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:

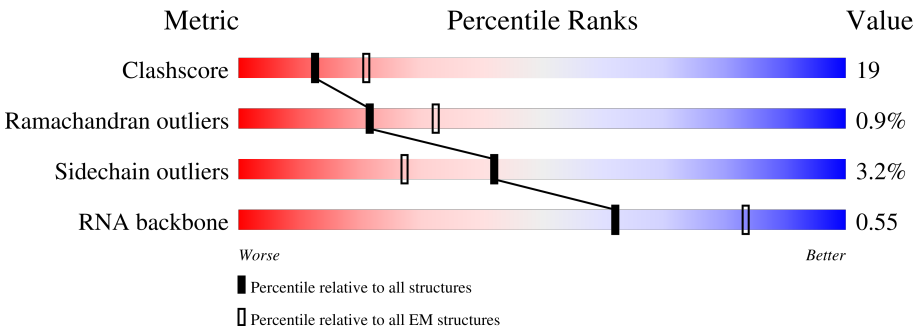
EMDB validation analysis	:	0.0.1.dev92
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	FAILED
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)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

1 Overall quality at a glance (i)

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
			Total	C	N	O	S		
7	G	151	1181	735	227	215	4	0	0

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

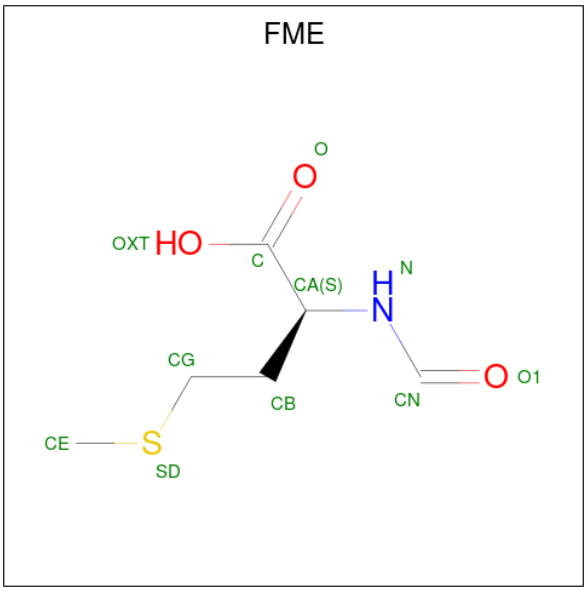
- Molecule 25 is a protein called Translation initiation factor IF-3.

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

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

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

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



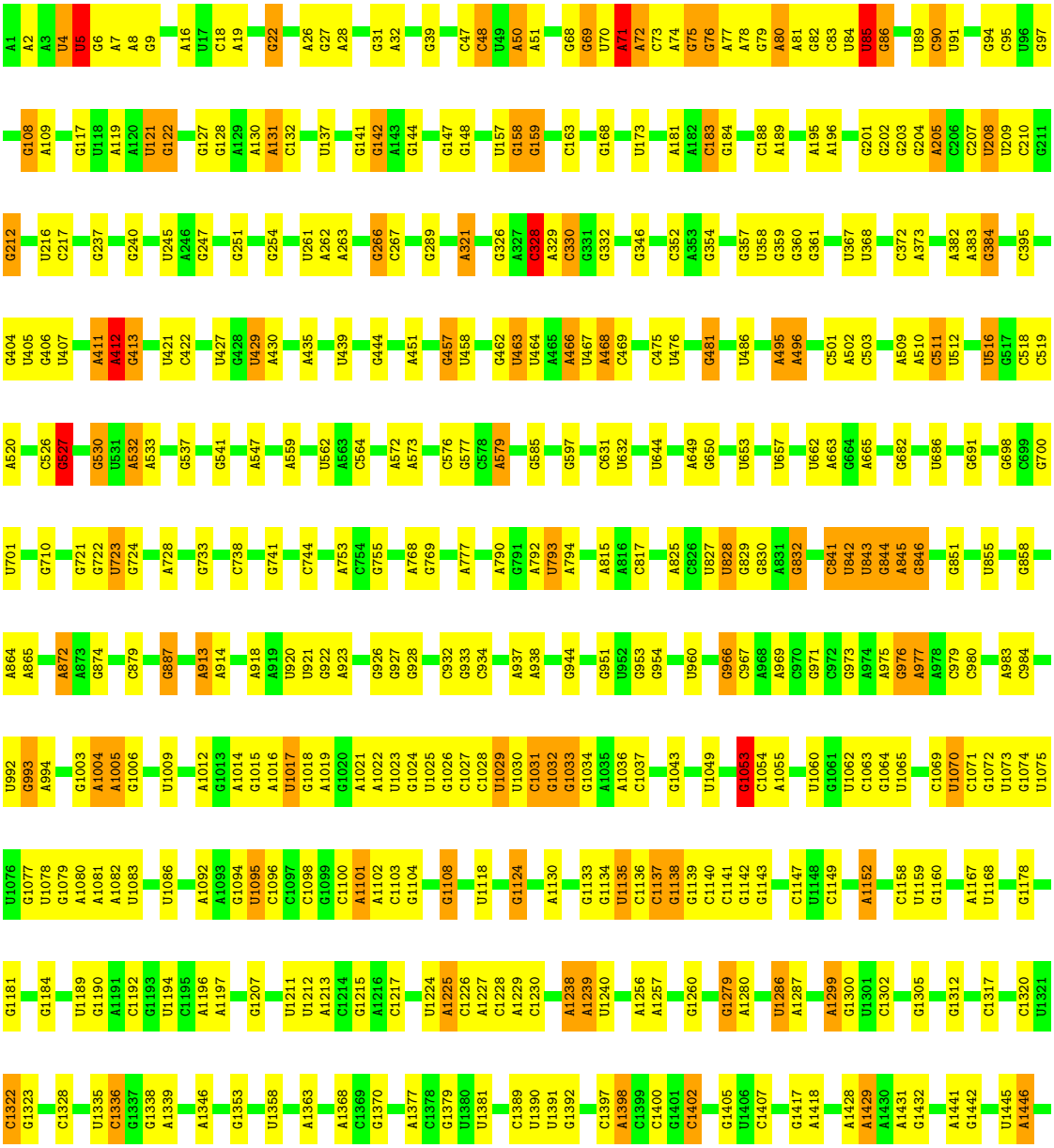
Mol	Chain	Residues	Atoms						AltConf
			Total	C	H	N	O	S	
27	X	1	10	6	1	1	1	1	0

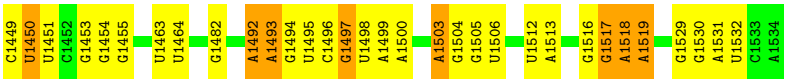
3 Residue-property plots (i)

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: 16S ribosomal RNA

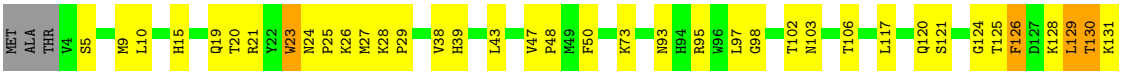
Chain A: 69% 24% 6%

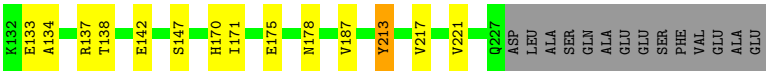




• Molecule 2: 30S ribosomal protein S2

Chain B:



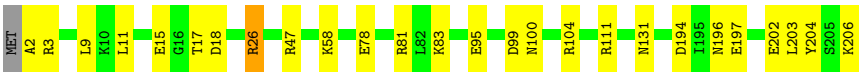


• Molecule 3: 30S ribosomal protein S3

Chain C:

• Molecule 4: 30S ribosomal protein S4

Chain D:

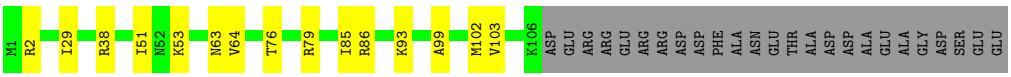


• Molecule 5: 30S ribosomal protein S5

Chain E:

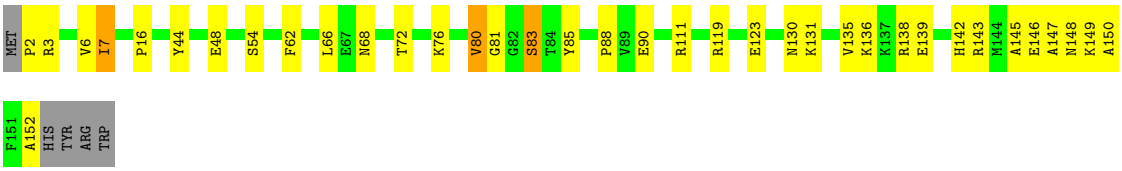
• Molecule 6: 30S ribosomal protein S6

Chain F:



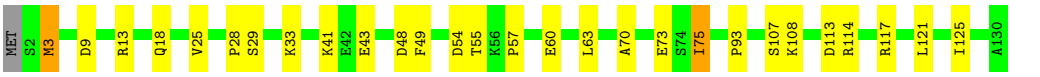
• Molecule 7: 30S ribosomal protein S7

Chain G: 73% 22%



- Molecule 8: 30S ribosomal protein S8

Chain H: 78% 20%

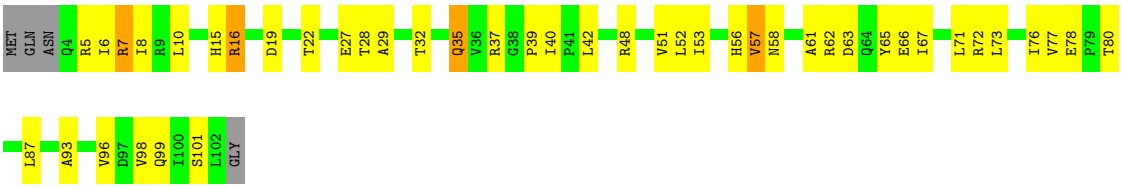


- Molecule 9: 30S ribosomal protein S9

Chain I: 72% 26%

- Molecule 10: 30S ribosomal protein S10

Chain J: 53% 39%

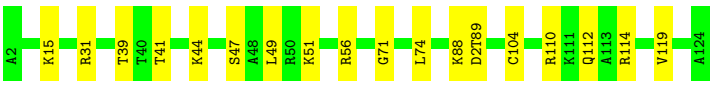


- Molecule 11: 30S ribosomal protein S11

Chain K: 71% 20% 9%

- Molecule 12: 30S ribosomal protein S12

Chain L: 85% 15%

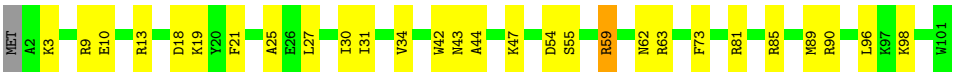


- Molecule 13: 30S ribosomal protein S13

Chain M: 65% 31%

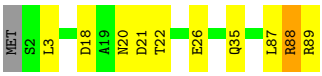
- Molecule 14: 30S ribosomal protein S14

Chain N:



- Molecule 15: 30S ribosomal protein S15

Chain O:

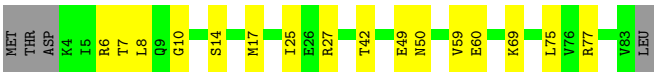


- Molecule 16: 30S ribosomal protein S16

Chain P:

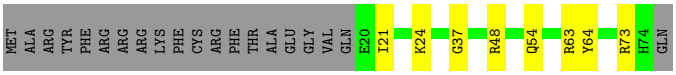
- Molecule 17: 30S ribosomal protein S17

Chain Q:



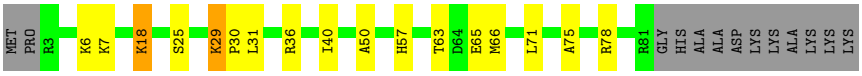
- Molecule 18: 30S ribosomal protein S18

Chain R:



- Molecule 19: 30S ribosomal protein S19

Chain S:



- Molecule 20: 30S ribosomal protein S20

Chain T: 80% 18%

MET A2 M27 M28 R29 I32 K33 E40 K44 A45 M54 I57 V58 D59 K64 K69 R74 H75 K76 A87

• Molecule 21: 30S ribosomal protein S21

Chain U: 61% 17% 21%

MET P2 V3 I4 K5 V6 F12 A15 R18 E31 V32 R33 R34 R35 P41 H56 A57 LYS LYS LEU ALA ARG GLU ASN ALA ARG ARG THR ARG LEU TYR

• Molecule 22: Translation initiation factor IF-1

Chain V: 17% 67% 15%

MET A1 K2 E3 K4 D5 T6 I7 R8 T9 E10 G11 T14 E15 A16 L17 P18 N19 A20 T21 F22 R23 V24 K25 L26 D27 S28 G29 P30 E31 I32 L33 A34 Y35 I36 S37 G38 K39 M40 R41 M42 H43 Y44 I45 R46 I47 L48 P49 G50 D51 R52 V53 V54 V55 E56 I57 T58 P59 Y60

D61 P62 T63 R64 G65 R66 I67 V68 Y69 R70 K71

• Molecule 23: Translation initiation factor IF-2

Chain W: 36% 19% 44%

MET THR ASP VAL THR ILE LYS THR LEU ALA ALA GLU ARG GLN THR SER VAL GLU ARG LEU VAL GLN GLN PHE ALA ASP ALA GLY ILE ARG LYS SER ALA ASP ASP SER VAL SER ALA GLN GLU LYS GLN THR LEU ILE ASP HIS LEU ASN GLN LYS ASN SER GLY PRO ASP LYS LEU THR

LEU GLN ARG LYS THR ARG SER THR LEU ASN ILE PRO GLY THR GLY GLY LYS SER LYS SER VAL GLN ILE GLU VAL ARG LYS LYS ARG THR PHE VAL LYS ARG ASP PRO GLN GLU ALA GLU ARG LEU ALA ALA GLU GLU GLN ALA GLN ARG GLU ALA GLU GLU GLN LYS GLU GLU ALA ARG ARG GLU ALA

GLU GLU SER ALA LYS ARG GLU ALA GLN GLN LYS ALA GLU ARG ARG GLU ALA ALA GLU GLN GLN ALA LYS ARG GLU ALA ALA GLN ALA ALA LYS ARG GLU ALA ALA GLU LYS ASP LYS VAL SER ASN GLN GLN ASP ASP MET THR LYS ASN ALA GLN ALA GLU LYS ALA ARG ARG GLU GLN GLU ALA

ALA GLU LEU LYS ARG LYS ALA GLU GLU GLU ALA ARG ARG LYS LEU GLU GLU GLU ALA ARG ARG VAL ALA GLU GLU ALA ARG ARG MET ALA GLU GLU GLU ASN LYS THR TRP THR ASP ASN ALA GLU PRO THR GLU ASP SER SER ASP TYR HIS VAL THR THR SER GLN HIS ALA ARG GLN GLU ALA

ASP GLU SER ASP ARG GLU VAL GLU GLY GLY ARG GLY ARG GLY ARG ASN ALA LYS ARG PRO LYS LYS GLY ASN LYS HIS ALA GLU SER LYS ALA ASP ARG GLU GLU ALA ALA ARG VAL ALA GLU GLY GLY LYS GLY GLY LYS ARG LYS GLY SER SER LEU GLN GLN GLY PHE GLN

LYS PRO ALA GLN ALA VAL ASN ARG ASP VAL VAL ILE GLY GLU THR ILE THR VAL GLY GLU LEU ALA ASN LYS MET ALA VAL LYS GLY SER GLN VAL ILE LYS ALA MET MET LYS LEU GLY ALA MET ALA THR ILE ASN GLN VAL ILE ASP GLN LEU VAL ALA GLU GLU

MET GLY HIS LYS VAL ILE LEU ARG ARG GLU ASN GLU LEU GLU GLU ALA VAL MET SER ASP ARG D382 A386 A387 E388 P389 R390 A391 P392 V393 V394 T395 I396 H399 V400 D401 H402 G403 K404 L408 T425 Q426 A430 L443 D444 T445 P446 G447 H448 F451 T452 S453 M454

R455 A456 R457 T462 D463 V466 L467 V468 V469 A470 A471 D472 D473 M476 P477 Q478 T479 I480 I483 Q484 H485 V493 V494 V495 A496 V497 N498 A505 D506 P507 K511 S515 I519 L520 W524 G525 G526 E527 F530 V531 H532 V533 S534 A537 G538 T539 G540 I541

D542 E543 L544 L545 L550 A559 V560 R561 A565 S566 G567 A568 V569 D575 K576 G577 R578 G579 P580 V584 L585 V586 R587 E588 G589 T590 L591 H592 L598 R607 A608 N611 E612 L613 G614 A620 G621 P622 S623 I624 P625 L629 A637 V644 E647 A650

R651 L666 A667 N676 M677 F678 K694 D706 K710 V716 I721 G724 G727 I728 T729 E730 T731 T734 L735 A738 V744 G745 F746 N747 V748 R749 A750 D751 A752 S753 V770 I771 Y772 N773 L774 I775 V778 K779 L786 S787 P788 E789 L790 K791 Q792

Q793 I794 I795 G796 L797 A798 E799 V800 F804 K805 I812 A813 G814 C815 M816 R824 V830 V836 I837 Y838 E839 L845 R846 R847 F848 D851 V855 M859 E860 C861 G862 I863 I877 E878 V879 F880 E881 I882 ILE GLU ILE GLN ARG THR ILE ALA

- Molecule 24: Translation initiation factor IF-3

Chain Y: 32% 11% • 56%

SER K3 Q21 L26 G27 I28 R41 N42 L43 D44 A49 V56 C57 R58 I59 M60 D61 Y62 G63 K64 F65 R66 F67 E68 Q69 Q70 K71 K72 E73 K74 E75 K78 LYS GLN LYS VAL ILE ASN VAL LYS GLU VAL ARG LEU SER PRO THR ILE GLU GLU HIS ASP PHE ASN

THR LYS LEU ARG ASN ALA ARG LYS PHE LEU GLU LYS GLY ASP LYS VAL LYS ALA THR ILE ARG PHE LYS GLY ARG ALA ILE THR HIS LYS GLU ILE GLY GLN ARG VAL LEU ASP ARG LEU SER GLU ALA CYS ALA ASP ILE ALA VAL VAL GLU THR ALA PRO LYS MET ASP GLY ARG ASN

MET PHE LEU VAL LEU ALA PRO LYS ASN ASP ASN LYS

- Molecule 25: Translation initiation factor IF-3

Chain Z: 31% 25% 7% • 37%

MET SER LEU ARG GLU ALA LEU GLU LYS ALA GLU GLU ALA GLY VAL ASP LEU VAL GLU ILE SER PRO ASN ALA GLU PRO PRO VAL CYS ARG ILE MET ASP TYR GLY LYS PHE LEU TYR GLU LYS SER LYS SER SER LYS GLU GLN LYS LYS LYS GLN LYS V90 I91 Q92 V93 K94 E95 I96

K97 F98 R99 P100 G101 T102 D103 E104 G105 D106 Y107 Q108 V109 I115 L118 K123 A124 K125 L128 R129 F130 R131 H137 G141 V144 L145 N146 R147 V148 K149 D150 D151 L152 Q153 E154 L155 A156 V157 V158 E159 S160 F161 P162 T163 K164 I165 V173 L174 A175 P176 K177 K178

K179 Q180

- Molecule 26: fMet-tRNA

Chain X: 13% 57% 21% 9%

C1 G2 C3 G4 G5 G6 G7 U8 G9 G10 A11 G12 C13 A14 G15 C16 C17 U17A G18 G19 U20 A21 G22 G23 U24 C25 G26 U27 C28 G29 G30 G31 C32 U33 C34 A35 U36 A37 A38 C39 C40 C41 G42 A46 U47 C48 G49 U50 C51 G52 G53 U54 U55 C56 A57 A58 A59 U60 C61

C62 G63 G64 C65 C66 C67 C68 C69 G70 C71 A72 A73 C74 C75 A76

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 (i)

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 (i)

This section was not generated.

6.2 Central slices (i)

This section was not generated.

6.3 Largest variance slices (i)

This section was not generated.

6.4 Orthogonal standard-deviation projections (False-color) (i)

This section was not generated.

6.5 Orthogonal surface views (i)

This section was not generated.

6.6 Mask visualisation (i)

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

7 Map analysis (i)

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

7.1 Map-value distribution (i)

This section was not generated.

7.2 Volume estimate versus contour level (i)

This section was not generated.

7.3 Rotationally averaged power spectrum (i)

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 (i)

This section was not generated.