



## wwPDB EM Validation Summary Report ⓘ

Nov 10, 2024 – 05:37 AM EST

PDB ID : 7KRA  
EMDB ID : EMD-23003  
Title : Cryo-EM structure of *Saccharomyces cerevisiae* ER membrane protein complex bound to Fab-DH4 in lipid nanodiscs  
Authors : Miller-Vedam, L.E.; Schirle Oakdale, N.S.; Braeuning, B.; Boydston, E.A.; Sevillano, N.; Popova, K.D.; Bonnar, J.L.; Shurtleff, M.J.; Prabu, J.R.; Stroud, R.M.; Craik, C.S.; Schulman, B.A.; Weissman, J.S.; Frost, A.  
Deposited on : 2020-11-19  
Resolution : 3.20 Å(reported)

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

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

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<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev113  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.39

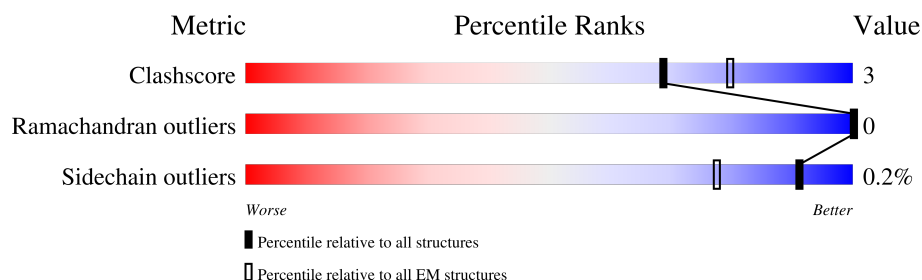
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.20 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.







Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion  $< 40\%$ ). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	760	
2	B	292	
3	C	253	
4	D	190	
5	E	182	
6	F	108	
7	G	234	
8	H	205	

Continued on next page...

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Mol	Chain	Length	Quality of chain
9	I	254	
10	J	234	
11	M	24	
11	N	24	

## 2 Entry composition

There are 13 unique types of molecules in this entry. The entry contains 17293 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 ER membrane protein complex subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	694	Total	C	N	O	S	0	0
			5637	3639	916	1067	15		

- Molecule 2 is a protein called ER membrane protein complex subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	290	Total	C	N	O	S	0	0
			2362	1518	380	452	12		

- Molecule 3 is a protein called ER membrane protein complex subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	188	Total	C	N	O	S	0	0
			1522	1003	243	265	11		

- Molecule 4 is a protein called ER membrane protein complex subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	68	Total	C	N	O	S	0	0
			515	338	87	86	4		

- Molecule 5 is a protein called ER membrane protein complex subunit 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	129	Total	C	N	O	S	0	0
			1028	671	166	188	3		

- Molecule 6 is a protein called ER membrane protein complex subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	95	Total	C	N	O	S	0	0
			780	528	121	129	2		

- Molecule 7 is a protein called Protein SOP4.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	151	Total	C	N	O	S	0	0
			1235	794	206	231	4		

- Molecule 8 is a protein called Endoplasmic reticulum membrane protein complex subunit 10.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	125	Total	C	N	O	S	0	0
			965	605	150	206	4		

- Molecule 9 is a protein called Fab DH4 heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	170	Total	C	N	O	S	0	0
			1309	842	218	245	4		

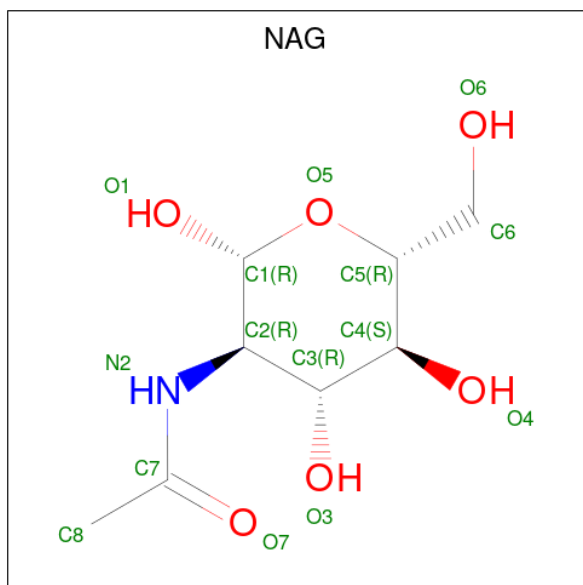
- Molecule 10 is a protein called Fab DH4 light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	209	Total	C	N	O	S	0	0
			1610	1003	276	323	8		

- Molecule 11 is a protein called Unassigned helix.

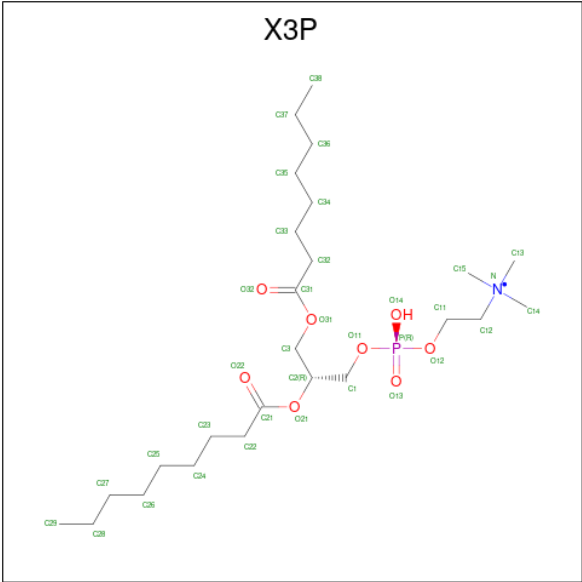
Mol	Chain	Residues	Atoms				AltConf	Trace
11	M	21	Total	C	N	O	0	0
			105	63	21	21		
11	N	24	Total	C	N	O	0	0
			120	72	24	24		

- Molecule 12 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).



Mol	Chain	Residues	Atoms				AltConf
12	A	1	Total	C	N	O	0
			14	8	1	5	
12	A	1	Total	C	N	O	0
			14	8	1	5	
12	A	1	Total	C	N	O	0
			14	8	1	5	
12	G	1	Total	C	N	O	0
			14	8	1	5	
12	G	1	Total	C	N	O	0
			14	8	1	5	

- Molecule 13 is [(2 {R})-1-octanoyloxy-3-[oxidanyl-2-(trimethyl- $\text{I}^{\{4\}}$ -azanyl)ethoxy]phosphoryl]oxy-propan-2-yl] nonanoate (three-letter code: X3P) (formula:  $\text{C}_{25}\text{H}_{51}\text{NO}_8\text{P}$ ).

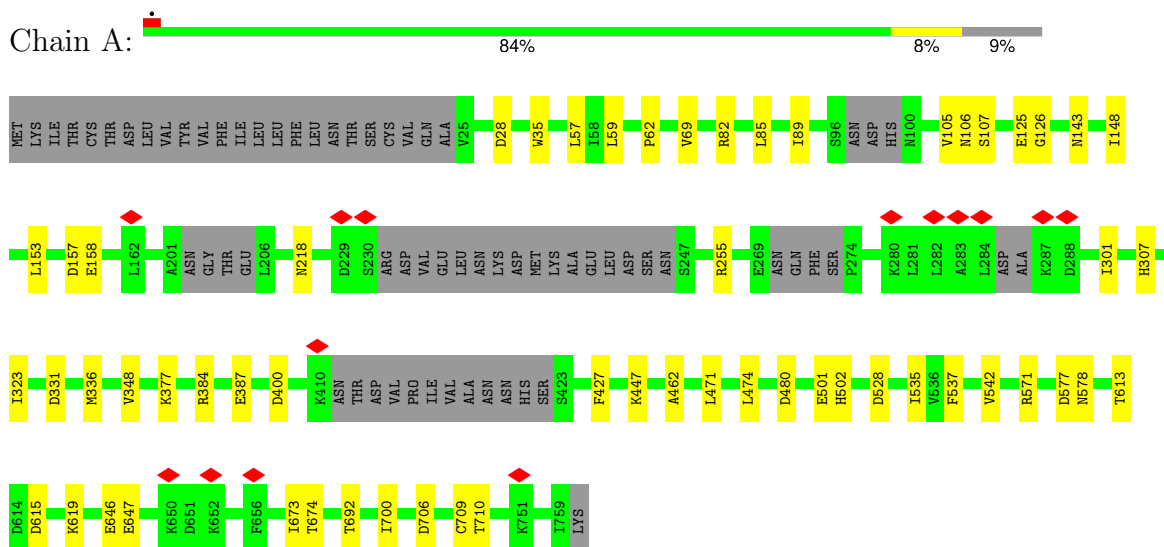


Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
13	C	1	35	25	1	8	1	0

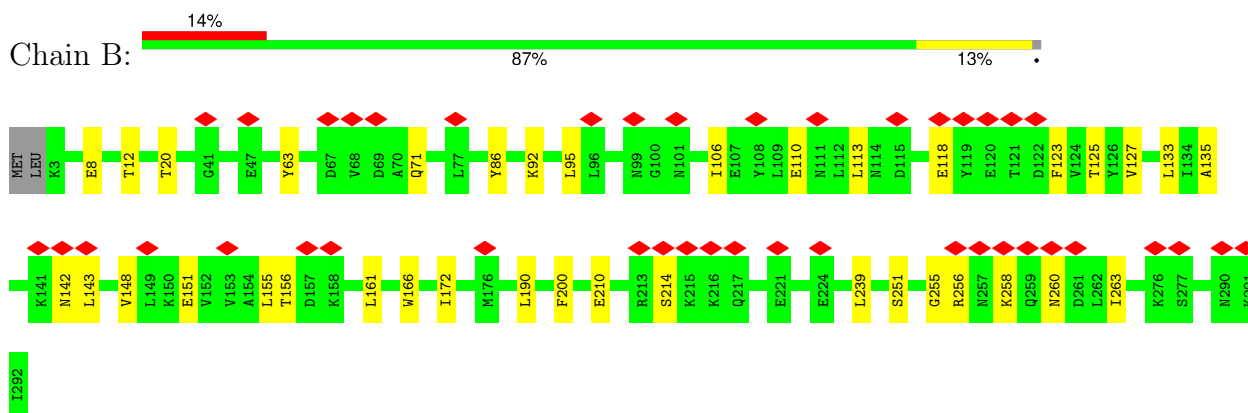
### 3 Residue-property plots [i](#)

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: ER membrane protein complex subunit 1



- Molecule 2: ER membrane protein complex subunit 2



- Molecule 3: ER membrane protein complex subunit 3







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

- Molecule 8: Endoplasmic reticulum membrane protein complex subunit 10

Chain H: 

MET LEU VAL ARG LEU VAL ILE LEU SER PHE VAL MET VAL CYS A18 D28 T40 T43 S44 D45 V50 D57 T70 K73 L74 V94 V102 T138 K139 T140 Y141 A142 ASP LYS LYS ALA SER LYS ASN LYS ASP GLY THR ALA GLN PHE

GLU GLU ASP VAL LYS VAL TRP PHE GLN LYS ASN TRP LYS MET LYS LEU LEU LEU GLY LEU ILE TYR ASN PHE VAL ALA GLY SER ALA LYS LYS GLN GLN GLY GLY ALA ASP GLN LYS THR GLU

- Molecule 9: Fab DH4 heavy chain


Chain I: 

MET A2 Q5 K15 E18 Y35 W36 S37 W38 I39 K45 I53 W62 PRO LEU LYS SER ARG VAL ILE THR SER V73 D74 S86 VAL THR ALA ALA D91 G105 S125 K129 F134 P135 L136 ALA PRO SER LYS SER THR SER GLY THR

ALA ALA G151 D156 S165 W166 ASN SER GLY ALA LEU THR SER GLY VAL H176 L182 G187 L190 V194 T195 VAL PRO SER SER LEU GLY THR THR T207 C208 N209 V210 K213 W216 T217 K218 V219 D220 K221 K222 V223 GLU PRO LYS

SER CYS ALA ALA HIS HIS HIS HIS HIS GLY ALA ALA GLN LYS LEU ILE SER GLU GLU ASP LEU LEU ASN GLY ALA ALA


- Molecule 10: Fab DH4 light chain

Chain J: 

LEU PHE ALA ILE PRO LEU VAL VAL PRO TYR SER HIS SER ALA LEU D17 E48 L54 L67 Y70 R82 F92 R98 Y99 E100 E125 R128 THR VAL ALA P133 T137 E143 G149 LYS LEU SER GLY T149 A150 A164 K165 V166 Q167 W168 K169

V170 D171 M172 A173 L174 Q175 S176 G177 M178 S179 Q180 E185 K189 D190 S191 T192 Y193 S197 T198 L201 S202 K203 A204 D205 Y206 E207 K208 H209 K210 V211 C214 E215 V216 T217 H218 L221 S222 S223 P224 V225 T226 K227 S228 F229 M230 R231 G232 E233 C234

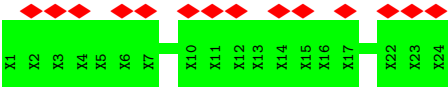
- Molecule 11: Unassigned helix

Chain M: 

X1 X2 X3 X4 X5 X6 X12 X13 X21 UNK UNK UNK

- Molecule 11: Unassigned helix

Chain N: 



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	230528	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 ( $e^-/\text{\AA}^2$ )	67	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	66.122	Depositor
Minimum map value	-33.508	Depositor
Average map value	0.008	Depositor
Map value standard deviation	1.036	Depositor
Recommended contour level	10.4	Depositor
Map size ( $\text{\AA}$ )	409.44, 409.44, 409.44	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	0.853, 0.853, 0.853	Depositor

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: X3P, NAG

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	0.31	0/5769	0.58	2/7838 (0.0%)
2	B	0.28	0/2397	0.50	0/3228
3	C	0.28	0/1556	0.53	0/2112
4	D	0.32	0/529	0.59	0/718
5	E	0.28	0/1051	0.49	0/1421
6	F	0.31	0/804	0.49	0/1094
7	G	0.32	0/1266	0.56	0/1713
8	H	0.31	0/979	0.58	0/1333
9	I	0.29	0/1342	0.56	0/1821
10	J	0.30	0/1644	0.58	0/2230
All	All	0.30	0/17337	0.55	2/23508 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	480	ASP	CB-CG-OD1	6.12	123.81	118.30
1	A	28	ASP	CB-CG-OD1	5.47	123.22	118.30

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	A	5637	0	5595	40	0
2	B	2362	0	2415	28	0
3	C	1522	0	1551	14	0
4	D	515	0	454	4	0
5	E	1028	0	1032	16	0
6	F	780	0	777	4	0
7	G	1235	0	1205	6	0
8	H	965	0	949	6	0
9	I	1309	0	1269	7	0
10	J	1610	0	1556	14	0
11	M	105	0	23	0	0
11	N	120	0	26	0	0
12	A	42	0	39	0	0
12	G	28	0	26	1	0
13	C	35	0	0	0	0
All	All	17293	0	16917	119	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 119 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)
2:B:86:TYR:HB3	2:B:125:THR:HG23	1.69	0.73
1:A:673:ILE:HG21	1:A:710:THR:HG21	1.70	0.71
8:H:70:ILE:HD12	8:H:74:LEU:HD22	1.73	0.71
10:J:206:TYR:OH	10:J:231:ARG:NH2	2.23	0.71
1:A:82:ARG:NH2	1:A:706:ASP:OD2	2.23	0.70

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	680/760 (90%)	652 (96%)	28 (4%)	0	100	100
2	B	288/292 (99%)	287 (100%)	1 (0%)	0	100	100
3	C	180/253 (71%)	178 (99%)	2 (1%)	0	100	100
4	D	64/190 (34%)	56 (88%)	8 (12%)	0	100	100
5	E	125/182 (69%)	123 (98%)	2 (2%)	0	100	100
6	F	93/108 (86%)	93 (100%)	0	0	100	100
7	G	149/234 (64%)	145 (97%)	4 (3%)	0	100	100
8	H	123/205 (60%)	114 (93%)	9 (7%)	0	100	100
9	I	156/254 (61%)	154 (99%)	2 (1%)	0	100	100
10	J	203/234 (87%)	200 (98%)	3 (2%)	0	100	100
All	All	2061/2712 (76%)	2002 (97%)	59 (3%)	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	A	646/707 (91%)	646 (100%)	0	100	100
2	B	262/264 (99%)	260 (99%)	2 (1%)	79	90
3	C	168/217 (77%)	168 (100%)	0	100	100
4	D	44/166 (26%)	44 (100%)	0	100	100
5	E	115/161 (71%)	114 (99%)	1 (1%)	75	89
6	F	83/95 (87%)	83 (100%)	0	100	100
7	G	135/204 (66%)	135 (100%)	0	100	100
8	H	111/178 (62%)	110 (99%)	1 (1%)	75	89
9	I	144/207 (70%)	144 (100%)	0	100	100
10	J	186/206 (90%)	186 (100%)	0	100	100
All	All	1894/2405 (79%)	1890 (100%)	4 (0%)	91	97

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	92	LYS
2	B	258	LYS
5	E	125	LYS
8	H	73	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 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](#)

6 ligands are modelled in this entry.

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	$\# Z  > 2$
12	NAG	A	803	1	14,14,15	0.19	0	17,19,21	0.44	0
12	NAG	G	302	7	14,14,15	0.39	0	17,19,21	0.54	0
12	NAG	A	801	1	14,14,15	0.27	0	17,19,21	0.58	0
12	NAG	A	802	1	14,14,15	0.26	0	17,19,21	0.38	0
13	X3P	C	301	-	34,34,34	1.43	7 (20%)	40,42,42	1.08	2 (5%)
12	NAG	G	301	7	14,14,15	0.38	0	17,19,21	0.37	0



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
12	NAG	A	803	1	-	2/6/23/26	0/1/1/1
12	NAG	G	302	7	-	2/6/23/26	0/1/1/1
12	NAG	A	801	1	-	1/6/23/26	0/1/1/1
12	NAG	A	802	1	-	1/6/23/26	0/1/1/1
13	X3P	C	301	-	-	17/38/38/38	-
12	NAG	G	301	7	-	1/6/23/26	0/1/1/1

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	C	301	X3P	O31-C31	3.42	1.43	1.33
13	C	301	X3P	O21-C21	3.41	1.43	1.34
13	C	301	X3P	O21-C2	-2.30	1.41	1.46
13	C	301	X3P	C12-C11	2.16	1.57	1.51
13	C	301	X3P	P-O11	2.10	1.67	1.59

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	C	301	X3P	O21-C21-C22	4.00	120.14	111.48
13	C	301	X3P	O31-C31-C32	2.34	118.97	111.83

There are no chirality outliers.

5 of 24 torsion outliers are listed below:

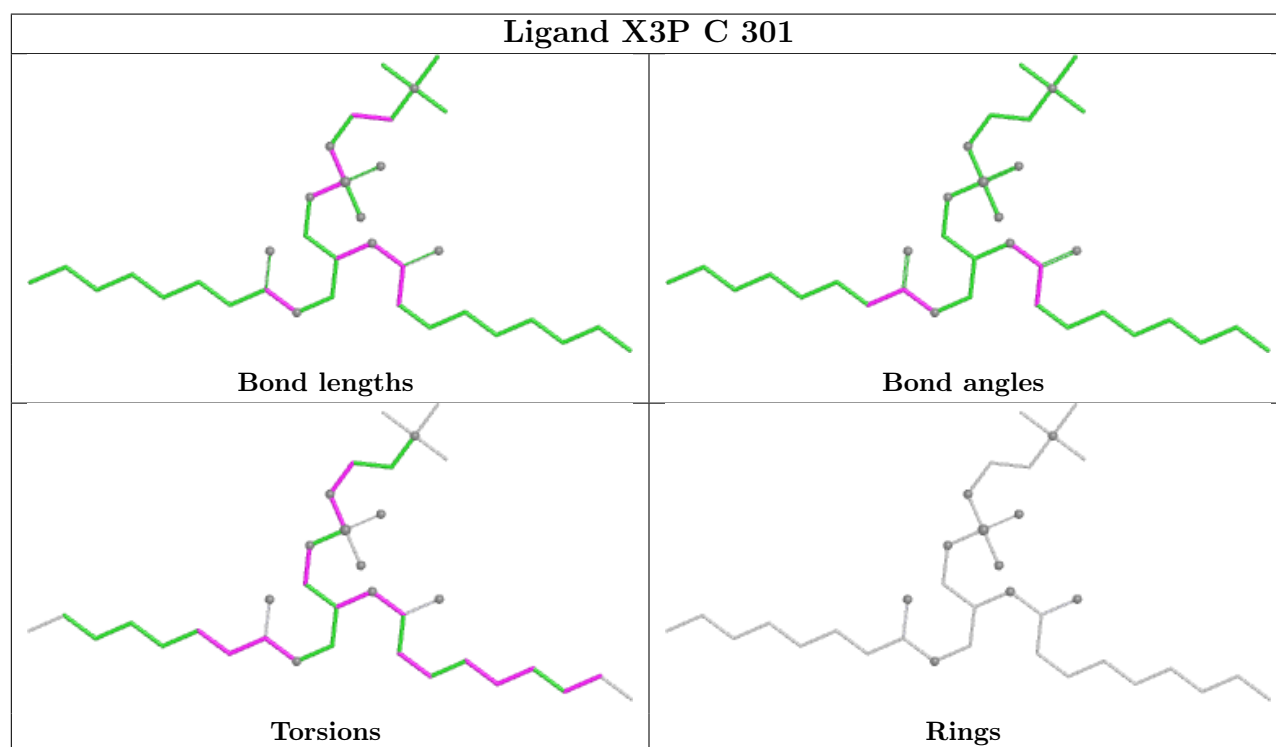
Mol	Chain	Res	Type	Atoms
13	C	301	X3P	C11-O12-P-O11
13	C	301	X3P	O32-C31-O31-C3
13	C	301	X3P	C32-C31-O31-C3
13	C	301	X3P	C31-C32-C33-C34
12	G	302	NAG	O5-C5-C6-O6

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	G	302	NAG	1	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 ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

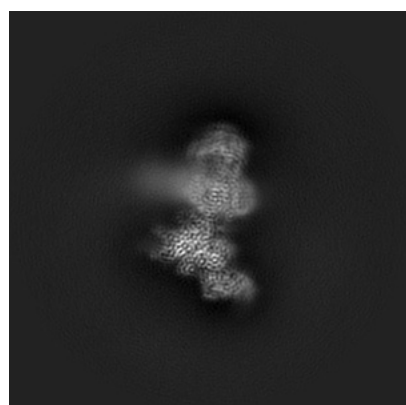
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-23003. These allow visual inspection of the internal detail of the map and identification of artifacts.

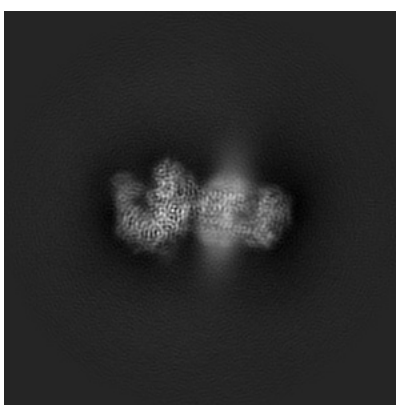
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

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

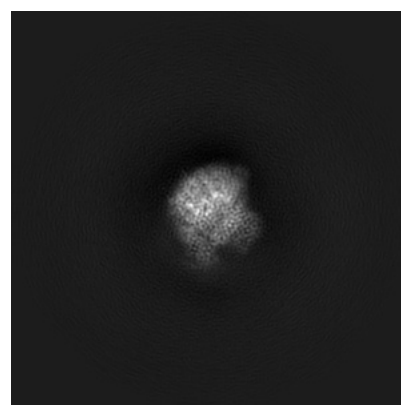
#### 6.1.1 Primary map



X



Y

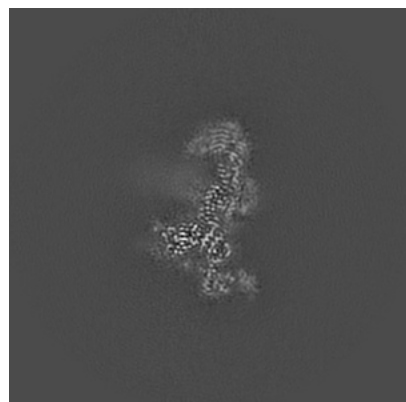


Z

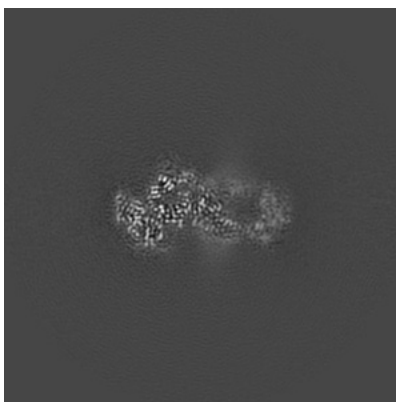
The images above show the map projected in three orthogonal directions.

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

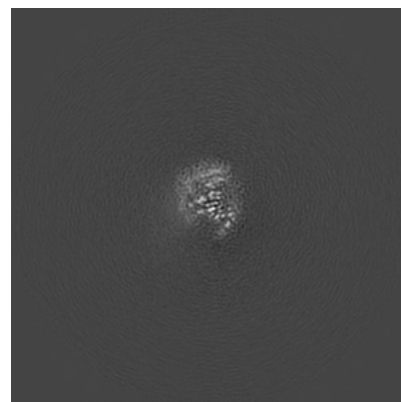
#### 6.2.1 Primary map



X Index: 240



Y Index: 240

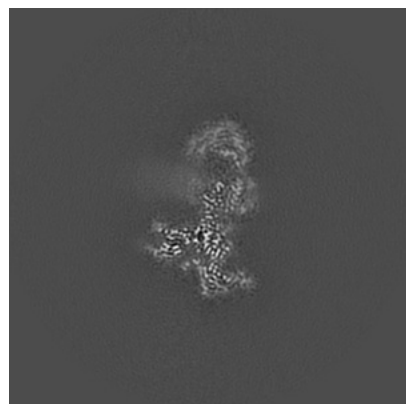


Z Index: 240

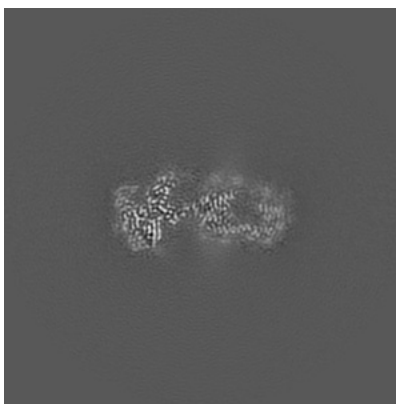
The images above show central slices of the map in three orthogonal directions.

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

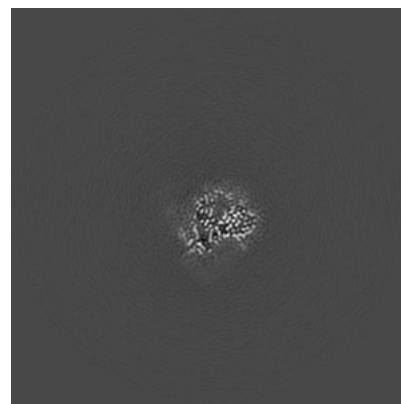
### 6.3.1 Primary map



X Index: 235



Y Index: 247



Z Index: 201

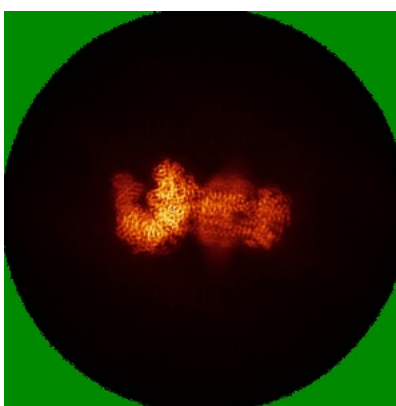
The images above show the largest variance slices of the map in three orthogonal directions.

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

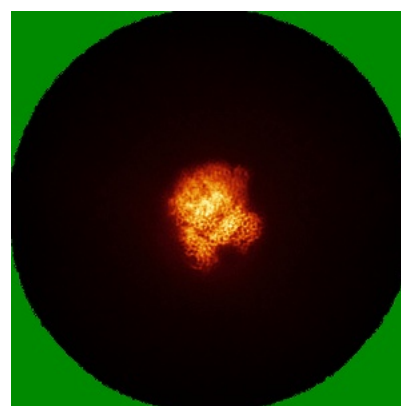
### 6.4.1 Primary map



X



Y

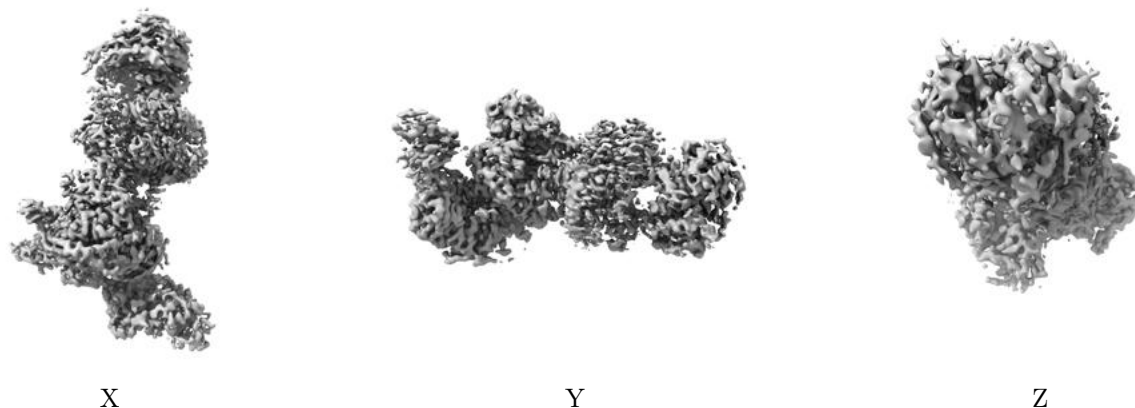


Z

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

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

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 10.4. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

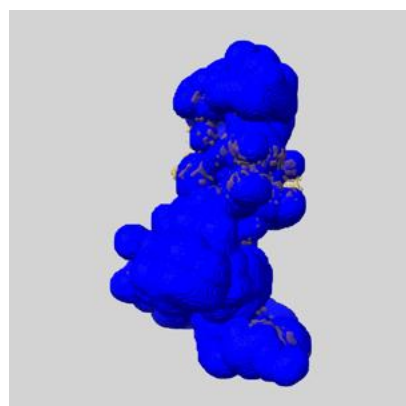
## 6.6 Mask visualisation [i](#)

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

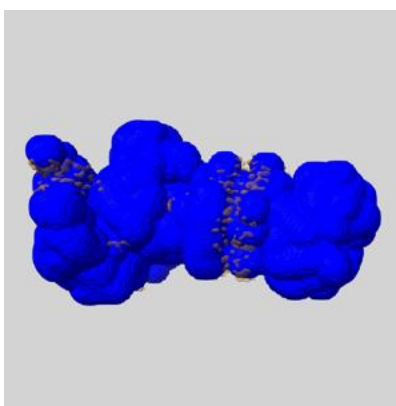
A mask typically either:

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

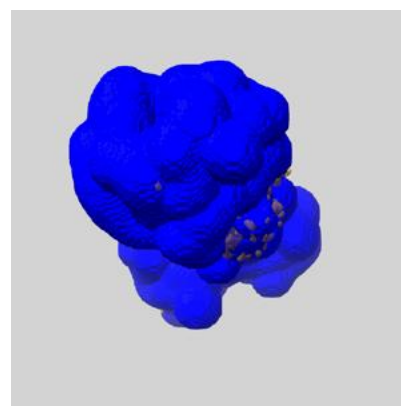
### 6.6.1 emd\_23003\_msk\_1.map [i](#)



X



Y

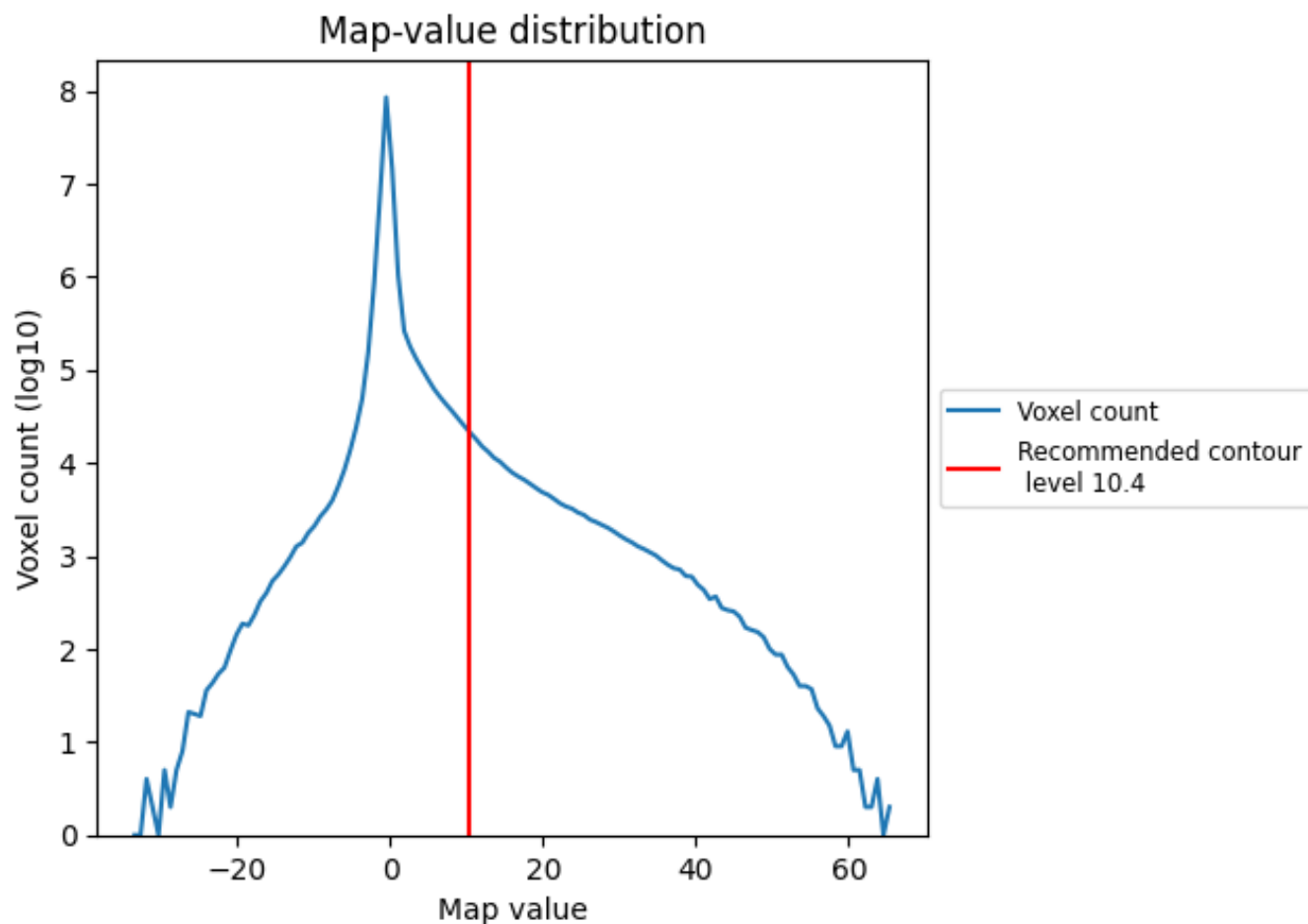


Z

## 7 Map analysis [i](#)

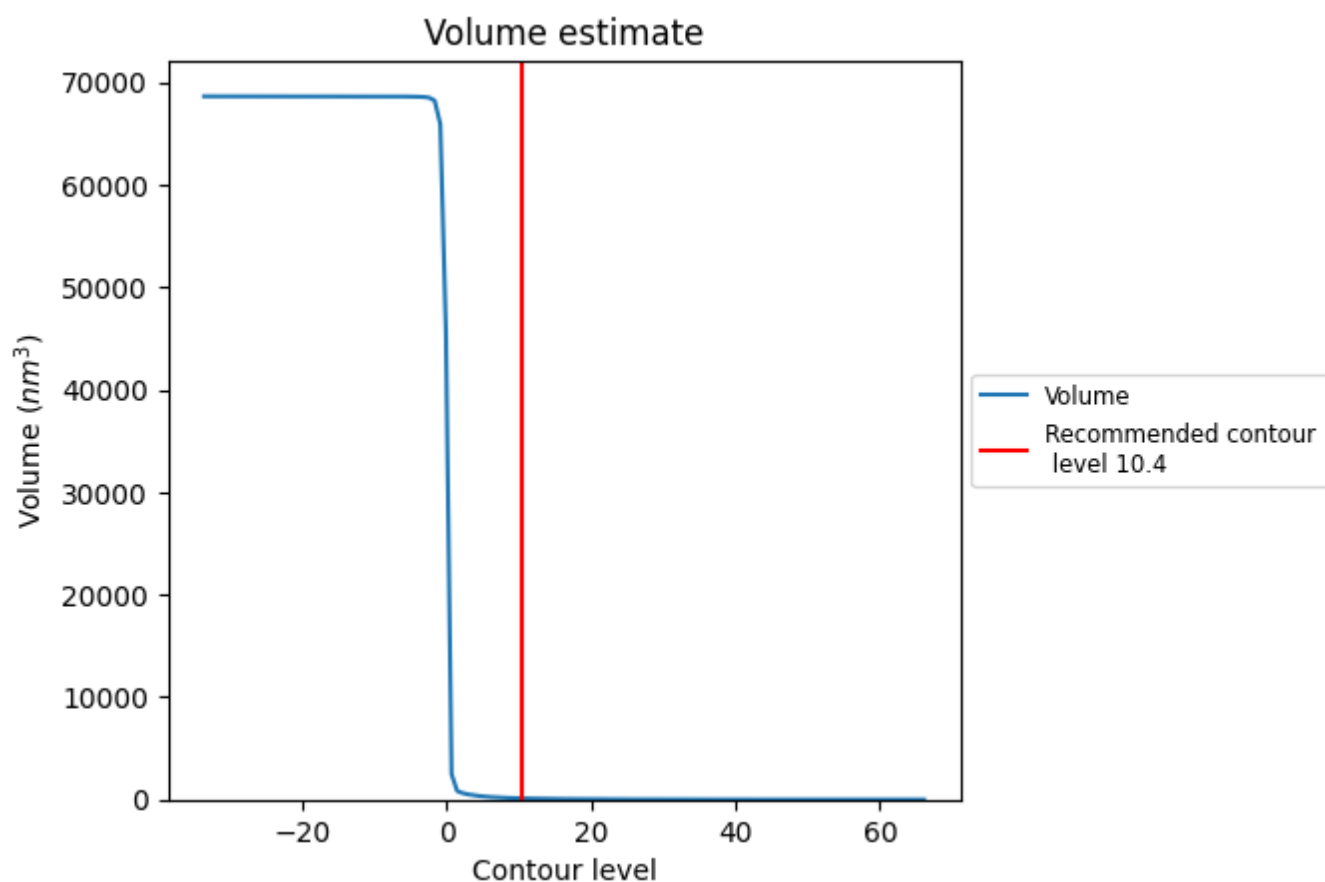
This section contains the results of statistical analysis of the map.

### 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](#)

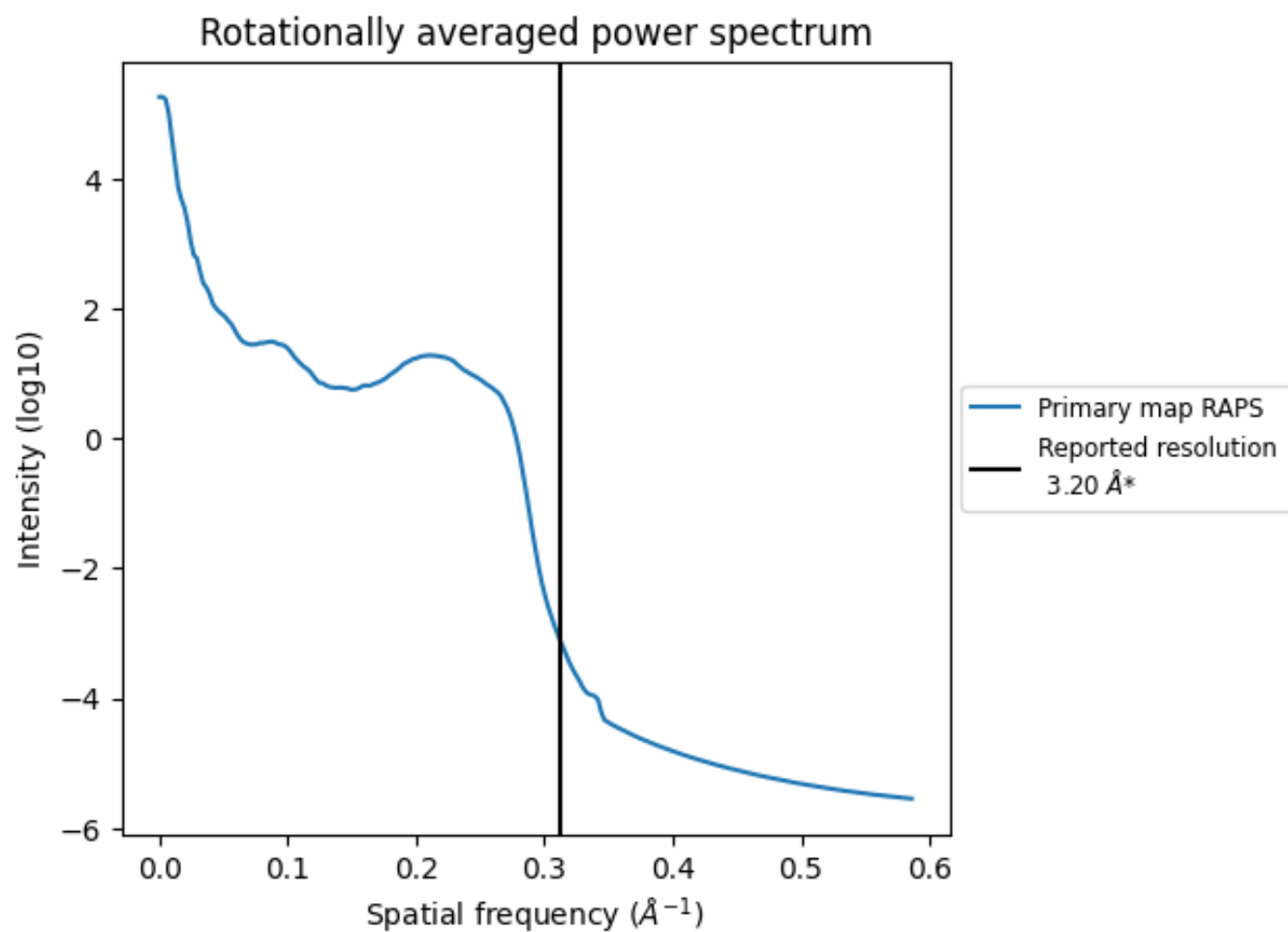


The volume at the recommended contour level is 118  $\text{nm}^3$ ; this corresponds to an approximate mass of 106 kDa.

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 ⓘ

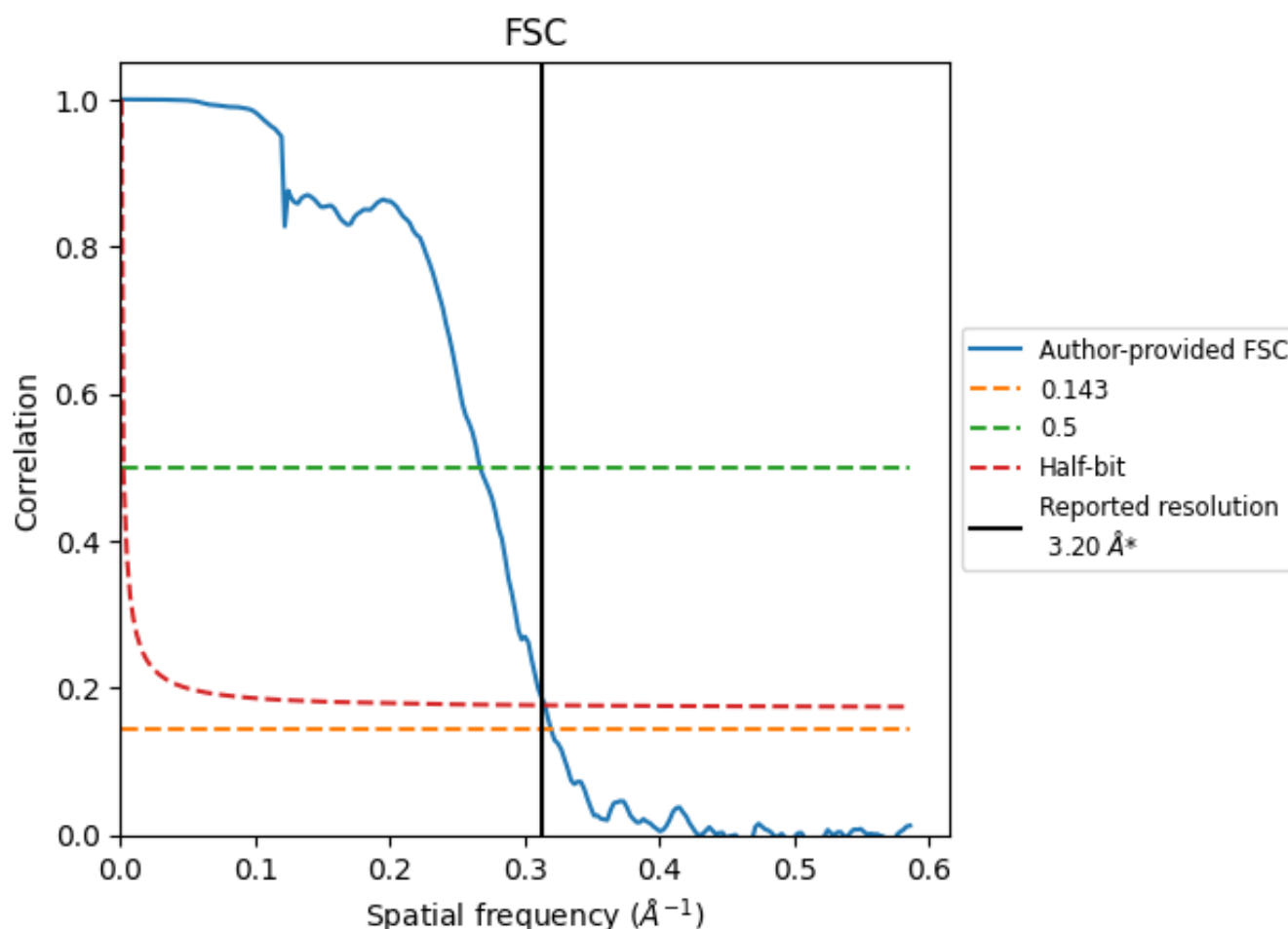


\*Reported resolution corresponds to spatial frequency of 0.312 Å<sup>-1</sup>

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

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

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of 0.312 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

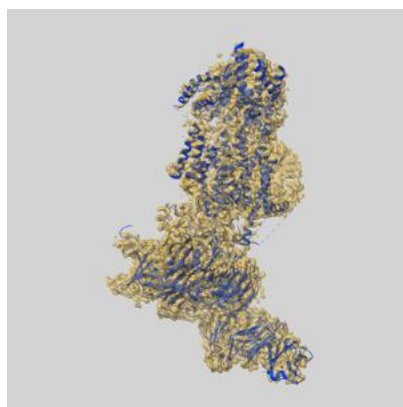
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.20	-	-
Author-provided FSC curve	3.13	3.74	3.17
Unmasked-calculated*	-	-	-

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

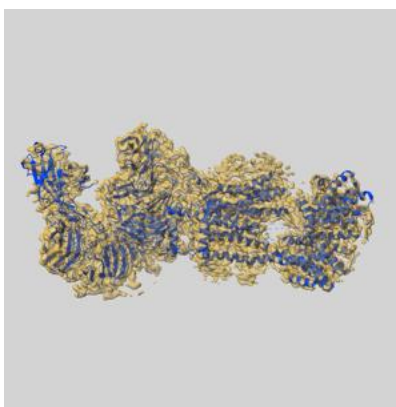
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-23003 and PDB model 7KRA. Per-residue inclusion information can be found in [section 3](#) on [page 8](#).

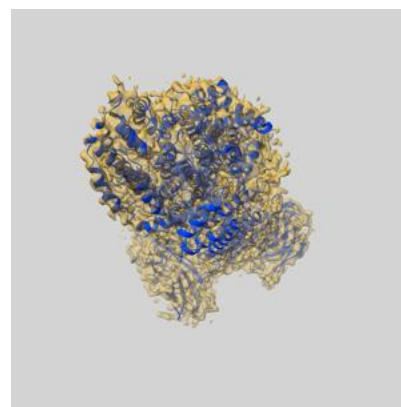
### 9.1 Map-model overlay [i](#)



X



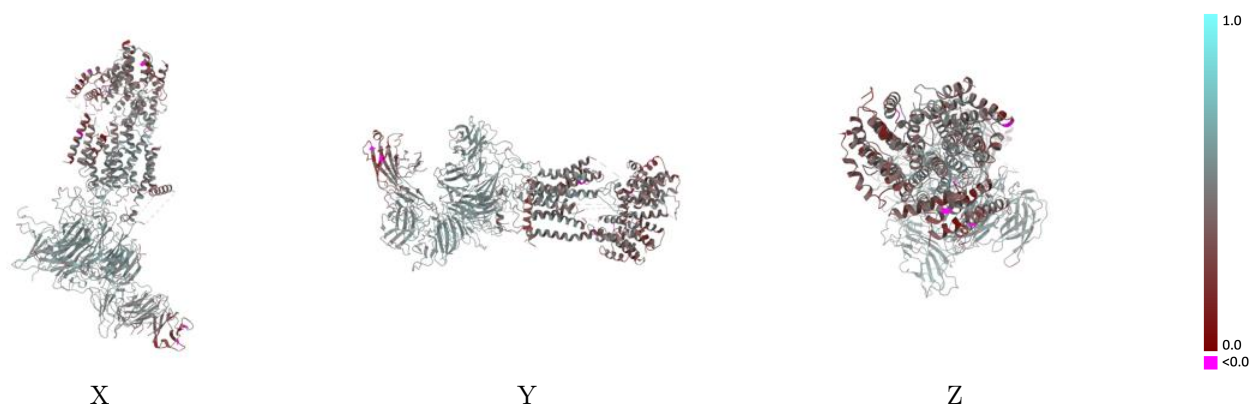
Y



Z

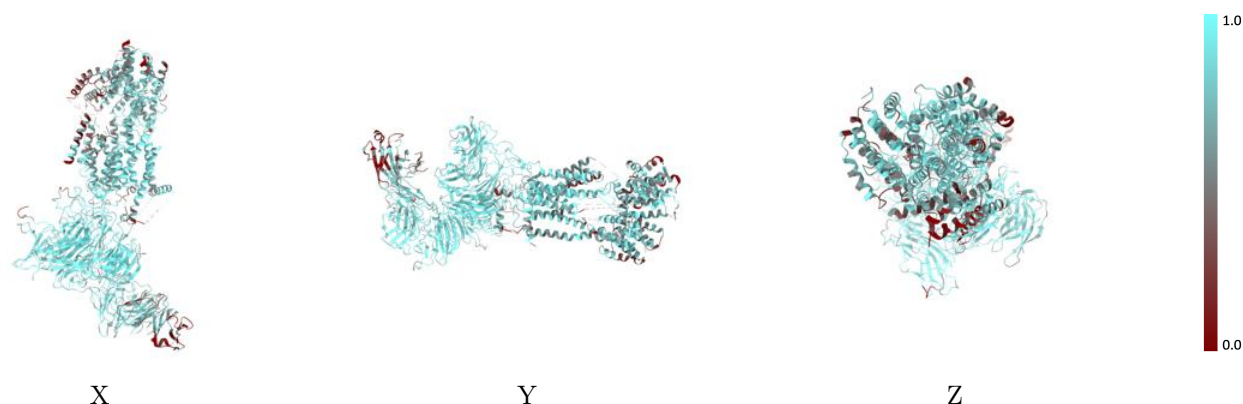
The images above show the 3D surface view of the map at the recommended contour level 10.4 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



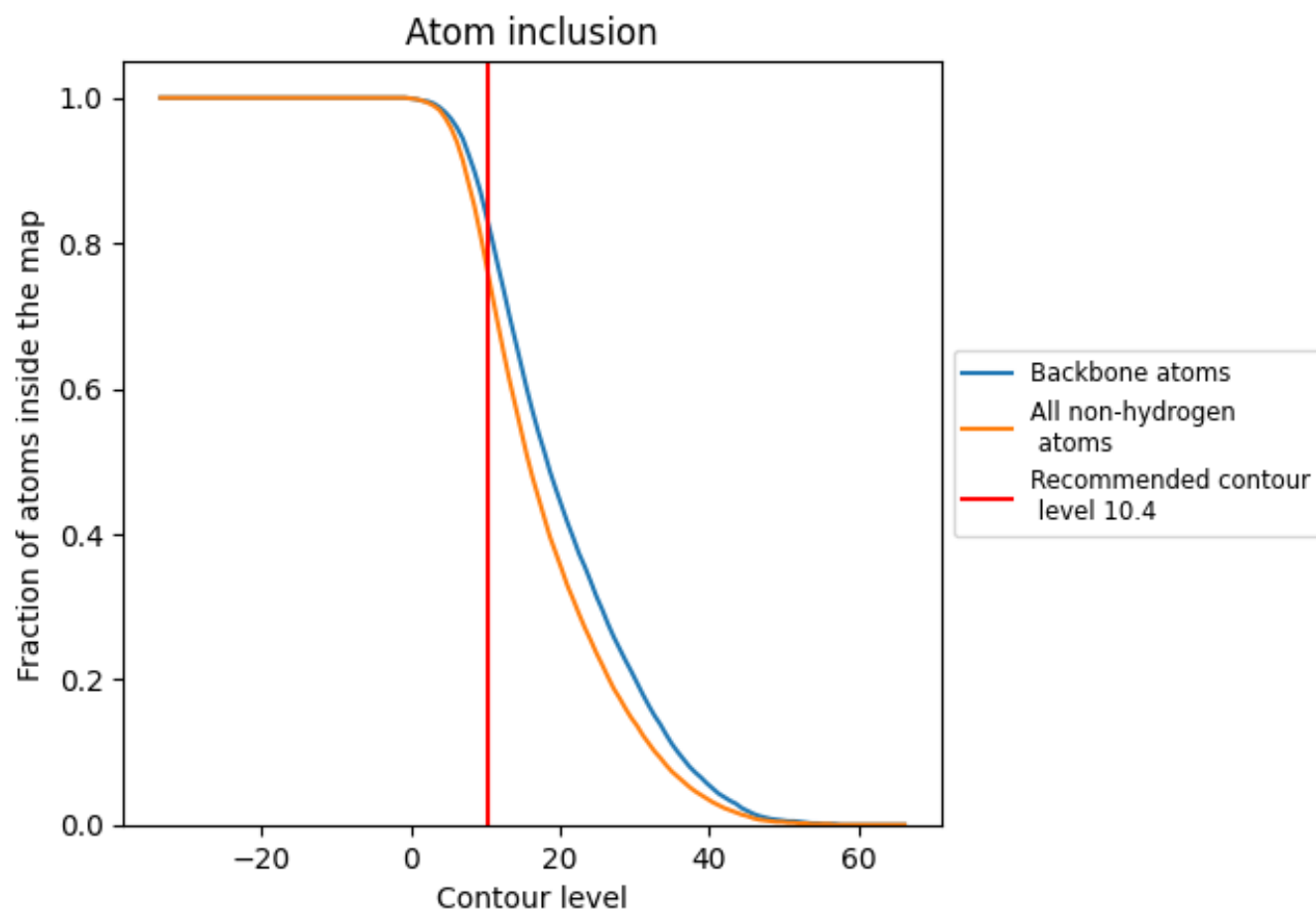
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (10.4).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 83% of all backbone atoms, 76% 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 (10.4) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.7550	<div></div> 0.4740
A	<div></div> 0.8420	<div></div> 0.5150
B	<div></div> 0.6580	<div></div> 0.4010
C	<div></div> 0.6200	<div></div> 0.4280
D	<div></div> 0.7700	<div></div> 0.4710
E	<div></div> 0.7410	<div></div> 0.4440
F	<div></div> 0.8530	<div></div> 0.5110
G	<div></div> 0.8640	<div></div> 0.5350
H	<div></div> 0.7900	<div></div> 0.5050
I	<div></div> 0.7460	<div></div> 0.4890
J	<div></div> 0.6140	<div></div> 0.4250
M	<div></div> 0.6380	<div></div> 0.3250
N	<div></div> 0.3920	<div></div> 0.2980

1.0

0.0

<0.0