wwPDB EM Map/Model Validation Report (i)

Apr 10, 2016 – 01:43 PM BST

PDB ID	:	2OM7
EMDB ID:	:	EMD-1315
Title	:	Structural Basis for Interaction of the Ribosome with the Switch Regions of GTP-bound Elongation Factors
Authors	:	Connell, S.R.; Wilson, D.N.; Rost, M.; Schueler, M.; Giesebrecht, J.; Dabrowski, M.; Mielke, T.; Fucini, P.; Spahn, C.M.T.
Deposited on	:	2007-01-21
Resolution	:	7.30 Å(reported)
Based on PDB ID	:	2j00, 1gix, 2j01, 1FNM, 1YL3,

This is a wwPDB EM Map/Model Validation Report for a publicly released PDB/EMDB entry.
For rigid body fitted models, validation errors reported here could
stem from errors in the original structure(s) used in the fitting.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
http://wwpdb.org/validation/2016/EMValidationReportHelp

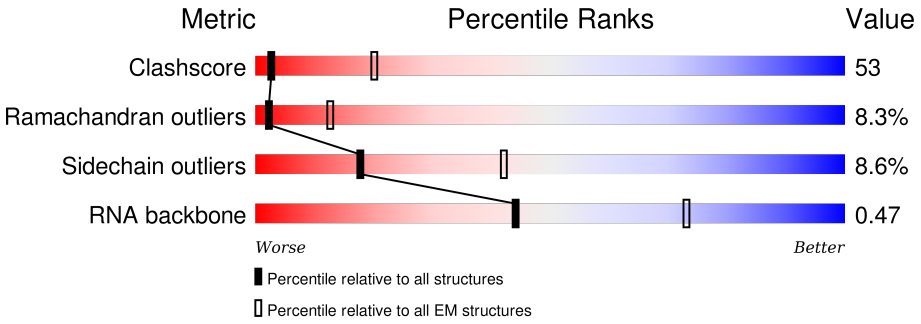
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk27241

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 7.30 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	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686
RNA backbone	3027	244

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. 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	12	33% 67%
2	B	28	7% 25% • 64%
3	C	96	23% 65% 11% •
4	D	303	• • 96%
5	F	29	14% 66% 17% •
6	G	54	35% 44% 20%
7	H	42	43% 38% 19%
8	I	58	• 34% 48% 16%

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Mol	Chain	Length	Quality of chain
9	J	102	16% 29% 26% 28%
10	M	74	5% 30% 42% 23%
11	E	135	33% 45% 13% 7%
12	K	229	38% 31% 13% 17%
13	L	691	48% 42% 5%
14	N	256	21% 54% 15% 8%

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
10	5MC	M	49	-	-	X	-
10	4SU	M	8	-	-	X	-

2 Entry composition

There are 14 unique types of molecules in this entry. The entry contains 19031 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 RNA chain called Fragment of 16S rRNA (h14).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	A	12	256	114	46	84	12	0	0

- Molecule 2 is a RNA chain called Fragment of 16S rRNA (h15).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
2	B	10	214	95	38	71	10	0	0

- Molecule 3 is a RNA chain called Fragment of 16S rRNA (h44).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
3	C	96	2069	919	387	667	96	0	0

- Molecule 4 is a RNA chain called 16S ribosomal RNA (H5).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
4	D	13	278	124	50	91	13	0	0

- Molecule 5 is a RNA chain called Fragment of23S rRNA (H95).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
5	F	29	624	278	116	201	29	0	0

- Molecule 6 is a RNA chain called Fragment of23S rRNA (H68).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
6	G	54	1172	521	228	369	54	0	0

- Molecule 7 is a RNA chain called Fragment of23S rRNA (H89).

Mol	Chain	Residues	Atoms					AltConf	Trace
7	H	42	Total	C	N	O	P	0	0
			898	399	161	296	42		

- Molecule 8 is a RNA chain called Fragment of23S rRNA (H42-44).

Mol	Chain	Residues	Atoms					AltConf	Trace
8	I	58	Total	C	N	O	P	0	0
			1241	554	224	405	58		

- Molecule 9 is a RNA chain called Fragment of23S rRNA (H76).

Mol	Chain	Residues	Atoms					AltConf	Trace
9	J	73	Total	C	N	O	P	0	0
			1569	696	284	516	73		

- Molecule 10 is a RNA chain called p/E-tRNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
10	M	74	Total	C	N	O	P	S	0	0
			1570	702	269	524	74	1		

- Molecule 11 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	E	125	Total	C	N	O	S	0	1
			971	611	196	163	1		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	2	VAL	-	INSERTION	UNP P17293
E	3	ALA	-	INSERTION	UNP P17293
E	4	LEU	-	INSERTION	UNP P17293

- Molecule 12 is a protein called 50S ribosomal protein L1.

Mol	Chain	Residues	Atoms				AltConf	Trace
12	K	191	Total	C	N	O	0	1
			1142	691	221	230		

- Molecule 13 is a protein called Elongation factor G.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	L	655	Total	C	N	O	S	0	0
			5126	3259	874	975	18		

- Molecule 14 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	235	Total	C	N	O	S	0	1
			1901	1213	342	341	5		

3 Residue-property plots (i)

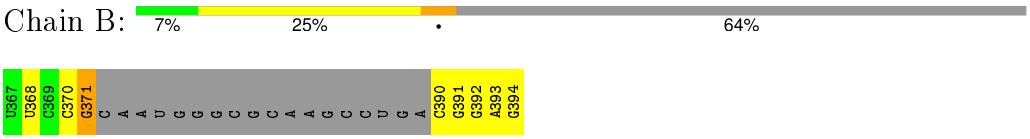
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric 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: Fragment of 16S rRNA (h14)

Chain A:

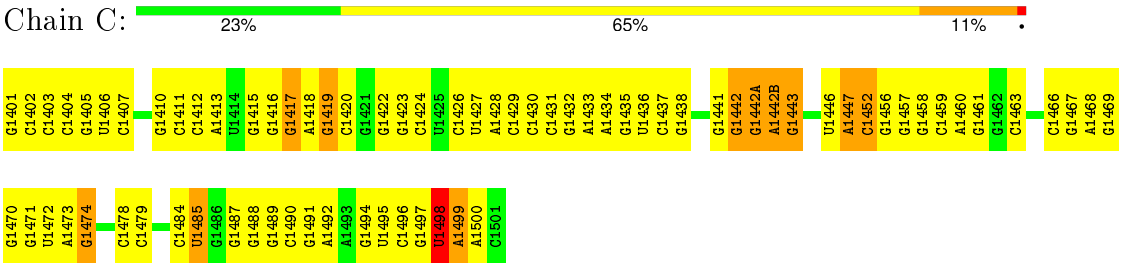
- Molecule 2: Fragment of 16S rRNA (h15)

Chain B:



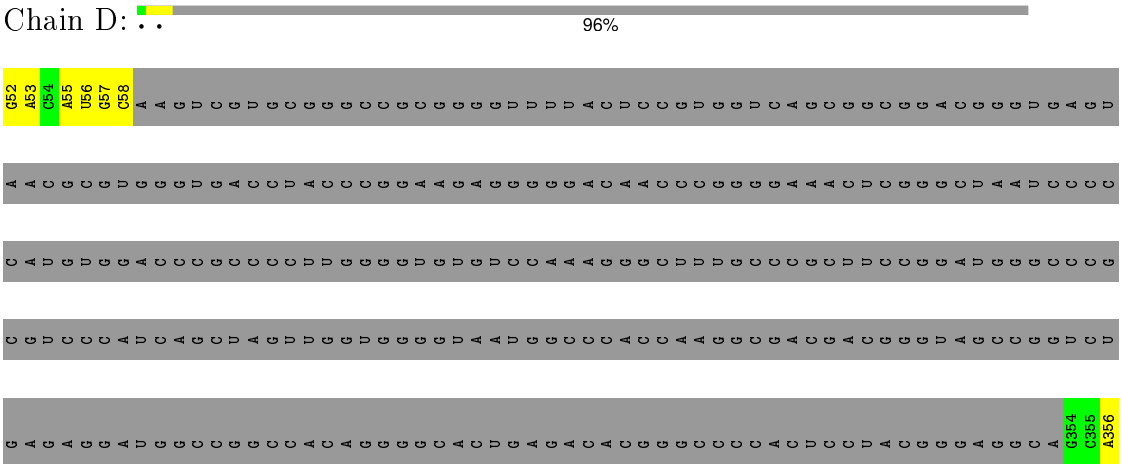
- Molecule 3: Fragment of 16S rRNA (h44)

Chain C:



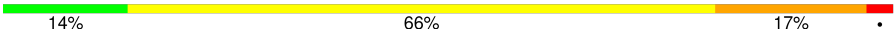
- Molecule 4: 16S ribosomal RNA (H5)

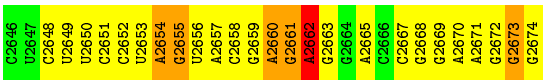
Chain D:



- Molecule 5: Fragment of23S rRNA (H95)

Chain F:





- Molecule 6: Fragment of23S rRNA (H68)

Chain G:

- Molecule 7: Fragment of23S rRNA (H89)

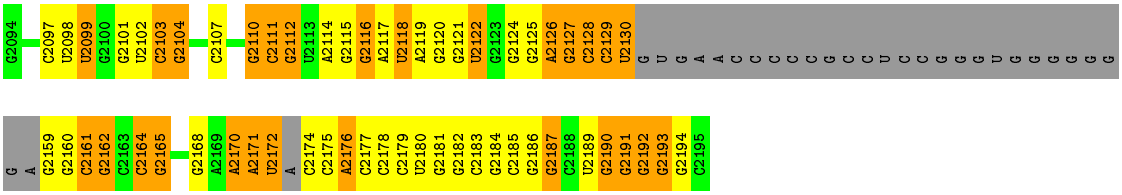
Chain H:

- Molecule 8: Fragment of23S rRNA (H42-44)

Chain I:

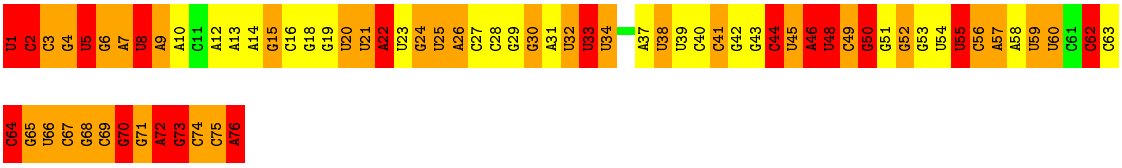
- Molecule 9: Fragment of23S rRNA (H76)

Chain J:



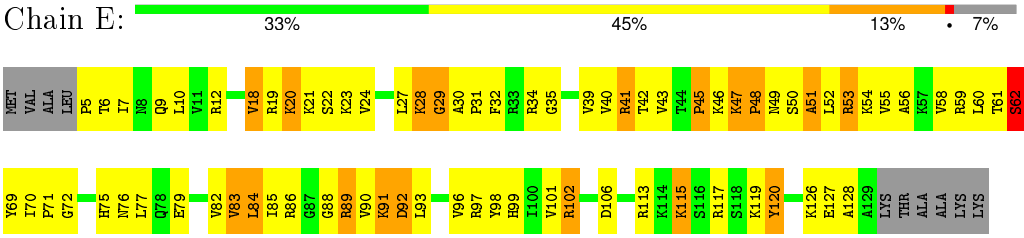
- Molecule 10: p/E-tRNA

Chain M:



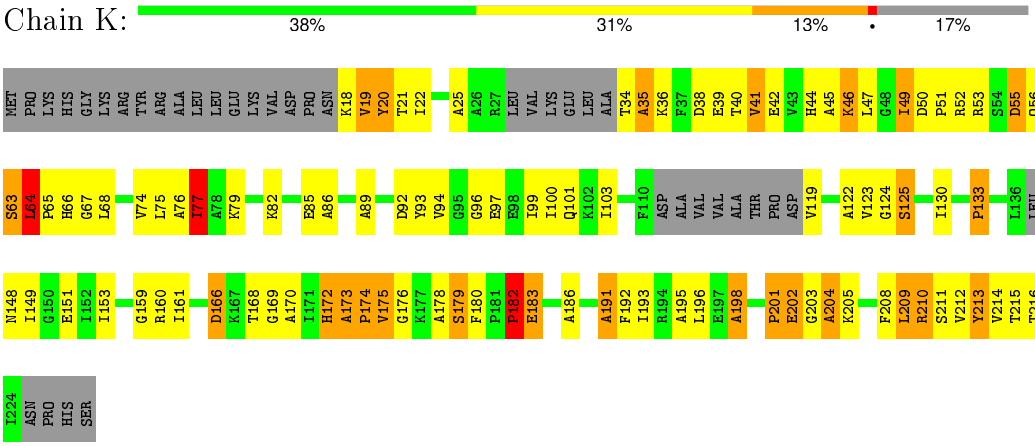
- Molecule 11: 30S ribosomal protein S12

Chain E:



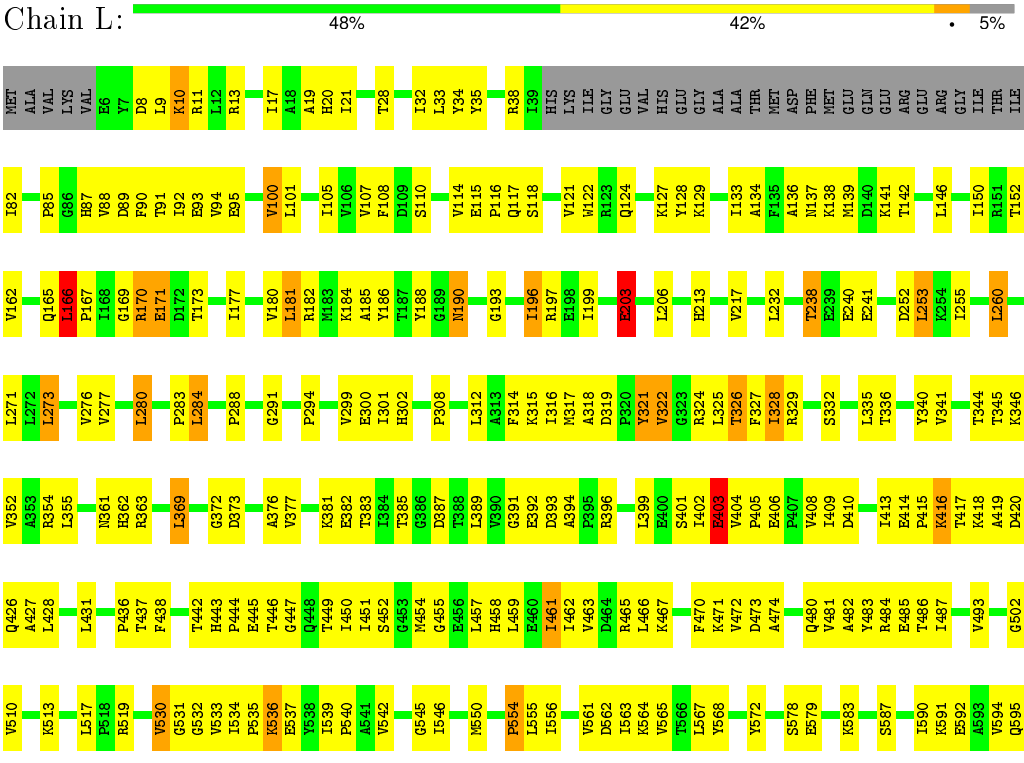
- Molecule 12: 50S ribosomal protein L1

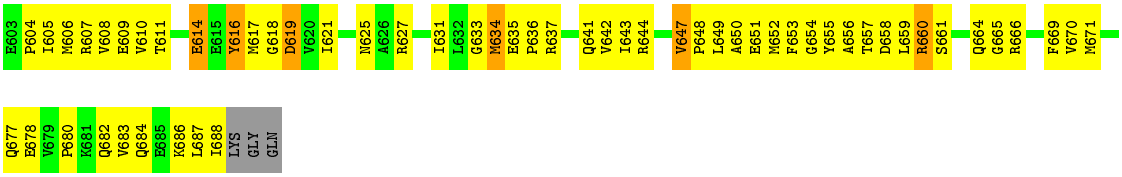
Chain K:



- Molecule 13: Elongation factor G

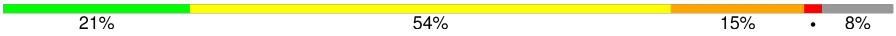
Chain L:

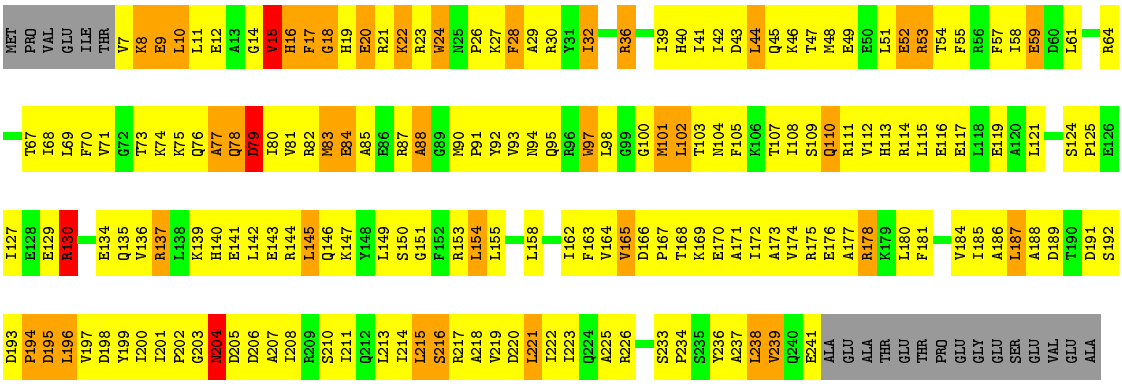




- Molecule 14: 30S ribosomal protein S2

Chain N:





4 Experimental information (i)

Property	Value	Source
Reconstruction method	Not provided	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of images	Not provided	Depositor
Resolution determination method	Not provided	Depositor
CTF correction method	defocus groups	Depositor
Microscope	FEI TECNAI F30	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	19	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	4000	Depositor
Magnification	39000	Depositor
Image detector	Kodak SO163 film	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 5MU, H2U, 4SU, 5MC, PSU

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	#$\|Z\|>2$	RMSZ	#$\|Z\|>2$
1	A	0.72	0/285	0.82	0/442
10	M	2.06	21/1616 (1.3%)	2.88	150/2512 (6.0%)
11	E	0.53	0/987	0.74	0/1322
12	K	0.48	0/1145	0.71	5/1556 (0.3%)
13	L	0.53	0/5219	0.80	6/7063 (0.1%)
14	N	0.48	0/1936	0.66	0/2611
2	B	0.82	0/237	0.84	0/365
3	C	0.88	0/2315	0.89	1/3613 (0.0%)
4	D	0.85	0/309	0.83	0/477
5	F	0.77	0/698	0.87	1/1087 (0.1%)
6	G	0.89	0/1314	0.92	0/2051
7	H	0.78	0/1002	0.88	0/1561
8	I	1.09	2/1388 (0.1%)	1.35	9/2162 (0.4%)
9	J	0.68	0/1753	0.85	1/2735 (0.0%)
All	All	0.90	23/20204 (0.1%)	1.18	173/29557 (0.6%)

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
2	B	0	1
3	C	0	7
5	F	1	0
7	H	0	1
8	I	0	5
9	J	1	0
All	All	2	14

The worst 5 of 23 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	M	33	U	O3'-P	31.01	1.98	1.61
10	M	15	G	O3'-P	23.54	1.89	1.61
10	M	26	A	O3'-P	-23.25	1.33	1.61
10	M	24	G	O3'-P	19.01	1.83	1.61
10	M	56	C	O3'-P	17.65	1.82	1.61

The worst 5 of 173 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	M	25	U	P-O3'-C3'	31.25	157.21	119.70
10	M	75	C	P-O3'-C3'	-29.62	84.16	119.70
10	M	8	4SU	O3'-P-O5'	-27.02	52.65	104.00
8	I	1084	A	O5'-P-OP2	-26.83	78.50	110.70
10	M	24	G	P-O3'-C3'	-24.75	90.00	119.70

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	F	2662	A	C1'
9	J	2191	G	C3'

5 of 14 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	371	G	Sidechain
3	C	1407	C	Sidechain
3	C	1417	G	Sidechain
3	C	1418	A	Sidechain
3	C	1434	A	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	256	0	131	5	0
2	B	214	0	110	24	0
3	C	2069	0	1046	86	0
4	D	278	0	141	28	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	F	624	0	314	85	0
6	G	1172	0	591	46	0
7	H	898	0	456	21	0
8	I	1241	0	625	313	0
9	J	1569	0	790	79	0
10	M	1570	0	800	112	0
11	E	971	0	1057	106	0
12	K	1142	0	865	113	0
13	L	5126	0	5163	628	0
14	N	1901	0	1951	251	0
All	All	19031	0	14040	1734	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 53.

The worst 5 of 1734 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)
4:D:55:A:C2	13:L:322:VAL:HG12	1.22	1.75
13:L:556:ILE:CD1	13:L:601:ILE:HD13	1.28	1.64
13:L:408:VAL:CG1	13:L:669:PHE:HE1	1.12	1.57
5:F:2661:G:N1	13:L:20:HIS:CE1	1.72	1.54
2:B:368:U:C5	13:L:354:ARG:CD	1.92	1.52

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
11	E	123/135 (91%)	83 (68%)	24 (20%)	16 (13%)	0 7
12	K	183/229 (80%)	90 (49%)	50 (27%)	43 (24%)	0 2

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
13	L	645/691 (93%)	583 (90%)	55 (8%)	7 (1%)	17 63
14	N	233/256 (91%)	150 (64%)	51 (22%)	32 (14%)	0 6
All	All	1184/1311 (90%)	906 (76%)	180 (15%)	98 (8%)	2 18

5 of 98 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
11	E	28	LYS
11	E	47	LYS
11	E	91	LYS
11	E	92	ASP
12	K	19	VAL

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
11	E	104/111 (94%)	95 (91%)	9 (9%)	13 45
12	K	61/181 (34%)	54 (88%)	7 (12%)	7 32
13	L	553/582 (95%)	510 (92%)	43 (8%)	16 51
14	N	202/220 (92%)	182 (90%)	20 (10%)	10 39
All	All	920/1094 (84%)	841 (91%)	79 (9%)	18 47

5 of 79 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
13	L	315	LYS
13	L	385	THR
14	N	178	ARG
13	L	321	TYR
13	L	352	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 25 such sidechains are listed below:

Mol	Chain	Res	Type
13	L	475	ASN
13	L	500	GLN
14	N	146	GLN
13	L	480	GLN
13	L	506	GLN

5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	11/12 (91%)	1 (9%)	0
10	M	73/74 (98%)	26 (35%)	2 (2%)
2	B	8/28 (28%)	0	0
3	C	95/96 (98%)	11 (11%)	2 (2%)
4	D	11/303 (3%)	0	0
5	F	28/29 (96%)	7 (25%)	1 (3%)
6	G	53/54 (98%)	12 (22%)	1 (1%)
7	H	41/42 (97%)	8 (19%)	1 (2%)
8	I	57/58 (98%)	34 (59%)	5 (8%)
9	J	72/102 (70%)	29 (40%)	2 (2%)
All	All	449/798 (56%)	128 (28%)	14 (3%)

5 of 128 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	345	C
3	C	1419	G
3	C	1442	G
3	C	1442(A)	G
3	C	1442(B)	A

5 of 14 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
8	I	1083	U
8	I	1085	A
9	J	2191	G
8	I	1069	A
9	J	2126	A

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

6 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	$\#\|Z\| > 2$
10	H2U	M	20	10	17,21,22	0.51	0	23,30,33	0.77	1 (4%)
10	H2U	M	21	10	17,21,22	0.61	0	23,30,33	0.88	1 (4%)
10	5MC	M	49	10	14,22,23	1.17	2 (14%)	17,32,35	1.36	5 (29%)
10	5MU	M	54	10	13,22,23	0.80	0	16,32,35	3.29	4 (25%)
10	PSU	M	55	10	15,21,22	1.66	4 (26%)	16,30,33	3.67	3 (18%)
10	4SU	M	8	10	12,21,22	1.66	2 (16%)	15,30,33	2.32	1 (6%)

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
10	H2U	M	20	10	-	0/7/38/39	0/2/2/2
10	H2U	M	21	10	-	0/7/38/39	0/2/2/2
10	5MC	M	49	10	-	0/3/25/26	0/2/2/2
10	5MU	M	54	10	-	0/3/25/26	0/2/2/2
10	PSU	M	55	10	-	0/7/25/26	0/2/2/2
10	4SU	M	8	10	-	0/3/25/26	0/2/2/2

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	M	55	PSU	C6-C5	-3.03	1.34	1.38
10	M	49	5MC	C6-C5	-2.83	1.32	1.40
10	M	55	PSU	C5-C1'	-2.25	1.50	1.52
10	M	55	PSU	C2'-C1'	-2.10	1.51	1.53
10	M	8	4SU	C6-C5	-2.10	1.33	1.38

The worst 5 of 15 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	M	8	4SU	C5-C4-N3	-8.75	114.28	123.56
10	M	54	5MU	C5-C4-N3	-7.86	118.75	125.35
10	M	55	PSU	C5-C1'-C2'	-2.74	110.78	115.44
10	M	21	H2U	N3-C2-N1	-2.46	114.36	116.64
10	M	20	H2U	N3-C2-N1	-2.38	114.44	116.64

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	M	20	H2U	2	0
10	M	49	5MC	7	0
10	M	54	5MU	2	0
10	M	55	PSU	3	0
10	M	8	4SU	8	0

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

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.