



## Full wwPDB EM Validation Report ⓘ

Nov 21, 2022 – 11:58 PM JST

PDB ID : 7DSD  
EMDB ID : EMD-30831  
Title : CALHM1 close state with disordered CTH  
Authors : Ren, Y.; Yang, X.; Shen, Y.Q.  
Deposited on : 2020-12-30  
Resolution : 2.90 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev43  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
MolProbity : 4.02b-467  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.9  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.31.3

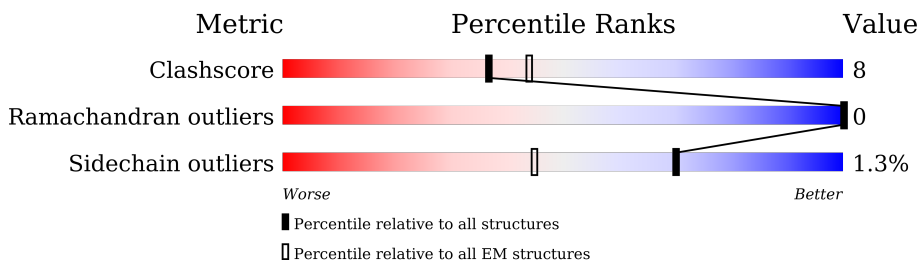
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 2.90 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	346	
1	B	346	
1	C	346	
1	D	346	
1	E	346	
1	F	346	
1	G	346	

## 2 Entry composition [i](#)

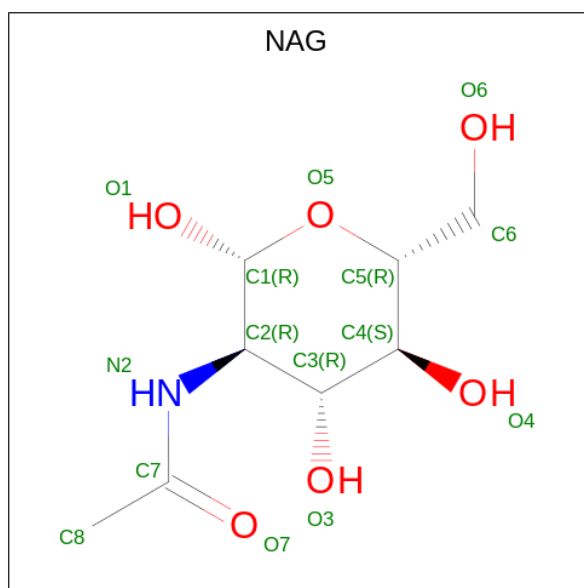
There are 2 unique types of molecules in this entry. The entry contains 10542 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Calcium homeostasis modulator 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	193	Total	C	N	O	S	0	0
			1492	974	241	264	13		
1	B	193	Total	C	N	O	S	0	0
			1492	974	241	264	13		
1	C	193	Total	C	N	O	S	0	0
			1492	974	241	264	13		
1	D	193	Total	C	N	O	S	0	0
			1492	974	241	264	13		
1	E	193	Total	C	N	O	S	0	0
			1492	974	241	264	13		
1	F	193	Total	C	N	O	S	0	0
			1492	974	241	264	13		
1	G	193	Total	C	N	O	S	0	0
			1492	974	241	264	13		

- Molecule 2 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).

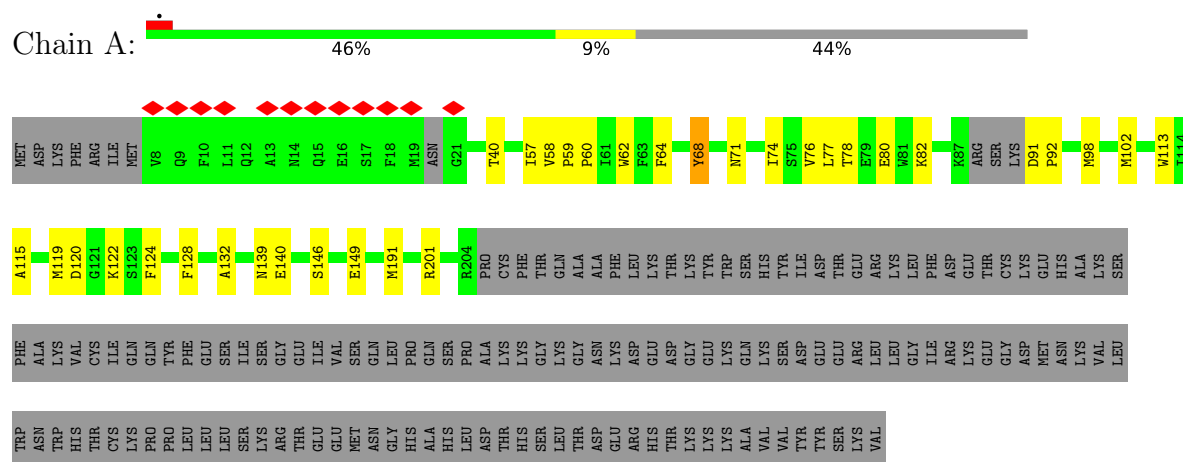


Mol	Chain	Residues	Atoms				AltConf
2	A	1	Total 14	C 8	N 1	O 5	0
2	B	1	Total 14	C 8	N 1	O 5	0
2	C	1	Total 14	C 8	N 1	O 5	0
2	D	1	Total 14	C 8	N 1	O 5	0
2	E	1	Total 14	C 8	N 1	O 5	0
2	F	1	Total 14	C 8	N 1	O 5	0
2	G	1	Total 14	C 8	N 1	O 5	0

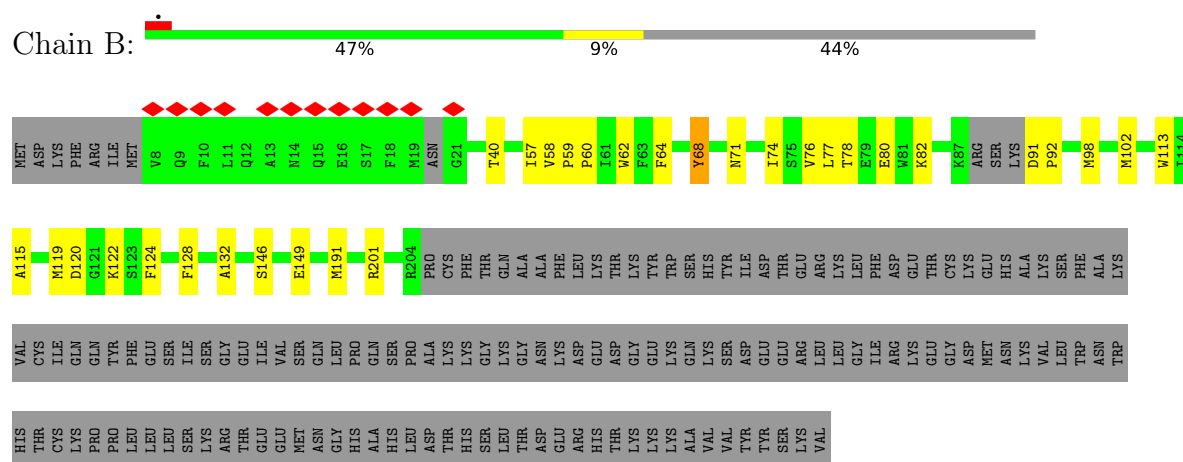
### 3 Residue-property plots

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.

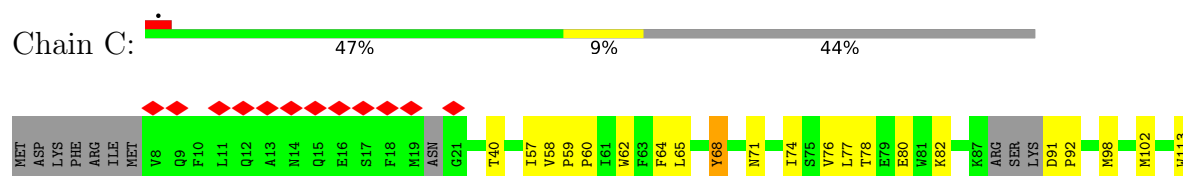
#### • Molecule 1: Calcium homeostasis modulator 1



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PHE	TRP	ALA	ASP	ASN	TRP	VAL	LYS	THR	ARG	CYS	THR	ILE	GLN	LYS	GLN	TYR	PHE	LEU	GLU	LEU	SER	ILE	SER	GLY	THR	ILE	GLU	VAL	SER	GLN	LEU	PRO	ALA	GLN	ASN	GLY	LEU	PRO	HIS	LEU	ASP	ALA	PRO	LEU	LYS	THR	LYS	GLY	LYS	THR	GLY	LYS	THR	GLY	ASN	GLY	ASP	ASN	LYS	GLU	ASP	ARG	HIS	THR	ASP	LYS	GLY	GLU	LYS	VAL	ALA	GLN	LYS	VAL	TYR	SER	GLU	ARG	LEU	LEU	LEU	GLY	ILE	TYL	ARG	LYS	GLY	GLY	ASP	MET	ASN	LYS	VAL	LEU
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

● Molecule 1: Calcium homeostasis modulator 1



ASN	TRP	HIS	THR	CYS	LYS	PRO	PRO	LEU	LEU	LEU	SER	LYS	ARG	THR	THR	GLU	GLU	VAL	MET	ASN	GLY	HIS	ALA	HIS	LEU	THR	HIS	LYS	THR	GLY	ASN	GLU	ARG	HIS	LYS	GLY	LYS	VAL	VAL	TYR	ASP	GLU	GLU	ARG	LEU	LEU	GLY	ILE	ARG	LYS	GLU	GLY	ASP	LYS	ASN	LYS	VAL	LEU	TRP	PHE			
ALA	LYS	VAL	CYS	ILE	GLN	GLN	TYR	PHE	GLU	SER	ILE	SER	GLY	GLU	ILE	VAL	SER	GLN	LEU	PRO	GLN	PRO	ALA	LYS	PHE	THR	GLN	ALA	ALA	PHE	LEU	LYS	THR	LYS	TYR	TRP	SER	HIS	TYR	ILE	ASP	THR	GLU	ARG	LEU	LEU	GLY	ILE	ARG	LYS	GLU	THR	CYS	LYS	ASP	MET	ASN	LYS	VAL	LEU	TRP	PHE	
I114	A115			M119	D120	G121	K122	S123	F124		M139	E140		S146	E149		M191		T194		R201		R204	PRO	CYS	PHE	THR	GLN	ALA	ALA	ALA	PHE	LEU	LYS	THR	TYR	TRP	SER	HIS	TYR	ILE	ASP	THR	GLU	ARG	LEU	LEU	GLY	ILE	ARG	LYS	GLU	THR	CYS	LYS	ASP	MET	ASN	LYS	VAL	LEU	TRP	PHE
MET	ASP	LYS	PHE	ARG	ILE	MET		V8	Q9	F10	L11	Q12	A13	N14	Q15	E16	S17	F18	M19	ASN	ASN	G21		T40		I57	V58	P59	P60	I61	W62	F63	F64	Y68		N71		I74	S75	V76	L77	T78	E79	E80	W81	K82		K87	ARG	SER	LYS		D91	P92		M98		M102	T103		W113		

## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	56801	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	50	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	1.390	Depositor
Minimum map value	-0.580	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	0.045	Depositor
Recommended contour level	0.154	Depositor
Map size ( $\text{\AA}$ )	263.64, 263.64, 263.64	wwPDB
Map dimensions	260, 260, 260	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	1.014, 1.014, 1.014	Depositor



## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.28	0/1526	0.41	0/2072
1	B	0.28	0/1526	0.41	0/2072
1	C	0.28	0/1526	0.41	0/2072
1	D	0.28	0/1526	0.41	0/2072
1	E	0.29	0/1526	0.41	0/2072
1	F	0.28	0/1526	0.41	0/2072
1	G	0.28	0/1526	0.41	0/2072
All	All	0.28	0/10682	0.41	0/14504

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	A	1492	0	1467	28	0
1	B	1492	0	1467	26	0
1	C	1492	0	1467	27	0
1	D	1492	0	1467	25	0
1	E	1492	0	1467	26	0
1	F	1492	0	1467	27	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	G	1492	0	1467	29	0
2	A	14	0	13	0	0
2	B	14	0	13	0	0
2	C	14	0	13	0	0
2	D	14	0	13	0	0
2	E	14	0	13	0	0
2	F	14	0	13	0	0
2	G	14	0	13	0	0
All	All	10542	0	10360	173	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 8.

All (173) 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:C:91:ASP:HB3	1:C:92:PRO:CD	1.83	1.09
1:B:91:ASP:HB3	1:B:92:PRO:CD	1.83	1.09
1:D:91:ASP:HB3	1:D:92:PRO:CD	1.83	1.09
1:E:91:ASP:HB3	1:E:92:PRO:CD	1.82	1.08
1:A:91:ASP:HB3	1:A:92:PRO:CD	1.83	1.08
1:F:91:ASP:HB3	1:F:92:PRO:CD	1.83	1.07
1:G:91:ASP:HB3	1:G:92:PRO:CD	1.82	1.06
1:C:91:ASP:HB3	1:C:92:PRO:HD2	1.01	1.01
1:D:91:ASP:HB3	1:D:92:PRO:HD2	1.01	1.01
1:A:91:ASP:HB3	1:A:92:PRO:HD2	1.01	1.00
1:B:91:ASP:HB3	1:B:92:PRO:HD2	1.01	1.00
1:E:91:ASP:CB	1:E:92:PRO:HD2	1.91	1.00
1:D:91:ASP:CB	1:D:92:PRO:HD2	1.92	1.00
1:F:91:ASP:CB	1:F:92:PRO:HD2	1.92	1.00
1:C:91:ASP:CB	1:C:92:PRO:HD2	1.92	0.99
1:G:91:ASP:HB3	1:G:92:PRO:HD2	1.01	0.99
1:G:91:ASP:CB	1:G:92:PRO:HD2	1.91	0.99
1:E:91:ASP:HB3	1:E:92:PRO:HD2	1.01	0.99
1:B:91:ASP:CB	1:B:92:PRO:HD2	1.92	0.99
1:A:91:ASP:CB	1:A:92:PRO:HD2	1.92	0.98
1:F:91:ASP:HB3	1:F:92:PRO:HD2	1.01	0.98
1:A:74:ILE:HD11	1:G:201:ARG:HB3	1.67	0.76
1:A:201:ARG:HB3	1:B:74:ILE:HD11	1.68	0.76
1:D:40:THR:HG23	1:D:40:THR:O	1.86	0.75
1:F:201:ARG:HB3	1:G:74:ILE:HD11	1.68	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:40:THR:HG23	1:G:40:THR:O	1.86	0.75
1:B:201:ARG:HB3	1:C:74:ILE:HD11	1.68	0.74
1:F:40:THR:O	1:F:40:THR:HG23	1.86	0.74
1:E:40:THR:O	1:E:40:THR:HG23	1.86	0.74
1:C:40:THR:HG23	1:C:40:THR:O	1.86	0.74
1:D:201:ARG:HB3	1:E:74:ILE:HD11	1.68	0.74
1:E:201:ARG:HB3	1:F:74:ILE:HD11	1.69	0.73
1:A:40:THR:O	1:A:40:THR:HG23	1.86	0.73
1:B:40:THR:O	1:B:40:THR:HG23	1.86	0.73
1:C:201:ARG:HB3	1:D:74:ILE:HD11	1.69	0.72
1:G:64:PHE:CZ	1:G:68:TYR:HE1	2.13	0.67
1:B:64:PHE:CZ	1:B:68:TYR:HE1	2.13	0.67
1:C:64:PHE:CZ	1:C:68:TYR:HE1	2.13	0.67
1:A:64:PHE:CZ	1:A:68:TYR:HE1	2.13	0.66
1:F:64:PHE:CZ	1:F:68:TYR:HE1	2.13	0.66
1:D:64:PHE:CZ	1:D:68:TYR:HE1	2.13	0.66
1:E:64:PHE:CZ	1:E:68:TYR:HE1	2.13	0.66
1:A:71:ASN:HD22	1:A:102:MET:HG3	1.63	0.64
1:E:71:ASN:HD22	1:E:102:MET:HG3	1.63	0.63
1:F:71:ASN:HD22	1:F:102:MET:HG3	1.63	0.63
1:C:71:ASN:HD22	1:C:102:MET:HG3	1.63	0.63
1:G:71:ASN:HD22	1:G:102:MET:HG3	1.63	0.63
1:B:71:ASN:HD22	1:B:102:MET:HG3	1.64	0.62
1:D:71:ASN:HD22	1:D:102:MET:HG3	1.64	0.62
1:G:64:PHE:CE1	1:G:68:TYR:HE1	2.21	0.59
1:A:64:PHE:CE1	1:A:68:TYR:HE1	2.21	0.58
1:E:64:PHE:CE1	1:E:68:TYR:HE1	2.21	0.58
1:C:64:PHE:CE1	1:C:68:TYR:HE1	2.21	0.58
1:B:191:MET:SD	1:C:62:TRP:HB2	2.44	0.58
1:A:191:MET:SD	1:B:62:TRP:HB2	2.44	0.58
1:F:64:PHE:CE1	1:F:68:TYR:HE1	2.21	0.58
1:B:64:PHE:CE1	1:B:68:TYR:HE1	2.21	0.58
1:D:64:PHE:CE1	1:D:68:TYR:HE1	2.21	0.58
1:D:191:MET:SD	1:E:62:TRP:HB2	2.44	0.58
1:C:191:MET:SD	1:D:62:TRP:HB2	2.44	0.57
1:A:62:TRP:HB2	1:G:191:MET:SD	2.44	0.56
1:F:191:MET:SD	1:G:62:TRP:HB2	2.44	0.56
1:E:191:MET:SD	1:F:62:TRP:HB2	2.45	0.56
1:D:64:PHE:CE1	1:D:68:TYR:CE1	2.94	0.56
1:B:91:ASP:CB	1:B:92:PRO:CD	2.62	0.56
1:A:64:PHE:CE1	1:A:68:TYR:CE1	2.94	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:64:PHE:CE1	1:C:68:TYR:CE1	2.94	0.56
1:E:68:TYR:HH	1:E:103:THR:HG1	1.52	0.56
1:G:64:PHE:CE1	1:G:68:TYR:CE1	2.94	0.56
1:F:64:PHE:CE1	1:F:68:TYR:CE1	2.94	0.55
1:E:64:PHE:CE1	1:E:68:TYR:CE1	2.94	0.55
1:B:64:PHE:CE1	1:B:68:TYR:CE1	2.94	0.55
1:G:68:TYR:HH	1:G:103:THR:HG1	1.52	0.55
1:E:120:ASP:OD2	1:E:122:LYS:NZ	2.36	0.55
1:F:120:ASP:OD2	1:F:122:LYS:NZ	2.36	0.54
1:A:40:THR:O	1:A:40:THR:CG2	2.55	0.54
1:D:120:ASP:OD2	1:D:122:LYS:NZ	2.36	0.54
1:B:120:ASP:OD2	1:B:122:LYS:NZ	2.36	0.54
1:A:120:ASP:OD2	1:A:122:LYS:NZ	2.36	0.53
1:F:40:THR:O	1:F:40:THR:CG2	2.56	0.53
1:G:120:ASP:OD2	1:G:122:LYS:NZ	2.36	0.53
1:D:40:THR:O	1:D:40:THR:CG2	2.56	0.53
1:C:40:THR:O	1:C:40:THR:CG2	2.56	0.53
1:A:91:ASP:CB	1:A:92:PRO:CD	2.62	0.52
1:E:40:THR:O	1:E:40:THR:CG2	2.55	0.51
1:D:91:ASP:CB	1:D:92:PRO:CD	2.62	0.51
1:G:40:THR:O	1:G:40:THR:CG2	2.55	0.51
1:C:91:ASP:CB	1:C:92:PRO:CD	2.62	0.51
1:C:120:ASP:OD2	1:C:122:LYS:NZ	2.36	0.51
1:B:40:THR:O	1:B:40:THR:CG2	2.55	0.50
1:E:91:ASP:CB	1:E:92:PRO:CD	2.62	0.49
1:A:60:PRO:HD3	1:A:113:TRP:CD1	2.48	0.49
1:B:60:PRO:HD3	1:B:113:TRP:CD1	2.48	0.49
1:F:91:ASP:CB	1:F:92:PRO:CD	2.62	0.49
1:A:146:SER:HB2	1:A:149:GLU:HG2	1.96	0.48
1:B:146:SER:HB2	1:B:149:GLU:HG2	1.96	0.48
1:G:60:PRO:HD3	1:G:113:TRP:CD1	2.48	0.48
1:G:91:ASP:CB	1:G:92:PRO:CD	2.62	0.48
1:F:60:PRO:HD3	1:F:113:TRP:CD1	2.48	0.48
1:G:146:SER:HB2	1:G:149:GLU:HG2	1.96	0.48
1:C:60:PRO:HD3	1:C:113:TRP:CD1	2.48	0.48
1:C:146:SER:HB2	1:C:149:GLU:HG2	1.96	0.48
1:D:60:PRO:HD3	1:D:113:TRP:CD1	2.48	0.48
1:D:146:SER:HB2	1:D:149:GLU:HG2	1.96	0.48
1:E:146:SER:HB2	1:E:149:GLU:HG2	1.96	0.47
1:E:60:PRO:HD3	1:E:113:TRP:CD1	2.48	0.47
1:F:146:SER:HB2	1:F:149:GLU:HG2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:115:ALA:O	1:D:119:MET:HG2	2.15	0.47
1:C:115:ALA:O	1:C:119:MET:HG2	2.15	0.46
1:A:115:ALA:O	1:A:119:MET:HG2	2.15	0.46
1:E:115:ALA:O	1:E:119:MET:HG2	2.15	0.46
1:G:115:ALA:O	1:G:119:MET:HG2	2.15	0.46
1:E:64:PHE:CZ	1:E:68:TYR:CE1	3.00	0.45
1:F:115:ALA:O	1:F:119:MET:HG2	2.15	0.45
1:B:115:ALA:O	1:B:119:MET:HG2	2.15	0.45
1:A:64:PHE:CZ	1:A:68:TYR:CE1	3.00	0.45
1:A:58:VAL:HB	1:A:59:PRO:HD3	1.99	0.45
1:B:64:PHE:CZ	1:B:68:TYR:CE1	3.00	0.45
1:G:71:ASN:ND2	1:G:102:MET:HG3	2.31	0.45
1:G:58:VAL:HB	1:G:59:PRO:HD3	1.99	0.44
1:F:58:VAL:HB	1:F:59:PRO:HD3	1.99	0.44
1:B:58:VAL:HB	1:B:59:PRO:HD3	1.99	0.44
1:E:58:VAL:HB	1:E:59:PRO:HD3	1.99	0.44
1:F:76:VAL:O	1:F:80:GLU:HG2	2.18	0.44
1:B:76:VAL:O	1:B:80:GLU:HG2	2.18	0.44
1:E:76:VAL:O	1:E:80:GLU:HG2	2.18	0.43
1:E:71:ASN:ND2	1:E:102:MET:HG3	2.31	0.43
1:F:71:ASN:ND2	1:F:102:MET:HG3	2.31	0.43
1:D:58:VAL:HB	1:D:59:PRO:HD3	1.99	0.43
1:G:76:VAL:O	1:G:80:GLU:HG2	2.18	0.43
1:A:76:VAL:O	1:A:80:GLU:HG2	2.18	0.43
1:D:76:VAL:O	1:D:80:GLU:HG2	2.18	0.43
1:E:77:LEU:HD21	1:E:98:MET:HG3	2.01	0.43
1:F:77:LEU:HD21	1:F:98:MET:HG3	2.01	0.43
1:G:64:PHE:CZ	1:G:68:TYR:CE1	3.00	0.43
1:A:71:ASN:ND2	1:A:102:MET:HG3	2.31	0.43
1:C:58:VAL:HB	1:C:59:PRO:HD3	1.99	0.43
1:C:64:PHE:CZ	1:C:68:TYR:CE1	3.00	0.43
1:C:76:VAL:O	1:C:80:GLU:HG2	2.18	0.43
1:D:77:LEU:HD21	1:D:98:MET:HG3	2.01	0.43
1:G:77:LEU:HD21	1:G:98:MET:HG3	2.01	0.43
1:C:77:LEU:HD21	1:C:98:MET:HG3	2.01	0.43
1:B:57:ILE:O	1:B:60:PRO:HG2	2.19	0.42
1:A:57:ILE:O	1:A:60:PRO:HG2	2.20	0.42
1:B:77:LEU:HD21	1:B:98:MET:HG3	2.01	0.42
1:A:77:LEU:HD21	1:A:98:MET:HG3	2.01	0.42
1:E:57:ILE:O	1:E:60:PRO:HG2	2.19	0.42
1:G:57:ILE:O	1:G:60:PRO:HG2	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:57:ILE:O	1:F:60:PRO:HG2	2.19	0.42
1:A:62:TRP:NE1	1:G:194:THR:OG1	2.50	0.42
1:D:57:ILE:O	1:D:60:PRO:HG2	2.20	0.42
1:B:71:ASN:ND2	1:B:102:MET:HG3	2.31	0.42
1:C:78:THR:O	1:C:82:LYS:HB2	2.20	0.42
1:D:71:ASN:ND2	1:D:102:MET:HG3	2.31	0.42
1:B:78:THR:O	1:B:82:LYS:HB2	2.20	0.41
1:D:78:THR:O	1:D:82:LYS:HB2	2.20	0.41
1:E:78:THR:O	1:E:82:LYS:HB2	2.20	0.41
1:F:78:THR:O	1:F:82:LYS:HB2	2.20	0.41
1:C:71:ASN:ND2	1:C:102:MET:HG3	2.31	0.41
1:G:57:ILE:HD13	1:G:57:ILE:HA	1.94	0.41
1:C:57:ILE:O	1:C:60:PRO:HG2	2.19	0.41
1:G:139:ASN:OD1	1:G:140:GLU:N	2.54	0.41
1:G:78:THR:O	1:G:82:LYS:HB2	2.20	0.41
1:A:78:THR:O	1:A:82:LYS:HB2	2.20	0.41
1:F:139:ASN:OD1	1:F:140:GLU:N	2.54	0.41
1:C:65:LEU:HD23	1:C:65:LEU:HA	1.95	0.40
1:C:128:PHE:O	1:C:132:ALA:HB2	2.22	0.40
1:A:139:ASN:OD1	1:A:140:GLU:N	2.54	0.40
1:F:128:PHE:O	1:F:132:ALA:HB2	2.22	0.40
1:A:128:PHE:O	1:A:132:ALA:HB2	2.22	0.40
1:B:128:PHE:O	1:B:132:ALA:HB2	2.22	0.40
1:D:64:PHE:CZ	1:D:68:TYR:CE1	3.00	0.40
1:F:64:PHE:CZ	1:F:68:TYR:CE1	3.00	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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	187/346 (54%)	182 (97%)	5 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	187/346 (54%)	182 (97%)	5 (3%)	0	100	100
1	C	187/346 (54%)	182 (97%)	5 (3%)	0	100	100
1	D	187/346 (54%)	182 (97%)	5 (3%)	0	100	100
1	E	187/346 (54%)	182 (97%)	5 (3%)	0	100	100
1	F	187/346 (54%)	182 (97%)	5 (3%)	0	100	100
1	G	187/346 (54%)	182 (97%)	5 (3%)	0	100	100
All	All	1309/2422 (54%)	1274 (97%)	35 (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	155/306 (51%)	153 (99%)	2 (1%)	69	90
1	B	155/306 (51%)	153 (99%)	2 (1%)	69	90
1	C	155/306 (51%)	153 (99%)	2 (1%)	69	90
1	D	155/306 (51%)	153 (99%)	2 (1%)	69	90
1	E	155/306 (51%)	153 (99%)	2 (1%)	69	90
1	F	155/306 (51%)	153 (99%)	2 (1%)	69	90
1	G	155/306 (51%)	153 (99%)	2 (1%)	69	90
All	All	1085/2142 (51%)	1071 (99%)	14 (1%)	70	90

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	68	TYR
1	A	124	PHE
1	B	68	TYR
1	B	124	PHE
1	C	68	TYR

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Mol	Chain	Res	Type
1	C	124	PHE
1	D	68	TYR
1	D	124	PHE
1	E	68	TYR
1	E	124	PHE
1	F	68	TYR
1	F	124	PHE
1	G	68	TYR
1	G	124	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	71	ASN
1	A	154	GLN
1	B	71	ASN
1	B	154	GLN
1	C	71	ASN
1	C	154	GLN
1	D	71	ASN
1	D	154	GLN
1	E	71	ASN
1	E	154	GLN
1	F	71	ASN
1	F	154	GLN
1	G	71	ASN
1	G	154	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.



## 5.6 Ligand geometry

7 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	$\# Z  > 2$
2	NAG	B	1001	1	14,14,15	0.28	0	17,19,21	0.51	0
2	NAG	C	1001	1	14,14,15	0.28	0	17,19,21	0.50	0
2	NAG	E	1001	1	14,14,15	0.28	0	17,19,21	0.51	0
2	NAG	G	1001	1	14,14,15	0.27	0	17,19,21	0.50	0
2	NAG	A	1001	1	14,14,15	0.27	0	17,19,21	0.50	0
2	NAG	F	1001	1	14,14,15	0.29	0	17,19,21	0.51	0
2	NAG	D	1001	1	14,14,15	0.27	0	17,19,21	0.52	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
2	NAG	B	1001	1	-	0/6/23/26	0/1/1/1
2	NAG	C	1001	1	-	0/6/23/26	0/1/1/1
2	NAG	E	1001	1	-	0/6/23/26	0/1/1/1
2	NAG	G	1001	1	-	0/6/23/26	0/1/1/1
2	NAG	A	1001	1	-	0/6/23/26	0/1/1/1
2	NAG	F	1001	1	-	0/6/23/26	0/1/1/1
2	NAG	D	1001	1	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

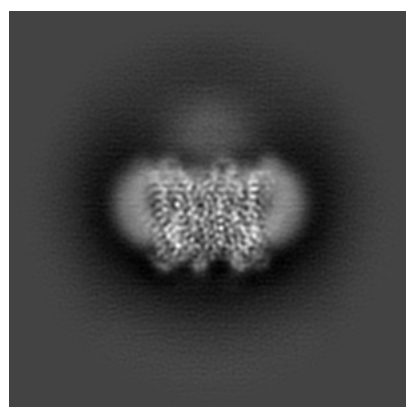
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-30831. These allow visual inspection of the internal detail of the map and identification of artifacts.

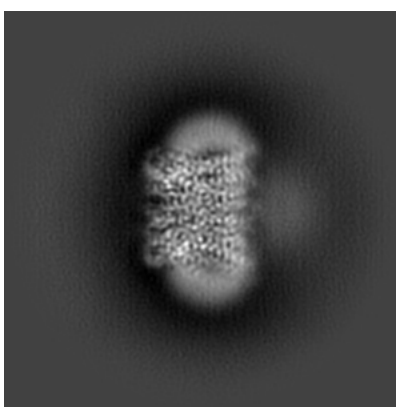
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

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

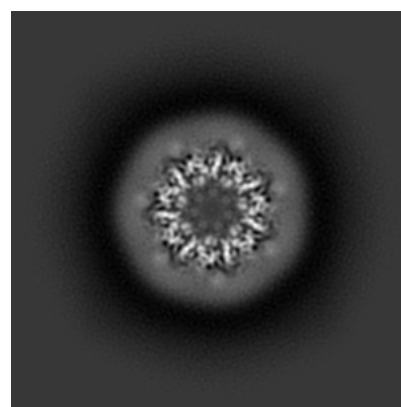
#### 6.1.1 Primary map



X



Y

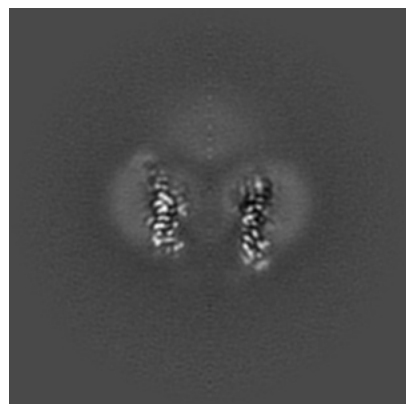


Z

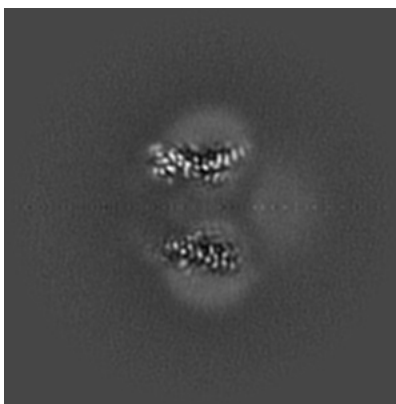
The images above show the map projected in three orthogonal directions.

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

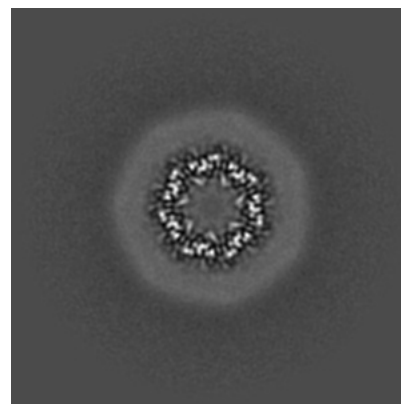
#### 6.2.1 Primary map



X Index: 130



Y Index: 130

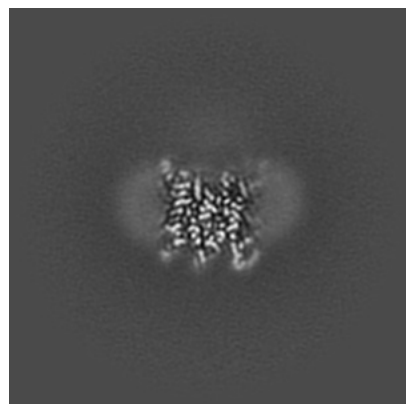


Z Index: 130

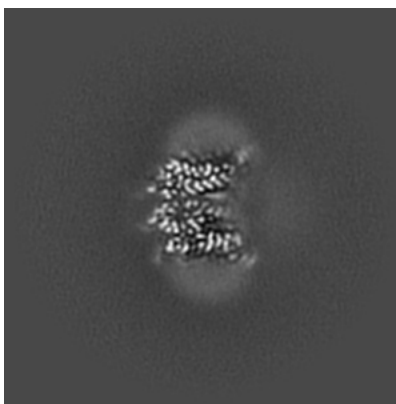
The images above show central slices of the map in three orthogonal directions.

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

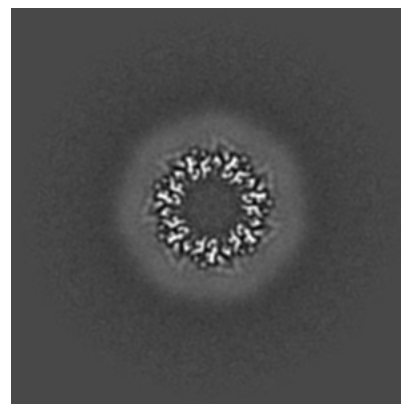
### 6.3.1 Primary map



X Index: 156



Y Index: 109

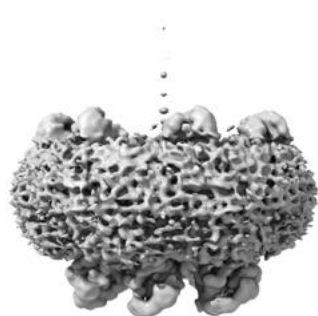


Z Index: 118

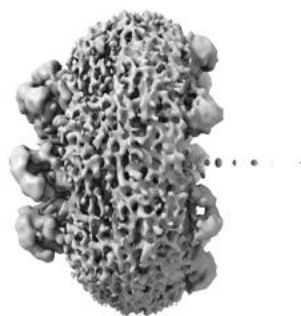
The images above show the largest variance slices of the map in three orthogonal directions.

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

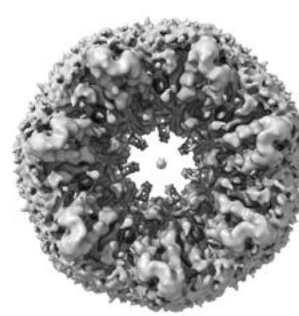
### 6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.154. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

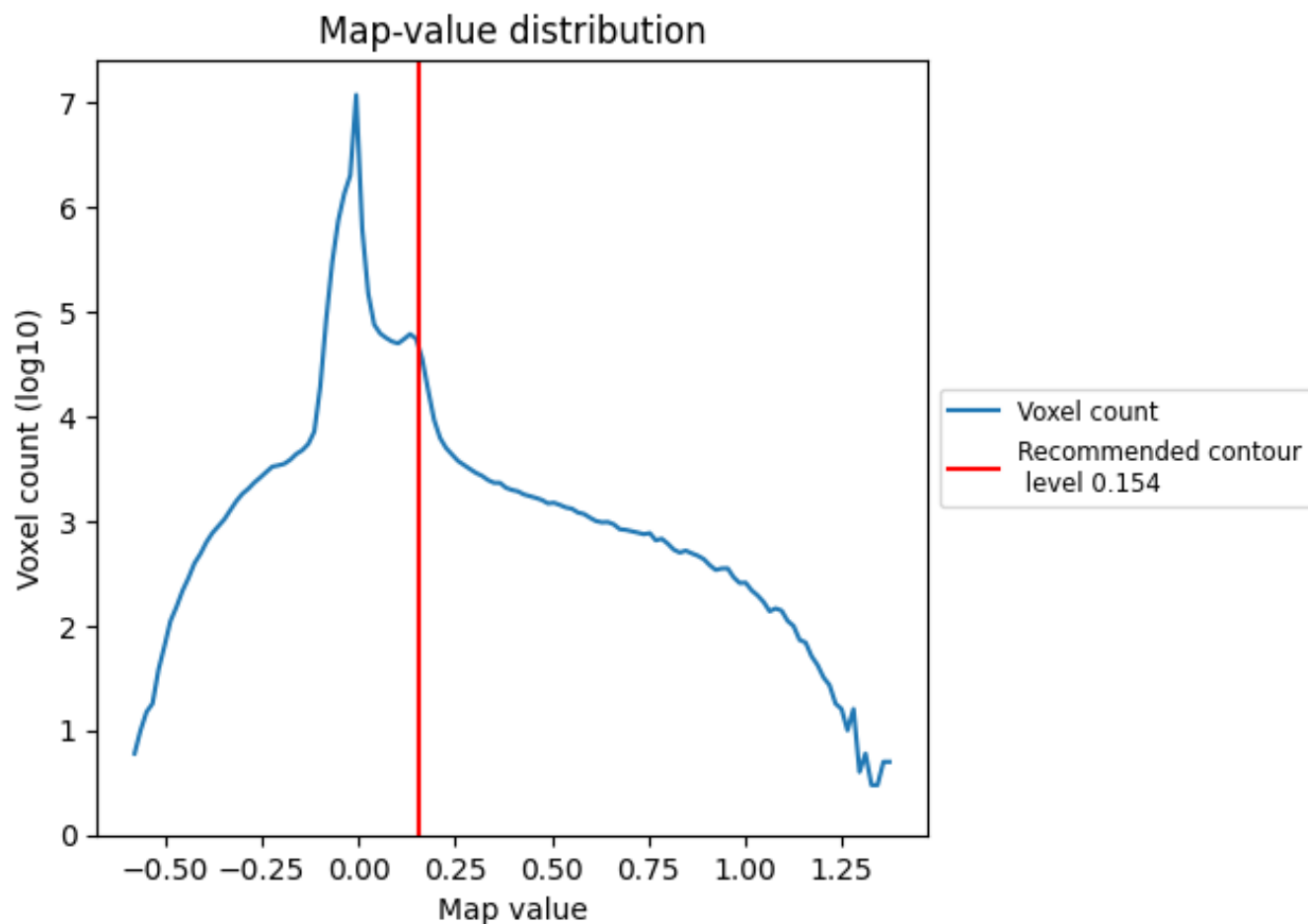
## 6.5 Mask visualisation

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

## 7 Map analysis [i](#)

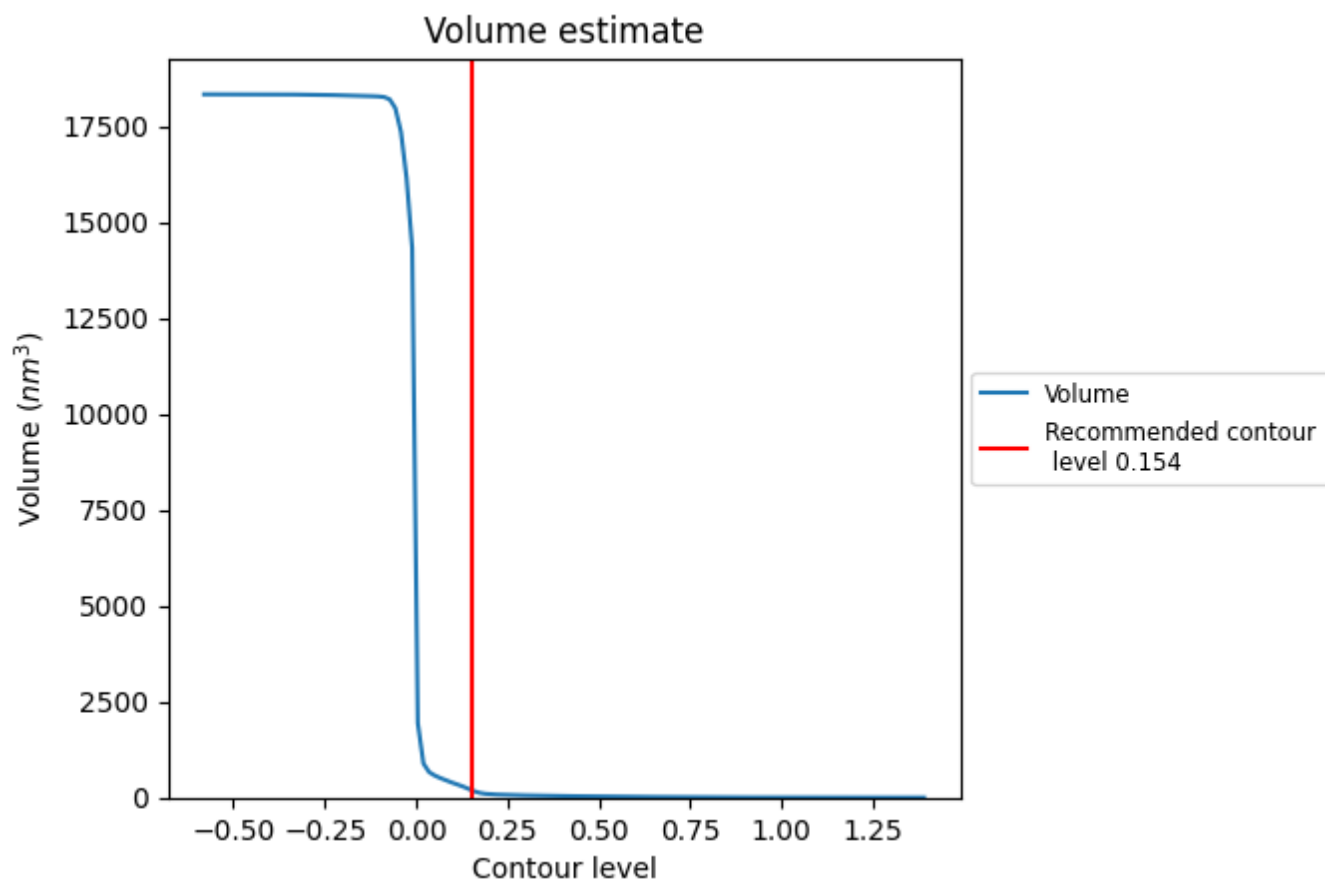
This section contains the results of statistical analysis of the map.

### 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.

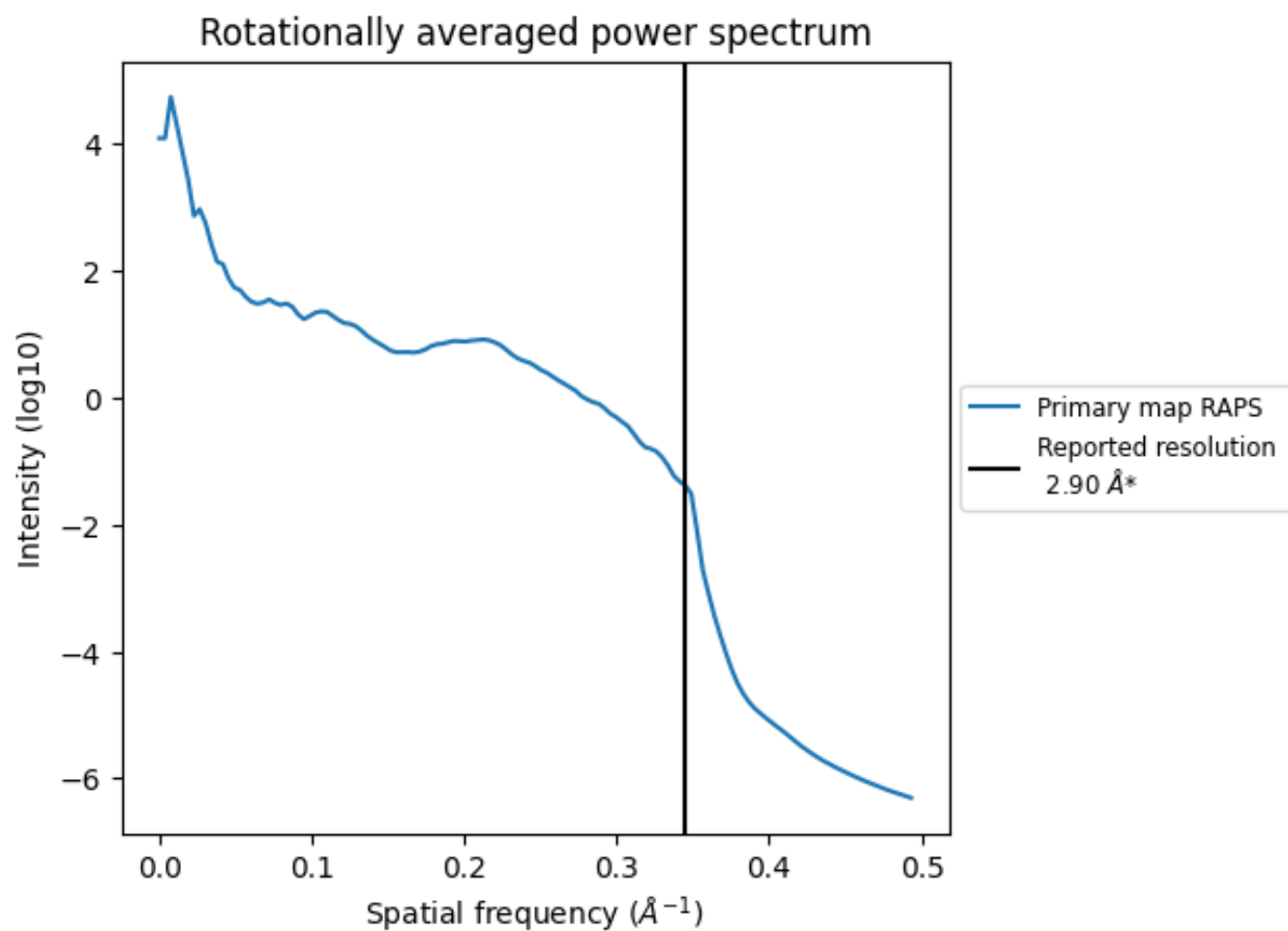
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 185 nm<sup>3</sup>; this corresponds to an approximate mass of 167 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 0.345 Å<sup>-1</sup>



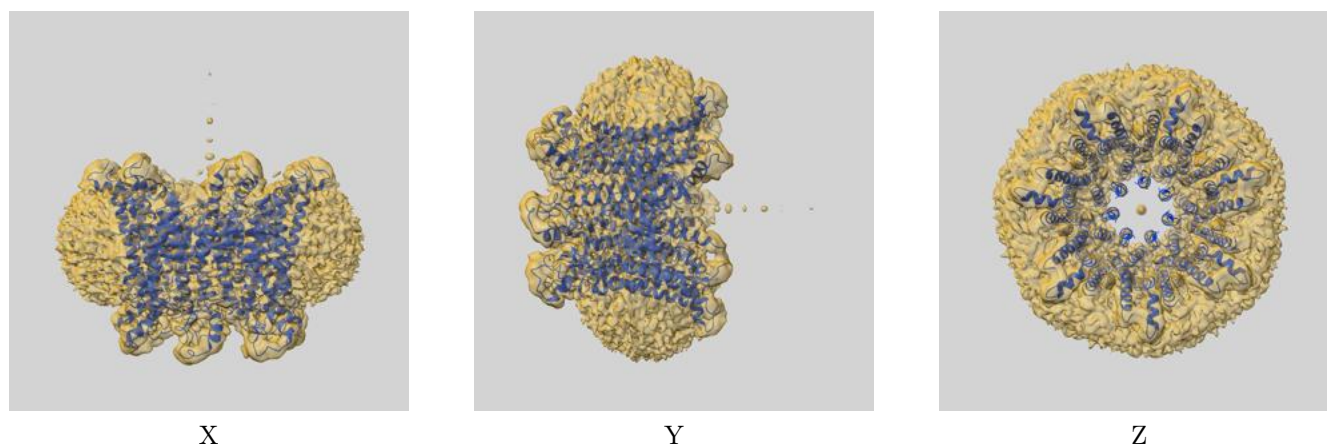
## 8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

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

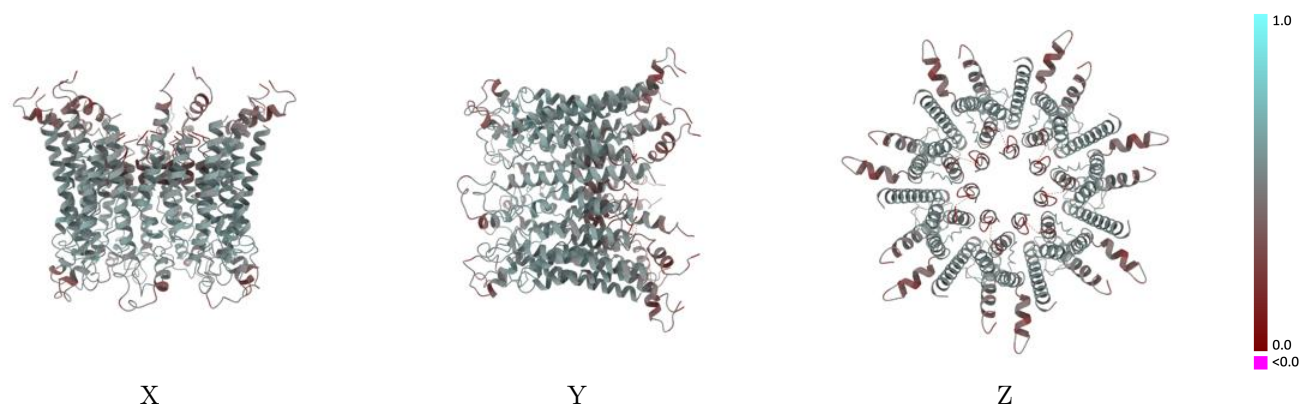
This section contains information regarding the fit between EMDB map EMD-30831 and PDB model 7DSD. Per-residue inclusion information can be found in section 3 on page 5.

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



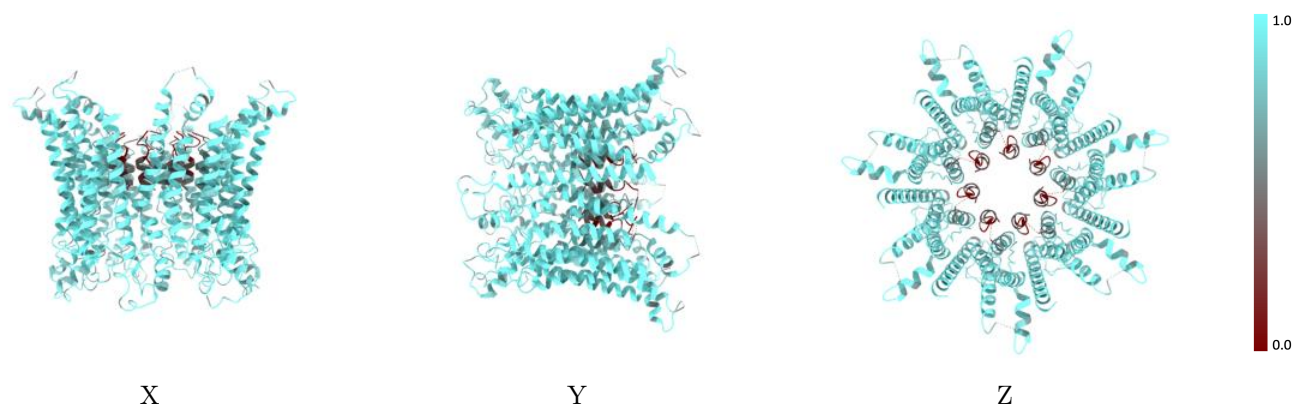
The images above show the 3D surface view of the map at the recommended contour level 0.154 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



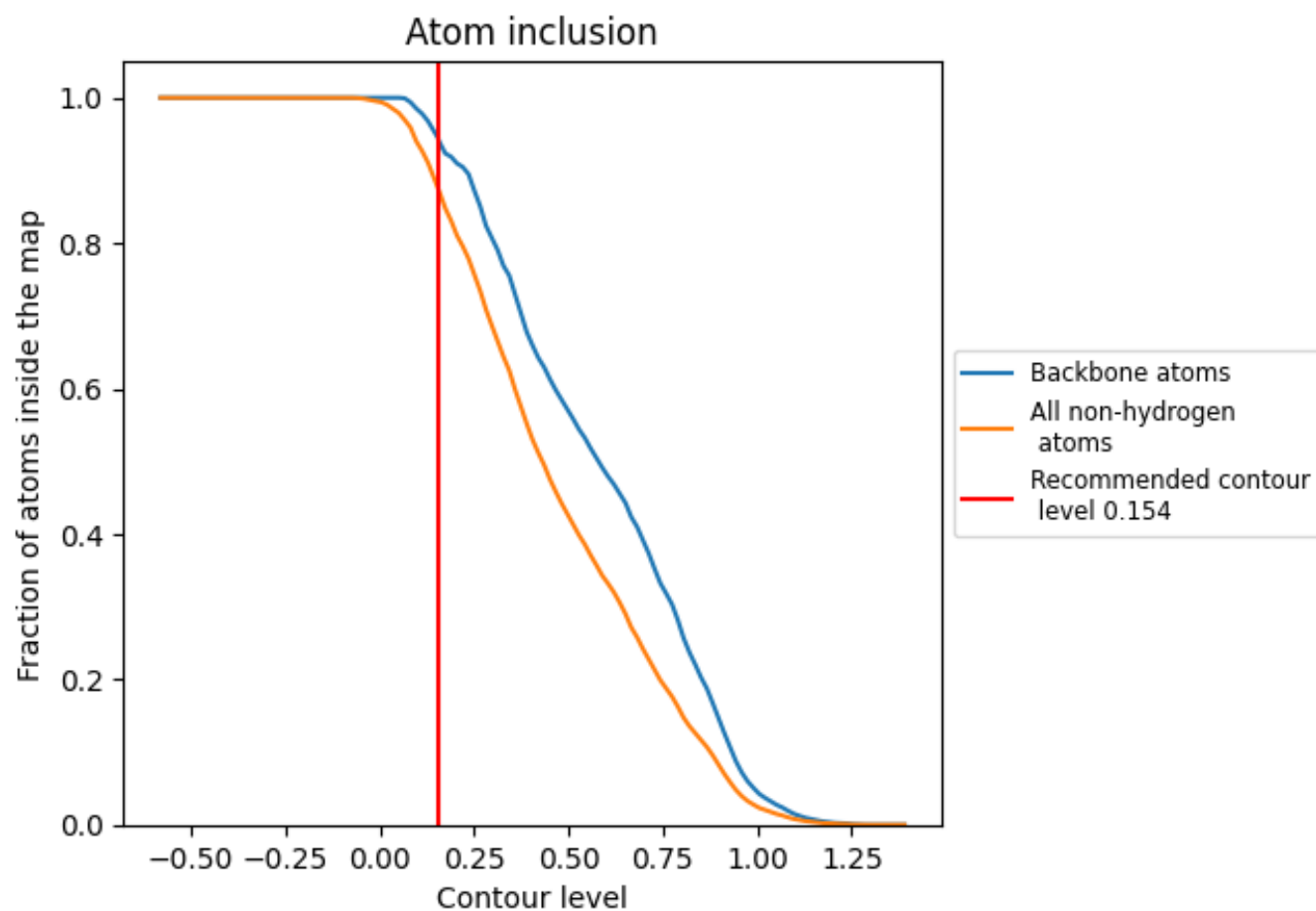
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.154).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 95% of all backbone atoms, 88% 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 (0.154) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div><div></div></div> 0.8760	<div><div></div></div> 0.4920
A	<div><div></div></div> 0.8748	<div><div></div></div> 0.4920
B	<div><div></div></div> 0.8762	<div><div></div></div> 0.4920
C	<div><div></div></div> 0.8762	<div><div></div></div> 0.4910
D	<div><div></div></div> 0.8755	<div><div></div></div> 0.4920
E	<div><div></div></div> 0.8762	<div><div></div></div> 0.4920
F	<div><div></div></div> 0.8748	<div><div></div></div> 0.4920
G	<div><div></div></div> 0.8782	<div><div></div></div> 0.4930

1.0

0.0

<0.0