wwPDB EM Map/Model Validation Report (i)

Apr 10, 2016 – 02:27 PM BST

PDB ID	:	3J80
EMDB ID:	:	EMD-2764
Title	:	CryoEM structure of 40S-eIF1-eIF1A preinitiation complex
Authors	:	Hussain, T.; Llacer, J.L.; Fernandez, I.S.; Savva, C.G.; Ramakrishnan, V.
Deposited on	:	2014-08-28
Resolution	:	3.75 Å(reported)
Based on PDB ID	:	3U5C, 3U5B

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

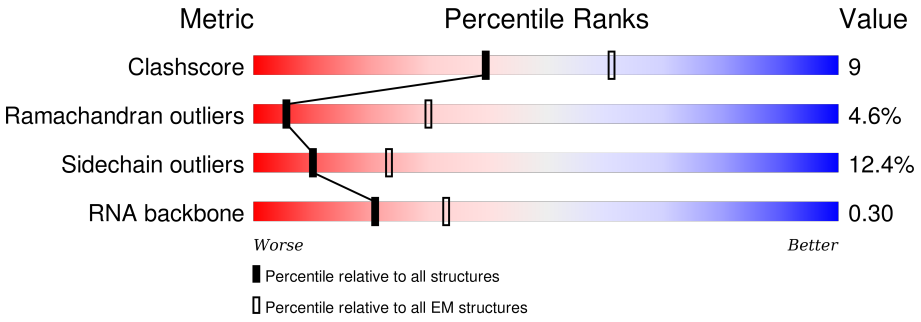
MolProbity	:	4.02b-467
Mogul	:	unknown
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk27241

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 3.75 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	29% 52% 17% •
2	A	254	52% 25% 5% 19%
3	B	255	59% 21% • • 16%
4	C	259	51% 27% 5% 16%
5	E	261	69% 25% 6%
6	G	236	69% 25% • •
7	H	190	63% 26% 7% •
8	I	201	59% 30% • • 6%

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Mol	Chain	Length	Quality of chain
9	J	188	56% 33% 8%
10	L	156	69% 25%
11	N	151	75% 21%
12	O	137	68% 22% 7%
13	V	87	63% 32% 5%
14	W	130	61% 31% 8%
15	X	145	67% 26% 6%
16	Y	135	67% 27%
17	a	119	58% 23% 18%
18	b	82	80% 17%
19	e	63	75% 10% 16%
20	D	237	67% 24% 6%
21	F	227	70% 19% 9%
22	K	106	68% 23% 9%
23	M	134	72% 18% 9%
24	P	140	69% 14% 12%
25	Q	143	69% 27%
26	R	136	65% 20% 12%
27	S	146	74% 23%
28	T	144	78% 19%
29	U	117	55% 32% 9%
30	Z	108	57% 5% 35%
31	c	67	85% 9% 6%
32	d	56	80% 14% 5%
33	f	150	37% 9% 54%

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Mol	Chain	Length	Quality of chain
34	g	326	91% 6%
35	h	25	88% 12%
36	i	153	58% 5% 37%
37	j	108	74% 6% 20%

2 Entry composition

There are 39 unique types of molecules in this entry. The entry contains 77716 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	1779	37775	16882	6653	12461	1779	0	0

- Molecule 2 is a protein called uS2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	A	206	1616	1035	285	294	2	0	0

- Molecule 3 is a protein called eS1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	B	214	1722	1089	313	317	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 eS4.

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

- Molecule 6 is a protein called eS6.

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

- Molecule 7 is a protein called eS7.

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

- Molecule 8 is a protein called eS8.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	I	188	Total	C	N	O	S	0	0
			1493	926	301	265	1		

- Molecule 9 is a protein called uS4.

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

- Molecule 10 is a protein called uS17.

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

- Molecule 11 is a protein called uS15.

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

- Molecule 12 is a protein called uS11.

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

- Molecule 13 is a protein called eS21.

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

- Molecule 14 is a protein called uS8.

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

- Molecule 15 is a protein called uS12.

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

- Molecule 16 is a protein called eS24.

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

- Molecule 17 is a protein called eS26.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	a	97	Total	C	N	O	S	0	0
			770	475	163	127	5		

- Molecule 18 is a protein called eS27.

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

- Molecule 19 is a protein called eS30.

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

- Molecule 20 is a protein called uS3.

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

- Molecule 21 is a protein called uS7.

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

- Molecule 22 is a protein called eS10.

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

- Molecule 23 is a protein called eS12.

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

- Molecule 24 is a protein called uS19.

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

- Molecule 25 is a protein called uS9.

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

- Molecule 26 is a protein called eS17.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	R	120	Total	C	N	O	S	0	0
			959	598	178	180	3		

- Molecule 27 is a protein called uS13.

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

- Molecule 28 is a protein called eS19.

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

- Molecule 29 is a protein called uS10.

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

- Molecule 30 is a protein called eS25.

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

- Molecule 31 is a protein called eS28.

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

- Molecule 32 is a protein called uS14.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	d	53	Total	C	N	O	S	0	0
			446	280	89	76	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	67	Total	Mg	0
			67	67	

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

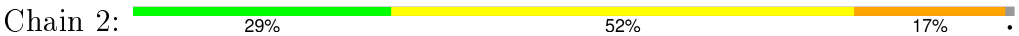
Mol	Chain	Residues	Atoms		AltConf
39	b	1	Total	Zn	0
			1	1	
39	a	1	Total	Zn	0
			1	1	
39	f	1	Total	Zn	0
			1	1	

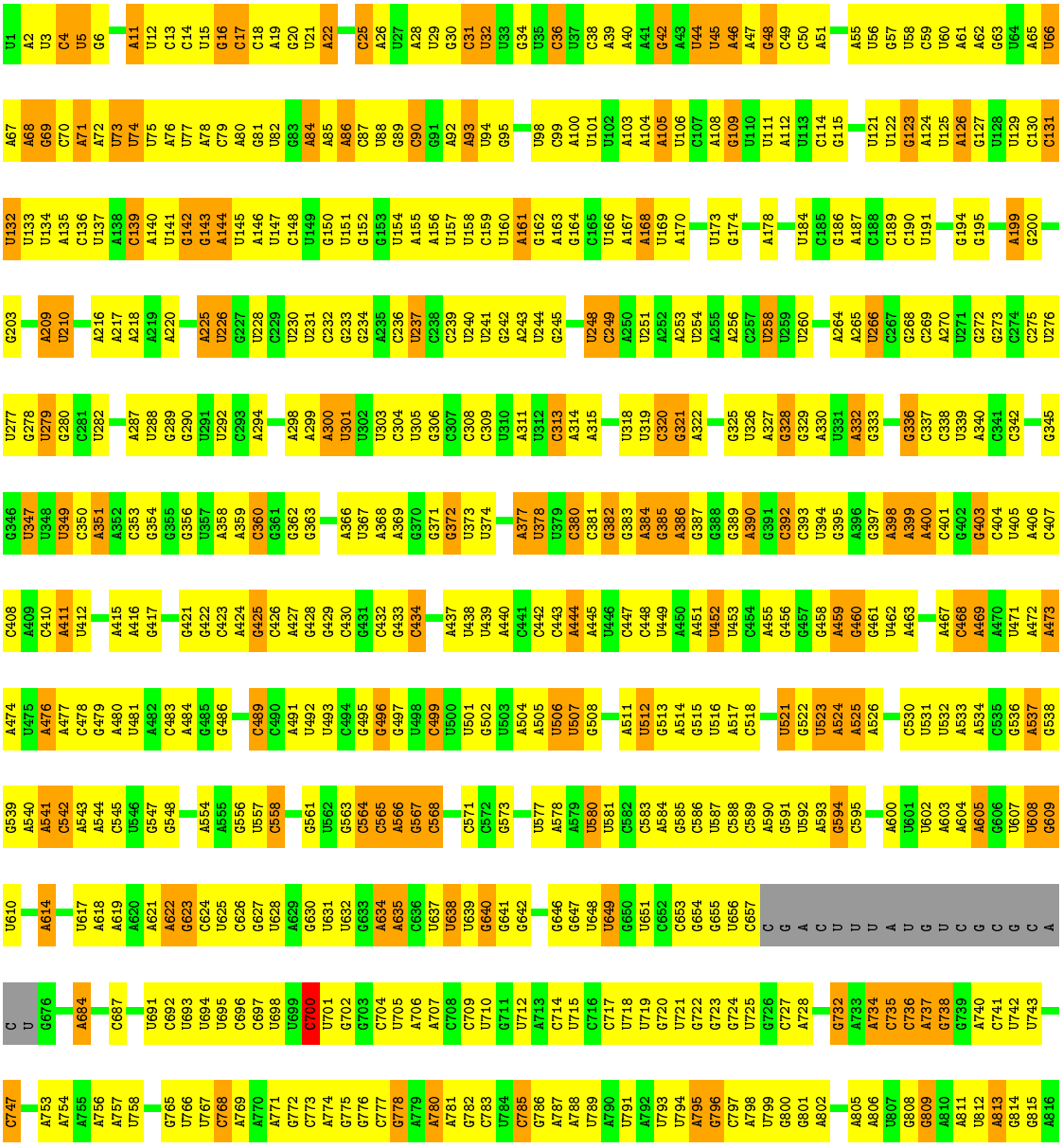
3 Residue-property plots (i)

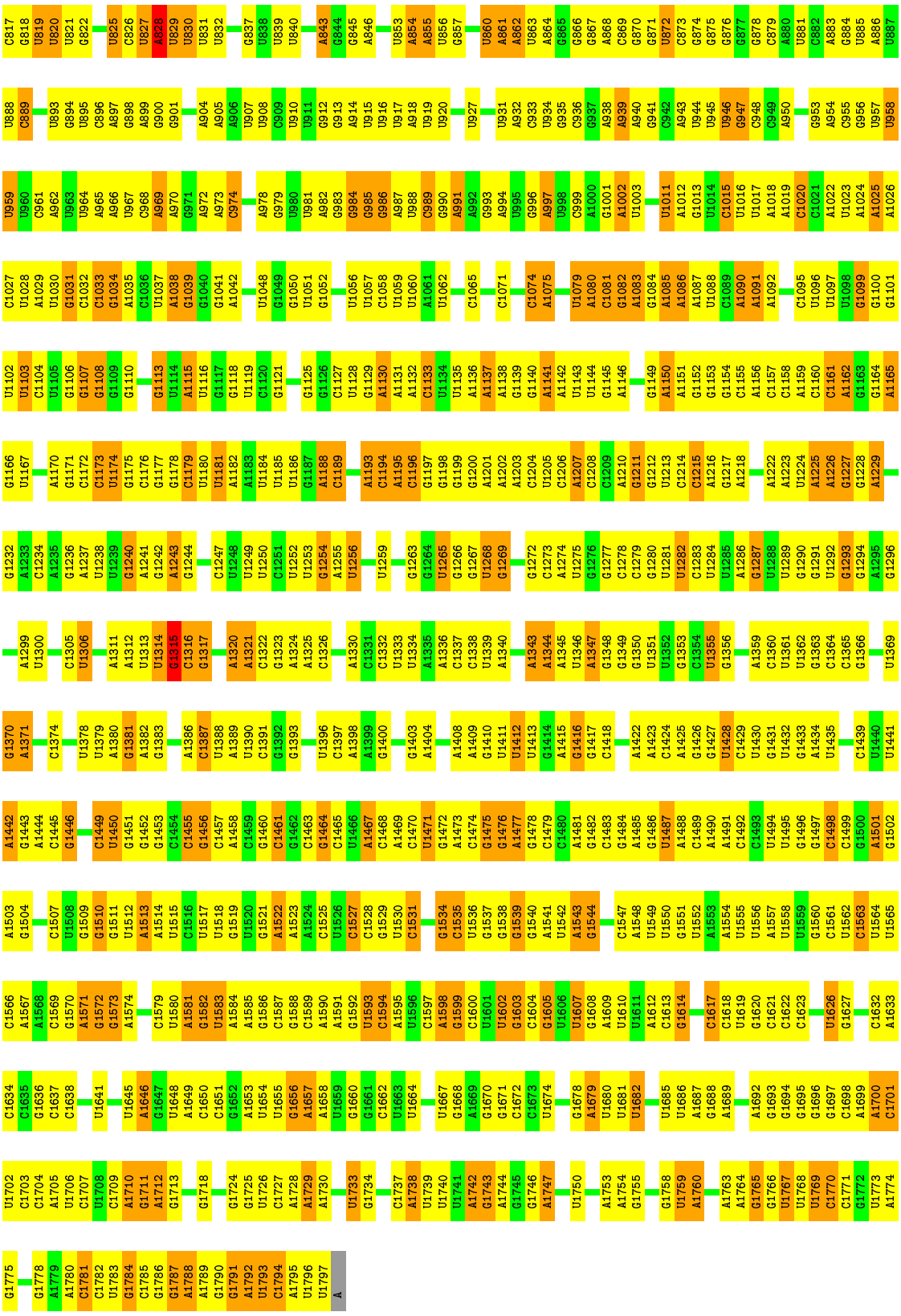
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric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

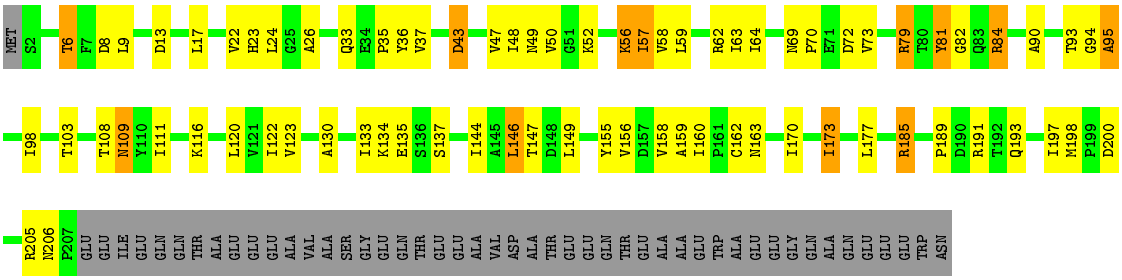






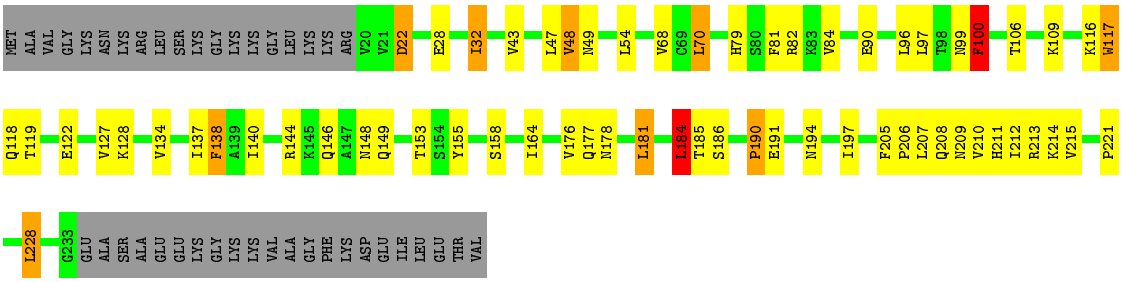
- Molecule 2: uS2

Chain A:



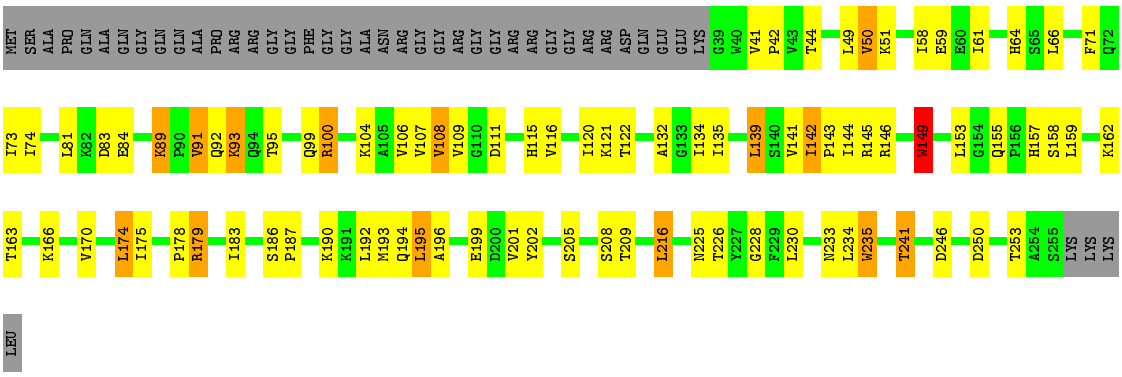
• Molecule 3: eS1

Chain B:



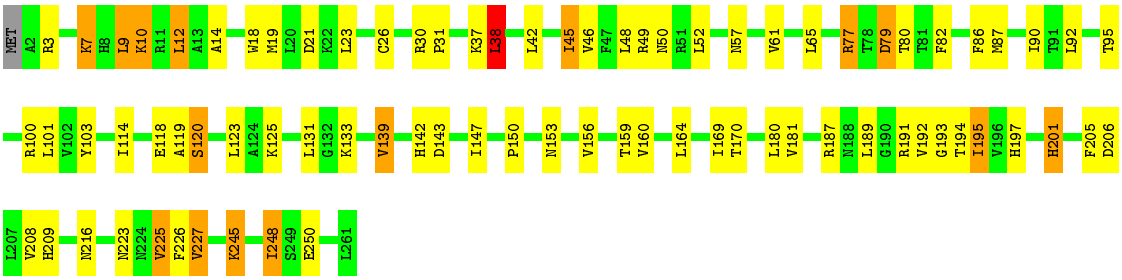
• Molecule 4: uS5

Chain C:



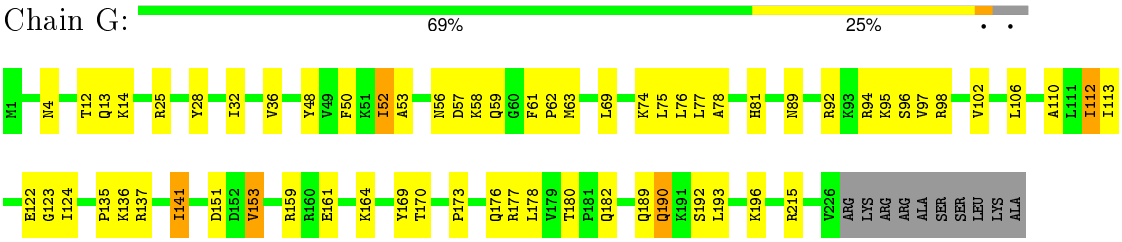
• Molecule 5: eS4

Chain E:



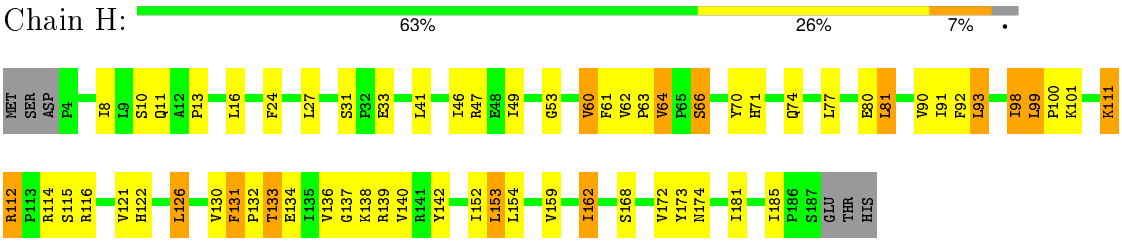
• Molecule 6: eS6

Chain G:



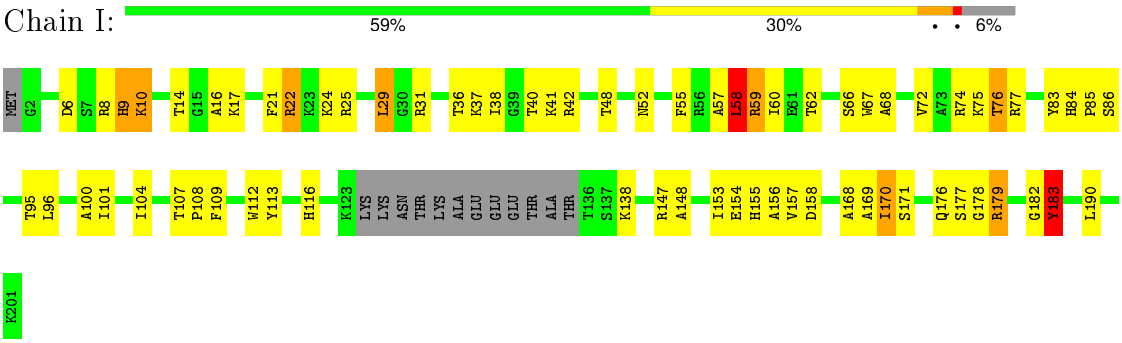
- Molecule 7: eS7

Chain H:



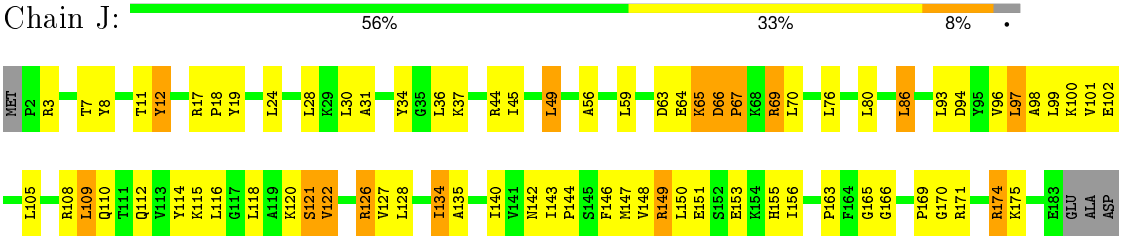
- Molecule 8: eS8

Chain I:



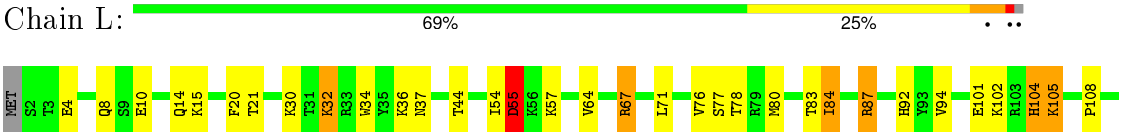
- Molecule 9: uS4

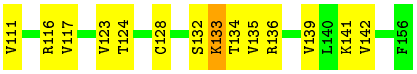
Chain J:



- Molecule 10: uS17

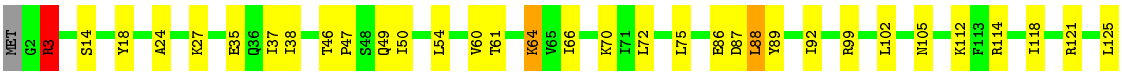
Chain L:





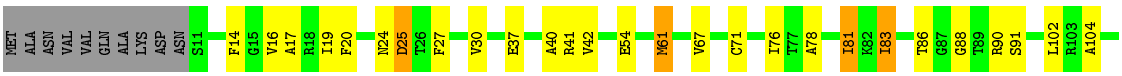
- Molecule 11: uS15

Chain N:



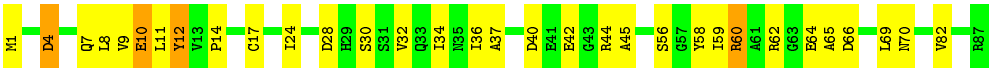
- Molecule 12: uS11

Chain O:



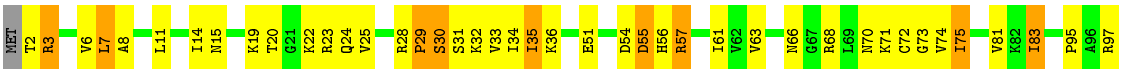
- Molecule 13: eS21

Chain V:



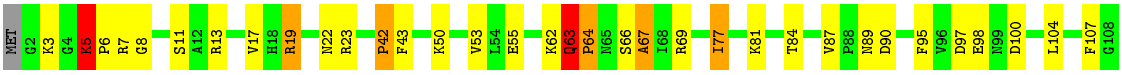
- Molecule 14: uS8

Chain W:



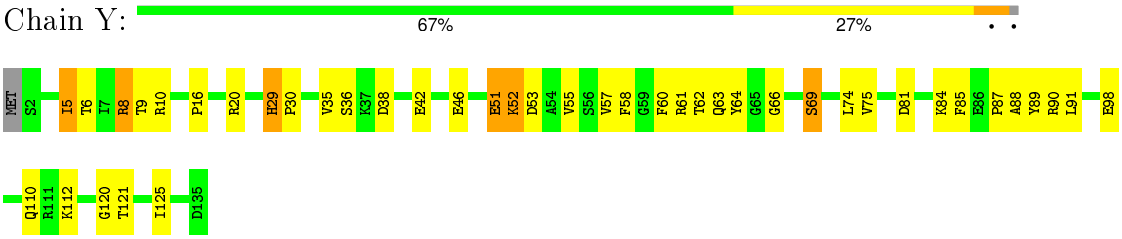
- Molecule 15: uS12

Chain X:



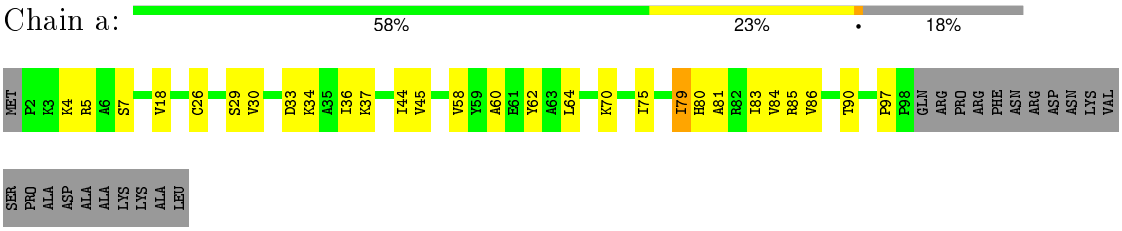
- Molecule 16: eS24

Chain Y:



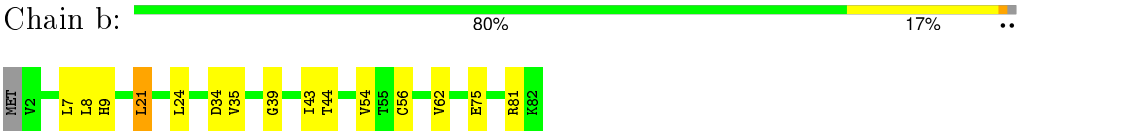
- Molecule 17: eS26

Chain a:



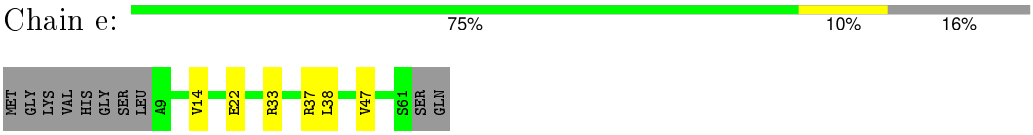
- Molecule 18: eS27

Chain b:



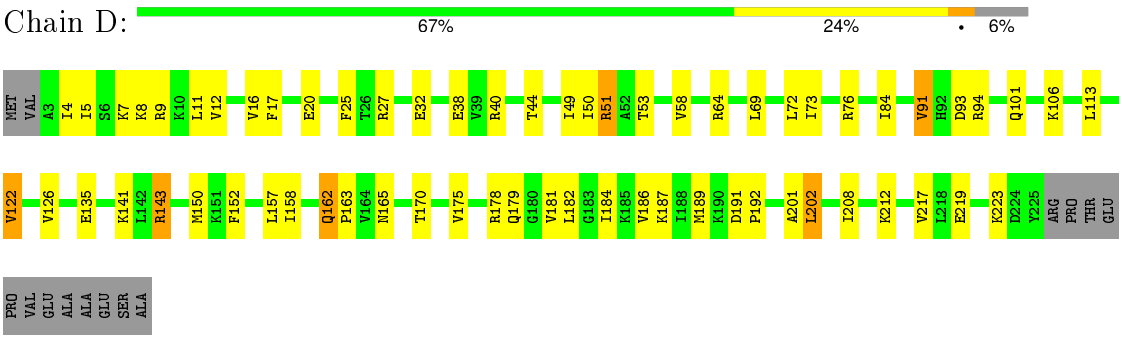
- Molecule 19: eS30

Chain e:



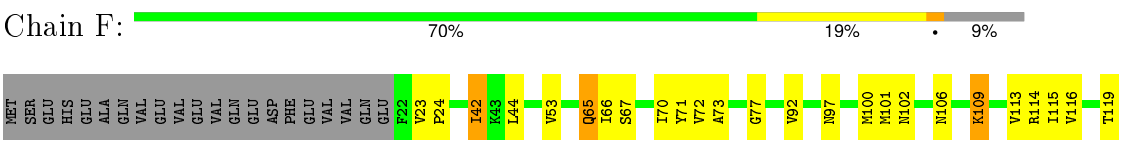
- Molecule 20: uS3

Chain D:



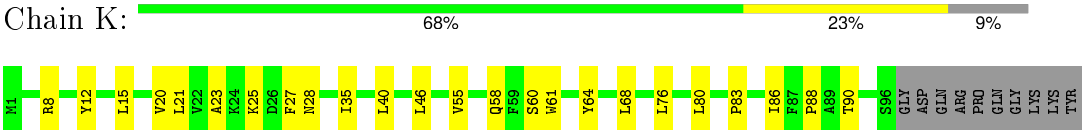
- Molecule 21: uS7

Chain F:



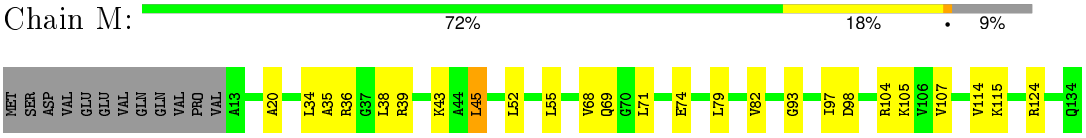
- Molecule 22: eS10

Chain K:



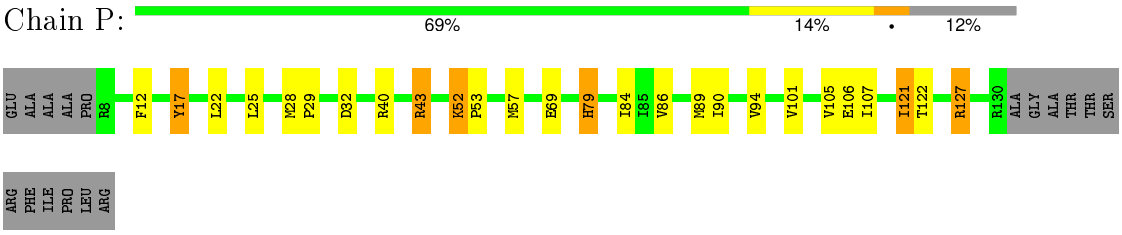
- Molecule 23: eS12

Chain M:



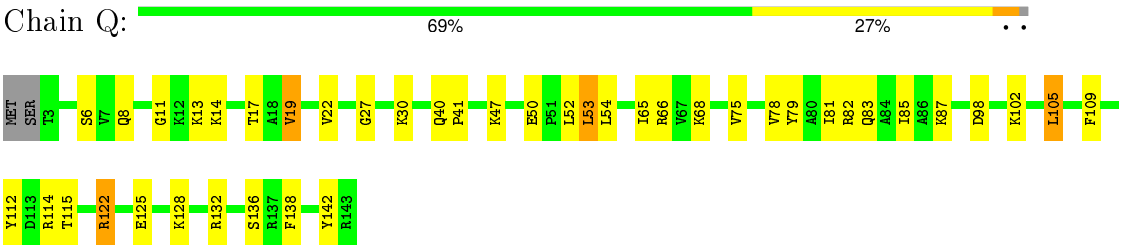
- Molecule 24: uS19

Chain P:



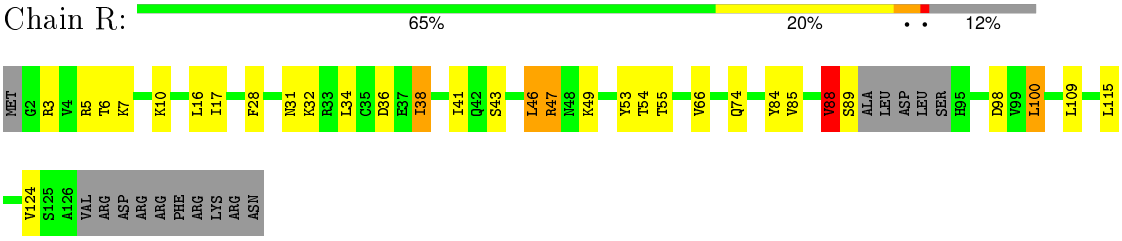
- Molecule 25: uS9

Chain Q:



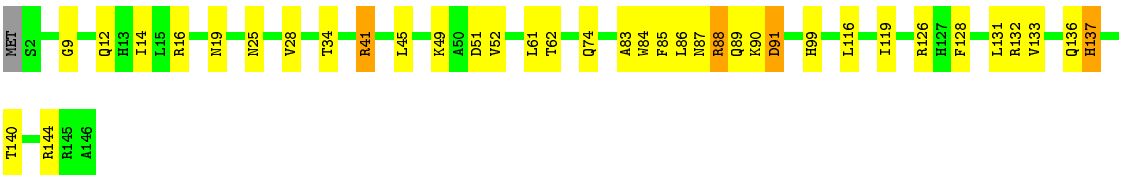
- Molecule 26: eS17

Chain R:



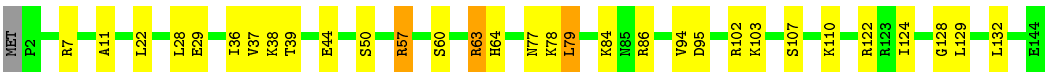
- Molecule 27: uS13

Chain S:



- Molecule 28: eS19

Chain T:



- Molecule 29: uS10

Chain U:

- Molecule 30: eS25

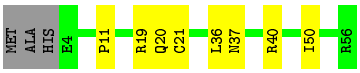
Chain Z:

- Molecule 31: eS28

Chain c:

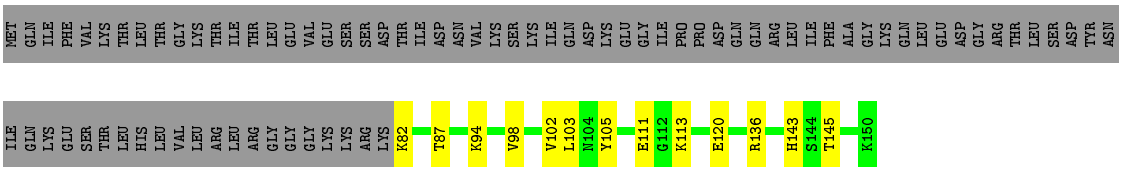
- Molecule 32: uS14

Chain d:



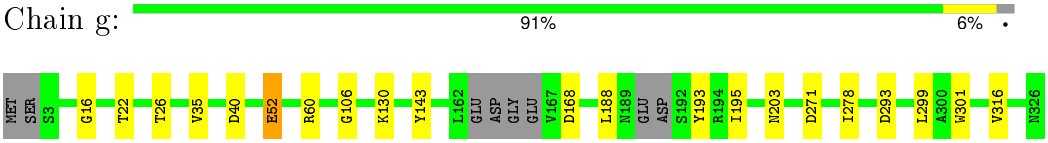
- Molecule 33: eS31

Chain f:



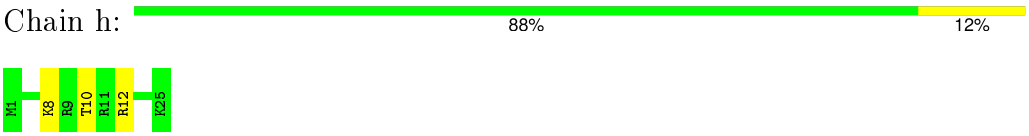
- Molecule 34: RACK1

Chain g:



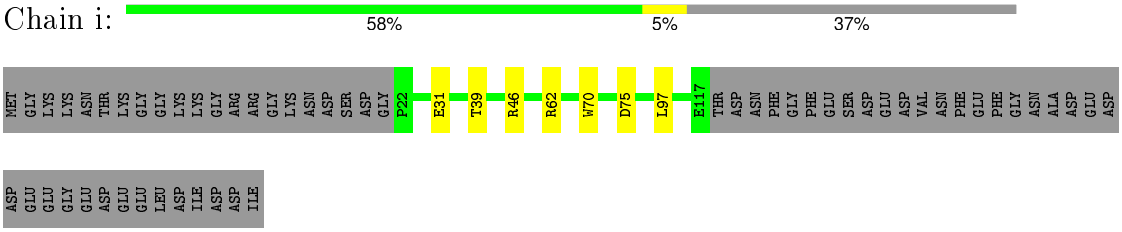
- Molecule 35: eL41

Chain h:



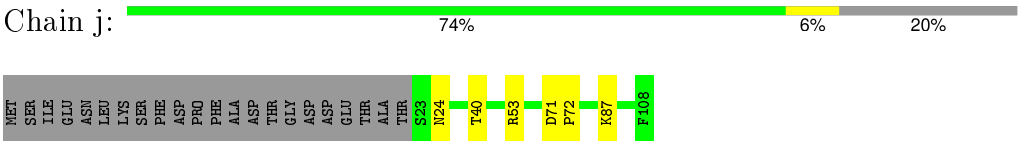
- Molecule 36: eIF1A

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	100709	Depositor
Resolution determination method	FSC 0.143	Depositor
CTF correction method	Each particle	Depositor
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	28	Depositor
Minimum defocus (nm)	1600	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	0.30	0/42244	0.70	5/65823 (0.0%)
10	L	0.45	0/1276	0.70	0/1718
11	N	0.45	0/1210	0.78	1/1628 (0.1%)
12	O	0.40	0/953	0.72	0/1279
13	V	0.43	0/696	0.73	0/938
14	W	0.50	0/1039	0.82	0/1399
15	X	0.48	0/1137	0.80	0/1516
16	Y	0.42	0/1075	0.72	0/1433
17	a	0.44	0/782	0.82	0/1047
18	b	0.40	0/619	0.70	0/837
19	e	0.39	0/435	0.70	0/579
2	A	0.43	0/1656	0.78	0/2264
20	D	0.43	0/1769	0.70	0/2378
21	F	0.40	0/1628	0.71	0/2198
22	K	0.46	0/831	0.67	0/1123
23	M	0.40	0/929	0.69	0/1255
24	P	0.43	0/1000	0.65	0/1343
25	Q	0.41	0/1125	0.69	0/1510
26	R	0.44	0/969	0.73	0/1299
27	S	0.39	0/1212	0.68	0/1629
28	T	0.39	0/1129	0.68	0/1520
29	U	0.43	0/857	0.73	0/1158
3	B	0.40	0/1747	0.72	1/2353 (0.0%)
30	Z	0.43	0/567	0.64	0/762
31	c	0.39	0/496	0.72	0/666
32	d	0.47	0/457	0.66	0/607
33	f	0.47	0/562	0.65	0/751
34	g	0.41	0/2521	0.61	0/3431
35	h	0.39	0/234	0.81	0/300
36	i	0.38	0/788	0.62	0/1051
37	j	0.41	0/703	0.66	0/938
4	C	0.45	0/1659	0.79	3/2252 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 2$	RMSZ	$\#\|Z\| > 2$
5	E	0.41	0/2122	0.71	1/2861 (0.0%)
6	G	0.39	0/1835	0.68	0/2451
7	H	0.43	0/1507	0.74	0/2028
8	I	0.44	0/1519	0.74	2/2033 (0.1%)
9	J	0.45	0/1495	0.82	2/2001 (0.1%)
All	All	0.37	0/82783	0.71	15/120359 (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
14	W	0	1
15	X	0	2
16	Y	0	1
17	a	0	1
25	Q	0	1
7	H	0	1
9	J	0	1
All	All	0	8

There are no bond length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	2	1315	G	C2'-C3'-O3'	7.15	125.23	109.50
9	J	49	LEU	CA-CB-CG	7.12	131.67	115.30
4	C	139	LEU	CA-CB-CG	6.41	130.05	115.30
3	B	184	LEU	CA-CB-CG	6.33	129.86	115.30
8	I	29	LEU	CA-CB-CG	6.22	129.61	115.30

There are no chirality outliers.

5 of 8 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
7	H	131	PHE	Peptide
9	J	12	TYR	Peptide
14	W	75	ILE	Peptide
15	X	11	SER	Peptide
15	X	63	GLN	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	37775	0	19004	704	0
2	A	1616	0	1636	35	0
3	B	1722	0	1795	27	0
4	C	1629	0	1710	41	0
5	E	2078	0	2157	37	0
6	G	1812	0	1911	32	0
7	H	1483	0	1579	29	0
8	I	1493	0	1515	29	0
9	J	1471	0	1554	43	0
10	L	1248	0	1311	25	0
11	N	1187	0	1251	17	0
12	O	942	0	979	16	0
13	V	687	0	682	14	0
14	W	1021	0	1056	34	0
15	X	1119	0	1198	21	0
16	Y	1061	0	1111	17	0
17	a	770	0	822	0	0
18	b	609	0	631	0	0
19	e	428	0	468	0	0
20	D	1744	0	1826	27	0
21	F	1609	0	1679	18	0
22	K	809	0	810	10	0
23	M	922	0	953	9	0
24	P	980	0	1026	10	0
25	Q	1105	0	1170	20	0
26	R	959	0	1006	12	0
27	S	1193	0	1217	19	0
28	T	1110	0	1124	16	0
29	U	845	0	913	14	0
30	Z	558	0	585	2	0
31	c	494	0	534	0	0
32	d	446	0	436	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	67	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	77716	0	60411	1161	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 9.

The worst 5 of 1161 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)
1:2:1037:U:H3	1:2:1091:A:N6	1.23	1.32
1:2:1290:G:N2	1:2:1323:G:H22	1.28	1.28
1:2:991:A:N1	1:2:1011:U:O4	1.78	1.15
1:2:991:A:N1	1:2:1011:U:C4	2.17	1.12
1:2:1290:G:H22	1:2:1323:G:N2	1.56	1.03

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	204/254 (80%)	167 (82%)	24 (12%)	13 (6%)	2 26
3	B	212/255 (83%)	175 (82%)	25 (12%)	12 (6%)	2 28
4	C	215/259 (83%)	182 (85%)	23 (11%)	10 (5%)	3 33
5	E	258/261 (99%)	215 (83%)	36 (14%)	7 (3%)	6 48
6	G	224/236 (95%)	196 (88%)	24 (11%)	4 (2%)	11 56
7	H	182/190 (96%)	152 (84%)	15 (8%)	15 (8%)	1 18

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
8	I	184/201 (92%)	146 (79%)	26 (14%)	12 (6%)	1 26
9	J	180/188 (96%)	148 (82%)	20 (11%)	12 (7%)	1 25
10	L	153/156 (98%)	129 (84%)	18 (12%)	6 (4%)	4 38
11	N	148/151 (98%)	127 (86%)	17 (12%)	4 (3%)	6 48
12	O	125/137 (91%)	98 (78%)	20 (16%)	7 (6%)	2 29
13	V	85/87 (98%)	67 (79%)	11 (13%)	7 (8%)	1 18
14	W	127/130 (98%)	109 (86%)	13 (10%)	5 (4%)	4 38
15	X	142/145 (98%)	115 (81%)	13 (9%)	14 (10%)	1 13
16	Y	132/135 (98%)	114 (86%)	10 (8%)	8 (6%)	2 27
17	a	95/119 (80%)	64 (67%)	21 (22%)	10 (10%)	1 12
18	b	79/82 (96%)	62 (78%)	12 (15%)	5 (6%)	2 26
19	e	51/63 (81%)	47 (92%)	3 (6%)	1 (2%)	9 54
20	D	221/237 (93%)	197 (89%)	18 (8%)	6 (3%)	6 48
21	F	204/227 (90%)	169 (83%)	25 (12%)	10 (5%)	3 32
22	K	94/106 (89%)	81 (86%)	11 (12%)	2 (2%)	9 53
23	M	120/134 (90%)	96 (80%)	20 (17%)	4 (3%)	5 44
24	P	121/140 (86%)	99 (82%)	16 (13%)	6 (5%)	3 32
25	Q	139/143 (97%)	120 (86%)	15 (11%)	4 (3%)	6 46
26	R	116/136 (85%)	93 (80%)	18 (16%)	5 (4%)	3 36
27	S	143/146 (98%)	113 (79%)	23 (16%)	7 (5%)	3 32
28	T	141/144 (98%)	123 (87%)	15 (11%)	3 (2%)	9 53
29	U	104/117 (89%)	91 (88%)	5 (5%)	8 (8%)	1 20
30	Z	68/108 (63%)	53 (78%)	10 (15%)	5 (7%)	1 21
31	c	61/67 (91%)	55 (90%)	6 (10%)	0	100 100
32	d	51/56 (91%)	41 (80%)	9 (18%)	1 (2%)	9 54
33	f	67/150 (45%)	43 (64%)	17 (25%)	7 (10%)	1 12
34	g	312/326 (96%)	256 (82%)	48 (15%)	8 (3%)	7 48
35	h	23/25 (92%)	23 (100%)	0	0	100 100
36	i	94/153 (61%)	86 (92%)	8 (8%)	0	100 100
37	j	84/108 (78%)	75 (89%)	8 (10%)	1 (1%)	16 63
All	All	4959/5572 (89%)	4127 (83%)	603 (12%)	229 (5%)	5 34

5 of 229 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	26	ALA
2	A	95	ALA
3	B	100	PHE
3	B	117	TRP
4	C	141	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%)	146 (84%)	28 (16%)	3 22
3	B	196/228 (86%)	176 (90%)	20 (10%)	9 43
4	C	176/203 (87%)	148 (84%)	28 (16%)	3 23
5	E	223/224 (100%)	189 (85%)	34 (15%)	3 25
6	G	192/200 (96%)	172 (90%)	20 (10%)	9 42
7	H	164/170 (96%)	140 (85%)	24 (15%)	4 27
8	I	148/159 (93%)	123 (83%)	25 (17%)	2 19
9	J	153/158 (97%)	129 (84%)	24 (16%)	3 24
10	L	136/137 (99%)	121 (89%)	15 (11%)	8 39
11	N	127/128 (99%)	114 (90%)	13 (10%)	9 43
12	O	96/104 (92%)	90 (94%)	6 (6%)	22 64
13	V	73/73 (100%)	59 (81%)	14 (19%)	2 13
14	W	110/111 (99%)	94 (86%)	16 (14%)	4 27
15	X	119/120 (99%)	104 (87%)	15 (13%)	5 32
16	Y	108/109 (99%)	88 (82%)	20 (18%)	2 15
17	a	82/100 (82%)	64 (78%)	18 (22%)	1 9
18	b	71/72 (99%)	60 (84%)	11 (16%)	3 24
19	e	47/55 (86%)	42 (89%)	5 (11%)	8 41
20	D	185/196 (94%)	161 (87%)	24 (13%)	5 32

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
21	F	174/194 (90%)	157 (90%)	17 (10%)	10 44
22	K	88/96 (92%)	79 (90%)	9 (10%)	9 43
23	M	97/109 (89%)	91 (94%)	6 (6%)	23 64
24	P	105/117 (90%)	92 (88%)	13 (12%)	6 33
25	Q	117/119 (98%)	102 (87%)	15 (13%)	5 32
26	R	109/124 (88%)	92 (84%)	17 (16%)	3 24
27	S	128/129 (99%)	110 (86%)	18 (14%)	4 29
28	T	117/118 (99%)	107 (92%)	10 (8%)	13 52
29	U	96/107 (90%)	82 (85%)	14 (15%)	4 27
30	Z	60/88 (68%)	57 (95%)	3 (5%)	30 70
31	c	55/59 (93%)	49 (89%)	6 (11%)	8 40
32	d	46/48 (96%)	39 (85%)	7 (15%)	3 25
33	f	58/133 (44%)	52 (90%)	6 (10%)	9 42
34	g	265/272 (97%)	251 (95%)	14 (5%)	28 69
35	h	23/23 (100%)	20 (87%)	3 (13%)	5 32
36	i	83/130 (64%)	76 (92%)	7 (8%)	14 53
37	j	77/96 (80%)	72 (94%)	5 (6%)	21 63
All	All	4278/4720 (91%)	3748 (88%)	530 (12%)	10 33

5 of 530 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
13	V	8	LEU
16	Y	81	ASP
32	d	20	GLN
13	V	59	ILE
15	X	19	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 51 such sidechains are listed below:

Mol	Chain	Res	Type
11	N	49	GLN
14	W	24	GLN
32	d	10	HIS
12	O	99	GLN

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Mol	Chain	Res	Type
15	X	22	ASN

5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	2	1777/1799 (98%)	836 (47%)	132 (7%)

5 of 836 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	2	2	A
1	2	3	U
1	2	4	C
1	2	5	U
1	2	11	A

5 of 132 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	2	747	C
1	2	1056	U
1	2	1655	U
1	2	812	U
1	2	896	C

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 70 ligands modelled in this entry, 70 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 (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.