



wwPDB EM Validation Summary Report ⓘ

Mar 8, 2026 – 03:39 PM UTC

PDB ID : 7YQ8 / pdb_00007yq8
EMDB ID : EMD-34022
Title : Cryo-EM structure of human topoisomerase II beta in complex with DNA and etoposide
Authors : Naganuma, M.; Ehara, H.; Kim, D.; Nakagawa, R.; Cong, A.; Bu, H.; Jeong, J.; Jang, J.; Schellenberg, M.J.; Bunch, H.; Sekine, S.
Deposited on : 2022-08-05
Resolution : 3.90 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 ⓘ 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

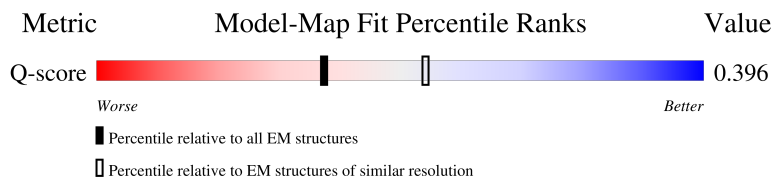
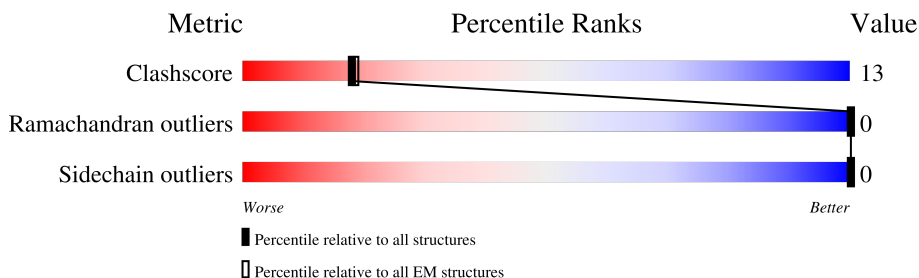
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.90 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	8855 (3.40 - 4.40)

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	A	1626	 31% 14% 55%
1	B	1626	 31% 14% 55%
2	C	50	 10% 14% 76%
2	D	50	 • 28% 68%

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Mol	Chain	Length	Quality of chain
3	E	50	16% 8% 76%
3	F	50	14% 18% 68%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 13036 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 DNA topoisomerase 2-beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	730	Total	C	N	O	S	0	0
			5901	3762	1016	1099	24		
1	B	730	Total	C	N	O	S	0	0
			5901	3762	1016	1099	24		

- Molecule 2 is a DNA chain called 50-mer DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	12	Total	C	N	O	P	0	0
			245	115	47	71	12		
2	D	16	Total	C	N	O	P	0	0
			332	156	66	94	16		

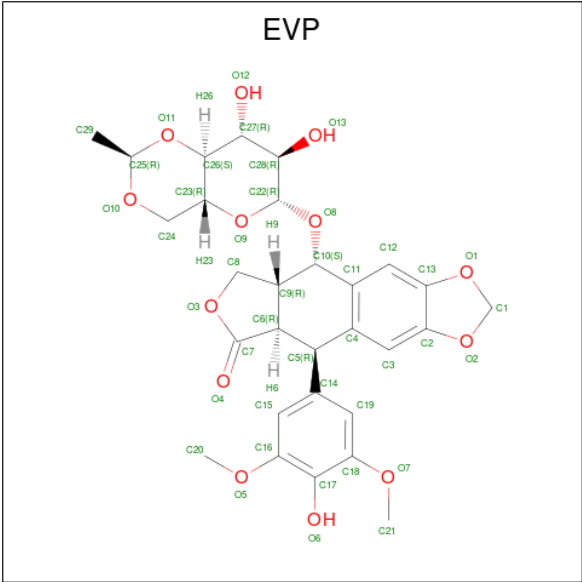
- Molecule 3 is a DNA chain called 50-mer DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	E	12	Total	C	N	O	P	0	0
			243	115	44	72	12		
3	F	16	Total	C	N	O	P	0	0
			328	155	58	99	16		

- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
4	A	1	Total	Mg	0
			1	1	
4	B	1	Total	Mg	0
			1	1	

- Molecule 5 is (5S,5aR,8aR,9R)-9-(4-hydroxy-3,5-dimethoxyphenyl)-8-oxo-5,5a,6,8,8a,9-hexahydrofuro[3',4':6,7]naphtho[2,3-d][1,3]dioxol-5-yl 4,6-O-[(1R)-ethylidene]-beta-D-glucopyranoside (CCD ID: EVP) (formula: C₂₉H₃₂O₁₃) (labeled as "Ligand of Interest" by depositor).

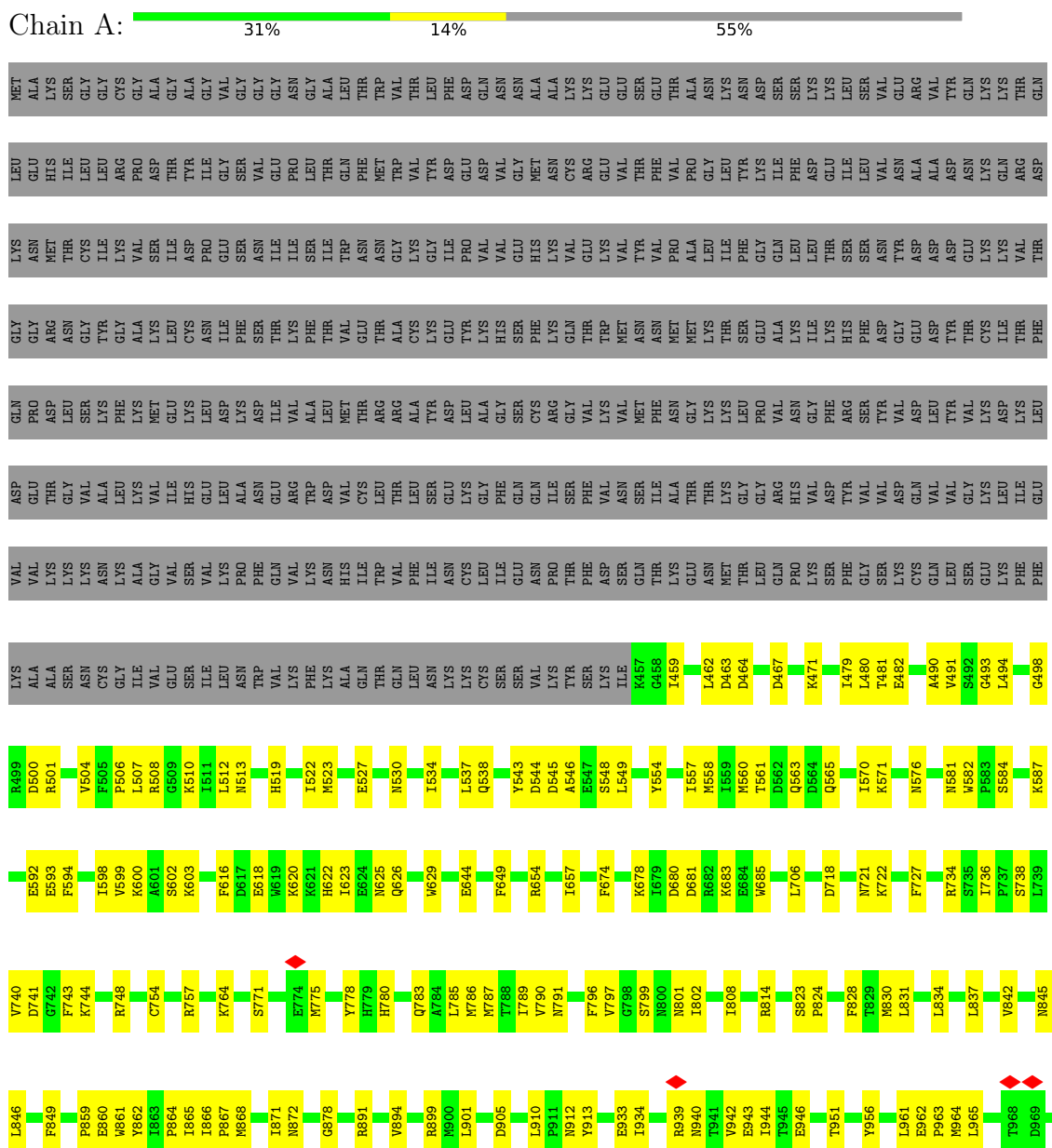


Mol	Chain	Residues	Atoms			AltConf
5	D	1	Total	C	O	0
			42	29	13	
5	F	1	Total	C	O	0
			42	29	13	

3 Residue-property plots

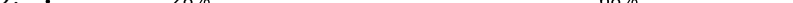
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: DNA topoisomerase 2-beta



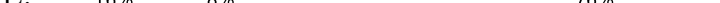
LYS	ALA	ALA	LYS	ASP	THR	GLN	PHE	ALA	PRO	ILE	Q165	K1083	D969	L850	K744	S602	D500	LYS
ALA	ALA	ALA	LYS	ASP	THR	THR	THR	ALA	LYS	PRO	Q166	I1086	E970	P859	R748	K603	R501	ALA
LYS	GLY	GLY	LYS	GLY	ILE	GLY	ILE	GLY	ARG	GLU	N1174	E1087	E860	V861	V504	F616	V504	SER
VAL	ARG	VAL	LYS	LYS	THR	LYS	THR	ALA	LYS	THR	K1177	P972	W861	T753	D617	D617	L507	CYS
LYS	LYS	LYS	LYS	LYS	ALA	LYS	ALA	MET	GLU	LYS	K1177	A973	Y862	T754	E618	E618	R508	GLY
ALA	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	S1182	L1094	P864	K764	E619	E619	G609	ILE
THR	THR	THR	THR	THR	LYS	LYS	LYS	LYS	LYS	LYS	D1183	L1098	I865	L768	K620	K620	G609	VAL
GLY	GLY	GLY	GLY	GLY	ASP	ASP	ASP	ASP	ASP	ASP	L1184	L1098	I866	L768	K621	K621	G609	GLY
GLY	GLY	GLY	GLY	GLY	ASP	ASP	ASP	ASP	ASP	ASP	W1185	L1098	I867	L768	K622	K622	G609	VAL
GLY	GLY	GLY	GLY	GLY	ASP	ASP	ASP	ASP	ASP	ASP	E1186	L1098	I868	L768	K623	K623	G609	VAL
GLY	GLY	GLY	GLY	GLY	ASP	ASP	ASP	ASP	ASP	ASP	E1187	L1098	I869	L768	K624	K624	G609	VAL
GLY	GLY	GLY	GLY	GLY	ASP	ASP	ASP	ASP	ASP	ASP	E1188	L1098	I870	L768	K625	K625	G609	VAL
GLY	GLY	GLY	GLY	GLY	ASP	ASP	ASP	ASP	ASP	ASP	E1189	L1098	I871	L768	K626	K626	G609	VAL
GLY	GLY	GLY	GLY	GLY	ASP	ASP	ASP	ASP	ASP	ASP	E1190	L1098	I872	L768	K627	K627	G609	VAL
GLY	GLY	GLY	GLY	GLY	ASP	ASP	ASP	ASP	ASP	ASP	E1191	L1098	I873	L768	K628	K628	G609	VAL
GLY	GLY	GLY	GLY	GLY	ASP	ASP	ASP	ASP	ASP	ASP	E1192	L1098	I874	L768	K629	K629	G609	VAL
GLY	GLY	GLY	GLY	GLY	ASP	ASP	ASP	ASP	ASP	ASP	E1193	L1098	I875	L768	K630	K630	G609	VAL
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GLY	GLY	GLY	GLY	GLY	ASP	ASP	ASP	ASP	ASP	ASP	E1195	L1098	I877	L768	K632	K632	G609	VAL
GLY	GLY	GLY	GLY	GLY	ASP	ASP	ASP	ASP	ASP	ASP	E1196	L1098	I878	L768	K633	K633	G609	VAL
GLY	GLY	GLY	GLY	GLY	ASP	ASP	ASP	ASP	ASP	ASP	E1197	L1098	I879	L768	K634	K634	G609	VAL
GLY	GLY	GLY	GLY	GLY	ASP	ASP	ASP	ASP	ASP	ASP	E1198	L1098	I880	L768	K635	K635	G609	VAL
GLY	GLY	GLY	GLY	GLY	ASP	ASP	ASP	ASP	ASP	ASP	E1199	L1098	I881	L768	K636	K636	G609	VAL
GLY	GLY	GLY	GLY	GLY	ASP	ASP	ASP	ASP	ASP	ASP	E1200	L1098	I882	L768	K637	K637	G609	VAL
GLY	GLY	GLY	GLY	GLY	ASP	ASP	ASP	ASP	ASP	ASP	E1201	L1098	I883	L768	K638	K638	G609	VAL
GLY	GLY	GLY	GLY	GLY	ASP	ASP	ASP	ASP	ASP	ASP	E1202	L1098	I884	L768	K639	K639	G609	VAL
GLY	GLY	GLY	GLY	GLY	ASP	ASP	ASP	ASP	ASP	ASP	E1203	L1098	I885	L768	K640	K640	G609	VAL
GLY	GLY	GLY	GLY	GLY	ASP	ASP	ASP	ASP	ASP	ASP	E1204	L1098	I886	L768	K641	K641	G609	VAL
GLY	GLY	GLY	GLY	GLY	ASP	ASP	ASP	ASP	ASP	ASP	E1205	L1098	I887	L768	K642	K642	G609	VAL
GLY	GLY	GLY	GLY	GLY	ASP	ASP	ASP	ASP	ASP	ASP	E1206	L1098	I888	L768	K643	K643	G609	VAL
GLY	GLY	GLY	GLY	GLY	ASP	ASP	ASP	ASP	ASP	ASP	E1207	L1098	I889	L768	K644	K644	G609	VAL
GLY	GLY	GLY	GLY	GLY	ASP	ASP	ASP	ASP	ASP	ASP	E1208	L1098	I890	L768	K645	K645	G609	VAL
GLY	GLY	GLY	GLY	GLY	ASP	ASP	ASP	ASP	ASP	ASP	E1209	L1098	I891	L768	K646	K646	G609	VAL
GLY	GLY	GLY	GLY	GLY	ASP	ASP	ASP	ASP	ASP	ASP	E1210	L1098	I892	L768	K647	K647	G609	VAL
GLY	GLY	GLY	GLY	GLY	ASP	ASP	ASP	ASP	ASP	ASP	E1211	L1098	I893	L768	K648	K648	G609	VAL
GLY	GLY	GLY	GLY	GLY	ASP	ASP	ASP	ASP	ASP	ASP	E1212	L1098	I894	L768	K649	K649	G609	VAL
GLY	GLY	GLY	GLY	GLY	ASP	ASP	ASP	ASP	ASP	ASP	E1213	L1098	I895	L768	K650	K650	G609	VAL
GLY	GLY	GLY	GLY	GLY	ASP	ASP	ASP	ASP	ASP	ASP	E1214	L1098	I896	L768	K651	K651	G609	VAL
GLY	GLY	GLY	GLY	GLY	ASP	ASP	ASP	ASP	ASP	ASP	E1215	L1098	I897	L768	K652	K652	G609	VAL
GLY	GLY	GLY	GLY	GLY	ASP	ASP	ASP	ASP	ASP	ASP	E1216	L1098	I898	L768	K653	K653	G609	VAL
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GLY	GLY	GLY	GLY	GLY	ASP	ASP	ASP	ASP	ASP	ASP	E1242	L1098	I924	L768	K679	K679	G609	VAL
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GLY	GLY	GLY	GLY	GLY	ASP	ASP	ASP	ASP	ASP	ASP	E1245	L1098	I927	L768	K682	K682	G609	VAL
GLY	GLY	GLY	GLY	GLY	ASP	ASP	ASP	ASP	ASP	ASP	E1246	L1098	I928	L768	K683	K683	G609	VAL
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GLY	GLY	GLY	GLY	GLY	ASP	ASP	ASP	ASP	ASP	ASP	E1253	L1098	I935	L768	K690	K690	G609	VAL
GLY	GLY	GLY	GLY	GLY	ASP	ASP	ASP	ASP	ASP	ASP	E1254	L1098	I936	L768	K691	K691	G609	VAL
GLY	GLY	GLY	GLY	GLY	ASP	ASP	ASP	ASP	ASP	ASP	E1255	L1098	I937	L768	K692	K692	G609	VAL
GLY	GLY	GLY	GLY	GLY	ASP	ASP	ASP	ASP	ASP	ASP	E1256	L1098	I938	L768	K693	K693	G609	VAL
GLY	GLY	GLY	GLY	GLY	ASP	ASP	ASP	ASP	ASP	ASP	E1257	L1098	I939	L768	K694	K694	G609	VAL
GLY	GLY	GLY	GLY	GLY	ASP	ASP	ASP	ASP	ASP	ASP	E1258	L1098	I940	L768	K695	K695	G609	VAL
GLY	GLY	GLY	GLY	GLY	ASP	ASP	ASP	ASP	ASP	ASP	E1259	L1098	I941	L768	K696	K696	G609	VAL
GLY	GLY	GLY	GLY	GLY	ASP	ASP	ASP	ASP	ASP	ASP	E1260	L1098	I942	L768	K697	K697	G609	VAL
GLY	GLY	GLY	GLY	GLY	ASP	ASP	ASP	ASP	ASP	ASP	E1261	L1098	I943	L768	K698	K698	G609	VAL
GLY	GLY	GLY	GLY	GLY	ASP	ASP	ASP	ASP	ASP	ASP	E1262	L1098	I944	L768	K699	K699	G609	VAL
GLY	GLY	GLY	GLY	GLY	ASP	ASP	ASP	ASP	ASP	ASP	E1263	L1098	I945	L768	K700	K700	G609	VAL
GLY	GLY	GLY	GLY	GLY	ASP	ASP	ASP</											

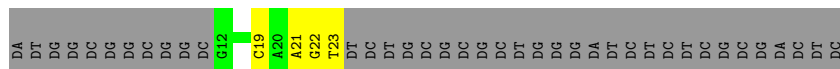
- Molecule 2: 50-mer DNA

Chain D:  28% 68%



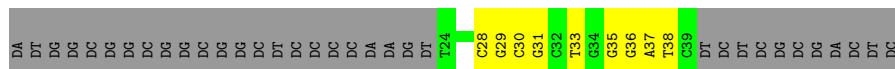
- Molecule 3: 50-mer DNA

Chain E:  16% 8% 76%



- Molecule 3: 50-mer DNA

Chain F: 14% 18% 68%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	26067	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	49	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.066	Depositor
Minimum map value	-0.027	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.0125	Depositor
Map size ($\text{\AA}$)	249.0, 249.0, 249.0	wwPDB
Map dimensions	200, 200, 200	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.245, 1.245, 1.245	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: MG, EVP

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	0.13	0/6020	0.29	0/8112
1	B	0.13	0/6020	0.31	0/8112
2	C	0.21	0/274	0.30	0/420
2	D	0.21	0/373	0.31	0/574
3	E	0.22	0/271	0.33	0/415
3	F	0.25	0/366	0.40	0/563
All	All	0.14	0/13324	0.31	0/18196

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	5901	0	5929	157	0
1	B	5901	0	5929	169	0
2	C	245	0	134	10	0
2	D	332	0	179	12	0
3	E	243	0	135	6	0
3	F	328	0	181	7	0
4	A	1	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	1	0	0	0	0
5	D	42	0	31	6	0
5	F	42	0	31	6	0
All	All	13036	0	12549	339	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 13.

The worst 5 of 339 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:B:753:THR:HG21	1:B:772:VAL:HG22	1.49	0.93
1:B:962:GLU:HG2	1:B:963:PRO:HD3	1.58	0.86
1:A:706:LEU:HD21	1:A:722:LYS:HD3	1.60	0.84
1:A:939:ARG:HH11	1:A:995:GLU:HB3	1.45	0.82
1:B:939:ARG:HH11	1:B:995:GLU:HB3	1.45	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	A	726/1626 (45%)	702 (97%)	24 (3%)	0	100	100
1	B	726/1626 (45%)	697 (96%)	29 (4%)	0	100	100
All	All	1452/3252 (45%)	1399 (96%)	53 (4%)	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	640/1425 (45%)	640 (100%)	0	100	100
1	B	640/1425 (45%)	640 (100%)	0	100	100
All	All	1280/2850 (45%)	1280 (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 10 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	695	GLN
1	B	1000	GLN
1	B	1144	ASN
1	A	1000	GLN
1	A	1072	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 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	$\# Z > 2$
5	EVP	D	101	-	48,48,48	1.73	14 (29%)	71,73,73	2.56	31 (43%)
5	EVP	F	101	-	48,48,48	1.82	12 (25%)	71,73,73	2.56	34 (47%)

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
5	EVP	D	101	-	-	0/12/76/76	0/7/7/7
5	EVP	F	101	-	-	0/12/76/76	0/7/7/7

The worst 5 of 26 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	F	101	EVP	C14-C5	4.41	1.57	1.52
5	F	101	EVP	C4-C5	4.05	1.57	1.51
5	F	101	EVP	O11-C26	-3.75	1.38	1.44
5	D	101	EVP	C4-C5	3.55	1.56	1.51
5	D	101	EVP	O4-C7	3.49	1.30	1.21

The worst 5 of 65 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	F	101	EVP	C24-O10-C25	7.99	119.49	111.67
5	D	101	EVP	O7-C18-C17	7.20	122.06	114.53
5	D	101	EVP	C24-O10-C25	6.70	118.22	111.67
5	F	101	EVP	O7-C18-C17	6.59	121.42	114.53
5	D	101	EVP	O1-C13-C12	6.38	136.33	127.86

There are no chirality outliers.

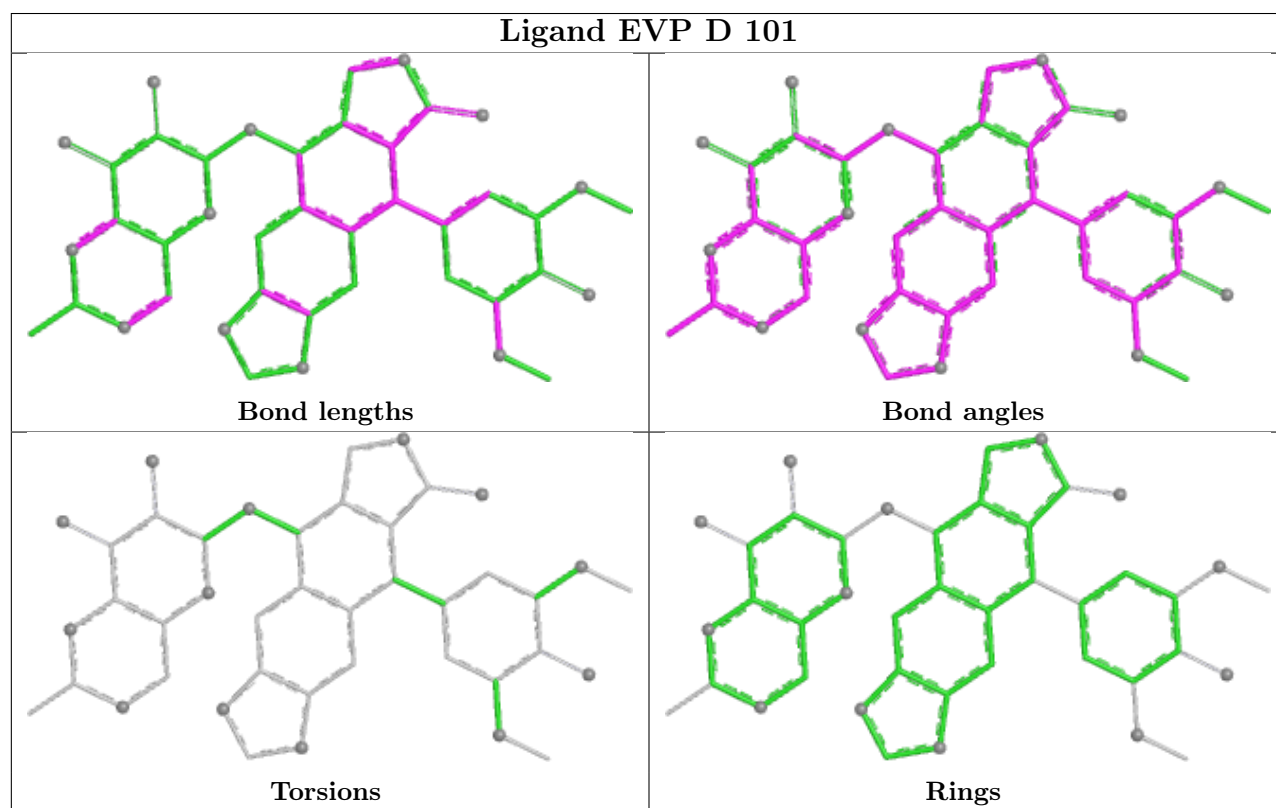
There are no torsion outliers.

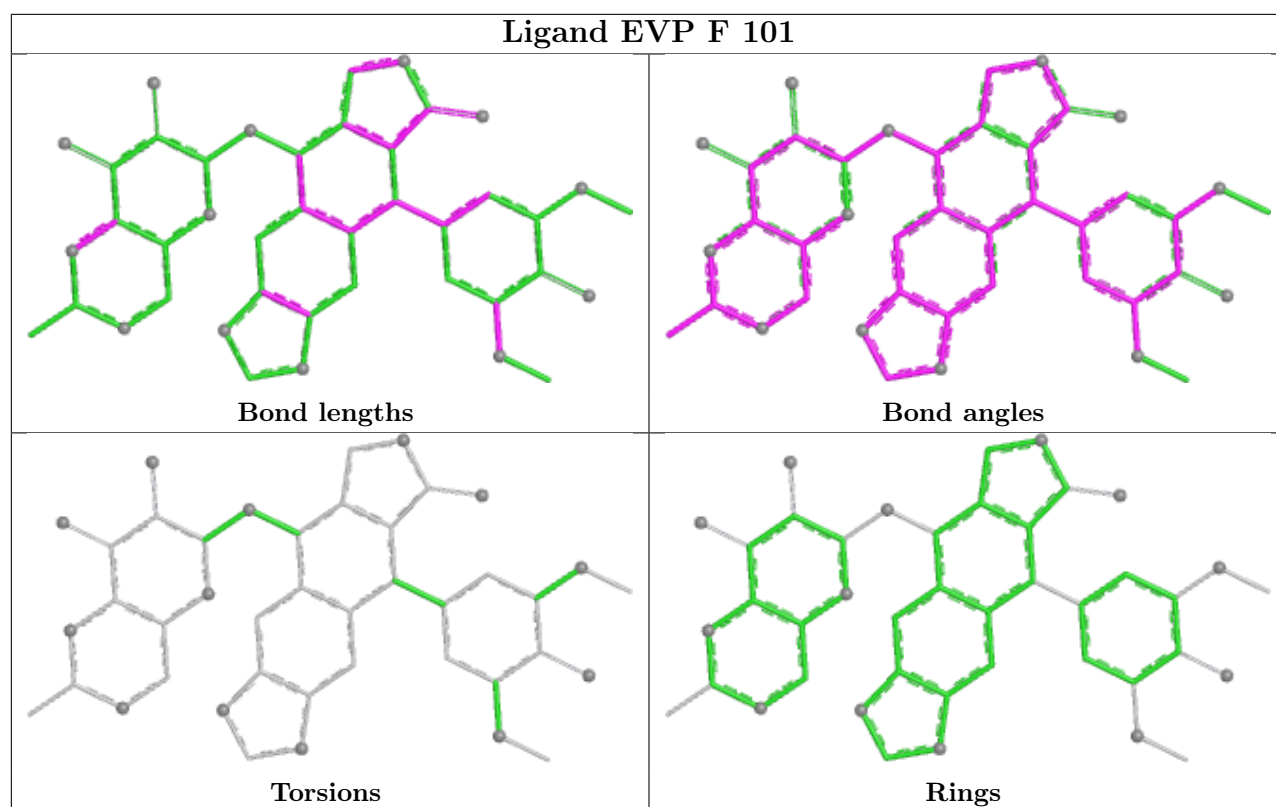
There are no ring outliers.

2 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	D	101	EVP	6	0
5	F	101	EVP	6	0

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 [i](#)

There are no chain breaks in this entry.

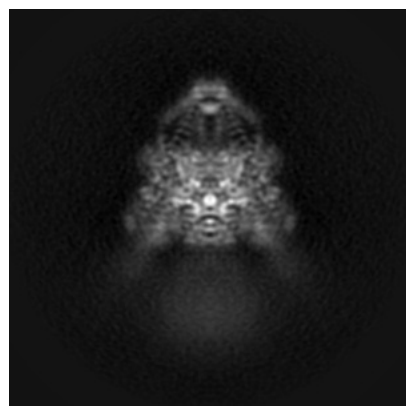
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-34022. These allow visual inspection of the internal detail of the map and identification of artifacts.

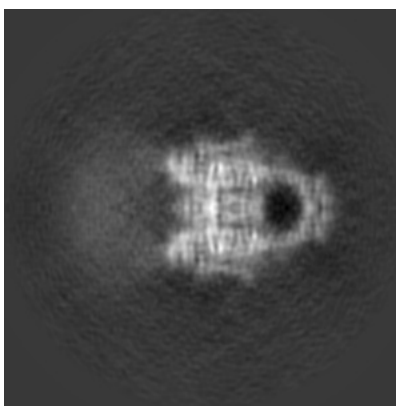
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

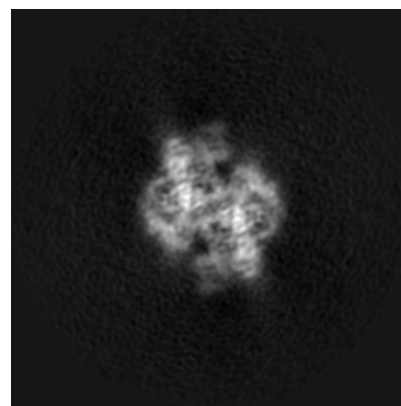
6.1.1 Primary map



X

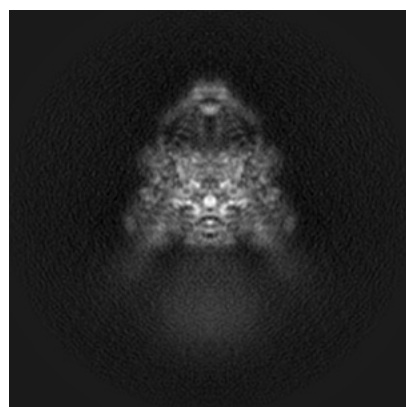


Y

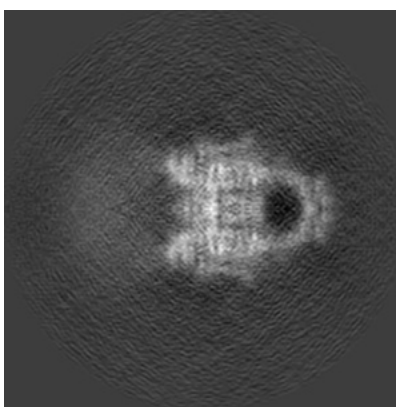


Z

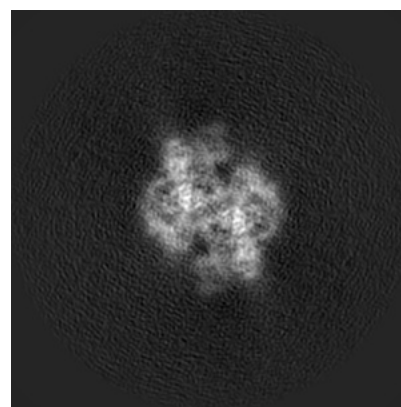
6.1.2 Raw map



X



Y

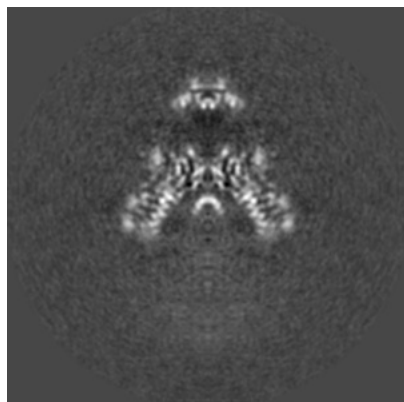


Z

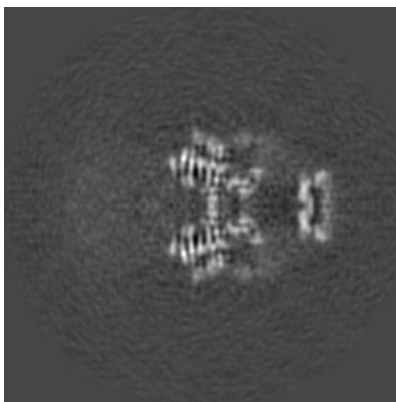
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

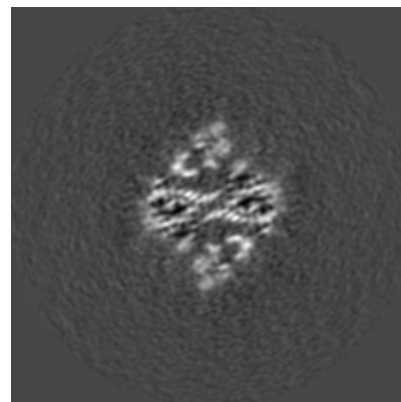
6.2.1 Primary map



X Index: 100

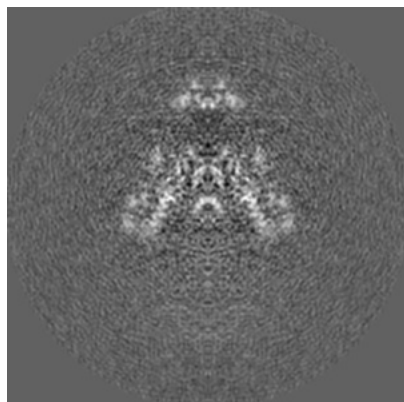


Y Index: 100

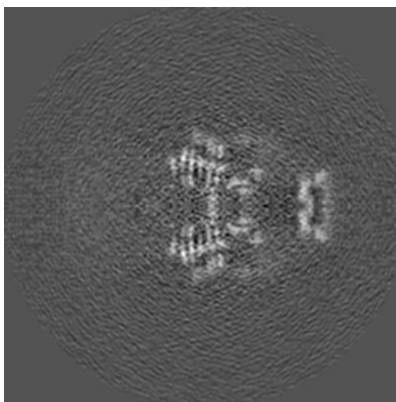


Z Index: 100

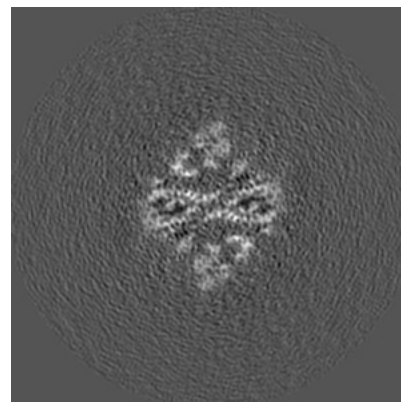
6.2.2 Raw map



X Index: 100



Y Index: 100

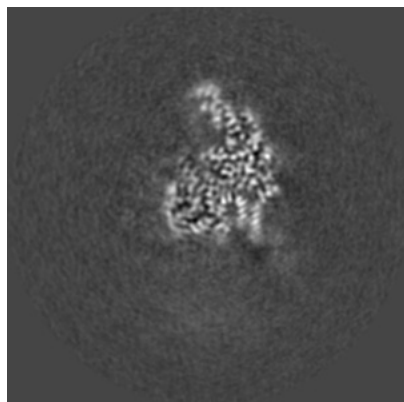


Z Index: 100

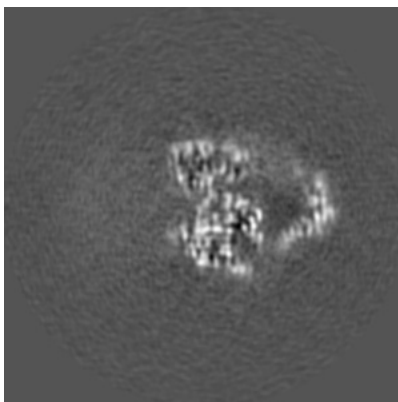
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

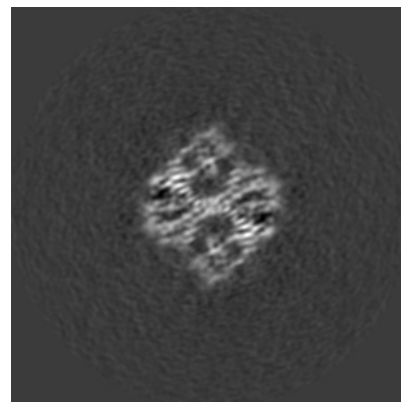
6.3.1 Primary map



X Index: 86

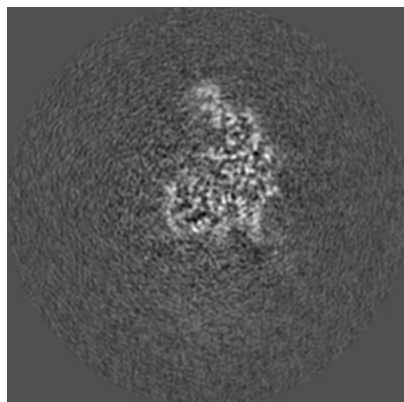


Y Index: 106

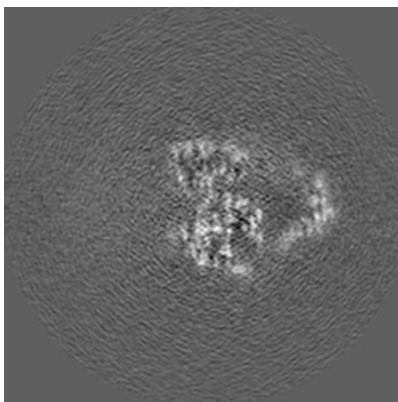


Z Index: 103

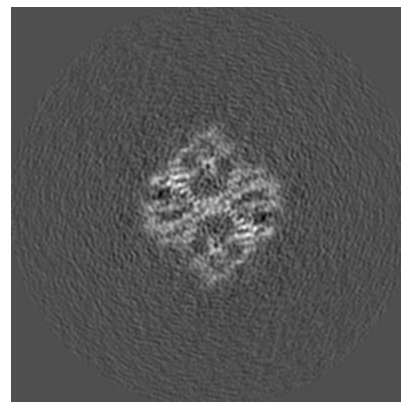
6.3.2 Raw map



X Index: 86



Y Index: 106

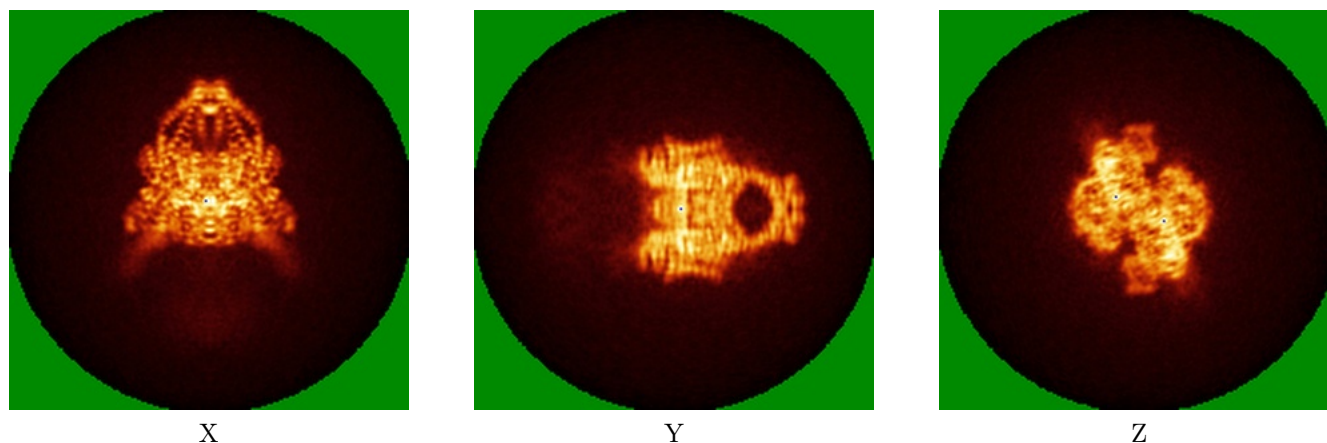


Z Index: 103

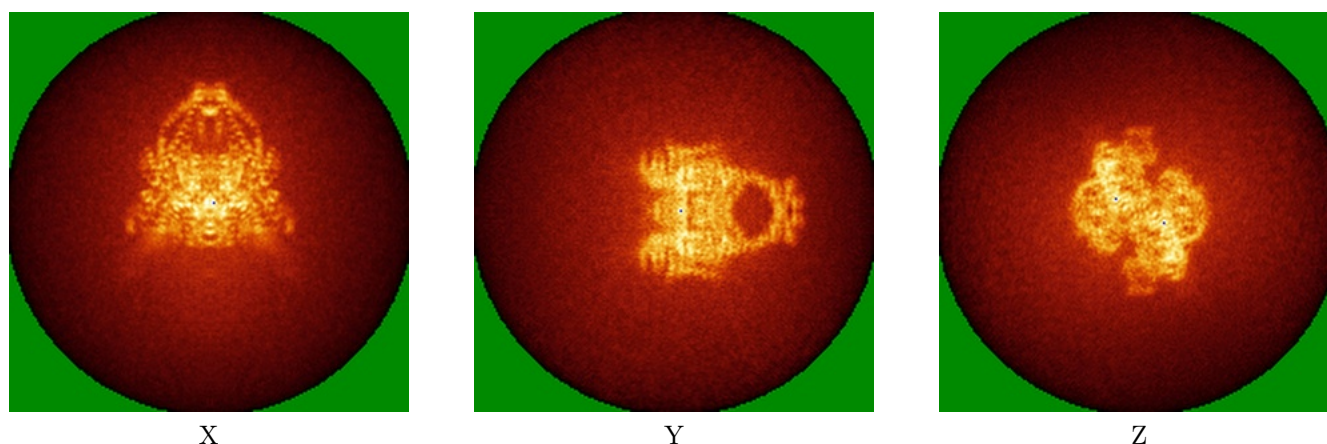
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



6.4.2 Raw map



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](#)

This section was not generated.

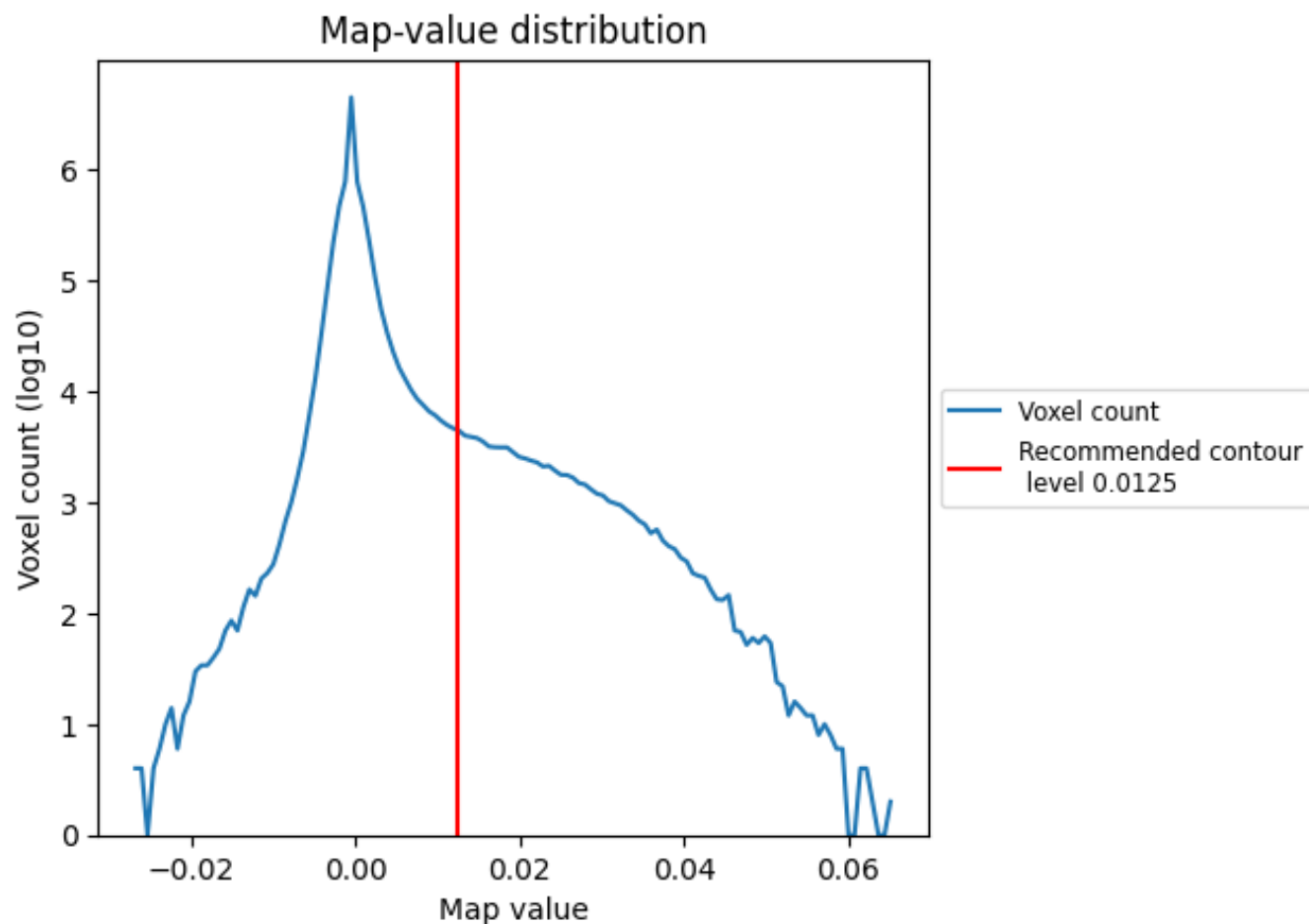
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

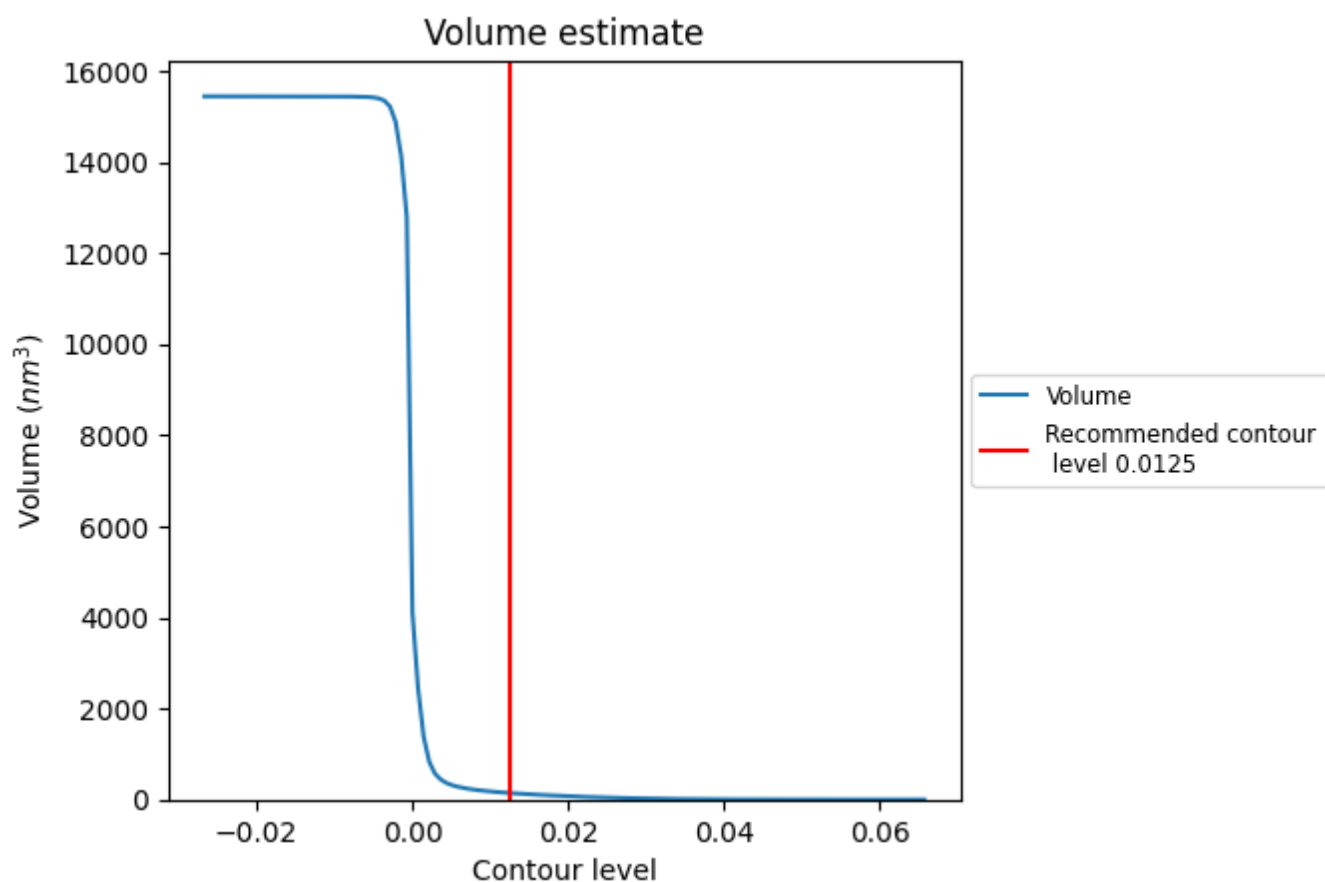
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

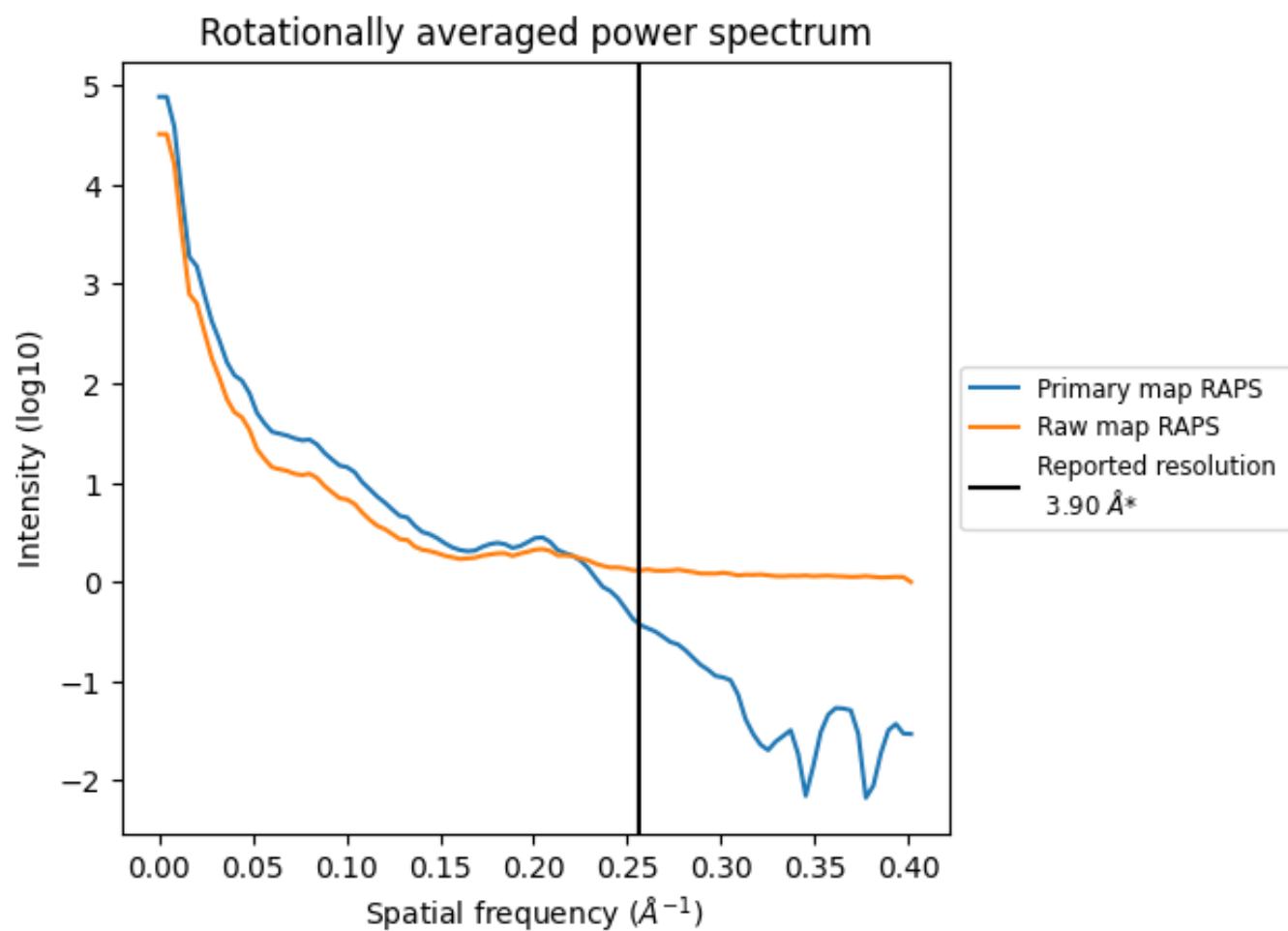
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 144 nm³; this corresponds to an approximate mass of 130 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 ⓘ

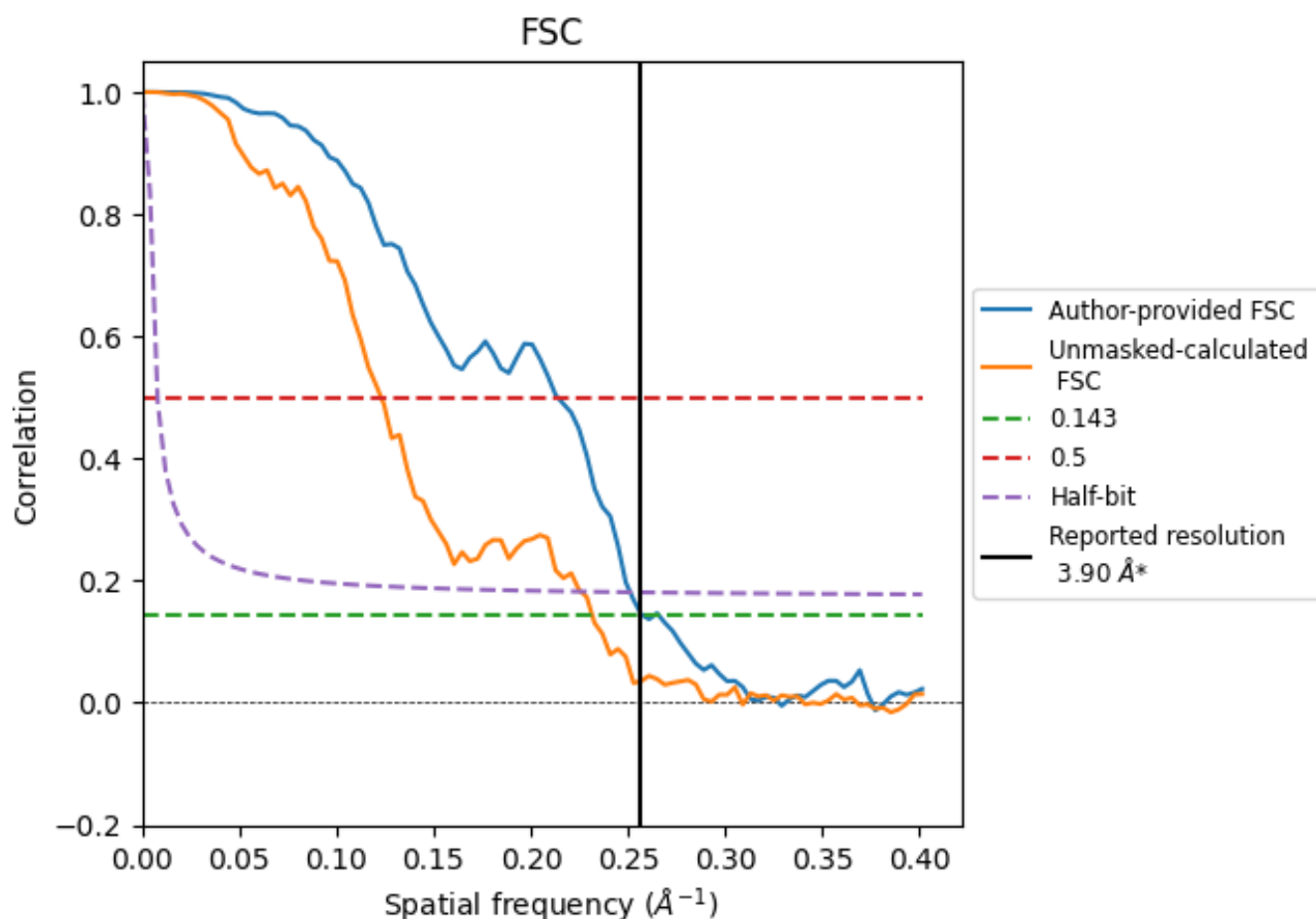


*Reported resolution corresponds to spatial frequency of 0.256 Å⁻¹

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 0.256 Å⁻¹

8.2 Resolution estimates [i](#)

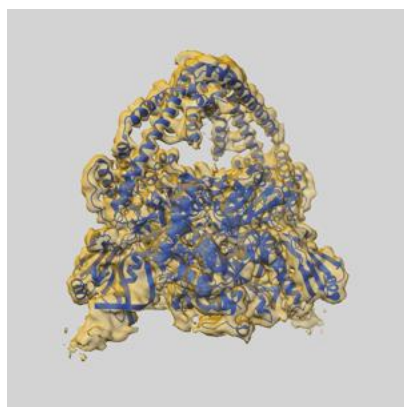
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.90	-	-
Author-provided FSC curve	3.88	4.68	3.98
Unmasked-calculated*	4.31	8.13	4.43

*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 4.31 differs from the reported value 3.9 by more than 10 %

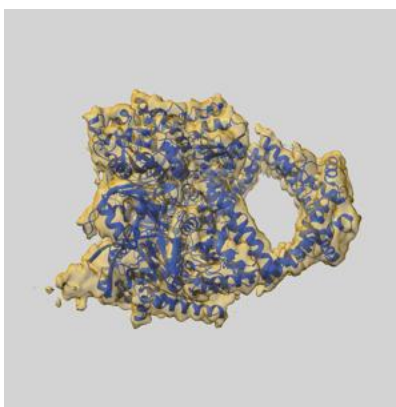
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-34022 and PDB model 7YQ8. Per-residue inclusion information can be found in section [3](#) on page [6](#).

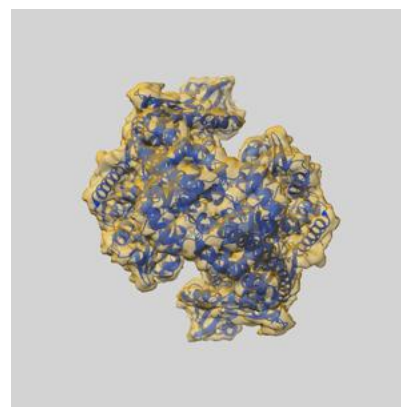
9.1 Map-model overlay [i](#)



X



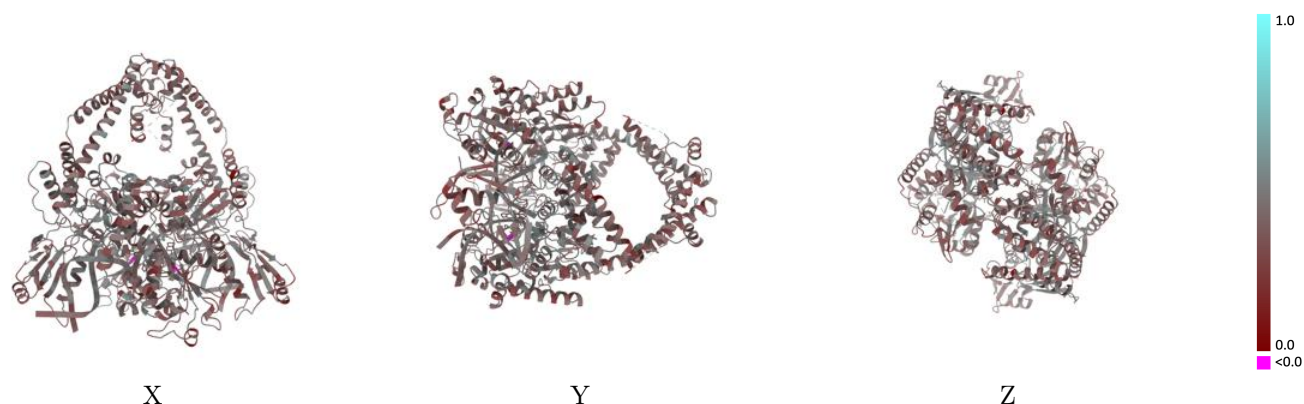
Y



Z

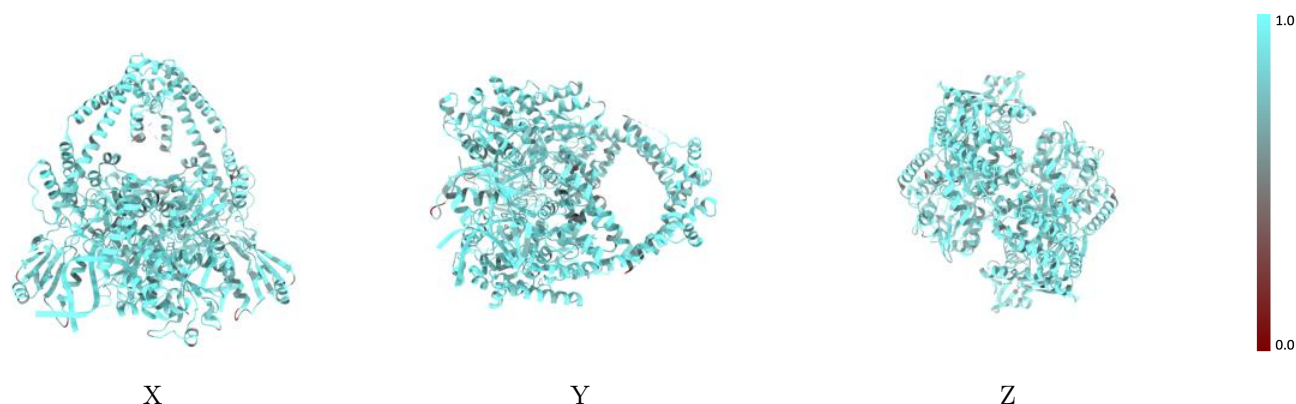
The images above show the 3D surface view of the map at the recommended contour level 0.0125 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



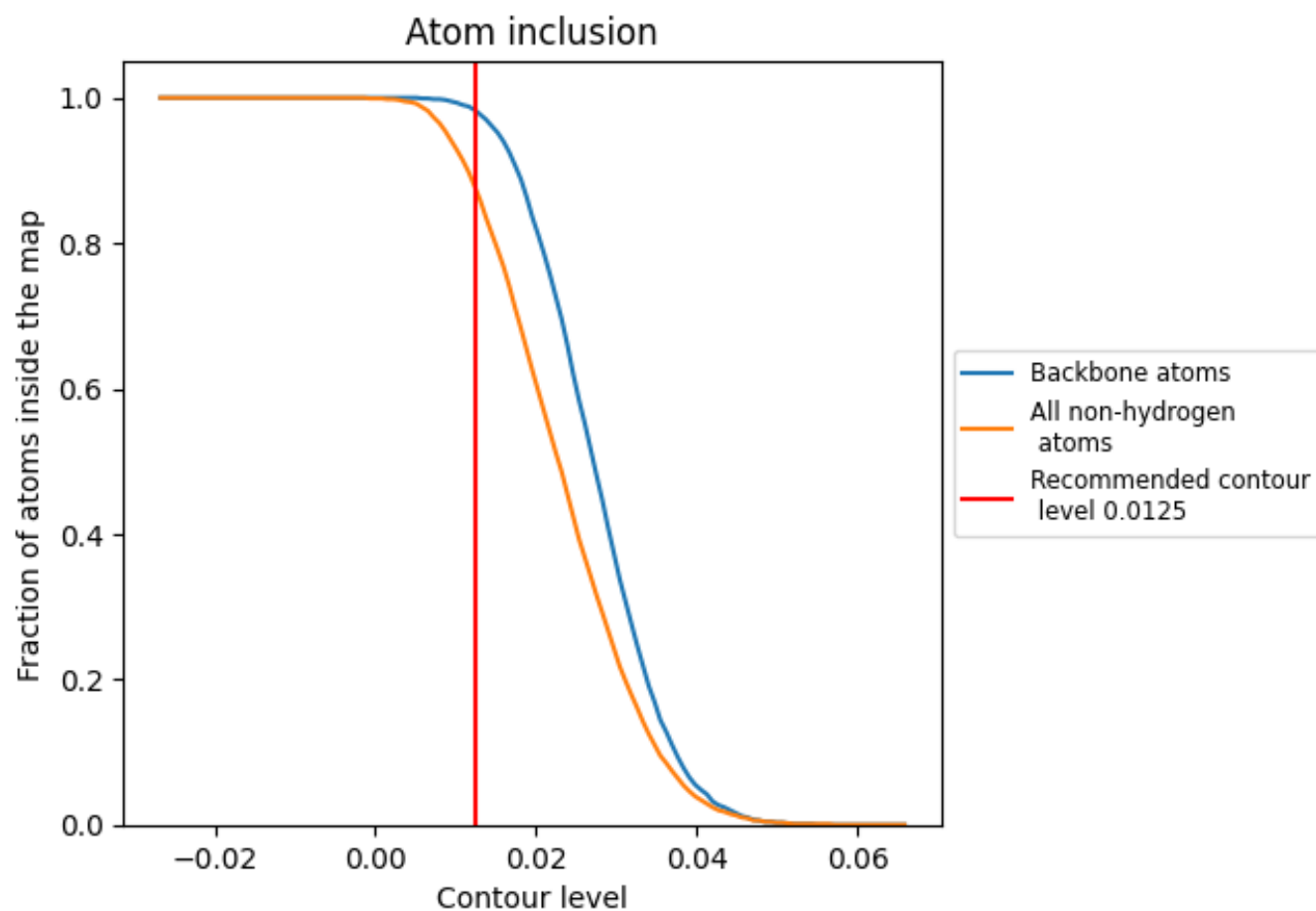
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0125).

9.4 Atom inclusion [i](#)



At the recommended contour level, 98% of all backbone atoms, 87% 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 (0.0125) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8740	0.3960
A	0.8640	0.3920
B	0.8630	0.3910
C	0.9880	0.4550
D	0.9730	0.4300
E	0.9880	0.4560
F	0.9680	0.4290

1.0

0.0

<0.0