

2 Entry composition (i)

There are 27 unique types of molecules in this entry. The entry contains 59063 atoms, of which 1 is hydrogen 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 RNA chain called 16S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	A	1534	32930	14694	6041	10661	1534	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	224	1753	1109	315	321	8	0	0

- Molecule 3 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	206	1624	1028	305	288	3	0	0

- Molecule 4 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	D	205	1643	1026	315	298	4	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	E	155	1144	711	216	211	6	0	0

- Molecule 6 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	F	106	862	545	156	154	7	0	0

- Molecule 7 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	151	Total	C	N	O	S	0	0
			1181	735	227	215	4		

- Molecule 8 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	129	Total	C	N	O	S	0	0
			979	616	173	184	6		

- Molecule 9 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	127	Total	C	N	O	S	0	0
			1022	634	206	179	3		

- Molecule 10 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	99	Total	C	N	O	S	0	0
			795	498	152	144	1		

- Molecule 11 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	117	Total	C	N	O	S	0	0
			877	540	174	160	3		

- Molecule 12 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	123	Total	C	N	O	S	0	0
			957	591	196	165	5		

- Molecule 13 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	114	Total	C	N	O	S	0	0
			883	546	178	156	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	100	Total	C	N	O	S	0	0
			805	499	164	139	3		

- Molecule 15 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	O	88	Total	C	N	O	S	0	0
			714	439	144	130	1		

- Molecule 16 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	P	82	Total	C	N	O	S	0	0
			649	406	128	114	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
17	Q	80	Total	C	N	O	S	0	0
			648	411	121	113	3		

- Molecule 18 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms				AltConf	Trace
18	R	55	Total	C	N	O	0	0
			455	288	86	81		

- Molecule 19 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	S	79	Total	C	N	O	S	0	0
			637	408	120	107	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
20	T	86	Total	C	N	O	S	0	0
			670	414	138	115	3		

- Molecule 21 is a protein called 30S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	U	56	Total	C	N	O	S	0	0
			465	290	96	78	1		

- Molecule 22 is a protein called Translation initiation factor IF-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	V	71	Total	C	N	O	S	0	0
			570	362	103	103	2		

- Molecule 23 is a protein called Translation initiation factor IF-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	W	501	Total	C	N	O	S	0	0
			3781	2368	663	735	15		

- Molecule 24 is a protein called Translation initiation factor IF-3.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	Y	76	Total	C	N	O	S	0	0
			623	390	119	112	2		

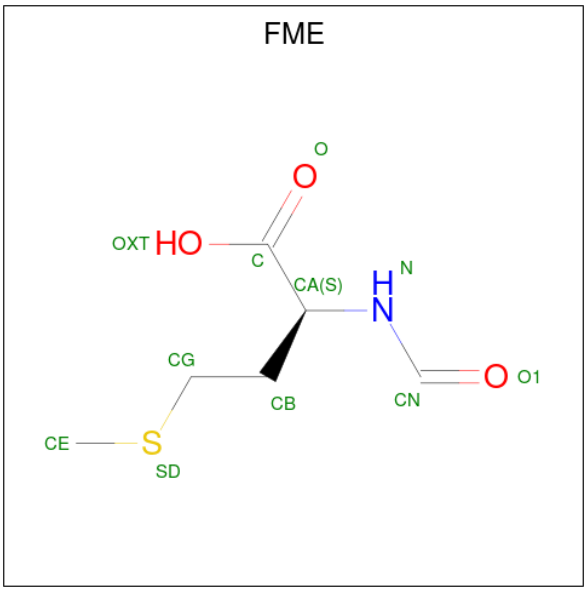
- Molecule 25 is a protein called Translation initiation factor IF-3.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	Z	91	Total	C	N	O	S	0	0
			743	470	135	134	4		

- Molecule 26 is a RNA chain called fMet-tRNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
26	X	77	Total	C	N	O	P	S	0	0
			1643	733	297	535	77	1		

- Molecule 27 is N-FORMYLMETHIONINE (three-letter code: FME) (formula: $C_6H_{11}NO_3S$).



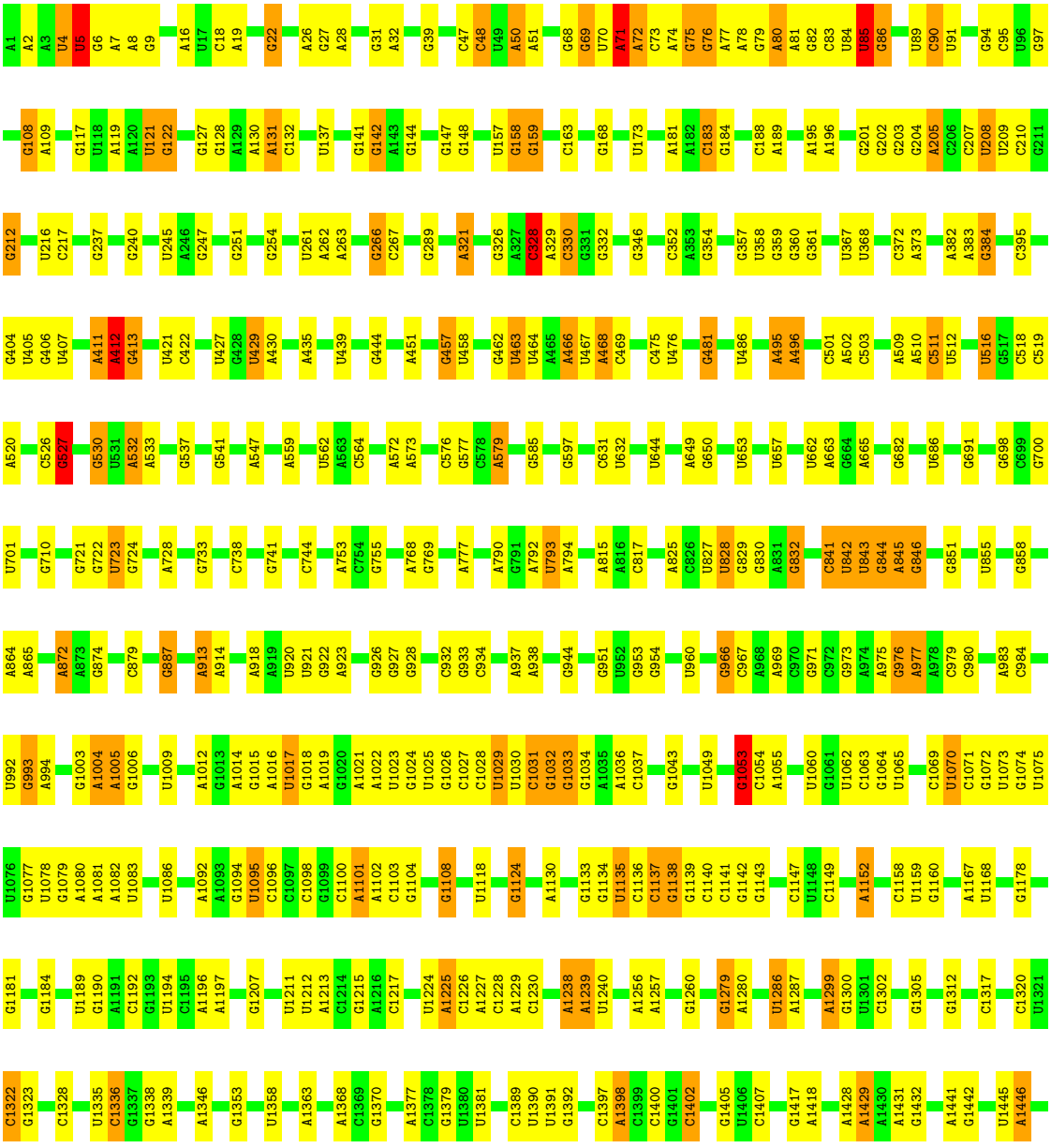
Mol	Chain	Residues	Atoms						AltConf
27	X	1	Total	C	H	N	O	S	0
			10	6	1	1	1	1	

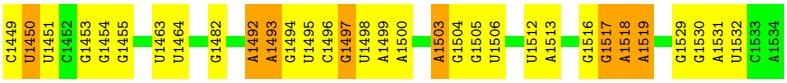
3 Residue-property plots (i)

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: 16S ribosomal RNA

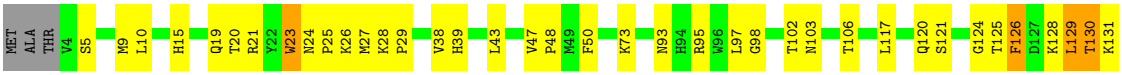
Chain A:

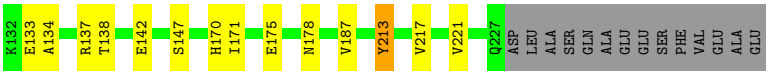




• Molecule 2: 30S ribosomal protein S2

Chain B:



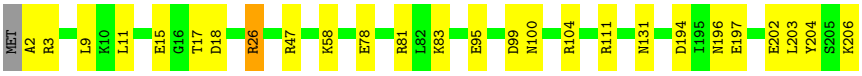


• Molecule 3: 30S ribosomal protein S3

Chain C:

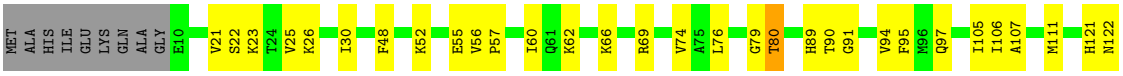
• Molecule 4: 30S ribosomal protein S4

Chain D:



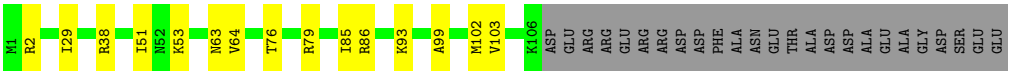
• Molecule 5: 30S ribosomal protein S5

Chain E:



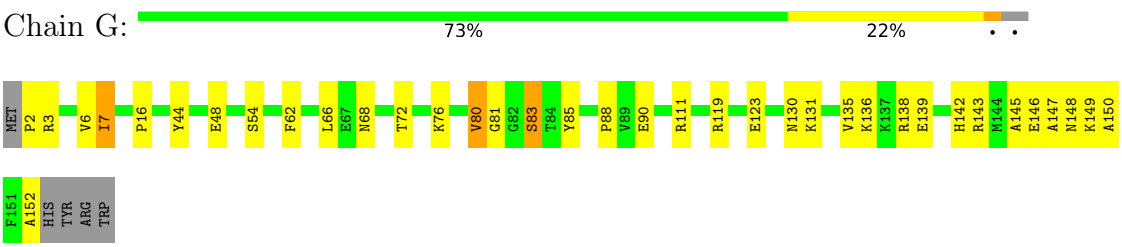
• Molecule 6: 30S ribosomal protein S6

Chain F:



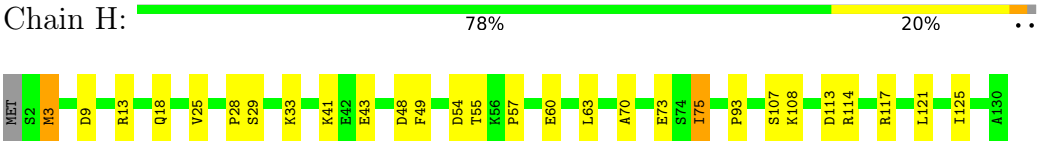
• Molecule 7: 30S ribosomal protein S7

Chain G:



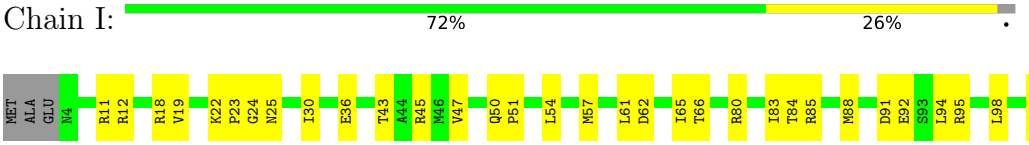
• Molecule 8: 30S ribosomal protein S8

Chain H:



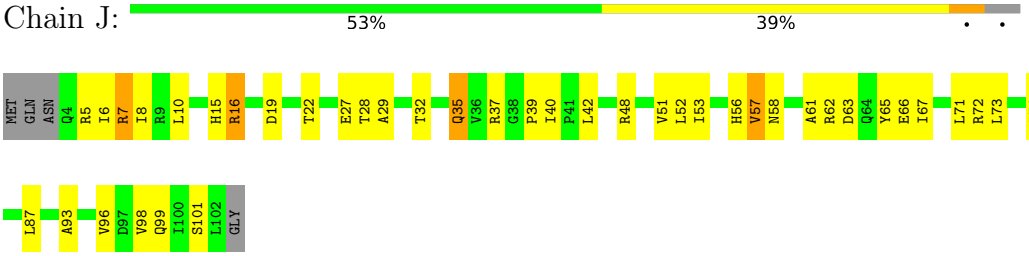
• Molecule 9: 30S ribosomal protein S9

Chain I:



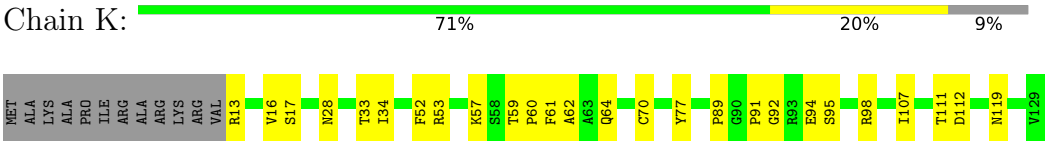
• Molecule 10: 30S ribosomal protein S10

Chain J:



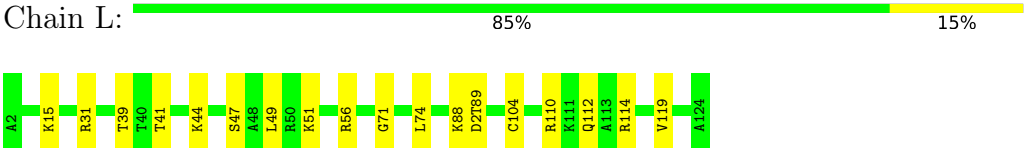
• Molecule 11: 30S ribosomal protein S11

Chain K:



• Molecule 12: 30S ribosomal protein S12

Chain L:

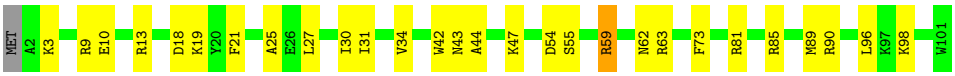


• Molecule 13: 30S ribosomal protein S13

Chain M:

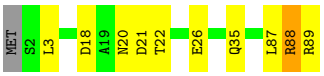
• Molecule 14: 30S ribosomal protein S14

Chain N:



• Molecule 15: 30S ribosomal protein S15

Chain O:

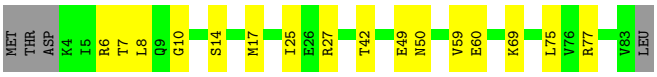


• Molecule 16: 30S ribosomal protein S16

Chain P:

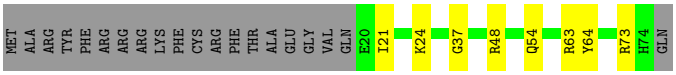
• Molecule 17: 30S ribosomal protein S17

Chain Q:



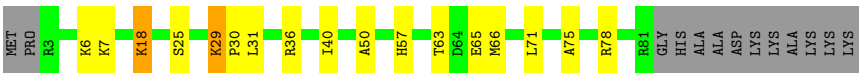
• Molecule 18: 30S ribosomal protein S18

Chain R:



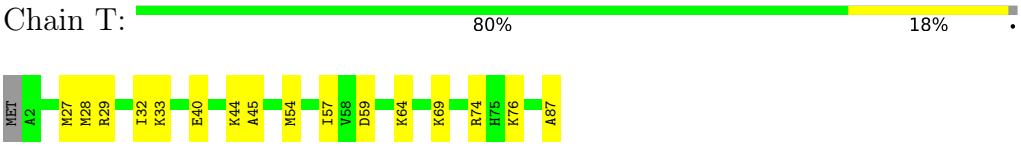
• Molecule 19: 30S ribosomal protein S19

Chain S:



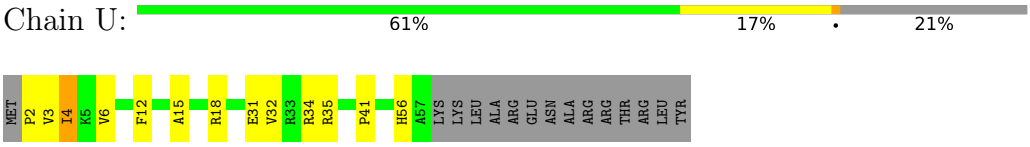
• Molecule 20: 30S ribosomal protein S20

Chain T:



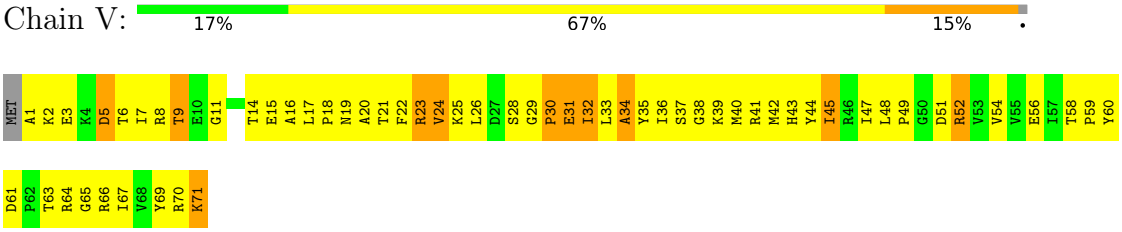
• Molecule 21: 30S ribosomal protein S21

Chain U:



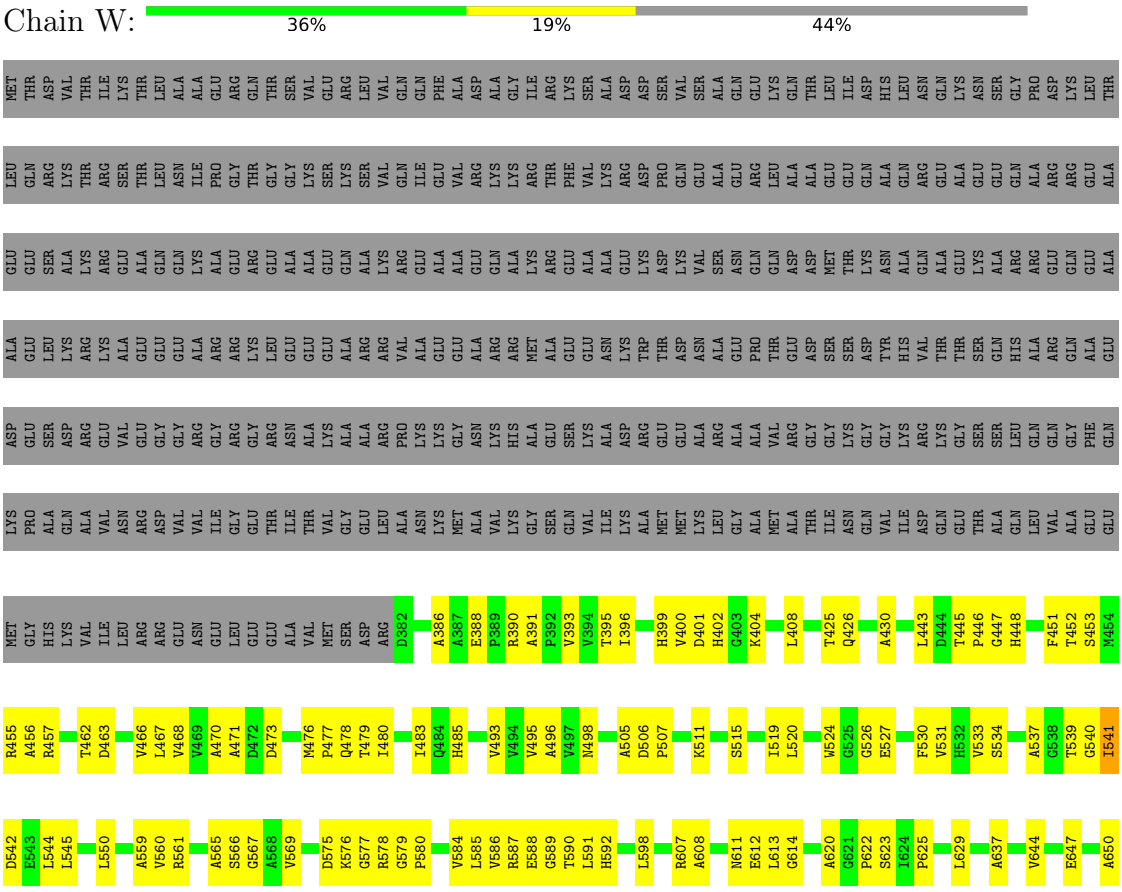
• Molecule 22: Translation initiation factor IF-1

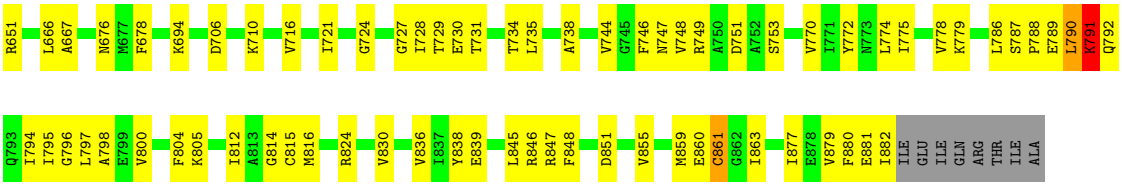
Chain V:



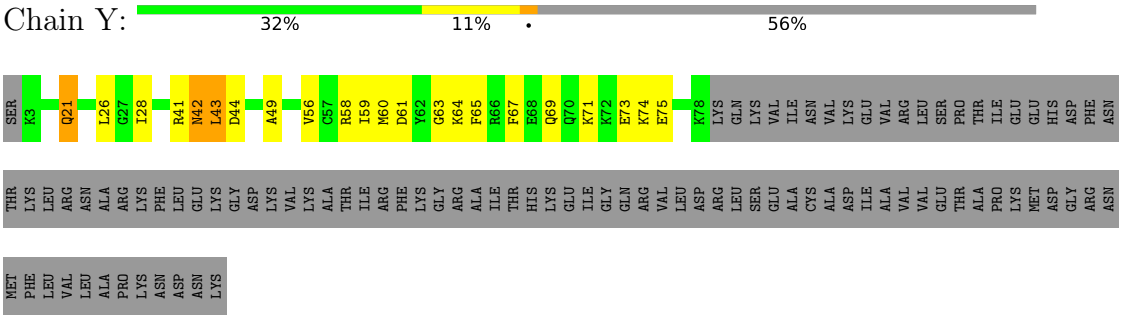
• Molecule 23: Translation initiation factor IF-2

Chain W:

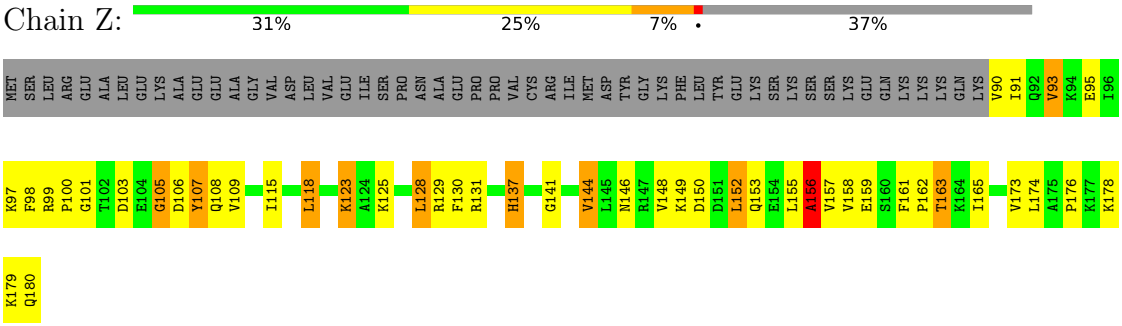




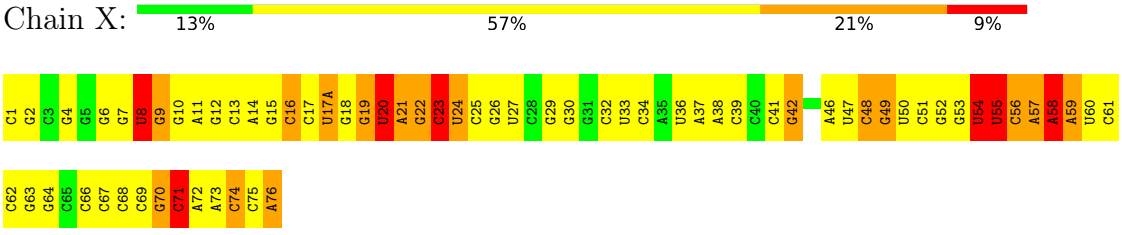
• Molecule 24: Translation initiation factor IF-3



• Molecule 25: Translation initiation factor IF-3



• Molecule 26: fMet-tRNA



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	26776	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	JEOL 2200FSC	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/Å^2$)	17	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	74183	Depositor
Image detector	GATAN ULTRASCAN 4000 (4k 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: UR3, 2MG, FME, MA6, PSU, G7M, H2U, 4OC, 5MC, 5MU, D2T, 4SU

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	0.58	0/36591	0.98	33/57073 (0.1%)
2	B	0.36	0/1784	0.55	0/2403
3	C	0.39	0/1651	0.55	0/2225
4	D	0.37	0/1665	0.53	0/2227
5	E	0.48	0/1157	0.61	0/1557
6	F	0.43	0/881	0.56	0/1189
7	G	0.35	0/1195	0.51	0/1602
8	H	0.43	0/989	0.58	0/1326
9	I	0.37	0/1034	0.60	0/1375
10	J	0.57	0/805	0.68	0/1089
11	K	0.39	0/893	0.54	0/1205
12	L	0.49	0/960	0.65	0/1286
13	M	0.38	0/892	0.63	0/1193
14	N	0.40	0/817	0.60	0/1088
15	O	0.42	0/722	0.52	0/964
16	P	0.40	0/659	0.59	0/884
17	Q	0.44	0/657	0.61	0/881
18	R	0.41	0/462	0.55	0/621
19	S	0.38	0/652	0.56	0/877
20	T	0.40	0/676	0.53	0/895
21	U	0.53	0/472	0.57	0/627
22	V	0.39	0/580	0.70	0/782
23	W	0.25	0/3829	0.46	1/5176 (0.0%)
24	Y	0.32	0/629	0.62	0/838
25	Z	1.18	0/751	1.61	13/999 (1.3%)
26	X	0.22	0/1746	0.81	5/2721 (0.2%)
All	All	0.52	0/63149	0.86	52/93103 (0.1%)

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
25	Z	0	6

There are no bond length outliers.

The worst 5 of 52 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	117	G	O5'-P-OP2	-9.51	97.14	105.70
25	Z	107	TYR	CB-CG-CD2	-8.11	116.13	121.00
26	X	71	C	N1-C1'-C2'	-7.46	103.80	112.00
25	Z	144	VAL	CA-CB-CG2	-7.42	99.77	110.90
25	Z	156	ALA	CB-CA-C	-6.93	99.71	110.10

There are no chirality outliers.

5 of 6 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
25	Z	103	ASP	Peptide
25	Z	107	TYR	Sidechain
25	Z	137	HIS	Peptide
25	Z	156	ALA	Peptide
25	Z	161	PHE	Sidechain

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	A	32930	0	16565	916	0
2	B	1753	0	1775	134	0
3	C	1624	0	1696	37	0
4	D	1643	0	1707	21	0
5	E	1144	0	1182	118	0
6	F	862	0	864	10	0
7	G	1181	0	1236	110	0
8	H	979	0	1031	18	0
9	I	1022	0	1068	36	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	J	795	0	836	39	0
11	K	877	0	887	103	0
12	L	957	0	1016	53	0
13	M	883	0	941	32	0
14	N	805	0	844	27	0
15	O	714	0	734	5	0
16	P	649	0	666	3	0
17	Q	648	0	691	11	0
18	R	455	0	478	7	0
19	S	637	0	665	16	0
20	T	670	0	719	12	0
21	U	465	0	491	8	0
22	V	570	0	592	201	0
23	W	3781	0	3836	318	0
24	Y	623	0	651	52	0
25	Z	743	0	773	185	0
26	X	1643	0	831	379	0
27	X	9	1	10	14	0
All	All	59062	1	42785	1891	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 19.

The worst 5 of 1891 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)
1:A:790:A:C8	26:X:38:A:H4'	1.24	1.71
1:A:790:A:C8	26:X:38:A:C4'	1.77	1.68
12:L:51:LYS:HE3	22:V:60:TYR:CD2	1.28	1.67
1:A:828:U:C2	2:B:25:PRO:CD	1.78	1.66
25:Z:91:ILE:HB	26:X:13:C:C4'	1.23	1.66

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
2	B	222/241 (92%)	209 (94%)	11 (5%)	2 (1%)	17 57
3	C	204/233 (88%)	193 (95%)	10 (5%)	1 (0%)	29 69
4	D	203/206 (98%)	199 (98%)	4 (2%)	0	100 100
5	E	153/167 (92%)	145 (95%)	8 (5%)	0	100 100
6	F	104/131 (79%)	96 (92%)	8 (8%)	0	100 100
7	G	149/156 (96%)	138 (93%)	10 (7%)	1 (1%)	22 63
8	H	127/130 (98%)	119 (94%)	8 (6%)	0	100 100
9	I	125/130 (96%)	111 (89%)	13 (10%)	1 (1%)	19 60
10	J	97/103 (94%)	88 (91%)	8 (8%)	1 (1%)	15 55
11	K	115/129 (89%)	104 (90%)	11 (10%)	0	100 100
12	L	120/123 (98%)	111 (92%)	9 (8%)	0	100 100
13	M	112/118 (95%)	101 (90%)	8 (7%)	3 (3%)	5 31
14	N	98/101 (97%)	91 (93%)	7 (7%)	0	100 100
15	O	86/89 (97%)	80 (93%)	3 (4%)	3 (4%)	3 25
16	P	80/102 (78%)	73 (91%)	6 (8%)	1 (1%)	12 48
17	Q	78/84 (93%)	73 (94%)	5 (6%)	0	100 100
18	R	53/75 (71%)	51 (96%)	1 (2%)	1 (2%)	8 38
19	S	77/92 (84%)	69 (90%)	7 (9%)	1 (1%)	12 48
20	T	84/87 (97%)	83 (99%)	1 (1%)	0	100 100
21	U	54/71 (76%)	53 (98%)	1 (2%)	0	100 100
22	V	69/72 (96%)	47 (68%)	15 (22%)	7 (10%)	0 9
23	W	499/890 (56%)	480 (96%)	17 (3%)	2 (0%)	34 72
24	Y	74/171 (43%)	73 (99%)	1 (1%)	0	100 100
25	Z	89/144 (62%)	76 (85%)	10 (11%)	3 (3%)	3 26
All	All	3072/3845 (80%)	2863 (93%)	182 (6%)	27 (1%)	21 57

5 of 27 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	130	THR
3	C	127	ARG
9	I	25	ASN

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Mol	Chain	Res	Type
10	J	57	VAL
13	M	5	ALA

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	
2	B	186/199 (94%)	180 (97%)	6 (3%)	39	61
3	C	170/190 (90%)	164 (96%)	6 (4%)	36	59
4	D	172/173 (99%)	167 (97%)	5 (3%)	42	64
5	E	118/126 (94%)	112 (95%)	6 (5%)	24	48
6	F	92/112 (82%)	91 (99%)	1 (1%)	73	84
7	G	124/129 (96%)	121 (98%)	3 (2%)	49	69
8	H	104/105 (99%)	100 (96%)	4 (4%)	33	57
9	I	105/107 (98%)	102 (97%)	3 (3%)	42	64
10	J	87/90 (97%)	81 (93%)	6 (7%)	15	40
11	K	90/99 (91%)	89 (99%)	1 (1%)	73	84
12	L	102/102 (100%)	101 (99%)	1 (1%)	76	86
13	M	92/96 (96%)	90 (98%)	2 (2%)	52	71
14	N	83/84 (99%)	82 (99%)	1 (1%)	71	83
15	O	76/77 (99%)	74 (97%)	2 (3%)	46	66
16	P	65/84 (77%)	63 (97%)	2 (3%)	40	62
17	Q	74/78 (95%)	72 (97%)	2 (3%)	44	65
18	R	48/65 (74%)	48 (100%)	0	100	100
19	S	70/79 (89%)	68 (97%)	2 (3%)	42	64
20	T	65/66 (98%)	63 (97%)	2 (3%)	40	62
21	U	48/61 (79%)	45 (94%)	3 (6%)	18	43
22	V	62/63 (98%)	54 (87%)	8 (13%)	4	18
23	W	402/713 (56%)	398 (99%)	4 (1%)	76	86

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
24	Y	66/149 (44%)	61 (92%)	5 (8%)	13 37
25	Z	81/128 (63%)	73 (90%)	8 (10%)	8 26
All	All	2582/3175 (81%)	2499 (97%)	83 (3%)	42 61

5 of 83 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
21	U	56	HIS
24	Y	26	LEU
22	V	23	ARG
22	V	71	LYS
25	Z	108	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 16 such sidechains are listed below:

Mol	Chain	Res	Type
25	Z	92	GLN
24	Y	21	GLN
23	W	426	GLN
23	W	498	ASN
23	W	402	HIS

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	1528/1534 (99%)	257 (16%)	9 (0%)
26	X	76/77 (98%)	24 (31%)	11 (14%)
All	All	1604/1611 (99%)	281 (17%)	20 (1%)

5 of 281 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	5	U
1	A	6	G
1	A	9	G
1	A	22	G
1	A	28	A

5 of 20 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
26	X	23	C
26	X	57	A
26	X	70	G
26	X	58	A
1	A	1024	G

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

16 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	$\#\|Z\| > 2$
1	4OC	A	1402	1	20,23,24	0.78	0	26,32,35	0.95	1 (3%)
1	MA6	A	1519	1	18,26,27	0.93	0	19,38,41	1.44	4 (21%)
26	H2U	X	20	26	18,21,22	0.81	0	21,30,33	1.13	2 (9%)
1	2MG	A	966	1,26	18,26,27	0.86	0	16,38,41	1.27	3 (18%)
12	D2T	L	89	12	7,9,10	1.57	2 (28%)	6,11,13	1.71	2 (33%)
1	G7M	A	527	1	20,26,27	1.17	2 (10%)	17,39,42	1.00	0
26	5MU	X	54	26	19,22,23	1.42	5 (26%)	28,32,35	2.15	7 (25%)
1	MA6	A	1518	1	18,26,27	0.94	1 (5%)	19,38,41	1.16	3 (15%)
1	2MG	A	1516	1	18,26,27	0.79	1 (5%)	16,38,41	1.37	3 (18%)
26	4SU	X	8	26	18,21,22	1.86	5 (27%)	26,30,33	2.53	11 (42%)
1	UR3	A	1498	1	19,22,23	0.96	1 (5%)	26,32,35	1.63	4 (15%)
1	PSU	A	516	1,22	18,21,22	0.94	2 (11%)	22,30,33	1.88	3 (13%)
1	5MC	A	1407	1	18,22,23	1.06	2 (11%)	26,32,35	1.14	2 (7%)
26	PSU	X	55	26	18,21,22	1.33	2 (11%)	22,30,33	2.04	4 (18%)
1	5MC	A	967	1	18,22,23	1.00	1 (5%)	26,32,35	1.12	2 (7%)
1	2MG	A	1207	1	18,26,27	0.85	1 (5%)	16,38,41	1.26	4 (25%)

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
1	4OC	A	1402	1	-	0/9/29/30	0/2/2/2
1	MA6	A	1519	1	-	1/7/29/30	0/3/3/3
26	H2U	X	20	26	-	3/7/38/39	0/2/2/2
1	2MG	A	966	1,26	-	2/5/27/28	0/3/3/3
12	D2T	L	89	12	-	1/7/12/14	-
1	G7M	A	527	1	-	0/3/25/26	0/3/3/3
26	5MU	X	54	26	-	3/7/25/26	0/2/2/2
1	MA6	A	1518	1	-	0/7/29/30	0/3/3/3
1	2MG	A	1516	1	-	0/5/27/28	0/3/3/3
26	4SU	X	8	26	-	3/7/25/26	0/2/2/2
1	UR3	A	1498	1	-	0/7/25/26	0/2/2/2
1	PSU	A	516	1,22	-	0/7/25/26	0/2/2/2
1	5MC	A	1407	1	-	0/7/25/26	0/2/2/2
26	PSU	X	55	26	-	1/7/25/26	0/2/2/2
1	5MC	A	967	1	-	0/7/25/26	0/2/2/2
1	2MG	A	1207	1	-	0/5/27/28	0/3/3/3

The worst 5 of 25 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	X	8	4SU	C4-S4	-4.47	1.59	1.68
26	X	8	4SU	C4-N3	-3.77	1.33	1.37
26	X	55	PSU	C6-C5	3.29	1.39	1.35
1	A	1407	5MC	C6-C5	3.01	1.39	1.34
1	A	967	5MC	C6-C5	2.99	1.39	1.34

The worst 5 of 55 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	X	8	4SU	C4-N3-C2	-6.62	120.91	127.34
1	A	1498	UR3	C4-N3-C2	-5.99	118.92	124.56
26	X	55	PSU	N1-C2-N3	5.91	121.82	115.13
26	X	8	4SU	C5-C4-N3	5.64	119.92	114.69
26	X	54	5MU	C4-N3-C2	-5.19	120.64	127.35

There are no chirality outliers.

5 of 14 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	966	2MG	N1-C2-N2-CM2

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Mol	Chain	Res	Type	Atoms
1	A	966	2MG	N3-C2-N2-CM2
26	X	8	4SU	O4'-C1'-N1-C2
26	X	8	4SU	O4'-C1'-N1-C6
26	X	20	H2U	O4'-C1'-N1-C6

There are no ring outliers.

10 monomers are involved in 51 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	1402	4OC	1	0
1	A	1519	MA6	3	0
26	X	20	H2U	5	0
1	A	966	2MG	21	0
1	A	527	G7M	2	0
26	X	54	5MU	5	0
1	A	1518	MA6	2	0
26	X	8	4SU	12	0
1	A	516	PSU	2	0
26	X	55	PSU	3	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

1 ligand is 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	$\#\|Z\| > 2$
27	FME	X	101	26	8,8,10	0.40	0	7,8,11	0.92	0

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
27	FME	X	101	26	-	0/7/7/11	-

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.

1 monomer is involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
27	X	101	FME	14	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	926:G	O3'	927:G	P	5.84
1	A	1390:U	O3'	1391:U	P	4.62

6 Map visualisation

This section contains visualisations of the EMDB entry EMD-3495. These allow visual inspection of the internal detail of the map and identification of artifacts.

Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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.