



wwPDB EM Map/Model Validation Report ⓘ

Apr 10, 2016 – 01:47 PM BST

PDB ID : 3J0Q
EMDB ID: : EMD-5329
Title : Core of mammalian 80S pre-ribosome in complex with tRNAs fitted to a 10.6A cryo-em map: rotated PRE state 2
Authors : Budkevich, T.; Giesebrecht, J.; Altman, R.; Munro, J.; Mielke, T.; Nierhaus, K.; Blanchard, S.; Spahn, C.M.
Deposited on : 2011-10-11
Resolution : 10.60 Å(reported)
Based on PDB ID : 2XZM, 3O58

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 : unknown
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

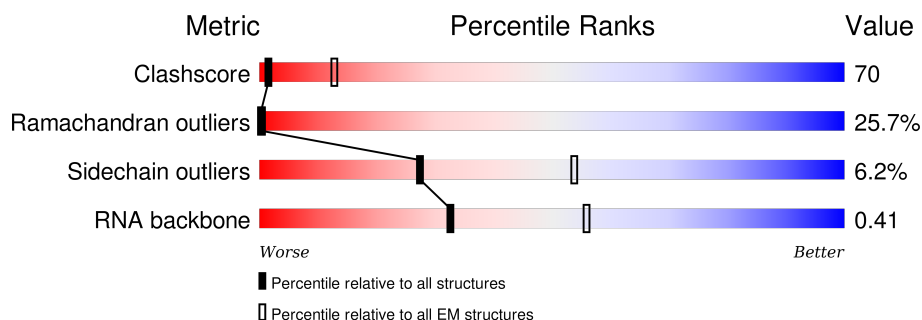
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 10.60 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.



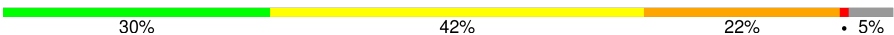
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686
RNA backbone	3027	244

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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	a	48	65% 25% 6% .
2	c	17	71% 29%
3	d	7	71% 14% 14%
4	g	31	71% 23% 6%
5	G	13	38% 46% 15%
6	f	21	76% 24%
7	h	111	88% 11% .
8	S	125	32% 62% 5% .

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Mol	Chain	Length	Quality of chain
9	L	141	
10	X	68	
11	2	112	
12	3	12	
13	9	19	
14	7	50	
15	B	213	
16	J	219	
17	k	165	
18	W	77	
18	Y	77	
19	y	3	
20	w	2	

2 Entry composition [i](#)

There are 20 unique types of molecules in this entry. The entry contains 18327 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 40S ribosomal RNA fragment.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	a	48	Total	C	N	O	P	0	0
			1029	459	190	332	48		

- Molecule 2 is a RNA chain called 40S ribosomal RNA fragment.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	c	17	Total	C	N	O	P	0	0
			362	162	66	117	17		

- Molecule 3 is a RNA chain called 40S ribosomal RNA fragment.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	d	7	Total	C	N	O	P	0	0
			155	69	33	46	7		

- Molecule 4 is a RNA chain called 40S ribosomal RNA fragment.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	g	31	Total	C	N	O	P	0	0
			660	295	118	216	31		

- Molecule 5 is a RNA chain called 40S ribosomal RNA fragment.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	G	13	Total	C	N	O	P	0	0
			276	123	49	91	13		

- Molecule 6 is a RNA chain called 40S ribosomal RNA fragment.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	f	21	Total	C	N	O	P	0	0
			452	200	79	152	21		

- Molecule 7 is a RNA chain called 40S ribosomal RNA fragment.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	h	111	Total	C	N	O	P	0	0
			2368	1060	431	766	111		

- Molecule 8 is a protein called Ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	S	125	Total	C	N	O	S	0	0
			985	632	173	176	4		

- Molecule 9 is a protein called Ribosomal protein S23.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	L	141	Total	C	N	O	S	0	0
			1097	691	221	180	5		

- Molecule 10 is a protein called Ribosomal protein S30.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	X	68	Total	C	N	O	S	0	0
			554	350	113	90	1		

- Molecule 11 is a RNA chain called 60S ribosomal RNA fragment.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	2	112	Total	C	N	O	P	0	0
			2392	1070	435	775	112		

- Molecule 12 is a RNA chain called 60S ribosomal RNA fragment.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	3	12	Total	C	N	O	P	0	0
			259	116	50	81	12		

- Molecule 13 is a RNA chain called 60S ribosomal RNA fragment.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	9	19	Total	C	N	O	P	0	0
			408	183	78	128	19		

- Molecule 14 is a RNA chain called 60S ribosomal RNA fragment.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	7	50	Total	C	N	O	P	0	0
			1054	471	173	360	50		

- Molecule 15 is a protein called Ribosomal protein L10a.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	B	213	Total	C	N	O		0	0
			1055	629	213	213			

- Molecule 16 is a protein called Ribosomal protein L10.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	J	208	Total	C	N	O		0	0
			1027	611	208	208			

- Molecule 17 is a protein called Ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	k	165	Total	C	N	O		0	0
			810	480	165	165			

- Molecule 18 is a RNA chain called tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	Y	77	Total	C	N	O	P	0	0
			1640	732	297	535	76		
18	W	77	Total	C	N	O	P	0	0
			1640	732	297	535	76		

- Molecule 19 is a RNA chain called mRNA fragment.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	y	3	Total	C	N	O	P	0	0
			60	27	7	23	3		

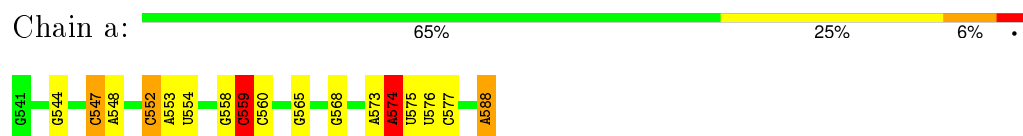
- Molecule 20 is a RNA chain called mRNA fragment.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	w	2	Total	C	N	O	P	0	0
			44	20	10	12	2		

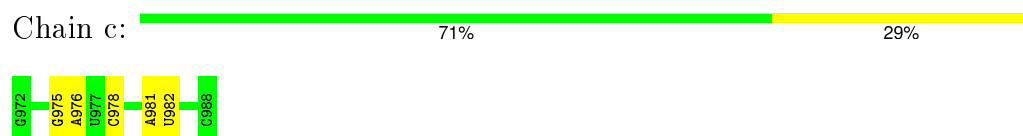
3 Residue-property plots [i](#)

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.

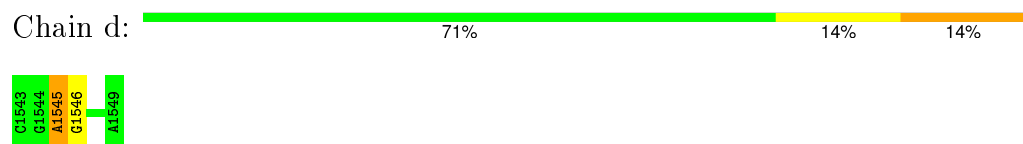
- Molecule 1: 40S ribosomal RNA fragment



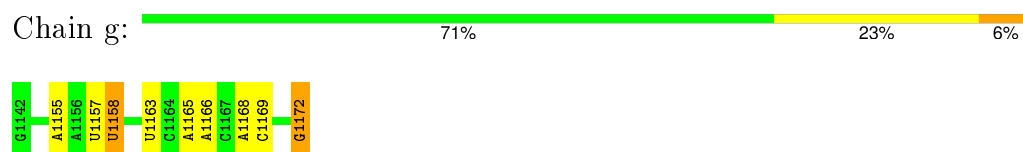
- Molecule 2: 40S ribosomal RNA fragment



- Molecule 3: 40S ribosomal RNA fragment



- Molecule 4: 40S ribosomal RNA fragment

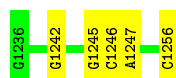


- Molecule 5: 40S ribosomal RNA fragment



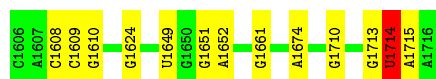
- Molecule 6: 40S ribosomal RNA fragment





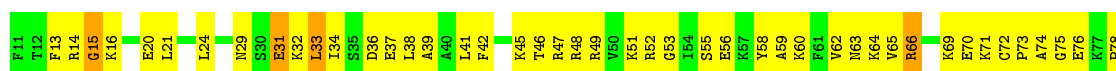
- Molecule 7: 40S ribosomal RNA fragment

Chain h: 88% 11%



- Molecule 8: Ribosomal protein S15

Chain S: 32% 62% 5%



- Molecule 9: Ribosomal protein S23

Chain L: 33% 51% 16%



- Molecule 10: Ribosomal protein S30

Chain X: 41% 51% 7%

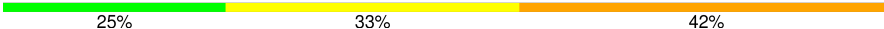


- Molecule 11: 60S ribosomal RNA fragment

Chain 2: 36% 49% 13%



- Molecule 12: 60S ribosomal RNA fragment

Chain 3: 

G2477
C2478
C2479
G2480
G2481
U2482
G2483
A2484
A2485
U2486
U2487
A2488

- Molecule 13: 60S ribosomal RNA fragment

Chain 9: 

U2668
G2669
G2670
A2671
G2672
G2673
A2674
C2675
A2676
G2677
A2678
A2679
A2680
U2681
U2682
U2683
C2684
C2685
A2686

- Molecule 14: 60S ribosomal RNA fragment

Chain 7: 

G2834
C2835
U2836
U2837
G2838
G2839
G2840
G2841
U2842
U2843
C2844
C2845
U2846
A2847
G2848
C2849
G2850
A2851
C2852
A2853
U2854
U2855
G2856
C2857
U2858
P2859
U2860
U2861
U2862
G2863
A2864
U2865
U2866
G2867
U2868
U2869
C2870
G2871
A2872
U2873

- Molecule 15: Ribosomal protein L10a

Chain B: 

I4
T5
H12
E22
T23
K24
K25
R26
N27
V32
V36
K39
N40
Y41
D42
P43
Q44
R45
D46
A2847
G2848
C2849
G2850
A2851
C2852
A2853
U2854
U2855
G2856
C2857
U2858
P2859
U2860
U2861
U2862
G2863
A2864
U2865
U2866
G2867
U2868
U2869
C2870
G2871
A2872
U2873

S104
K105
Y107
M108
A109
A112
V115
L116
I117
V120
P121
R122
L123
L124
G125
P126
Q127
L128
S129
K130
A131
G132
P135
T136
P137
D143
L144
Y145
V146
V148
V151
R152
S153
T154
I155
K156
L158
A159
V167
A168
V169
M174
D177
V178
N181
Q182
S186
V187

M188
F189
V190
V191
S192
L193
L194
K195
M197
V201
G202
S203
L204
V205
V206
K207
S208
S209
M210
G211
P212
A213
L216

- Molecule 16: Ribosomal protein L10

Chain J: 

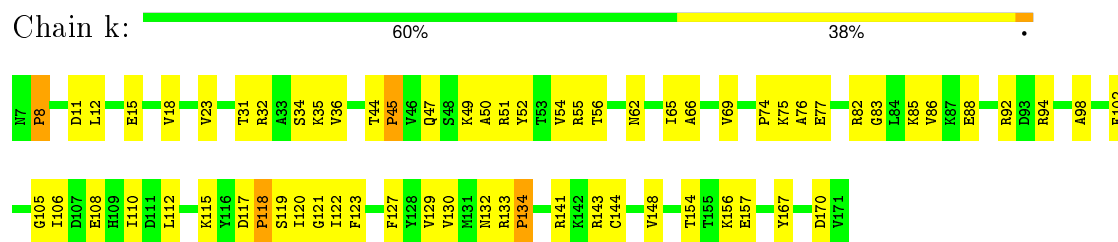
R3
R4
P5
A6
R7
C8
Y9
R10
Y11
Q12
K13
N14
K15
P16
Y17
P18
R19
S20
R21
Y22
M23
R24
A25
V26
P27
D28
S29

C71
A72
M73
K74
Y75
M76
T77
Y78
V79
D83
A84
R85
R86
L87
R88
V89
R90
V91
R92
P93
F94
R95
A96
V97
L97
R98
M99
M100
K101
M102
LEU
SER
CYS
ALA
GLY
ASP
ARG
LEU
GLN
Q113
G114
M115
R116
G117
G120
K121
P122
H123
A126
L127
R128
A129
V130
D131
I131
T135
R136

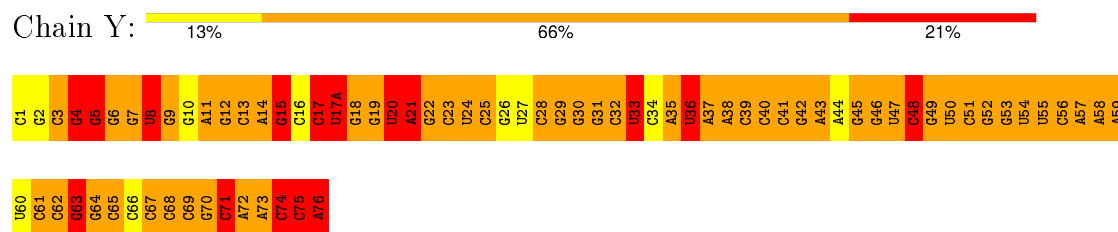
S137
V138
R139
T140
K141
D142
S143
M144
K145
V146
D147
A148
V149
E150
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R152
R153
R154
A155
K158
F159
P160
G161
Q162
Q163
K164
I165
K169
K170
W171
G172
F173
T174
N175
L176
D177
R178
P179
Y181
K184
R185
E186
E189
V190
K191
D192
D193
G194
A195
F196
S201
K202
K203
G204

S205
L206
E207
M208
E212
F213
F214
E215
F216
F217
A218
A219
Q220
A221

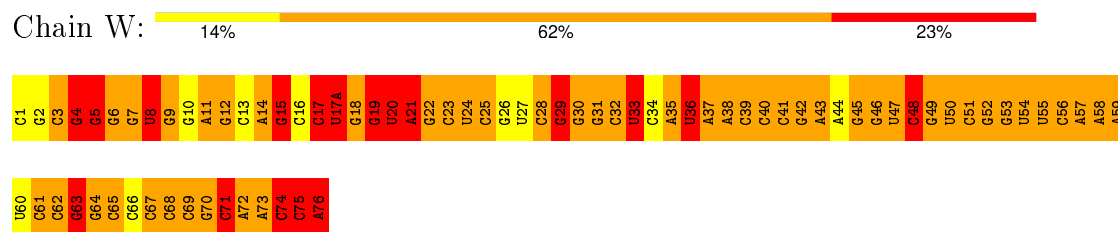
- Molecule 17: Ribosomal protein L11



- Molecule 18: tRNA



- Molecule 18: tRNA



- Molecule 19: mRNA fragment



There are no outlier residues recorded for this chain.

- Molecule 20: mRNA fragment



There are no outlier residues recorded for this chain.

4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of images	23347	Depositor
Resolution determination method	Not provided	Depositor
CTF correction method	CTF CORRECTION OF EACH DEFOCUS GROUP VOLUME PRIOR TO BACK PROJECTION	Depositor
Microscope	FEI POLARA	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	20	Depositor
Minimum defocus (nm)	2000	Depositor
Maximum defocus (nm)	4000	Depositor
Magnification	39000	Depositor
Image detector	KODAK SO163 FILM	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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	0.69	2/1151 (0.2%)	0.99	8/1793 (0.4%)
10	X	0.35	0/566	0.71	0/753
11	2	1.10	4/2677 (0.1%)	1.68	69/4170 (1.7%)
12	3	0.19	0/290	0.43	0/450
13	9	1.04	0/457	2.15	29/710 (4.1%)
14	7	1.07	2/1174 (0.2%)	2.34	33/1825 (1.8%)
15	B	0.34	0/1054	0.63	9/1468 (0.6%)
16	J	0.66	0/1025	0.89	8/1424 (0.6%)
17	k	0.56	0/809	0.86	5/1122 (0.4%)
18	W	2.74	133/1832 (7.3%)	2.54	183/2855 (6.4%)
18	Y	2.74	134/1832 (7.3%)	2.54	181/2855 (6.3%)
19	y	0.41	0/65	0.70	0/98
2	c	0.63	0/404	0.91	1/627 (0.2%)
20	w	0.40	0/49	0.79	0/74
3	d	0.49	0/174	0.84	0/270
4	g	0.60	0/737	0.87	2/1146 (0.2%)
5	G	0.52	0/307	0.82	0/476
6	f	0.58	0/504	0.87	0/785
7	h	0.45	0/2650	0.74	1/4127 (0.0%)
8	S	0.39	0/1003	0.66	1/1342 (0.1%)
9	L	0.43	0/1114	0.74	0/1485
All	All	1.34	275/19874 (1.4%)	1.56	530/29855 (1.8%)

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
1	a	0	3
17	k	0	1
18	W	0	5
18	Y	0	5

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Mol	Chain	#Chirality outliers	#Planarity outliers
3	d	0	1
4	g	0	2
7	h	0	2
All	All	0	19

The worst 5 of 275 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	Y	59	A	N9-C4	-13.26	1.29	1.37
18	W	59	A	N9-C4	-13.23	1.29	1.37
18	Y	2	G	C8-N7	-13.20	1.23	1.30
18	W	2	G	C8-N7	-13.15	1.23	1.30
18	W	40	C	N1-C6	-12.03	1.29	1.37

The worst 5 of 530 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	7	2845	A	N1-C6-N6	39.32	142.19	118.60
14	7	2845	A	C6-N1-C2	38.58	141.75	118.60
14	7	2845	A	C5-C6-N1	-33.94	100.73	117.70
14	7	2845	A	N1-C2-N3	-22.70	117.95	129.30
13	9	2681	U	C2-N1-C1'	14.58	135.19	117.70

There are no chirality outliers.

5 of 19 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	a	547	C	Sidechain
1	a	559	C	Sidechain
1	a	574	A	Sidechain
3	d	1545	A	Sidechain
4	g	1157	U	Sidechain

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of 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	1029	0	521	0	0
2	c	362	0	185	0	0
3	d	155	0	77	0	0
4	g	660	0	335	0	0
5	G	276	0	142	10	0
6	f	452	0	226	0	0
7	h	2368	0	1196	0	0
8	S	985	0	1026	98	0
9	L	1097	0	1169	102	0
10	X	554	0	604	42	0
11	2	2392	0	1208	402	0
12	3	259	0	125	92	0
13	9	408	0	199	109	0
14	7	1054	0	529	186	0
15	B	1055	0	449	125	0
16	J	1027	0	468	105	0
17	k	810	0	353	0	0
18	W	1640	0	825	117	0
18	Y	1640	0	825	146	0
19	y	60	0	31	0	0
20	w	44	0	23	0	0
All	All	18327	0	10516	1371	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 70.

The worst 5 of 1371 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)
12:3:2481:G:O5'	15:B:102:LYS:CB	1.65	1.44
12:3:2484:A:H5'	15:B:122:ARG:C	1.34	1.43
11:2:2253:G:OP1	18:Y:13:C:C4'	1.64	1.43
14:7:2828:G:N1	18:Y:76:A:H1'	1.33	1.39
12:3:2481:G:H8	15:B:102:LYS:CB	1.34	1.39

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	
8	S	123/125 (98%)	90 (73%)	25 (20%)	8 (6%)	1	25
9	L	139/141 (99%)	106 (76%)	18 (13%)	15 (11%)	0	11
10	X	66/68 (97%)	48 (73%)	12 (18%)	6 (9%)	1	17
15	B	211/213 (99%)	76 (36%)	67 (32%)	68 (32%)	0	0
16	J	204/219 (93%)	80 (39%)	52 (26%)	72 (35%)	0	0
17	k	163/165 (99%)	57 (35%)	42 (26%)	64 (39%)	0	0
All	All	906/931 (97%)	457 (50%)	216 (24%)	233 (26%)	0	1

5 of 233 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
8	S	15	GLY
9	L	45	ALA
9	L	62	GLN
9	L	87	PRO
9	L	88	MET

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	
8	S	105/105 (100%)	101 (96%)	4 (4%)	40	73
9	L	113/113 (100%)	102 (90%)	11 (10%)	10	40
10	X	57/57 (100%)	55 (96%)	2 (4%)	43	74

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	275/275 (100%)	258 (94%)	17 (6%)	27 60

5 of 17 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
9	L	55	LYS
9	L	69	LYS
9	L	106	LEU
9	L	33	LEU
9	L	132	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 7 such sidechains are listed below:

Mol	Chain	Res	Type
9	L	62	GLN
10	X	42	ASN
9	L	78	ASN
8	S	84	HIS
9	L	98	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	a	47/48 (97%)	15 (31%)	0
11	2	111/112 (99%)	54 (48%)	9 (8%)
12	3	11/12 (91%)	6 (54%)	1 (9%)
13	9	18/19 (94%)	13 (72%)	1 (5%)
14	7	49/50 (98%)	29 (59%)	5 (10%)
18	W	76/77 (98%)	17 (22%)	0
18	Y	76/77 (98%)	17 (22%)	0
19	y	2/3 (66%)	0	0
2	c	16/17 (94%)	4 (25%)	0
20	w	1/2 (50%)	0	0
3	d	6/7 (85%)	2 (33%)	0
4	g	30/31 (96%)	8 (26%)	0
5	G	12/13 (92%)	2 (16%)	1 (8%)
6	f	20/21 (95%)	5 (25%)	0
7	h	110/111 (99%)	12 (10%)	0
All	All	585/600 (97%)	184 (31%)	17 (2%)

5 of 184 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	a	544	G
1	a	547	C
1	a	548	A
1	a	552	C
1	a	553	A

5 of 17 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
11	2	2281	A
11	2	2290	C
14	7	2850	G
11	2	2280	A
14	7	2851	A

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

There are no non-standard protein/DNA/RNA residues in this entry.

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.