



# wwPDB EM Validation Summary Report ⓘ

Feb 13, 2024 – 05:12 PM EST

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 initial models : 3U5C, 3U5B

This is a wwPDB EM Validation Summary Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto: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.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

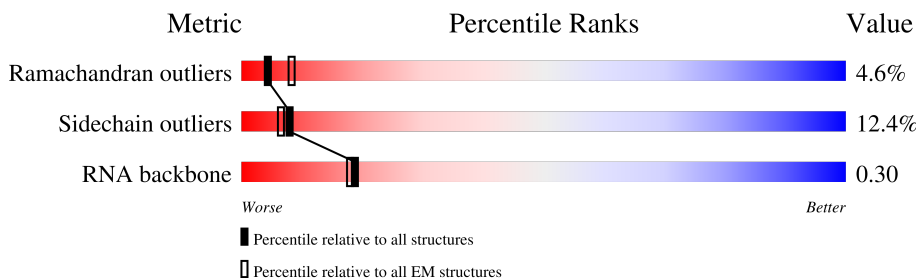
EMDB validation analysis : 0.0.1.dev70  
MolProbity : 4.02b-467  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.9  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.36

# 1 Overall quality at a glance

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

The reported resolution of this entry is 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)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. 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  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion  $< 40\%$ ). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	2	1799	6% (red), 51% (green), 48% (yellow), . (grey)
2	A	254	. (red), 66% (green), 15% (yellow), . (grey), 19% (grey)
3	B	255	. (red), 72% (green), 11% (yellow), . (grey), 16% (grey)
4	C	259	. (red), 68% (green), 15% (yellow), 16% (grey)
5	E	261	. (red), 85% (green), 14% (yellow), . (grey)
6	G	236	. (red), 86% (green), 10% (yellow), . (grey)
7	H	190	. (red), 76% (green), 20% (yellow), . (grey), . (grey)
8	I	201	7% (red), 76% (green), 15% (yellow), . (grey), 6% (grey)

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Mol	Chain	Length	Quality of chain
9	J	188	77% 20%
10	L	156	87% 12%
11	N	151	88% 11%
12	O	137	83% 9% 7%
13	V	87	78% 20%
14	W	130	83% 15%
15	X	145	80% 18%
16	Y	135	79% 19%
17	a	119	58% 23% 18%
18	b	82	80% 17%
19	e	63	75% 10% 16%
20	D	237	82% 12% 6%
21	F	227	79% 11% 9%
22	K	106	80% 10% 9%
23	M	134	84% 7% 9%
24	P	140	75% 12% 12%
25	Q	143	85% 14%
26	R	136	74% 13% 12%
27	S	146	82% 17%
28	T	144	90% 9%
29	U	117	73% 17% 9%
30	Z	108	59% 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	
35	h	25	
36	i	153	
37	j	108	

## 2 Entry composition [i](#)

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
			Total	C	N	O		
7	H	184	1483	950	270	263	0	0

- Molecule 8 is a protein called eS8.

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

- Molecule 9 is a protein called uS4.

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

- Molecule 10 is a protein called uS17.

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

- Molecule 11 is a protein called uS15.

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

- Molecule 12 is a protein called uS11.

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

- Molecule 13 is a protein called eS21.

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

- 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
			Total	C	N	O	S		
35	h	25	233	142	63	27	1	0	0

- Molecule 36 is a protein called eIF1A.

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

- Molecule 37 is a protein called eIF1.

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

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

Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
38	2	67	67	67	0

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

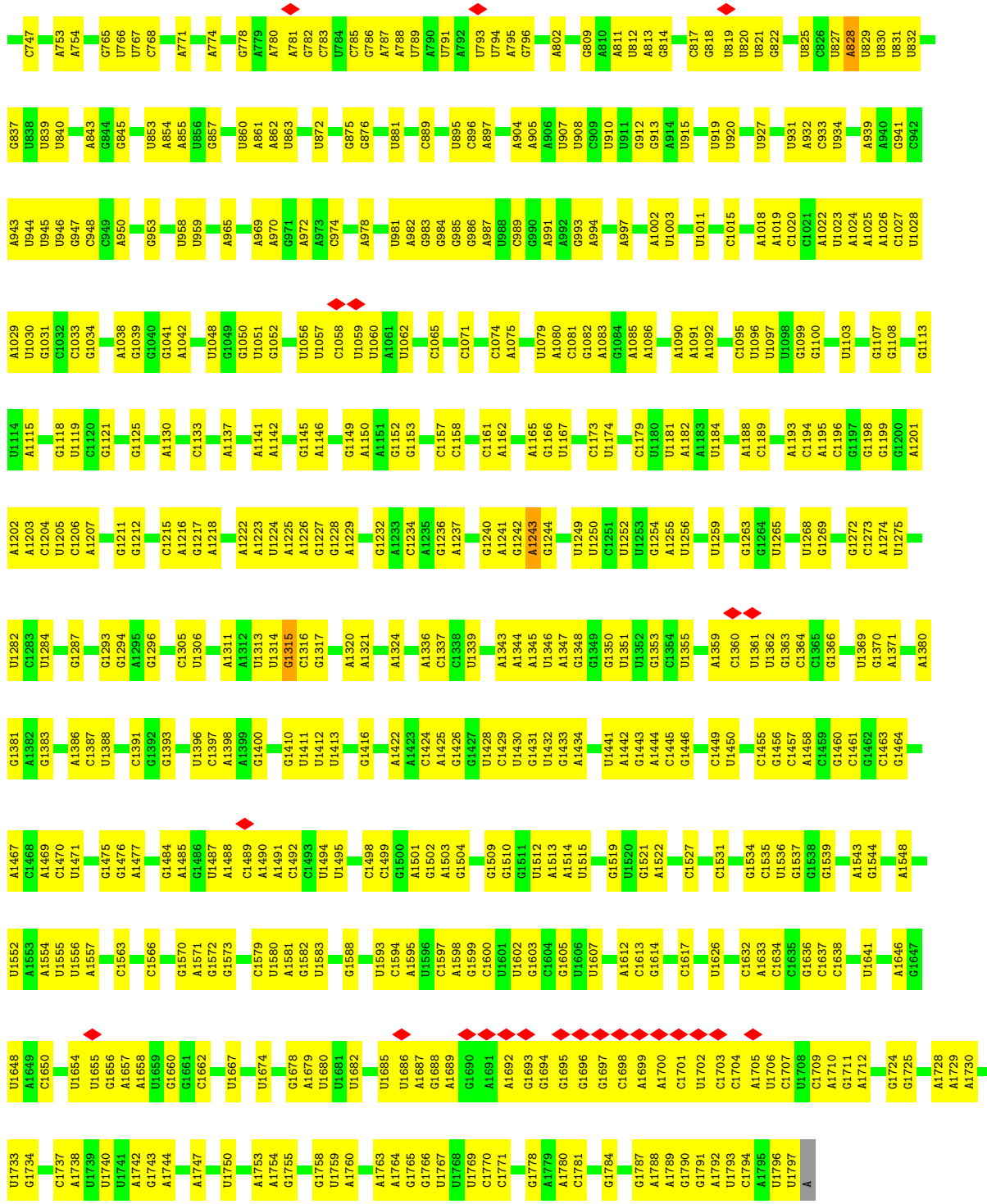
Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
39	a	1	1	1	0
39	b	1	1	1	0
39	f	1	1	1	0

### 3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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 and atom inclusion in map density. 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. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). 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.

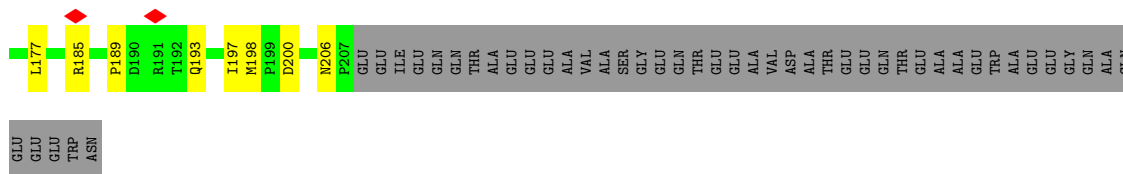
- Molecule 1: 18S rRNA



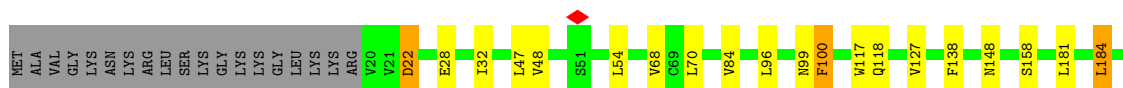


• Molecule 2: uS2

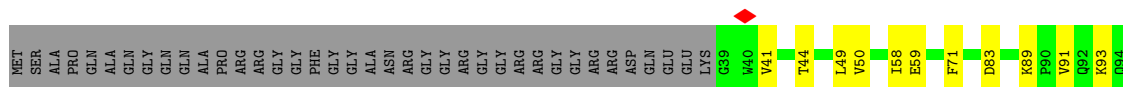




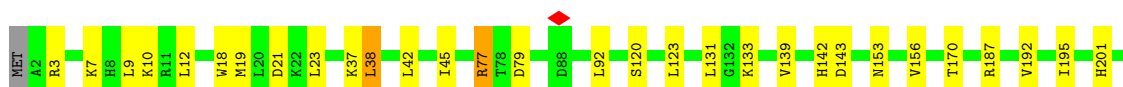
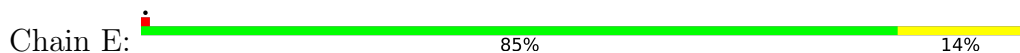
• Molecule 3: eS1



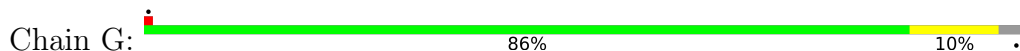
• Molecule 4: uS5



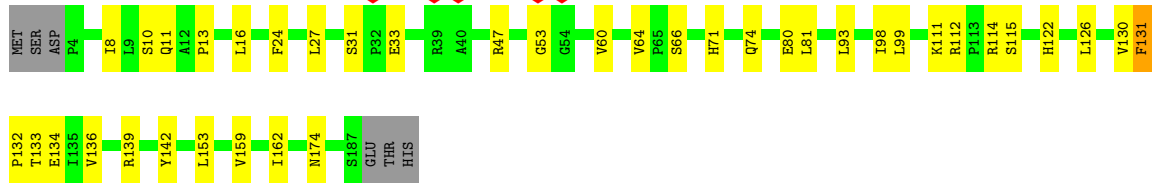
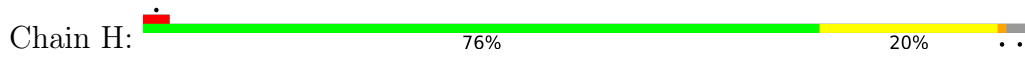
• Molecule 5: eS4



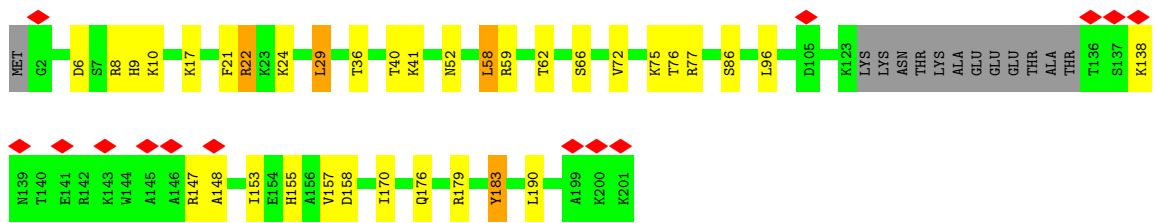
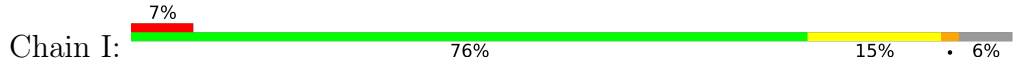
• Molecule 6: eS6



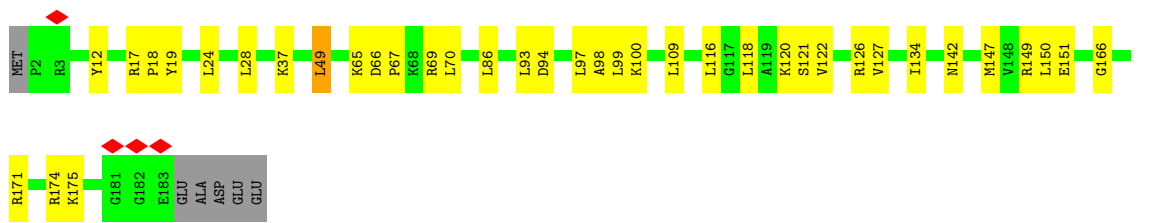
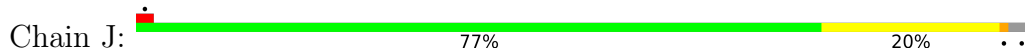
• Molecule 7: eS7



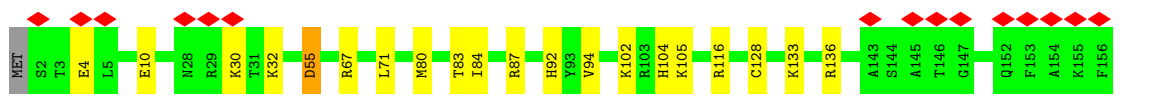
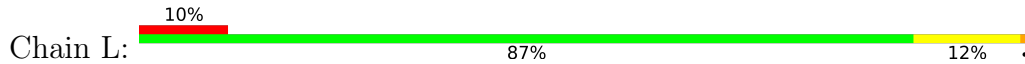
• Molecule 8: eS8



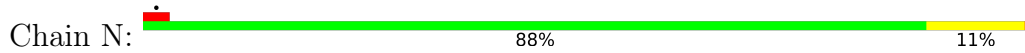
• Molecule 9: uS4



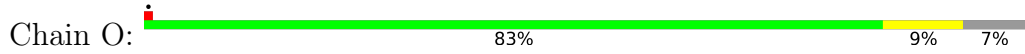
• Molecule 10: uS17



• Molecule 11: uS15

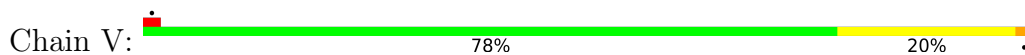


• Molecule 12: uS11

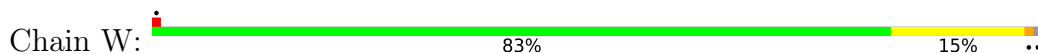




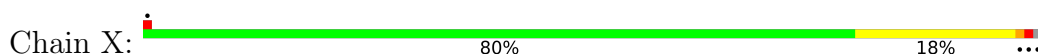
• Molecule 13: eS21



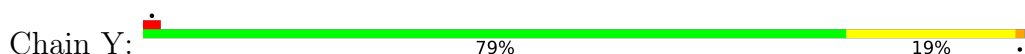
• Molecule 14: uS8



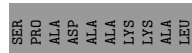
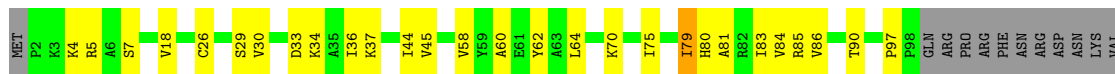
• Molecule 15: uS12



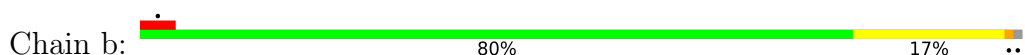
• Molecule 16: eS24



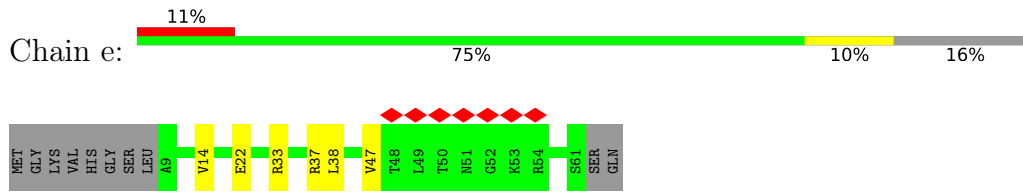
• Molecule 17: eS26



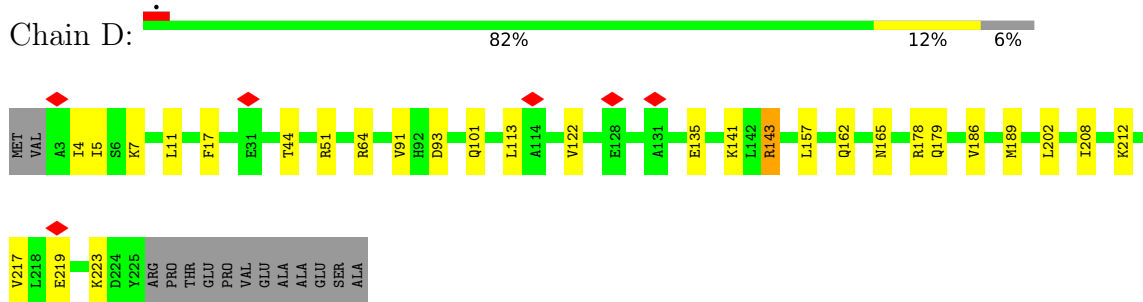
• Molecule 18: eS27



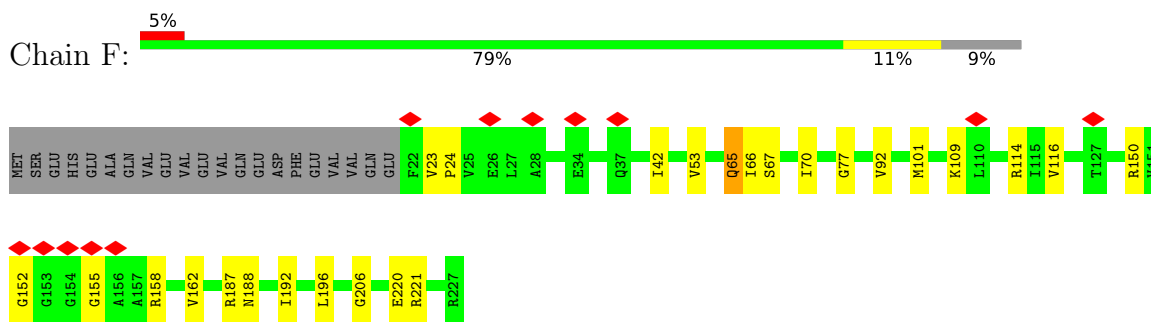
• Molecule 19: eS30



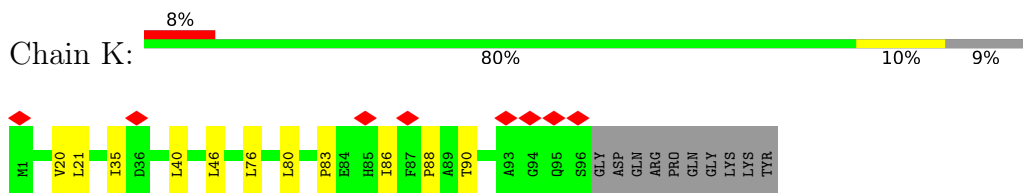
• Molecule 20: uS3



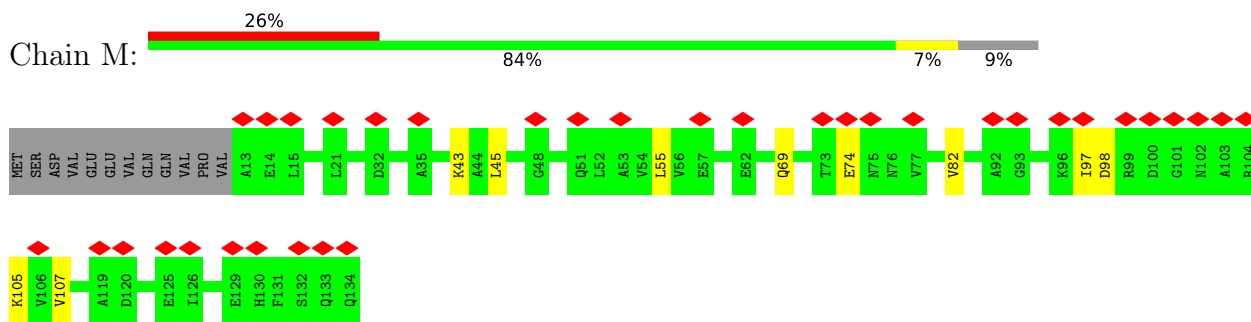
• Molecule 21: uS7



• Molecule 22: eS10

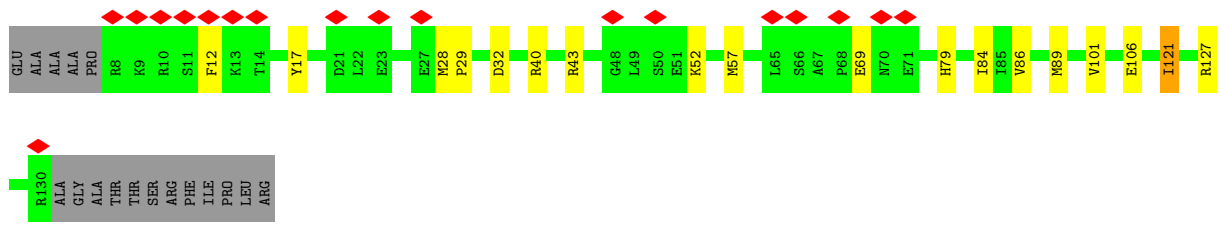
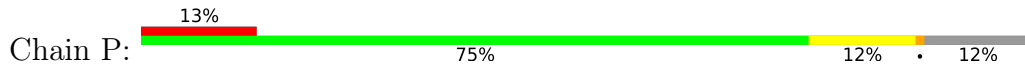


• Molecule 23: eS12

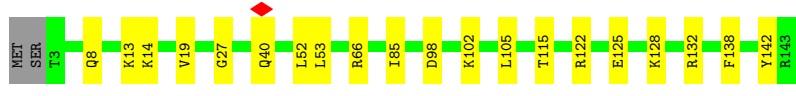
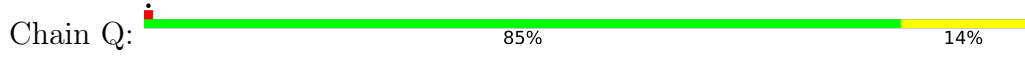


• Molecule 24: uS19

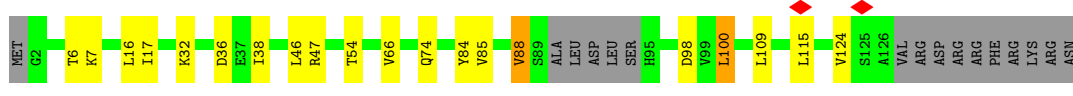
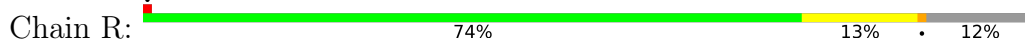




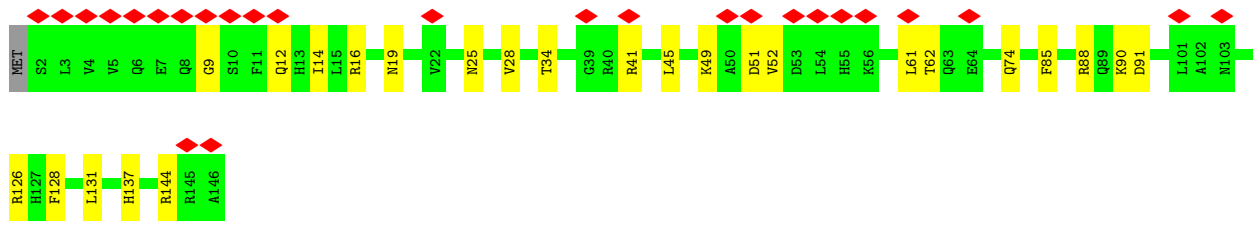
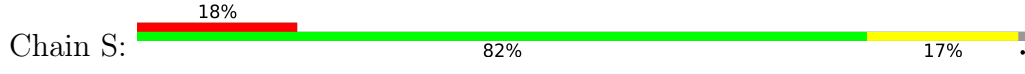
• Molecule 25: uS9



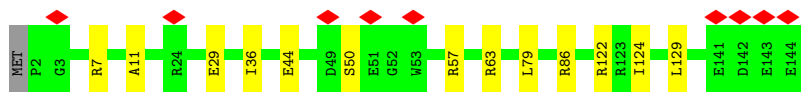
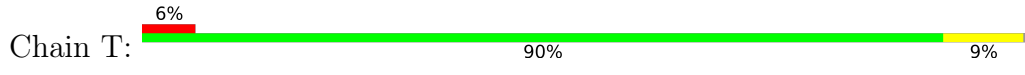
• Molecule 26: eS17



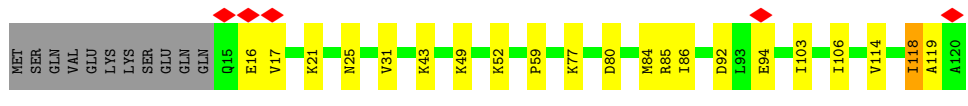
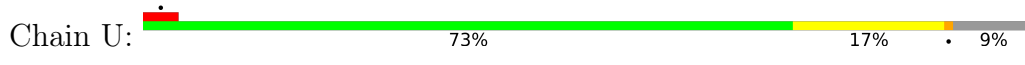
• Molecule 27: uS13



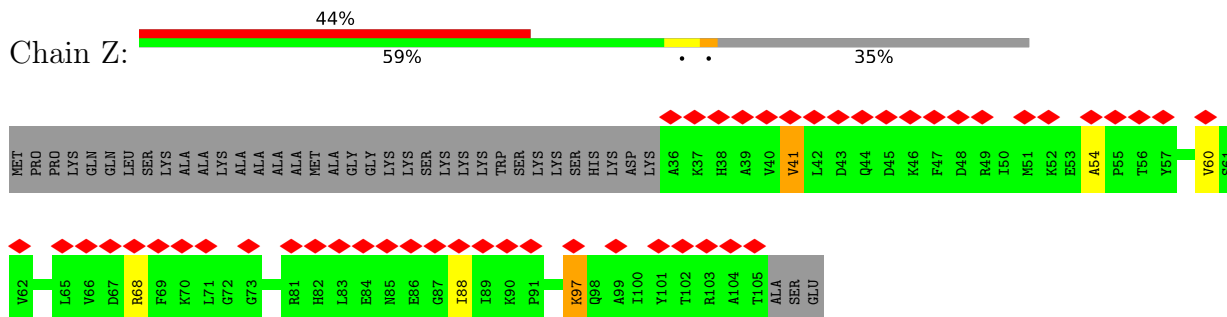
• Molecule 28: eS19



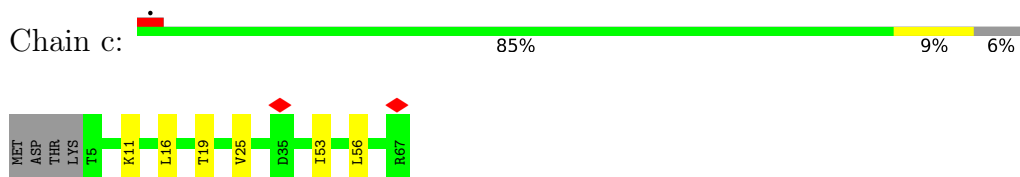
• Molecule 29: uS10



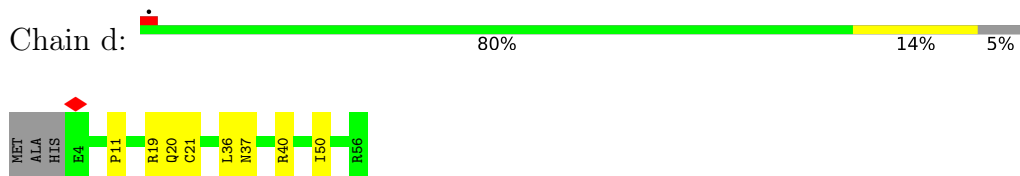
- Molecule 30: eS25



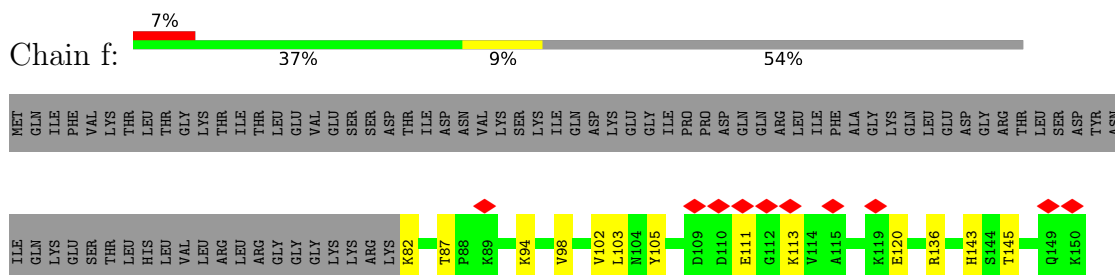
- Molecule 31: eS28



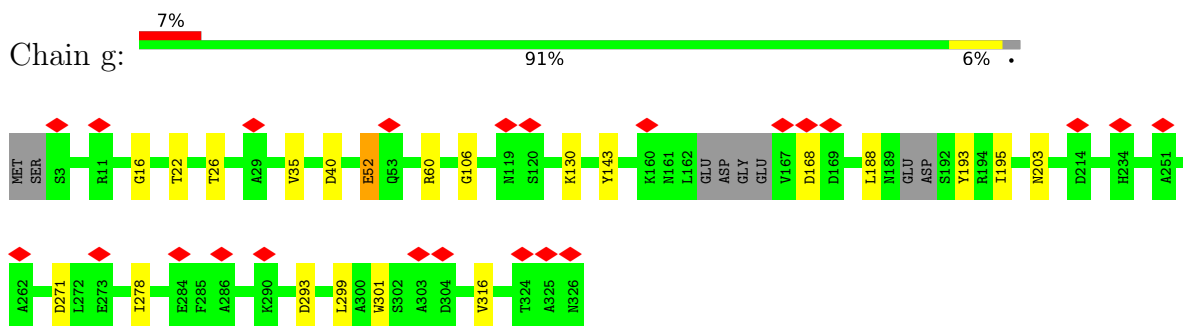
- Molecule 32: uS14



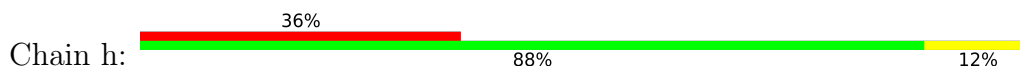
- Molecule 33: eS31



- Molecule 34: RACK1

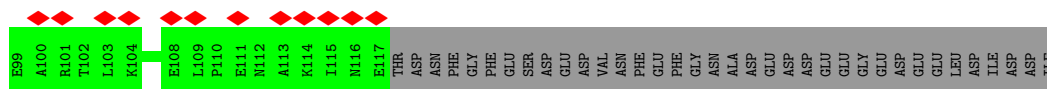
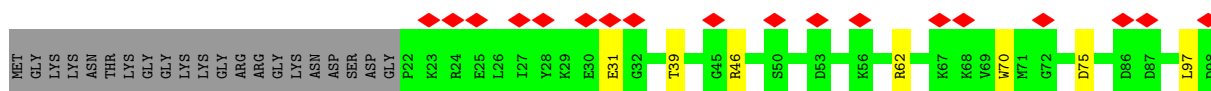


- Molecule 35: eL41

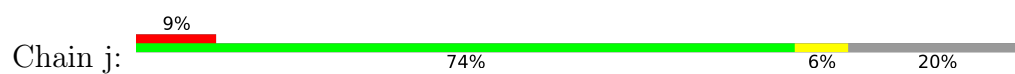




- Molecule 36: eIF1A



- Molecule 37: eIF1



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	100709	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	Each particle	Depositor
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	28	Depositor
Minimum defocus (nm)	1600	Depositor
Maximum defocus (nm)	4000	Depositor
Magnification	104478	Depositor
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	0.602	Depositor
Minimum map value	-0.221	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.024	Depositor
Recommended contour level	0.065	Depositor
Map size ( $\text{\AA}$ )	402.0, 402.0, 402.0	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	1.34, 1.34, 1.34	Depositor

## 5 Model quality

### 5.1 Standard geometry

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

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  >5	RMSZ	# Z  >5
1	2	0.30	0/42244	0.70	5/65823 (0.0%)
2	A	0.43	0/1656	0.78	0/2264
3	B	0.40	0/1747	0.72	1/2353 (0.0%)
4	C	0.45	0/1659	0.79	3/2252 (0.1%)
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%)
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
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
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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
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
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
7	H	0	1
9	J	0	1
14	W	0	1
15	X	0	2
16	Y	0	1
17	a	0	1
25	Q	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(°)	Ideal(°)
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](#)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

## 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%)	1	19
3	B	212/255 (83%)	175 (82%)	25 (12%)	12 (6%)	1	20
4	C	215/259 (83%)	182 (85%)	23 (11%)	10 (5%)	2	24
5	E	258/261 (99%)	215 (83%)	36 (14%)	7 (3%)	5	35
6	G	224/236 (95%)	196 (88%)	24 (11%)	4 (2%)	8	42
7	H	182/190 (96%)	152 (84%)	15 (8%)	15 (8%)	1	12
8	I	184/201 (92%)	146 (79%)	26 (14%)	12 (6%)	1	19
9	J	180/188 (96%)	148 (82%)	20 (11%)	12 (7%)	1	18
10	L	153/156 (98%)	129 (84%)	18 (12%)	6 (4%)	3	28
11	N	148/151 (98%)	127 (86%)	17 (12%)	4 (3%)	5	35
12	O	125/137 (91%)	98 (78%)	20 (16%)	7 (6%)	2	21
13	V	85/87 (98%)	67 (79%)	11 (13%)	7 (8%)	1	12
14	W	127/130 (98%)	109 (86%)	13 (10%)	5 (4%)	3	28
15	X	142/145 (98%)	115 (81%)	13 (9%)	14 (10%)	0	9
16	Y	132/135 (98%)	114 (86%)	10 (8%)	8 (6%)	1	19
17	a	95/119 (80%)	64 (67%)	21 (22%)	10 (10%)	0	8
18	b	79/82 (96%)	62 (78%)	12 (15%)	5 (6%)	1	19
19	e	51/63 (81%)	47 (92%)	3 (6%)	1 (2%)	7	41
20	D	221/237 (93%)	197 (89%)	18 (8%)	6 (3%)	5	35
21	F	204/227 (90%)	169 (83%)	25 (12%)	10 (5%)	2	23
22	K	94/106 (89%)	81 (86%)	11 (12%)	2 (2%)	7	40

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
23	M	120/134 (90%)	96 (80%)	20 (17%)	4 (3%)	4	32
24	P	121/140 (86%)	99 (82%)	16 (13%)	6 (5%)	2	23
25	Q	139/143 (97%)	120 (86%)	15 (11%)	4 (3%)	4	34
26	R	116/136 (85%)	93 (80%)	18 (16%)	5 (4%)	2	26
27	S	143/146 (98%)	113 (79%)	23 (16%)	7 (5%)	2	23
28	T	141/144 (98%)	123 (87%)	15 (11%)	3 (2%)	7	40
29	U	104/117 (89%)	91 (88%)	5 (5%)	8 (8%)	1	14
30	Z	68/108 (63%)	53 (78%)	10 (15%)	5 (7%)	1	15
31	c	61/67 (91%)	55 (90%)	6 (10%)	0	100	100
32	d	51/56 (91%)	41 (80%)	9 (18%)	1 (2%)	7	41
33	f	67/150 (45%)	43 (64%)	17 (25%)	7 (10%)	0	8
34	g	312/326 (96%)	256 (82%)	48 (15%)	8 (3%)	5	36
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%)	13	49
All	All	4959/5572 (89%)	4127 (83%)	603 (12%)	229 (5%)	4	24

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%)	2	16

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	B	196/228 (86%)	176 (90%)	20 (10%)	7	32
4	C	176/203 (87%)	148 (84%)	28 (16%)	2	16
5	E	223/224 (100%)	189 (85%)	34 (15%)	3	18
6	G	192/200 (96%)	172 (90%)	20 (10%)	7	31
7	H	164/170 (96%)	140 (85%)	24 (15%)	3	19
8	I	148/159 (93%)	123 (83%)	25 (17%)	2	14
9	J	153/158 (97%)	129 (84%)	24 (16%)	2	17
10	L	136/137 (99%)	121 (89%)	15 (11%)	6	29
11	N	127/128 (99%)	114 (90%)	13 (10%)	7	32
12	O	96/104 (92%)	90 (94%)	6 (6%)	18	49
13	V	73/73 (100%)	59 (81%)	14 (19%)	1	9
14	W	110/111 (99%)	94 (86%)	16 (14%)	3	19
15	X	119/120 (99%)	104 (87%)	15 (13%)	4	24
16	Y	108/109 (99%)	88 (82%)	20 (18%)	1	10
17	a	82/100 (82%)	64 (78%)	18 (22%)	1	6
18	b	71/72 (99%)	60 (84%)	11 (16%)	2	17
19	e	47/55 (86%)	42 (89%)	5 (11%)	6	30
20	D	185/196 (94%)	161 (87%)	24 (13%)	4	23
21	F	174/194 (90%)	157 (90%)	17 (10%)	8	33
22	K	88/96 (92%)	79 (90%)	9 (10%)	7	32
23	M	97/109 (89%)	91 (94%)	6 (6%)	18	50
24	P	105/117 (90%)	92 (88%)	13 (12%)	4	24
25	Q	117/119 (98%)	102 (87%)	15 (13%)	4	23
26	R	109/124 (88%)	92 (84%)	17 (16%)	2	17
27	S	128/129 (99%)	110 (86%)	18 (14%)	3	21
28	T	117/118 (99%)	107 (92%)	10 (8%)	10	40
29	U	96/107 (90%)	82 (85%)	14 (15%)	3	19
30	Z	60/88 (68%)	57 (95%)	3 (5%)	24	55
31	c	55/59 (93%)	49 (89%)	6 (11%)	6	29
32	d	46/48 (96%)	39 (85%)	7 (15%)	3	18
33	f	58/133 (44%)	52 (90%)	6 (10%)	7	31

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
34	g	265/272 (97%)	251 (95%)	14 (5%)	22	54
35	h	23/23 (100%)	20 (87%)	3 (13%)	4	23
36	i	83/130 (64%)	76 (92%)	7 (8%)	11	41
37	j	77/96 (80%)	72 (94%)	5 (6%)	17	49
All	All	4278/4720 (91%)	3748 (88%)	530 (12%)	8	24

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

Mol	Chain	Res	Type
28	T	124	ILE
29	U	103	ILE
28	T	122	ARG
36	i	46	ARG
9	J	122	VAL

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

Mol	Chain	Res	Type
14	W	24	GLN
21	F	102	ASN
36	i	112	ASN
15	X	22	ASN
16	Y	29	HIS

### 5.3.3 RNA [i](#)

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	1570	G
1	2	1613	C
1	2	1788	A
1	2	577	U
1	2	566	A

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

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

#### 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

#### 5.6 Ligand geometry [i](#)

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.

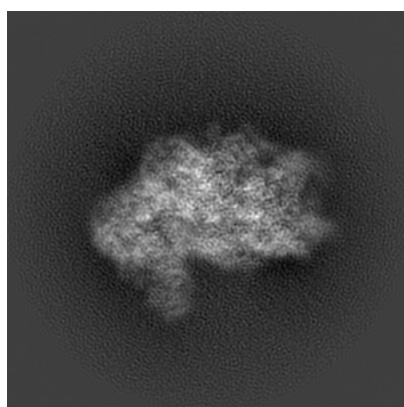
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-2764. These allow visual inspection of the internal detail of the map and identification of artifacts.

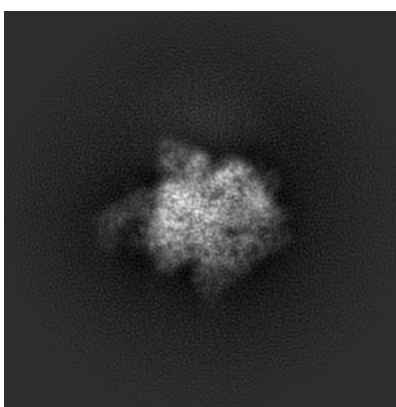
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

### 6.1 Orthogonal projections [i](#)

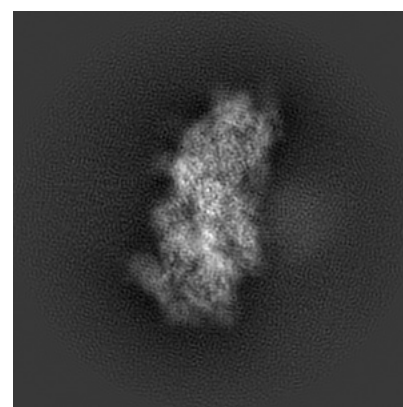
#### 6.1.1 Primary map



X



Y

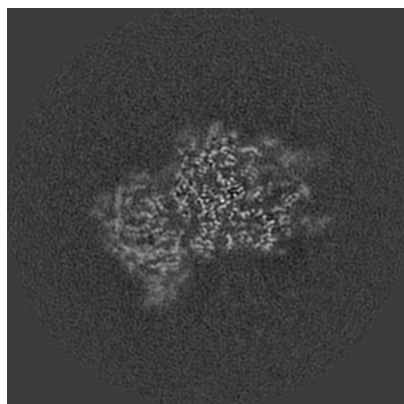


Z

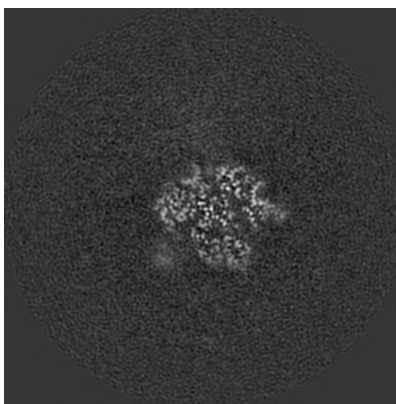
The images above show the map projected in three orthogonal directions.

### 6.2 Central slices [i](#)

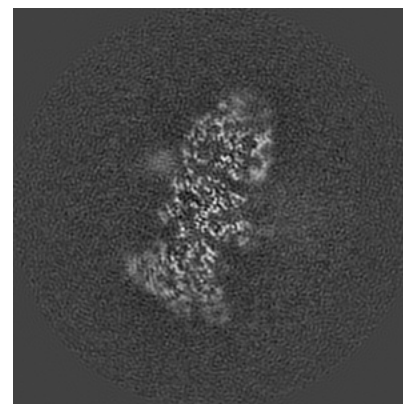
#### 6.2.1 Primary map



X Index: 150



Y Index: 150

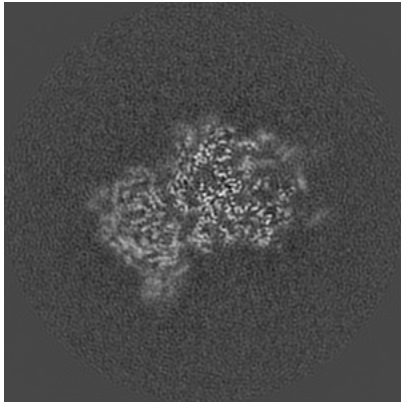


Z Index: 150

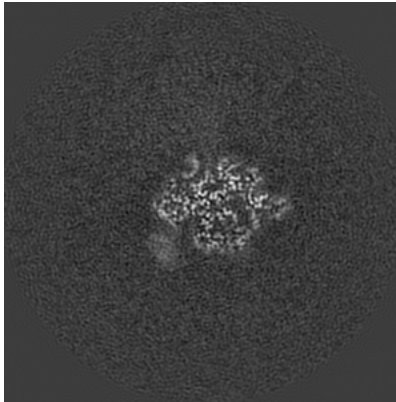
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

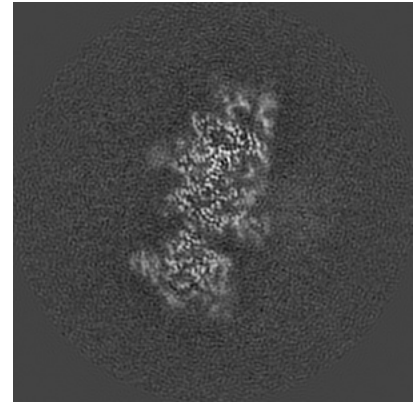
### 6.3.1 Primary map



X Index: 149



Y Index: 153

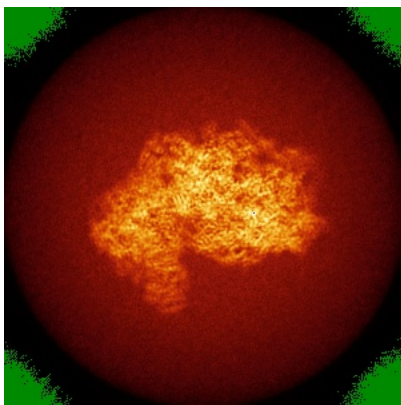


Z Index: 145

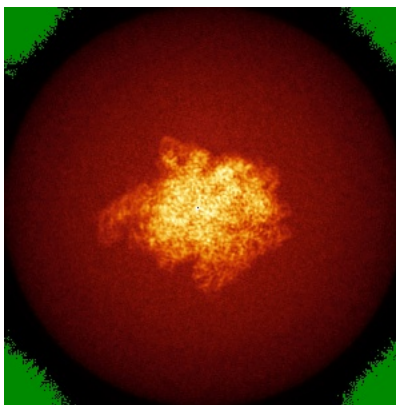
The images above show the largest variance slices of the map in three orthogonal directions.

## 6.4 Orthogonal standard-deviation projections (False-color) [i](#)

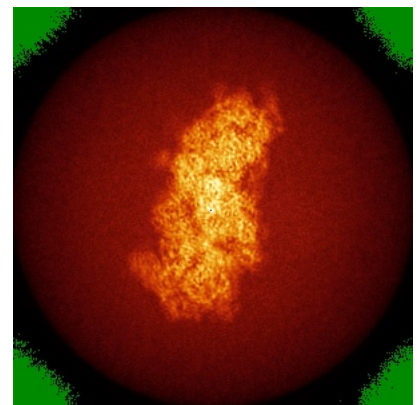
### 6.4.1 Primary map



X



Y

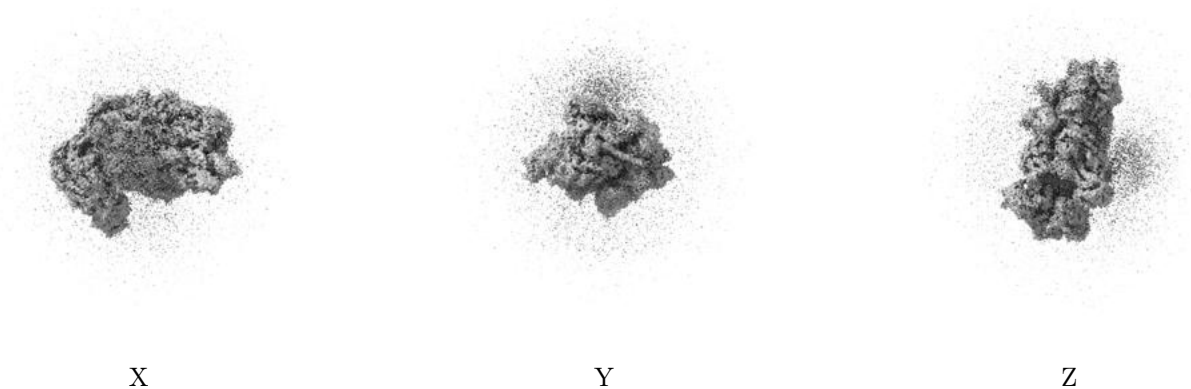


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.065. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

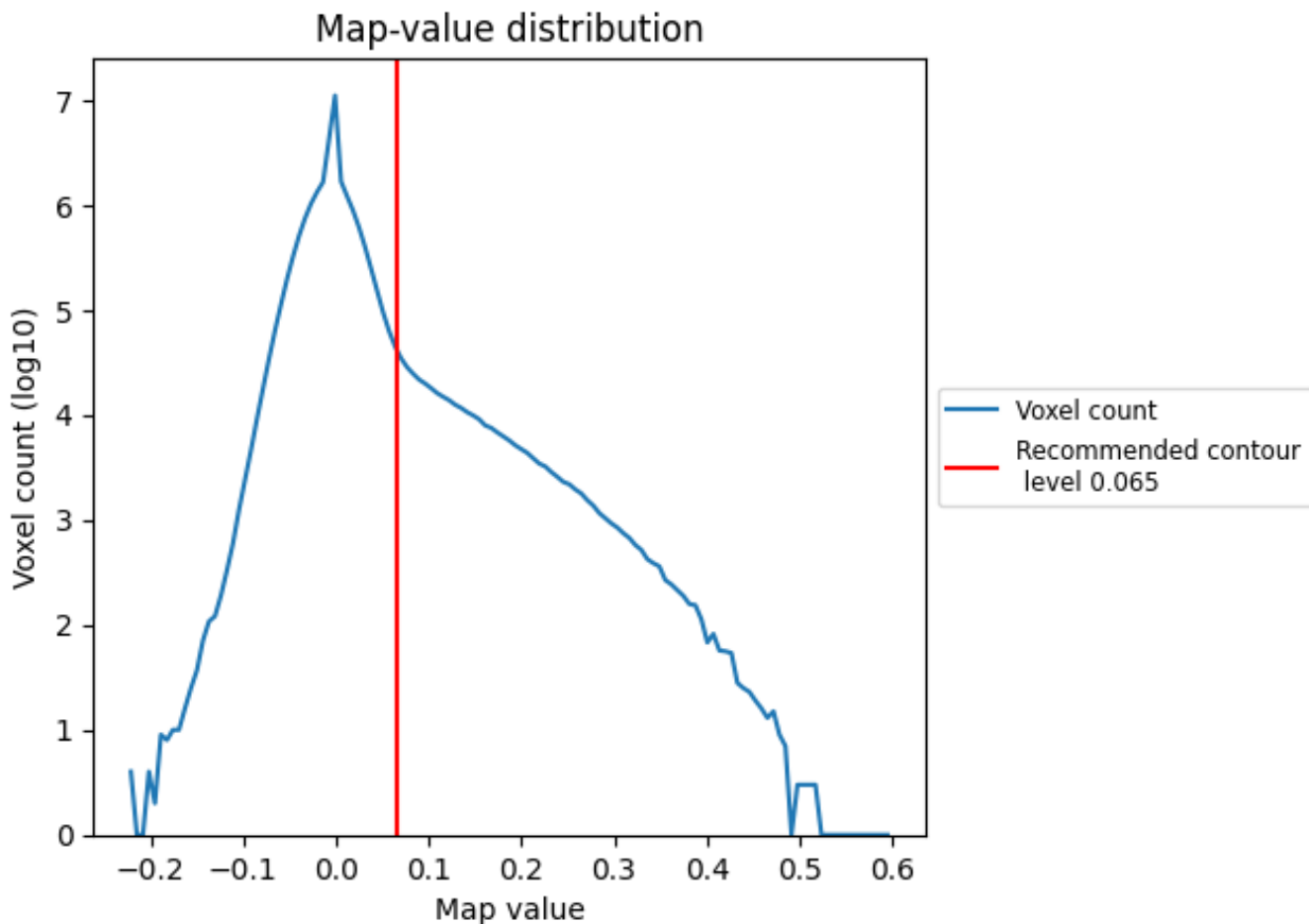
## 6.6 Mask visualisation [i](#)

This section was not generated. No masks/segmentation were deposited.

## 7 Map analysis [i](#)

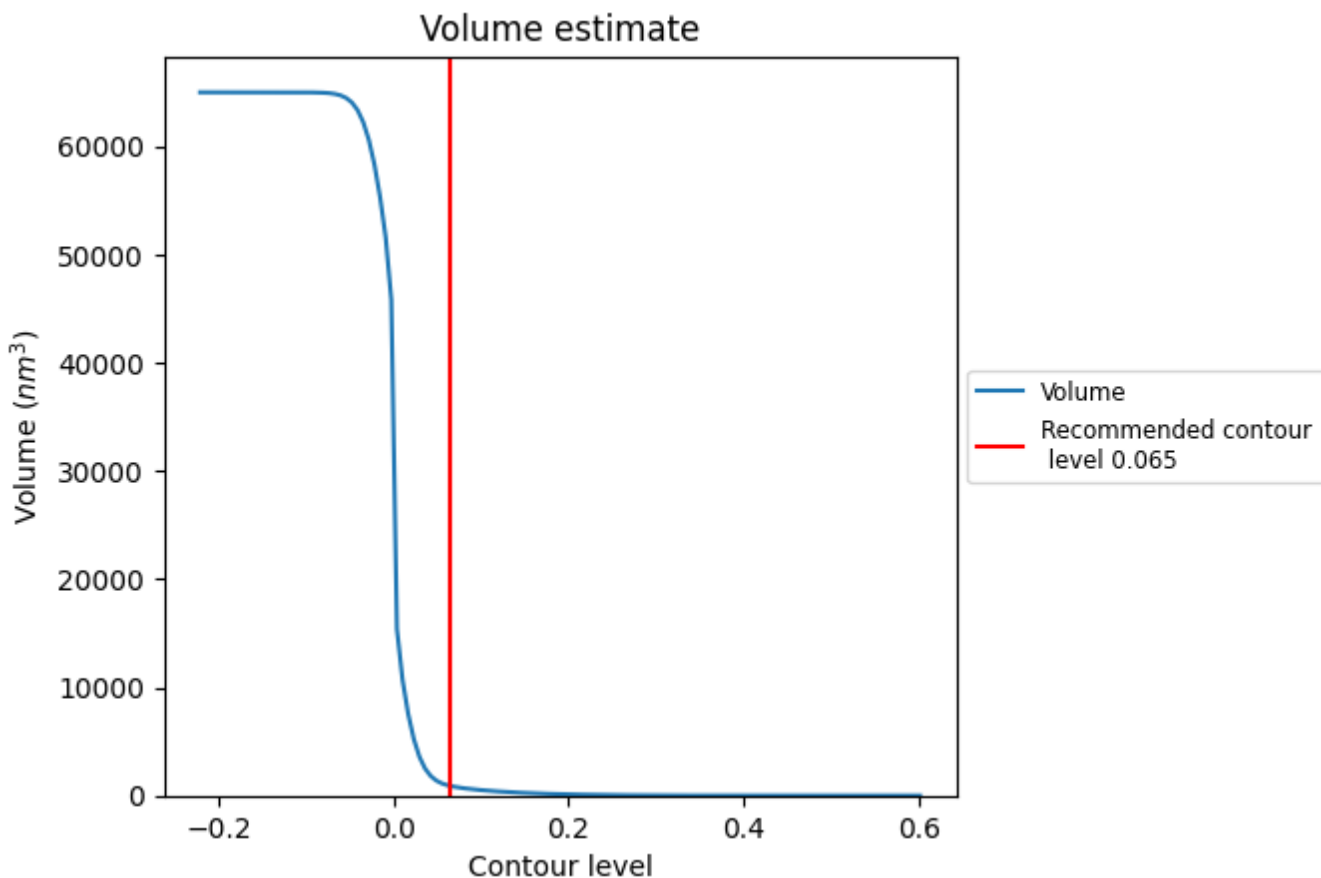
This section contains the results of statistical analysis of the map.

### 7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

## 7.2 Volume estimate [i](#)

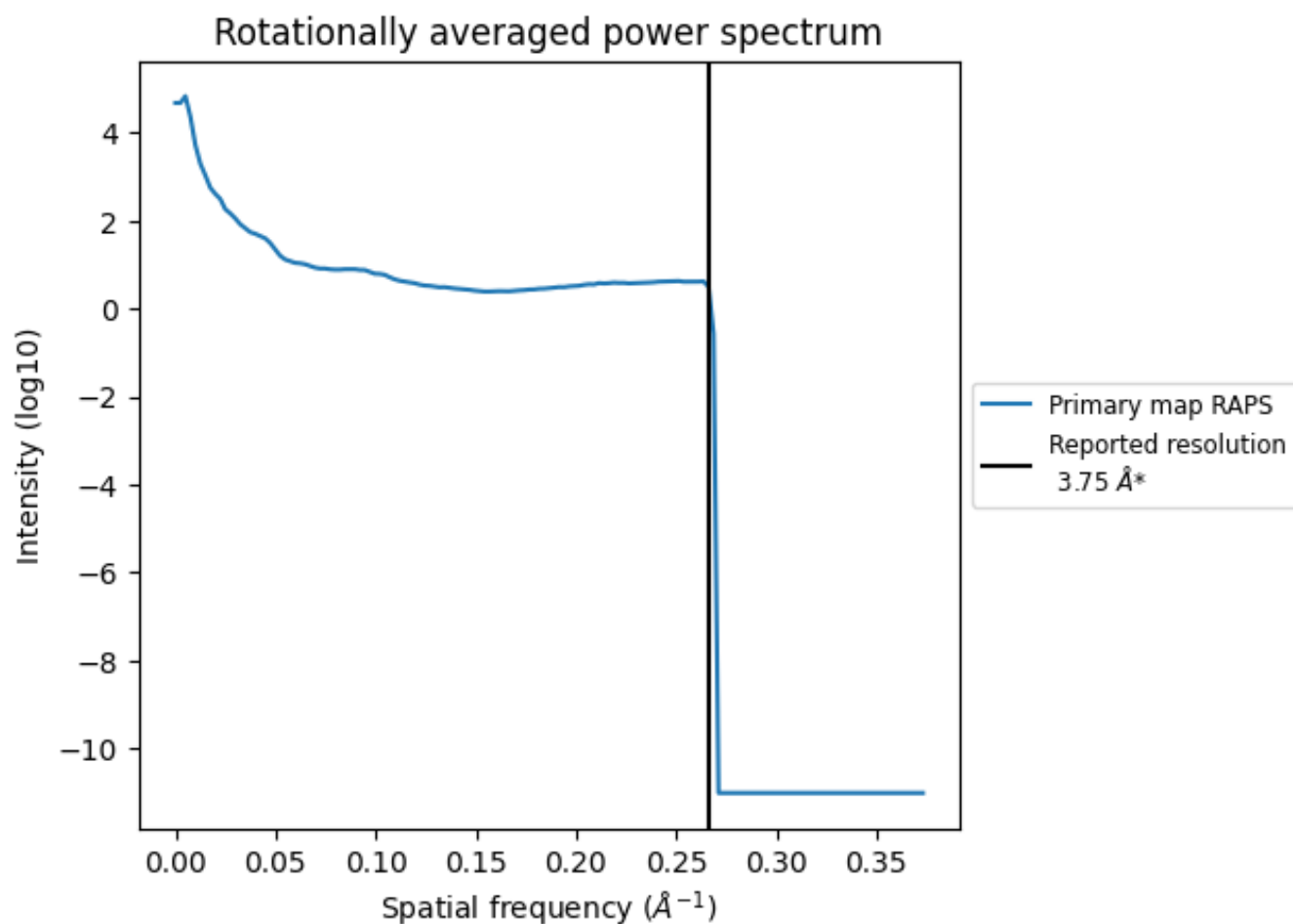


The volume at the recommended contour level is 888  $\text{nm}^3$ ; this corresponds to an approximate mass of 802 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.



### 7.3 Rotationally averaged power spectrum [\(i\)](#)

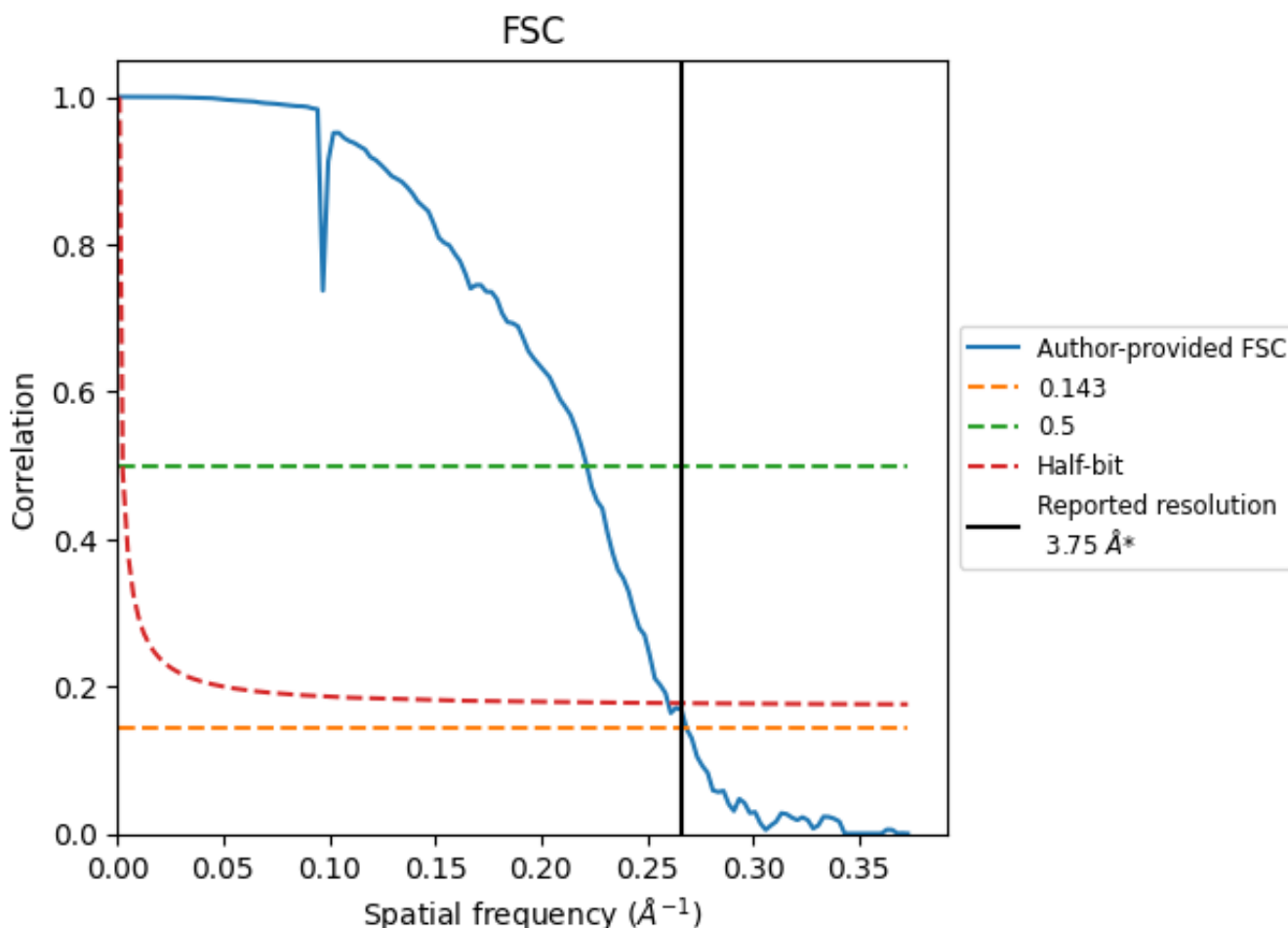


\*Reported resolution corresponds to spatial frequency of 0.267 Å<sup>-1</sup>

## 8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of 0.267 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

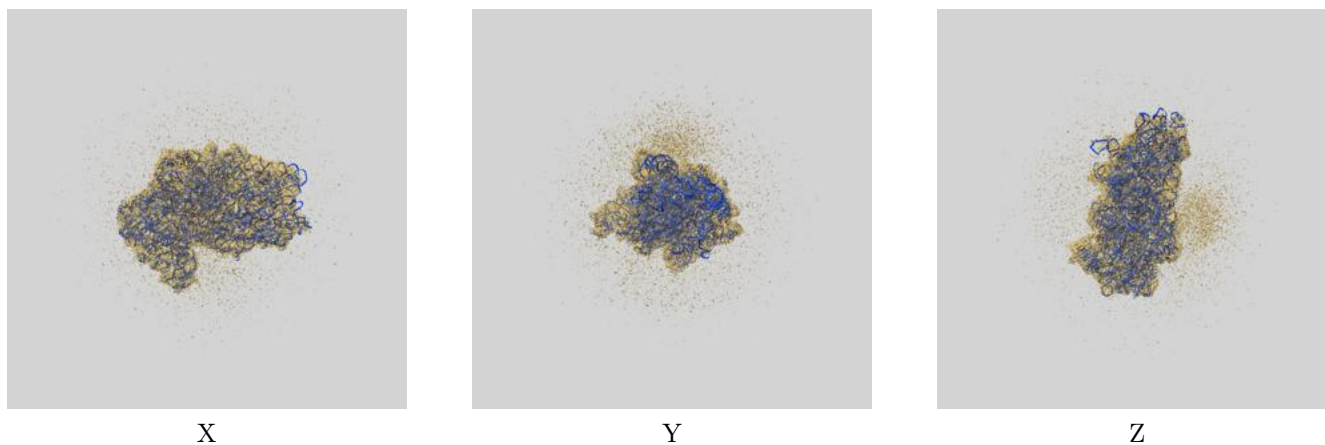
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.75	-	-
Author-provided FSC curve	3.72	4.51	3.85
Unmasked-calculated*	-	-	-

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

## 9 Map-model fit [i](#)

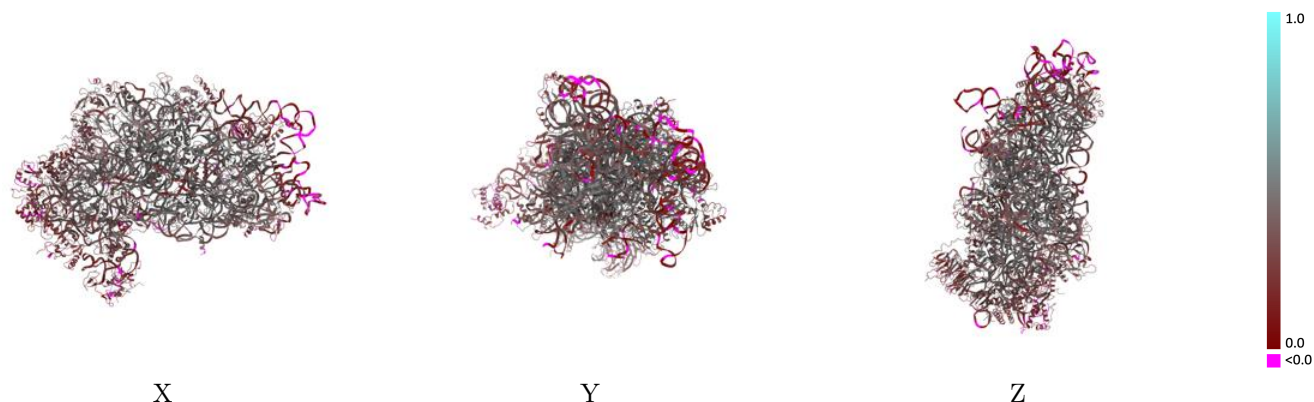
This section contains information regarding the fit between EMDB map EMD-2764 and PDB model 3J80. Per-residue inclusion information can be found in section 3 on page 11.

### 9.1 Map-model overlay [i](#)



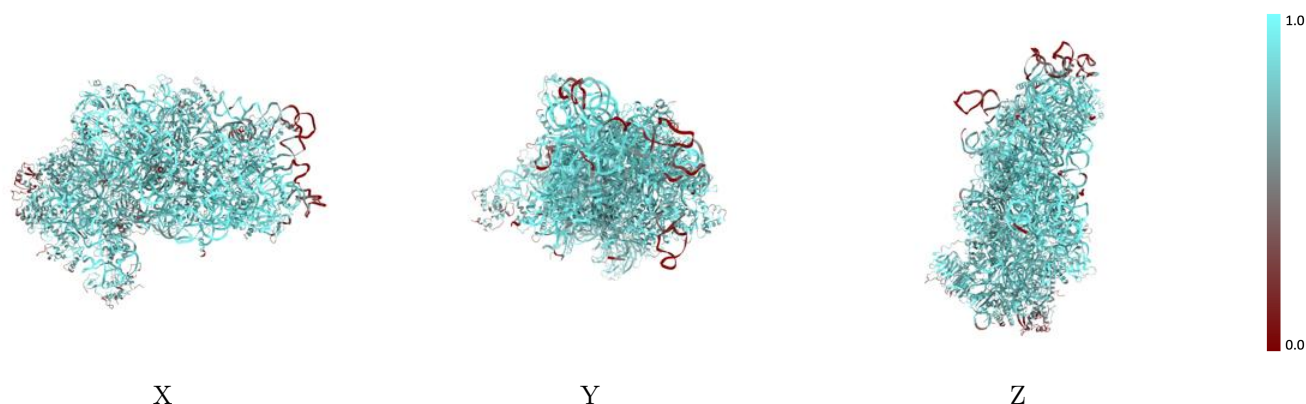
The images above show the 3D surface view of the map at the recommended contour level 0.065 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

## 9.2 Q-score mapped to coordinate model [i](#)



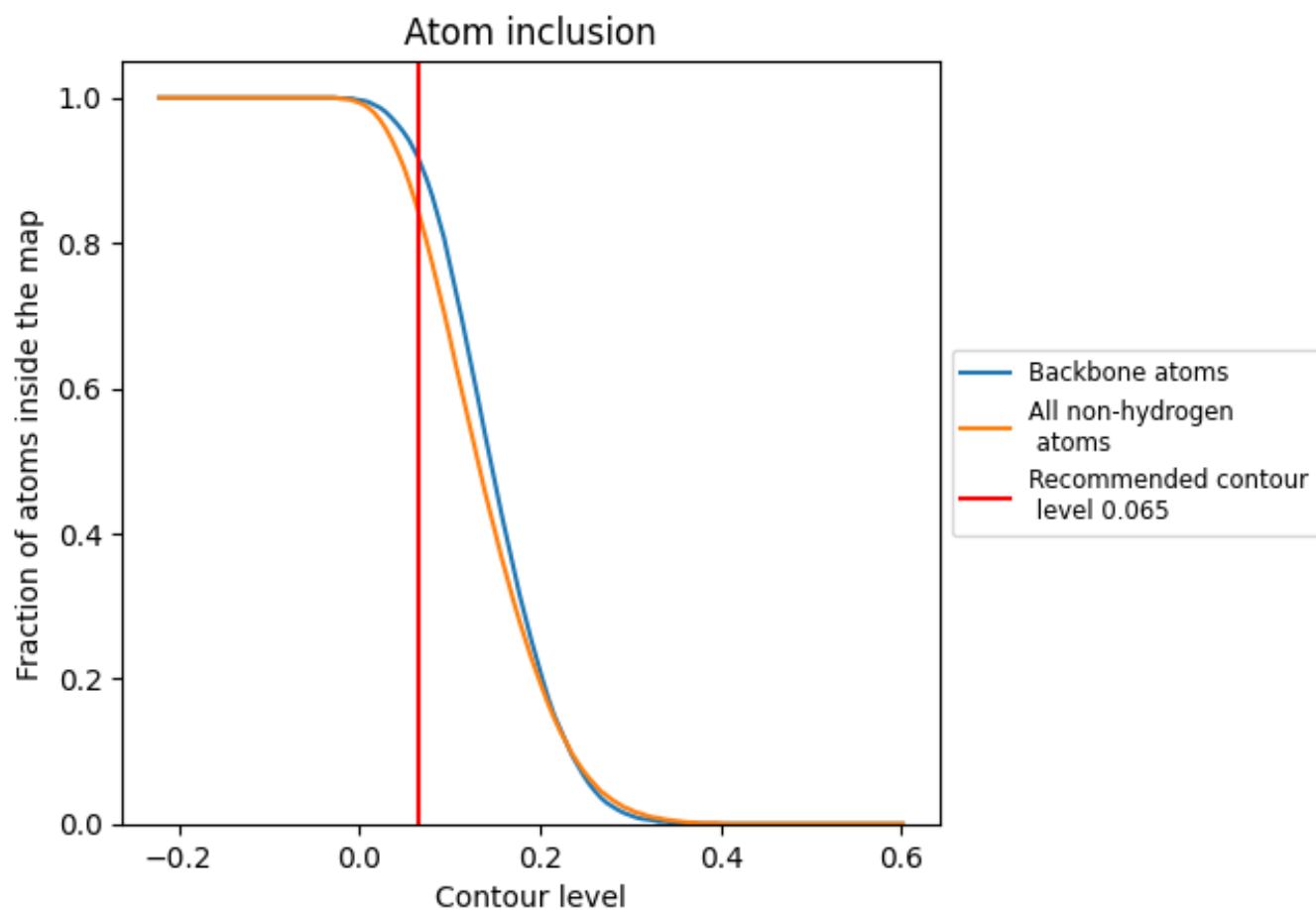
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

## 9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.065).







































































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 92% of all backbone atoms, 84% of all non-hydrogen atoms, are inside the map.

## 9.5 Map-model fit summary







The table lists the average atom inclusion at the recommended contour level (0.065) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8450	 0.3520
2	 0.9050	 0.3540
A	 0.8570	 0.3850
B	 0.8540	 0.3740
C	 0.8300	 0.4160
D	 0.7950	 0.3480
E	 0.8200	 0.4300
F	 0.7520	 0.3020
G	 0.8220	 0.3550
H	 0.8350	 0.3620
I	 0.8140	 0.3700
J	 0.8500	 0.4050
K	 0.7700	 0.3070
L	 0.7970	 0.4240
M	 0.5660	 0.1740
N	 0.8310	 0.3940
O	 0.8300	 0.3670
P	 0.7000	 0.2230
Q	 0.8010	 0.3540
R	 0.8100	 0.3420
S	 0.6330	 0.1820
T	 0.7560	 0.2730
U	 0.7690	 0.3710
V	 0.8280	 0.3890
W	 0.8720	 0.4450
X	 0.8880	 0.4490
Y	 0.8470	 0.3980
Z	 0.2820	 0.1170
a	 0.8660	 0.4390
b	 0.8610	 0.4120
c	 0.7720	 0.3420
d	 0.8690	 0.4280
e	 0.8070	 0.3920
f	 0.6930	 0.1990
g	 0.7810	 0.2890



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Chain	Atom inclusion	Q-score
h	 0.5420	 0.3260
i	 0.5330	 0.2640
j	 0.6930	 0.3040