



wwPDB/EMDataBank EM Map/Model Validation Summary Report ⓘ

Feb 19, 2018 – 07:57 am GMT

PDB ID : 4D5L
EMDB ID: : EMD-2810
Title : Cryo-EM structures of ribosomal 80S complexes with termination factors and cricket paralysis virus IRES reveal the IRES in the translocated state
Authors : Muhs, M.; Hilal, T.; Mielke, T.; Skabkin, M.A.; Sanbonmatsu, K.Y.; Pestova, T.V.; Spahn, C.M.T.
Deposited on : 2014-11-05
Resolution : 9.00 Å(reported)
Based on PDB ID : 4CXC

This is a wwPDB/EMDataBank EM Map/Model Validation Summary Report
for a publicly released PDB/EMDB 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 ⓘ symbol.

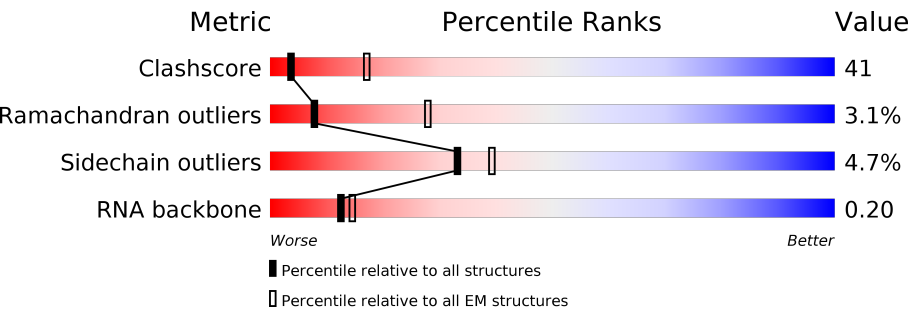
MolProbity : 4.02b-467
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : trunk30686

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 9.00 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.














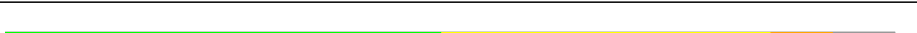


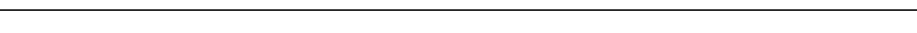




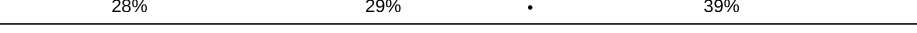





Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	136279	1886
Ramachandran outliers	132675	1663
Sidechain outliers	132484	1531
RNA backbone	3744	458

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	1	1869	6% 38% 47% • 7%
2	A	295	42% 31% • 26%
3	B	264	33% 41% 6% • 19%
4	C	293	49% 23% • 24%
5	D	243	52% 34% • 13%
6	E	263	54% 40% • •
7	F	204	49% 38% 6% 8%
8	G	249	51% 39% • 7%

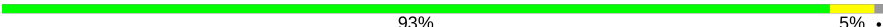
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Mol	Chain	Length	Quality of chain
9	H	194	
10	I	208	
11	J	194	
12	K	165	
13	L	158	
14	M	132	
15	N	151	
16	O	151	
17	P	145	
18	Q	146	
19	R	135	
20	S	152	
21	T	145	
22	U	119	
23	V	83	
24	W	130	
25	X	142	
26	Y	133	
27	Z	125	
28	a	115	
29	b	84	
30	c	69	
31	d	56	
32	e	59	
33	f	156	

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Mol	Chain	Length	Quality of chain
34	g	317	 93%5% •

2 Entry composition

There are 34 unique types of molecules in this entry. The entry contains 75320 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 18S RRNA 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	1	1742	Total	C	N	O	P	0	0
			37159	16589	6665	12164	1741		

- Molecule 2 is a protein called 40S RIBOSOMAL PROTEIN ES26.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A	218	Total	C	N	O	S	0	0
			1719	1091	301	319	8		

- Molecule 3 is a protein called 40S RIBOSOMAL PROTEIN ES27.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	B	213	Total	C	N	O	S	0	0
			1729	1098	309	308	14		

- Molecule 4 is a protein called 40S RIBOSOMAL PROTEIN ES28.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	C	222	Total	C	N	O	S	0	0
			1724	1114	296	304	10		

- Molecule 5 is a protein called 40S RIBOSOMAL PROTEIN US14.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	D	212	Total	C	N	O	S	0	0
			1646	1050	299	290	7		

- Molecule 6 is a protein called 40S RIBOSOMAL PROTEIN ES30.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	E	257	Total	C	N	O	S	0	0
			2031	1298	381	344	8		

- Molecule 7 is a protein called 40S RIBOSOMAL PROTEIN ES31.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	F	188	Total	C	N	O	S	0	0
			1486	930	283	266	7		

- Molecule 8 is a protein called 40S RIBOSOMAL PROTEIN RACK1.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	G	232	Total	C	N	O	S	0	0
			1884	1176	379	322	7		

- Molecule 9 is a protein called 40S RIBOSOMAL PROTEIN ES7.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	H	191	Total	C	N	O	S	0	0
			1535	978	282	274	1		

- Molecule 10 is a protein called 40S RIBOSOMAL PROTEIN ES8.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	I	207	Total	C	N	O	S	0	0
			1695	1064	334	292	5		

- Molecule 11 is a protein called 40S RIBOSOMAL PROTEIN US4.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	J	179	Total	C	N	O	S	0	0
			1495	953	299	241	2		

- Molecule 12 is a protein called 40S RIBOSOMAL PROTEIN ES10.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	K	94	Total	C	N	O	S	0	0
			791	519	138	129	5		

- Molecule 13 is a protein called 40S RIBOSOMAL PROTEIN US17.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	L	146	Total	C	N	O	S	0	0
			1199	764	224	205	6		

- Molecule 14 is a protein called 40S RIBOSOMAL PROTEIN ES12.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	M	120	Total	C	N	O	S	0	0
			931	584	164	174	9		

- Molecule 15 is a protein called 40S RIBOSOMAL PROTEIN US15.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	N	150	Total	C	N	O	S	0	0
			1207	773	229	204	1		

- Molecule 16 is a protein called 40S RIBOSOMAL PROTEIN US11.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	O	137	Total	C	N	O	S	0	0
			1023	627	200	190	6		

- Molecule 17 is a protein called 40S RIBOSOMAL PROTEIN US19.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	P	118	Total	C	N	O	S	0	0
			981	625	183	166	7		

- Molecule 18 is a protein called 40S RIBOSOMAL PROTEIN US9.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	Q	139	Total	C	N	O	S	0	0
			1108	704	210	191	3		

- Molecule 19 is a protein called 40S RIBOSOMAL PROTEIN ES17.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	R	109	Total	C	N	O	S	0	0
			893	561	170	159	3		

- Molecule 20 is a protein called 40S RIBOSOMAL PROTEIN US13.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	S	142	Total	C	N	O	S	0	0
			1172	736	236	199	1		

- Molecule 21 is a protein called 40S RIBOSOMAL PROTEIN ES19.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	T	143	Total	C	N	O	S	0	0
			1112	697	214	198	3		

- Molecule 22 is a protein called 40S RIBOSOMAL PROTEIN US10.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	U	101	Total	C	N	O	S	0	0
			803	502	153	144	4		

- Molecule 23 is a protein called 40S RIBOSOMAL PROTEIN ES21.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	V	83	Total	C	N	O	S	0	0
			636	393	117	121	5		

- Molecule 24 is a protein called 40S RIBOSOMAL PROTEIN US8.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	W	129	Total	C	N	O	S	0	0
			1033	659	193	175	6		

- Molecule 25 is a protein called 40S RIBOSOMAL PROTEIN US12.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	X	134	Total	C	N	O	S	0	0
			1046	663	205	176	2		

- Molecule 26 is a protein called 40S RIBOSOMAL PROTEIN ES24.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	Y	122	Total	C	N	O	S	0	0
			1002	635	196	166	5		

- Molecule 27 is a protein called 40S RIBOSOMAL PROTEIN ES25.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	Z	76	Total	C	N	O	S	0	0
			605	387	112	105	1		

- Molecule 28 is a protein called 40S RIBOSOMAL PROTEIN US2.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	a	96	Total	C	N	O	S	0	0
			767	476	159	127	5		

- Molecule 29 is a protein called 40S RIBOSOMAL PROTEIN ES1.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	b	80	Total	C	N	O	S	0	0
			625	391	116	111	7		

- Molecule 30 is a protein called 40S RIBOSOMAL PROTEIN US5.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	c	62	Total	C	N	O	S	0	0
			490	298	99	91	2		

- Molecule 31 is a protein called 40S RIBOSOMAL PROTEIN US3.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	d	53	Total	C	N	O	S	0	0
			444	278	90	71	5		

- Molecule 32 is a protein called 40S RIBOSOMAL PROTEIN ES4.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	e	51	Total	C	N	O	S	0	0
			412	258	90	63	1		

- Molecule 33 is a protein called 40S RIBOSOMAL PROTEIN US7.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	f	61	Total	C	N	O	S	0	0
			497	312	94	84	7		

- Molecule 34 is a protein called 40S RIBOSOMAL PROTEIN ES6.

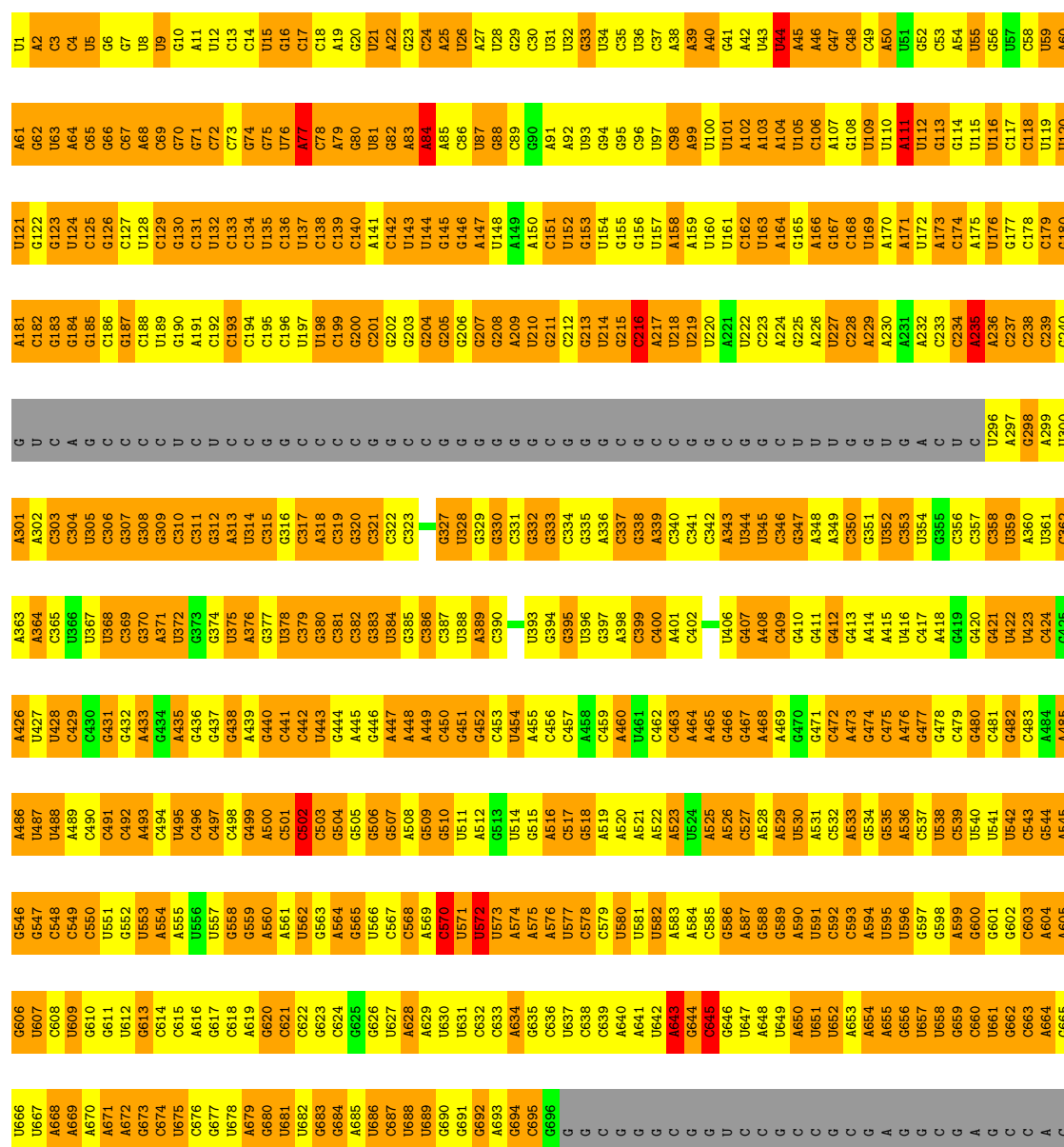
Mol	Chain	Residues	Atoms					AltConf	Trace
34	g	314	Total	C	N	O	S	0	0
			2440	1537	425	466	12		

3 Residue-property plots

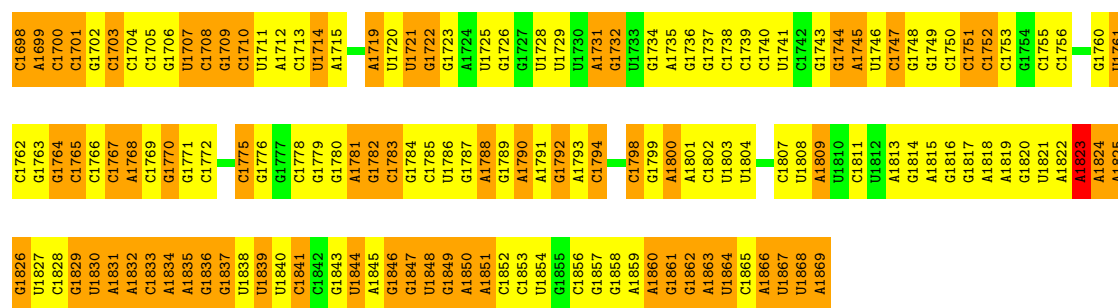
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according 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: 18S RRNA 2

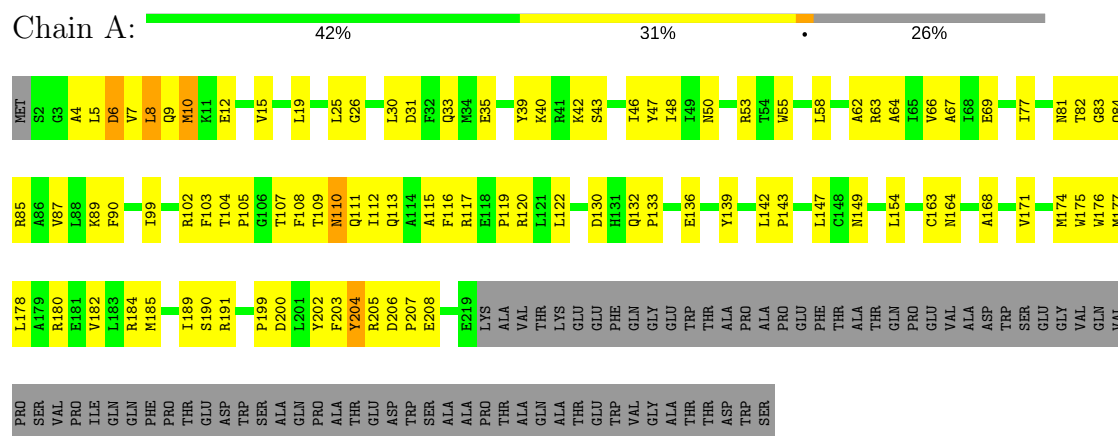
Chain 1: 



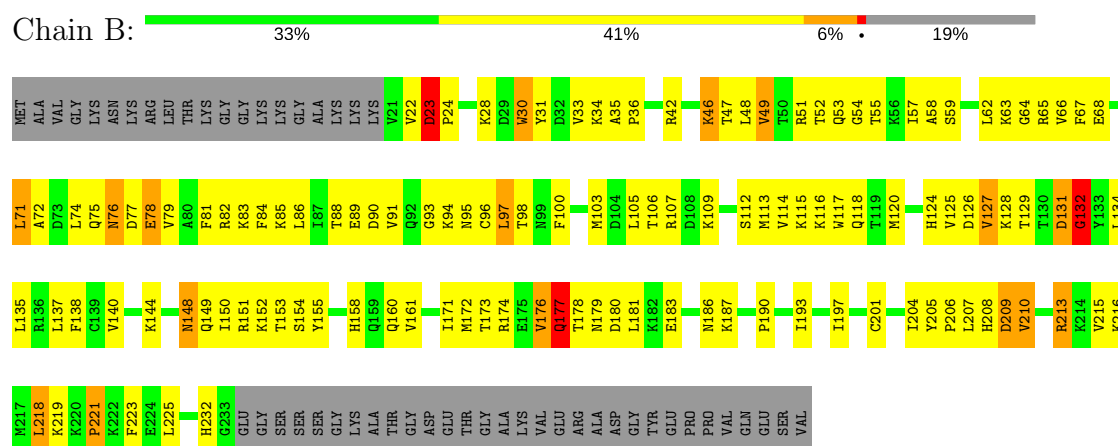


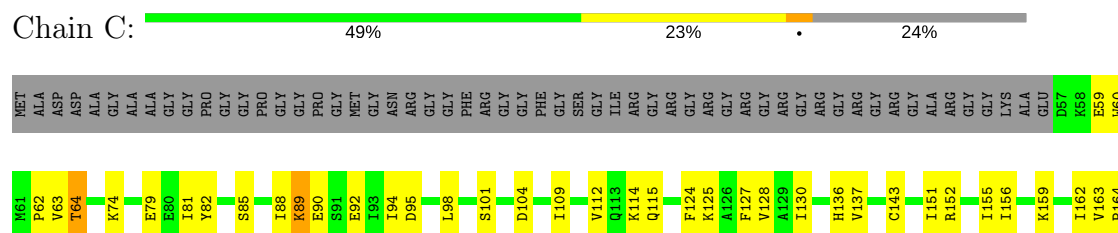
• Molecule 2: 40S RIBOSOMAL PROTEIN ES26

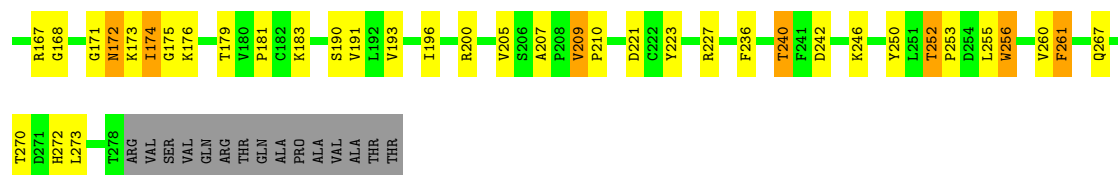


• Molecule 3: 40S RIBOSOMAL PROTEIN ES27



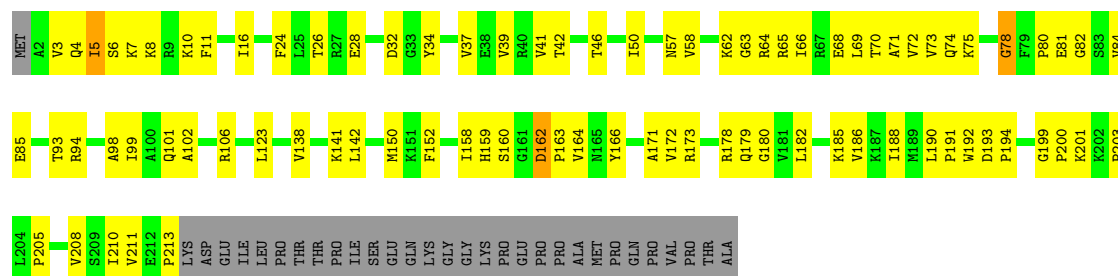
• Molecule 4: 40S RIBOSOMAL PROTEIN ES28





• Molecule 5: 40S RIBOSOMAL PROTEIN US14

Chain D: 52% 34% 13%



• Molecule 6: 40S RIBOSOMAL PROTEIN ES30

Chain E: 54% 40%



• Molecule 7: 40S RIBOSOMAL PROTEIN ES31

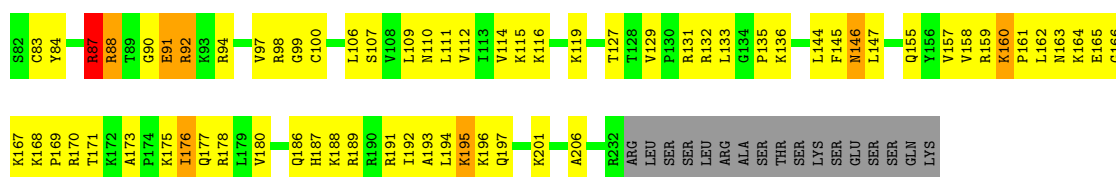
Chain F: 49% 38% 6% 8%



• Molecule 8: 40S RIBOSOMAL PROTEIN RACK1

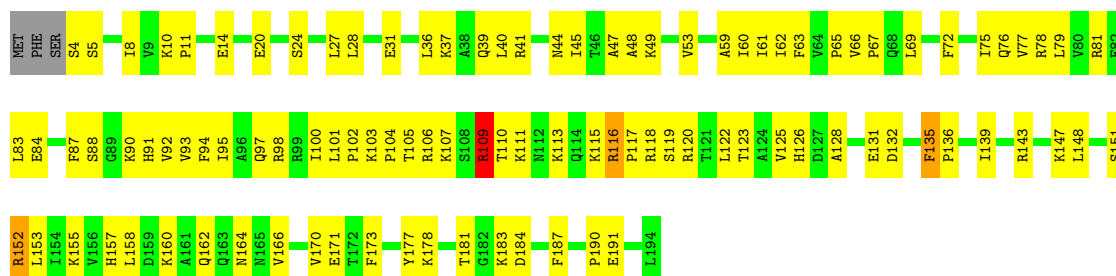
Chain G: 51% 39% 7%





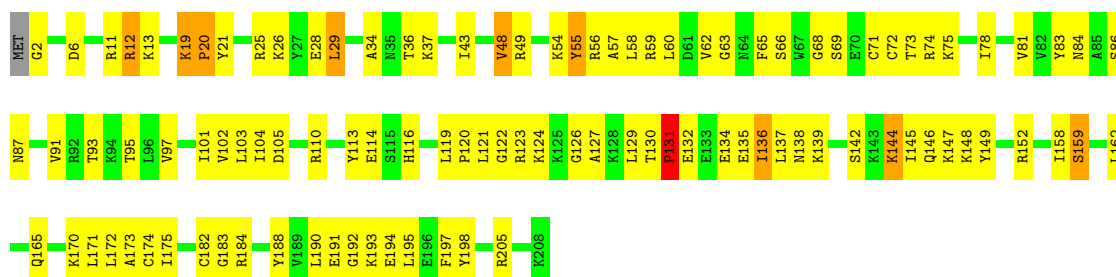
• Molecule 9: 40S RIBOSOMAL PROTEIN ES7

Chain H:  46% 51% ...



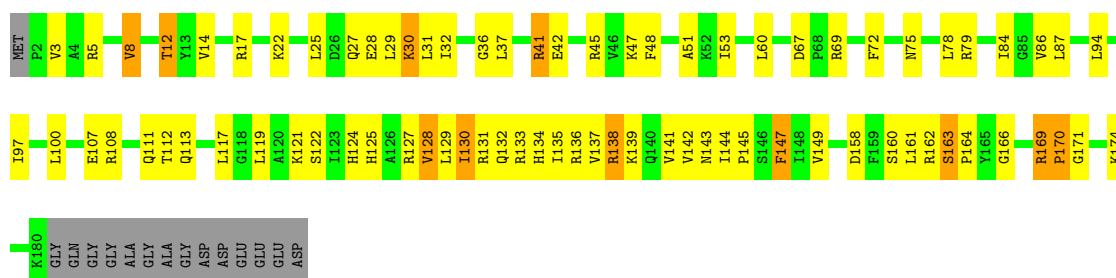
- Molecule 10: 40S RIBOSOMAL PROTEIN ES8

Chain I:  50% 45% .

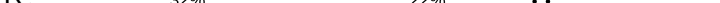


• Molecule 11: 40S RIBOSOMAL PROTEIN US4

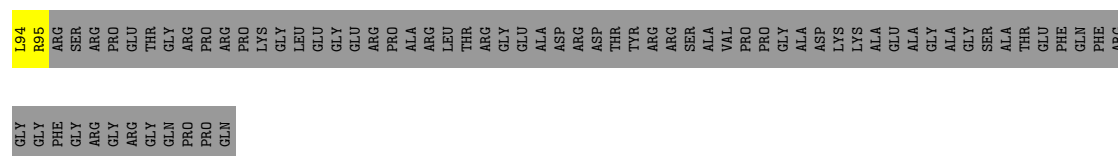
Chain J: 52% 35% 6% 8%



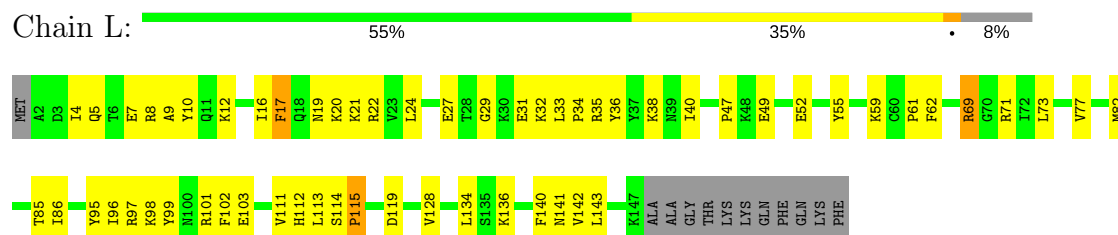
- Molecule 12: 40S RIBOSOMAL PROTEIN ES10

Chain K:  32% 22% .. 43%

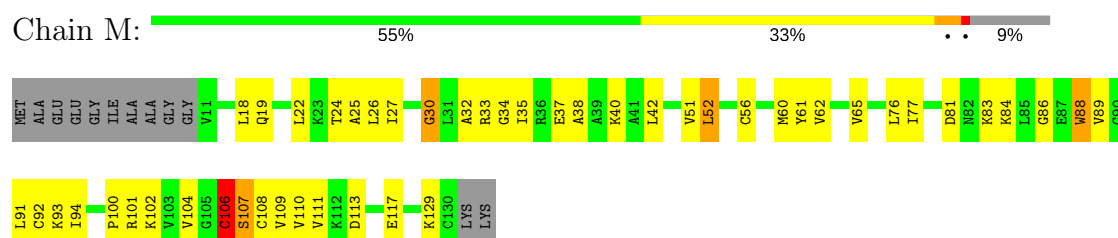




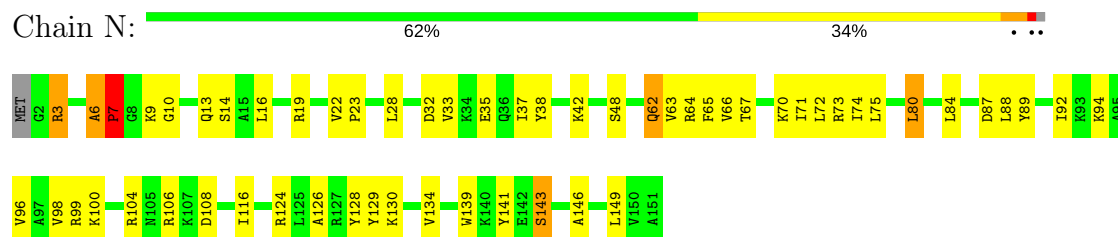
• Molecule 13: 40S RIBOSOMAL PROTEIN US17



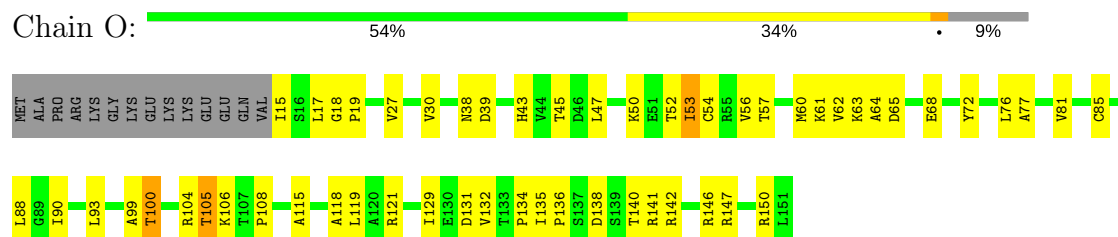
• Molecule 14: 40S RIBOSOMAL PROTEIN ES12



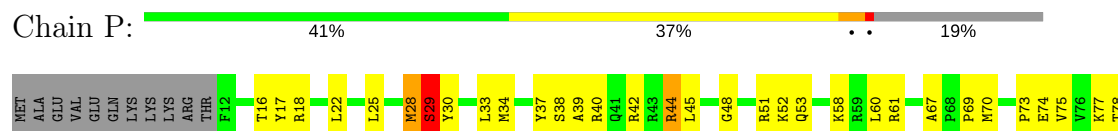
• Molecule 15: 40S RIBOSOMAL PROTEIN US15



• Molecule 16: 40S RIBOSOMAL PROTEIN US11



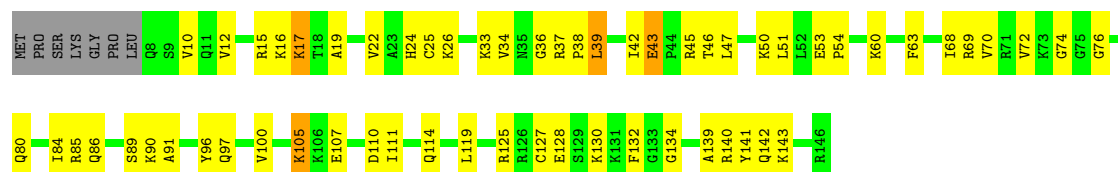
• Molecule 17: 40S RIBOSOMAL PROTEIN US19





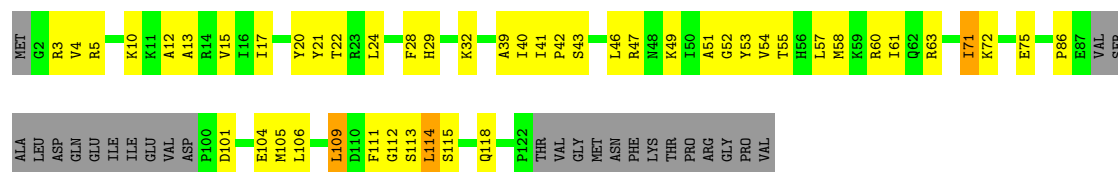
• Molecule 18: 40S RIBOSOMAL PROTEIN US9

Chain Q: 54% 38% 5%



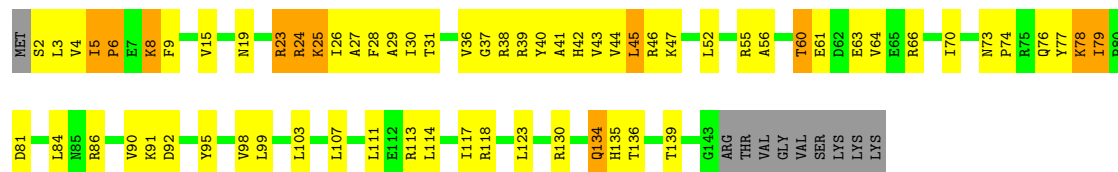
• Molecule 19: 40S RIBOSOMAL PROTEIN ES17

Chain R: 45% 33% 19%



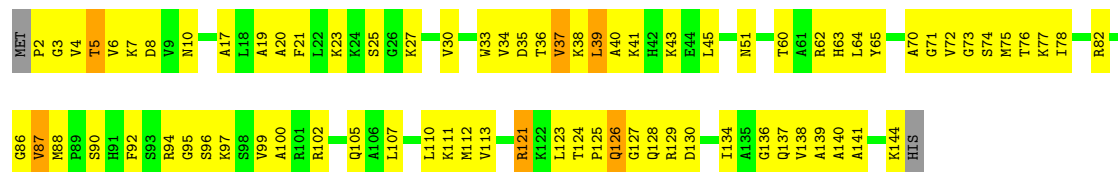
• Molecule 20: 40S RIBOSOMAL PROTEIN US13

Chain S: 49% 37% 7% 7%



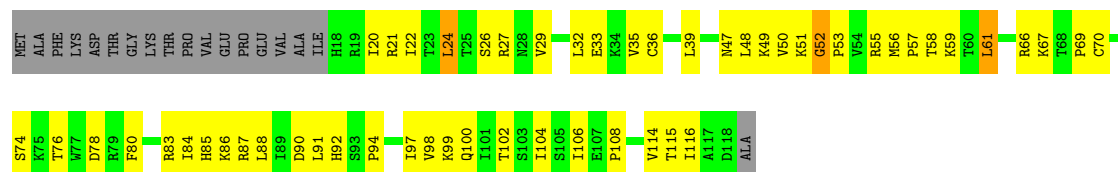
• Molecule 21: 40S RIBOSOMAL PROTEIN ES19

Chain T: 45% 50% 2%



• Molecule 22: 40S RIBOSOMAL PROTEIN US10

Chain U: 39% 43% 15%



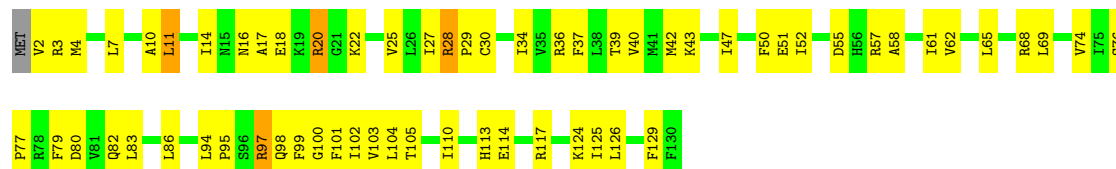
• Molecule 23: 40S RIBOSOMAL PROTEIN ES21

Chain V:  61% 37%



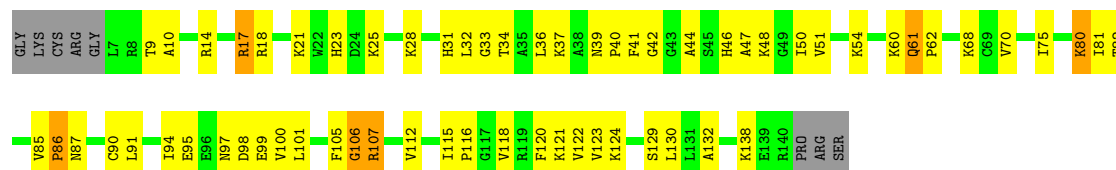
- Molecule 24: 40S RIBOSOMAL PROTEIN US8

Chain W:  51% 45% .



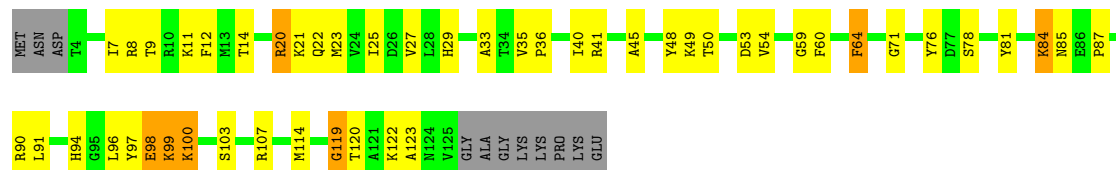
• Molecule 25: 40S RIBOSOMAL PROTEIN US12

Chain X:  50% 40% 6%




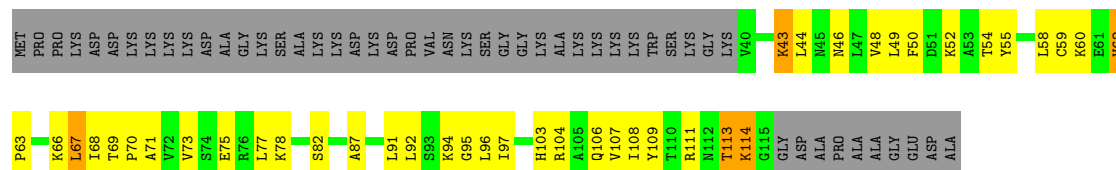
• Molecule 26: 40S RIBOSOMAL PROTEIN ES24

Chain Y: 



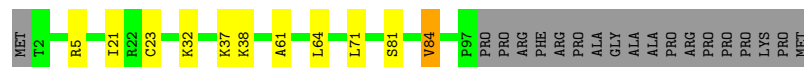
● Molecule 27: 40S RIBOSOMAL PROTEIN ES25

Chain Z:  28% 29% . 42%



● Molecule 28: 40S RIBOSOMAL PROTEIN US2

Chain a:  74% 9% • 17%




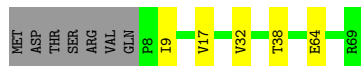
- Molecule 29: 40S RIBOSOMAL PROTEIN ES1

Chain b:  90% 5% 5%




- Molecule 30: 40S RIBOSOMAL PROTEIN US5

Chain c:  83% 7% 10%




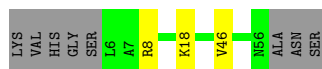
- Molecule 31: 40S RIBOSOMAL PROTEIN US3

Chain d:  88% 7% 5%



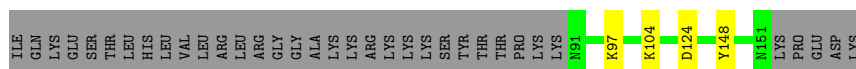
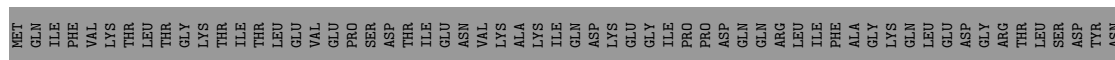
- Molecule 32: 40S RIBOSOMAL PROTEIN ES4

Chain e:  81% 5% 14%



- Molecule 33: 40S RIBOSOMAL PROTEIN US7

Chain f:  37% 61%



- Molecule 34: 40S RIBOSOMAL PROTEIN ES6

Chain g:  93% 5% 2%



4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	109596	Depositor
Resolution determination method	Not provided	Depositor
CTF correction method	DEFOCUS GROUP	Depositor
Microscope	FEI TECNAI F20	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	20	Depositor
Minimum defocus (nm)	2000	Depositor
Maximum defocus (nm)	4000	Depositor
Magnification	65520	Depositor
Image detector	KODAK SO-163 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	1	0.37	2/41550 (0.0%)	0.80	6/64763 (0.0%)
10	I	0.48	0/1724	0.72	0/2298
11	J	0.45	0/1520	0.77	0/2030
12	K	0.48	0/815	0.68	0/1101
13	L	0.45	0/1220	0.72	0/1633
14	M	0.48	0/941	0.72	0/1264
15	N	0.43	0/1231	0.73	1/1656 (0.1%)
16	O	0.46	0/1036	0.71	0/1391
17	P	0.43	0/1000	0.67	0/1335
18	Q	0.43	0/1125	0.66	0/1506
19	R	0.42	0/904	0.67	0/1208
2	A	0.51	0/1756	0.68	0/2386
20	S	0.42	0/1190	0.68	0/1594
21	T	0.44	0/1131	0.69	0/1515
22	U	0.50	0/813	0.70	0/1092
23	V	0.47	0/643	0.71	0/860
24	W	0.44	0/1050	0.69	0/1406
25	X	0.46	0/1063	0.70	0/1421
26	Y	0.45	0/1019	0.70	0/1354
27	Z	0.46	0/611	0.71	0/820
28	a	0.48	0/778	0.75	1/1041 (0.1%)
29	b	0.48	0/637	0.68	0/854
3	B	0.51	0/1756	0.75	1/2350 (0.0%)
30	c	0.46	0/492	0.74	0/657
31	d	0.51	0/454	0.77	0/603
32	e	0.45	0/417	0.69	0/548
33	f	0.53	0/507	0.84	1/673 (0.1%)
34	g	0.45	0/2497	0.67	0/3399
4	C	0.42	0/1761	0.65	0/2379
5	D	0.41	0/1672	0.66	0/2250
6	E	0.47	0/2072	0.70	0/2793
7	F	0.43	0/1507	0.74	0/2026
8	G	0.48	0/1907	0.74	0/2538
9	H	0.46	0/1558	0.74	1/2087 (0.0%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >2	RMSZ	# Z >2
All	All	0.42	2/80357 (0.0%)	0.76	11/116831 (0.0%)

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	1	0	24

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	992	A	C6-N6	-6.31	1.28	1.33
1	1	1286	G	C2-N2	-5.29	1.29	1.34

The worst 5 of 11 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	502	C	C3'-C2'-C1'	-6.04	96.66	101.50
1	1	1441	U	C3'-C2'-C1'	-5.56	97.06	101.50
1	1	645	C	C3'-C2'-C1'	-5.51	97.09	101.50
15	N	6	ALA	N-CA-C	-5.40	96.41	111.00
9	H	109	ARG	N-CA-CB	5.26	120.08	110.60

There are no chirality outliers.

5 of 24 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	1	111	A	Sidechain
1	1	44	U	Sidechain
1	1	77	A	Sidechain
1	1	84	A	Sidechain
1	1	88	G	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	1	37159	0	18780	3647	0
2	A	1719	0	1717	129	0
3	B	1729	0	1803	135	0
4	C	1724	0	1808	63	0
5	D	1646	0	1737	81	0
6	E	2031	0	2138	116	0
7	F	1486	0	1545	99	0
8	G	1884	0	2044	151	0
9	H	1535	0	1632	130	0
10	I	1695	0	1785	113	0
11	J	1495	0	1615	89	0
12	K	791	0	811	45	0
13	L	1199	0	1269	69	0
14	M	931	0	961	40	0
15	N	1207	0	1294	63	0
16	O	1023	0	1050	51	0
17	P	981	0	1026	55	0
18	Q	1108	0	1174	73	0
19	R	893	0	946	57	0
20	S	1172	0	1229	77	0
21	T	1112	0	1146	116	0
22	U	803	0	866	68	0
23	V	636	0	637	42	0
24	W	1033	0	1080	61	0
25	X	1046	0	1110	68	0
26	Y	1002	0	1075	65	0
27	Z	605	0	665	58	0
28	a	767	0	816	0	0
29	b	625	0	642	0	0
30	c	490	0	520	0	0
31	d	444	0	442	0	0
32	e	412	0	463	0	0
33	f	497	0	497	0	0
34	g	2440	0	2396	0	0
All	All	75320	0	58719	5138	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 41.

The worst 5 of 5138 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)
1:1:1431:G:H2'	1:1:1432:U:C6	1.77	1.18
1:1:377:G:H4'	10:I:97:VAL:HG13	1.24	1.18
1:1:571:U:H3'	1:1:572:U:C5'	1.77	1.15
1:1:569:A:H2'	1:1:570:C:H5''	1.24	1.14
1:1:1547:C:H3'	1:1:1548:G:H5''	1.29	1.14

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	A	216/295 (73%)	209 (97%)	5 (2%)	2 (1%)	19	61
3	B	211/264 (80%)	176 (83%)	18 (8%)	17 (8%)	1	16
4	C	220/293 (75%)	213 (97%)	2 (1%)	5 (2%)	7	41
5	D	210/243 (86%)	201 (96%)	4 (2%)	5 (2%)	6	40
6	E	255/263 (97%)	237 (93%)	13 (5%)	5 (2%)	8	45
7	F	186/204 (91%)	163 (88%)	13 (7%)	10 (5%)	2	24
8	G	230/249 (92%)	216 (94%)	5 (2%)	9 (4%)	3	30
9	H	189/194 (97%)	178 (94%)	7 (4%)	4 (2%)	8	43
10	I	205/208 (99%)	184 (90%)	14 (7%)	7 (3%)	4	33
11	J	177/194 (91%)	168 (95%)	6 (3%)	3 (2%)	10	49
12	K	92/165 (56%)	84 (91%)	1 (1%)	7 (8%)	1	17
13	L	144/158 (91%)	133 (92%)	5 (4%)	6 (4%)	3	29
14	M	118/132 (89%)	111 (94%)	1 (1%)	6 (5%)	2	25
15	N	148/151 (98%)	138 (93%)	5 (3%)	5 (3%)	4	33
16	O	135/151 (89%)	129 (96%)	3 (2%)	3 (2%)	7	42
17	P	116/145 (80%)	106 (91%)	5 (4%)	5 (4%)	3	28

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
18	Q	137/146 (94%)	129 (94%)	6 (4%)	2 (2%)	11	51
19	R	105/135 (78%)	99 (94%)	4 (4%)	2 (2%)	9	46
20	S	140/152 (92%)	125 (89%)	7 (5%)	8 (6%)	2	23
21	T	141/145 (97%)	135 (96%)	4 (3%)	2 (1%)	12	52
22	U	99/119 (83%)	95 (96%)	3 (3%)	1 (1%)	17	60
23	V	81/83 (98%)	78 (96%)	1 (1%)	2 (2%)	6	39
24	W	127/130 (98%)	118 (93%)	7 (6%)	2 (2%)	11	50
25	X	132/142 (93%)	120 (91%)	5 (4%)	7 (5%)	2	25
26	Y	120/133 (90%)	114 (95%)	2 (2%)	4 (3%)	4	33
27	Z	74/125 (59%)	71 (96%)	0	3 (4%)	3	29
28	a	94/115 (82%)	85 (90%)	5 (5%)	4 (4%)	3	28
29	b	78/84 (93%)	70 (90%)	8 (10%)	0	100	100
30	c	60/69 (87%)	57 (95%)	1 (2%)	2 (3%)	4	33
31	d	51/56 (91%)	44 (86%)	7 (14%)	0	100	100
32	e	49/59 (83%)	43 (88%)	5 (10%)	1 (2%)	8	45
33	f	59/156 (38%)	53 (90%)	6 (10%)	0	100	100
34	g	312/317 (98%)	291 (93%)	14 (4%)	7 (2%)	7	42
All	All	4711/5475 (86%)	4373 (93%)	192 (4%)	146 (3%)	8	35

5 of 146 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	B	76	ASN
3	B	132	GLY
3	B	148	ASN
3	B	154	SER
3	B	176	VAL

5.3.2 Protein sidechains ⓘ

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	A	181/243 (74%)	176 (97%)	5 (3%)	47	71
3	B	194/231 (84%)	183 (94%)	11 (6%)	23	53
4	C	188/225 (84%)	181 (96%)	7 (4%)	37	65
5	D	175/202 (87%)	166 (95%)	9 (5%)	26	57
6	E	220/225 (98%)	208 (94%)	12 (6%)	24	55
7	F	158/170 (93%)	151 (96%)	7 (4%)	31	60
8	G	202/218 (93%)	195 (96%)	7 (4%)	39	66
9	H	171/174 (98%)	167 (98%)	4 (2%)	53	76
10	I	179/180 (99%)	167 (93%)	12 (7%)	18	48
11	J	160/168 (95%)	150 (94%)	10 (6%)	20	50
12	K	85/136 (62%)	82 (96%)	3 (4%)	39	66
13	L	133/142 (94%)	131 (98%)	2 (2%)	67	85
14	M	102/108 (94%)	97 (95%)	5 (5%)	27	58
15	N	130/131 (99%)	128 (98%)	2 (2%)	67	85
16	O	107/119 (90%)	100 (94%)	7 (6%)	19	49
17	P	107/130 (82%)	102 (95%)	5 (5%)	29	59
18	Q	115/121 (95%)	111 (96%)	4 (4%)	39	66
19	R	99/122 (81%)	94 (95%)	5 (5%)	26	57
20	S	123/132 (93%)	114 (93%)	9 (7%)	15	46
21	T	113/115 (98%)	106 (94%)	7 (6%)	20	51
22	U	93/107 (87%)	89 (96%)	4 (4%)	32	61
23	V	67/67 (100%)	66 (98%)	1 (2%)	67	85
24	W	112/113 (99%)	107 (96%)	5 (4%)	30	60
25	X	108/114 (95%)	103 (95%)	5 (5%)	29	59
26	Y	107/115 (93%)	101 (94%)	6 (6%)	23	54
27	Z	67/103 (65%)	63 (94%)	4 (6%)	21	52
28	a	83/98 (85%)	76 (92%)	7 (8%)	12	40
29	b	72/76 (95%)	68 (94%)	4 (6%)	23	54
30	c	55/62 (89%)	52 (94%)	3 (6%)	24	55
31	d	47/49 (96%)	43 (92%)	4 (8%)	12	40
32	e	42/48 (88%)	40 (95%)	2 (5%)	28	58
33	f	54/140 (39%)	51 (94%)	3 (6%)	23	54

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
34	g	272/275 (99%)	260 (96%)	12 (4%)	31	60
All	All	4121/4659 (88%)	3928 (95%)	193 (5%)	33	59

5 of 193 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
13	L	17	PHE
18	Q	39	LEU
33	f	97	LYS
14	M	52	LEU
16	O	100	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 86 such sidechains are listed below:

Mol	Chain	Res	Type
12	K	44	HIS
18	Q	11	GLN
32	e	44	ASN
13	L	5	GLN
15	N	105	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1	1738/1869 (92%)	1037 (59%)	152 (8%)

5 of 1037 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1	2	A
1	1	3	C
1	1	4	C
1	1	5	U
1	1	6	G

5 of 152 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	1	834	C

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Mol	Chain	Res	Type
1	1	1150	A
1	1	1721	U
1	1	899	U
1	1	1021	U

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.