wwPDB EM Map/Model Validation Report (i)

Apr 10, 2016 – 02:15 PM BST

PDB ID	:	3JAM
EMDB ID:	:	EMD-3047
Title	:	CryoEM structure of 40S-eIF1A-eIF1 complex from yeast
Authors	:	Llacer, J.L.; Hussain, T.; Ramakrishnan, V.
Deposited on	:	2015-06-17
Resolution	:	3.46 Å(reported)
Based on PDB ID	:	3J80

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

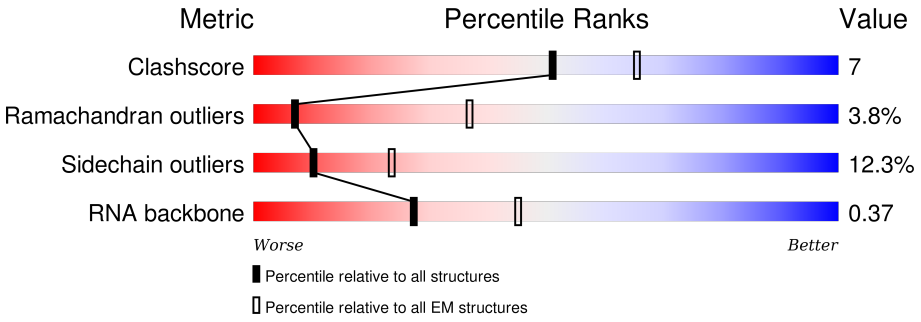
MolProbity	:	4.02b-467
Mogul	:	unknown
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk27241

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.46 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	2	1799	40% 45% 14% •
2	A	254	57% 20% 5% 18%
3	B	255	64% 20% • 13%
4	C	259	66% 15% • 16%
5	D	237	69% 21% • 6%
6	E	261	74% 22% •
7	F	227	69% 20% • 9%
8	G	236	75% 19% • •

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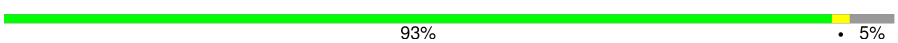
Mol	Chain	Length	Quality of chain
9	H	190	
10	I	201	
11	J	188	
12	K	106	
13	L	156	
14	M	134	
15	N	151	
16	O	137	
17	P	142	
18	Q	143	
19	R	136	
20	S	146	
21	T	144	
22	U	117	
23	V	87	
24	W	130	
25	X	145	
26	Y	135	
27	Z	108	
28	a	119	
29	b	82	
30	c	67	
31	d	56	
32	e	63	
33	f	150	

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Mol	Chain	Length	Quality of chain
34	g	326	86% 11%
35	h	25	92% 8%
36	i	153	57% 6% 37%
37	j	108	69% 10% 20%

2 Entry composition

There are 39 unique types of molecules in this entry. The entry contains 77850 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.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	2	1780	37797	16892	6658	12467	1780	0	0

- Molecule 2 is a protein called uS2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	A	208	1626	1040	286	298	2	0	0

- Molecule 3 is a protein called eS1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	B	223	1774	1120	325	326	3	0	0

- Molecule 4 is a protein called uS5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	C	217	1629	1041	287	297	4	0	0

- Molecule 5 is a protein called uS3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	D	223	1744	1108	313	318	5	0	0

- Molecule 6 is a protein called eS4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	E	260	2078	1322	393	359	4	0	0

- Molecule 7 is a protein called uS7.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	F	206	Total	C	N	O	S	0	0
			1609	1008	298	300	3		

- Molecule 8 is a protein called eS6.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	G	226	Total	C	N	O	S	0	0
			1812	1134	348	326	4		

- Molecule 9 is a protein called eS7.

Mol	Chain	Residues	Atoms				AltConf	Trace
9	H	184	Total	C	N	O	0	0
			1483	950	270	263		

- Molecule 10 is a protein called eS8.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	I	188	Total	C	N	O	S	0	0
			1489	923	300	265	1		

- Molecule 11 is a protein called uS4.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	J	182	Total	C	N	O	S	0	0
			1471	929	287	254	1		

- Molecule 12 is a protein called eS10.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	K	96	Total	C	N	O	S	0	0
			809	533	129	146	1		

- Molecule 13 is a protein called uS17.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	L	155	Total	C	N	O	S	0	0
			1248	798	237	210	3		

- Molecule 14 is a protein called eS12.

Mol	Chain	Residues	Atoms				AltConf	Trace
14	M	122	Total 922	C 575	N 167	O 180	0	0

- Molecule 15 is a protein called uS15.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	N	150	Total 1187	C 756	N 223	O 206	S 2	0	0

- Molecule 16 is a protein called uS11.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	O	127	Total 942	C 578	N 188	O 173	S 3	0	0

- Molecule 17 is a protein called uS19.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	P	123	Total 980	C 628	N 179	O 168	S 5	0	0

- Molecule 18 is a protein called uS9.

Mol	Chain	Residues	Atoms				AltConf	Trace
18	Q	141	Total 1105	C 709	N 204	O 192	0	0

- Molecule 19 is a protein called eS17.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	R	125	Total 991	C 619	N 182	O 187	S 3	0	0

- Molecule 20 is a protein called uS13.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	S	145	Total 1193	C 741	N 240	O 210	S 2	0	0

- Molecule 21 is a protein called eS19.

Mol	Chain	Residues	Atoms				AltConf	Trace
21	T	143	Total	C	N	O	0	0
			1110	693	210	207		

- Molecule 22 is a protein called uS10.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	U	106	Total	C	N	O	S	0	0
			845	540	152	152	1		

- Molecule 23 is a protein called eS21.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	V	87	Total	C	N	O	S	0	0
			687	424	126	135	2		

- Molecule 24 is a protein called uS8.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	W	129	Total	C	N	O	S	0	0
			1021	651	187	180	3		

- Molecule 25 is a protein called uS12.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	X	144	Total	C	N	O	S	0	0
			1119	708	218	191	2		

- Molecule 26 is a protein called eS24.

Mol	Chain	Residues	Atoms				AltConf	Trace
26	Y	134	Total	C	N	O	0	0
			1061	665	207	189		

- Molecule 27 is a protein called eS25.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	Z	70	Total	C	N	O	S	0	0
			558	355	104	98	1		

- Molecule 28 is a protein called eS26.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	a	98	Total	C	N	O	S	0	0
			779	480	165	129	5		

- Molecule 29 is a protein called eS27.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	b	81	Total	C	N	O	S	0	0
			609	379	112	113	5		

- Molecule 30 is a protein called eS28.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	c	63	Total	C	N	O	S	0	0
			494	305	98	90	1		

- Molecule 31 is a protein called uS14.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	d	53	Total	C	N	O	S	0	0
			446	280	89	76	1		

- Molecule 32 is a protein called eS30.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	e	53	Total	C	N	O	S	0	0
			428	268	87	72	1		

- Molecule 33 is a protein called eS31.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	f	69	Total	C	N	O	S	0	0
			549	352	102	91	4		

- Molecule 34 is a protein called RACK1.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	g	318	Total	C	N	O	S	0	0
			2466	1561	430	470	5		

- Molecule 35 is a protein called eL41.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	h	25	Total	C	N	O	S	0	0
			233	142	63	27	1		

- Molecule 36 is a protein called eIF1A.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	i	96	Total	C	N	O	S	0	0
			778	482	144	147	5		

- Molecule 37 is a protein called eIF1.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	j	86	Total	C	N	O	S	0	0
			695	439	128	124	4		

- Molecule 38 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
38	2	78	Total	Mg	0
			78	78	
38	J	1	Total	Mg	0
			1	1	
38	f	1	Total	Mg	0
			1	1	

- Molecule 39 is ZINC ION (three-letter code: ZN) (formula: Zn).

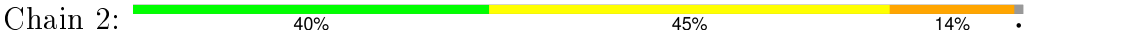
Mol	Chain	Residues	Atoms		AltConf
39	b	1	Total	Zn	0
			1	1	
39	a	1	Total	Zn	0
			1	1	
39	f	1	Total	Zn	0
			1	1	

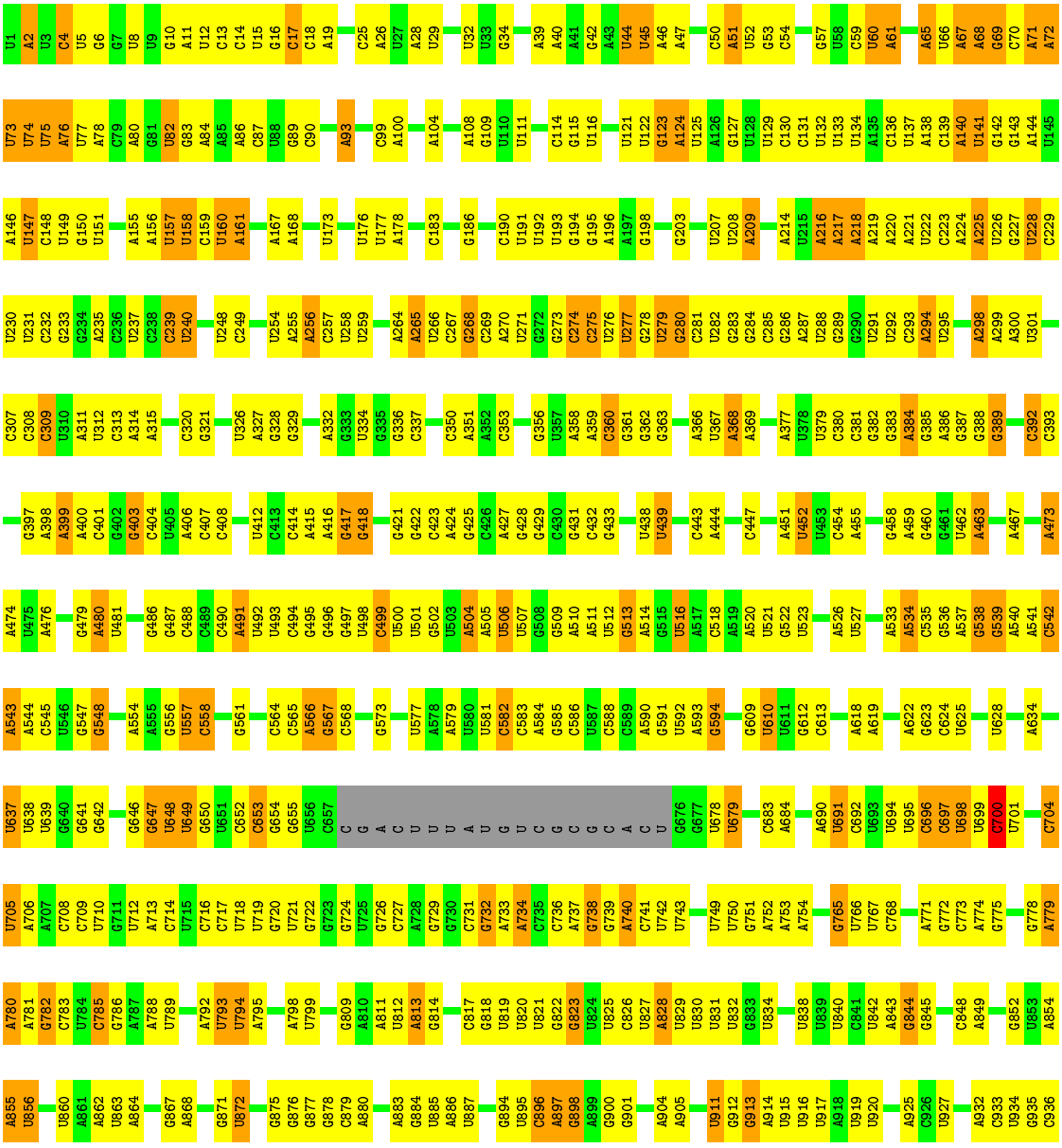
3 Residue-property plots (i)

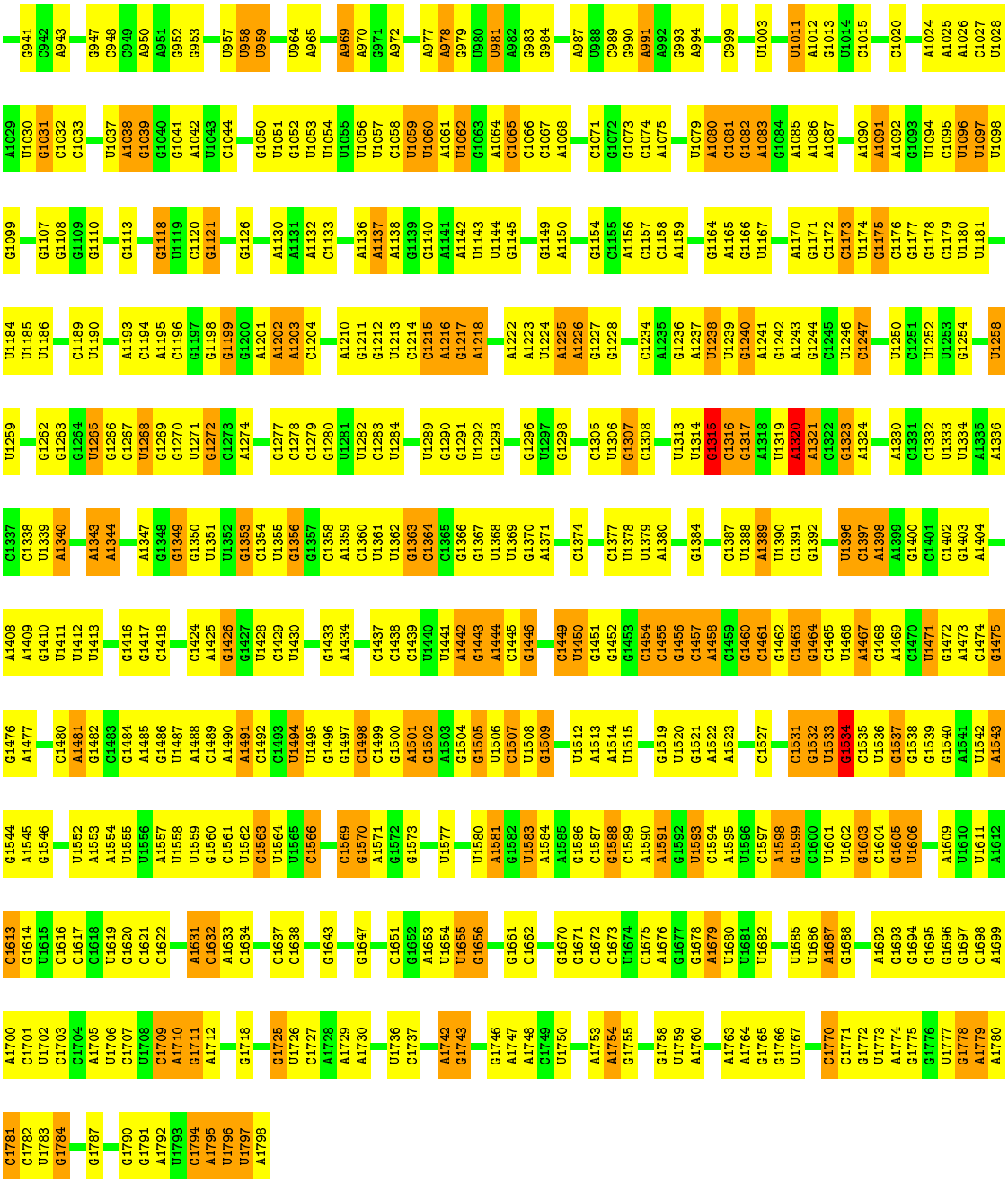
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric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

Chain 2:

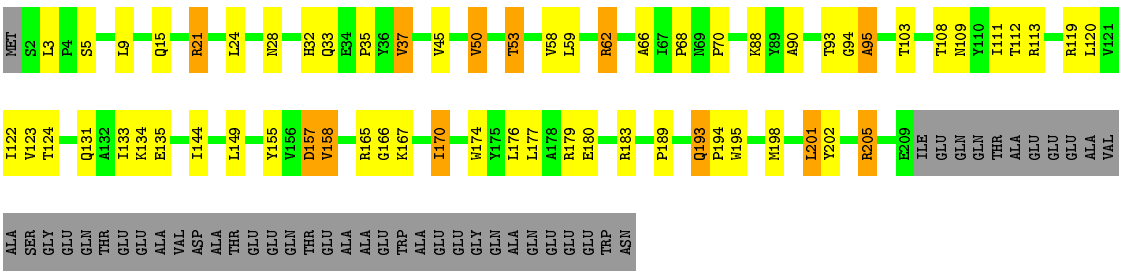






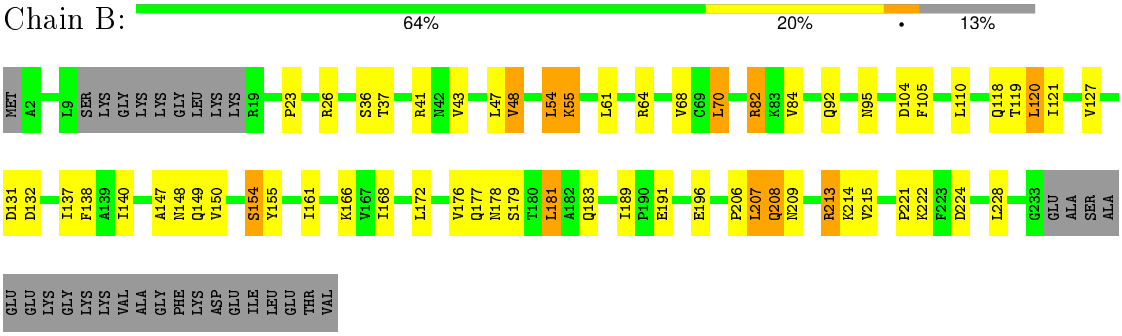
- Molecule 2: uS2

Chain A:



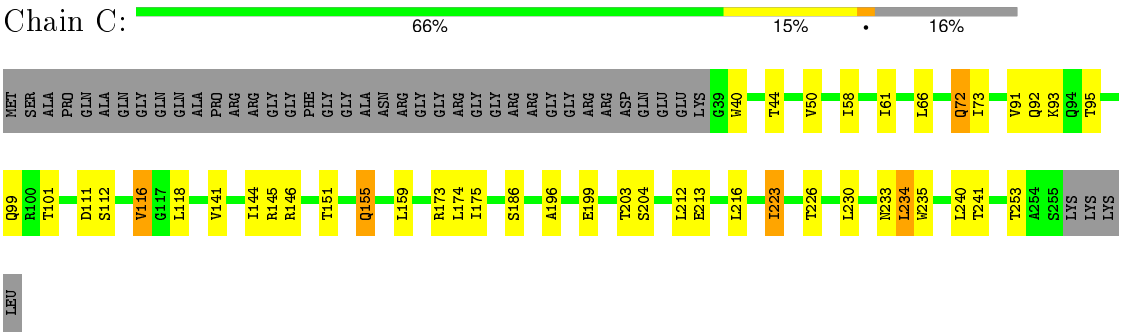
- Molecule 3: eS1

Chain B:



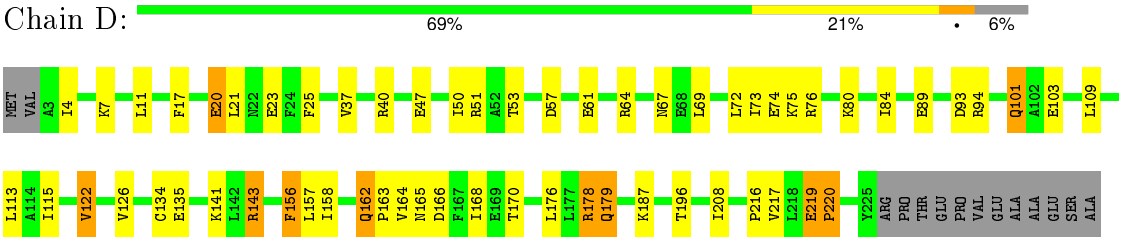
- Molecule 4: uS5

Chain C:



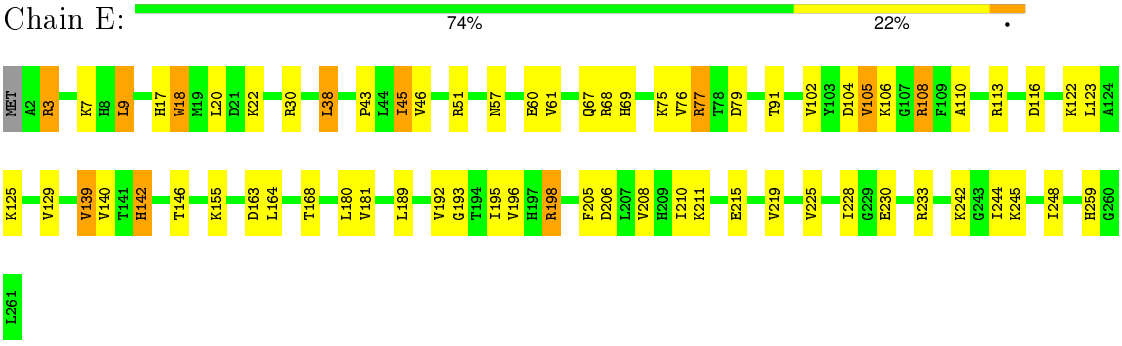
- Molecule 5: uS3

Chain D:



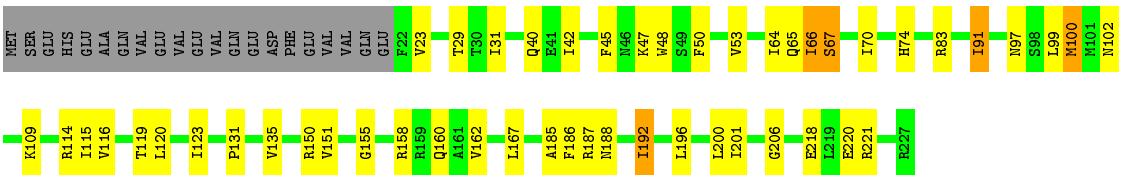
- Molecule 6: eS4

Chain E:



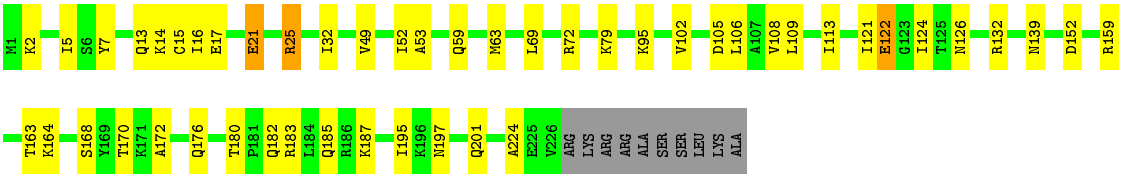
- Molecule 7: uS7

Chain F:



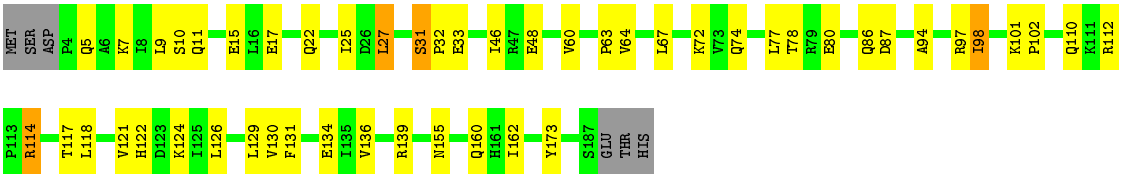
- Molecule 8: eS6

Chain G:



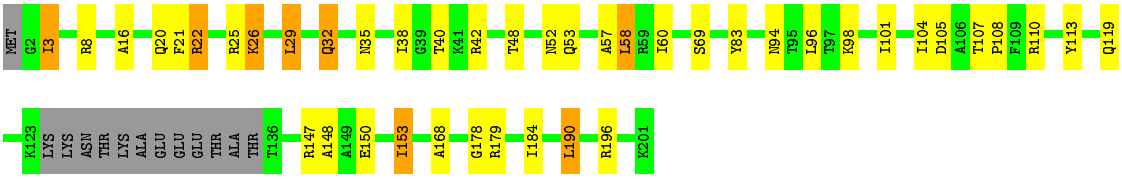
- Molecule 9: eS7

Chain H:



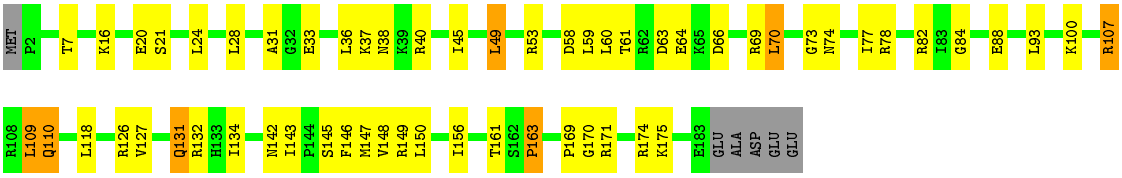
- Molecule 10: eS8

Chain I:



- Molecule 11: uS4

Chain J:



- Molecule 12: eS10

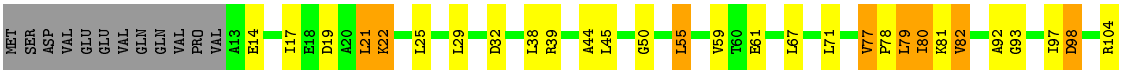
Chain K:

- Molecule 13: uS17

Chain L:

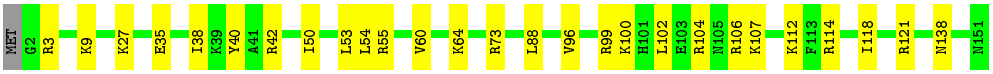
- Molecule 14: eS12

Chain M:



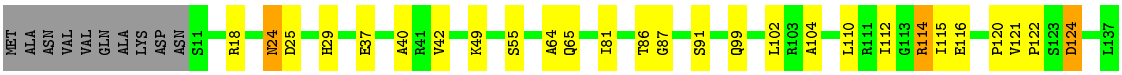
- Molecule 15: uS15

Chain N:



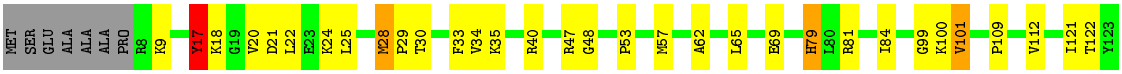
- Molecule 16: uS11

Chain O:



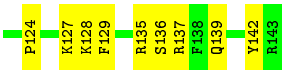
- Molecule 17: uS19

Chain P:



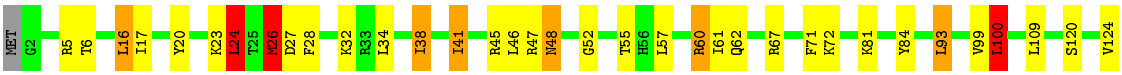
- Molecule 18: uS9

Chain Q:



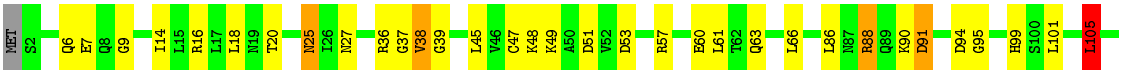
- Molecule 19: eS17

Chain R:



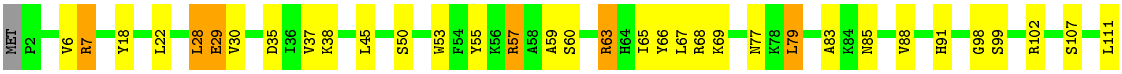
- Molecule 20: uS13

Chain S:



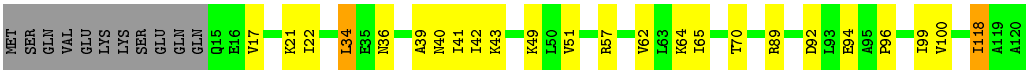
- Molecule 21: eS19

Chain T:



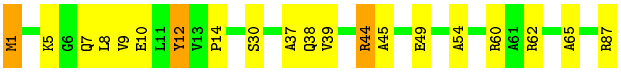
- Molecule 22: uS10

Chain U:



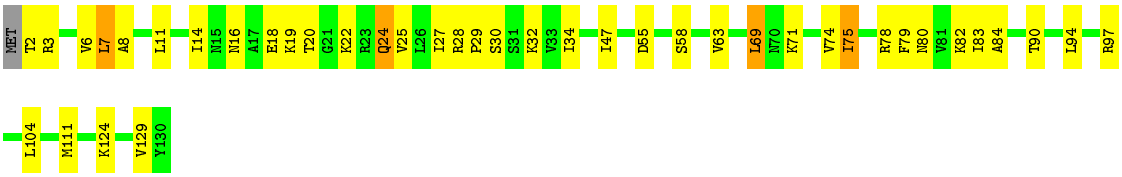
- Molecule 23: eS21

Chain V:



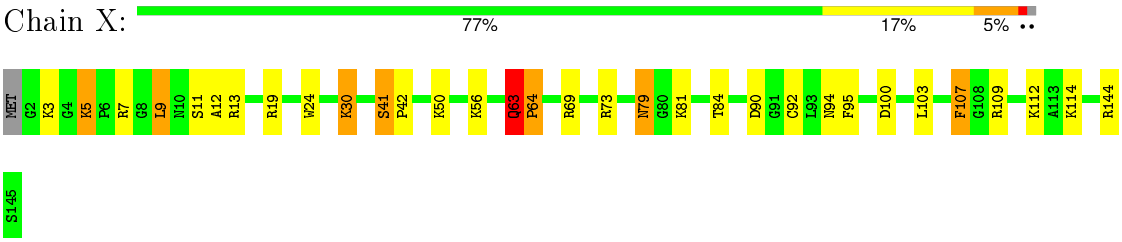
- Molecule 24: uS8

Chain W:



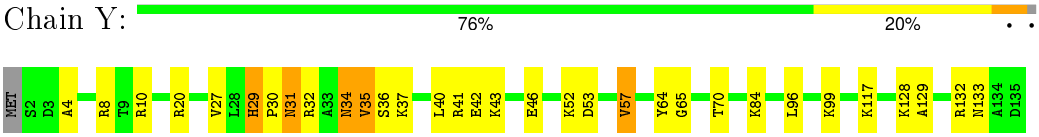
- Molecule 25: uS12

Chain X:



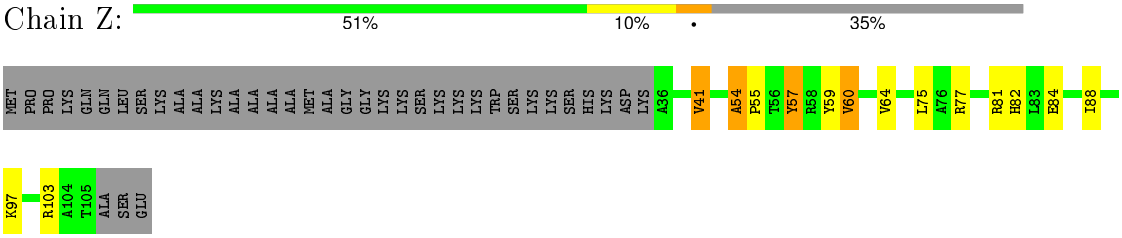
- Molecule 26: eS24

Chain Y:



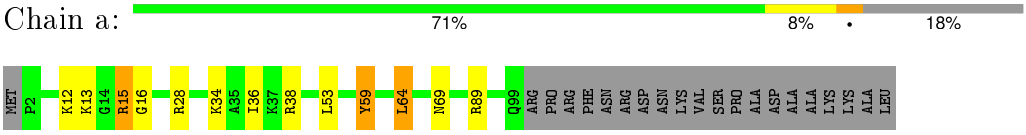
- Molecule 27: eS25

Chain Z:



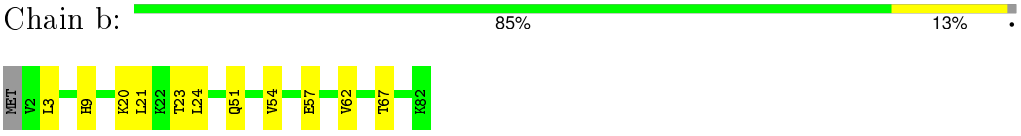
- Molecule 28: eS26

Chain a:



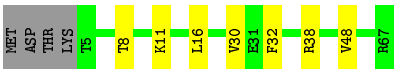
- Molecule 29: eS27

Chain b:



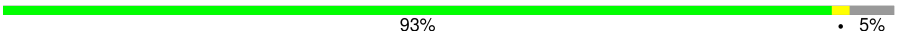
- Molecule 30: eS28

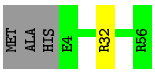
Chain c:



- Molecule 31: uS14

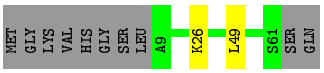
Chain d:





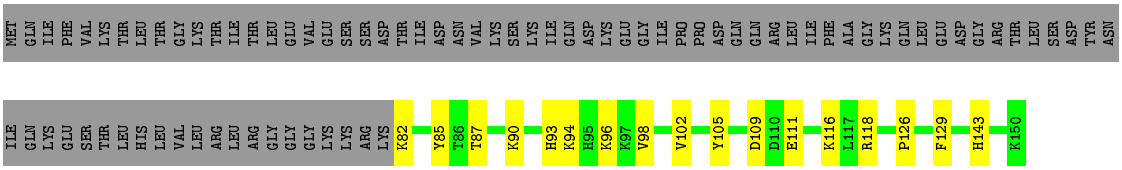
- Molecule 32: eS30

Chain e:



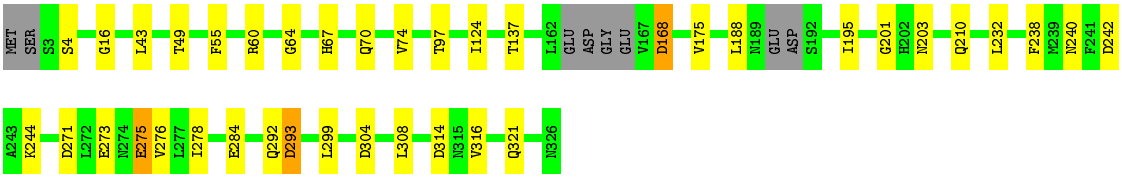
- Molecule 33: eS31

Chain f:



- Molecule 34: RACK1

Chain g:

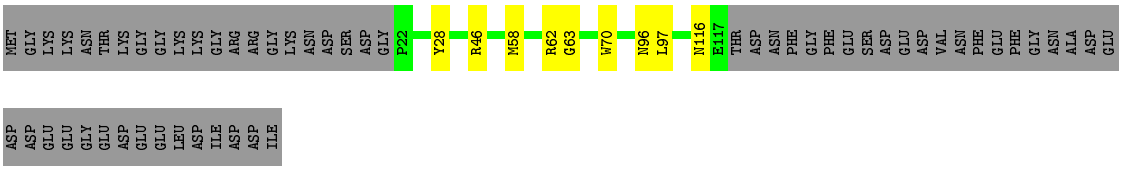


- Molecule 35: eL41

Chain h:

- Molecule 36: eIF1A

Chain i:



- Molecule 37: eIF1

Chain j:

4 Experimental information (i)

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of images	86055	Depositor
Resolution determination method	FSC 0.143	Depositor
CTF correction method	Not provided	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	27	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	4000	Depositor
Magnification	78000	Depositor
Image detector	FEI FALCON II (4k x 4k)	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, MG

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	2	0.27	0/42269	0.69	8/65862 (0.0%)
10	I	0.42	0/1515	0.74	2/2029 (0.1%)
11	J	0.43	0/1495	0.82	1/2001 (0.0%)
12	K	0.49	0/831	0.74	0/1123
13	L	0.41	0/1276	0.64	0/1718
14	M	0.46	0/929	0.77	0/1255
15	N	0.44	0/1210	0.77	0/1628
16	O	0.41	0/953	0.73	0/1279
17	P	0.46	0/1000	0.72	0/1343
18	Q	0.44	0/1125	0.74	1/1510 (0.1%)
19	R	0.43	0/1002	0.82	2/1346 (0.1%)
2	A	0.44	0/1666	0.78	1/2279 (0.0%)
20	S	0.42	0/1212	0.75	1/1629 (0.1%)
21	T	0.45	0/1129	0.79	1/1520 (0.1%)
22	U	0.40	0/857	0.69	0/1158
23	V	0.40	0/696	0.72	0/938
24	W	0.39	0/1039	0.77	2/1399 (0.1%)
25	X	0.41	0/1137	0.74	0/1516
26	Y	0.41	0/1075	0.72	0/1433
27	Z	0.48	0/567	0.70	0/762
28	a	0.38	0/791	0.69	0/1059
29	b	0.39	0/619	0.65	0/837
3	B	0.41	0/1798	0.73	2/2421 (0.1%)
30	c	0.42	0/496	0.73	0/666
31	d	0.44	0/457	0.67	0/607
32	e	0.40	0/435	0.72	0/579
33	f	0.50	0/562	0.70	0/751
34	g	0.44	0/2521	0.63	0/3431
35	h	0.43	0/234	0.88	0/300
36	i	0.40	0/788	0.67	0/1051
37	j	0.43	0/703	0.69	0/938
4	C	0.42	0/1659	0.71	0/2252

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 2$	RMSZ	$\#\|Z\| > 2$
5	D	0.44	0/1769	0.72	0/2378
6	E	0.39	0/2122	0.70	1/2861 (0.0%)
7	F	0.44	0/1628	0.78	0/2198
8	G	0.41	0/1835	0.71	0/2451
9	H	0.44	0/1507	0.76	2/2028 (0.1%)
All	All	0.36	0/82907	0.71	24/120536 (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
12	K	0	1
17	P	0	1
18	Q	0	1
25	X	0	1
26	Y	0	1
All	All	0	5

There are no bond length outliers.

The worst 5 of 24 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	2	1315	G	C2'-C3'-O3'	7.09	125.10	109.50
20	S	105	LEU	CA-CB-CG	7.01	131.42	115.30
10	I	29	LEU	CA-CB-CG	6.92	131.22	115.30
3	B	181	LEU	CA-CB-CG	6.79	130.92	115.30
1	2	1534	G	C2'-C3'-O3'	6.15	123.53	113.70

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
12	K	87	PHE	Peptide
17	P	28	MET	Peptide
18	Q	40	GLN	Peptide
25	X	63	GLN	Peptide
26	Y	29	HIS	Peptide

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	2	37797	0	19016	570	0
2	A	1626	0	1633	28	0
3	B	1774	0	1834	18	0
4	C	1629	0	1710	20	0
5	D	1744	0	1826	18	0
6	E	2078	0	2157	20	0
7	F	1609	0	1679	22	0
8	G	1812	0	1911	21	0
9	H	1483	0	1579	16	0
10	I	1489	0	1504	17	0
11	J	1471	0	1554	22	0
12	K	809	0	810	12	0
13	L	1248	0	1311	15	0
14	M	922	0	953	9	0
15	N	1187	0	1251	6	0
16	O	942	0	979	10	0
17	P	980	0	1026	15	0
18	Q	1105	0	1170	23	0
19	R	991	0	1039	15	0
20	S	1193	0	1217	20	0
21	T	1110	0	1124	18	0
22	U	845	0	913	9	0
23	V	687	0	682	12	0
24	W	1021	0	1056	19	0
25	X	1119	0	1198	14	0
26	Y	1061	0	1111	11	0
27	Z	558	0	585	6	0
28	a	779	0	828	0	0
29	b	609	0	631	0	0
30	c	494	0	534	0	0
31	d	446	0	436	0	0
32	e	428	0	468	0	0
33	f	549	0	564	0	0
34	g	2466	0	2406	0	0
35	h	233	0	284	0	0
36	i	778	0	779	0	0
37	j	695	0	729	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
38	2	78	0	0	0	0
38	J	1	0	0	0	0
38	f	1	0	0	0	0
39	a	1	0	0	0	0
39	b	1	0	0	0	0
39	f	1	0	0	0	0
All	All	77850	0	60487	893	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 7.

The worst 5 of 893 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)
1:2:51:A:N6	1:2:439:U:H3	1.05	1.41
1:2:1593:U:H3	1:2:1598:A:N6	1.13	1.40
1:2:480:A:N1	1:2:506:U:O4	1.62	1.33
1:2:628:U:N3	1:2:969:A:N6	1.77	1.32
1:2:1079:U:O4	1:2:1090:A:N1	1.66	1.25

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	206/254 (81%)	171 (83%)	27 (13%)	8 (4%)	4 33
3	B	219/255 (86%)	187 (85%)	20 (9%)	12 (6%)	2 23
4	C	215/259 (83%)	192 (89%)	17 (8%)	6 (3%)	6 41
5	D	221/237 (93%)	195 (88%)	17 (8%)	9 (4%)	3 32
6	E	258/261 (99%)	226 (88%)	25 (10%)	7 (3%)	6 42

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
7	F	204/227 (90%)	167 (82%)	28 (14%)	9 (4%)	3 29
8	G	224/236 (95%)	205 (92%)	15 (7%)	4 (2%)	11 51
9	H	182/190 (96%)	157 (86%)	16 (9%)	9 (5%)	3 26
10	I	184/201 (92%)	168 (91%)	9 (5%)	7 (4%)	4 33
11	J	180/188 (96%)	154 (86%)	20 (11%)	6 (3%)	5 37
12	K	94/106 (89%)	79 (84%)	9 (10%)	6 (6%)	2 19
13	L	153/156 (98%)	131 (86%)	19 (12%)	3 (2%)	9 49
14	M	120/134 (90%)	95 (79%)	18 (15%)	7 (6%)	2 21
15	N	148/151 (98%)	138 (93%)	9 (6%)	1 (1%)	26 71
16	O	125/137 (91%)	108 (86%)	11 (9%)	6 (5%)	3 27
17	P	121/142 (85%)	100 (83%)	12 (10%)	9 (7%)	1 15
18	Q	139/143 (97%)	128 (92%)	8 (6%)	3 (2%)	8 47
19	R	123/136 (90%)	104 (85%)	14 (11%)	5 (4%)	3 32
20	S	143/146 (98%)	116 (81%)	17 (12%)	10 (7%)	1 16
21	T	141/144 (98%)	125 (89%)	12 (8%)	4 (3%)	6 41
22	U	104/117 (89%)	93 (89%)	9 (9%)	2 (2%)	10 49
23	V	85/87 (98%)	70 (82%)	10 (12%)	5 (6%)	2 21
24	W	127/130 (98%)	115 (91%)	7 (6%)	5 (4%)	4 33
25	X	142/145 (98%)	121 (85%)	15 (11%)	6 (4%)	3 31
26	Y	132/135 (98%)	119 (90%)	7 (5%)	6 (4%)	3 29
27	Z	68/108 (63%)	51 (75%)	13 (19%)	4 (6%)	2 21
28	a	96/119 (81%)	82 (85%)	8 (8%)	6 (6%)	2 19
29	b	79/82 (96%)	68 (86%)	8 (10%)	3 (4%)	4 33
30	c	61/67 (91%)	55 (90%)	6 (10%)	0	100 100
31	d	51/56 (91%)	47 (92%)	4 (8%)	0	100 100
32	e	51/63 (81%)	45 (88%)	5 (10%)	1 (2%)	9 49
33	f	67/150 (45%)	40 (60%)	20 (30%)	7 (10%)	1 8
34	g	312/326 (96%)	253 (81%)	51 (16%)	8 (3%)	7 43
35	h	23/25 (92%)	23 (100%)	0	0	100 100
36	i	94/153 (61%)	83 (88%)	9 (10%)	2 (2%)	9 48
37	j	84/108 (78%)	70 (83%)	11 (13%)	3 (4%)	4 35

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	4976/5574 (89%)	4281 (86%)	506 (10%)	189 (4%)	7 33

5 of 189 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	95	ALA
3	B	55	LYS
3	B	148	ASN
4	C	141	VAL
5	D	217	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
2	A	174/211 (82%)	145 (83%)	29 (17%)	3 15
3	B	198/228 (87%)	173 (87%)	25 (13%)	5 27
4	C	176/203 (87%)	157 (89%)	19 (11%)	8 36
5	D	185/196 (94%)	155 (84%)	30 (16%)	3 16
6	E	223/224 (100%)	186 (83%)	37 (17%)	3 15
7	F	174/194 (90%)	154 (88%)	20 (12%)	7 31
8	G	192/200 (96%)	174 (91%)	18 (9%)	11 43
9	H	164/170 (96%)	145 (88%)	19 (12%)	7 31
10	I	147/159 (92%)	129 (88%)	18 (12%)	6 28
11	J	153/158 (97%)	130 (85%)	23 (15%)	3 20
12	K	88/96 (92%)	75 (85%)	13 (15%)	4 20
13	L	136/137 (99%)	128 (94%)	8 (6%)	24 64
14	M	97/109 (89%)	80 (82%)	17 (18%)	2 13
15	N	127/128 (99%)	110 (87%)	17 (13%)	5 25
16	O	96/104 (92%)	85 (88%)	11 (12%)	7 31
17	P	105/119 (88%)	93 (89%)	12 (11%)	7 32

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
18	Q	117/119 (98%)	100 (86%)	17 (14%)	4 21
19	R	112/124 (90%)	92 (82%)	20 (18%)	2 11
20	S	128/129 (99%)	109 (85%)	19 (15%)	4 20
21	T	117/118 (99%)	103 (88%)	14 (12%)	6 29
22	U	96/107 (90%)	85 (88%)	11 (12%)	7 31
23	V	73/73 (100%)	69 (94%)	4 (6%)	27 66
24	W	110/111 (99%)	97 (88%)	13 (12%)	6 30
25	X	119/120 (99%)	108 (91%)	11 (9%)	11 44
26	Y	108/109 (99%)	98 (91%)	10 (9%)	11 44
27	Z	60/88 (68%)	55 (92%)	5 (8%)	14 49
28	a	83/100 (83%)	73 (88%)	10 (12%)	6 29
29	b	71/72 (99%)	63 (89%)	8 (11%)	7 32
30	c	55/59 (93%)	48 (87%)	7 (13%)	5 27
31	d	46/48 (96%)	45 (98%)	1 (2%)	60 86
32	e	47/55 (86%)	46 (98%)	1 (2%)	61 86
33	f	58/133 (44%)	48 (83%)	10 (17%)	2 14
34	g	265/272 (97%)	231 (87%)	34 (13%)	5 27
35	h	23/23 (100%)	21 (91%)	2 (9%)	13 47
36	i	83/130 (64%)	76 (92%)	7 (8%)	14 49
37	j	77/96 (80%)	69 (90%)	8 (10%)	9 38
All	All	4283/4722 (91%)	3755 (88%)	528 (12%)	10 28

5 of 528 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
12	K	14	HIS
16	O	49	LYS
34	g	168	ASP
12	K	40	LEU
14	M	61	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 69 such sidechains are listed below:

Mol	Chain	Res	Type
16	O	12	GLN
19	R	62	GLN
29	b	42	ASN
16	O	29	HIS
17	P	79	HIS

5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	2	1778/1799 (98%)	675 (37%)	113 (6%)

5 of 675 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	2	2	A
1	2	4	C
1	2	17	C
1	2	25	C
1	2	26	A

5 of 113 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	2	708	C
1	2	854	A
1	2	1655	U
1	2	710	U
1	2	779	A

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 83 ligands modelled in this entry, 83 are monoatomic - leaving 0 for Mogul analysis.

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.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.