



wwPDB EM Validation Summary Report ⓘ

Mar 26, 2026 – 10:52 PM UTC

PDB ID : 7O4K / pdb_00007o4k
EMDB ID : EMD-12721
Title : Yeast TFIIDH in the contracted state within the pre-initiation complex
Authors : Schilbach, S.; Aibara, S.; Dienemann, C.; Grabbe, F.; Cramer, P.
Deposited on : 2021-04-06
Resolution : 3.60 Å (reported)
Based on initial model : 5OQJ

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 ⓘ 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 ⓘ](#)) were used in the production of this report:

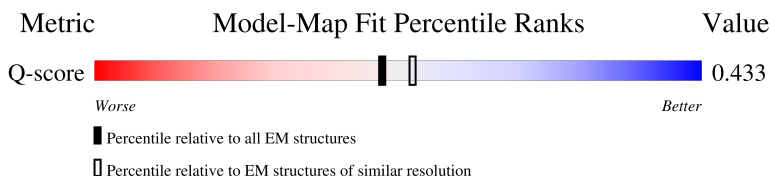
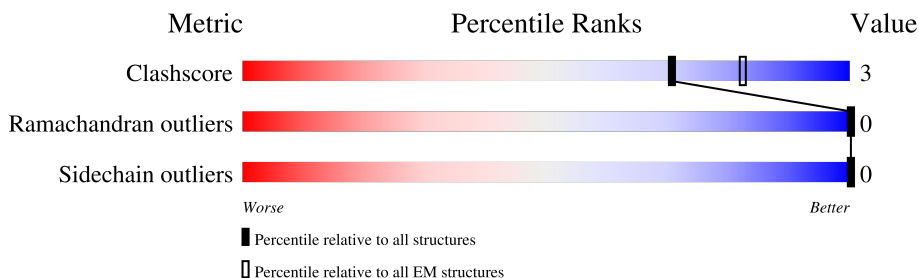
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDb archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

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 3.60 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	12797 (3.10 - 4.10)

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 $\leq 5\%$. 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	0	778	 14% 89% 8% .
2	1	645	 21% 76% 5% 19%
3	2	517	 37% 77% 9% 14%
4	3	324	 37% 60% .

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Mol	Chain	Length	Quality of chain
5	4	341	
6	5	76	
7	6	464	
8	7	843	
9	A	1733	
10	B	1224	
11	D	221	
12	F	155	
13	G	177	
14	N	106	
15	T	106	
16	W	492	
17	X	328	

2 Entry composition

There are 22 unique types of molecules in this entry. The entry contains 34264 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 General transcription and DNA repair factor IIH helicase subunit XPD.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	0	752	Total	C	N	O	S	0	0
			6091	3882	1029	1142	38		

- Molecule 2 is a protein called General transcription and DNA repair factor IIH subunit TFB1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	1	522	Total	C	N	O	S	0	0
			4214	2660	734	798	22		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
1	-2	GLY	-	expression tag	UNP P32776
1	-1	GLY	-	expression tag	UNP P32776
1	0	SER	-	expression tag	UNP P32776

- Molecule 3 is a protein called General transcription and DNA repair factor IIH subunit TFB2.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	2	445	Total	C	N	O	S	0	0
			3597	2327	591	663	16		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
2	-3	GLY	-	expression tag	UNP Q02939
2	-2	PRO	-	expression tag	UNP Q02939
2	-1	GLY	-	expression tag	UNP Q02939
2	0	SER	-	expression tag	UNP Q02939

- Molecule 4 is a protein called RNA polymerase II transcription factor B subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	3	130	Total	C	N	O	S	0	0
			1081	688	178	207	8		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
3	-2	GLY	-	expression tag	UNP Q03290
3	-1	PRO	-	expression tag	UNP Q03290
3	0	HIS	-	expression tag	UNP Q03290

- Molecule 5 is a protein called General transcription and DNA repair factor IIH subunit TFB4.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	4	292	Total	C	N	O	S	0	0
			2267	1449	376	428	14		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
4	-2	SER	-	expression tag	UNP Q12004
4	-1	ASN	-	expression tag	UNP Q12004
4	0	ALA	-	expression tag	UNP Q12004

- Molecule 6 is a protein called General transcription and DNA repair factor IIH subunit TFB5.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	5	65	Total	C	N	O	S	0	0
			514	326	90	95	3		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
5	-3	GLY	-	expression tag	UNP Q3E7C1
5	-2	PRO	-	expression tag	UNP Q3E7C1
5	-1	GLY	-	expression tag	UNP Q3E7C1
5	0	SER	-	expression tag	UNP Q3E7C1

- Molecule 7 is a protein called General transcription and DNA repair factor IIH subunit SSL1.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	6	355	Total	C	N	O	S	0	0
			2786	1765	481	512	28		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
6	-2	GLY	-	expression tag	UNP Q04673
6	-1	GLY	-	expression tag	UNP Q04673
6	0	SER	-	expression tag	UNP Q04673

- Molecule 8 is a protein called General transcription and DNA repair factor IIIH helicase subunit XPB.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	7	608	Total	C	N	O	S	0	0
			4889	3110	847	906	26		

- Molecule 9 is a protein called DNA-directed RNA polymerase II subunit RPB1.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	A	167	Total	C	N	O	S	0	0
			1298	812	218	255	13		

- Molecule 10 is a protein called DNA-directed RNA polymerase II subunit RPB2.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	B	71	Total	C	N	O	S	0	0
			569	366	98	98	7		

- Molecule 11 is a protein called DNA-directed RNA polymerase II subunit RPB4.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	D	163	Total	C	N	O	S	0	0
			1305	808	232	263	2		

- Molecule 12 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC2.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	F	28	Total	C	N	O	S	0	0
			228	147	43	37	1		

- Molecule 13 is a protein called DNA-directed RNA polymerase II subunit RPB7.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	G	171	Total	C	N	O	S	0	0
			1339	861	222	248	8		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	172	HIS	-	expression tag	UNP P34087
G	173	HIS	-	expression tag	UNP P34087
G	174	HIS	-	expression tag	UNP P34087
G	175	HIS	-	expression tag	UNP P34087
G	176	HIS	-	expression tag	UNP P34087
G	177	HIS	-	expression tag	UNP P34087

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

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	10	Total	C	N	O	P	0	0
			206	99	36	61	10		

- Molecule 15 is a DNA chain called Template DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	T	10	Total	C	N	O	P	0	0
			204	98	37	59	10		

- Molecule 16 is a protein called Transcription initiation factor IIE subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	W	312	Total	C	N	O	S	0	0
			2532	1595	442	488	7		

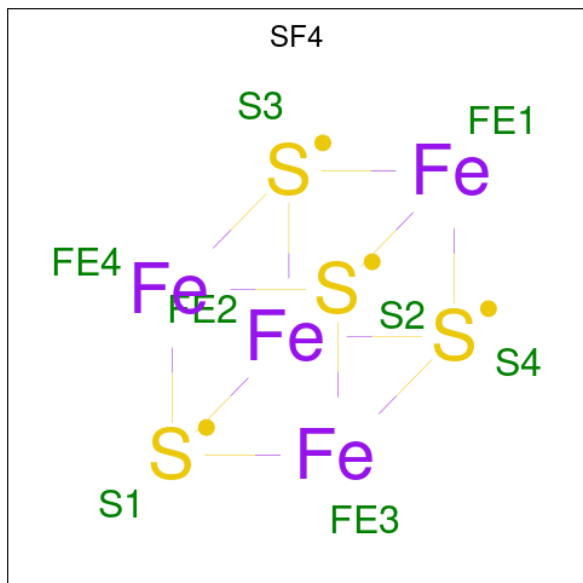
There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
W	483	ALA	-	expression tag	UNP P36100
W	484	ALA	-	expression tag	UNP P36100
W	485	ALA	-	expression tag	UNP P36100
W	486	LEU	-	expression tag	UNP P36100
W	487	GLU	-	expression tag	UNP P36100
W	488	HIS	-	expression tag	UNP P36100
W	489	HIS	-	expression tag	UNP P36100
W	490	HIS	-	expression tag	UNP P36100
W	491	HIS	-	expression tag	UNP P36100
W	492	HIS	-	expression tag	UNP P36100

- Molecule 17 is a protein called Transcription initiation factor IIE subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	X	135	Total	C	N	O	S	0	0
			1094	694	190	205	5		

- Molecule 18 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).

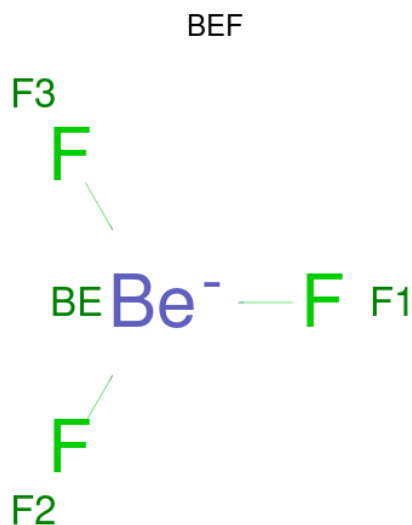


Mol	Chain	Residues	Atoms			AltConf
18	0	1	Total	Fe	S	0
			8	4	4	

- Molecule 19 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
19	3	2	Total	Zn	0
			2	2	
19	4	1	Total	Zn	0
			1	1	
19	6	4	Total	Zn	0
			4	4	
19	A	1	Total	Zn	0
			1	1	
19	B	1	Total	Zn	0
			1	1	
19	W	1	Total	Zn	0
			1	1	

- Molecule 20 is BERYLLIUM TRIFLUORIDE ION (CCD ID: BEF) (formula: BeF_3).

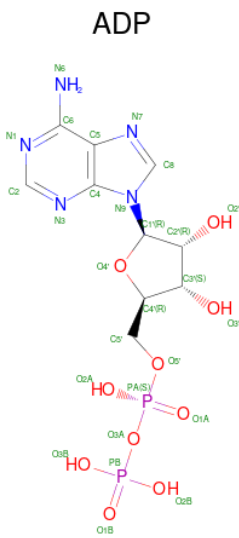


Mol	Chain	Residues	Atoms			AltConf
20	7	1	Total 4	Be 1	F 3	0

- Molecule 21 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	AltConf
21	7	1	Total Mg 1 1	0

- Molecule 22 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).

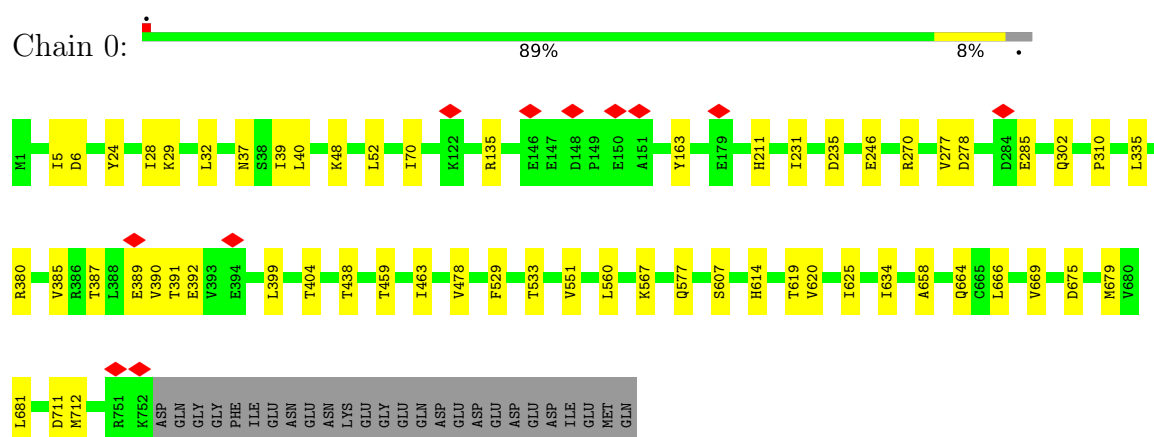


Mol	Chain	Residues	Atoms					AltConf
22	7	1	Total	C	N	O	P	0
			27	10	5	10	2	

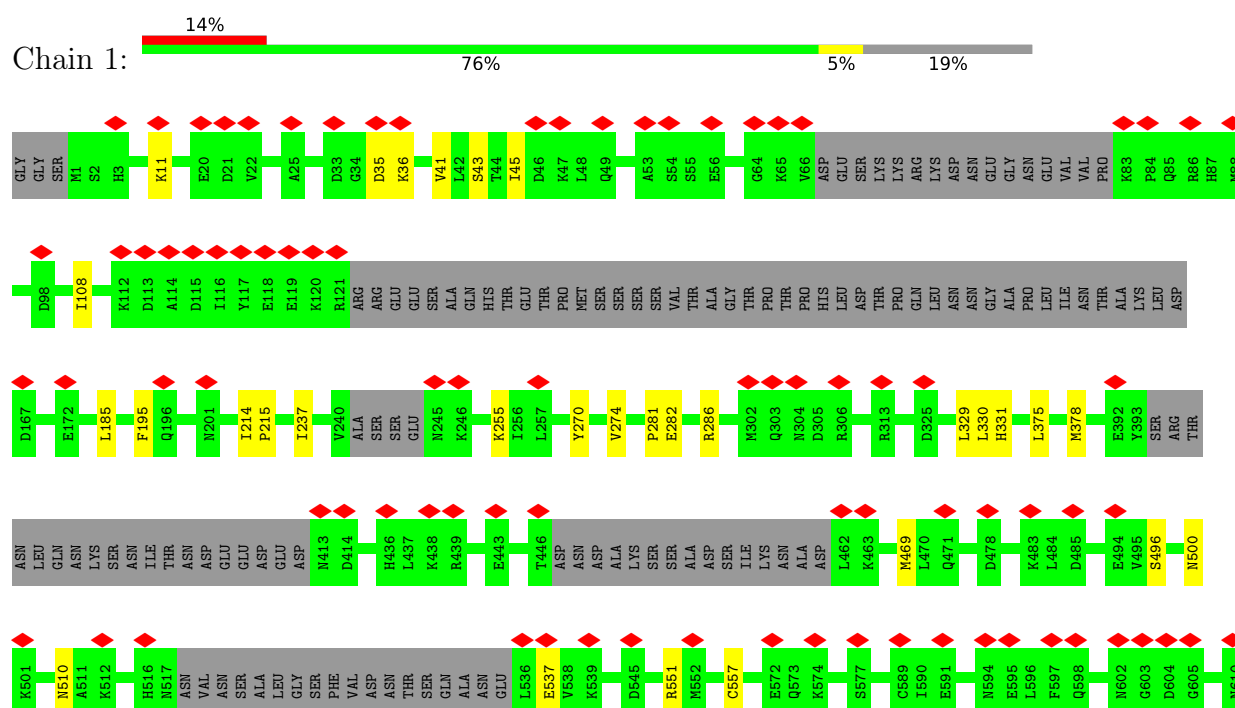
3 Residue-property plots

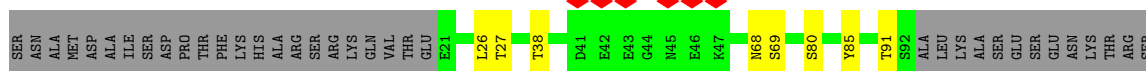
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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.

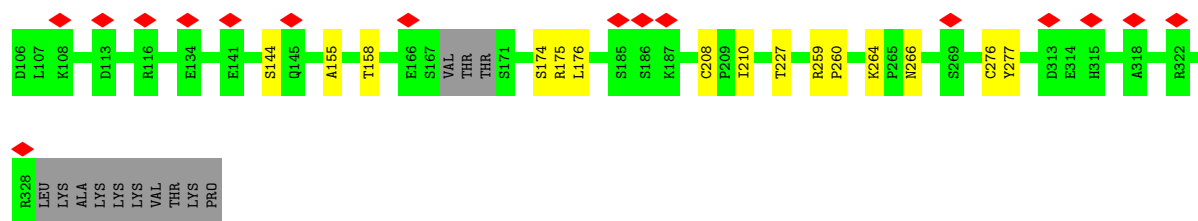
- Molecule 1: General transcription and DNA repair factor IIH helicase subunit XPD



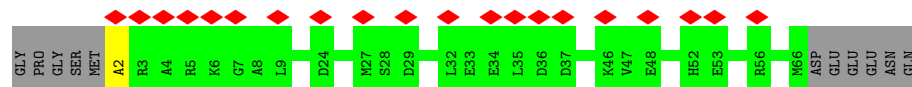
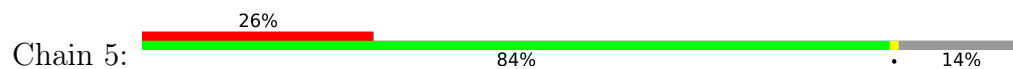
- Molecule 2: General transcription and DNA repair factor IIH subunit TFB1



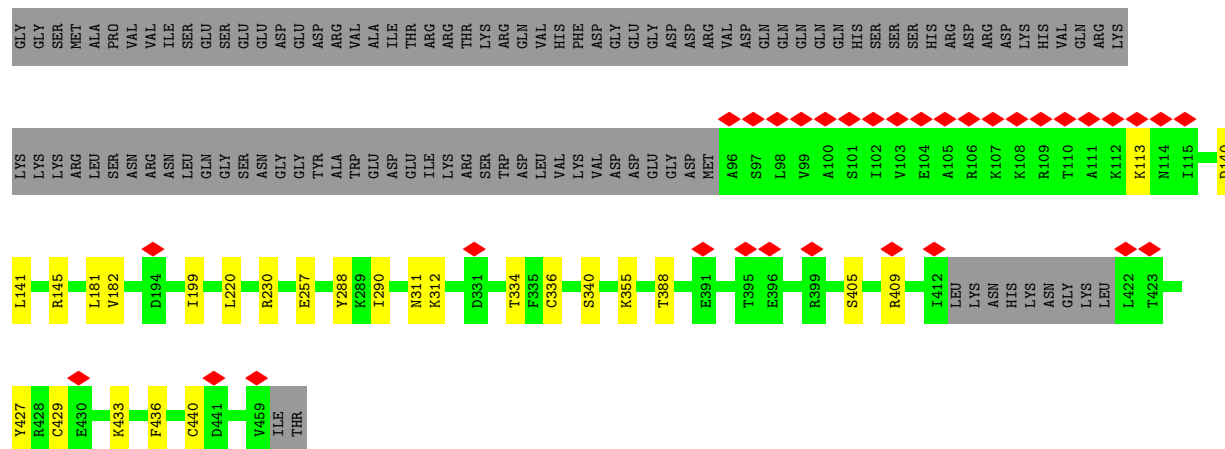




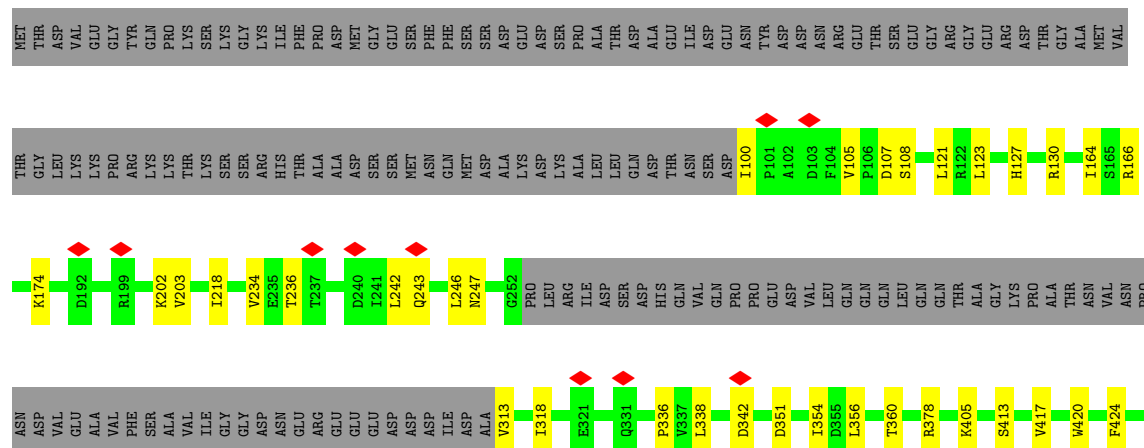
- Molecule 6: General transcription and DNA repair factor IIH subunit TFB5

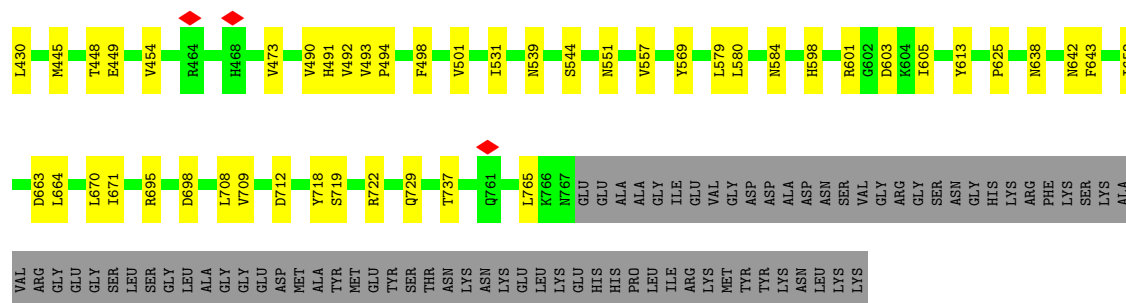


- Molecule 7: General transcription and DNA repair factor IIH subunit SSL1



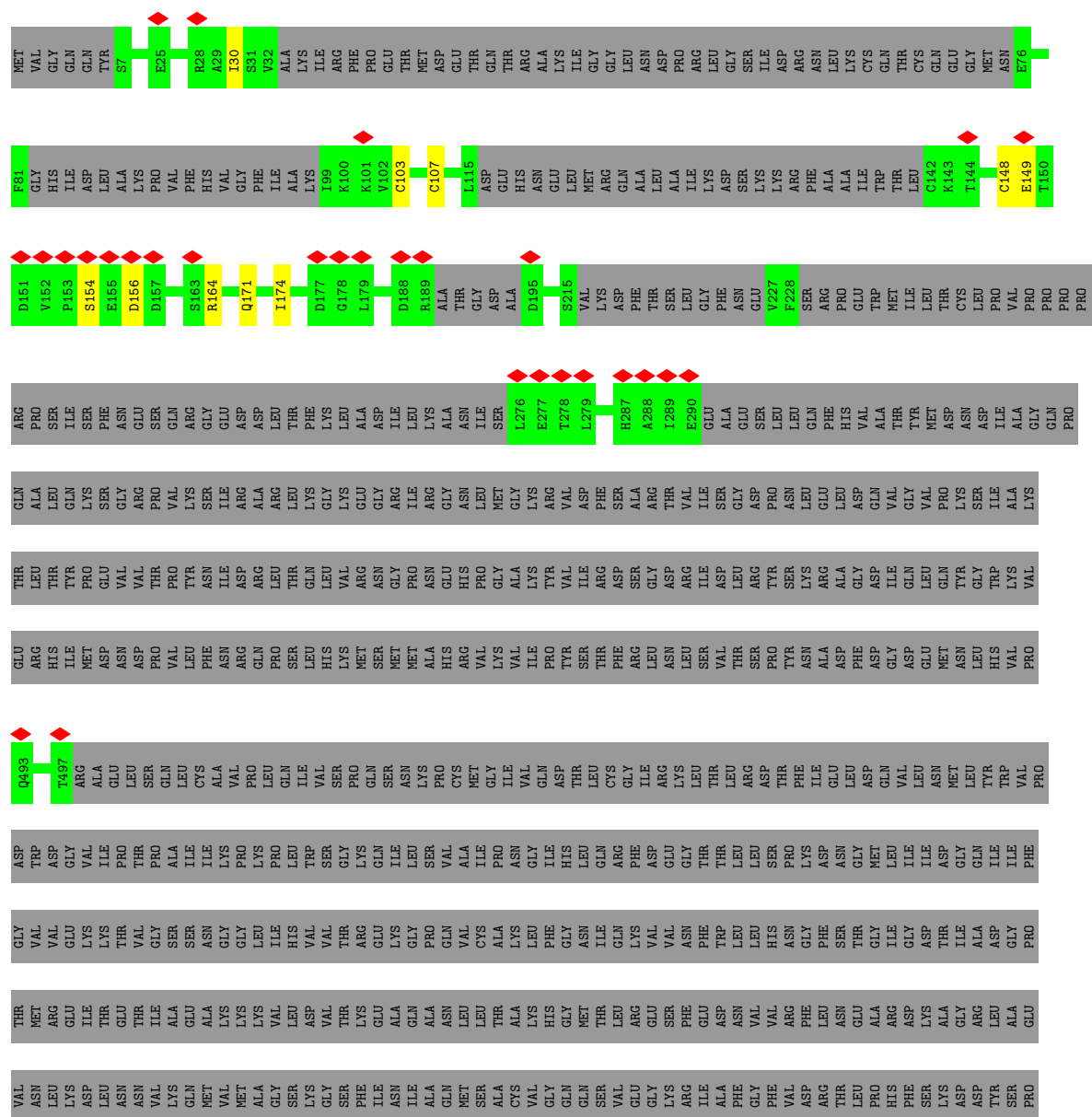
- Molecule 8: General transcription and DNA repair factor IIH helicase subunit XPB



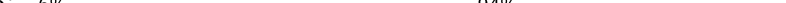


● Molecule 9: DNA-directed RNA polymerase II subunit RPB1

Chain A: 9% 90%

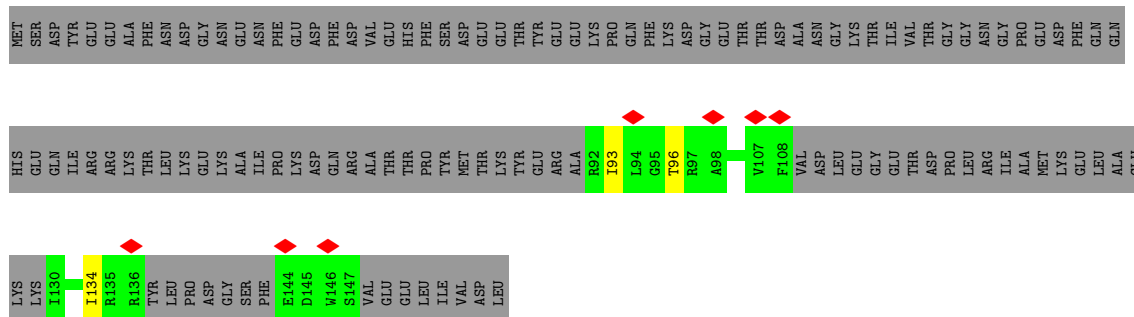


- Molecule 10: DNA-directed RNA polymerase II subunit RPB2

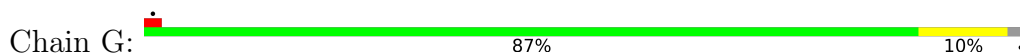
Chain B:  6% 94%

[illegible]

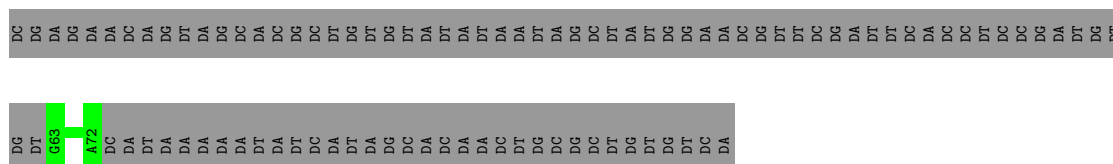
- Molecule 12: DNA-directed RNA polymerases I, II, and III subunit RPABC2



- Molecule 13: DNA-directed RNA polymerase II subunit RPB7



- Molecule 14: Non-template DNA

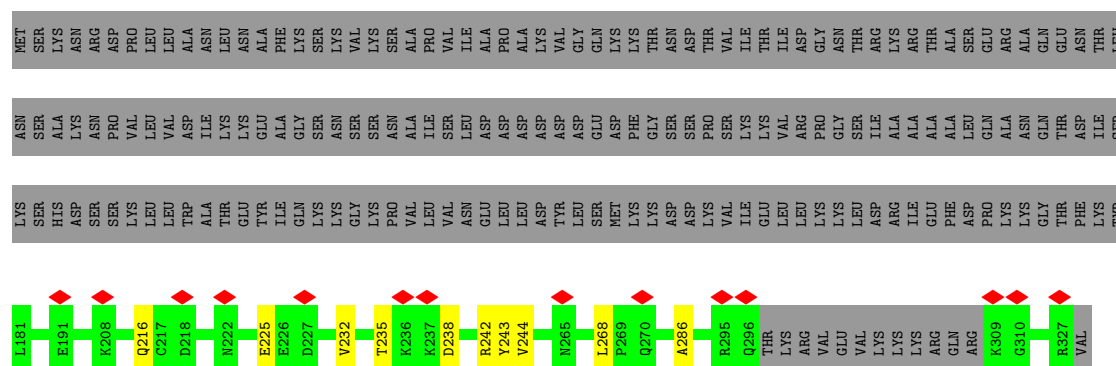


- Molecule 15: Template DNA



- Molecule 16: Transcription initiation factor IIE subunit alpha





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	24671	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 ($e^-/\text{\AA}^2$)	43.6	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	4000	Depositor
Magnification	130000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	89.137	Depositor
Minimum map value	-52.303	Depositor
Average map value	0.027	Depositor
Map value standard deviation	0.977	Depositor
Recommended contour level	3.8	Depositor
Map size (Å)	398.99997, 398.99997, 398.99997	wwPDB
Map dimensions	380, 380, 380	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.05, 1.05, 1.05	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ADP, BEF, ZN, SF4, 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	0	0.13	0/6209	0.28	0/8384
2	1	0.10	0/4277	0.26	0/5755
3	2	0.09	0/3664	0.25	0/4952
4	3	0.09	0/1101	0.22	0/1481
5	4	0.10	0/2305	0.26	0/3117
6	5	0.10	0/520	0.28	0/701
7	6	0.10	0/2843	0.25	0/3845
8	7	0.10	0/4992	0.28	0/6754
9	A	0.09	0/1310	0.23	0/1751
10	B	0.11	0/579	0.27	0/777
11	D	0.10	0/1313	0.27	0/1761
12	F	0.11	0/230	0.27	0/308
13	G	0.11	0/1367	0.25	0/1844
14	N	0.17	0/230	0.44	0/353
15	T	0.18	0/228	0.42	0/349
16	W	0.09	0/2575	0.26	0/3473
17	X	0.11	0/1115	0.31	0/1502
All	All	0.10	0/34858	0.27	0/47107

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

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	0	6091	0	6155	40	0
2	1	4214	0	4288	23	0
3	2	3597	0	3687	35	0
4	3	1081	0	1063	6	0
5	4	2267	0	2323	16	0
6	5	514	0	541	1	0
7	6	2786	0	2804	16	0
8	7	4889	0	4877	50	0
9	A	1298	0	1276	6	0
10	B	569	0	574	2	0
11	D	1305	0	1327	13	0
12	F	228	0	240	3	0
13	G	1339	0	1357	13	0
14	N	206	0	115	0	0
15	T	204	0	114	0	0
16	W	2532	0	2529	33	0
17	X	1094	0	1114	8	0
18	0	8	0	0	0	0
19	3	2	0	0	0	0
19	4	1	0	0	0	0
19	6	4	0	0	0	0
19	A	1	0	0	0	0
19	B	1	0	0	0	0
19	W	1	0	0	0	0
20	7	4	0	0	0	0
21	7	1	0	0	0	0
22	7	27	0	12	0	0
All	All	34264	0	34396	238	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 3.

The worst 5 of 238 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)
8:7:351:ASP:OD1	8:7:405:LYS:NZ	2.19	0.76
11:D:32:GLU:O	13:G:5:LYS:NZ	2.18	0.76
1:0:335:LEU:HD21	1:0:399:LEU:HD12	1.68	0.75
1:0:607:SER:O	1:0:664:GLN:NE2	2.19	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:7:166:ARG:NH1	8:7:539:ASN:OD1	2.19	0.75

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	0	750/778 (96%)	730 (97%)	20 (3%)	0	100	100
2	1	508/645 (79%)	503 (99%)	5 (1%)	0	100	100
3	2	435/517 (84%)	426 (98%)	9 (2%)	0	100	100
4	3	128/324 (40%)	127 (99%)	1 (1%)	0	100	100
5	4	286/341 (84%)	286 (100%)	0	0	100	100
6	5	63/76 (83%)	62 (98%)	1 (2%)	0	100	100
7	6	351/464 (76%)	348 (99%)	3 (1%)	0	100	100
8	7	604/843 (72%)	587 (97%)	17 (3%)	0	100	100
9	A	145/1733 (8%)	142 (98%)	3 (2%)	0	100	100
10	B	67/1224 (6%)	66 (98%)	1 (2%)	0	100	100
11	D	159/221 (72%)	157 (99%)	2 (1%)	0	100	100
12	F	22/155 (14%)	22 (100%)	0	0	100	100
13	G	169/177 (96%)	165 (98%)	4 (2%)	0	100	100
16	W	304/492 (62%)	295 (97%)	9 (3%)	0	100	100
17	X	131/328 (40%)	125 (95%)	6 (5%)	0	100	100
All	All	4122/8318 (50%)	4041 (98%)	81 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	0	684/707 (97%)	684 (100%)	0	100	100
2	1	483/590 (82%)	483 (100%)	0	100	100
3	2	408/470 (87%)	408 (100%)	0	100	100
4	3	124/305 (41%)	124 (100%)	0	100	100
5	4	259/302 (86%)	259 (100%)	0	100	100
6	5	59/68 (87%)	59 (100%)	0	100	100
7	6	322/419 (77%)	322 (100%)	0	100	100
8	7	540/737 (73%)	540 (100%)	0	100	100
9	A	150/1520 (10%)	150 (100%)	0	100	100
10	B	62/1061 (6%)	62 (100%)	0	100	100
11	D	145/200 (72%)	145 (100%)	0	100	100
12	F	25/137 (18%)	25 (100%)	0	100	100
13	G	152/158 (96%)	152 (100%)	0	100	100
16	W	281/436 (64%)	281 (100%)	0	100	100
17	X	125/295 (42%)	125 (100%)	0	100	100
All	All	3819/7405 (52%)	3819 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 23 such sidechains are listed below:

Mol	Chain	Res	Type
8	7	611	ASN
8	7	697	ASN
8	7	672	GLN
11	D	37	GLN
3	2	55	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 14 ligands modelled in this entry, 11 are monoatomic - leaving 3 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	$\# Z > 2$
22	ADP	7	903	20,21	28,29,29	0.49	0	43,45,45	0.54	0
18	SF4	0	801	1	0,12,12	-	-	-		
20	BEF	7	901	22	0,3,3	-	-	-		

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
22	ADP	7	903	20,21	-	2/16/32/32	0/3/3/3
18	SF4	0	801	1	-	-	0/6/5/5

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

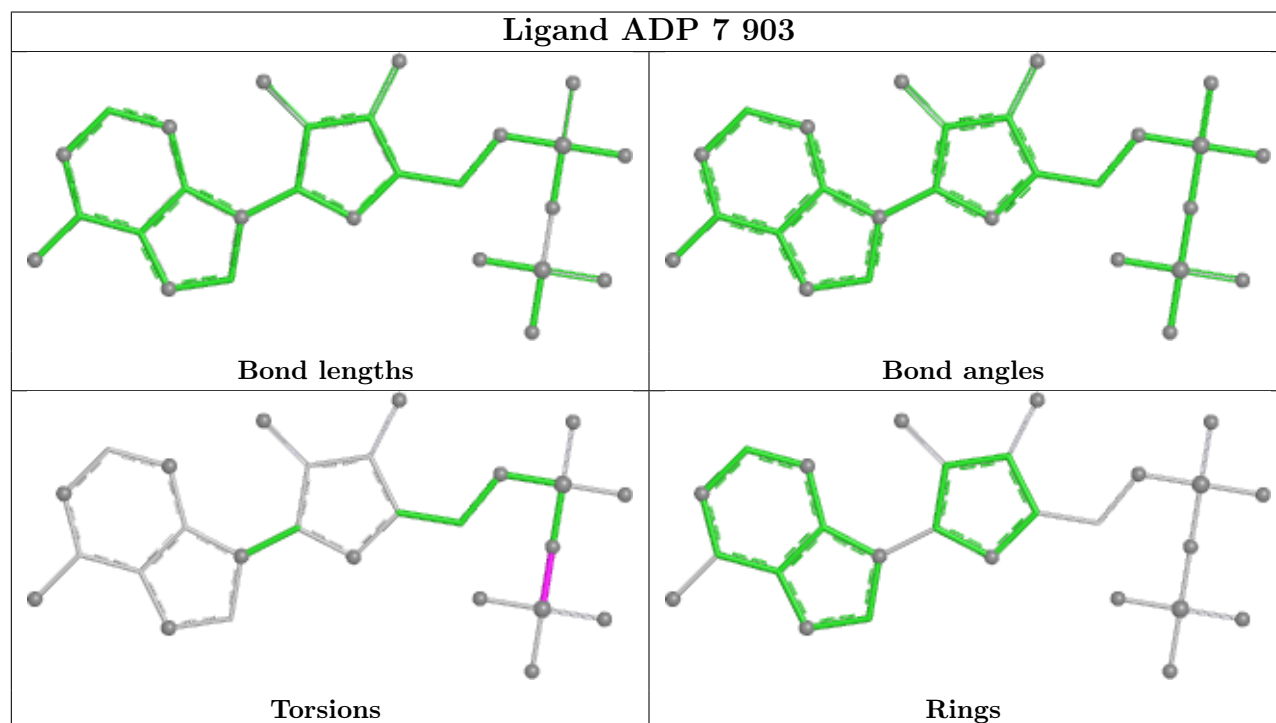
All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
22	7	903	ADP	PA-O3A-PB-O3B
22	7	903	ADP	PA-O3A-PB-O2B

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

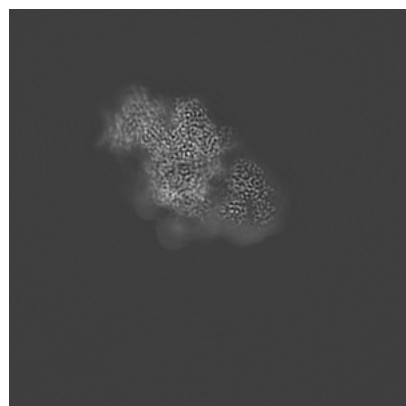
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-12721. These allow visual inspection of the internal detail of the map and identification of artifacts.

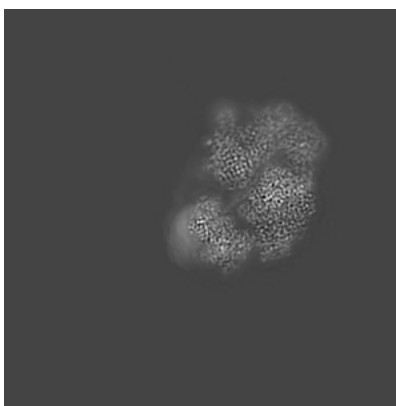
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

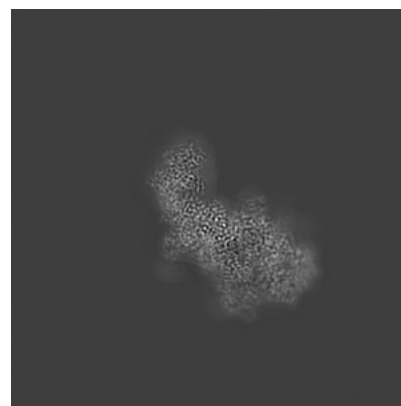
6.1.1 Primary map



X

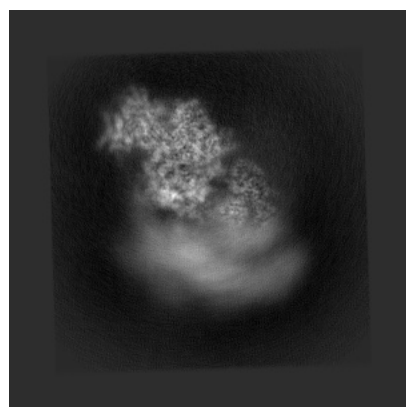


Y

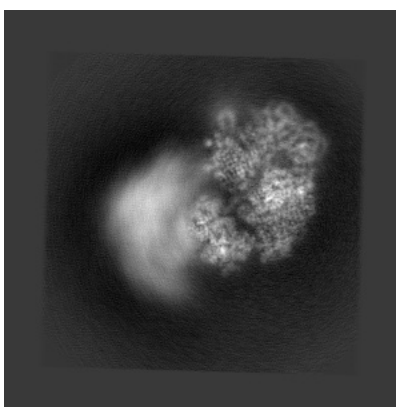


Z

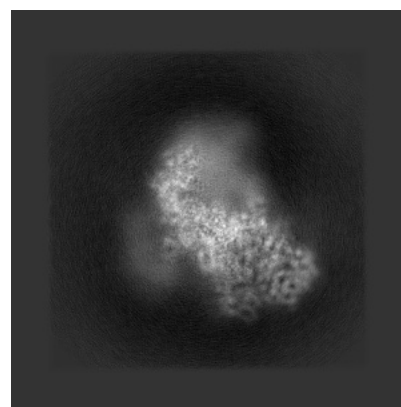
6.1.2 Raw map



X



Y

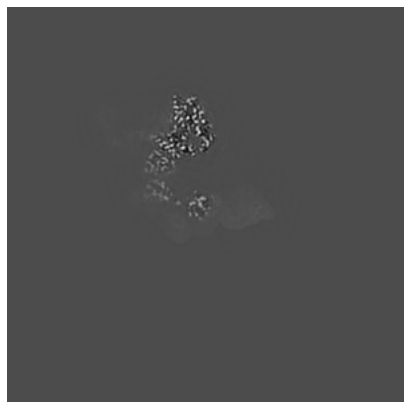


Z

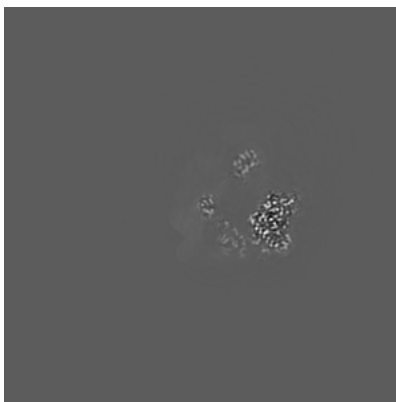
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

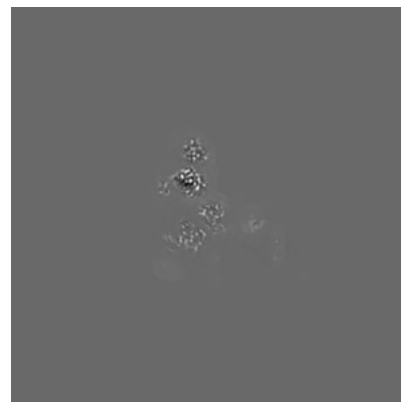
6.2.1 Primary map



X Index: 190

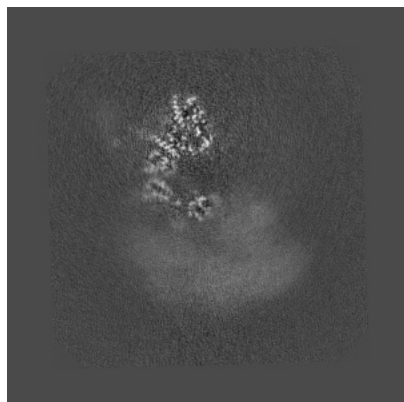


Y Index: 190

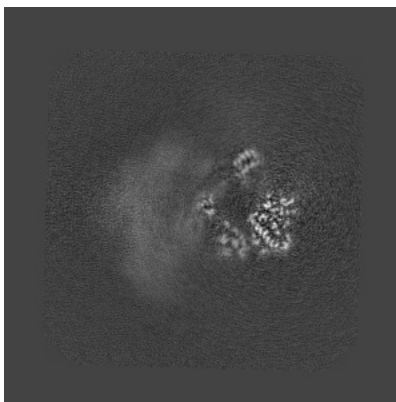


Z Index: 190

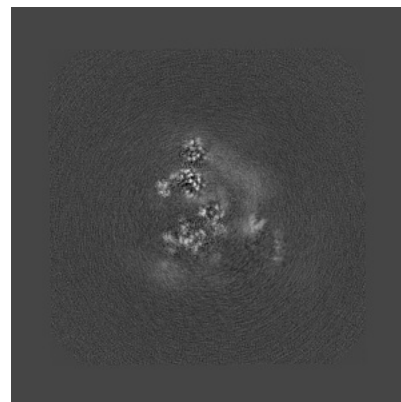
6.2.2 Raw map



X Index: 190



Y Index: 190



Z Index: 190

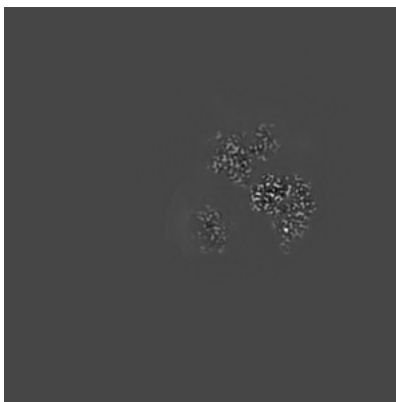
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

6.3.1 Primary map



X Index: 199

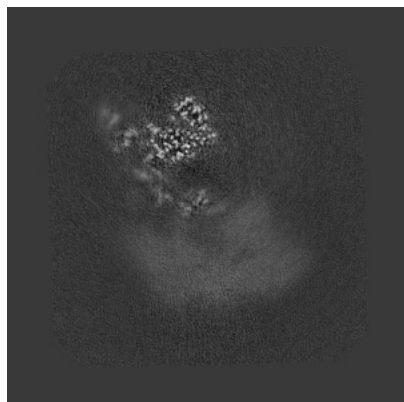


Y Index: 162

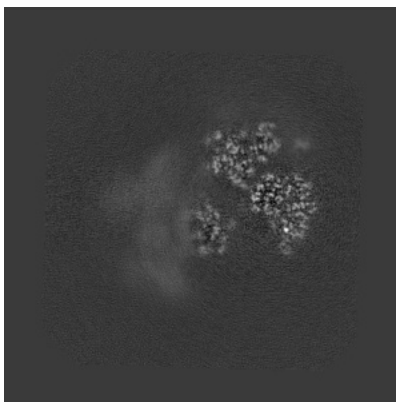


Z Index: 256

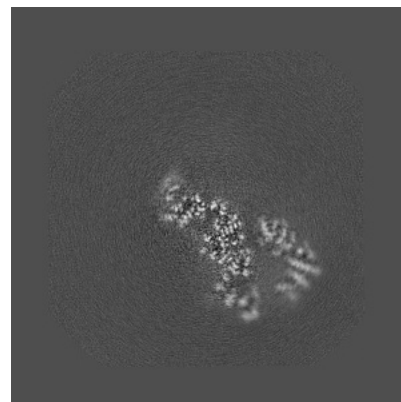
6.3.2 Raw map



X Index: 198



Y Index: 162

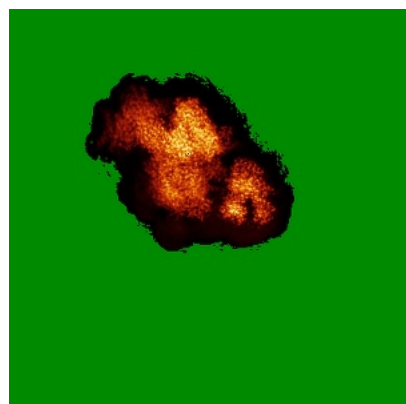


Z Index: 252

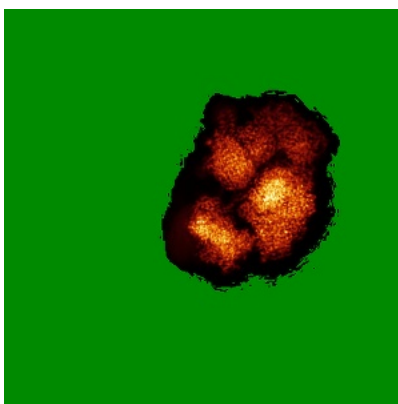
The images above show the largest variance slices of the map in three orthogonal directions.

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

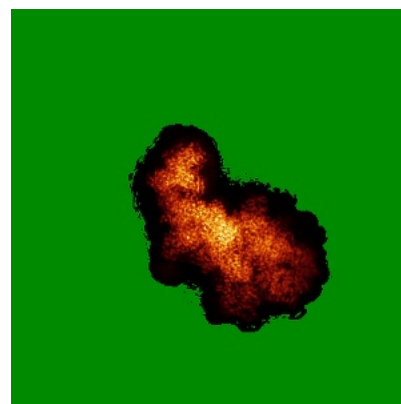
6.4.1 Primary map



X



Y

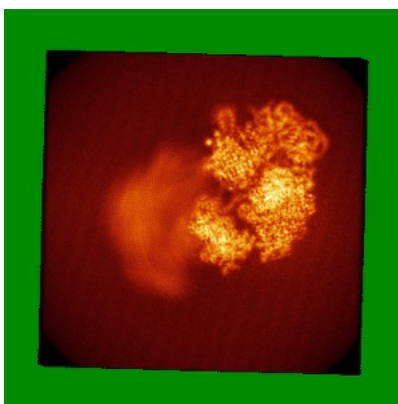


Z

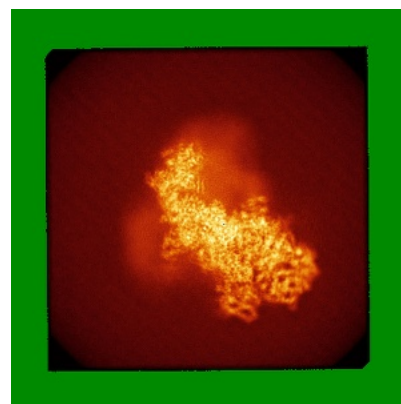
6.4.2 Raw map



X



Y

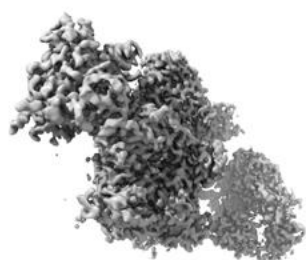


Z

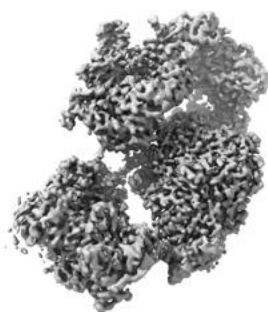
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

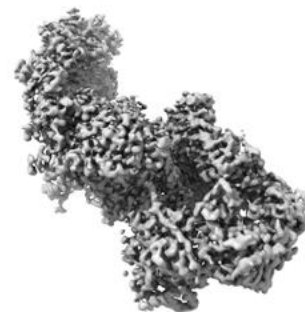
6.5.1 Primary map



X



Y



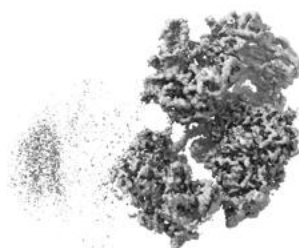
Z

The images above show the 3D surface view of the map at the recommended contour level 3.8. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

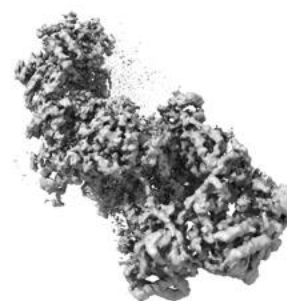
6.5.2 Raw map



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.

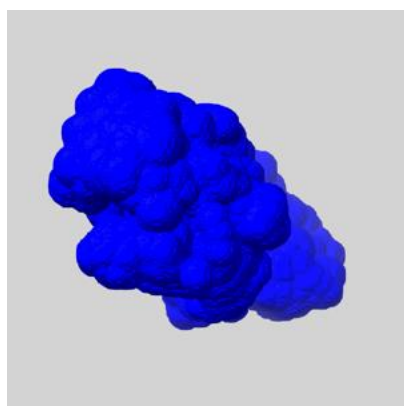
6.6 Mask visualisation [i](#)

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

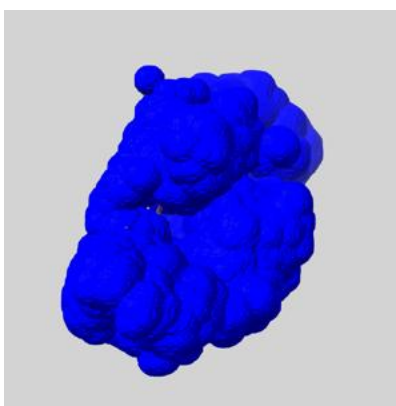
A mask typically either:

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

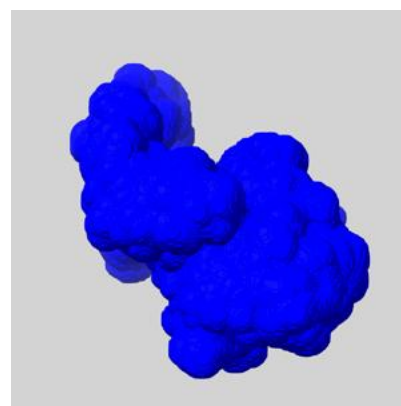
6.6.1 emd_12721_msk_1.map [i](#)



X



Y

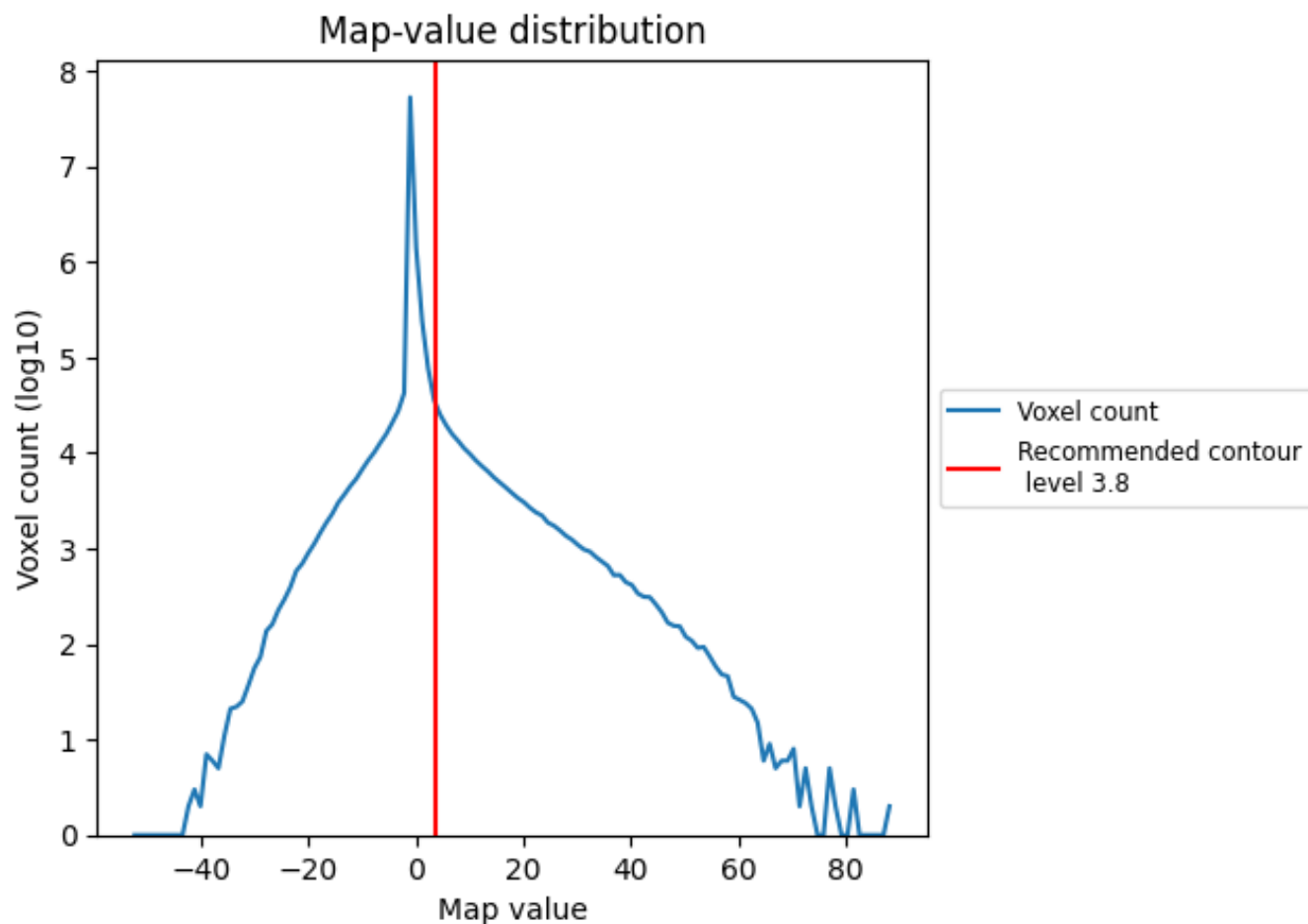


Z

7 Map analysis [i](#)

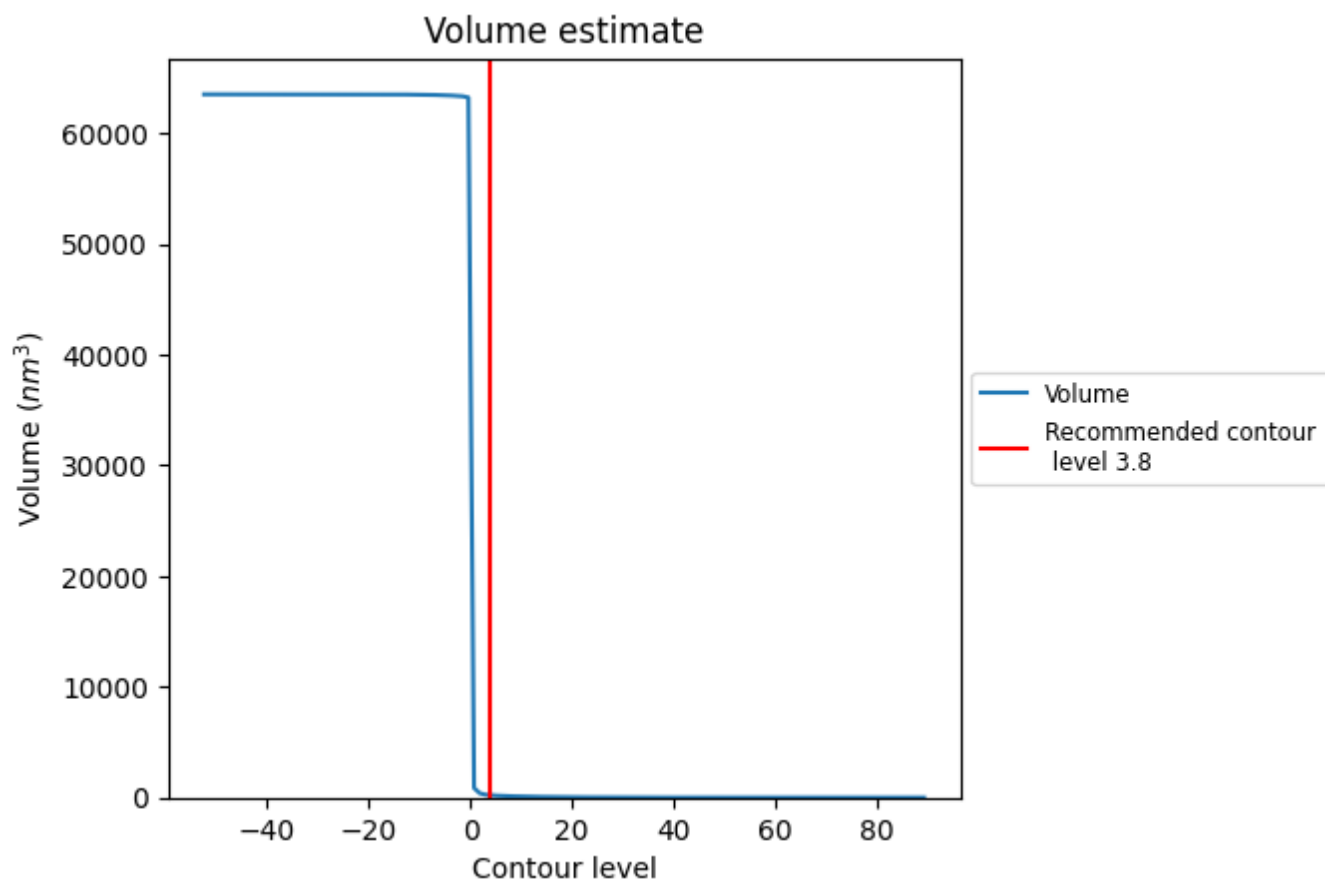
This section contains the results of statistical analysis of the map.

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.

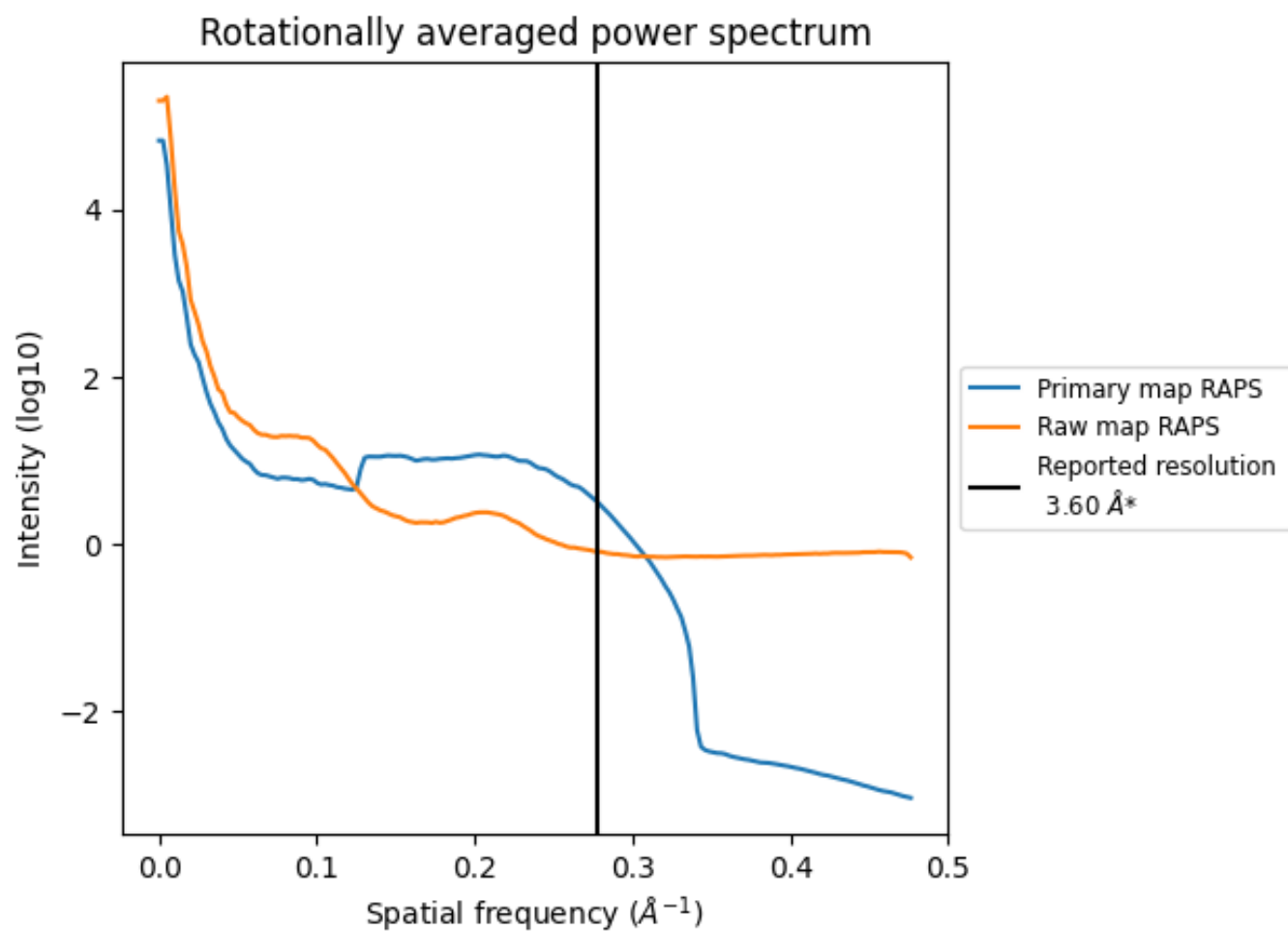
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 219 nm^3 ; this corresponds to an approximate mass of 198 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 ⓘ

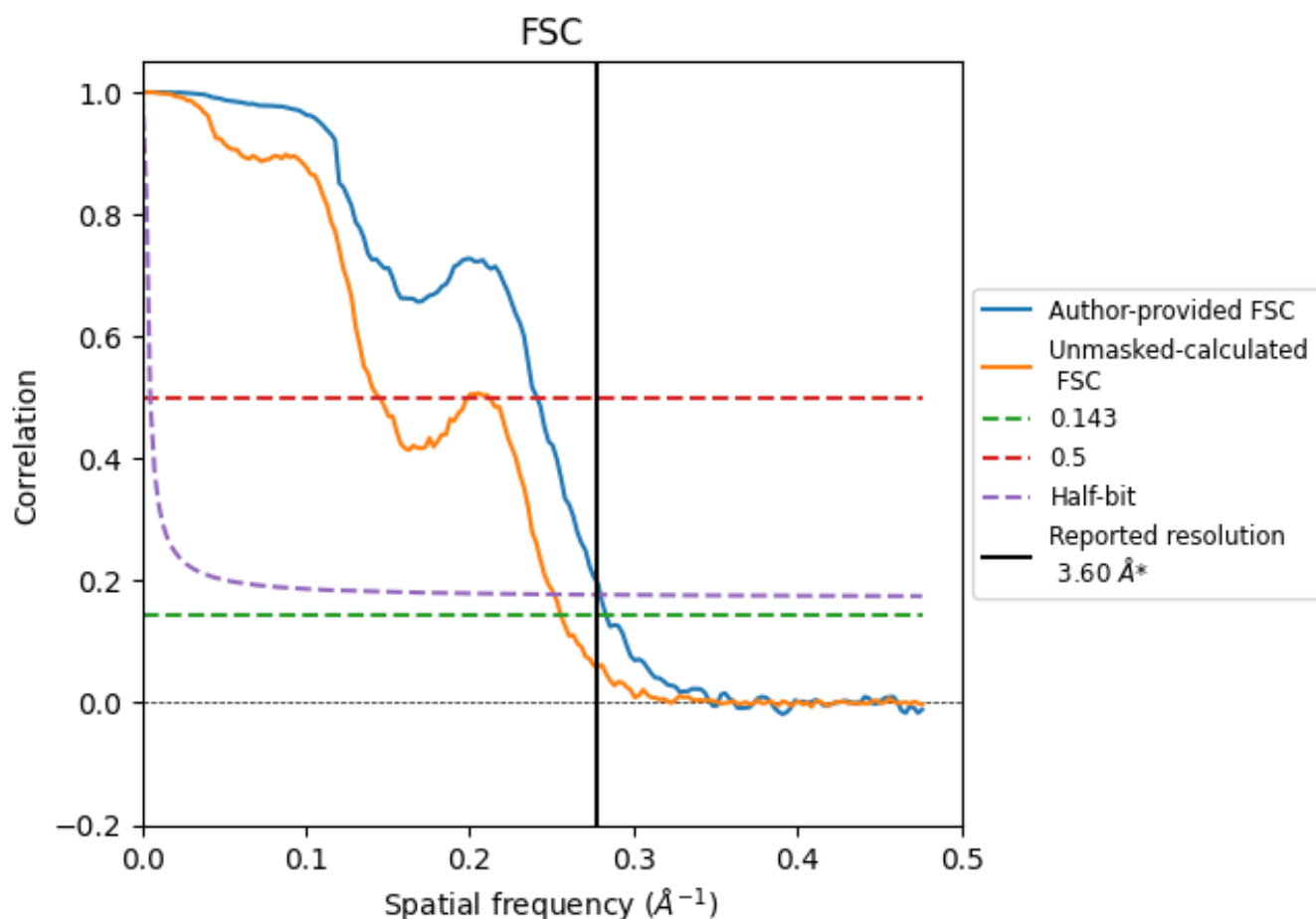


*Reported resolution corresponds to spatial frequency of 0.278 $\text{\AA}^{-1}$

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 0.278 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

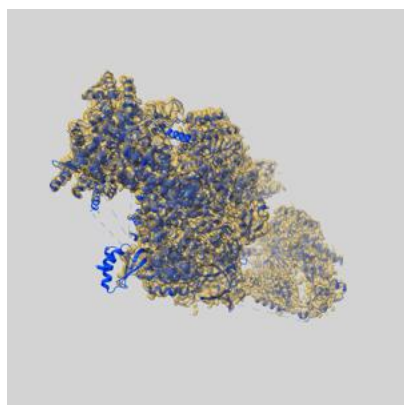
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.60	-	-
Author-provided FSC curve	3.53	4.15	3.57
Unmasked-calculated*	3.91	6.91	3.98

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

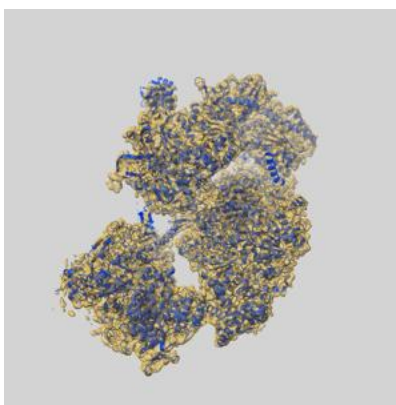
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-12721 and PDB model 7O4K. Per-residue inclusion information can be found in section [3](#) on page [11](#).

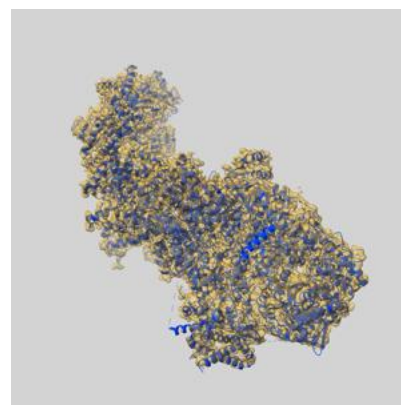
9.1 Map-model overlay [i](#)



X



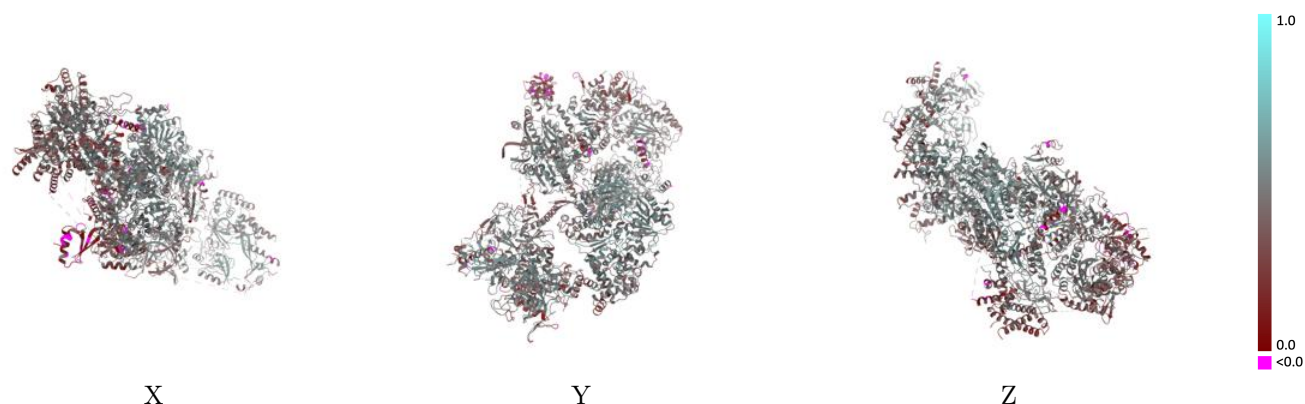
Y



Z

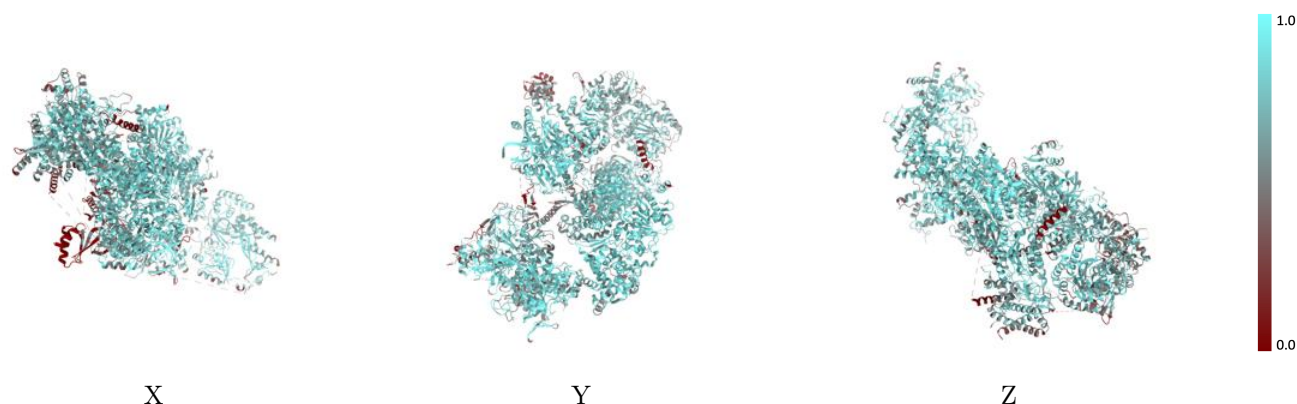
The images above show the 3D surface view of the map at the recommended contour level 3.8 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



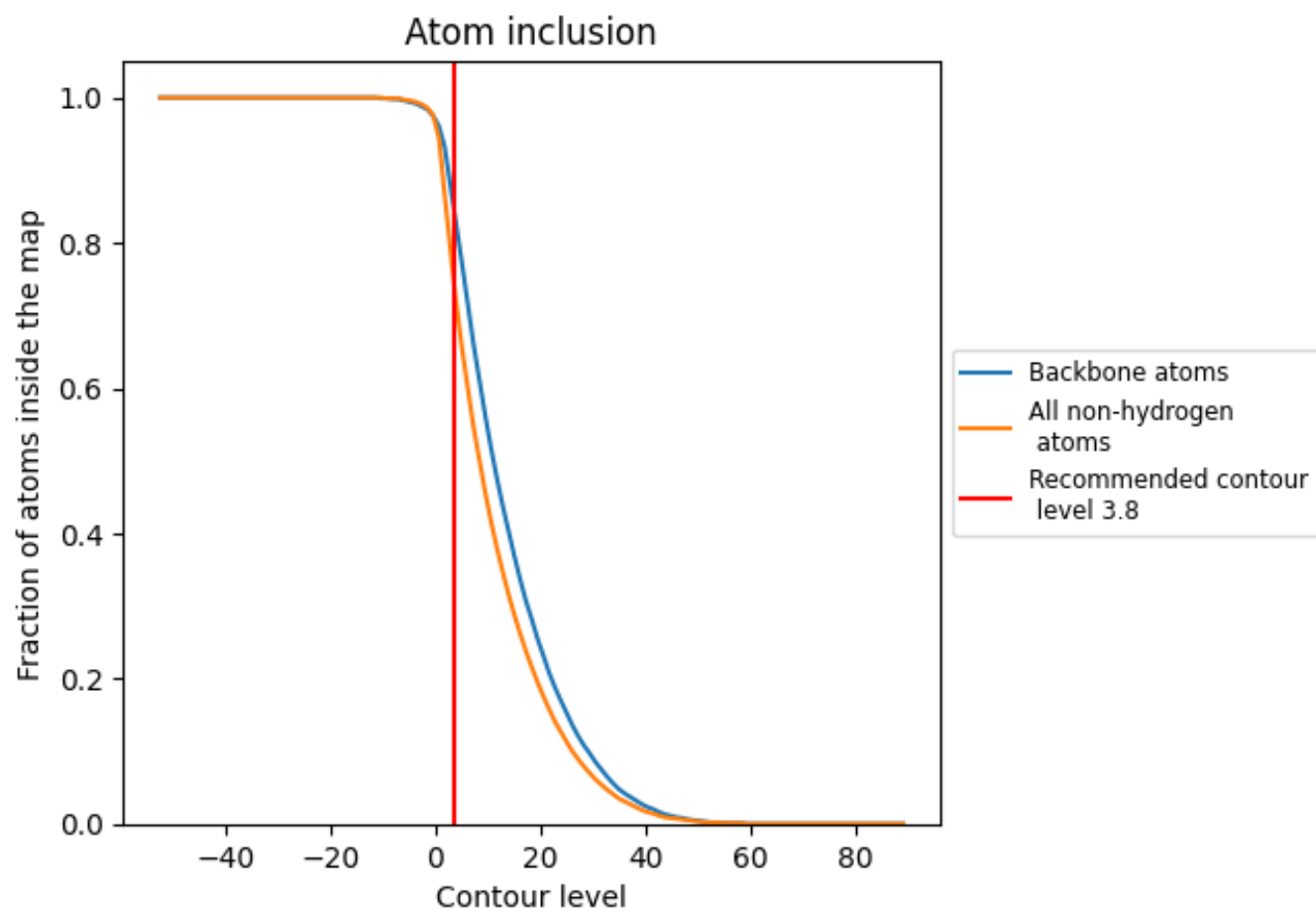
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (3.8).

9.4 Atom inclusion [i](#)



At the recommended contour level, 84% of all backbone atoms, 73% 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 (3.8) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7310	 0.4330
0	 0.8490	 0.5130
1	 0.6380	 0.3760
2	 0.5820	 0.3400
3	 0.7370	 0.4070
4	 0.7410	 0.4320
5	 0.5400	 0.2980
6	 0.7670	 0.4670
7	 0.8070	 0.4620
A	 0.6320	 0.4280
B	 0.7770	 0.4920
D	 0.7300	 0.4230
F	 0.6260	 0.4070
G	 0.8340	 0.4920
N	 0.8450	 0.3950
T	 0.8820	 0.4450
W	 0.6500	 0.4000
X	 0.6760	 0.3960

