



# wwPDB EM Validation Summary Report ⓘ

May 6, 2025 – 05:14 AM EDT

PDB ID : 8UMH / pdb\_00008umh  
EMDB ID : EMD-42379  
Title : Consensus map of PICdeltaTFIIK form2  
Authors : Yang, C.; Murakami, K.  
Deposited on : 2023-10-17  
Resolution : 4.10 Å(reported)

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.dev118  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4-5-2 with Phenix2.0rc1  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.43.1

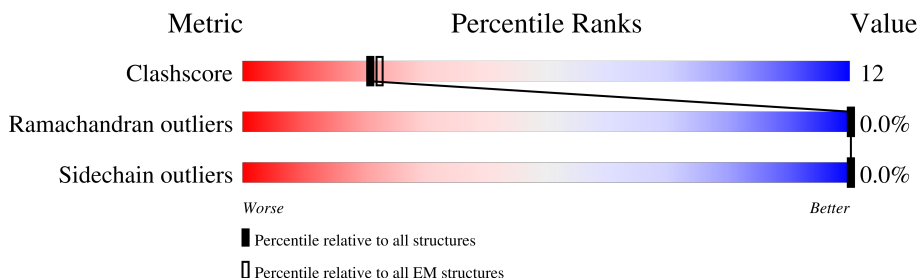
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*


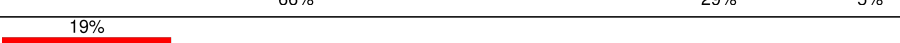

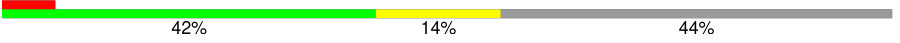

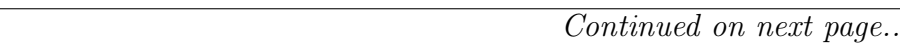

The reported resolution of this entry is 4.10 Å.

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	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	M	345	
2	A	1733	
3	B	1224	
4	C	318	
5	E	215	
6	F	155	
7	H	146	
8	I	122	

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Mol	Chain	Length	Quality of chain
9	J	70	
10	K	120	
11	L	70	
12	Q	735	
13	P	400	
14	S	309	
15	O	240	
16	U	286	
17	V	122	
18	W	482	
19	X	328	
20	D	221	
21	G	171	
22	0	778	
23	1	642	
24	4	338	
25	6	461	
26	7	843	
27	2	513	
28	5	72	
29	N	64	
30	T	64	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
33	SF4	0	801	-	-	X	-

## 2 Entry composition

There are 33 unique types of molecules in this entry. The entry contains 70481 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 protein called Transcription initiation factor IIB.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	M	279	Total	C	N	O	S	0	0
			2175	1382	373	403	17		

- Molecule 2 is a protein called DNA-directed RNA polymerase subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A	1425	Total	C	N	O	S	0	0
			11167	7036	1948	2121	62		

- Molecule 3 is a protein called DNA-directed RNA polymerase subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	B	1166	Total	C	N	O	S	0	0
			9227	5823	1619	1729	56		

- Molecule 4 is a protein called DNA-directed RNA polymerase II subunit RPB3.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	C	265	Total	C	N	O	S	0	0
			2086	1312	347	414	13		

- Molecule 5 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC1.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	214	Total	C	N	O	S	0	0
			1752	1111	309	321	11		

- Molecule 6 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC2.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	87	Total	C	N	O	S	0	0
			705	451	119	132	3		

- Molecule 7 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC3.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	H	135	Total	C	N	O	S	0	0
			1080	679	182	214	5		

- Molecule 8 is a protein called DNA-directed RNA polymerase II subunit RPB9.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	I	114	Total	C	N	O	S	0	0
			927	571	168	178	10		

- Molecule 9 is a protein called DNA-directed RNA polymerases II subunit RPABC5.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	J	66	Total	C	N	O	S	0	0
			540	345	94	95	6		

- Molecule 10 is a protein called DNA-directed RNA polymerase II subunit RPB11.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	K	115	Total	C	N	O	S	0	0
			924	593	157	172	2		

- Molecule 11 is a protein called DNA-directed RNA polymerases II subunit RPABC4.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	L	44	Total	C	N	O	S	0	0
			352	217	70	61	4		

- Molecule 12 is a protein called Transcription initiation factor IIF subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	Q	214	Total	C	N	O	S	0	0
			1619	1017	297	299	6		

- Molecule 13 is a protein called Transcription initiation factor IIF subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	P	179	Total	C	N	O	S	0	0
			1484	941	258	279	6		

- Molecule 14 is a protein called Transcription elongation factor.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	S	164	Total	C	N	O	S	0	0
			1294	809	230	247	8		

- Molecule 15 is a protein called TATA-box-binding protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	O	181	Total	C	N	O	S	0	0
			1422	925	243	248	6		

- Molecule 16 is a protein called Transcription initiation factor IIA large subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	U	107	Total	C	N	O	S	0	0
			885	559	147	176	3		

- Molecule 17 is a protein called Transcription initiation factor IIA subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	V	104	Total	C	N	O	S	0	0
			815	511	136	164	4		

- Molecule 18 is a protein called Transcription initiation factor IIE subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	W	247	Total	C	N	O	S	0	0
			2010	1275	347	381	7		

- Molecule 19 is a protein called Transcription initiation factor IIE subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	X	160	Total	C	N	O	S	0	0
			1288	826	212	245	5		

- Molecule 20 is a protein called DNA-directed RNA polymerase II subunit RPB4.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	D	168	Total	C	N	O	S	0	0
			1331	822	237	270	2		

- Molecule 21 is a protein called DNA-directed RNA polymerase II subunit RPB7.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	G	171	Total	C	N	O	S	0	0
			1335	858	221	248	8		

- Molecule 22 is a protein called General transcription and DNA repair factor IIIH helicase subunit XPD.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	0	752	Total	C	N	O	S	0	0
			6091	3882	1029	1142	38		

- Molecule 23 is a protein called TFB1 isoform 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	1	417	Total	C	N	O	S	0	0
			3382	2139	587	640	16		

- Molecule 24 is a protein called General transcription and DNA repair factor IIIH subunit TFB4.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	4	292	Total	C	N	O	S	0	0
			2267	1449	376	428	14		

- Molecule 25 is a protein called General transcription and DNA repair factor IIIH.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	6	355	Total	C	N	O	S	0	0
			2786	1765	481	512	28		

- Molecule 26 is a protein called General transcription and DNA repair factor IIIH helicase subunit XPB.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	7	608	Total	C	N	O	S	0	0
			4889	3110	847	906	26		

- Molecule 27 is a protein called RNA polymerase II transcription factor B subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	2	445	Total	C	N	O	S	0	0
			3546	2291	585	654	16		

- Molecule 28 is a protein called General transcription and DNA repair factor IIIH subunit



TFB5.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	5	66	Total	C	N	O	S	0	0
			498	314	89	93	2		

- Molecule 29 is a DNA chain called DNA (63-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
29	N	63	Total	C	N	O	P	0	0
			1288	621	225	380	62		

- Molecule 30 is a DNA chain called DNA (63-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
30	T	63	Total	C	N	O	P	0	0
			1291	619	236	373	63		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
T	-10	DC	DT	conflict	GB 2567904391

- Molecule 31 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
31	M	1	Total	Zn	0
			1	1	
31	A	2	Total	Zn	0
			2	2	
31	B	1	Total	Zn	0
			1	1	
31	C	1	Total	Zn	0
			1	1	
31	I	2	Total	Zn	0
			2	2	
31	J	1	Total	Zn	0
			1	1	
31	L	1	Total	Zn	0
			1	1	
31	S	1	Total	Zn	0
			1	1	
31	4	1	Total	Zn	0
			1	1	

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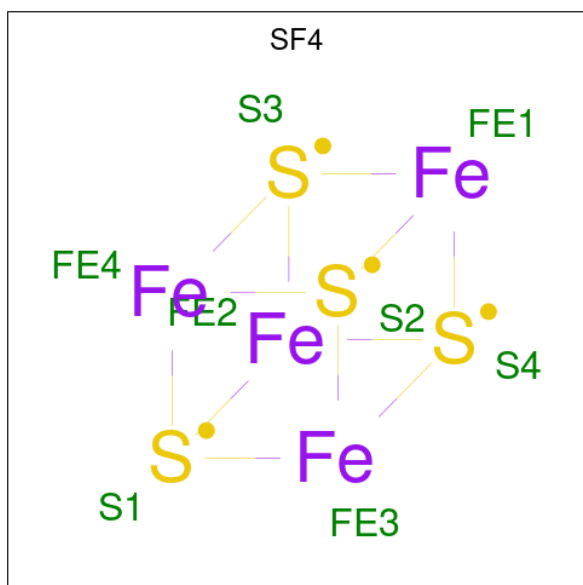
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Mol	Chain	Residues	Atoms		AltConf
31	6	4	Total	Zn	0
			4	4	

- Molecule 32 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
32	A	1	Total	Mg	0
			1	1	
32	7	1	Total	Mg	0
			1	1	

- Molecule 33 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe<sub>4</sub>S<sub>4</sub>).

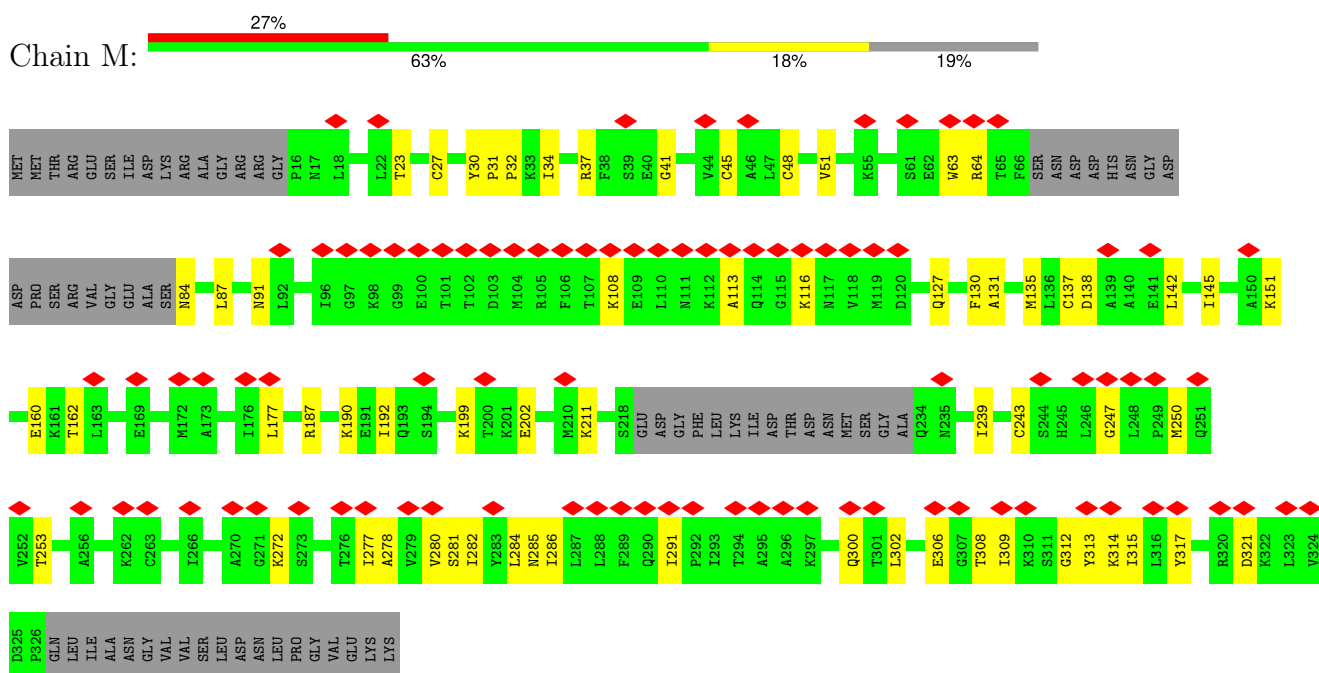


Mol	Chain	Residues	Atoms			AltConf
33	0	1	Total	Fe	S	0
			8	4	4	

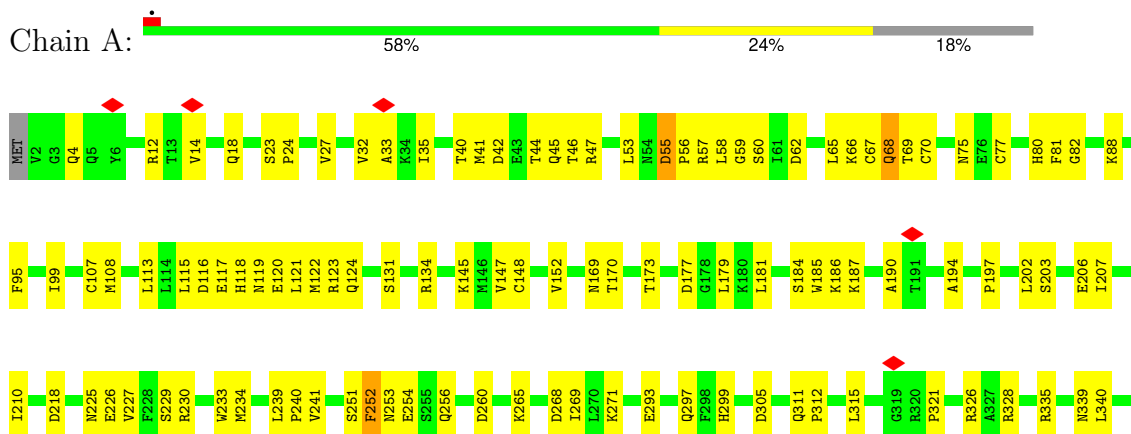
### 3 Residue-property plots

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.

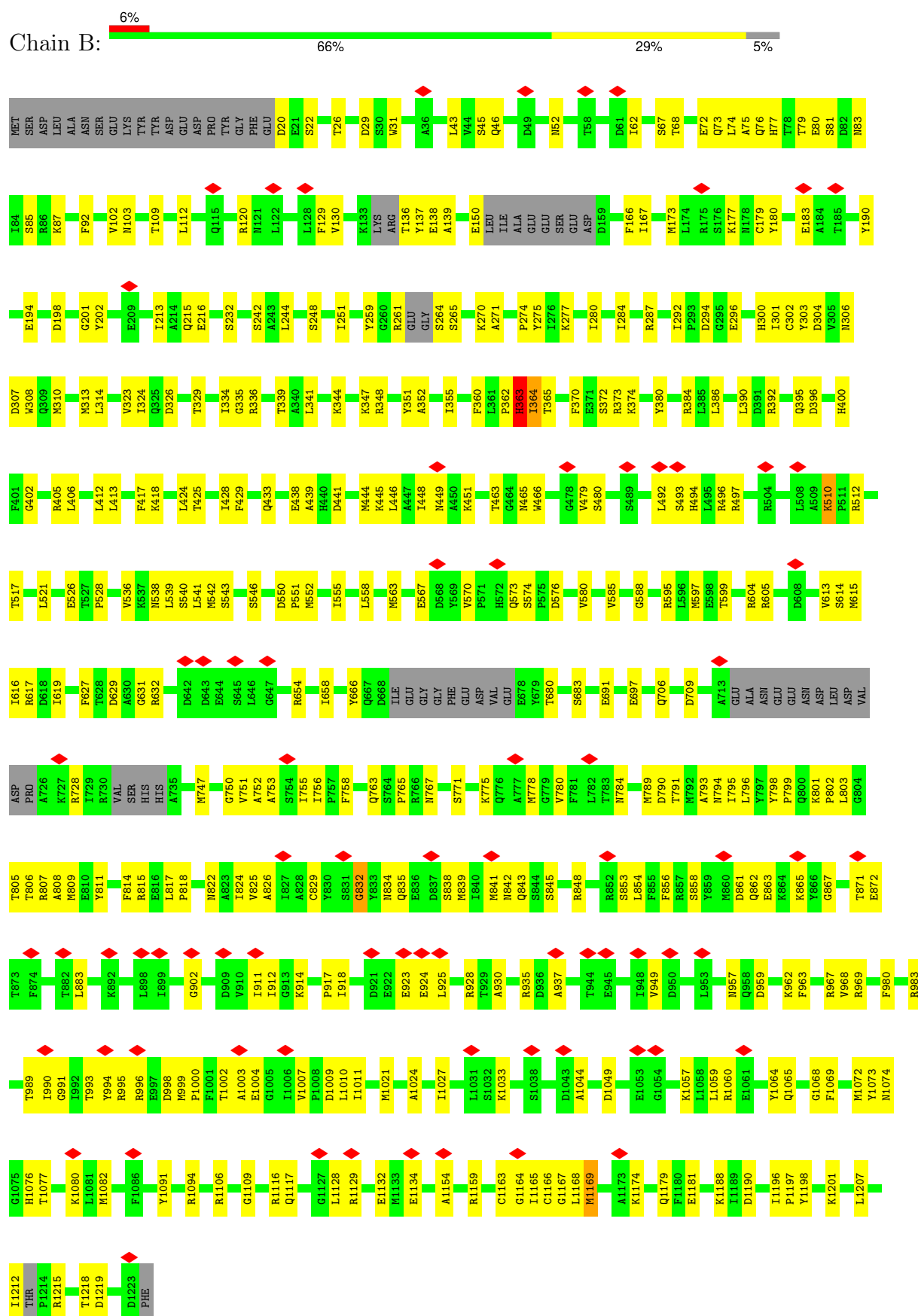
#### • Molecule 1: Transcription initiation factor IIB



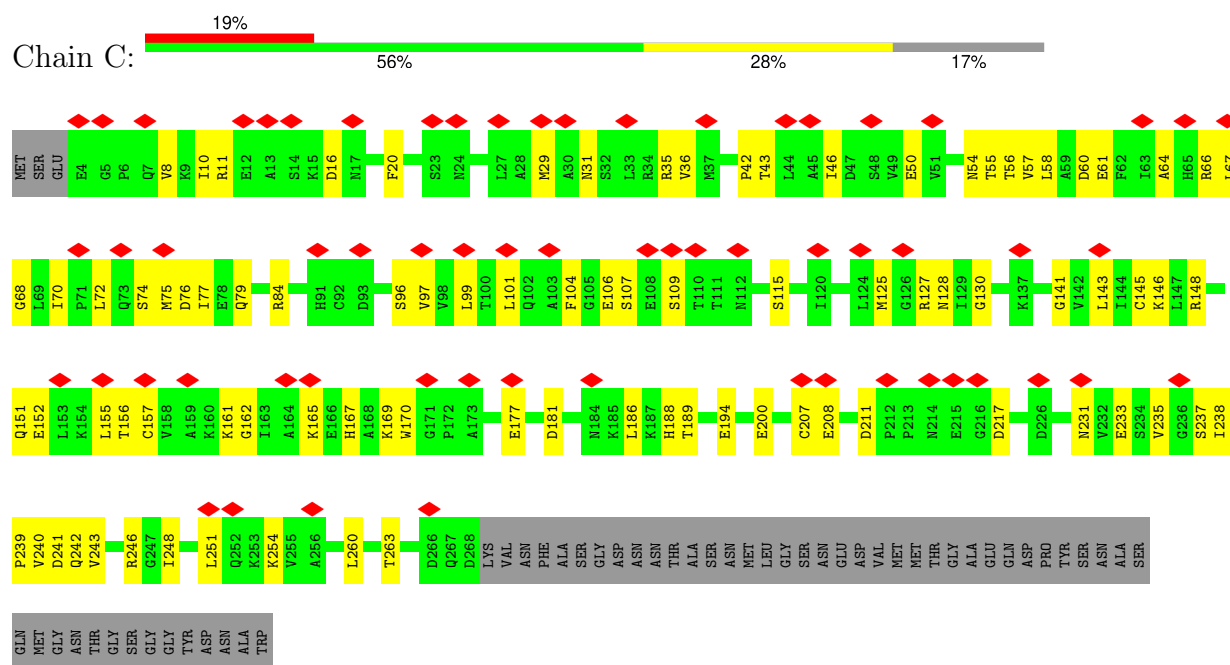
#### • Molecule 2: DNA-directed RNA polymerase subunit



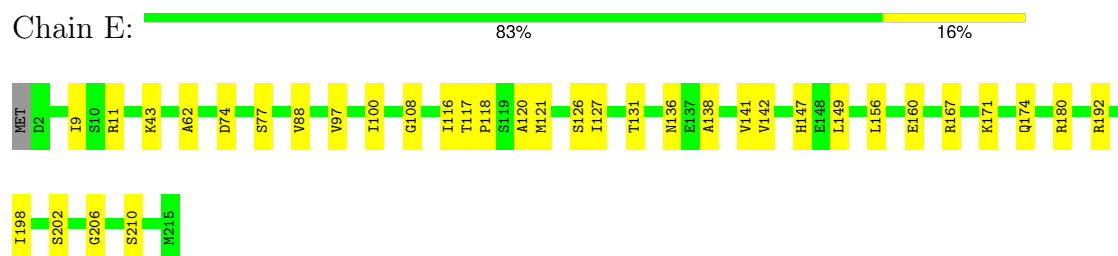




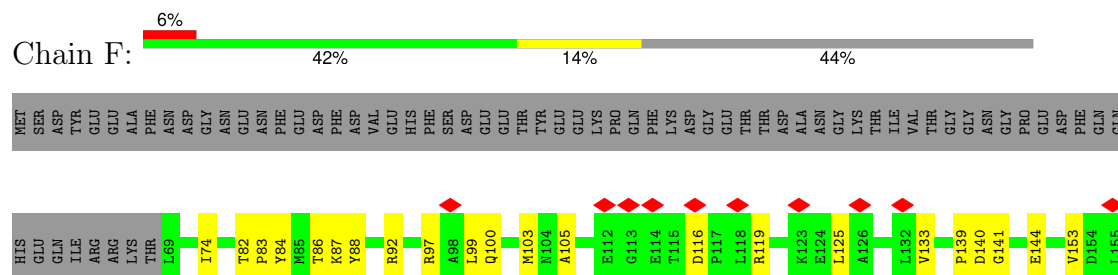
- Molecule 4: DNA-directed RNA polymerase II subunit RPB3



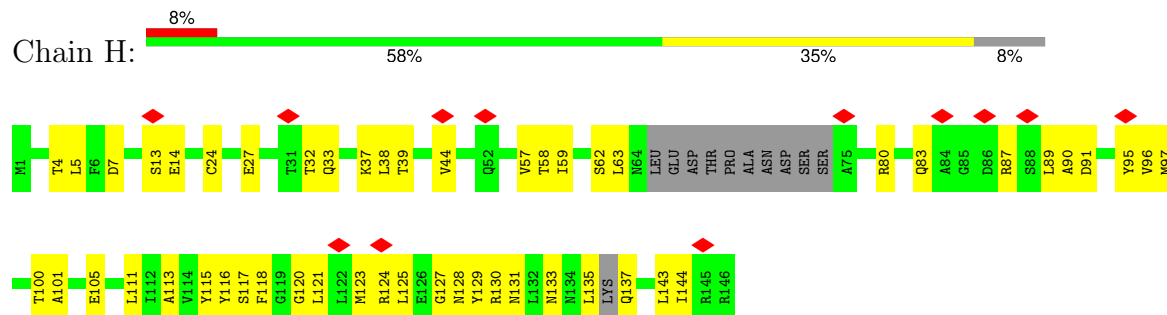
- Molecule 5: DNA-directed RNA polymerases I, II, and III subunit RPABC1



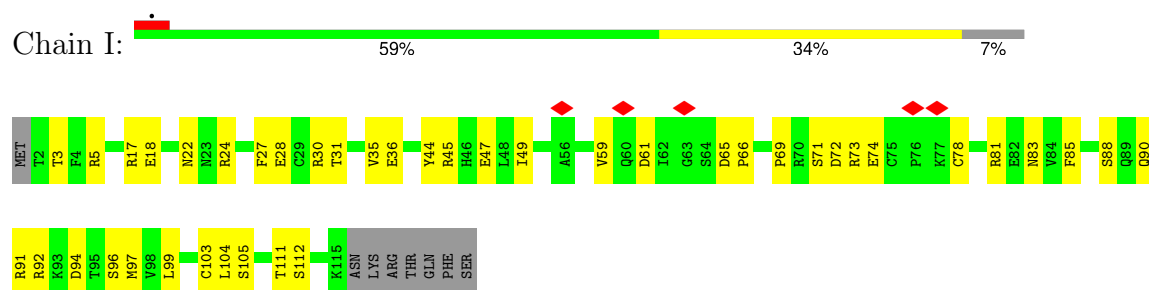
- Molecule 6: DNA-directed RNA polymerases I, II, and III subunit RPABC2



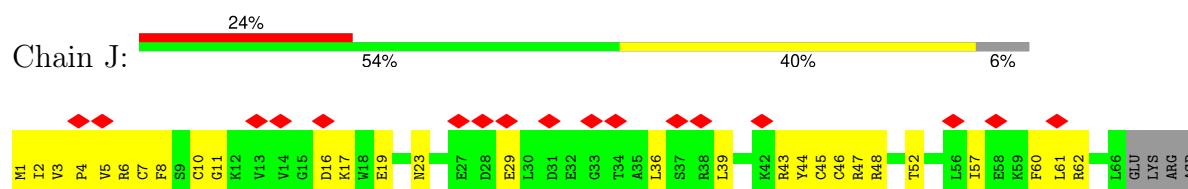
- Molecule 7: DNA-directed RNA polymerases I, II, and III subunit RPABC3



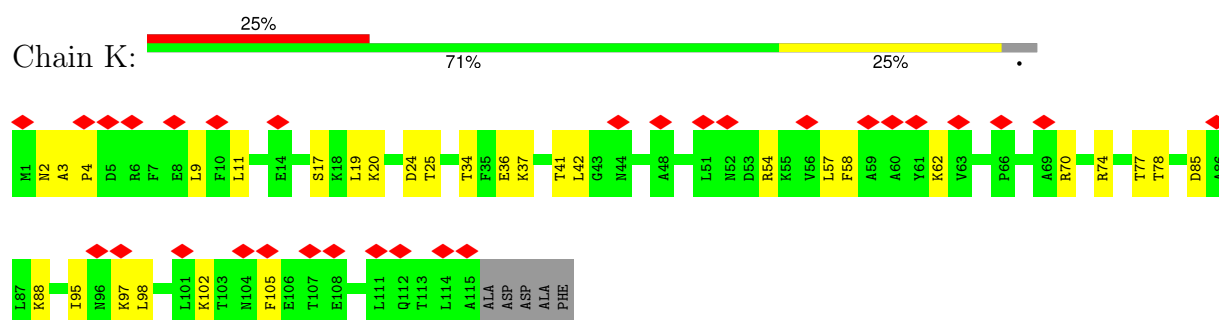
- Molecule 8: DNA-directed RNA polymerase II subunit RPB9



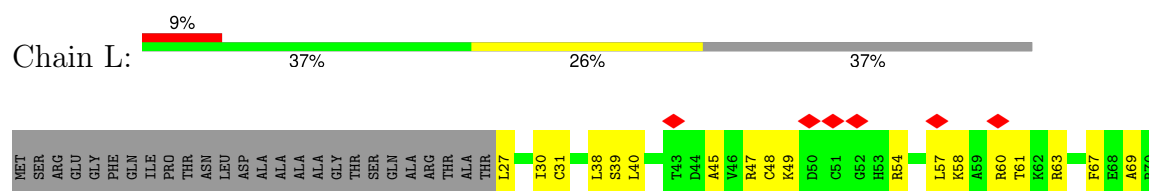
- Molecule 9: DNA-directed RNA polymerase II subunit RPABC5



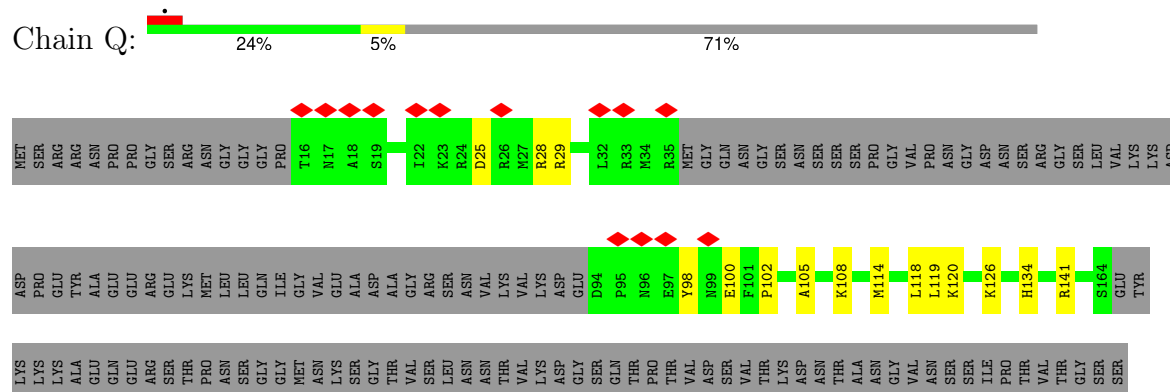
- Molecule 10: DNA-directed RNA polymerase II subunit RPB11

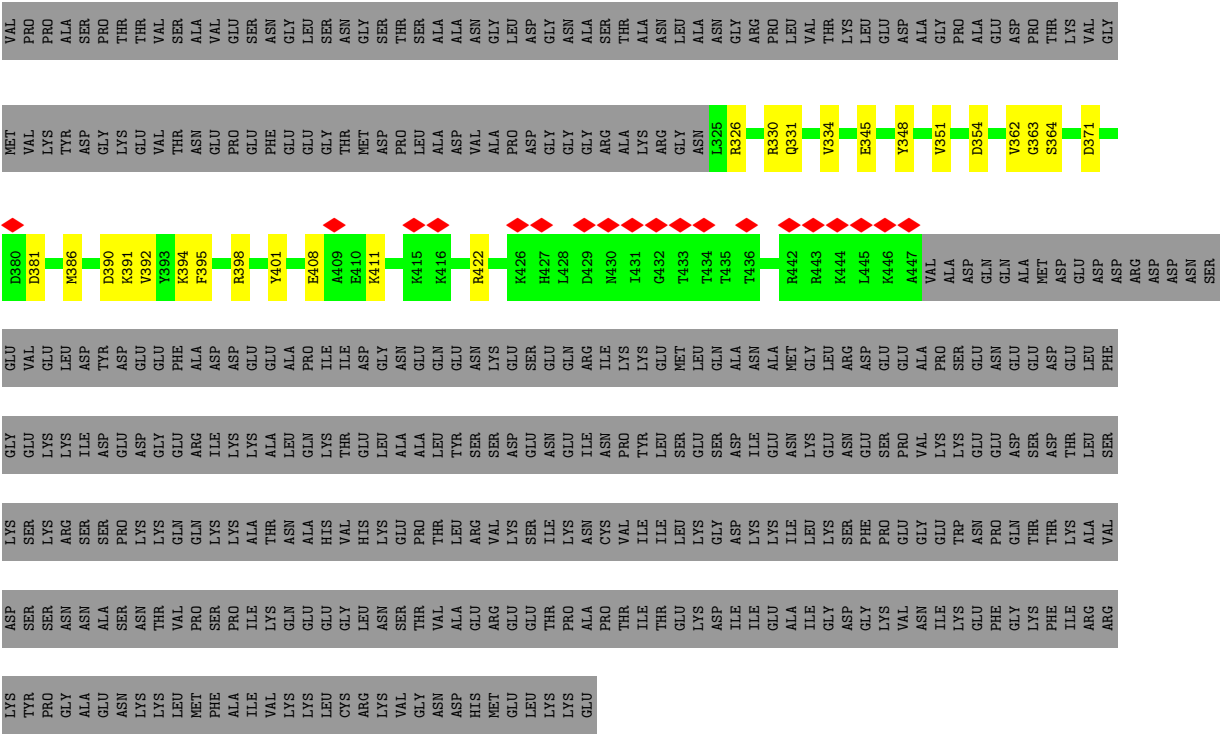


- Molecule 11: DNA-directed RNA polymerase II subunit RPABC4

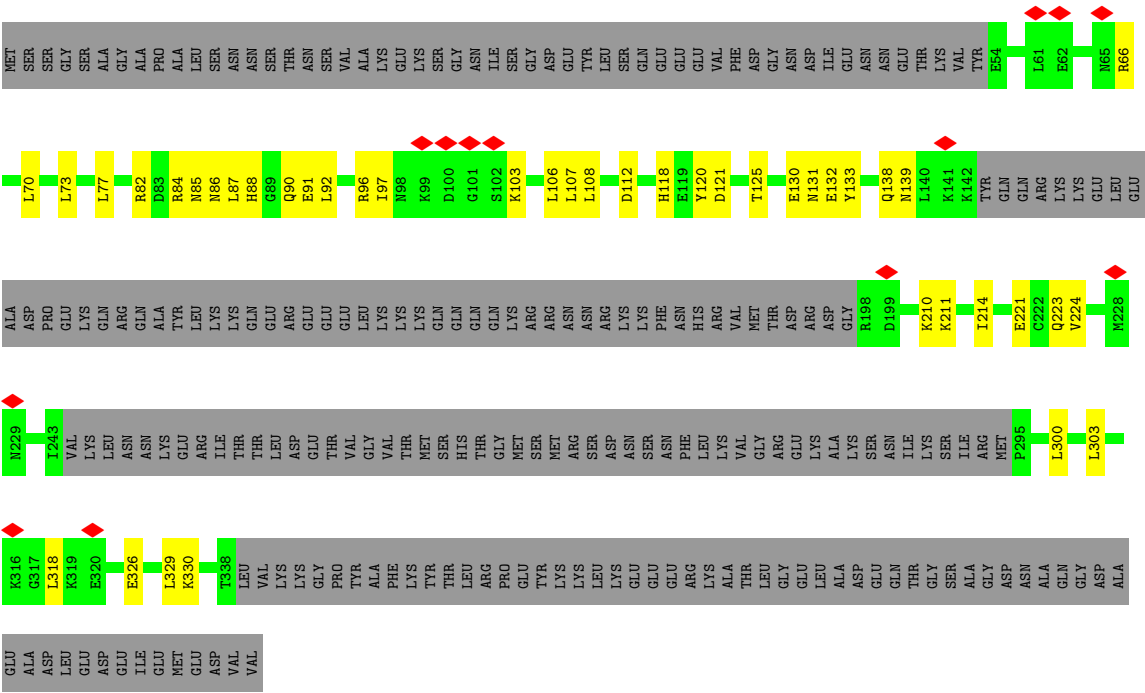
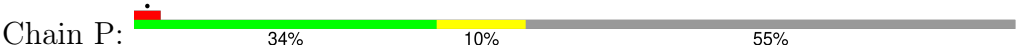


- Molecule 12: Transcription initiation factor IIF subunit alpha

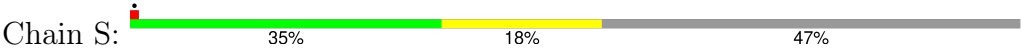




• Molecule 13: Transcription initiation factor IIF subunit beta

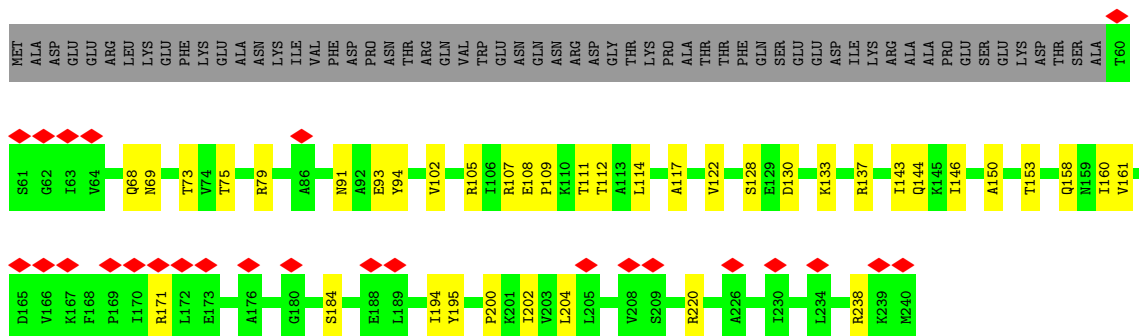


• Molecule 14: Transcription elongation factor

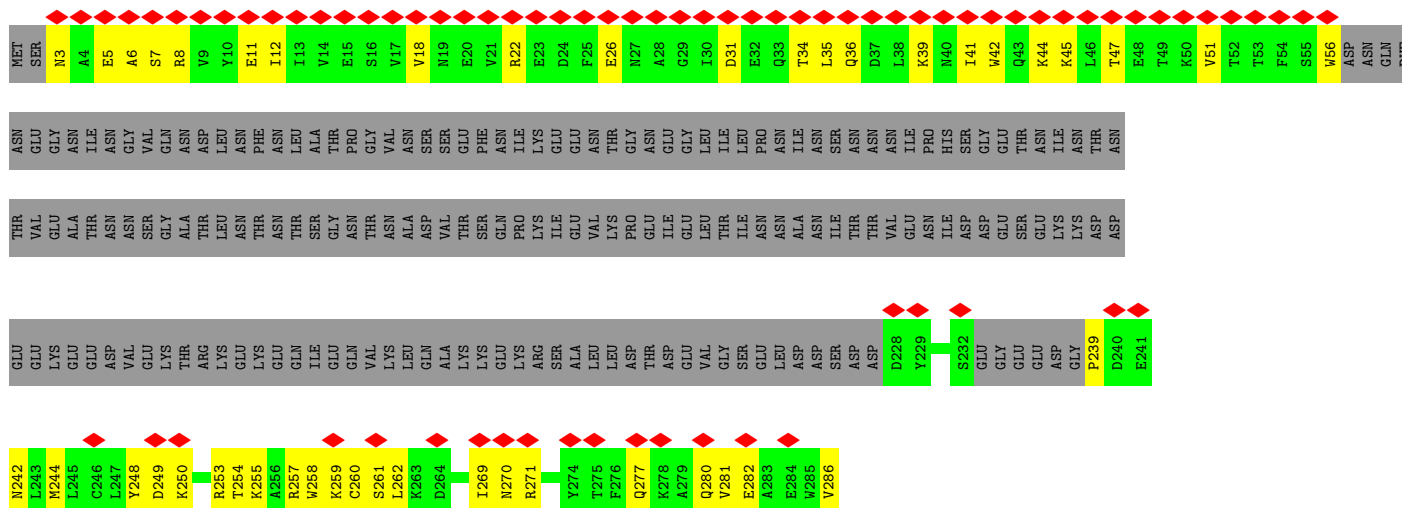




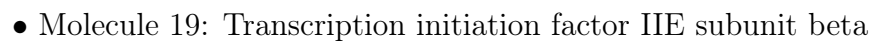
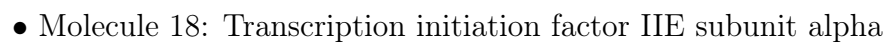
- Molecule 15: TATA-box-binding protein

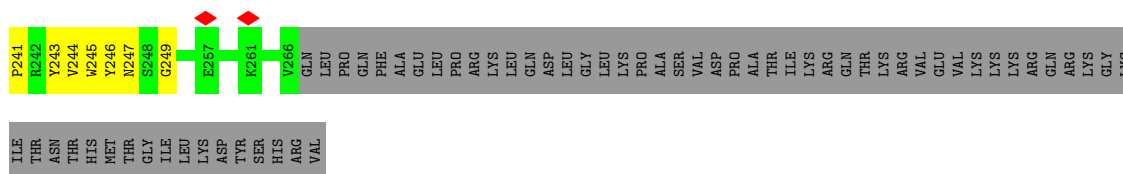


- Molecule 16: Transcription initiation factor IIA large subunit

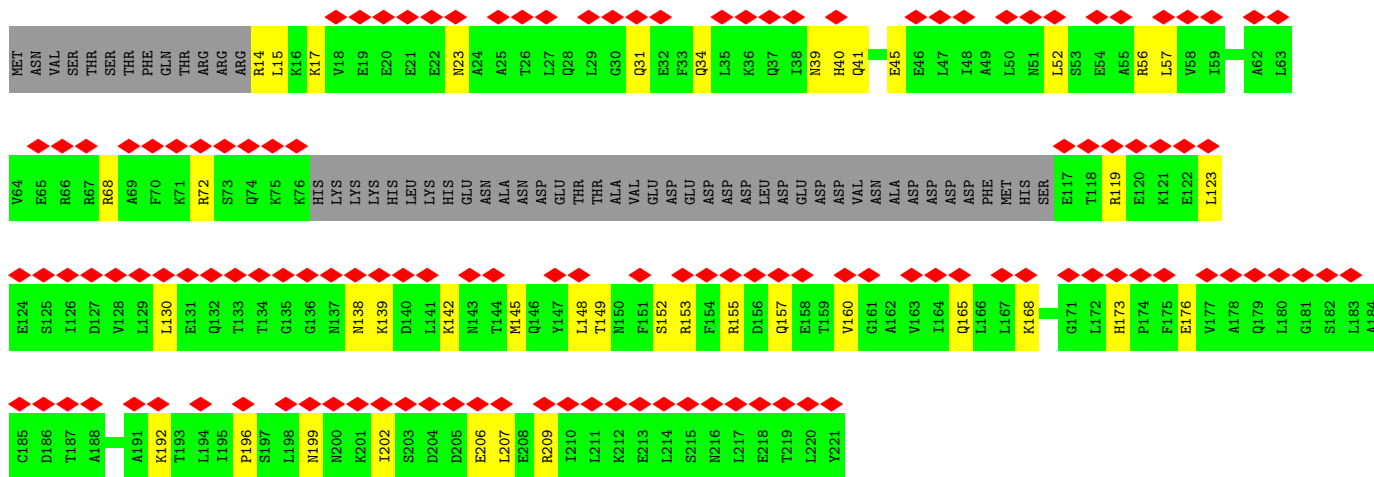


- Molecule 17: Transcription initiation factor IIA subunit 2

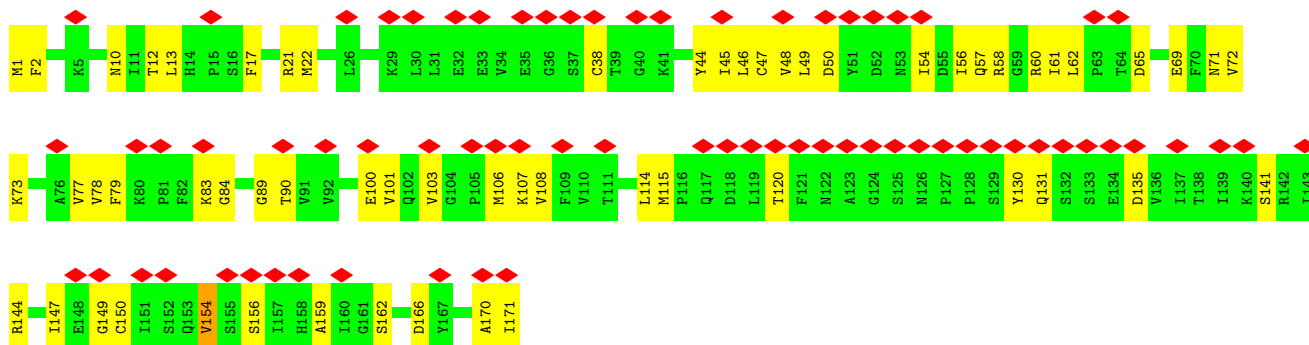
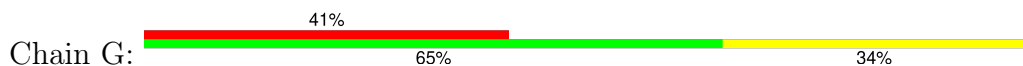




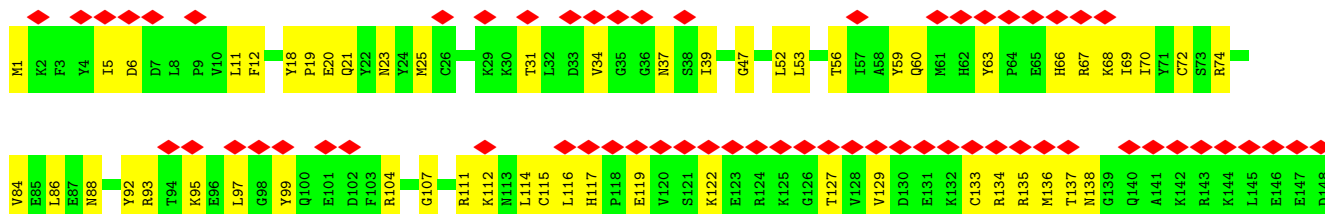
• Molecule 20: DNA-directed RNA polymerase II subunit RPB4



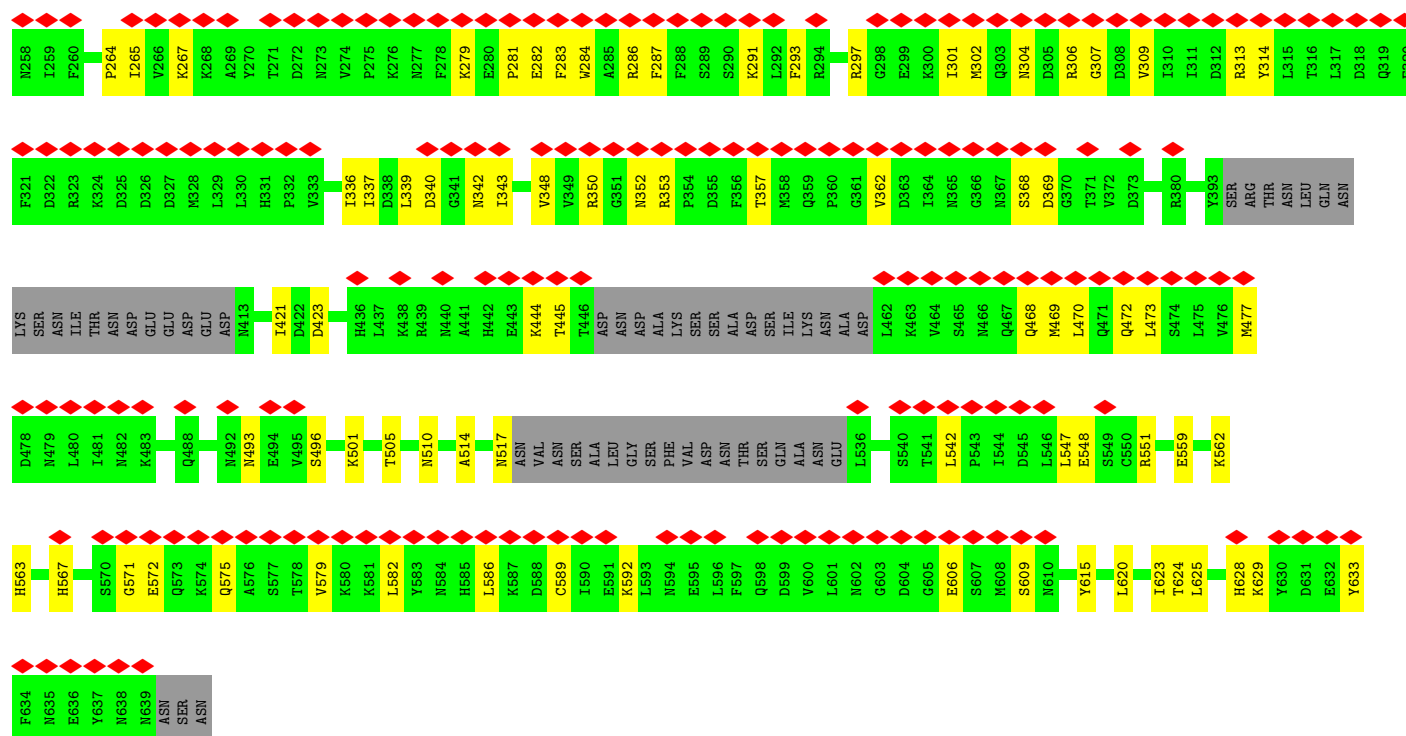
• Molecule 21: DNA-directed RNA polymerase II subunit RPB7



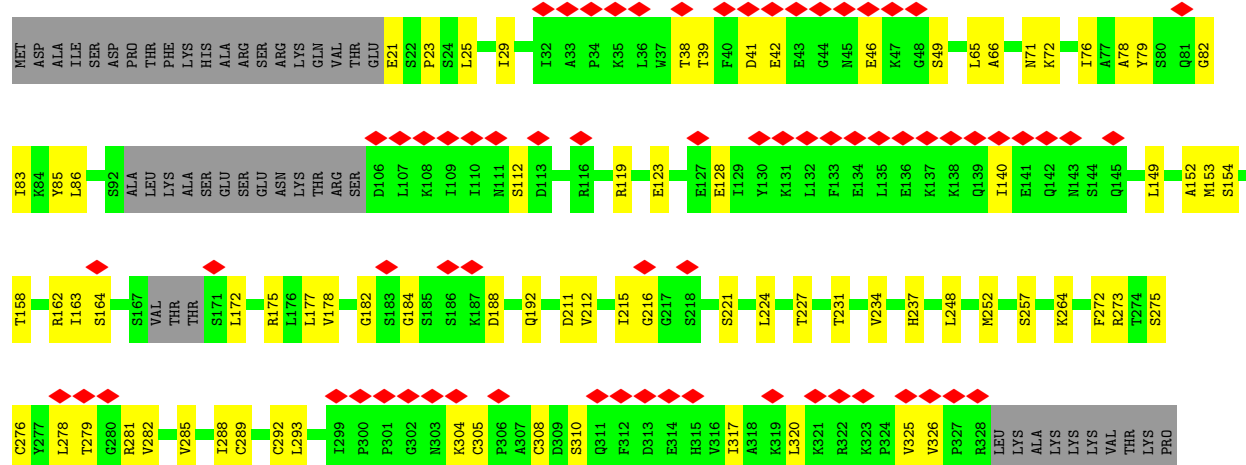
• Molecule 22: General transcription and DNA repair factor IIH helicase subunit XPD





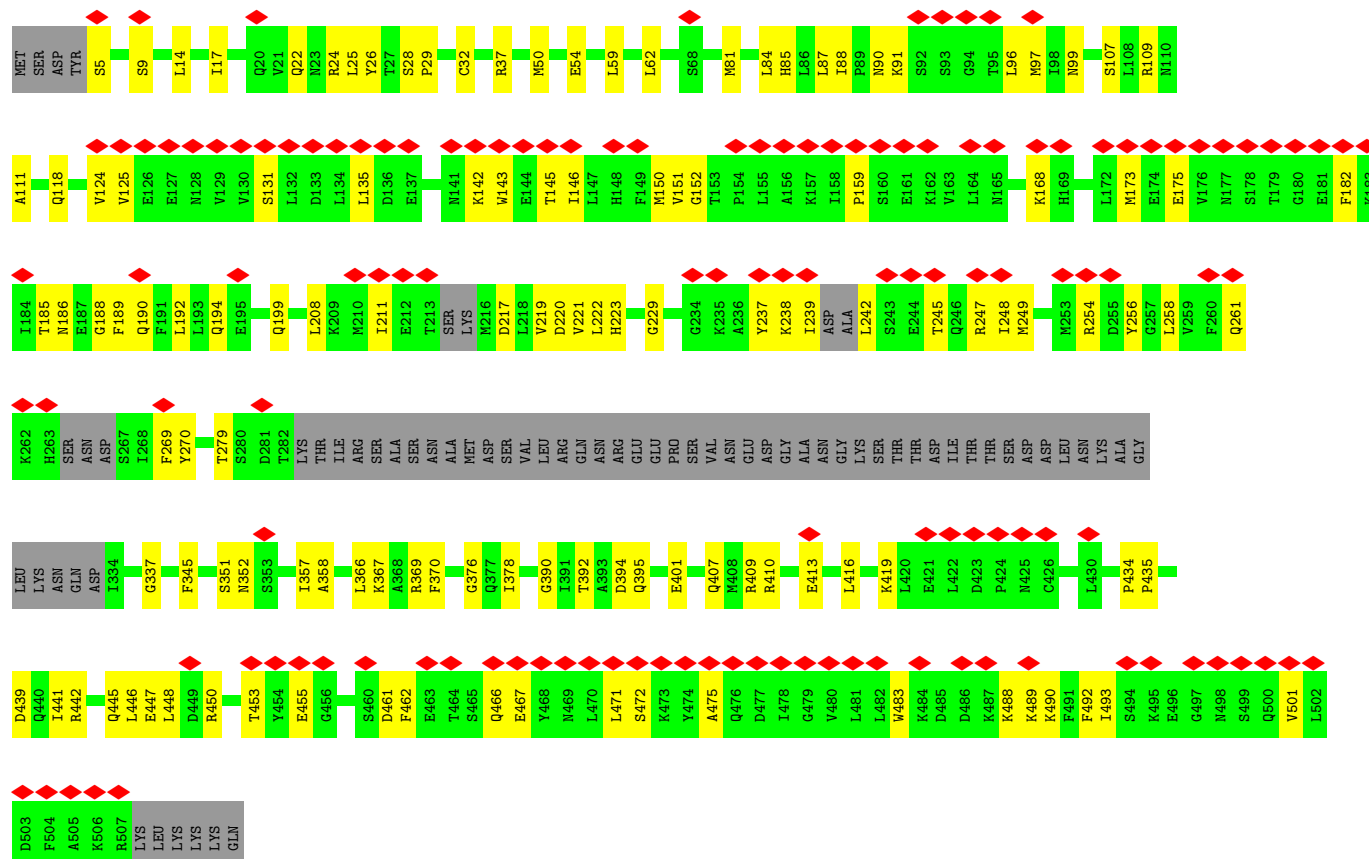


• Molecule 24: General transcription and DNA repair factor IIH subunit TFB4

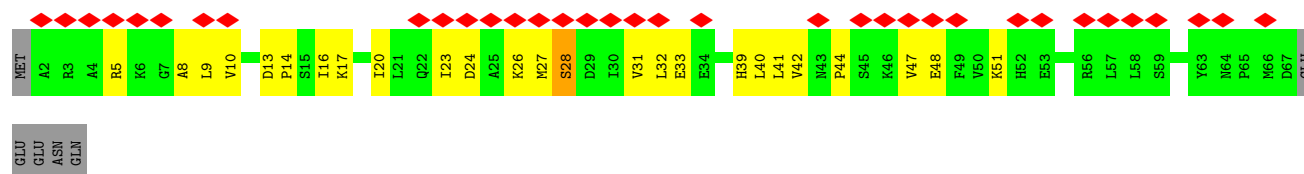




- Molecule 27: RNA polymerase II transcription factor B subunit 2



- Molecule 28: General transcription and DNA repair factor IIH subunit TFB5

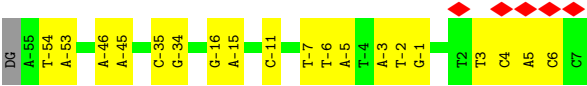


- Molecule 29: DNA (63-MER)





• Molecule 30: DNA (63-MER)





## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	90136	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	1.25	Depositor
Minimum defocus (nm)	750	Depositor
Maximum defocus (nm)	1750	Depositor
Magnification	81000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.078	Depositor
Minimum map value	-0.023	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.0098	Depositor
Map size ( $\text{\AA}$ )	414.72003, 414.72003, 414.72003	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	1.08, 1.08, 1.08	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, SF4, 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	M	0.23	0/2204	0.62	0/2963
2	A	0.35	0/11368	0.69	5/15383 (0.0%)
3	B	0.37	0/9402	0.71	12/12680 (0.1%)
4	C	0.37	0/2124	0.65	0/2879
5	E	0.29	0/1788	0.60	0/2406
6	F	0.34	0/717	0.71	0/967
7	H	0.35	0/1097	0.70	0/1484
8	I	0.28	0/945	0.54	0/1273
9	J	0.48	0/549	0.85	1/738 (0.1%)
10	K	0.35	0/942	0.58	0/1272
11	L	0.35	0/354	0.90	2/468 (0.4%)
12	Q	0.23	0/1648	0.52	0/2226
13	P	0.22	0/1511	0.56	0/2035
14	S	0.25	0/1317	0.66	0/1778
15	O	0.21	0/1449	0.51	0/1952
16	U	0.23	0/898	0.59	0/1212
17	V	0.22	0/822	0.59	0/1109
18	W	0.19	0/2045	0.47	0/2757
19	X	0.18	0/1312	0.44	0/1767
20	D	0.19	0/1339	0.54	0/1793
21	G	0.24	0/1363	0.64	0/1840
22	0	0.21	0/6209	0.50	0/8384
23	1	0.20	0/3434	0.52	0/4624
24	4	0.19	0/2305	0.48	0/3117
25	6	0.20	0/2843	0.49	0/3845
26	7	0.21	0/4992	0.54	0/6754
27	2	0.21	0/3611	0.55	2/4881 (0.0%)
28	5	0.27	0/502	0.78	2/677 (0.3%)
29	N	0.37	0/1443	0.61	0/2226
30	T	0.37	0/1449	0.61	0/2233
All	All	0.28	0/71982	0.61	24/97723 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	M	0	3
2	A	0	7
3	B	0	5
5	E	0	1
11	L	0	1
14	S	0	2
21	G	0	1
All	All	0	20

There are no bond length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1107	VAL	CA-C-N	7.67	135.50	121.70
2	A	1107	VAL	C-N-CA	7.67	135.50	121.70
3	B	79	THR	CA-C-N	7.49	135.18	121.70
3	B	79	THR	C-N-CA	7.49	135.18	121.70
27	2	125	VAL	N-CA-C	-7.25	105.72	112.96

There are no chirality outliers.

5 of 20 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	A	55	ASP	Peptide
2	A	65	LEU	Peptide
1	M	272	LYS	Peptide
1	M	30	TYR	Peptide
1	M	31	PRO	Peptide

## 5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	M	2175	0	2283	40	0
2	A	11167	0	11189	295	0
3	B	9227	0	9200	260	0
4	C	2086	0	2045	64	0
5	E	1752	0	1776	24	0
6	F	705	0	731	18	0
7	H	1080	0	1049	42	0
8	I	927	0	880	34	0
9	J	540	0	553	21	0
10	K	924	0	934	29	0
11	L	352	0	375	13	0
12	Q	1619	0	1452	36	0
13	P	1484	0	1480	35	0
14	S	1294	0	1289	32	0
15	O	1422	0	1500	28	0
16	U	885	0	866	34	0
17	V	815	0	822	30	0
18	W	2010	0	2026	46	0
19	X	1288	0	1307	24	0
20	D	1331	0	1345	27	0
21	G	1335	0	1346	34	0
22	0	6091	0	6155	189	0
23	1	3382	0	3436	67	0
24	4	2267	0	2323	54	0
25	6	2786	0	2804	70	0
26	7	4889	0	4876	129	0
27	2	3546	0	3593	87	0
28	5	498	0	506	14	0
29	N	1288	0	719	16	0
30	T	1291	0	713	16	0
31	4	1	0	0	0	0
31	6	4	0	0	0	0
31	A	2	0	0	0	0
31	B	1	0	0	0	0
31	C	1	0	0	0	0
31	I	2	0	0	0	0
31	J	1	0	0	0	0
31	L	1	0	0	0	0
31	M	1	0	0	0	0
31	S	1	0	0	0	0
32	7	1	0	0	0	0
32	A	1	0	0	0	0
33	0	8	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	70481	0	69573	1636	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 12.

The worst 5 of 1636 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)
25:6:406:CYS:HB3	25:6:440:CYS:SG	2.01	0.99
11:L:27:LEU:N	11:L:39:SER:HG	1.68	0.91
22:0:134:ARG:O	22:0:138:ASN:HB2	1.72	0.88
11:L:31:CYS:SG	11:L:48:CYS:HB3	2.16	0.84
2:A:107:CYS:SG	2:A:148:CYS:HB2	2.18	0.82

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	
1	M	273/345 (79%)	239 (88%)	34 (12%)	0	100	100
2	A	1417/1733 (82%)	1240 (88%)	177 (12%)	0	100	100
3	B	1150/1224 (94%)	990 (86%)	158 (14%)	2 (0%)	44	77
4	C	263/318 (83%)	225 (86%)	38 (14%)	0	100	100
5	E	212/215 (99%)	193 (91%)	19 (9%)	0	100	100
6	F	85/155 (55%)	76 (89%)	9 (11%)	0	100	100
7	H	129/146 (88%)	108 (84%)	21 (16%)	0	100	100
8	I	112/122 (92%)	98 (88%)	14 (12%)	0	100	100
9	J	64/70 (91%)	53 (83%)	11 (17%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
10	K	113/120 (94%)	106 (94%)	7 (6%)	0	100	100
11	L	42/70 (60%)	31 (74%)	11 (26%)	0	100	100
12	Q	208/735 (28%)	201 (97%)	7 (3%)	0	100	100
13	P	173/400 (43%)	163 (94%)	10 (6%)	0	100	100
14	S	162/309 (52%)	143 (88%)	18 (11%)	1 (1%)	22	59
15	O	179/240 (75%)	168 (94%)	11 (6%)	0	100	100
16	U	101/286 (35%)	96 (95%)	5 (5%)	0	100	100
17	V	100/122 (82%)	99 (99%)	1 (1%)	0	100	100
18	W	241/482 (50%)	229 (95%)	12 (5%)	0	100	100
19	X	158/328 (48%)	147 (93%)	11 (7%)	0	100	100
20	D	164/221 (74%)	159 (97%)	5 (3%)	0	100	100
21	G	169/171 (99%)	155 (92%)	14 (8%)	0	100	100
22	0	750/778 (96%)	709 (94%)	41 (6%)	0	100	100
23	1	407/642 (63%)	393 (97%)	14 (3%)	0	100	100
24	4	286/338 (85%)	276 (96%)	10 (4%)	0	100	100
25	6	351/461 (76%)	337 (96%)	14 (4%)	0	100	100
26	7	604/843 (72%)	564 (93%)	40 (7%)	0	100	100
27	2	435/513 (85%)	412 (95%)	23 (5%)	0	100	100
28	5	64/72 (89%)	56 (88%)	8 (12%)	0	100	100
All	All	8412/11459 (73%)	7666 (91%)	743 (9%)	3 (0%)	100	100

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	B	364	ILE
3	B	363	HIS
14	S	167	PRO

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	M	245/299 (82%)	244 (100%)	1 (0%)	89	91
2	A	1235/1520 (81%)	1234 (100%)	1 (0%)	92	95
3	B	1000/1061 (94%)	1000 (100%)	0	100	100
4	C	233/274 (85%)	233 (100%)	0	100	100
5	E	196/197 (100%)	196 (100%)	0	100	100
6	F	77/137 (56%)	77 (100%)	0	100	100
7	H	118/128 (92%)	118 (100%)	0	100	100
8	I	108/116 (93%)	108 (100%)	0	100	100
9	J	61/65 (94%)	61 (100%)	0	100	100
10	K	99/102 (97%)	99 (100%)	0	100	100
11	L	39/57 (68%)	39 (100%)	0	100	100
12	Q	147/641 (23%)	147 (100%)	0	100	100
13	P	166/363 (46%)	166 (100%)	0	100	100
14	S	141/274 (52%)	141 (100%)	0	100	100
15	O	153/205 (75%)	153 (100%)	0	100	100
16	U	99/260 (38%)	99 (100%)	0	100	100
17	V	94/108 (87%)	94 (100%)	0	100	100
18	W	224/429 (52%)	224 (100%)	0	100	100
19	X	144/295 (49%)	144 (100%)	0	100	100
20	D	146/200 (73%)	146 (100%)	0	100	100
21	G	151/152 (99%)	151 (100%)	0	100	100
22	0	684/707 (97%)	684 (100%)	0	100	100
23	1	389/589 (66%)	389 (100%)	0	100	100
24	4	259/300 (86%)	259 (100%)	0	100	100
25	6	322/418 (77%)	322 (100%)	0	100	100
26	7	540/737 (73%)	540 (100%)	0	100	100
27	2	394/468 (84%)	394 (100%)	0	100	100
28	5	53/66 (80%)	53 (100%)	0	100	100
All	All	7517/10168 (74%)	7515 (100%)	2 (0%)	100	100

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	M	300	GLN
2	A	68	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 80 such sidechains are listed below:

Mol	Chain	Res	Type
23	1	575	GLN
26	7	672	GLN
24	4	71	ASN
26	7	423	GLN
27	2	148	HIS

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

## 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 oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 18 ligands modelled in this entry, 17 are monoatomic - leaving 1 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
33	SF4	0	801	22	0,12,12	-	-	-		



In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
33	SF4	0	801	22	-	-	0/6/5/5

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.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
33	0	801	SF4	2	0

## 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.

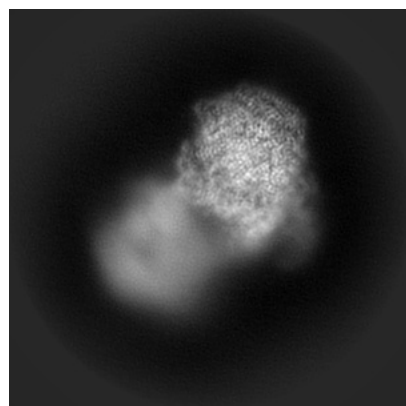
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-42379. These allow visual inspection of the internal detail of the map and identification of artifacts.

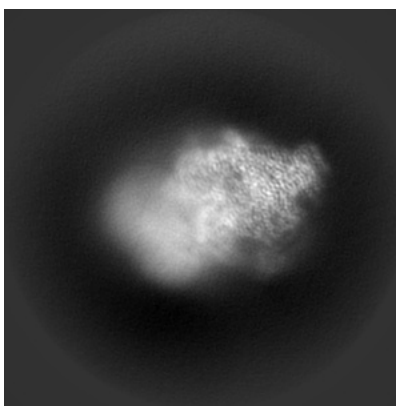
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

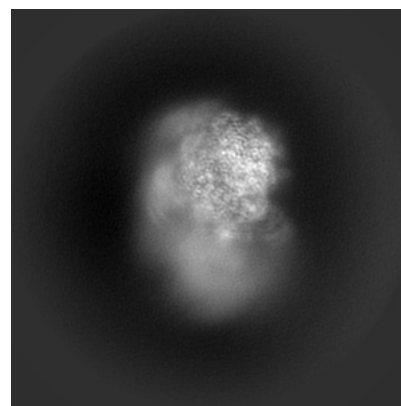
#### 6.1.1 Primary map



X

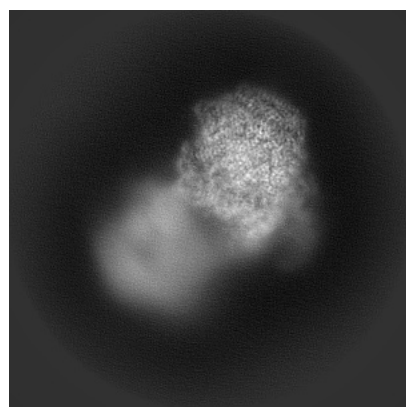


Y

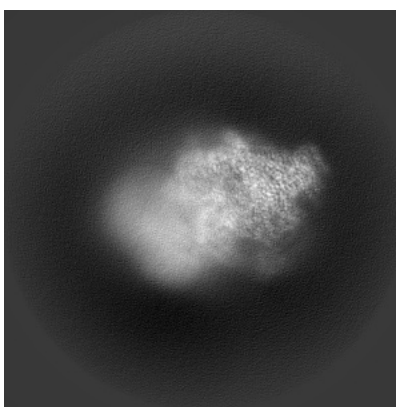


Z

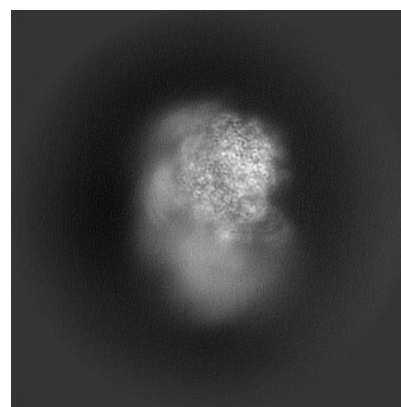
#### 6.1.2 Raw map



X



Y

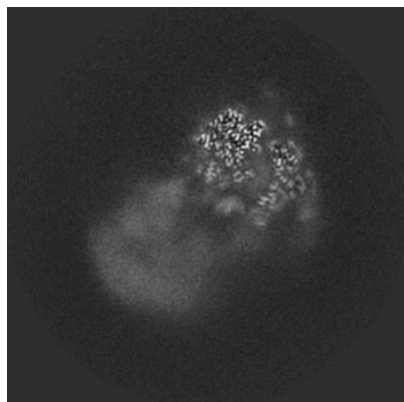


Z

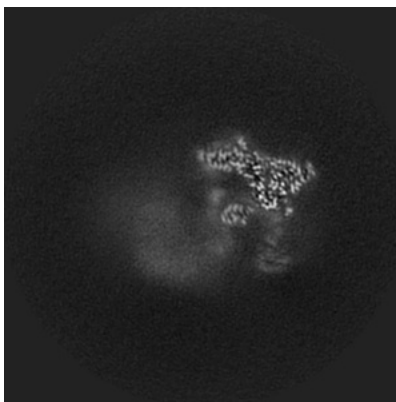
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

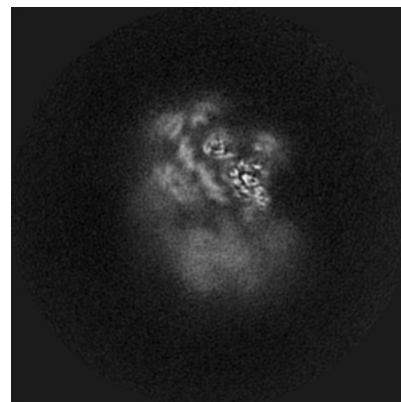
### 6.2.1 Primary map



X Index: 192

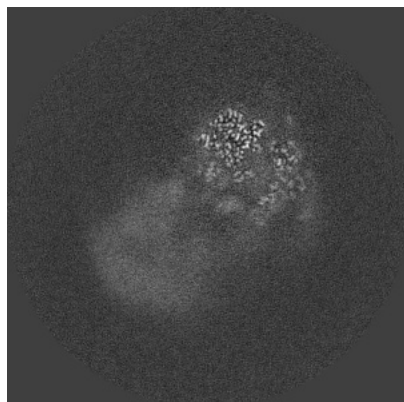


Y Index: 192

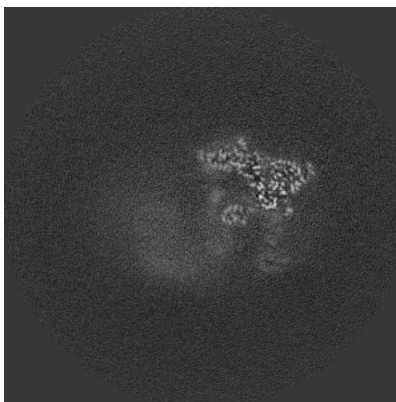


Z Index: 192

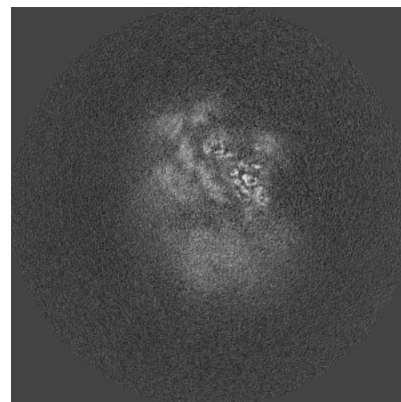
### 6.2.2 Raw map



X Index: 192



Y Index: 192

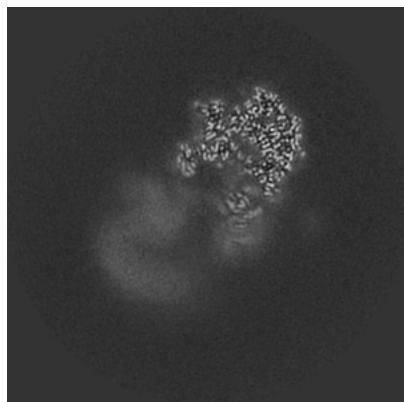


Z Index: 192

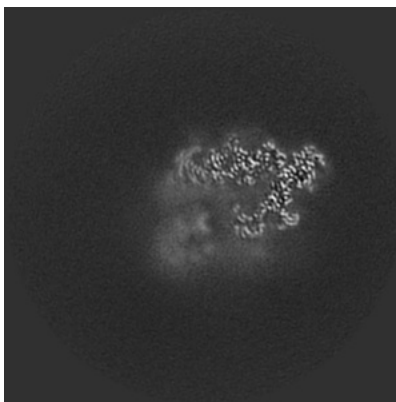
The images above show central slices of the map in three orthogonal directions.

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

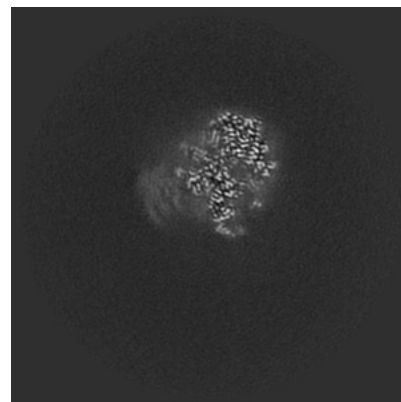
### 6.3.1 Primary map



X Index: 215

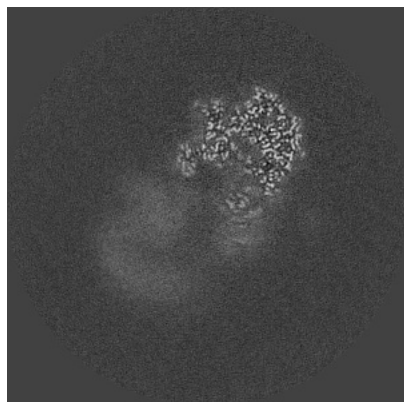


Y Index: 232

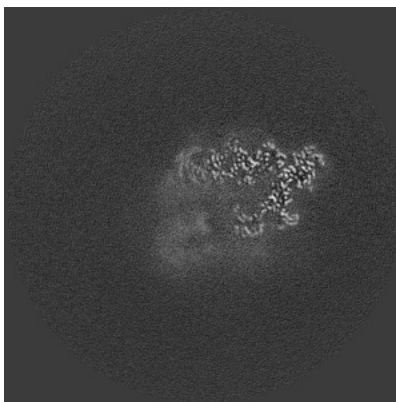


Z Index: 253

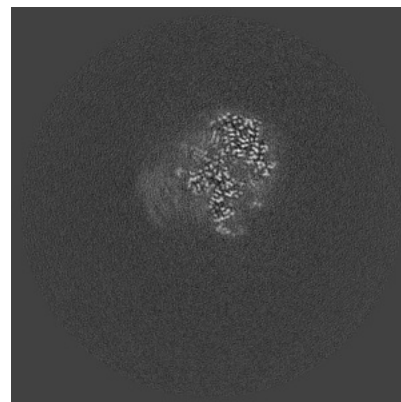
### 6.3.2 Raw map



X Index: 215



Y Index: 232

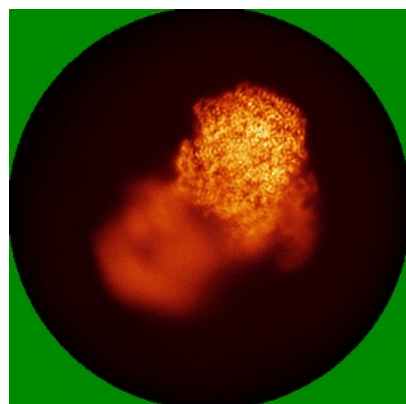


Z Index: 253

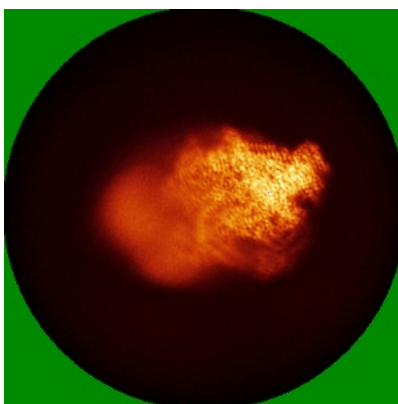
The images above show the largest variance slices of the map in three orthogonal directions.

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

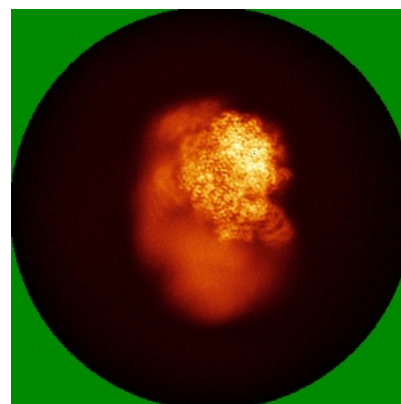
### 6.4.1 Primary map



X

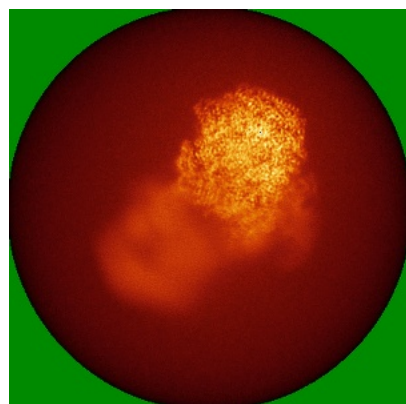


Y

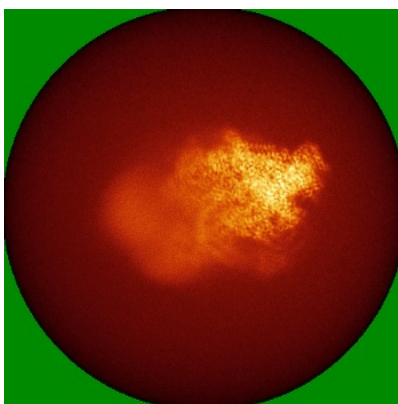


Z

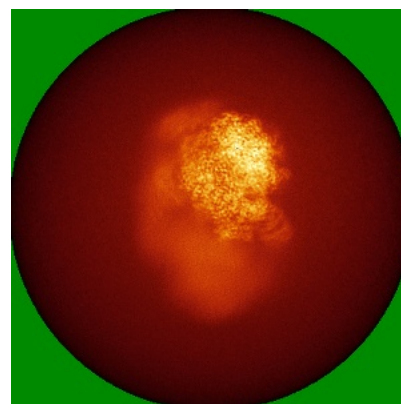
### 6.4.2 Raw map



X



Y



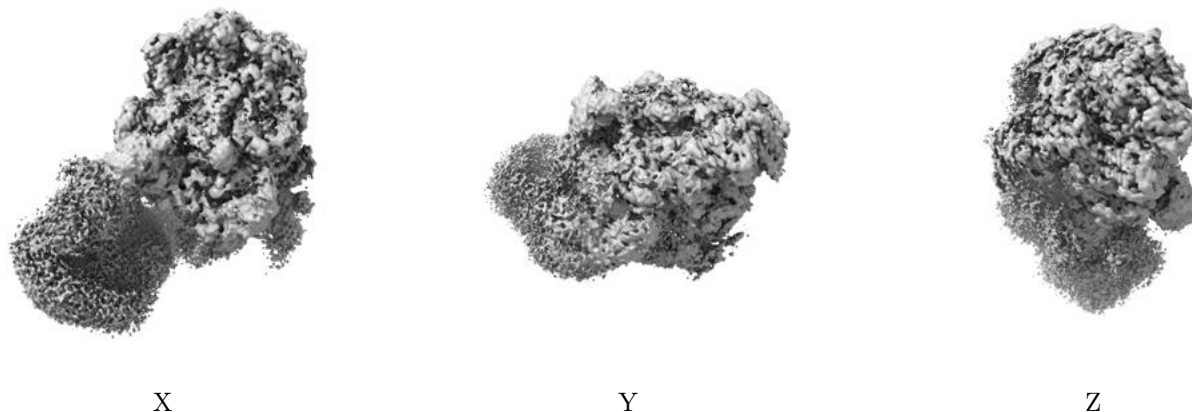
Z

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.



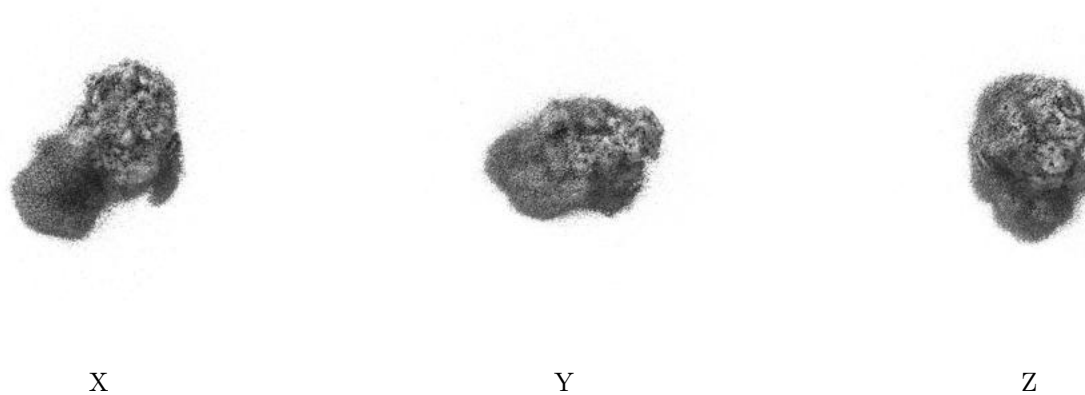
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0098. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

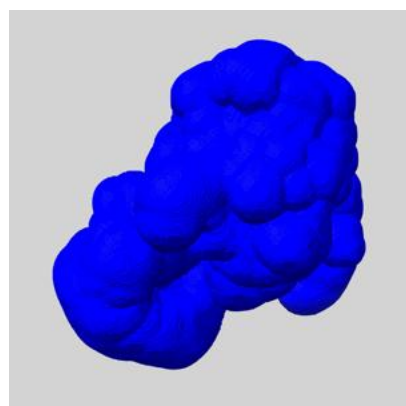
## 6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

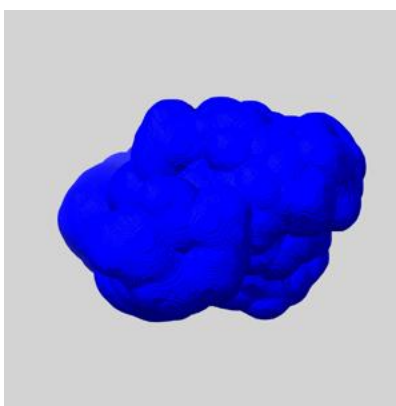
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

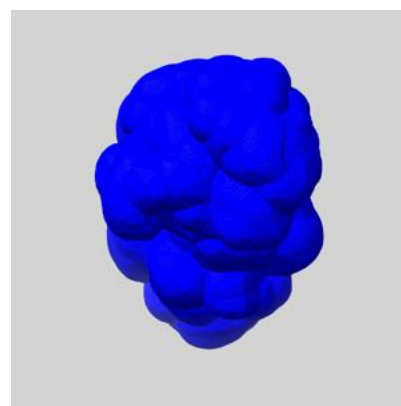
### 6.6.1 emd\_42379\_msk\_1.map [i](#)



X



Y

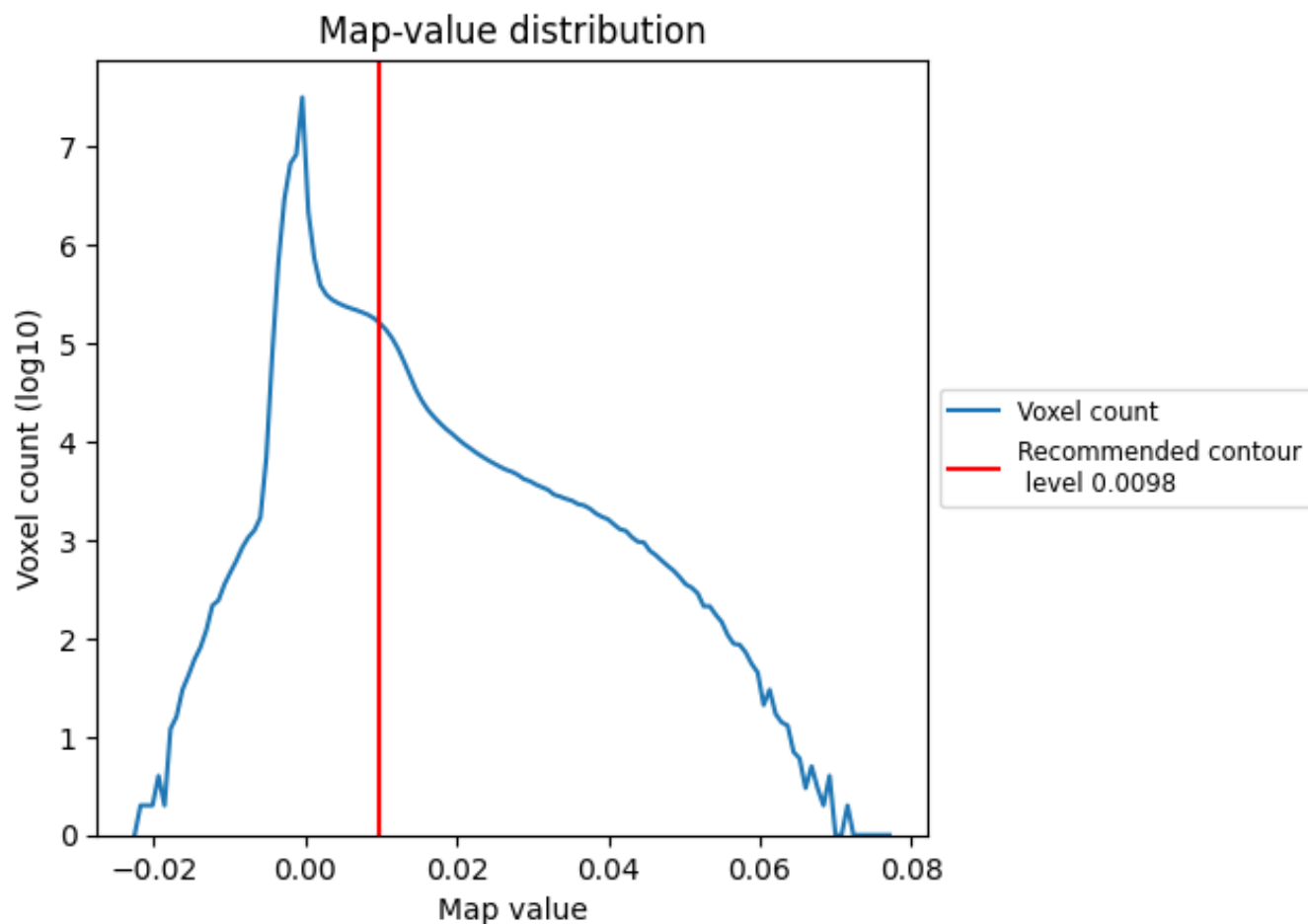


Z

## 7 Map analysis [i](#)

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

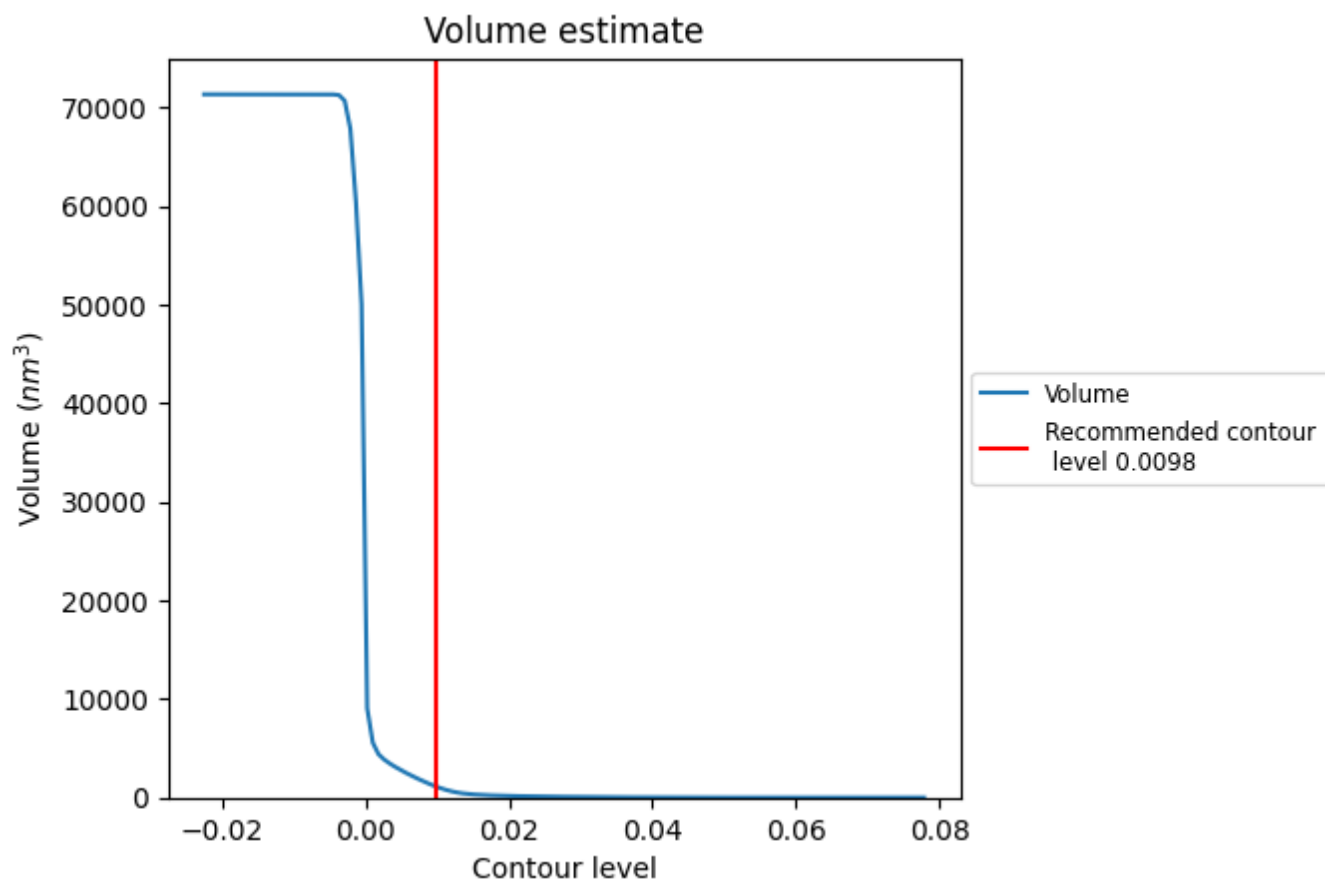
### 7.1 Map-value distribution [i](#)



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.



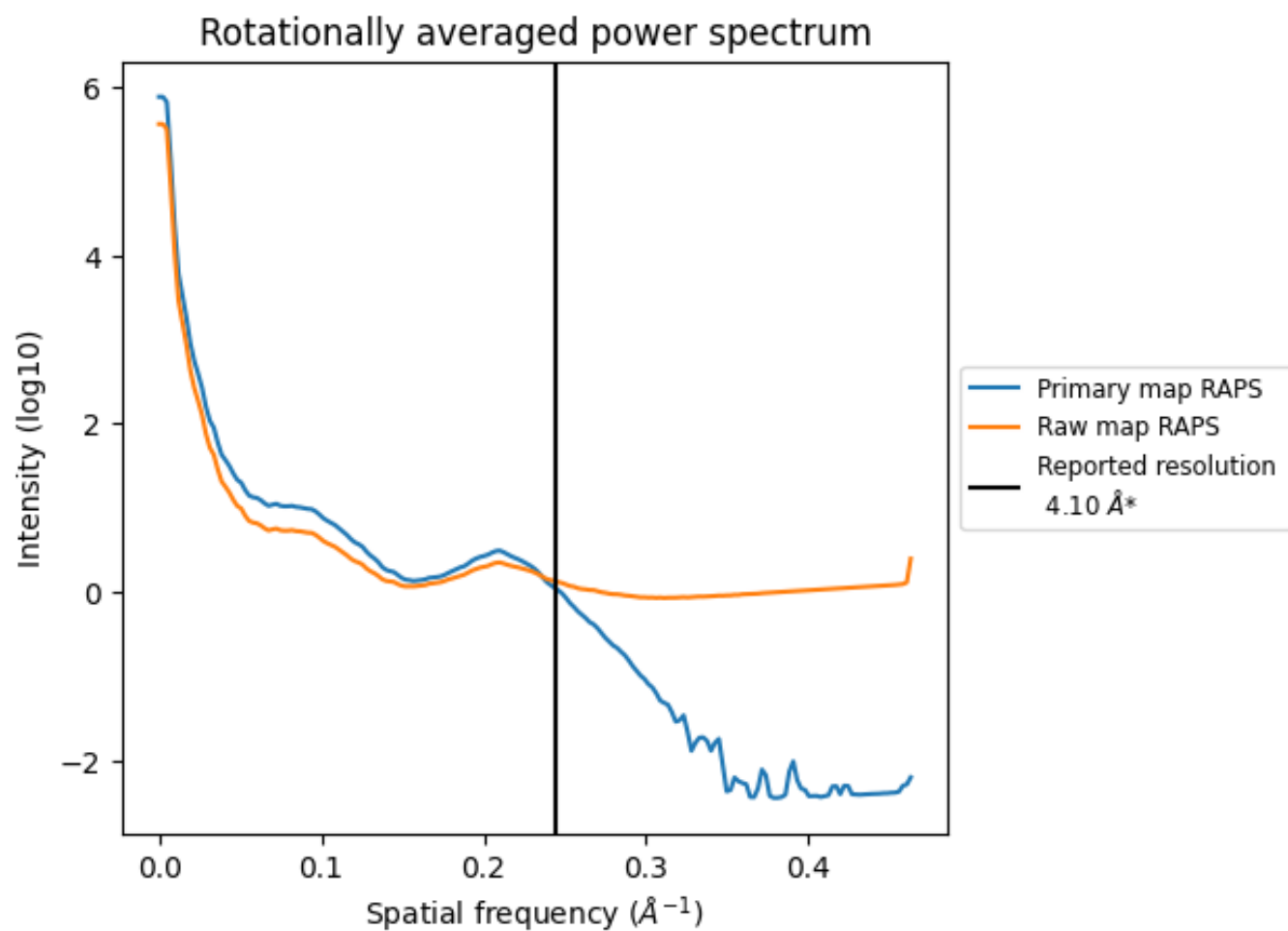
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1130 nm<sup>3</sup>; this corresponds to an approximate mass of 1021 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 ⓘ

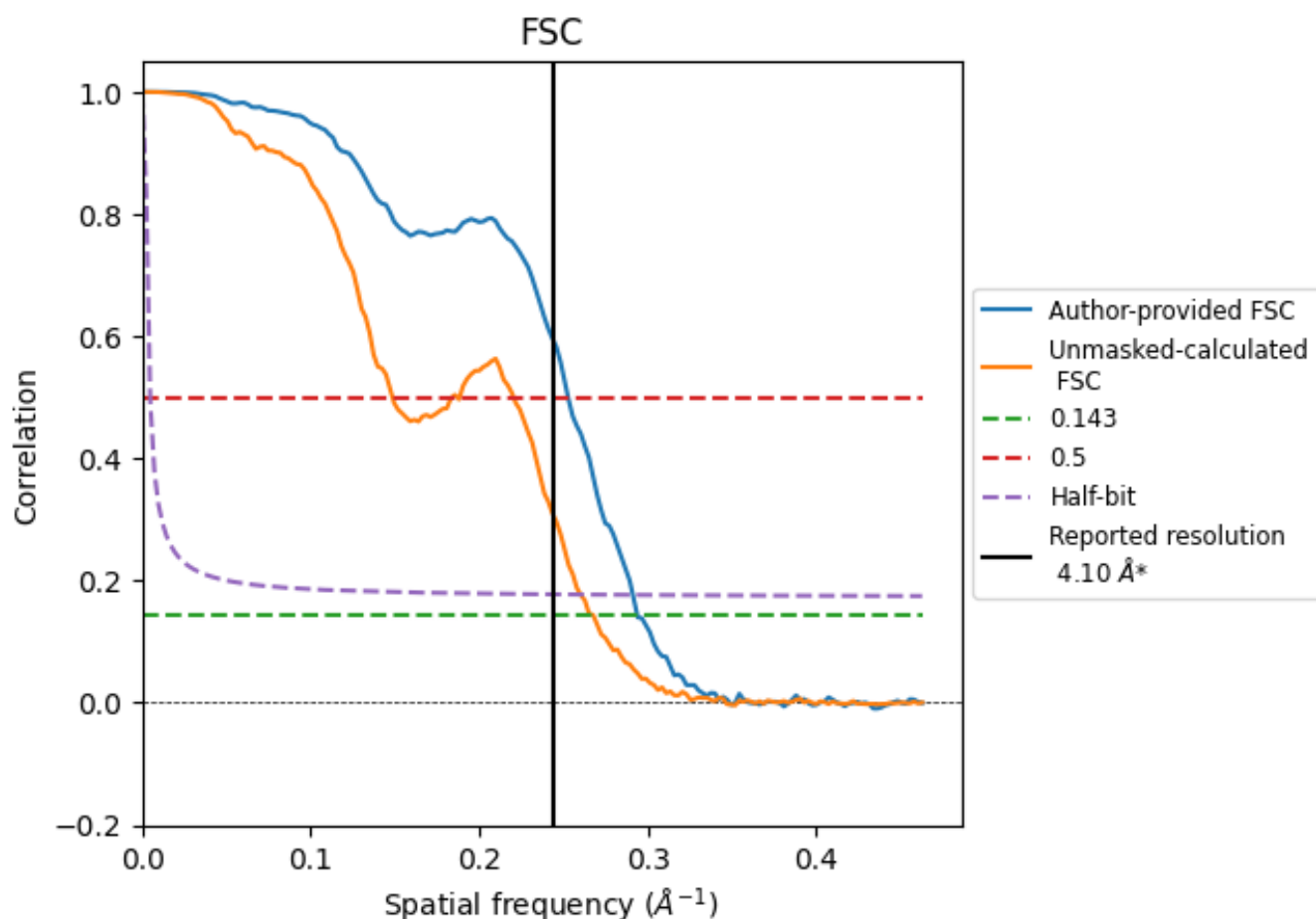


\*Reported resolution corresponds to spatial frequency of  $0.244 \text{ \AA}^{-1}$

## 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 0.244  $\text{\AA}^{-1}$

## 8.2 Resolution estimates [i](#)

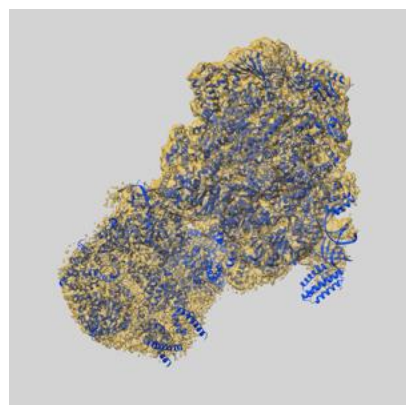
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.10	-	-
Author-provided FSC curve	3.40	3.96	3.43
Unmasked-calculated*	3.74	6.73	3.84

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from author-provided FSC intersecting FSC 0.143 CUT-OFF 3.40 differs from the reported value 4.1 by more than 10 %

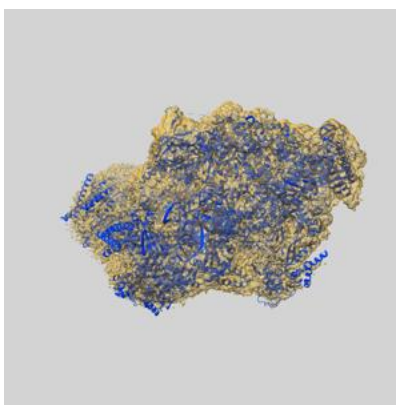
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-42379 and PDB model 8UMH. Per-residue inclusion information can be found in section [3](#) on page [11](#).

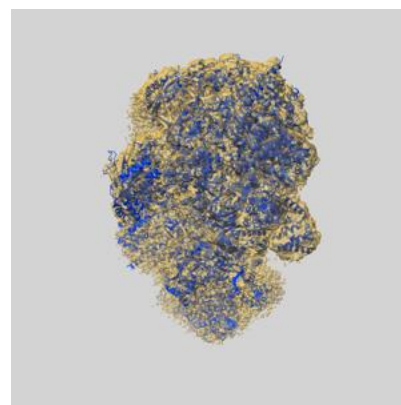
### 9.1 Map-model overlay [i](#)



X



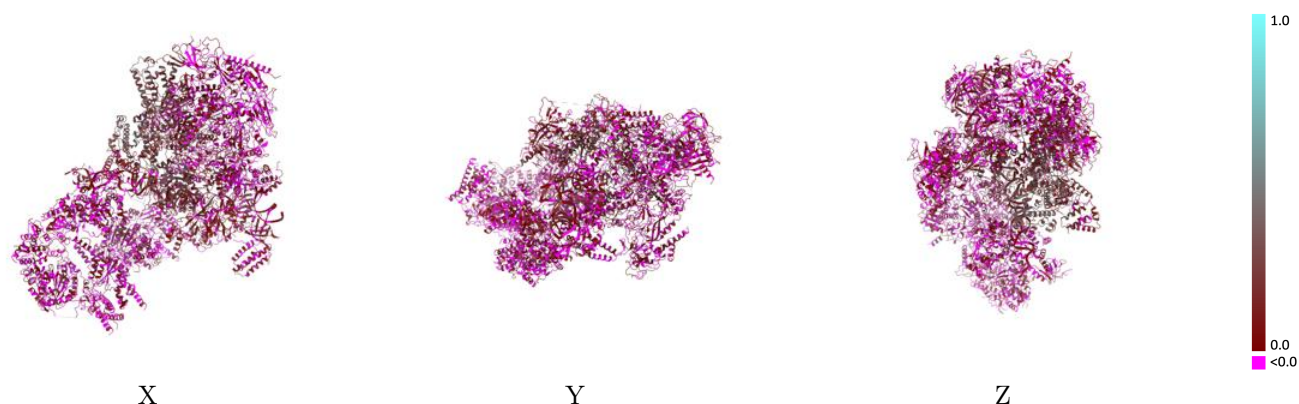
Y



Z

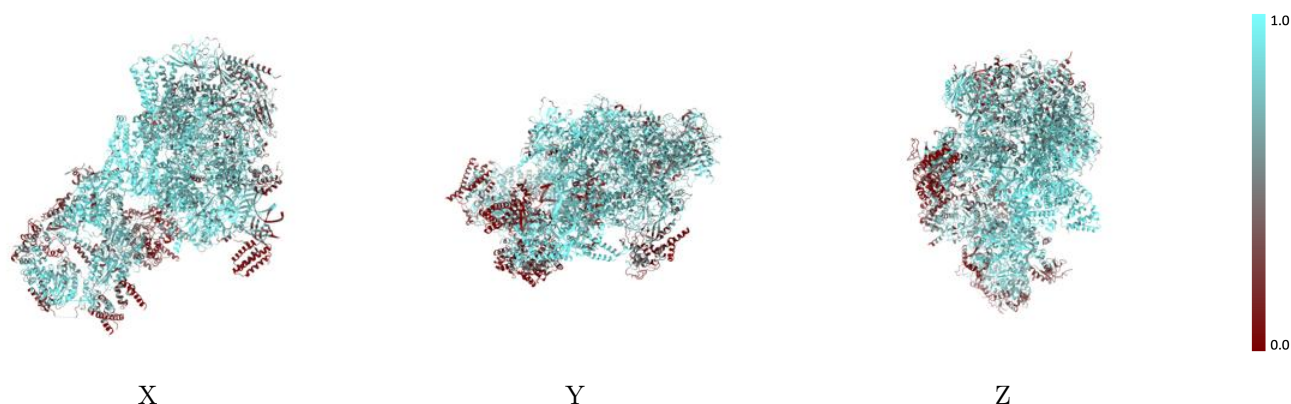
The images above show the 3D surface view of the map at the recommended contour level 0.0098 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



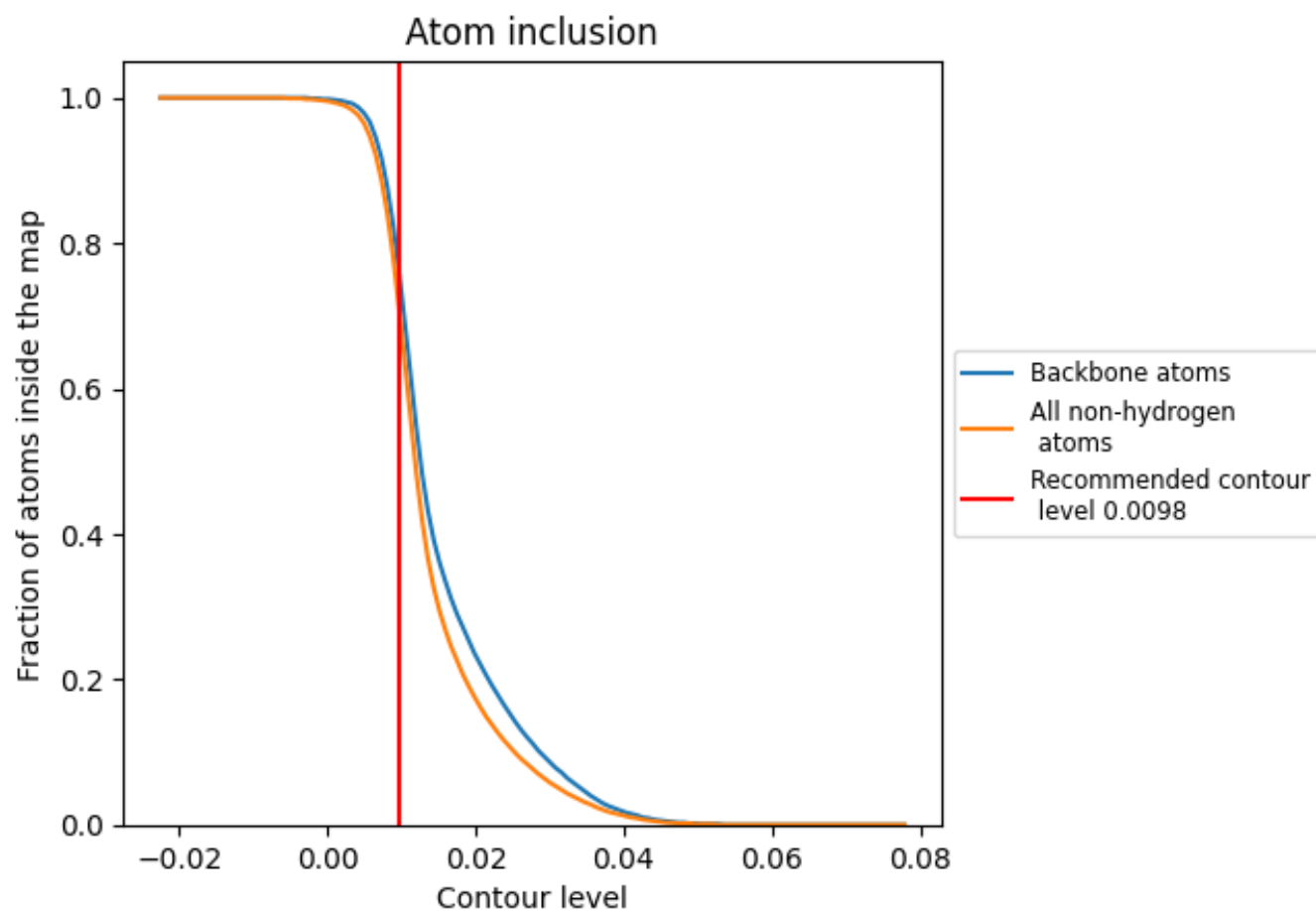
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0098).































































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 75% of all backbone atoms, 70% 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 (0.0098) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6980	 0.0810
0	 0.4800	 0.0170
1	 0.3720	 -0.0050
2	 0.6150	 0.0270
4	 0.6940	 0.0080
5	 0.3900	 0.0130
6	 0.8040	 0.0050
7	 0.7630	 0.0210
A	 0.8460	 0.1840
B	 0.7780	 0.0990
C	 0.6130	 -0.0030
D	 0.2250	 0.0310
E	 0.9600	 0.3580
F	 0.7700	 0.1480
G	 0.4540	 0.0510
H	 0.7480	 0.0840
I	 0.8470	 0.1730
J	 0.6040	 -0.0140
K	 0.6420	 0.0220
L	 0.7380	 0.0420
M	 0.5740	 0.0270
N	 0.8830	 0.1380
O	 0.7930	 0.0210
P	 0.8560	 0.1120
Q	 0.7570	 0.1470
S	 0.8770	 0.1340
T	 0.8120	 0.1040
U	 0.2700	 0.0460
V	 0.3060	 0.0670
W	 0.7430	 0.0810
X	 0.8720	 0.0790

