wwPDB EM Validation Summary Report (i)

Jul 3, 2024 – 11:59 am BST

PDB ID	:	7NVT
EMDB ID	:	EMD-12612
Title	:	RNA polymerase II core pre-initiation complex with closed promoter DNA in distal position
Authors	:	Aibara, S.; Schilbach, S.; Cramer, P.
Deposited on	:	2021-03-16
Resolution	:	2.90 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*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

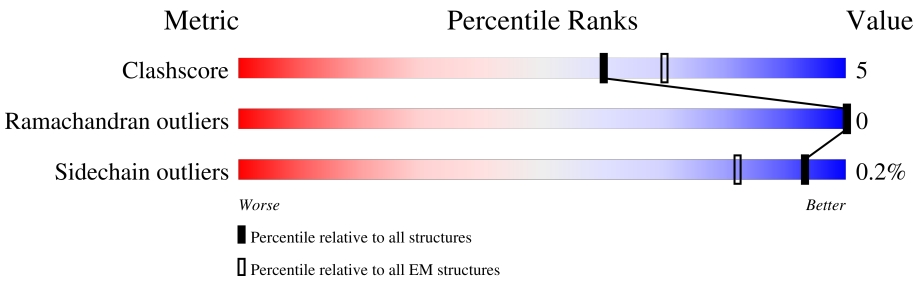
EMDB validation analysis	:	0.0.1.dev92
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 2.90 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	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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 >=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 <=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	A	1970	63% 9% 28%
2	B	1174	85% 11%
3	C	275	83% 10% 7%
4	D	142	51% 82% 8% 10%
5	E	210	78% 21%
6	F	127	54% 8% 38%
7	G	172	25% 89% 10%
8	H	150	90% 9%

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Mol	Chain	Length	Quality of chain
9	I	125	79% 12% 9%
10	J	67	78% 18%
11	K	117	82% 16%
12	L	58	71% 5% 24%
13	M	316	73% 6% 20%
14	N	106	11% 34% 13% 53%
15	O	339	47% 6% 47%
16	Q	517	24% 73%
17	R	249	22% 82% 7% 11%
18	T	106	8% 40% 8% 53%
19	U	376	28% 27% 70%
20	V	109	87% 79% 12% 9%
21	W	439	24% 35% 8% 57%
22	X	291	47% 52% 7% 41%

2 Entry composition (i)

There are 24 unique types of molecules in this entry. The entry contains 44114 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 RPB1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	1423	11274	7092	2016	2094	72	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	1136	9076	5739	1597	1676	64	0	0

- Molecule 3 is a protein called DNA-directed RNA polymerase II subunit RPB3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	257	2059	1294	351	408	6	0	0

- Molecule 4 is a protein called RPOL4c domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	D	128	1050	656	178	212	4	0	0

- Molecule 5 is a protein called DNA-directed RNA polymerase II subunit E.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	E	209	1721	1089	300	324	8	0	0

- Molecule 6 is a protein called DNA-directed RNA polymerase II subunit F.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	F	79	636	406	108	117	5	0	0

- Molecule 7 is a protein called DNA-directed RNA polymerase II subunit RPB7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	G	171	1351	875	219	249	8	0	0

- Molecule 8 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	H	148	1186	750	194	237	5	0	0

- Molecule 9 is a protein called DNA-directed RNA polymerase II subunit RPB9.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	I	114	928	571	166	180	11	0	0

- Molecule 10 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	J	64	507	328	86	87	6	0	0

- Molecule 11 is a protein called RNA_pol_L_2 domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	K	115	920	593	152	173	2	0	0

- Molecule 12 is a protein called RNA polymerase II subunit K.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	L	44	373	231	72	64	6	0	0

- Molecule 13 is a protein called Transcription initiation factor IIB.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	M	252	1953	1224	346	366	17	0	0

- Molecule 14 is a DNA chain called Non-Template DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
14	N	50	1034	489	195	301	49	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
15	O	179	1422	923	251	241	7	0	0

- Molecule 16 is a protein called General transcription factor IIF subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
16	Q	138	1138	719	208	208	3	0	0

- Molecule 17 is a protein called General transcription factor IIF subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
17	R	222	1788	1127	320	338	3	0	0

- Molecule 18 is a DNA chain called Template DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
18	T	50	1013	480	186	297	50	0	0

- Molecule 19 is a protein called Transcription initiation factor IIA subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
19	U	113	930	585	152	189	4	0	0

- Molecule 20 is a protein called Transcription initiation factor IIA subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
20	V	99	806	510	142	151	3	0	0

- Molecule 21 is a protein called General transcription factor IIE subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
21	W	187	1535	964	275	285	11	0	0

- Molecule 22 is a protein called Transcription initiation factor IIE subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
22	X	171	1403	895	243	261	4	0	0

- Molecule 23 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
23	A	2	2	2	0
23	B	1	1	1	0
23	C	1	1	1	0
23	I	2	2	2	0
23	J	1	1	1	0
23	L	1	1	1	0
23	M	1	1	1	0
23	W	1	1	1	0

- Molecule 24 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

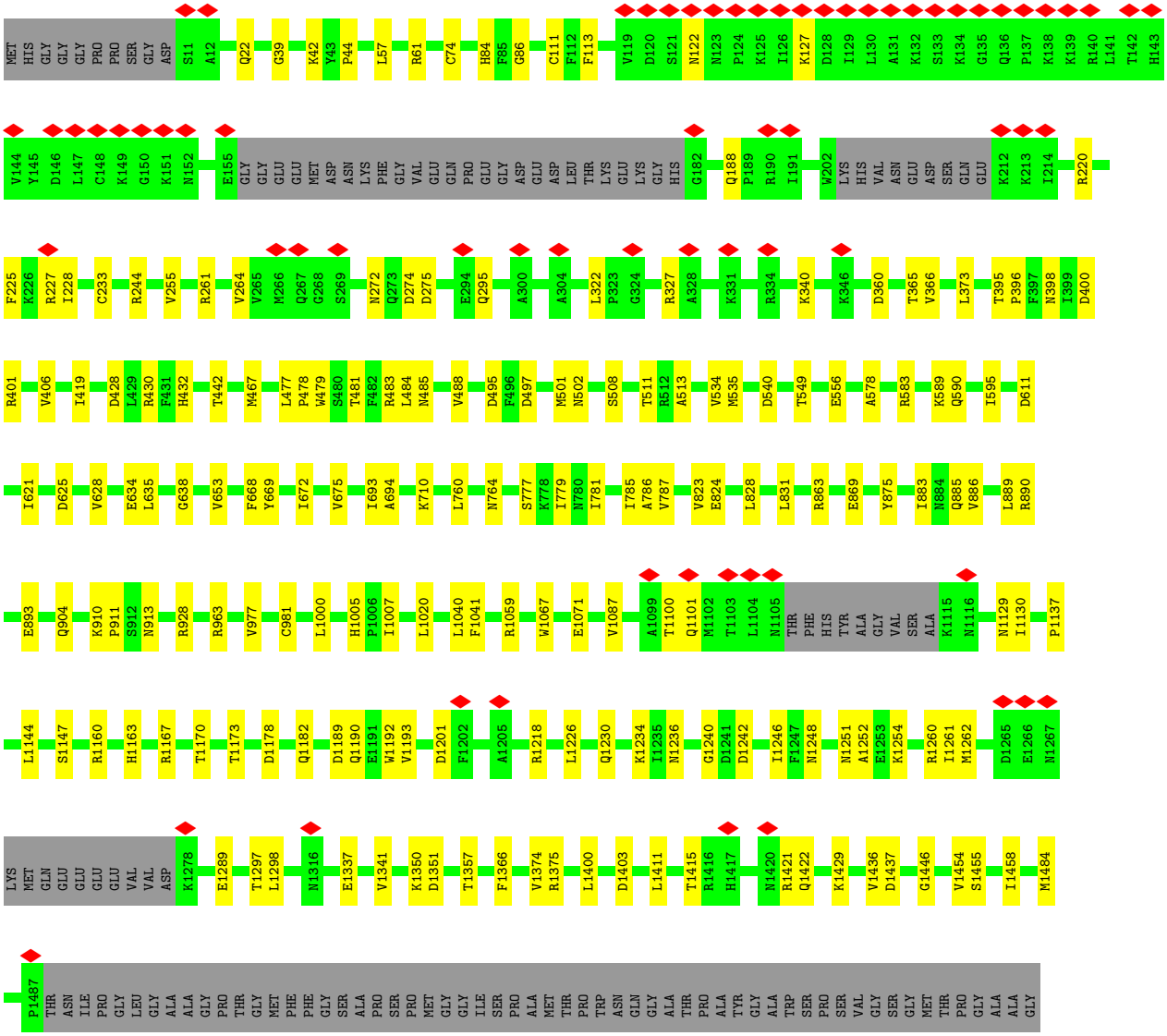
Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
24	A	1	1	1	0

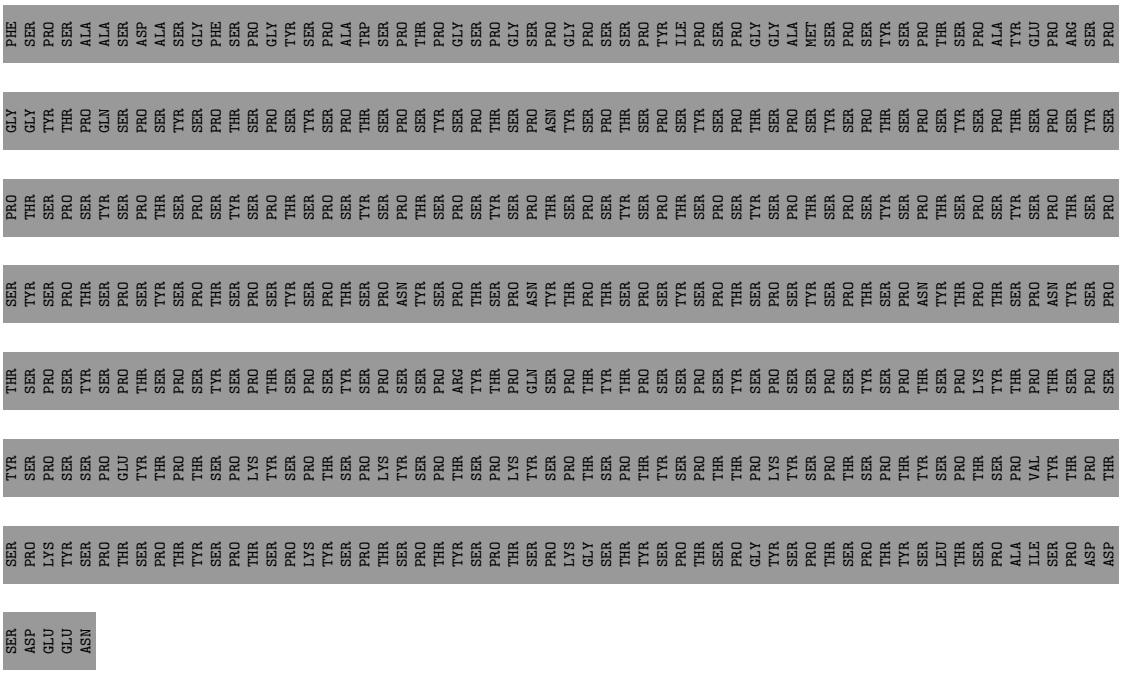
3 Residue-property plots (i)

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: RPB1

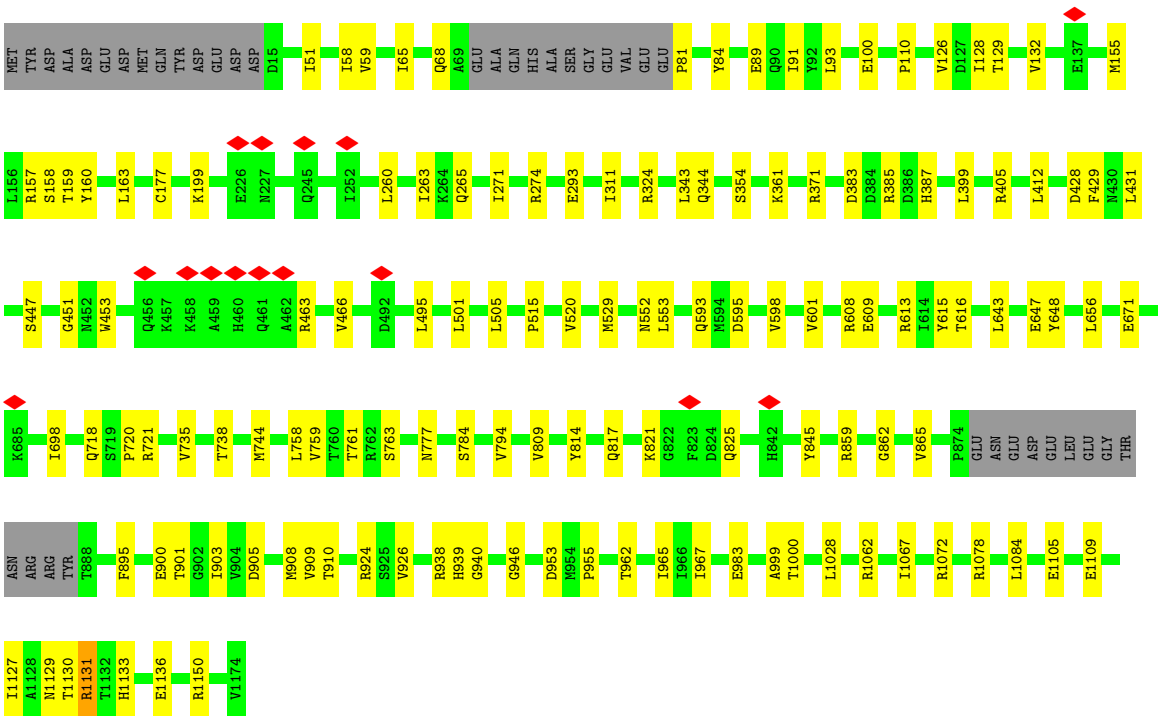
Chain A:





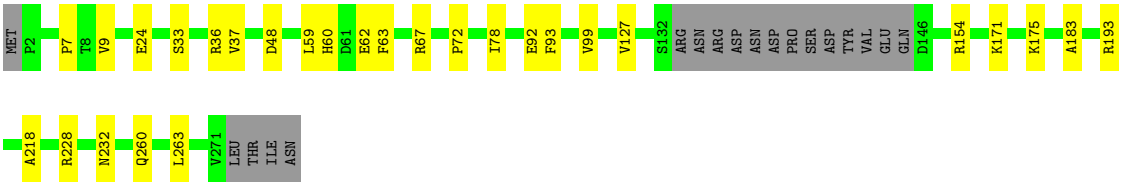
- Molecule 2: DNA-directed RNA polymerase subunit beta

Chain B:



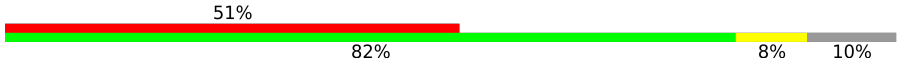
- Molecule 3: DNA-directed RNA polymerase II subunit RPB3

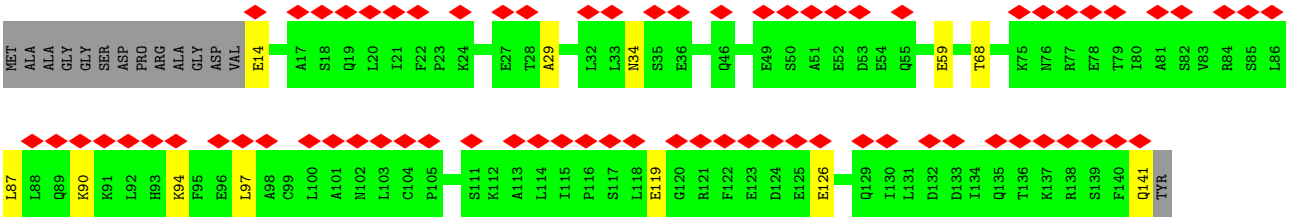
Chain C:



• Molecule 4: RPOL4c domain-containing protein

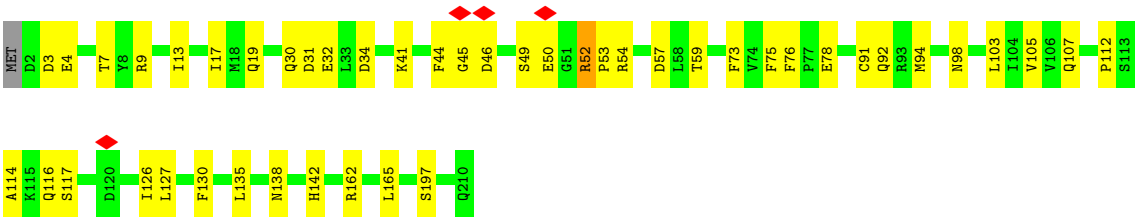
Chain D:





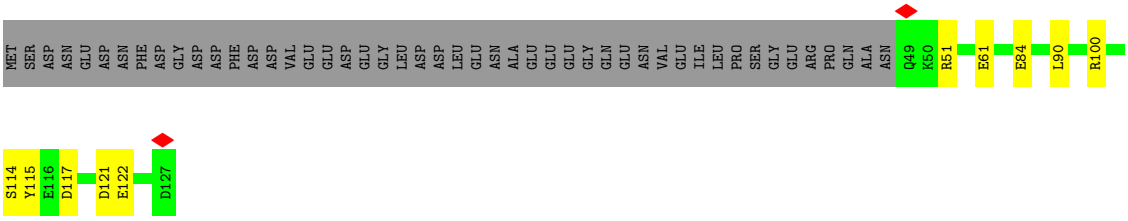
• Molecule 5: DNA-directed RNA polymerase II subunit E

Chain E:



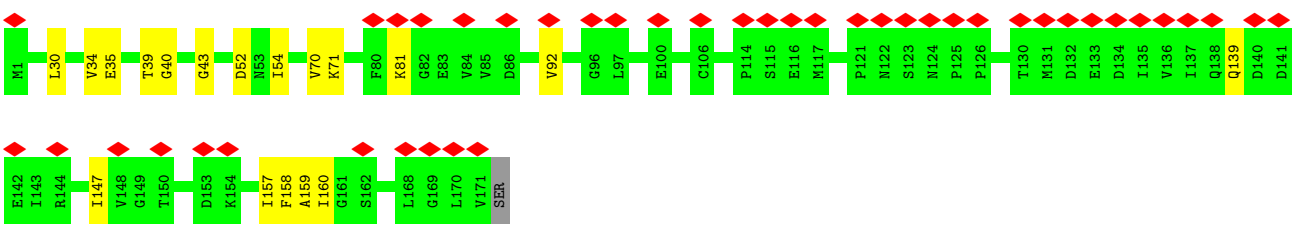
• Molecule 6: DNA-directed RNA polymerase II subunit F

Chain F:



• Molecule 7: DNA-directed RNA polymerase II subunit RPB7

Chain G:

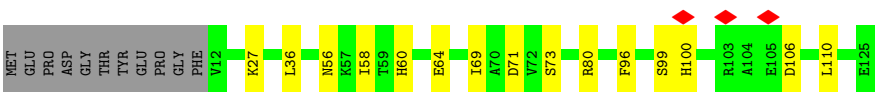


• Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC3

Chain H:

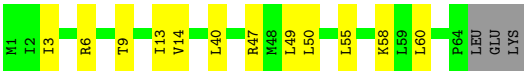
• Molecule 9: DNA-directed RNA polymerase II subunit RPB9

Chain I:



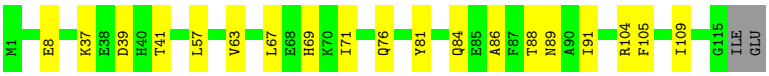
• Molecule 10: DNA-directed RNA polymerases I, II, and III subunit RPABC5

Chain J:



• Molecule 11: RNA_pol_L_2 domain-containing protein

Chain K:

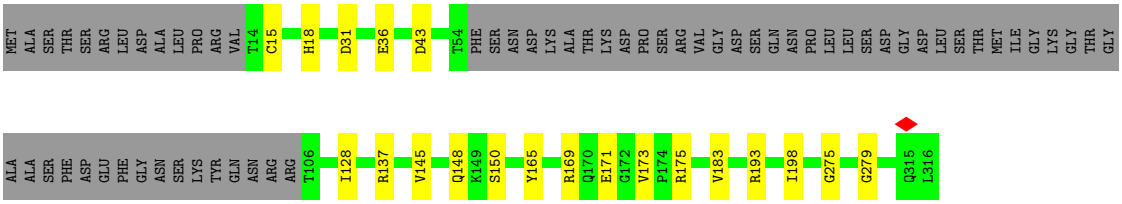


• Molecule 12: RNA polymerase II subunit K

Chain L:

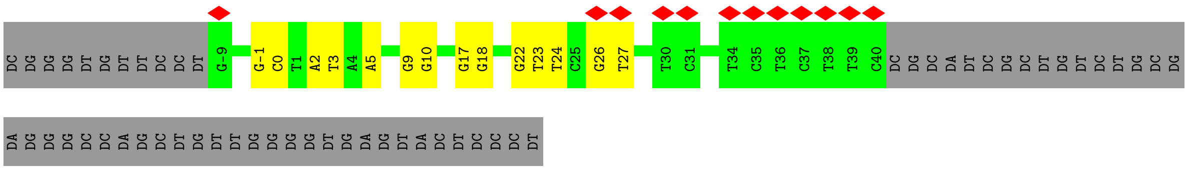
• Molecule 13: Transcription initiation factor IIB

Chain M:

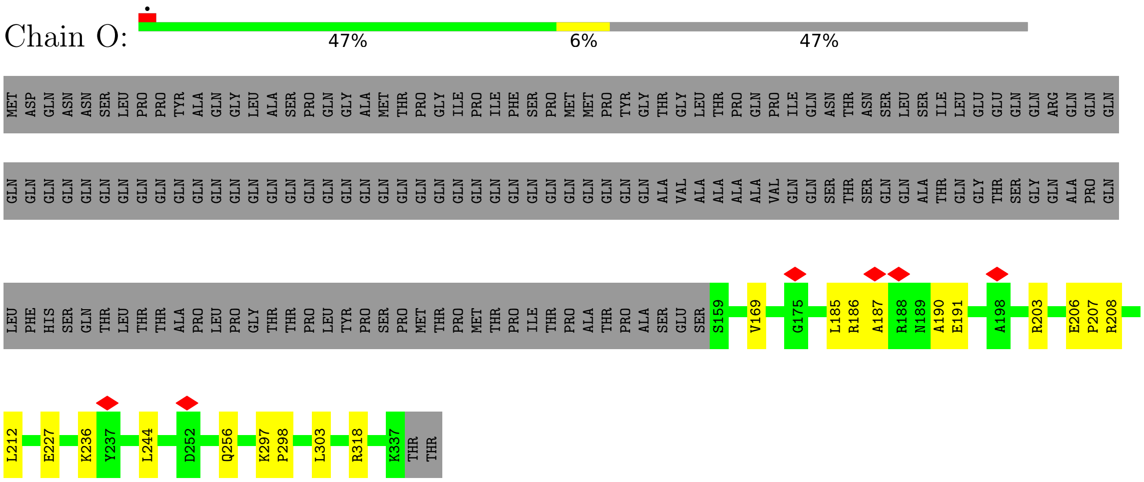


• Molecule 14: Non-Template DNA

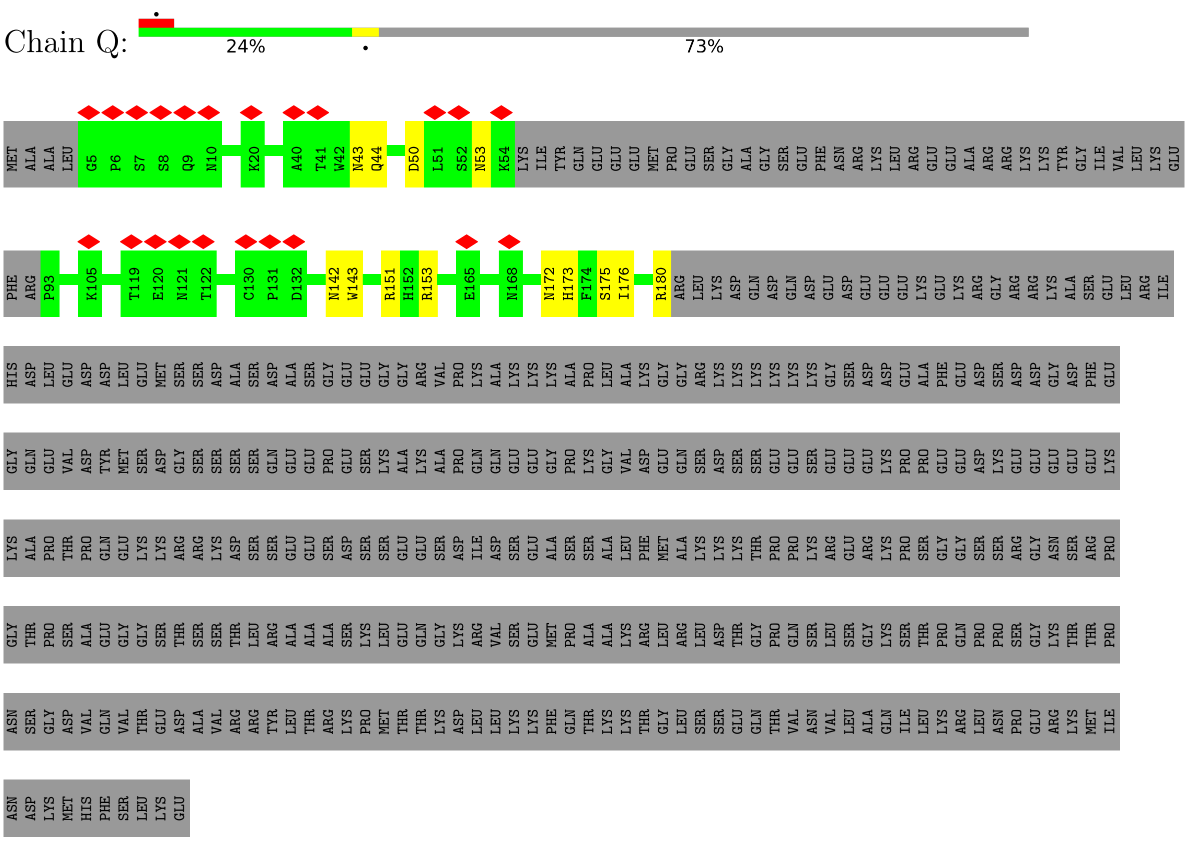
Chain N:



• Molecule 15: TATA-box-binding protein

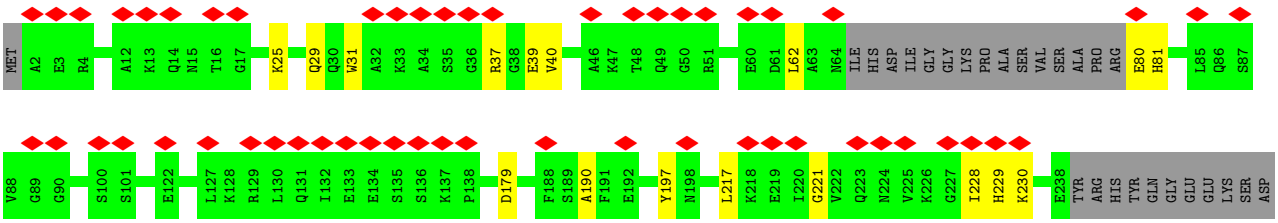


• Molecule 16: General transcription factor IIF subunit 1



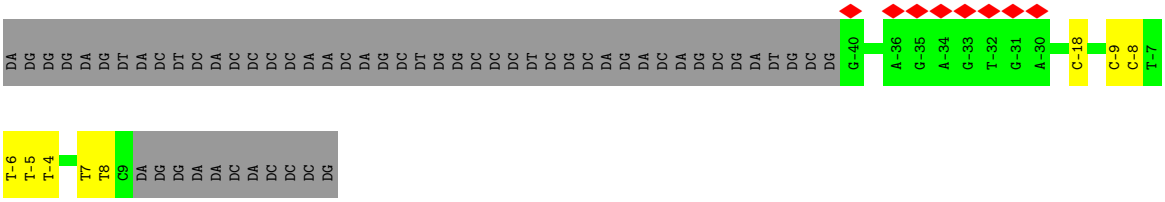
• Molecule 17: General transcription factor IIF subunit 2

Chain R:



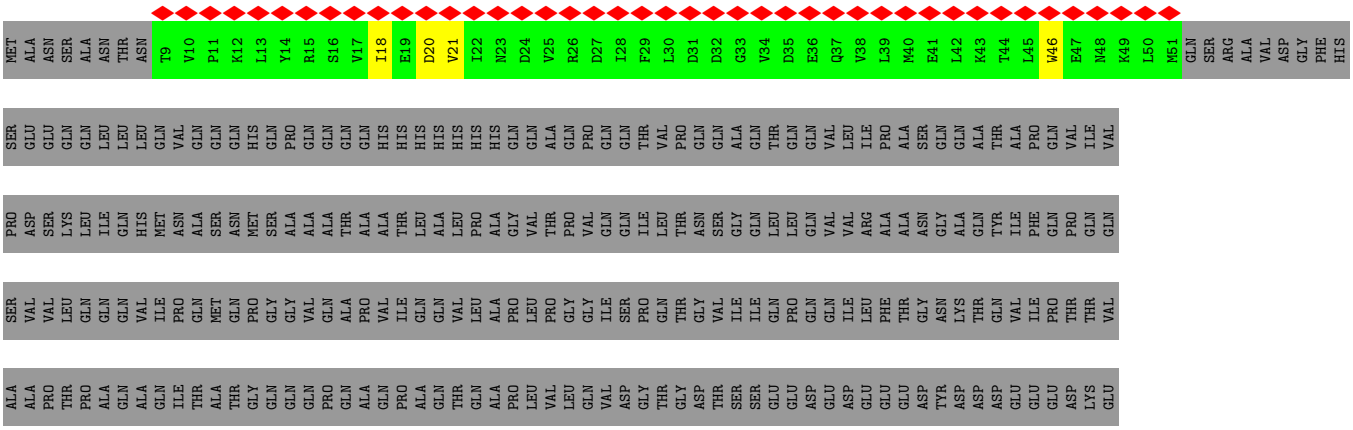
- Molecule 18: Template DNA

Chain T:



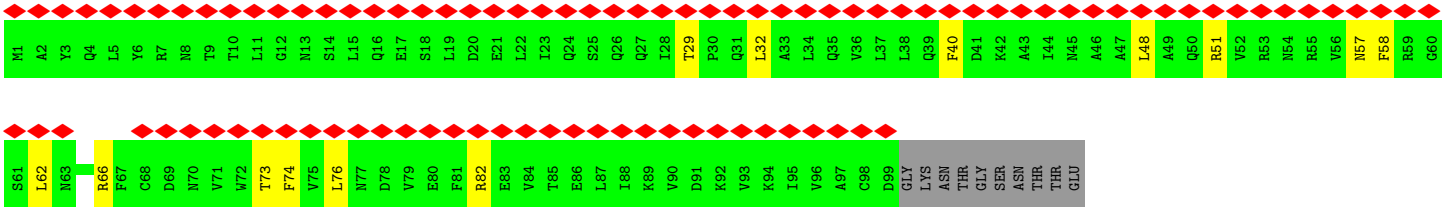
- Molecule 19: Transcription initiation factor IIA subunit 1

Chain U:



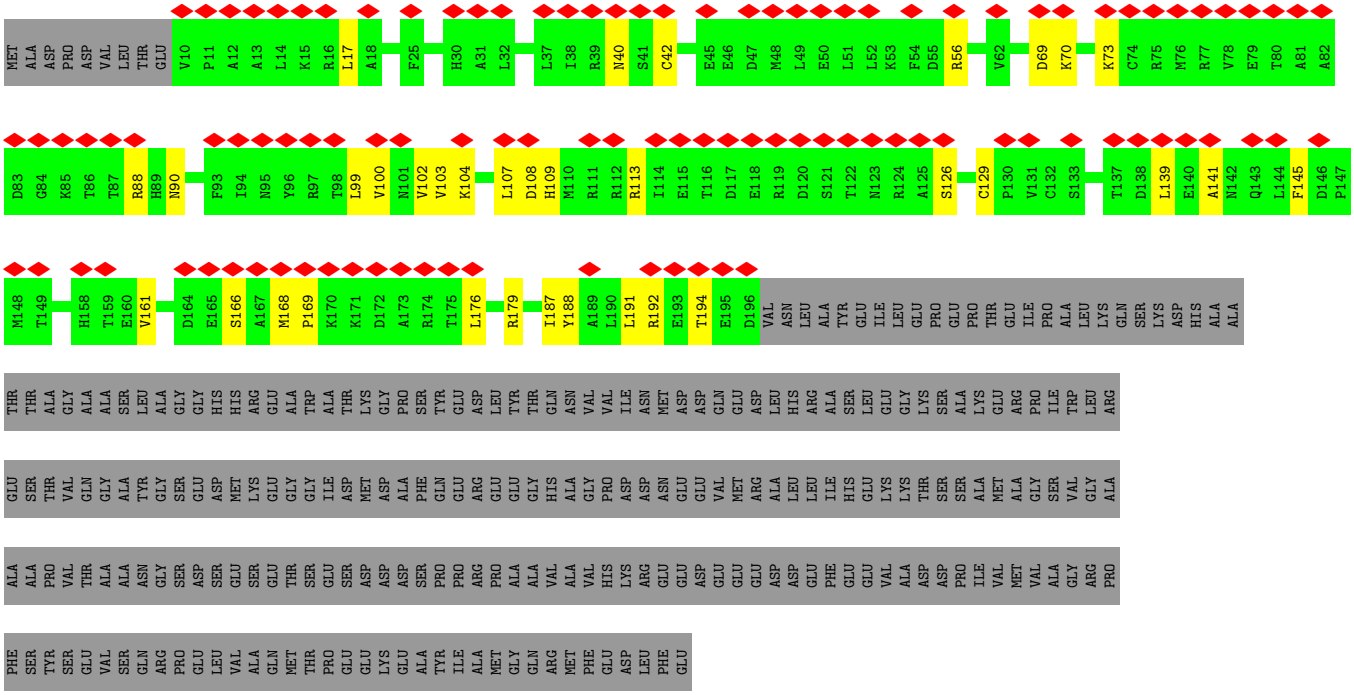
- Molecule 20: Transcription initiation factor IIA subunit 2

Chain V:



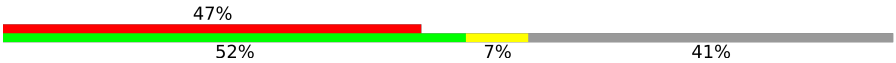
- Molecule 21: General transcription factor IIE subunit 1

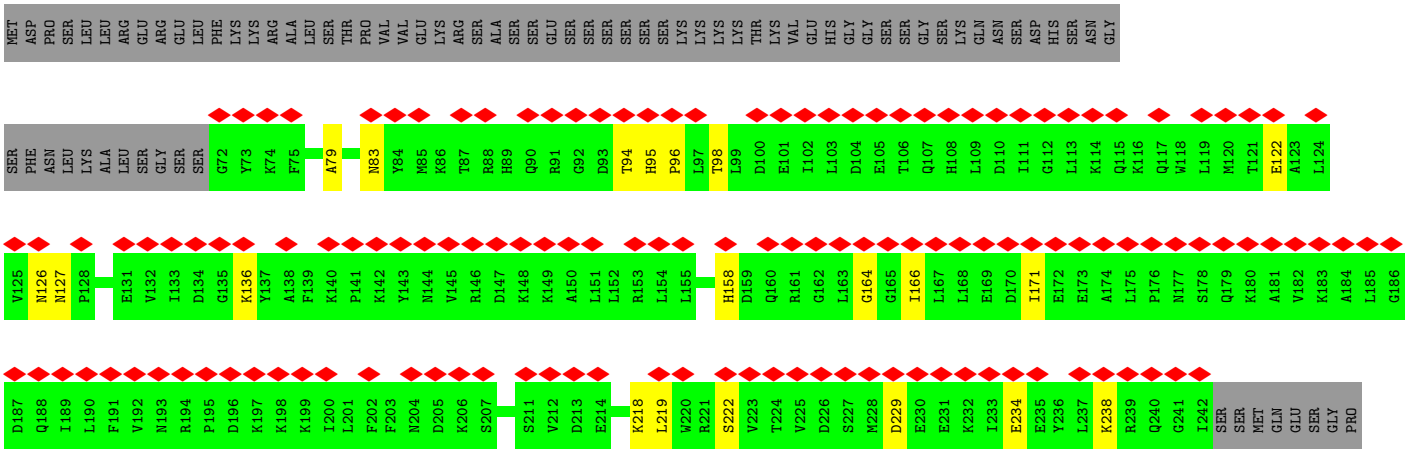
Chain W:



- Molecule 22: Transcription initiation factor IIE subunit beta

Chain X:





LYS LYS VAL ALA PRO ILE GLN ARG ARG LYS LYS PRO ALA SER GLN LYS LYS ARG ARG PHE LYS THR HIS ASN GLU HIS LEU ALA GLY VAL LEU LYS ASP TYR SER ASP ILE THR SER SER LYS

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	50177	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	41.1	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	75.645	Depositor
Minimum map value	-51.877	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	0.975	Depositor
Recommended contour level	4.5	Depositor
Map size (Å)	472.49997, 472.49997, 472.49997	wwPDB
Map dimensions	450, 450, 450	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.05, 1.05, 1.05	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

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	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
1	A	0.26	0/11479	0.41	0/15496
2	B	0.28	0/9257	0.42	0/12493
3	C	0.28	0/2102	0.44	0/2857
4	D	0.24	0/1064	0.35	0/1428
5	E	0.25	0/1752	0.41	0/2366
6	F	0.26	0/646	0.41	0/871
7	G	0.25	0/1382	0.40	0/1874
8	H	0.29	0/1207	0.45	0/1628
9	I	0.25	0/949	0.44	0/1284
10	J	0.30	0/516	0.43	0/696
11	K	0.28	0/939	0.41	0/1271
12	L	0.31	0/378	0.40	0/500
13	M	0.24	0/1983	0.39	0/2679
14	N	0.49	0/1161	0.88	0/1794
15	O	0.25	0/1448	0.41	0/1948
16	Q	0.24	0/1167	0.39	0/1576
17	R	0.24	0/1817	0.39	0/2445
18	T	0.52	0/1134	0.85	0/1744
19	U	0.23	0/945	0.40	0/1274
20	V	0.24	0/816	0.39	0/1105
21	W	0.23	0/1560	0.37	0/2097
22	X	0.23	0/1427	0.36	0/1916
All	All	0.28	0/45129	0.45	0/61342

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	A	11274	0	11406	122	0
2	B	9076	0	9116	89	0
3	C	2059	0	2007	24	0
4	D	1050	0	1033	8	0
5	E	1721	0	1737	32	0
6	F	636	0	665	7	0
7	G	1351	0	1358	14	0
8	H	1186	0	1147	8	0
9	I	928	0	859	11	0
10	J	507	0	523	15	0
11	K	920	0	942	17	0
12	L	373	0	378	3	0
13	M	1953	0	1987	13	0
14	N	1034	0	563	12	0
15	O	1422	0	1514	14	0
16	Q	1138	0	1103	6	0
17	R	1788	0	1819	10	0
18	T	1013	0	559	8	0
19	U	930	0	888	11	0
20	V	806	0	818	9	0
21	W	1535	0	1540	25	0
22	X	1403	0	1428	12	0
23	A	2	0	0	0	0
23	B	1	0	0	0	0
23	C	1	0	0	0	0
23	I	2	0	0	0	0
23	J	1	0	0	0	0
23	L	1	0	0	0	0
23	M	1	0	0	0	0
23	W	1	0	0	0	0
24	A	1	0	0	0	0
All	All	44114	0	43390	409	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 5.

The worst 5 of 409 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:A:911:PRO:O	1:A:963:ARG:NH2	2.06	0.89
7:G:160:ILE:HD11	21:W:139:LEU:HD11	1.59	0.85
1:A:513:ALA:HB2	6:F:90:LEU:HD21	1.58	0.82
3:C:36:ARG:NH1	11:K:41:THR:OG1	2.14	0.81
17:R:190:ALA:O	17:R:197:TYR:OH	1.98	0.81

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	A	1413/1970 (72%)	1374 (97%)	39 (3%)	0	100	100
2	B	1130/1174 (96%)	1092 (97%)	38 (3%)	0	100	100
3	C	253/275 (92%)	246 (97%)	7 (3%)	0	100	100
4	D	126/142 (89%)	123 (98%)	3 (2%)	0	100	100
5	E	207/210 (99%)	203 (98%)	4 (2%)	0	100	100
6	F	77/127 (61%)	75 (97%)	2 (3%)	0	100	100
7	G	169/172 (98%)	165 (98%)	4 (2%)	0	100	100
8	H	146/150 (97%)	141 (97%)	5 (3%)	0	100	100
9	I	112/125 (90%)	103 (92%)	9 (8%)	0	100	100
10	J	62/67 (92%)	60 (97%)	2 (3%)	0	100	100
11	K	113/117 (97%)	112 (99%)	1 (1%)	0	100	100
12	L	42/58 (72%)	39 (93%)	3 (7%)	0	100	100
13	M	248/316 (78%)	241 (97%)	7 (3%)	0	100	100
15	O	177/339 (52%)	175 (99%)	2 (1%)	0	100	100
16	Q	134/517 (26%)	129 (96%)	5 (4%)	0	100	100
17	R	218/249 (88%)	213 (98%)	5 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
19	U	109/376 (29%)	103 (94%)	6 (6%)	0	100	100
20	V	97/109 (89%)	95 (98%)	2 (2%)	0	100	100
21	W	185/439 (42%)	184 (100%)	1 (0%)	0	100	100
22	X	169/291 (58%)	167 (99%)	2 (1%)	0	100	100
All	All	5187/7223 (72%)	5040 (97%)	147 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	
1	A	1254/1749 (72%)	1253 (100%)	1 (0%)	93	98
2	B	994/1027 (97%)	992 (100%)	2 (0%)	93	98
3	C	234/252 (93%)	234 (100%)	0	100	100
4	D	118/126 (94%)	118 (100%)	0	100	100
5	E	191/192 (100%)	189 (99%)	2 (1%)	76	92
6	F	69/111 (62%)	69 (100%)	0	100	100
7	G	152/153 (99%)	151 (99%)	1 (1%)	84	95
8	H	129/131 (98%)	129 (100%)	0	100	100
9	I	103/112 (92%)	103 (100%)	0	100	100
10	J	53/56 (95%)	53 (100%)	0	100	100
11	K	104/106 (98%)	104 (100%)	0	100	100
12	L	41/55 (74%)	41 (100%)	0	100	100
13	M	215/268 (80%)	215 (100%)	0	100	100
15	O	154/293 (53%)	154 (100%)	0	100	100
16	Q	121/448 (27%)	120 (99%)	1 (1%)	81	94
17	R	196/218 (90%)	195 (100%)	1 (0%)	88	96
19	U	105/324 (32%)	105 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
20	V	90/98 (92%)	89 (99%)	1 (1%)	73	92
21	W	169/373 (45%)	168 (99%)	1 (1%)	86	96
22	X	154/261 (59%)	154 (100%)	0	100	100
All	All	4646/6353 (73%)	4636 (100%)	10 (0%)	93	98

5 of 10 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
17	R	230	LYS
20	V	82	ARG
21	W	56	ARG
5	E	52	ARG
5	E	162	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	344	GLN
2	B	980	HIS
2	B	1049	GLN

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 11 ligands modelled in this entry, 11 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.

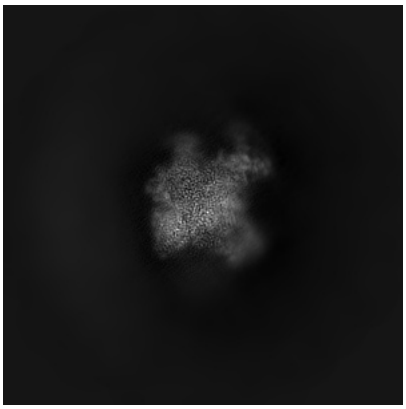
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-12612. These allow visual inspection of the internal detail of the map and identification of artifacts.

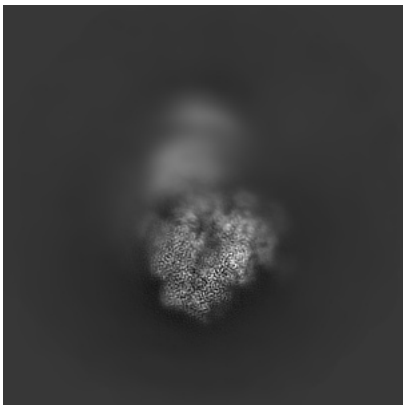
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections (i)

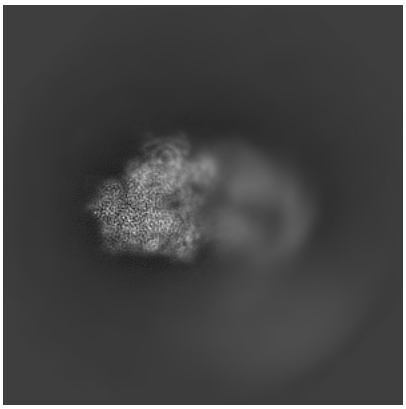
6.1.1 Primary map



X

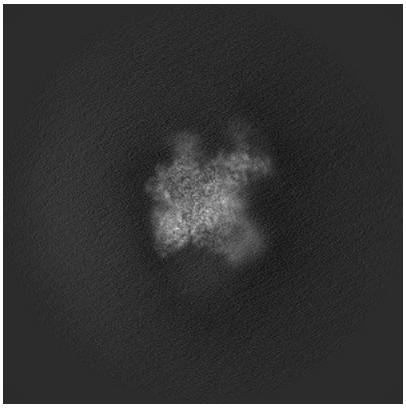


Y

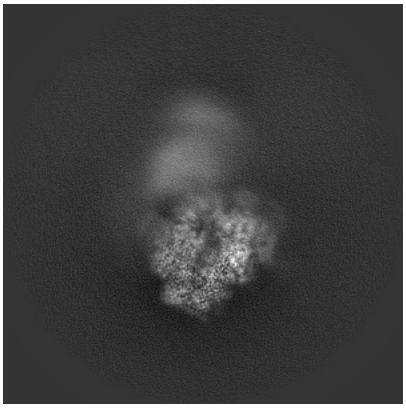


Z

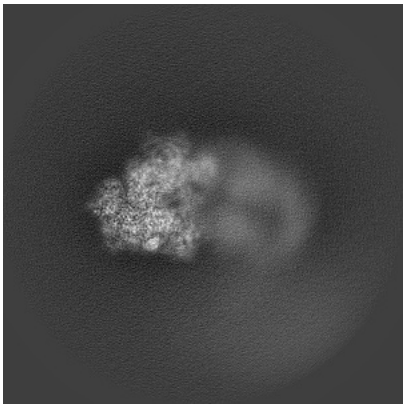
6.1.2 Raw map



X



Y

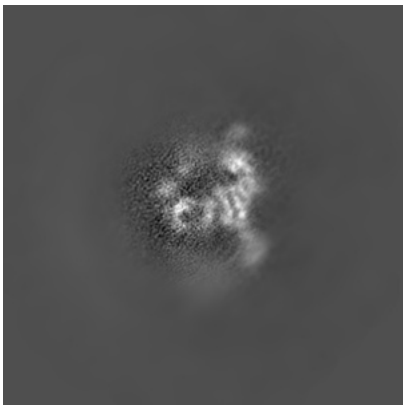


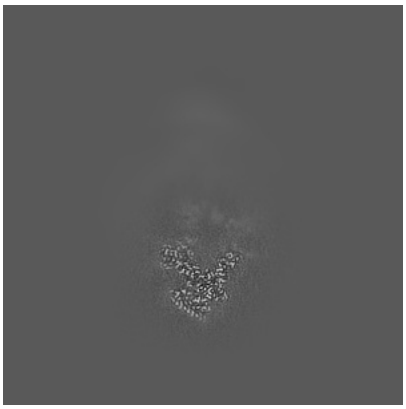
Z

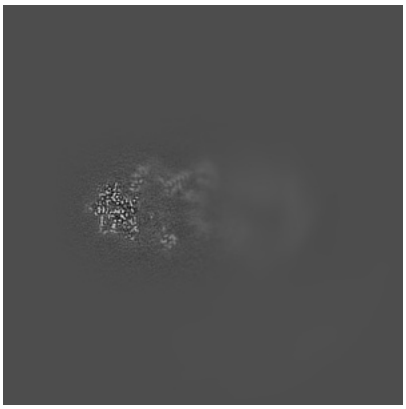
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

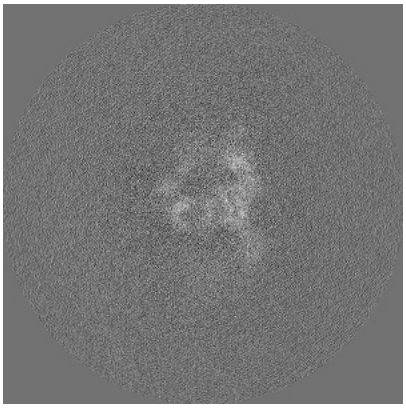
6.2.1 Primary map

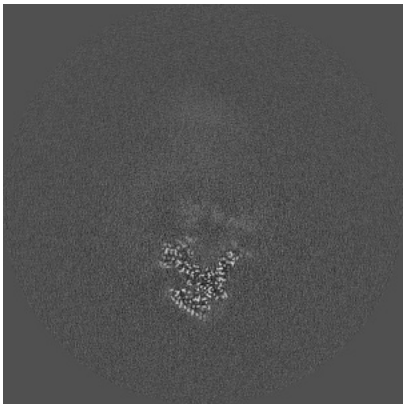

X Index: 225

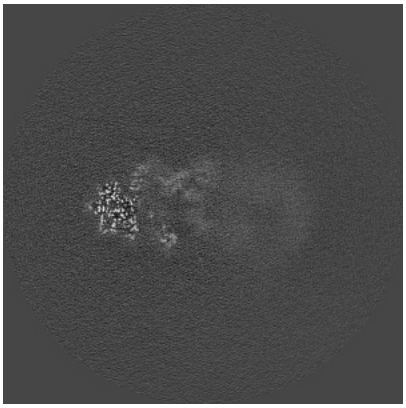

Y Index: 225


Z Index: 225

6.2.2 Raw map


X Index: 225

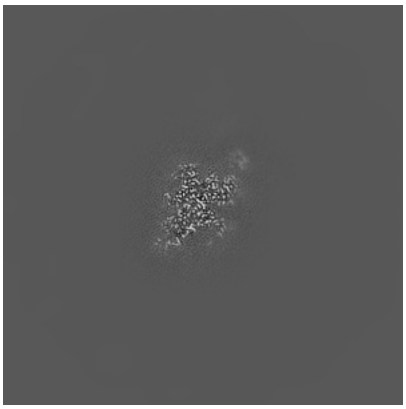

Y Index: 225


Z Index: 225

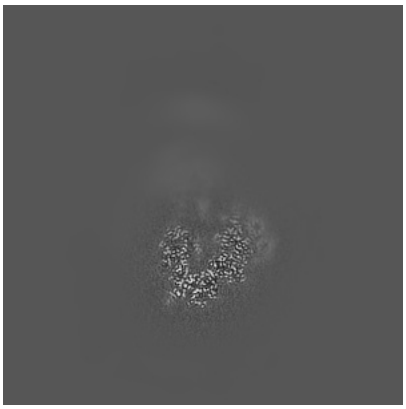
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

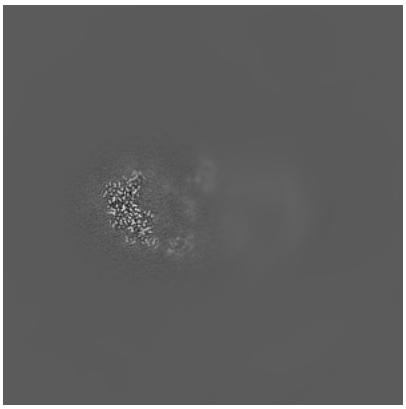
6.3.1 Primary map



X Index: 144

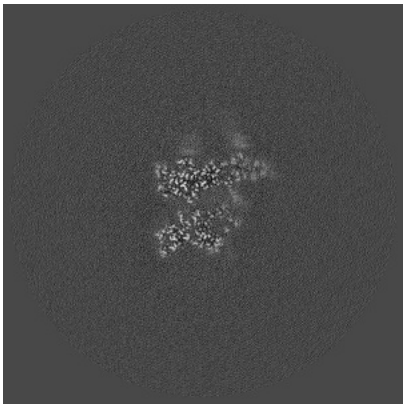


Y Index: 204

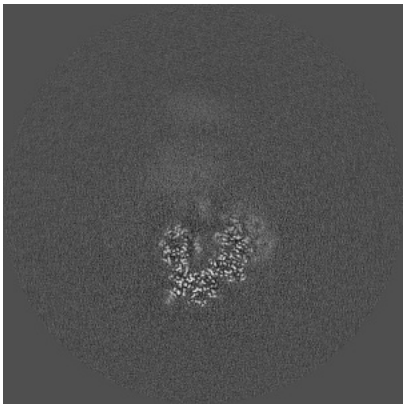


Z Index: 235

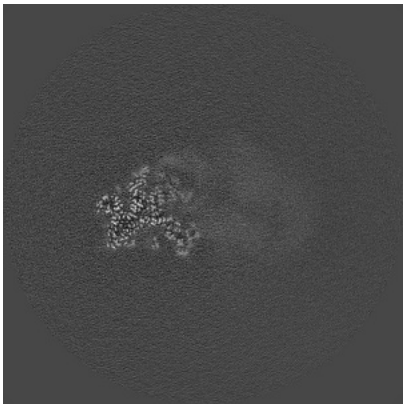
6.3.2 Raw map



X Index: 163



Y Index: 204

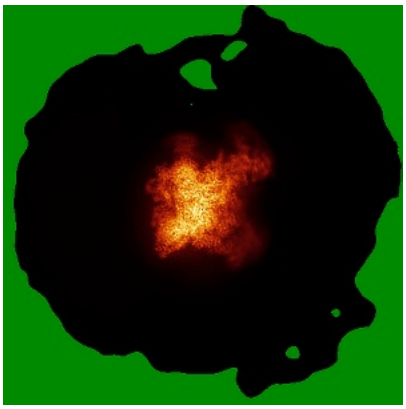


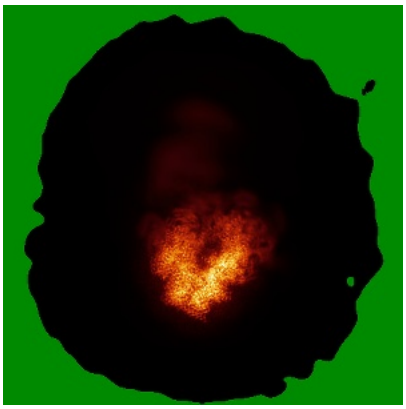
Z Index: 203

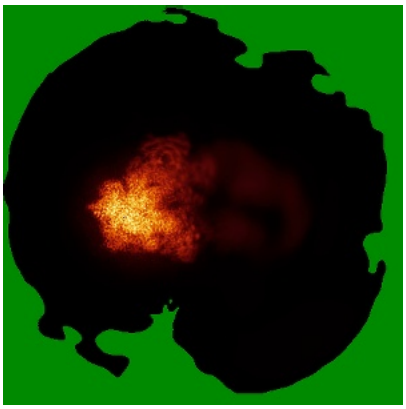
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

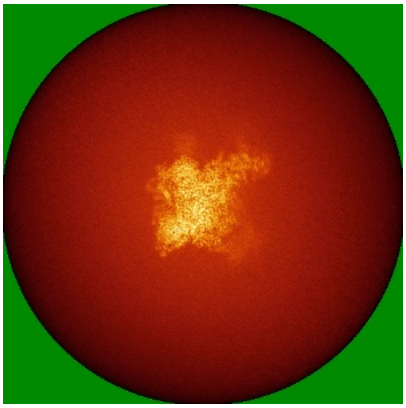
6.4.1 Primary map

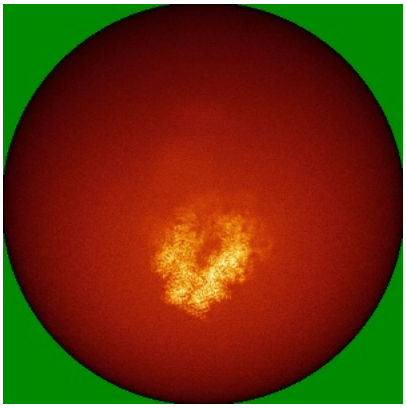

X

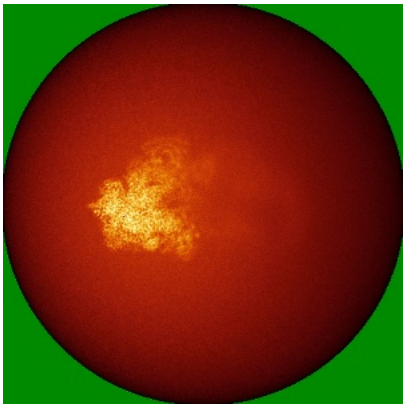

Y


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.

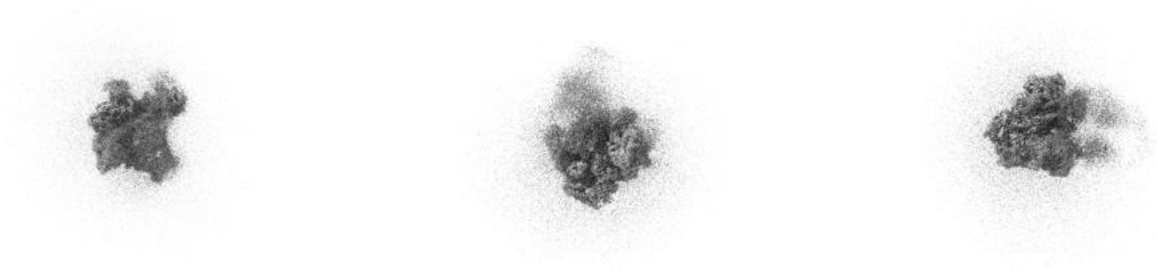
6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 4.5. 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



X Y Z

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.

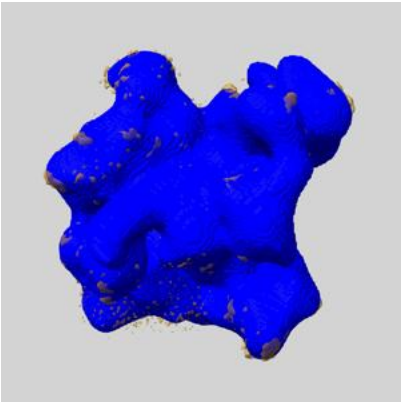
6.6 Mask visualisation (i)

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

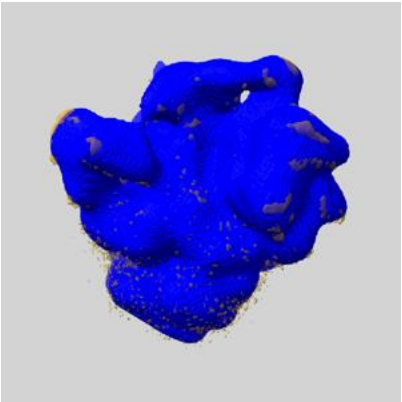
A mask typically either:

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

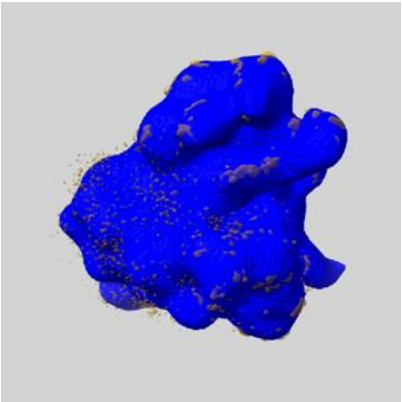
6.6.1 emd_12612_msk_1.map (i)



X



Y

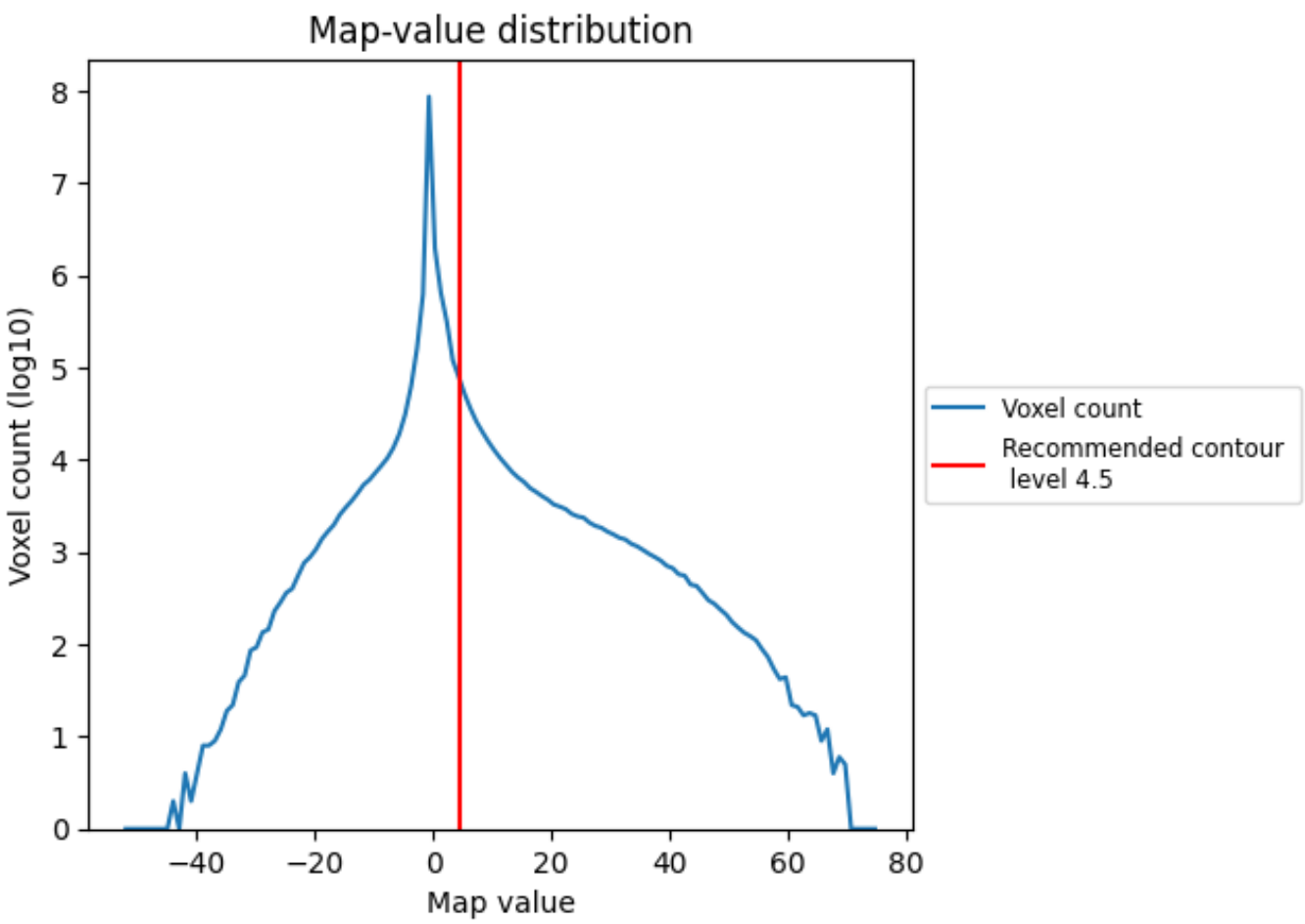


Z

7 Map analysis (i)

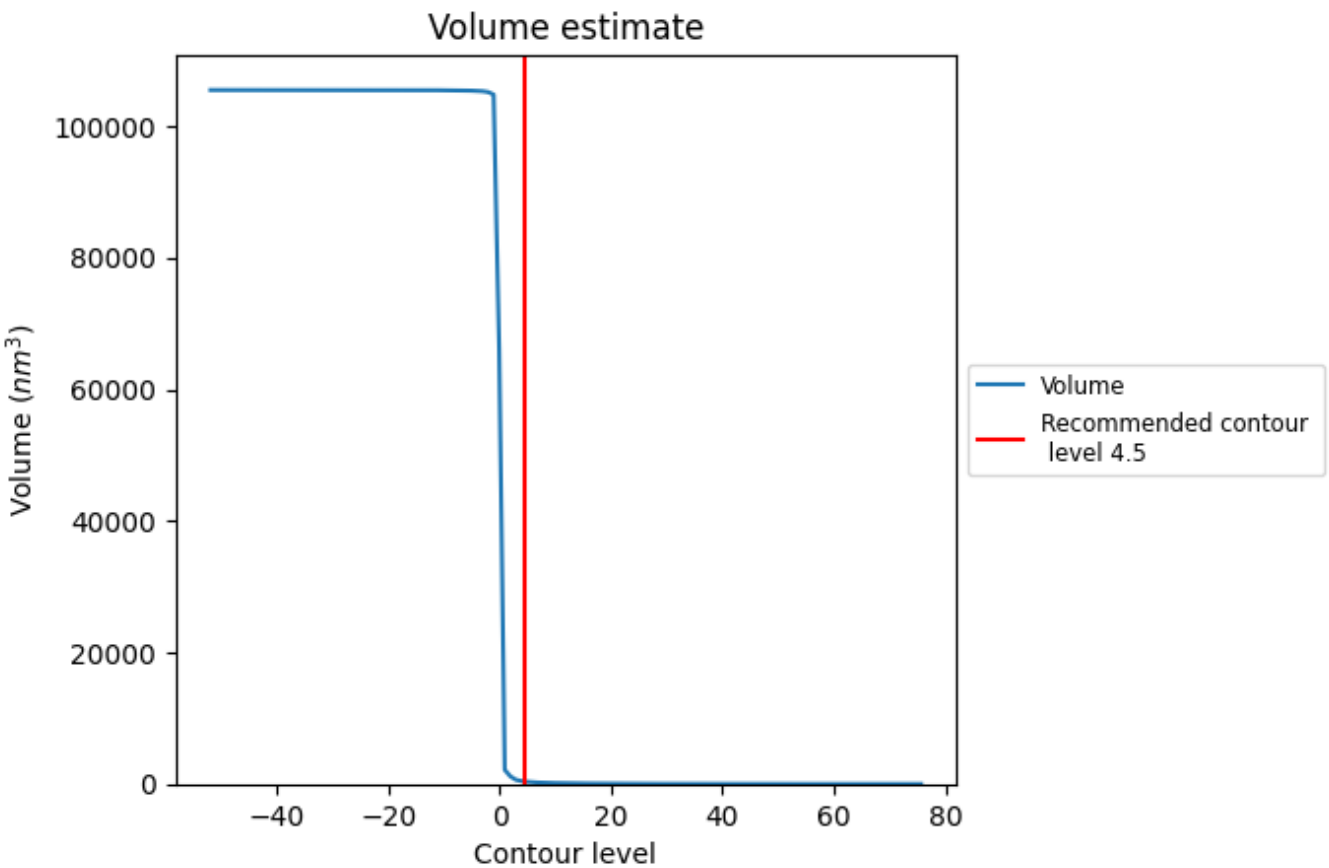
This section contains the results of statistical analysis of the map.

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.

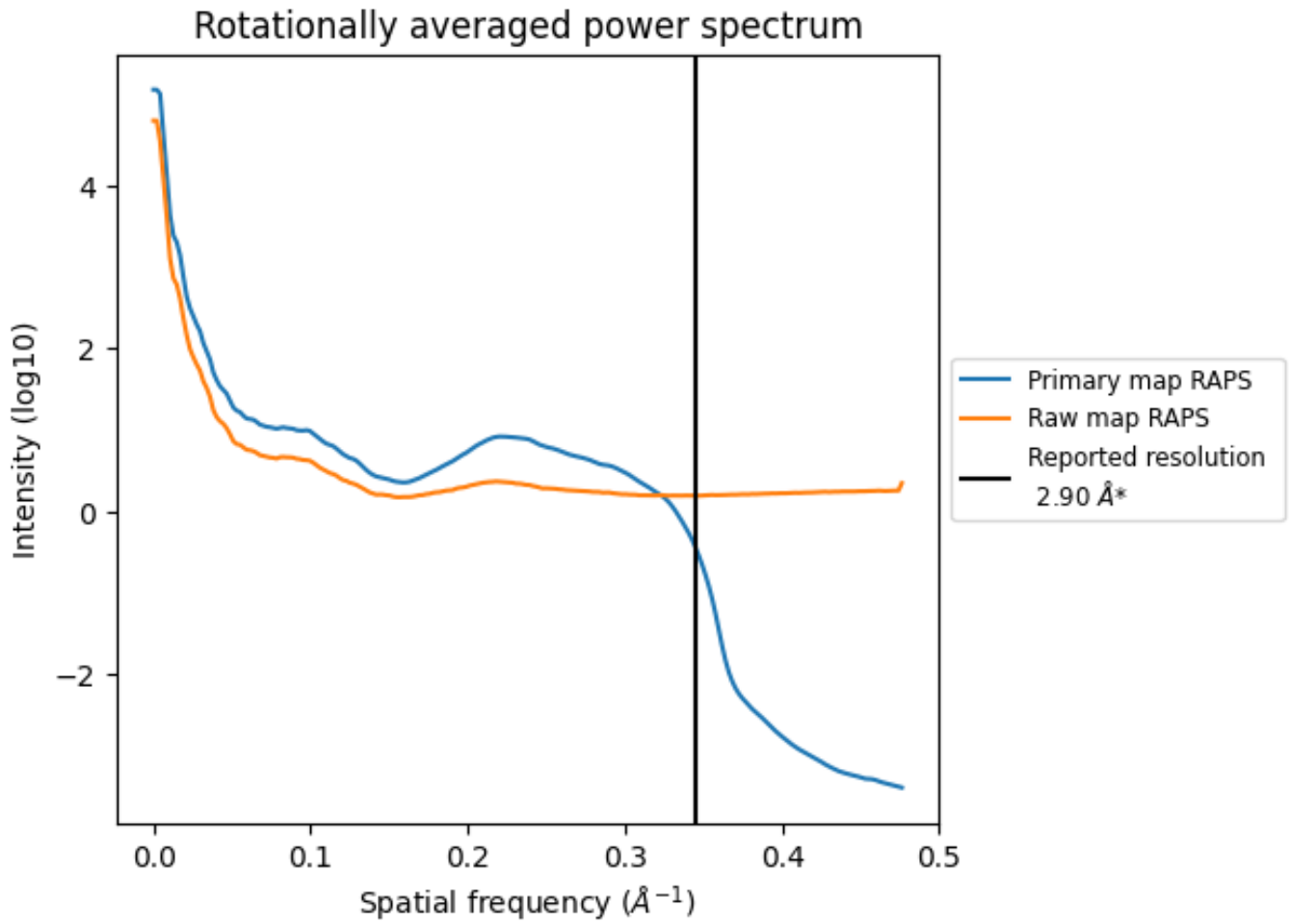
7.2 Volume estimate (i)



The volume at the recommended contour level is 381 nm^3; this corresponds to an approximate mass of 344 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)

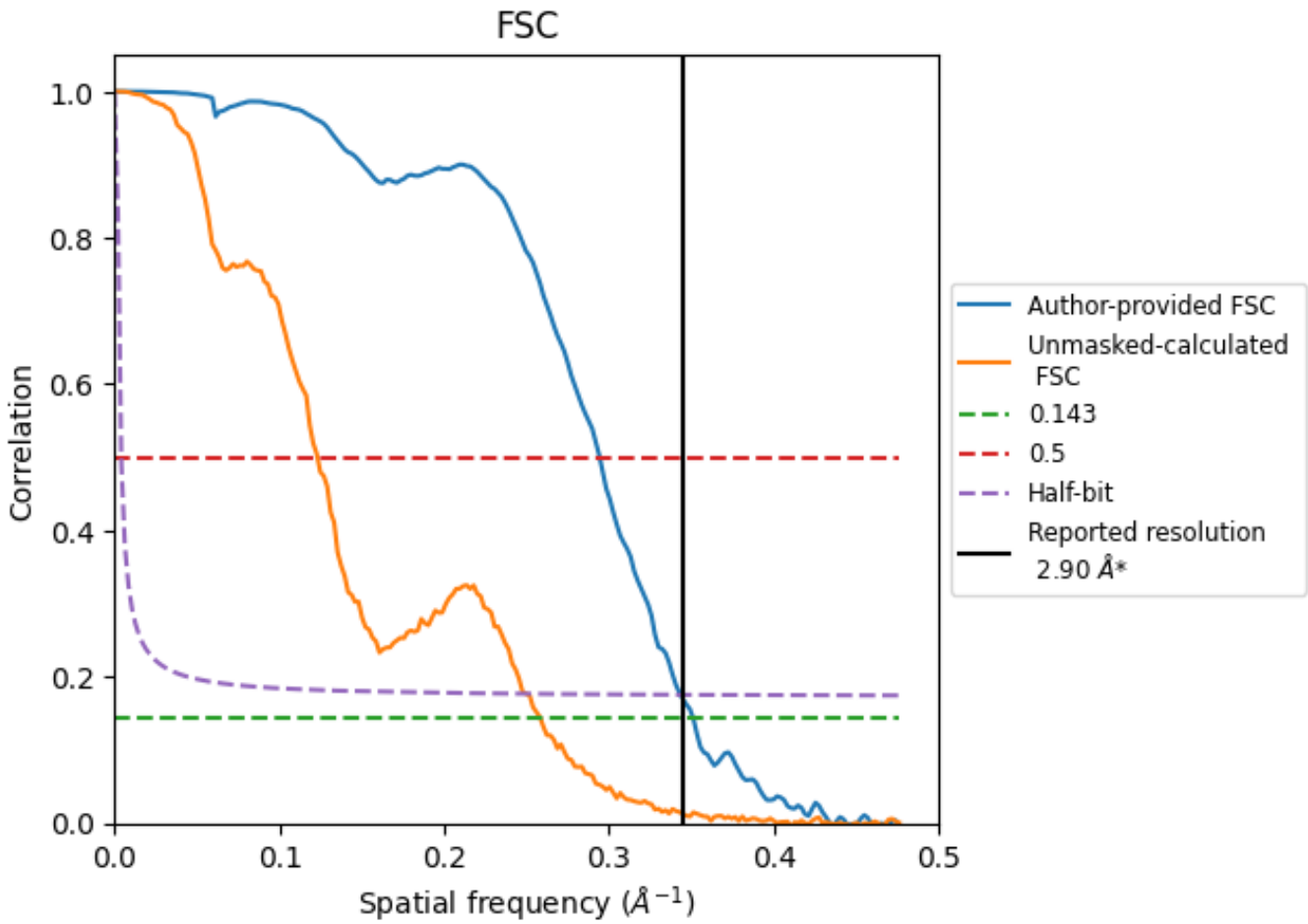


*Reported resolution corresponds to spatial frequency of 0.345 Å^{-1}

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 0.345 Å^{-1}

8.2 Resolution estimates (i)

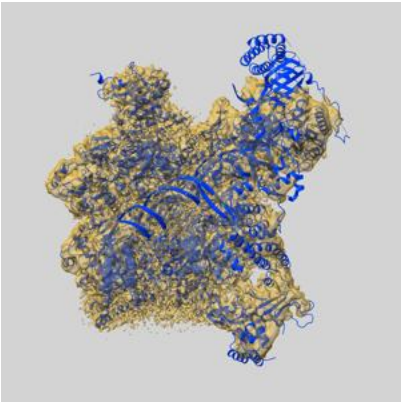
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.90	-	-
Author-provided FSC curve	2.85	3.40	2.91
Unmasked-calculated*	3.87	8.12	4.00

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.87 differs from the reported value 2.9 by more than 10 %

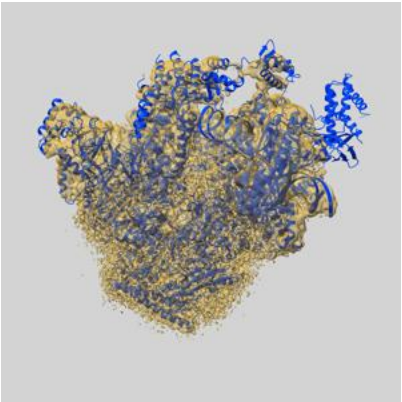
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-12612 and PDB model 7NVT. Per-residue inclusion information can be found in section 3 on page 8.

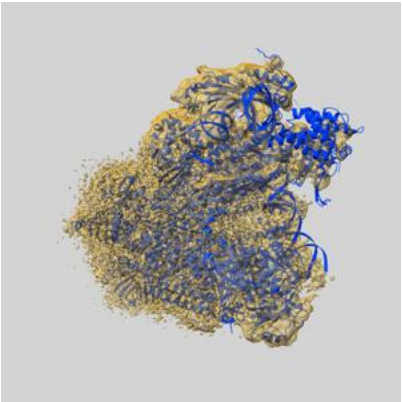
9.1 Map-model overlay (i)



X



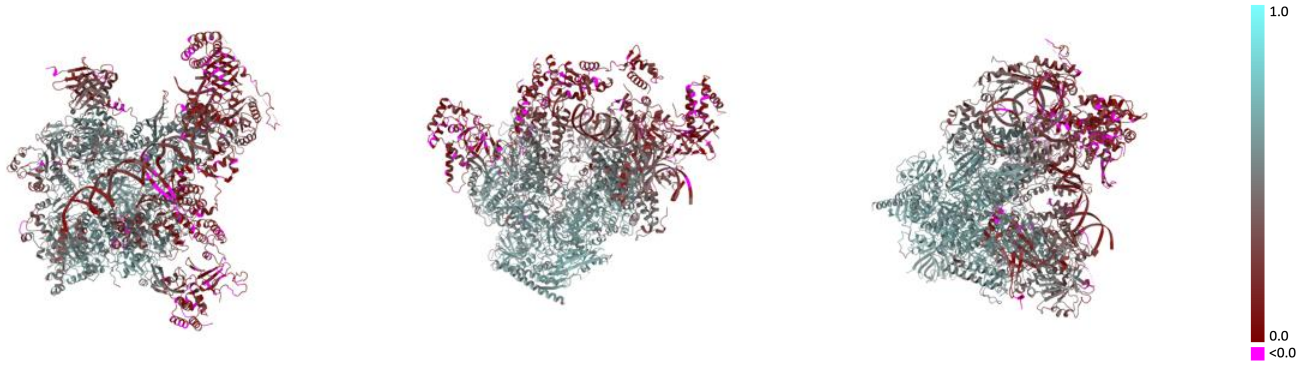
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 4.5 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.

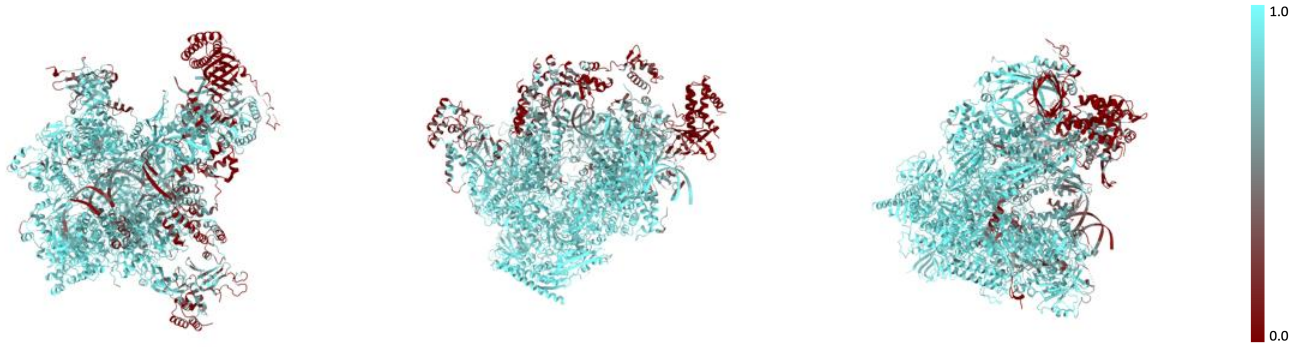
9.2 Q-score mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according 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.

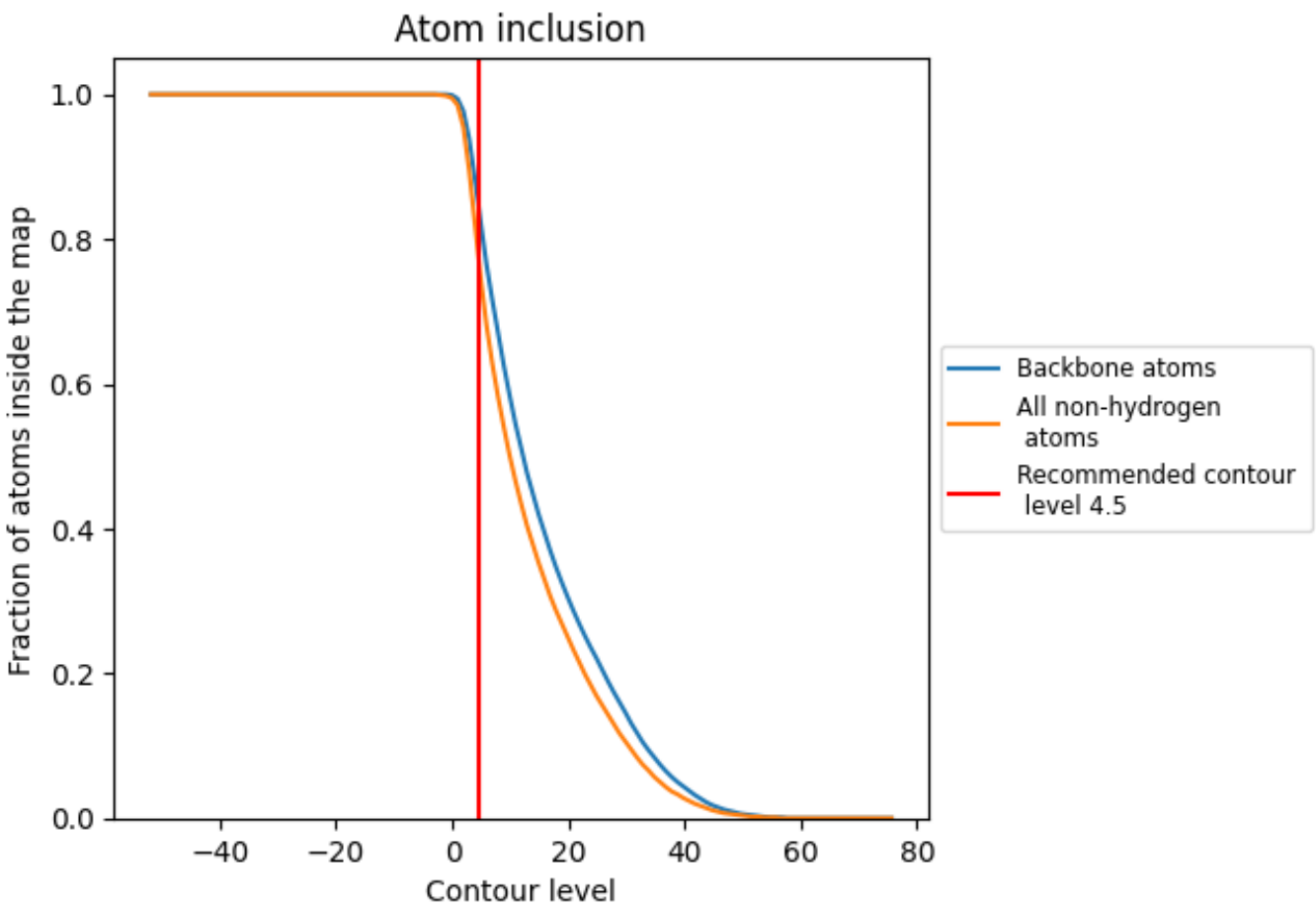
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

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 (4.5).

9.4 Atom inclusion (i)



At the recommended contour level, 85% of all backbone atoms, 78% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (4.5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7760	0.4330
A	0.8700	0.4990
B	0.9270	0.5650
C	0.9630	0.6060
D	0.3790	0.1370
E	0.8700	0.4620
F	0.9300	0.5840
G	0.6550	0.2620
H	0.9530	0.5750
I	0.8790	0.4850
J	0.9700	0.6220
K	0.9700	0.6080
L	0.9020	0.5280
M	0.8680	0.4720
N	0.7160	0.2550
O	0.7800	0.2980
Q	0.6510	0.2880
R	0.6020	0.2550
T	0.7190	0.2440
U	0.0590	0.1130
V	0.0480	0.0990
W	0.3450	0.1310
X	0.1940	0.1390