



Full wwPDB EM Validation Report ⓘ

Mar 6, 2026 – 04:25 PM UTC

PDB ID : 9Y45 / pdb_00009y45
EMDB ID : EMD-72471
Title : His-tagged beta galactosidase (LacZ) on a Ni-NTA lipid monolayer grid
Authors : Baker, R.W.; Strauss, J.D.
Deposited on : 2025-09-02
Resolution : 2.41 Å(reported)
Based on initial model : 1PX3

This is a Full wwPDB EM Validation 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
MolProbity : 4-5-2 with Phenix2.0
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

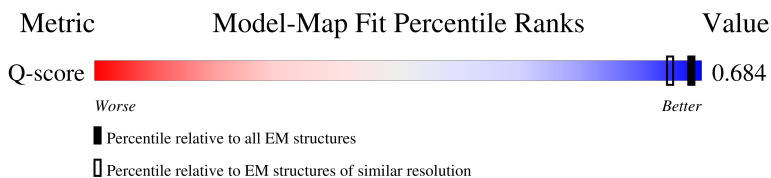
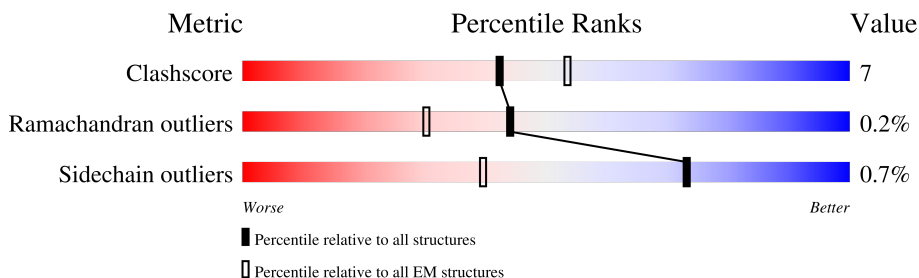
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.41 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	5662 (1.92 - 2.91)

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	1030	 81% 17% .
1	B	1030	 82% 17% .
1	C	1030	 82% 17% .
1	D	1030	 81% 17% .

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 32612 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 Beta-galactosidase.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1014	Total	C	N	O	S	0	0
			8147	5153	1440	1515	39		
1	B	1014	Total	C	N	O	S	0	0
			8147	5153	1440	1515	39		
1	C	1014	Total	C	N	O	S	0	0
			8147	5153	1440	1515	39		
1	D	1014	Total	C	N	O	S	0	0
			8147	5153	1440	1515	39		

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1025	HIS	-	expression tag	UNP P00722
A	1026	HIS	-	expression tag	UNP P00722
A	1027	HIS	-	expression tag	UNP P00722
A	1028	HIS	-	expression tag	UNP P00722
A	1029	HIS	-	expression tag	UNP P00722
A	1030	HIS	-	expression tag	UNP P00722
B	1025	HIS	-	expression tag	UNP P00722
B	1026	HIS	-	expression tag	UNP P00722
B	1027	HIS	-	expression tag	UNP P00722
B	1028	HIS	-	expression tag	UNP P00722
B	1029	HIS	-	expression tag	UNP P00722
B	1030	HIS	-	expression tag	UNP P00722
C	1025	HIS	-	expression tag	UNP P00722
C	1026	HIS	-	expression tag	UNP P00722
C	1027	HIS	-	expression tag	UNP P00722
C	1028	HIS	-	expression tag	UNP P00722
C	1029	HIS	-	expression tag	UNP P00722
C	1030	HIS	-	expression tag	UNP P00722
D	1025	HIS	-	expression tag	UNP P00722
D	1026	HIS	-	expression tag	UNP P00722
D	1027	HIS	-	expression tag	UNP P00722
D	1028	HIS	-	expression tag	UNP P00722

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Chain	Residue	Modelled	Actual	Comment	Reference
D	1029	HIS	-	expression tag	UNP P00722
D	1030	HIS	-	expression tag	UNP P00722

- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

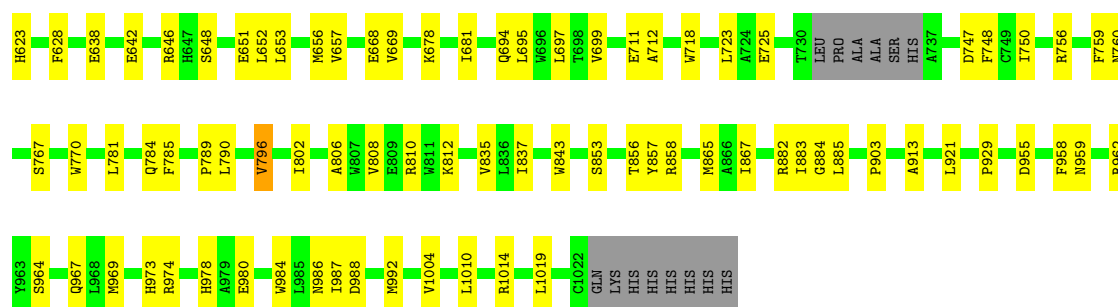
Mol	Chain	Residues	Atoms	AltConf
2	A	2	Total Mg 2 2	0
2	B	2	Total Mg 2 2	0
2	C	2	Total Mg 2 2	0
2	D	2	Total Mg 2 2	0

- Molecule 3 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms	AltConf
3	A	1	Total Na 1 1	0
3	B	1	Total Na 1 1	0
3	C	1	Total Na 1 1	0
3	D	1	Total Na 1 1	0

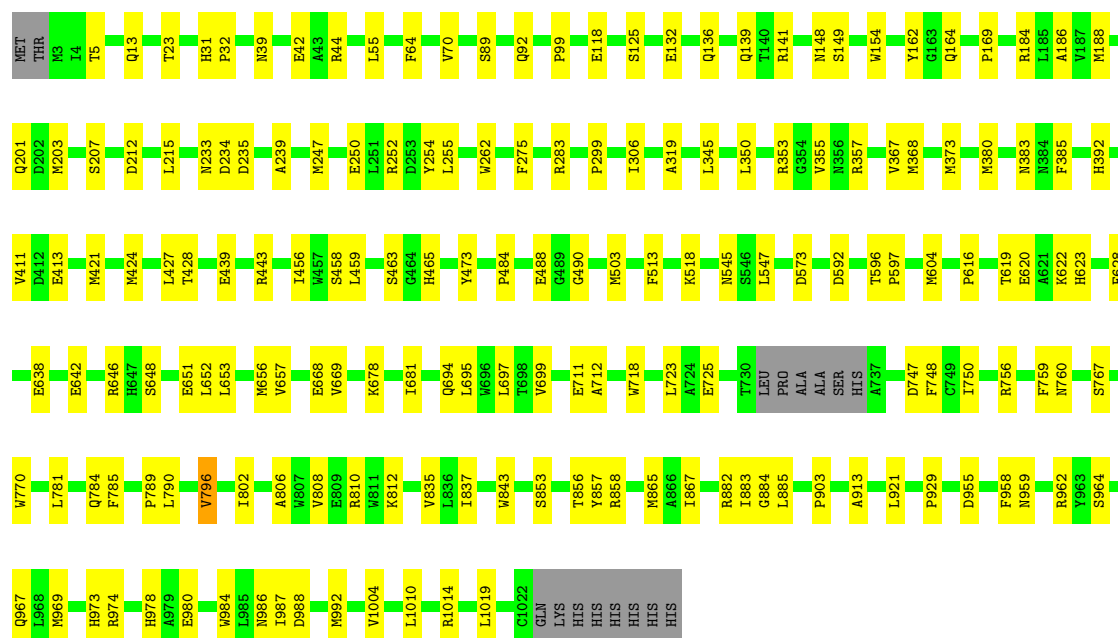
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	AltConf
4	A	3	Total O 3 3	0
4	B	3	Total O 3 3	0
4	C	3	Total O 3 3	0
4	D	3	Total O 3 3	0



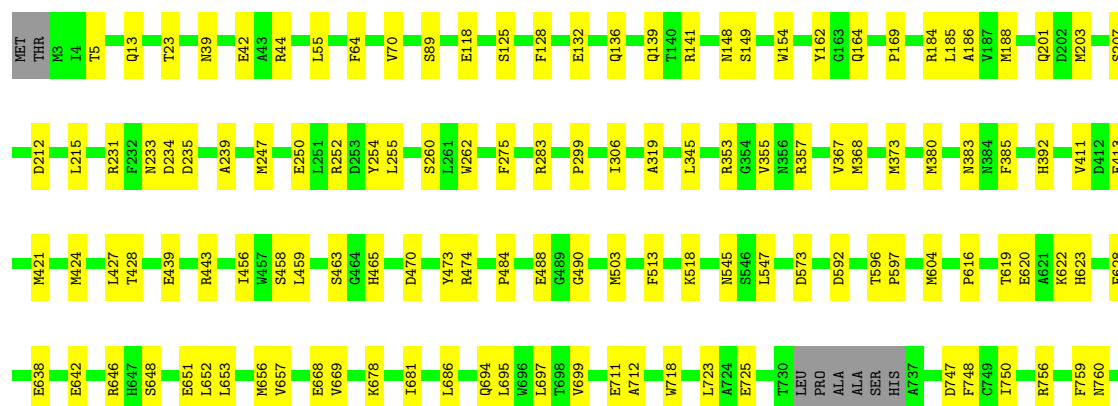
• Molecule 1: Beta-galactosidase

Chain C: 82% 17% .



• Molecule 1: Beta-galactosidase

Chain D: 81% 17% .



S767	W770	L781	Q784	F785	P789	L790	V796	I802	A806	W807	V808	E809	R810	W811	K812	V835	L836	I837	W843	S853	T856	Y857	R858	M865	A866	I867	A874	T877	R882	I883	G884	L885	P903	A913	L921	P929	D955	F958
N959	R962	Y963	S964	Q967	L968	N969	H973	R974	H978	A979	E980	W984	L985	N986	L987	D988	N992	V1004	L1010	R1014	L1019	C1022	GLN	LYS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, D2	Depositor
Number of particles used	515041	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS TALOS	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	55	Depositor
Minimum defocus (nm)	400	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	2.720	Depositor
Minimum map value	-1.857	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.066	Depositor
Recommended contour level	0.1	Depositor
Map size ($\text{\AA}$)	384.428, 384.428, 384.428	wwPDB
Map dimensions	440, 440, 440	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.8737, 0.8737, 0.8737	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: NA, MG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.22	0/8386	0.40	0/11440
1	B	0.22	0/8386	0.40	0/11440
1	C	0.22	0/8386	0.40	0/11440
1	D	0.22	0/8386	0.40	0/11440
All	All	0.22	0/33544	0.40	0/45760

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	8147	0	7743	111	0
1	B	8147	0	7743	110	0
1	C	8147	0	7743	109	0
1	D	8147	0	7743	109	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
3	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	3	0	0	0	0
4	B	3	0	0	0	0
4	C	3	0	0	0	0
4	D	3	0	0	0	0
All	All	32612	0	30972	425	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 7.

All (425) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:865:MET:HE3	1:A:867:ILE:HD11	1.67	0.76
1:B:865:MET:HE3	1:B:867:ILE:HD11	1.67	0.76
1:C:865:MET:HE3	1:C:867:ILE:HD11	1.67	0.76
1:D:865:MET:HE3	1:D:867:ILE:HD11	1.67	0.76
1:C:955:ASP:OD2	1:D:1014:ARG:NH2	2.22	0.73
1:A:1014:ARG:NH2	1:B:955:ASP:OD2	2.23	0.72
1:C:1014:ARG:NH2	1:D:955:ASP:OD2	2.22	0.71
1:C:789:PRO:HD2	1:C:969:MET:HG3	1.72	0.71
1:A:789:PRO:HD2	1:A:969:MET:HG3	1.72	0.71
1:A:955:ASP:OD2	1:B:1014:ARG:NH2	2.23	0.71
1:D:789:PRO:HD2	1:D:969:MET:HG3	1.72	0.71
1:B:789:PRO:HD2	1:B:969:MET:HG3	1.72	0.71
1:D:694:GLN:NE2	1:D:723:LEU:O	2.25	0.69
1:A:694:GLN:NE2	1:A:723:LEU:O	2.25	0.69
1:A:148:ASN:HB3	1:A:207:SER:HA	1.75	0.69
1:B:694:GLN:NE2	1:B:723:LEU:O	2.25	0.69
1:C:694:GLN:NE2	1:C:723:LEU:O	2.25	0.69
1:C:148:ASN:HB3	1:C:207:SER:HA	1.75	0.69
1:A:883:ILE:HD12	1:A:1010:LEU:HD13	1.76	0.69
1:B:148:ASN:HB3	1:B:207:SER:HA	1.75	0.69
1:D:148:ASN:HB3	1:D:207:SER:HA	1.75	0.68
1:D:883:ILE:HD12	1:D:1010:LEU:HD13	1.76	0.68
1:B:883:ILE:HD12	1:B:1010:LEU:HD13	1.76	0.68
1:C:883:ILE:HD12	1:C:1010:LEU:HD13	1.76	0.67
1:A:357:ARG:HD2	1:A:380:MET:HE1	1.77	0.67
1:D:357:ARG:HD2	1:D:380:MET:HE1	1.77	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:459:LEU:HD11	1:A:473:TYR:HB2	1.76	0.67
1:D:459:LEU:HD11	1:D:473:TYR:HB2	1.76	0.66
1:B:357:ARG:HD2	1:B:380:MET:HE1	1.77	0.66
1:C:357:ARG:HD2	1:C:380:MET:HE1	1.77	0.66
1:B:459:LEU:HD11	1:B:473:TYR:HB2	1.76	0.66
1:C:459:LEU:HD11	1:C:473:TYR:HB2	1.76	0.66
1:A:13:GLN:HG3	1:D:5:THR:HG21	1.77	0.65
1:A:5:THR:HG21	1:D:13:GLN:HG3	1.77	0.65
1:B:652:LEU:HD21	1:B:668:GLU:HG2	1.79	0.65
1:C:652:LEU:HD21	1:C:668:GLU:HG2	1.79	0.65
1:A:652:LEU:HD21	1:A:668:GLU:HG2	1.79	0.65
1:D:652:LEU:HD21	1:D:668:GLU:HG2	1.79	0.65
1:B:13:GLN:HG3	1:C:5:THR:HG21	1.79	0.64
1:B:5:THR:HG21	1:C:13:GLN:HG3	1.80	0.63
1:B:39:ASN:HD22	1:B:42:GLU:H	1.47	0.62
1:C:39:ASN:HD22	1:C:42:GLU:H	1.47	0.62
1:B:154:TRP:HB2	1:B:186:ALA:HB3	1.81	0.62
1:C:154:TRP:HB2	1:C:186:ALA:HB3	1.81	0.62
1:D:39:ASN:HD22	1:D:42:GLU:H	1.47	0.61
1:A:39:ASN:HD22	1:A:42:GLU:H	1.47	0.60
1:A:154:TRP:HB2	1:A:186:ALA:HB3	1.81	0.60
1:D:154:TRP:HB2	1:D:186:ALA:HB3	1.81	0.60
1:A:513:PHE:HE2	1:A:518:LYS:HE2	1.67	0.60
1:D:513:PHE:HE2	1:D:518:LYS:HE2	1.67	0.60
1:B:967:GLN:HE22	1:B:978:HIS:H	1.49	0.60
1:C:967:GLN:HE22	1:C:978:HIS:H	1.49	0.60
1:B:513:PHE:HE2	1:B:518:LYS:HE2	1.67	0.59
1:C:653:LEU:HD11	1:C:699:VAL:HB	1.84	0.59
1:C:513:PHE:HE2	1:C:518:LYS:HE2	1.67	0.59
1:B:653:LEU:HD11	1:B:699:VAL:HB	1.84	0.59
1:A:653:LEU:HD11	1:A:699:VAL:HB	1.83	0.59
1:B:39:ASN:HD22	1:B:42:GLU:HG3	1.68	0.59
1:C:39:ASN:HD22	1:C:42:GLU:HG3	1.68	0.59
1:D:653:LEU:HD11	1:D:699:VAL:HB	1.84	0.59
1:D:39:ASN:HD22	1:D:42:GLU:HG3	1.68	0.58
1:A:39:ASN:HD22	1:A:42:GLU:HG3	1.68	0.58
1:A:967:GLN:HE22	1:A:978:HIS:H	1.49	0.58
1:D:967:GLN:HE22	1:D:978:HIS:H	1.49	0.58
1:A:748:PHE:HB2	1:A:759:PHE:HB2	1.85	0.58
1:D:748:PHE:HB2	1:D:759:PHE:HB2	1.85	0.58
1:B:748:PHE:HB2	1:B:759:PHE:HB2	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:748:PHE:HB2	1:C:759:PHE:HB2	1.85	0.58
1:C:929:PRO:HB2	1:C:974:ARG:HH11	1.69	0.56
1:A:929:PRO:HB2	1:A:974:ARG:HH11	1.69	0.56
1:B:70:VAL:HG21	1:B:188:MET:HE2	1.87	0.56
1:B:929:PRO:HB2	1:B:974:ARG:HH11	1.69	0.56
1:C:70:VAL:HG21	1:C:188:MET:HE2	1.87	0.56
1:D:929:PRO:HB2	1:D:974:ARG:HH11	1.70	0.56
1:B:424:MET:HE2	1:C:283:ARG:HG2	1.86	0.56
1:D:962:ARG:NH2	1:D:980:GLU:O	2.37	0.56
1:A:962:ARG:NH2	1:A:980:GLU:O	2.37	0.56
1:A:162:TYR:OH	1:A:164:GLN:NE2	2.39	0.56
1:B:306:ILE:HD11	1:B:646:ARG:HB3	1.88	0.56
1:D:162:TYR:OH	1:D:164:GLN:NE2	2.39	0.56
1:A:139:GLN:HE22	1:A:141:ARG:HB3	1.71	0.56
1:B:283:ARG:HG2	1:C:424:MET:HE2	1.87	0.56
1:B:162:TYR:OH	1:B:164:GLN:NE2	2.39	0.55
1:B:962:ARG:NH2	1:B:980:GLU:O	2.37	0.55
1:C:306:ILE:HD11	1:C:646:ARG:HB3	1.88	0.55
1:C:962:ARG:NH2	1:C:980:GLU:O	2.37	0.55
1:D:139:GLN:HE22	1:D:141:ARG:HB3	1.71	0.55
1:A:424:MET:HE2	1:D:283:ARG:HG2	1.88	0.55
1:C:139:GLN:HE22	1:C:141:ARG:HB3	1.71	0.55
1:C:162:TYR:OH	1:C:164:GLN:NE2	2.39	0.55
1:C:592:ASP:OD2	1:C:973:HIS:NE2	2.39	0.55
1:A:283:ARG:HG2	1:D:424:MET:HE2	1.89	0.55
1:B:139:GLN:HE22	1:B:141:ARG:HB3	1.71	0.55
1:B:592:ASP:OD2	1:B:973:HIS:NE2	2.39	0.55
1:A:70:VAL:HG21	1:A:188:MET:HE2	1.87	0.55
1:B:252:ARG:H	1:B:255:LEU:HD12	1.71	0.55
1:C:252:ARG:H	1:C:255:LEU:HD12	1.71	0.55
1:D:70:VAL:HG21	1:D:188:MET:HE2	1.87	0.55
1:A:669:VAL:HG11	1:A:681:ILE:HD13	1.89	0.55
1:D:669:VAL:HG11	1:D:681:ILE:HD13	1.89	0.55
1:D:306:ILE:HD11	1:D:646:ARG:HB3	1.88	0.54
1:A:306:ILE:HD11	1:A:646:ARG:HB3	1.88	0.54
1:B:383:ASN:HA	1:B:622:LYS:HG3	1.88	0.54
1:C:383:ASN:HA	1:C:622:LYS:HG3	1.88	0.54
1:D:383:ASN:HA	1:D:622:LYS:HG3	1.88	0.54
1:B:669:VAL:HG11	1:B:681:ILE:HD13	1.89	0.54
1:C:669:VAL:HG11	1:C:681:ILE:HD13	1.89	0.54
1:A:383:ASN:HA	1:A:622:LYS:HG3	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:252:ARG:H	1:A:255:LEU:HD12	1.71	0.54
1:D:592:ASP:OD2	1:D:973:HIS:NE2	2.39	0.54
1:A:592:ASP:OD2	1:A:973:HIS:NE2	2.39	0.54
1:D:252:ARG:H	1:D:255:LEU:HD12	1.71	0.54
1:A:638:GLU:OE2	1:A:678:LYS:HD3	2.08	0.53
1:D:638:GLU:OE2	1:D:678:LYS:HD3	2.08	0.53
1:A:89:SER:HA	1:A:367:VAL:HG21	1.90	0.53
1:B:421:MET:HE3	1:B:427:LEU:HD11	1.91	0.53
1:D:89:SER:HA	1:D:367:VAL:HG21	1.90	0.53
1:A:421:MET:HE3	1:A:427:LEU:HD11	1.91	0.53
1:C:421:MET:HE3	1:C:427:LEU:HD11	1.91	0.53
1:C:978:HIS:O	1:C:978:HIS:ND1	2.42	0.53
1:D:421:MET:HE3	1:D:427:LEU:HD11	1.91	0.53
1:B:978:HIS:O	1:B:978:HIS:ND1	2.42	0.53
1:C:638:GLU:OE2	1:C:678:LYS:HD3	2.08	0.53
1:B:89:SER:HA	1:B:367:VAL:HG21	1.90	0.52
1:B:368:MET:HB3	1:B:373:MET:HE2	1.92	0.52
1:C:89:SER:HA	1:C:367:VAL:HG21	1.90	0.52
1:C:368:MET:HB3	1:C:373:MET:HE2	1.92	0.52
1:B:596:THR:HB	1:B:597:PRO:HD2	1.92	0.52
1:B:638:GLU:OE2	1:B:678:LYS:HD3	2.08	0.52
1:C:596:THR:HB	1:C:597:PRO:HD2	1.91	0.52
1:A:596:THR:HB	1:A:597:PRO:HD2	1.91	0.52
1:C:233:ASN:ND2	1:C:235:ASP:OD1	2.43	0.52
1:B:233:ASN:ND2	1:B:235:ASP:OD1	2.43	0.52
1:D:596:THR:HB	1:D:597:PRO:HD2	1.91	0.52
1:A:233:ASN:ND2	1:A:235:ASP:OD1	2.43	0.52
1:D:233:ASN:ND2	1:D:235:ASP:OD1	2.43	0.52
1:A:39:ASN:HB3	1:A:42:GLU:HG3	1.92	0.51
1:A:201:GLN:HG2	1:A:392:HIS:CB	2.41	0.51
1:A:695:LEU:HB3	1:A:723:LEU:HB2	1.92	0.51
1:D:39:ASN:HB3	1:D:42:GLU:HG3	1.92	0.51
1:A:368:MET:HB3	1:A:373:MET:HE2	1.92	0.51
1:A:882:ARG:HB2	1:A:988:ASP:OD2	2.11	0.51
1:D:201:GLN:HG2	1:D:392:HIS:CB	2.41	0.51
1:D:368:MET:HB3	1:D:373:MET:HE2	1.92	0.51
1:D:695:LEU:HB3	1:D:723:LEU:HB2	1.92	0.51
1:C:39:ASN:HB3	1:C:42:GLU:HG3	1.92	0.51
1:D:882:ARG:HB2	1:D:988:ASP:OD2	2.11	0.51
1:B:858:ARG:HG2	1:B:858:ARG:HH11	1.75	0.51
1:A:573:ASP:HB3	1:A:604:MET:HG2	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:39:ASN:HB3	1:B:42:GLU:HG3	1.92	0.51
1:C:858:ARG:HH11	1:C:858:ARG:HG2	1.75	0.51
1:D:573:ASP:HB3	1:D:604:MET:HG2	1.93	0.51
1:C:44:ARG:HD2	1:C:262:TRP:CD2	2.45	0.51
1:B:44:ARG:HD2	1:B:262:TRP:CD2	2.45	0.51
1:A:858:ARG:HG2	1:A:858:ARG:HH11	1.75	0.50
1:D:858:ARG:HG2	1:D:858:ARG:HH11	1.75	0.50
1:A:992:MET:HE2	1:A:1004:VAL:HG21	1.94	0.50
1:B:882:ARG:HB2	1:B:988:ASP:OD2	2.11	0.50
1:D:992:MET:HE2	1:D:1004:VAL:HG21	1.94	0.50
1:A:44:ARG:HD2	1:A:262:TRP:CD2	2.45	0.50
1:B:992:MET:HE2	1:B:1004:VAL:HG21	1.94	0.50
1:C:992:MET:HE2	1:C:1004:VAL:HG21	1.94	0.50
1:C:695:LEU:HB3	1:C:723:LEU:HB2	1.92	0.50
1:C:882:ARG:HB2	1:C:988:ASP:OD2	2.11	0.50
1:D:44:ARG:HD2	1:D:262:TRP:CD2	2.45	0.50
1:A:411:VAL:HG22	1:A:456:ILE:HB	1.94	0.50
1:B:695:LEU:HB3	1:B:723:LEU:HB2	1.92	0.50
1:C:201:GLN:HG2	1:C:392:HIS:CB	2.41	0.50
1:D:411:VAL:HG22	1:D:456:ILE:HB	1.94	0.50
1:B:201:GLN:HG2	1:B:392:HIS:CB	2.41	0.49
1:A:837:ILE:HB	1:A:857:TYR:HB2	1.94	0.49
1:D:837:ILE:HB	1:D:857:TYR:HB2	1.94	0.49
1:B:837:ILE:HB	1:B:857:TYR:HB2	1.94	0.49
1:C:987:ILE:HG21	1:C:1019:LEU:HD11	1.94	0.49
1:A:125:SER:OG	1:A:184:ARG:NH2	2.45	0.49
1:C:837:ILE:HB	1:C:857:TYR:HB2	1.94	0.49
1:B:573:ASP:HB3	1:B:604:MET:HG2	1.93	0.49
1:B:987:ILE:HG21	1:B:1019:LEU:HD11	1.95	0.49
1:C:411:VAL:HG22	1:C:456:ILE:HB	1.94	0.49
1:D:125:SER:OG	1:D:184:ARG:NH2	2.45	0.49
1:A:139:GLN:NE2	1:A:141:ARG:HB3	2.28	0.49
1:C:573:ASP:HB3	1:C:604:MET:HG2	1.93	0.49
1:D:139:GLN:NE2	1:D:141:ARG:HB3	2.28	0.49
1:B:411:VAL:HG22	1:B:456:ILE:HB	1.94	0.49
1:C:125:SER:OG	1:C:184:ARG:NH2	2.45	0.49
1:D:978:HIS:O	1:D:978:HIS:ND1	2.42	0.49
1:A:978:HIS:O	1:A:978:HIS:ND1	2.42	0.49
1:B:125:SER:OG	1:B:184:ARG:NH2	2.45	0.49
1:B:139:GLN:NE2	1:B:141:ARG:HB3	2.28	0.48
1:C:139:GLN:NE2	1:C:141:ARG:HB3	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:616:PRO:O	1:B:619:THR:HG22	2.14	0.48
1:B:656:MET:HG2	1:B:657:VAL:N	2.29	0.48
1:C:656:MET:HG2	1:C:657:VAL:N	2.29	0.48
1:C:616:PRO:O	1:C:619:THR:HG22	2.14	0.47
1:D:987:ILE:HG21	1:D:1019:LEU:HD11	1.95	0.47
1:A:656:MET:HG2	1:A:657:VAL:N	2.29	0.47
1:A:987:ILE:HG21	1:A:1019:LEU:HD11	1.95	0.47
1:D:656:MET:HG2	1:D:657:VAL:N	2.29	0.47
1:A:750:ILE:HG12	1:A:835:VAL:HG11	1.97	0.47
1:D:750:ILE:HG12	1:D:835:VAL:HG11	1.97	0.47
1:A:648:SER:HB2	1:A:651:GLU:HB2	1.97	0.47
1:D:648:SER:HB2	1:D:651:GLU:HB2	1.97	0.47
1:B:648:SER:HB2	1:B:651:GLU:HB2	1.97	0.47
1:C:648:SER:HB2	1:C:651:GLU:HB2	1.97	0.47
1:A:843:TRP:HZ3	1:A:853:SER:HB3	1.80	0.47
1:D:843:TRP:HZ3	1:D:853:SER:HB3	1.80	0.47
1:B:750:ILE:HG12	1:B:835:VAL:HG11	1.97	0.46
1:C:750:ILE:HG12	1:C:835:VAL:HG11	1.97	0.46
1:D:616:PRO:O	1:D:619:THR:HG22	2.14	0.46
1:A:616:PRO:O	1:A:619:THR:HG22	2.14	0.46
1:D:55:LEU:HD11	1:D:215:LEU:HG	1.97	0.46
1:A:55:LEU:HD11	1:A:215:LEU:HG	1.97	0.46
1:C:239:ALA:HB2	1:C:299:PRO:HG3	1.97	0.46
1:A:39:ASN:ND2	1:A:42:GLU:HG3	2.31	0.46
1:A:428:THR:HG21	1:A:463:SER:HB3	1.97	0.46
1:C:55:LEU:HD11	1:C:215:LEU:HG	1.97	0.46
1:C:148:ASN:HA	1:C:149:SER:HA	1.59	0.46
1:D:39:ASN:ND2	1:D:42:GLU:HG3	2.31	0.46
1:A:201:GLN:HG2	1:A:392:HIS:HB2	1.98	0.46
1:B:239:ALA:HB2	1:B:299:PRO:HG3	1.97	0.46
1:B:620:GLU:HA	1:B:913:ALA:HB2	1.98	0.46
1:D:201:GLN:HG2	1:D:392:HIS:HB2	1.98	0.46
1:D:428:THR:HG21	1:D:463:SER:HB3	1.97	0.46
1:B:55:LEU:HD11	1:B:215:LEU:HG	1.97	0.46
1:C:620:GLU:HA	1:C:913:ALA:HB2	1.98	0.46
1:C:806:ALA:O	1:C:810:ARG:HG3	2.17	0.45
1:B:39:ASN:ND2	1:B:42:GLU:HG3	2.31	0.45
1:C:39:ASN:ND2	1:C:42:GLU:HG3	2.31	0.45
1:D:620:GLU:HA	1:D:913:ALA:HB2	1.98	0.45
1:A:247:MET:HB3	1:A:275:PHE:CZ	2.51	0.45
1:A:465:HIS:HB2	1:A:490:GLY:HA3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:620:GLU:HA	1:A:913:ALA:HB2	1.98	0.45
1:A:653:LEU:HD22	1:A:681:ILE:HD12	1.99	0.45
1:B:247:MET:HB3	1:B:275:PHE:CZ	2.51	0.45
1:B:653:LEU:HD22	1:B:681:ILE:HD12	1.99	0.45
1:B:806:ALA:O	1:B:810:ARG:HG3	2.17	0.45
1:C:653:LEU:HD22	1:C:681:ILE:HD12	1.99	0.45
1:D:247:MET:HB3	1:D:275:PHE:CZ	2.51	0.45
1:D:653:LEU:HD22	1:D:681:ILE:HD12	1.99	0.45
1:A:250:GLU:OE1	1:A:252:ARG:NE	2.43	0.45
1:B:148:ASN:HA	1:B:149:SER:HA	1.59	0.45
1:B:784:GLN:HG2	1:B:882:ARG:HD2	1.97	0.45
1:D:784:GLN:HG2	1:D:882:ARG:HD2	1.97	0.45
1:A:784:GLN:HG2	1:A:882:ARG:HD2	1.97	0.45
1:B:756:ARG:HB2	1:B:770:TRP:HB2	1.99	0.45
1:C:247:MET:HB3	1:C:275:PHE:CZ	2.51	0.45
1:C:756:ARG:HB2	1:C:770:TRP:HB2	1.99	0.45
1:D:239:ALA:HB2	1:D:299:PRO:HG3	1.97	0.45
1:D:465:HIS:HB2	1:D:490:GLY:HA3	1.98	0.45
1:B:958:PHE:HA	1:B:986:ASN:O	2.17	0.45
1:C:784:GLN:HG2	1:C:882:ARG:HD2	1.97	0.45
1:D:250:GLU:OE1	1:D:252:ARG:NE	2.43	0.45
1:A:239:ALA:HB2	1:A:299:PRO:HG3	1.97	0.45
1:C:843:TRP:HZ3	1:C:853:SER:HB3	1.80	0.45
1:D:958:PHE:HA	1:D:986:ASN:O	2.17	0.45
1:A:958:PHE:HA	1:A:986:ASN:O	2.17	0.45
1:B:250:GLU:OE1	1:B:252:ARG:NE	2.43	0.45
1:C:958:PHE:HA	1:C:986:ASN:O	2.17	0.45
1:D:132:GLU:O	1:D:136:GLN:HG3	2.16	0.45
1:D:201:GLN:HB2	1:D:203:MET:HE2	1.99	0.45
1:A:201:GLN:HB2	1:A:203:MET:HE2	1.99	0.45
1:A:756:ARG:HB2	1:A:770:TRP:HB2	1.99	0.45
1:B:843:TRP:HZ3	1:B:853:SER:HB3	1.80	0.45
1:D:756:ARG:HB2	1:D:770:TRP:HB2	1.99	0.45
1:A:132:GLU:O	1:A:136:GLN:HG3	2.16	0.45
1:C:465:HIS:HB2	1:C:490:GLY:HA3	1.98	0.45
1:A:148:ASN:HA	1:A:149:SER:HA	1.58	0.44
1:A:596:THR:O	1:A:597:PRO:C	2.60	0.44
1:B:428:THR:HG21	1:B:463:SER:HB3	1.97	0.44
1:C:428:THR:HG21	1:C:463:SER:HB3	1.97	0.44
1:D:596:THR:O	1:D:597:PRO:C	2.60	0.44
1:B:456:ILE:HG12	1:B:484:PRO:HG2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:132:GLU:O	1:C:136:GLN:HG3	2.16	0.44
1:C:250:GLU:OE1	1:C:252:ARG:NE	2.43	0.44
1:B:465:HIS:HB2	1:B:490:GLY:HA3	1.98	0.44
1:D:747:ASP:C	1:D:747:ASP:OD1	2.61	0.44
1:A:747:ASP:C	1:A:747:ASP:OD1	2.61	0.44
1:B:132:GLU:O	1:B:136:GLN:HG3	2.16	0.44
1:B:201:GLN:HG2	1:B:392:HIS:HB2	1.98	0.44
1:B:545:ASN:HB3	1:B:790:LEU:HD22	1.99	0.44
1:B:747:ASP:OD1	1:B:747:ASP:C	2.61	0.44
1:C:201:GLN:HG2	1:C:392:HIS:HB2	1.98	0.44
1:C:353:ARG:NH2	1:C:642:GLU:OE1	2.50	0.44
1:C:355:VAL:HB	1:C:385:PHE:CE1	2.52	0.44
1:C:456:ILE:HG12	1:C:484:PRO:HG2	1.99	0.44
1:C:747:ASP:OD1	1:C:747:ASP:C	2.61	0.44
1:B:353:ARG:NH2	1:B:642:GLU:OE1	2.50	0.44
1:B:355:VAL:HB	1:B:385:PHE:CE1	2.52	0.44
1:A:545:ASN:HB3	1:A:790:LEU:HD22	1.99	0.44
1:A:234:ASP:OD1	1:A:235:ASP:N	2.50	0.44
1:C:234:ASP:OD1	1:C:235:ASP:N	2.50	0.44
1:C:254:TYR:O	1:C:319:ALA:N	2.51	0.44
1:C:545:ASN:HB3	1:C:790:LEU:HD22	1.99	0.44
1:D:234:ASP:OD1	1:D:235:ASP:N	2.50	0.44
1:A:413:GLU:HA	1:A:458:SER:HB3	1.99	0.44
1:A:964:SER:HB3	1:A:984:TRP:CE2	2.53	0.44
1:B:254:TYR:O	1:B:319:ALA:N	2.51	0.44
1:B:711:GLU:CD	1:B:712:ALA:H	2.26	0.44
1:D:545:ASN:HB3	1:D:790:LEU:HD22	1.99	0.44
1:D:964:SER:HB3	1:D:984:TRP:CE2	2.53	0.44
1:B:234:ASP:OD1	1:B:235:ASP:N	2.50	0.44
1:B:596:THR:O	1:B:597:PRO:C	2.60	0.44
1:C:711:GLU:CD	1:C:712:ALA:H	2.26	0.44
1:D:413:GLU:HA	1:D:458:SER:HB3	1.99	0.44
1:A:355:VAL:HB	1:A:385:PHE:CE1	2.52	0.43
1:C:596:THR:O	1:C:597:PRO:C	2.60	0.43
1:D:355:VAL:HB	1:D:385:PHE:CE1	2.52	0.43
1:A:456:ILE:HG12	1:A:484:PRO:HG2	1.99	0.43
1:B:474:ARG:HA	1:B:474:ARG:HD2	1.89	0.43
1:C:201:GLN:HB2	1:C:203:MET:HE2	1.99	0.43
1:C:964:SER:HB3	1:C:984:TRP:CE2	2.53	0.43
1:A:806:ALA:O	1:A:810:ARG:HG3	2.17	0.43
1:B:964:SER:HB3	1:B:984:TRP:CE2	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:118:GLU:HA	1:A:118:GLU:OE1	2.19	0.43
1:D:353:ARG:NH2	1:D:642:GLU:OE1	2.50	0.43
1:D:456:ILE:HG12	1:D:484:PRO:HG2	1.99	0.43
1:B:23:THR:O	1:B:164:GLN:HB2	2.18	0.43
1:B:201:GLN:HB2	1:B:203:MET:HE2	1.99	0.43
1:C:169:PRO:O	1:C:443:ARG:NH2	2.51	0.43
1:D:118:GLU:OE1	1:D:118:GLU:HA	2.19	0.43
1:D:806:ALA:O	1:D:810:ARG:HG3	2.17	0.43
1:A:353:ARG:NH2	1:A:642:GLU:OE1	2.50	0.43
1:B:169:PRO:O	1:B:443:ARG:NH2	2.51	0.43
1:C:23:THR:O	1:C:164:GLN:HB2	2.18	0.43
1:C:623:HIS:HB2	1:C:718:TRP:CZ2	2.54	0.43
1:D:254:TYR:O	1:D:319:ALA:N	2.51	0.43
1:D:808:VAL:HG22	1:D:812:LYS:HD2	2.01	0.43
1:A:254:TYR:O	1:A:319:ALA:N	2.51	0.43
1:B:623:HIS:HB2	1:B:718:TRP:CZ2	2.54	0.43
1:C:808:VAL:HG22	1:C:812:LYS:HD2	2.01	0.43
1:D:858:ARG:HG2	1:D:858:ARG:NH1	2.34	0.43
1:A:808:VAL:HG22	1:A:812:LYS:HD2	2.01	0.43
1:C:488:GLU:HG3	1:C:503:MET:HG3	2.01	0.43
1:A:858:ARG:HG2	1:A:858:ARG:NH1	2.34	0.43
1:B:413:GLU:HA	1:B:458:SER:HB3	1.99	0.43
1:B:488:GLU:HG3	1:B:503:MET:HG3	2.01	0.43
1:B:808:VAL:HG22	1:B:812:LYS:HD2	2.01	0.43
1:D:711:GLU:CD	1:D:712:ALA:H	2.26	0.43
1:A:711:GLU:CD	1:A:712:ALA:H	2.26	0.42
1:B:884:GLY:HA3	1:B:988:ASP:HA	2.00	0.42
1:A:64:PHE:CD2	1:A:70:VAL:HG22	2.54	0.42
1:A:169:PRO:O	1:A:443:ARG:NH2	2.51	0.42
1:A:413:GLU:OE1	1:A:458:SER:OG	2.33	0.42
1:A:628:PHE:CZ	1:A:651:GLU:HG2	2.54	0.42
1:B:858:ARG:HG2	1:B:858:ARG:NH1	2.34	0.42
1:C:413:GLU:HA	1:C:458:SER:HB3	1.99	0.42
1:C:884:GLY:HA3	1:C:988:ASP:HA	2.01	0.42
1:D:64:PHE:CD2	1:D:70:VAL:HG22	2.54	0.42
1:D:169:PRO:O	1:D:443:ARG:NH2	2.51	0.42
1:D:628:PHE:CZ	1:D:651:GLU:HG2	2.54	0.42
1:A:903:PRO:HB2	1:A:921:LEU:HD11	2.02	0.42
1:B:903:PRO:HB2	1:B:921:LEU:HD11	2.01	0.42
1:D:884:GLY:HA3	1:D:988:ASP:HA	2.01	0.42
1:B:413:GLU:OE1	1:B:458:SER:OG	2.33	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:413:GLU:OE1	1:C:458:SER:OG	2.33	0.42
1:C:858:ARG:HG2	1:C:858:ARG:NH1	2.34	0.42
1:C:903:PRO:HB2	1:C:921:LEU:HD11	2.02	0.42
1:D:903:PRO:HB2	1:D:921:LEU:HD11	2.02	0.42
1:A:23:THR:O	1:A:164:GLN:HB2	2.18	0.42
1:A:884:GLY:HA3	1:A:988:ASP:HA	2.01	0.42
1:C:118:GLU:HA	1:C:118:GLU:OE1	2.19	0.42
1:B:118:GLU:OE1	1:B:118:GLU:HA	2.19	0.42
1:C:628:PHE:CZ	1:C:651:GLU:HG2	2.54	0.42
1:D:623:HIS:HB2	1:D:718:TRP:CZ2	2.54	0.42
1:A:102:THR:OG1	1:A:105:THR:O	2.30	0.42
1:A:488:GLU:HG3	1:A:503:MET:HG3	2.01	0.42
1:B:695:LEU:HD23	1:B:695:LEU:HA	1.94	0.42
1:C:781:LEU:HD11	1:C:885:LEU:HB3	2.01	0.42
1:D:23:THR:O	1:D:164:GLN:HB2	2.18	0.42
1:A:623:HIS:HB2	1:A:718:TRP:CZ2	2.54	0.42
1:A:781:LEU:HD11	1:A:885:LEU:HB3	2.01	0.42
1:B:31:HIS:ND1	1:B:32:PRO:O	2.36	0.42
1:B:628:PHE:CZ	1:B:651:GLU:HG2	2.54	0.42
1:B:781:LEU:HD11	1:B:885:LEU:HB3	2.01	0.42
1:B:959:ASN:HD21	1:B:986:ASN:HD22	1.67	0.42
1:C:31:HIS:ND1	1:C:32:PRO:O	2.36	0.42
1:D:488:GLU:HG3	1:D:503:MET:HG3	2.01	0.42
1:D:781:LEU:HD11	1:D:885:LEU:HB3	2.01	0.42
1:D:697:LEU:HB2	1:D:723:LEU:HD11	2.02	0.42
1:A:212:ASP:OD1	1:A:212:ASP:N	2.52	0.41
1:A:697:LEU:HB2	1:A:723:LEU:HD11	2.02	0.41
1:C:64:PHE:CD2	1:C:70:VAL:HG22	2.54	0.41
1:C:959:ASN:HD21	1:C:986:ASN:HD22	1.67	0.41
1:D:212:ASP:OD1	1:D:212:ASP:N	2.52	0.41
1:B:64:PHE:CD2	1:B:70:VAL:HG22	2.54	0.41
1:B:212:ASP:OD1	1:B:212:ASP:N	2.52	0.41
1:C:201:GLN:HG2	1:C:392:HIS:HB3	2.02	0.41
1:C:695:LEU:HD23	1:C:695:LEU:HA	1.94	0.41
1:B:201:GLN:HG2	1:B:392:HIS:HB3	2.02	0.41
1:A:785:PHE:HA	1:A:882:ARG:O	2.20	0.41
1:C:212:ASP:OD1	1:C:212:ASP:N	2.52	0.41
1:B:697:LEU:HB2	1:B:723:LEU:HD11	2.02	0.41
1:D:148:ASN:HA	1:D:149:SER:HA	1.59	0.41
1:D:474:ARG:HA	1:D:474:ARG:HD2	1.89	0.41
1:D:785:PHE:HA	1:D:882:ARG:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:470:ASP:HB3	1:D:474:ARG:HG3	2.02	0.41
1:A:474:ARG:HA	1:A:474:ARG:HD2	1.89	0.41
1:A:874:ALA:O	1:A:877:THR:HG22	2.21	0.41
1:C:697:LEU:HB2	1:C:723:LEU:HD11	2.02	0.41
1:A:474:ARG:HG3	1:D:470:ASP:HB3	2.03	0.41
1:A:959:ASN:HD21	1:A:986:ASN:HD22	1.67	0.41
1:C:978:HIS:HD1	1:C:978:HIS:C	2.28	0.41
1:D:874:ALA:O	1:D:877:THR:HG22	2.21	0.41
1:D:959:ASN:HD21	1:D:986:ASN:HD22	1.67	0.41
1:A:694:GLN:OE1	1:A:725:GLU:HB2	2.21	0.41
1:C:760:ASN:HB2	1:C:767:SER:OG	2.20	0.41
1:D:686:LEU:HD23	1:D:686:LEU:HA	1.92	0.41
1:D:694:GLN:OE1	1:D:725:GLU:HB2	2.21	0.41
1:B:694:GLN:OE1	1:B:725:GLU:HB2	2.21	0.41
1:B:760:ASN:HB2	1:B:767:SER:OG	2.20	0.41
1:B:785:PHE:HA	1:B:882:ARG:O	2.20	0.41
1:B:978:HIS:HD1	1:B:978:HIS:C	2.28	0.41
1:C:350:LEU:HD23	1:C:350:LEU:HA	1.96	0.41
1:C:694:GLN:OE1	1:C:725:GLU:HB2	2.21	0.41
1:C:785:PHE:HA	1:C:882:ARG:O	2.20	0.41
1:A:695:LEU:HD23	1:A:695:LEU:HA	1.94	0.41
1:B:92:GLN:HB3	1:B:99:PRO:HD3	2.03	0.40
1:B:350:LEU:HD23	1:B:350:LEU:HA	1.96	0.40
1:C:92:GLN:HB3	1:C:99:PRO:HD3	2.03	0.40
1:A:686:LEU:HD23	1:A:686:LEU:HA	1.92	0.40
1:D:760:ASN:HB2	1:D:767:SER:OG	2.20	0.40
1:A:760:ASN:HB2	1:A:767:SER:OG	2.20	0.40
1:D:695:LEU:HD23	1:D:695:LEU:HA	1.94	0.40
1:A:128:PHE:HE1	1:A:185:LEU:HG	1.87	0.40
1:D:128:PHE:HE1	1:D:185:LEU:HG	1.87	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	1010/1030 (98%)	977 (97%)	31 (3%)	2 (0%)	43	57
1	B	1010/1030 (98%)	977 (97%)	31 (3%)	2 (0%)	43	57
1	C	1010/1030 (98%)	977 (97%)	31 (3%)	2 (0%)	43	57
1	D	1010/1030 (98%)	977 (97%)	31 (3%)	2 (0%)	43	57
All	All	4040/4120 (98%)	3908 (97%)	124 (3%)	8 (0%)	44	57

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	796	VAL
1	B	796	VAL
1	C	796	VAL
1	D	796	VAL
1	A	802	ILE
1	B	802	ILE
1	C	802	ILE
1	D	802	ILE

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	868/882 (98%)	862 (99%)	6 (1%)	76	87
1	B	868/882 (98%)	862 (99%)	6 (1%)	76	87
1	C	868/882 (98%)	863 (99%)	5 (1%)	78	88
1	D	868/882 (98%)	861 (99%)	7 (1%)	73	85
All	All	3472/3528 (98%)	3448 (99%)	24 (1%)	73	87

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	260	SER
1	A	345	LEU
1	A	439	GLU
1	A	547	LEU
1	A	796	VAL
1	A	856	THR
1	B	260	SER
1	B	345	LEU
1	B	439	GLU
1	B	547	LEU
1	B	796	VAL
1	B	856	THR
1	C	345	LEU
1	C	439	GLU
1	C	547	LEU
1	C	796	VAL
1	C	856	THR
1	D	231	ARG
1	D	260	SER
1	D	345	LEU
1	D	439	GLU
1	D	547	LEU
1	D	796	VAL
1	D	856	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (95) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	39	ASN
1	A	136	GLN
1	A	164	GLN
1	A	246	GLN
1	A	446	GLN
1	A	511	GLN
1	A	623	HIS
1	A	624	GLN
1	A	625	GLN
1	A	635	GLN
1	A	647	HIS
1	A	719	GLN
1	A	758	GLN
1	A	760	ASN
1	A	762	GLN

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Mol	Chain	Res	Type
1	A	844	GLN
1	A	845	HIS
1	A	897	ASN
1	A	946	ASN
1	A	951	GLN
1	A	957	GLN
1	A	959	ASN
1	A	967	GLN
1	A	991	HIS
1	A	1018	GLN
1	B	39	ASN
1	B	136	GLN
1	B	164	GLN
1	B	246	GLN
1	B	511	GLN
1	B	623	HIS
1	B	624	GLN
1	B	635	GLN
1	B	719	GLN
1	B	758	GLN
1	B	760	ASN
1	B	762	GLN
1	B	844	GLN
1	B	845	HIS
1	B	897	ASN
1	B	946	ASN
1	B	951	GLN
1	B	957	GLN
1	B	959	ASN
1	B	967	GLN
1	B	991	HIS
1	B	1016	HIS
1	B	1018	GLN
1	C	39	ASN
1	C	136	GLN
1	C	164	GLN
1	C	246	GLN
1	C	511	GLN
1	C	623	HIS
1	C	624	GLN
1	C	635	GLN
1	C	719	GLN

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Mol	Chain	Res	Type
1	C	758	GLN
1	C	760	ASN
1	C	762	GLN
1	C	844	GLN
1	C	845	HIS
1	C	897	ASN
1	C	946	ASN
1	C	951	GLN
1	C	957	GLN
1	C	959	ASN
1	C	967	GLN
1	C	991	HIS
1	C	1018	GLN
1	D	39	ASN
1	D	136	GLN
1	D	164	GLN
1	D	246	GLN
1	D	446	GLN
1	D	511	GLN
1	D	623	HIS
1	D	624	GLN
1	D	625	GLN
1	D	635	GLN
1	D	647	HIS
1	D	719	GLN
1	D	758	GLN
1	D	760	ASN
1	D	762	GLN
1	D	844	GLN
1	D	845	HIS
1	D	897	ASN
1	D	946	ASN
1	D	951	GLN
1	D	957	GLN
1	D	959	ASN
1	D	967	GLN
1	D	991	HIS
1	D	1018	GLN

5.3.3 RNA ⓘ

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 12 ligands modelled in this entry, 12 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

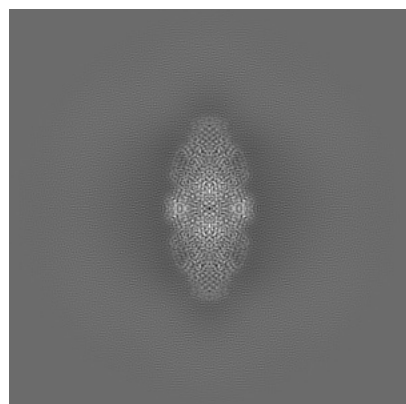
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-72471. These allow visual inspection of the internal detail of the map and identification of artifacts.

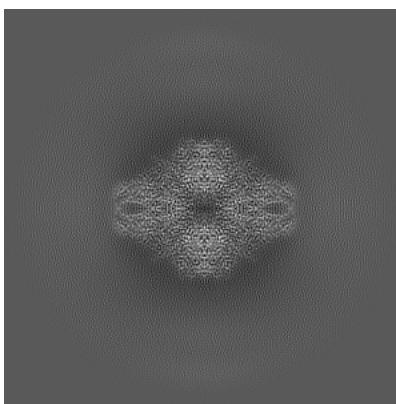
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

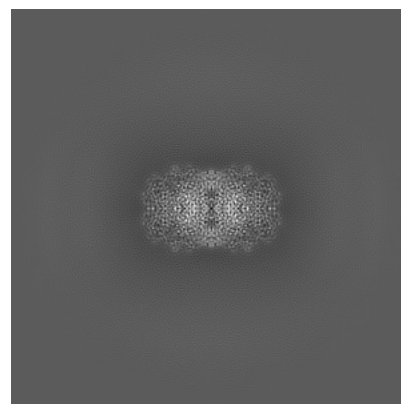
6.1.1 Primary map



X

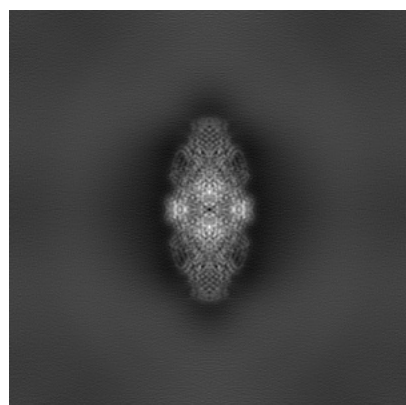


Y

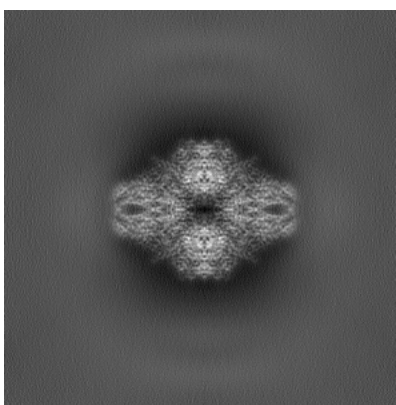


Z

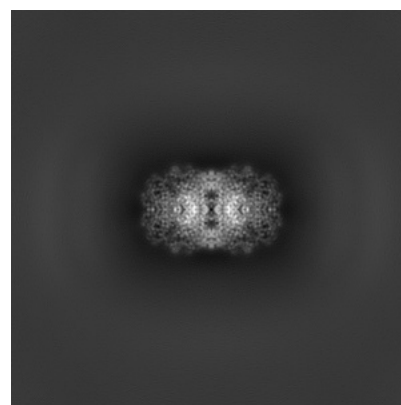
6.1.2 Raw map



X



Y

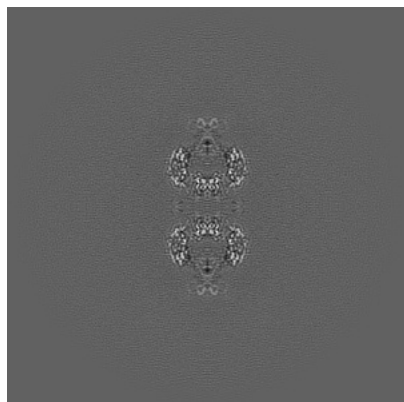


Z

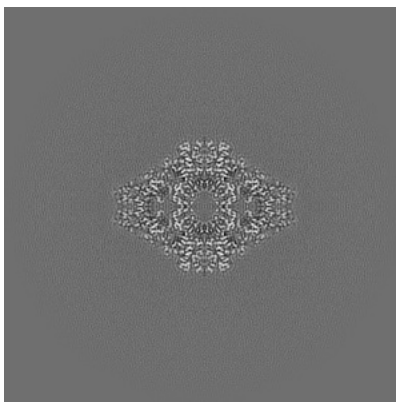
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

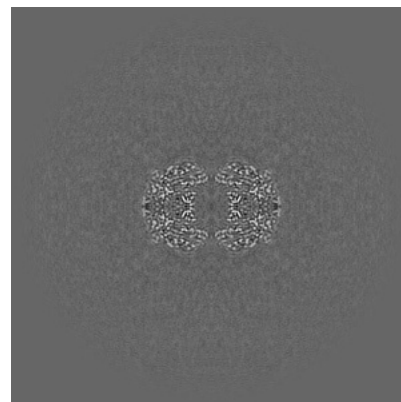
6.2.1 Primary map



X Index: 220

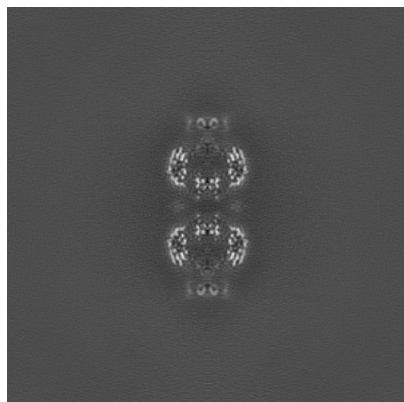


Y Index: 220

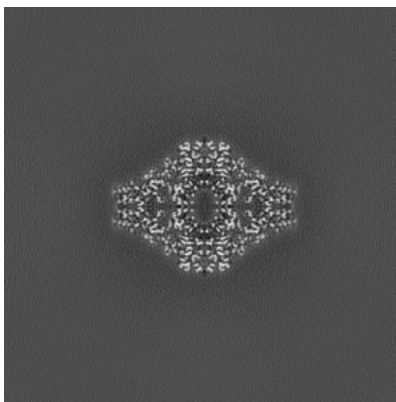


Z Index: 220

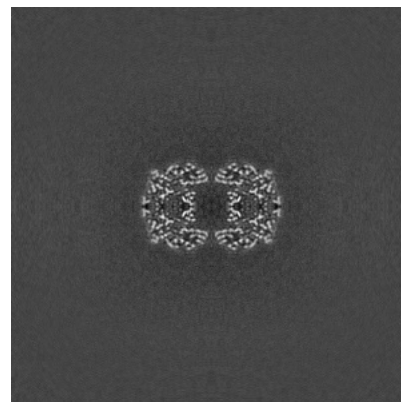
6.2.2 Raw map



X Index: 220



Y Index: 220

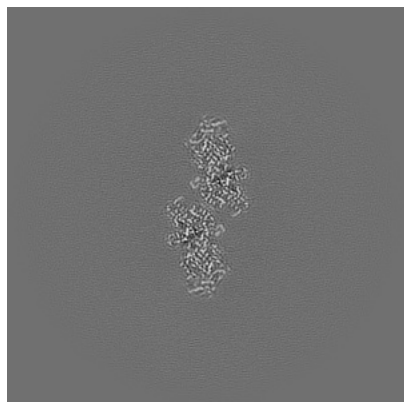


Z Index: 220

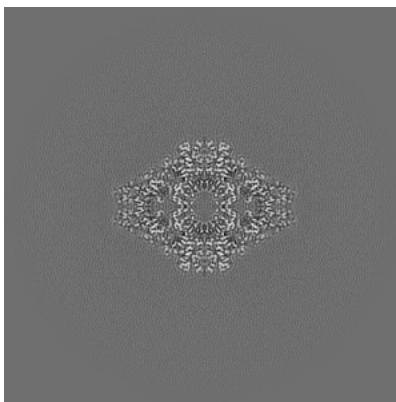
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

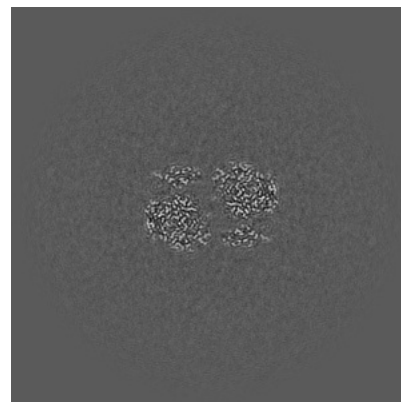
6.3.1 Primary map



X Index: 201

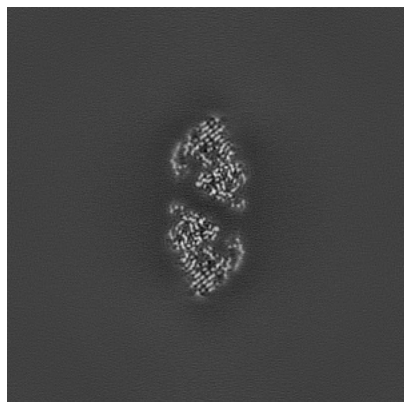


Y Index: 220

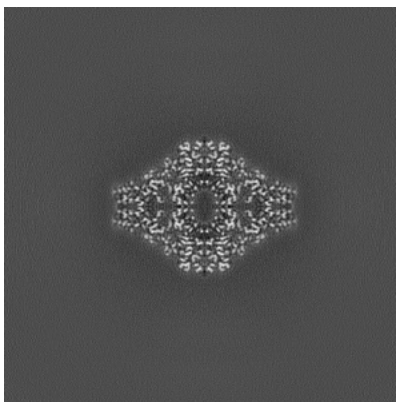


Z Index: 214

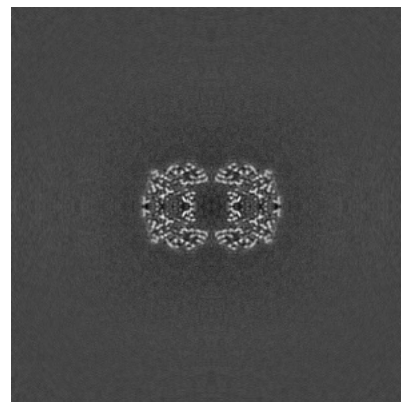
6.3.2 Raw map



X Index: 211



Y Index: 220

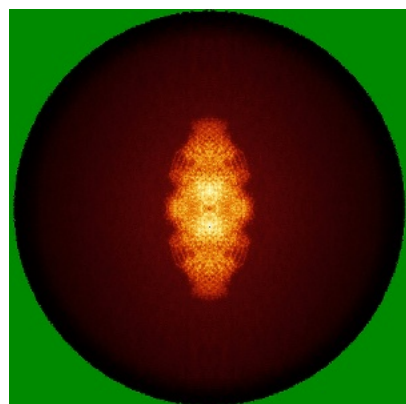


Z Index: 220

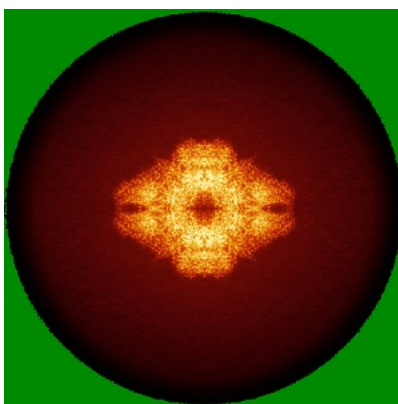
The images above show the largest variance slices of the map in three orthogonal directions.

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

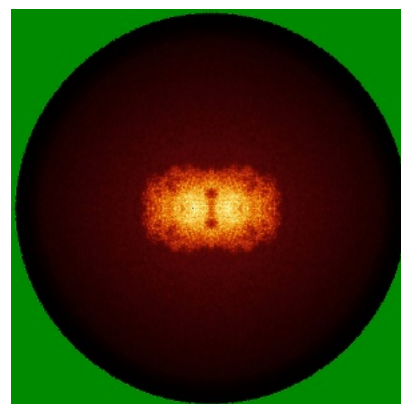
6.4.1 Primary map



X

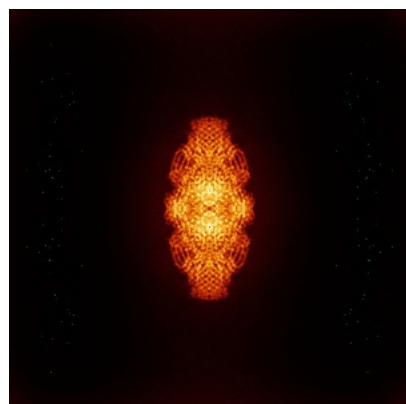


Y

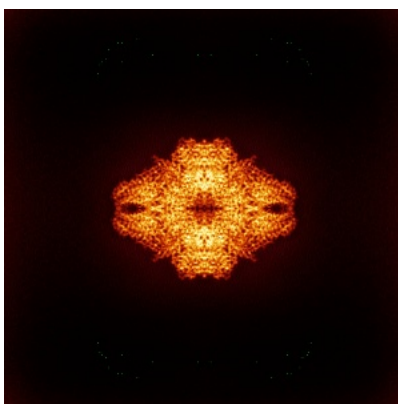


Z

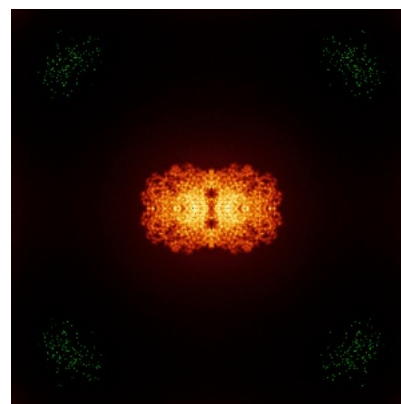
6.4.2 Raw map



X



Y

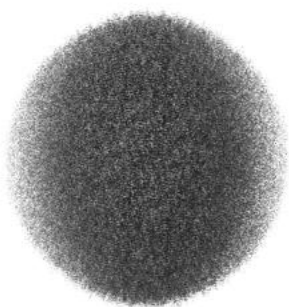


Z

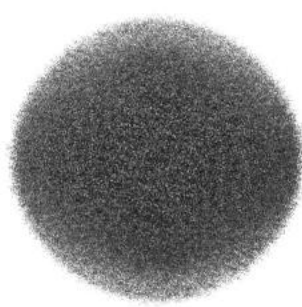
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



X



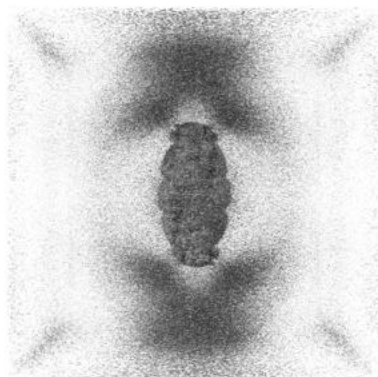
Y



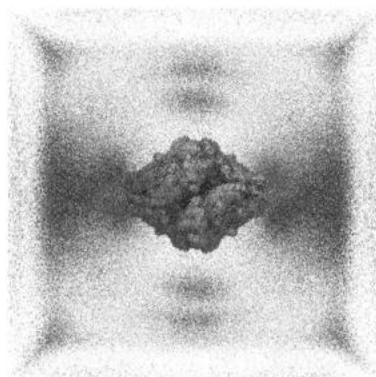
Z

The images above show the 3D surface view of the map at the recommended contour level 0.1. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

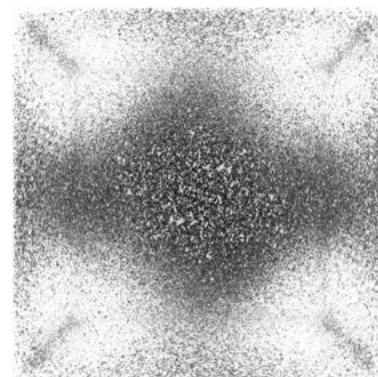
6.5.2 Raw map



X



Y



Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

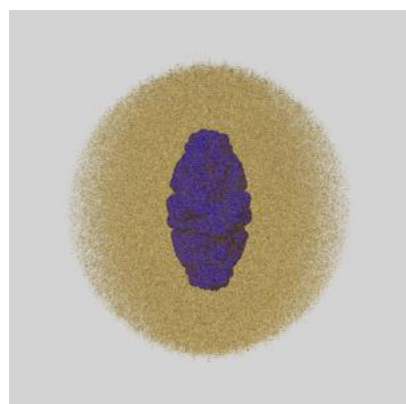
6.6 Mask visualisation [i](#)

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

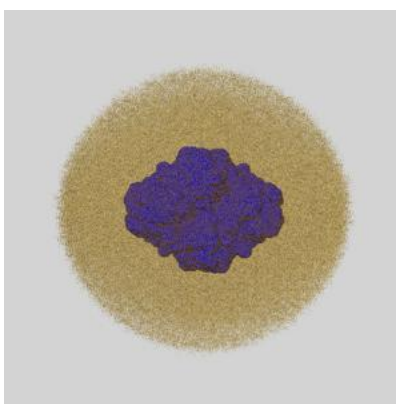
A mask typically either:

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

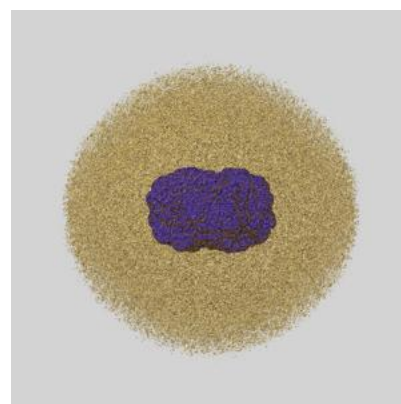
6.6.1 emd_72471_msk_1.map [i](#)



X

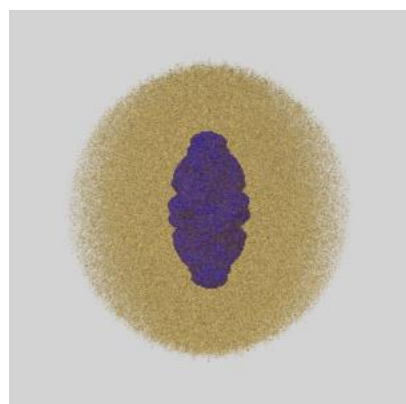


Y

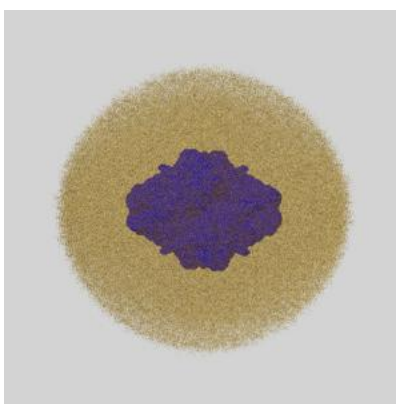


Z

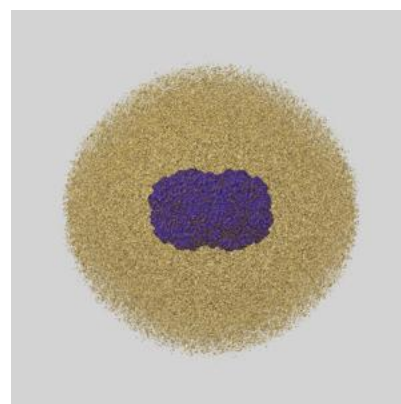
6.6.2 emd_72471_msk_2.map [i](#)



X



Y

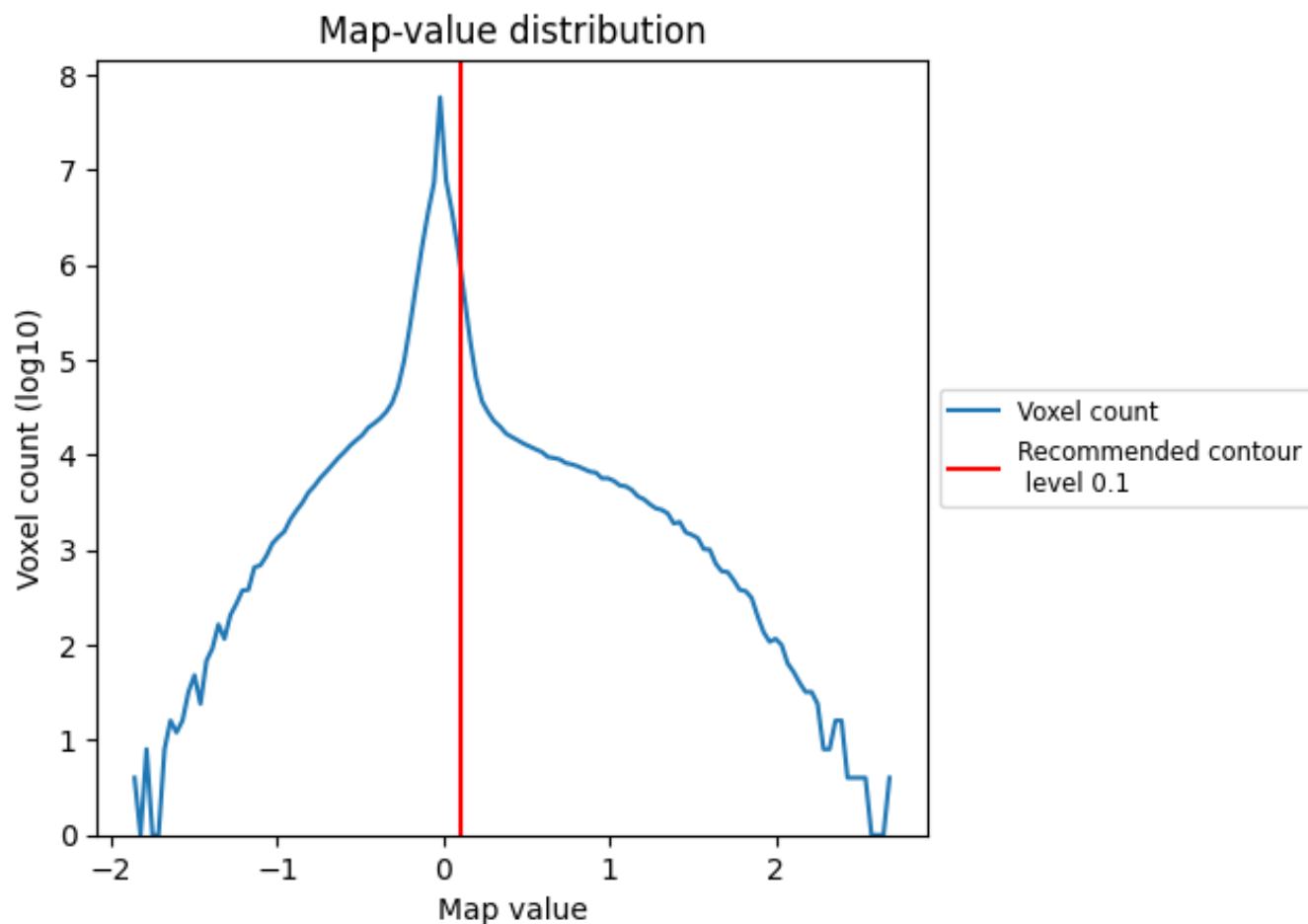


Z

7 Map analysis [i](#)

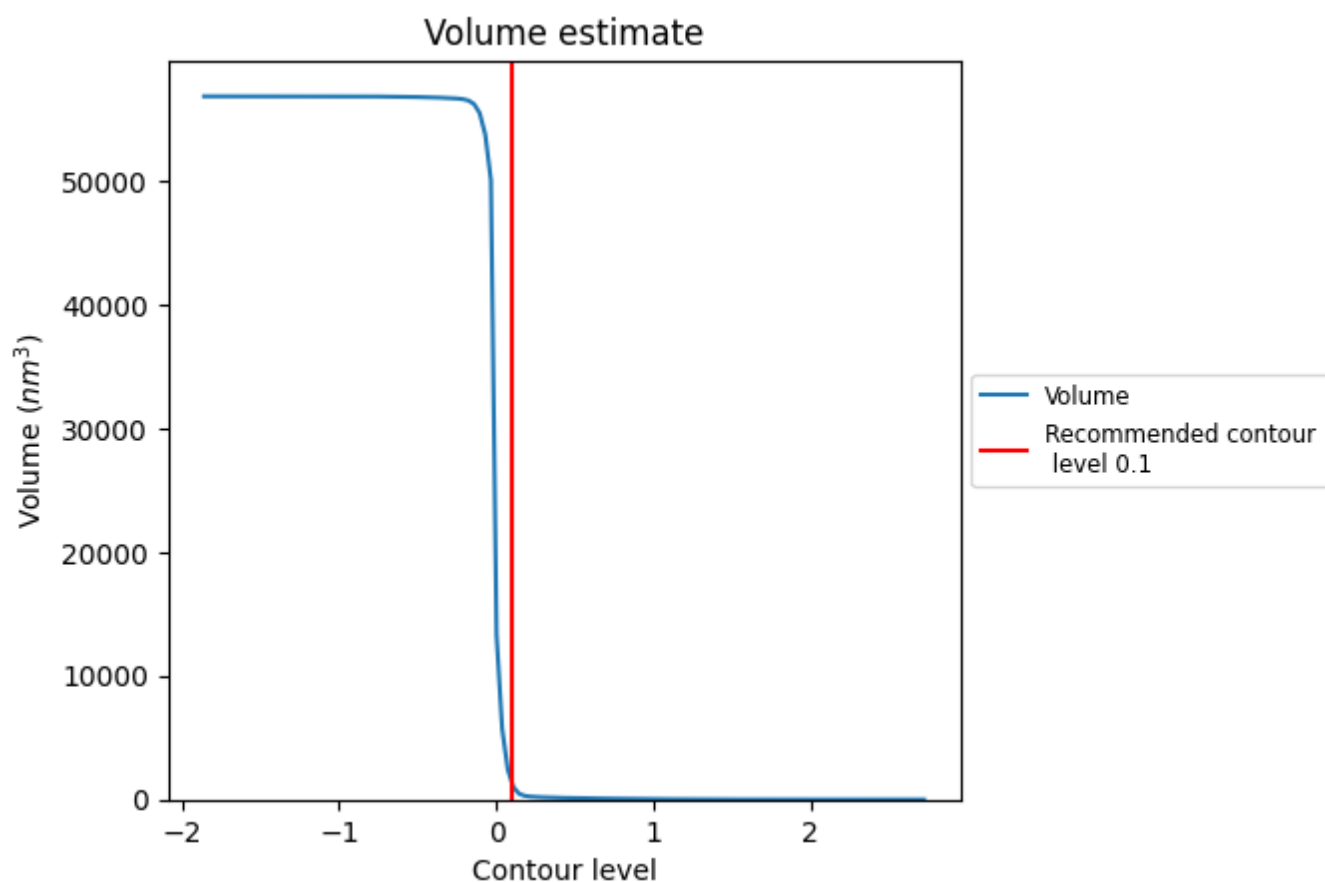
This section contains the results of statistical analysis of the map.

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.

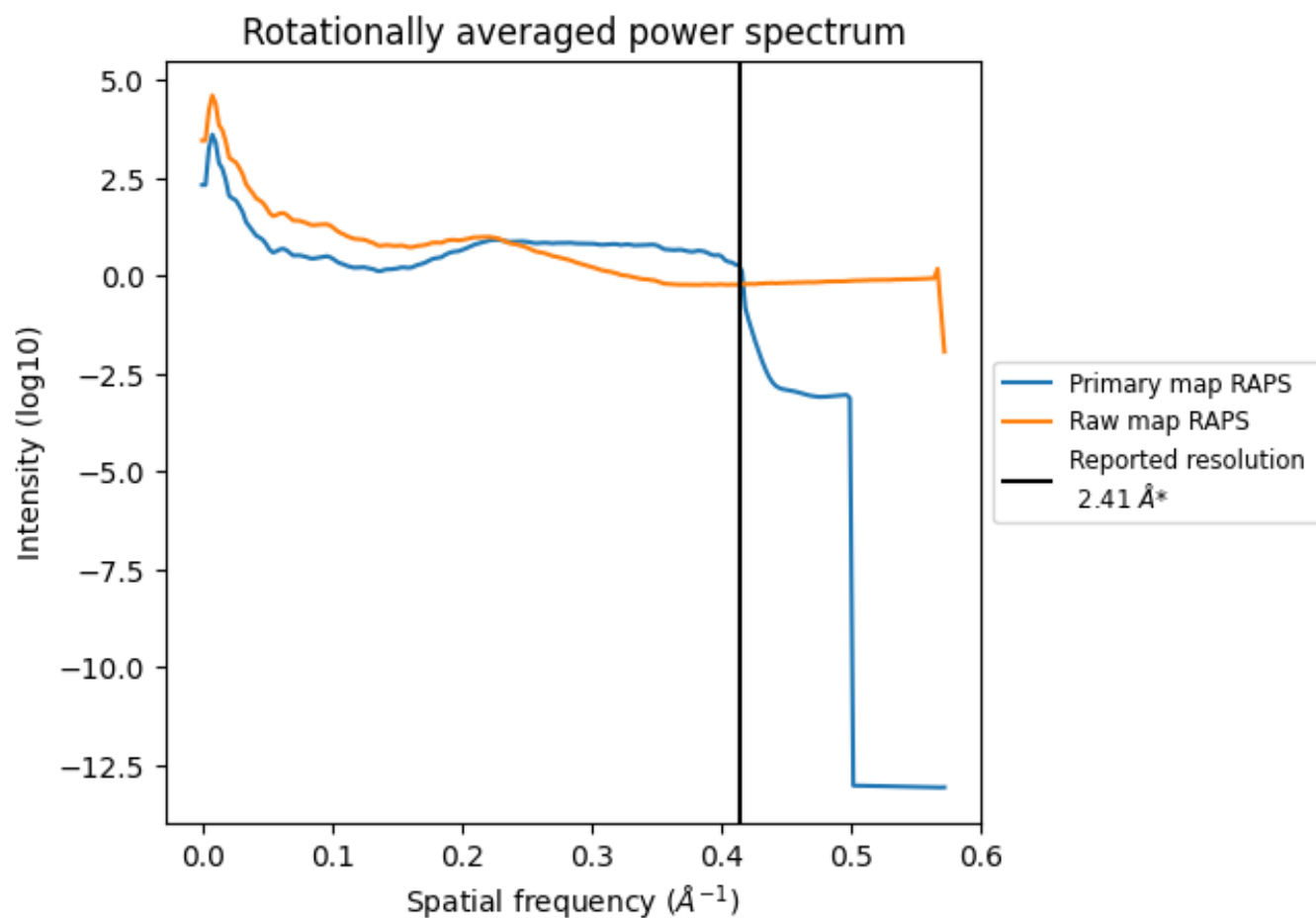
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1378 nm^3 ; this corresponds to an approximate mass of 1245 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 ⓘ

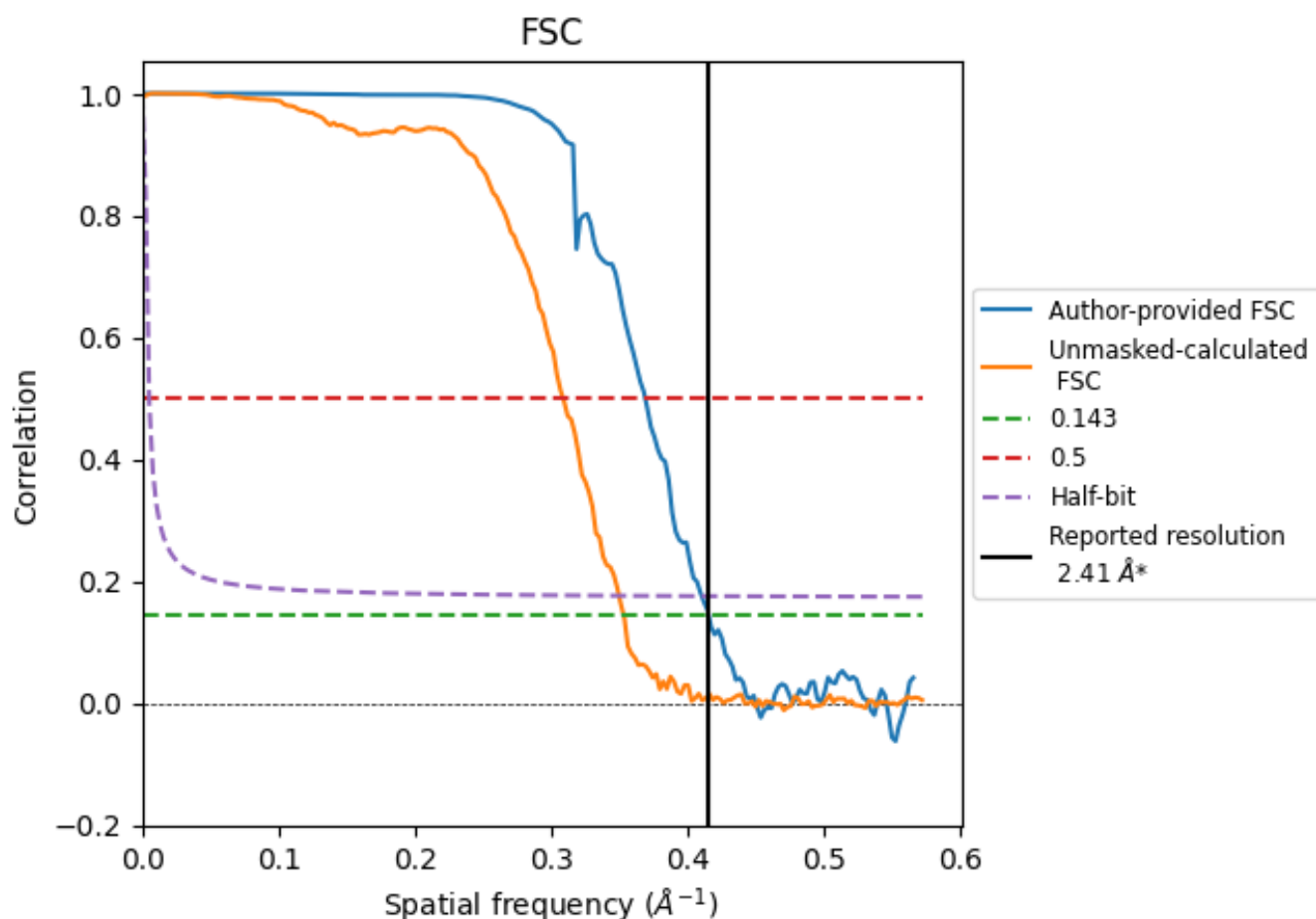


*Reported resolution corresponds to spatial frequency of 0.415 $\text{\AA}^{-1}$

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of $0.415 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

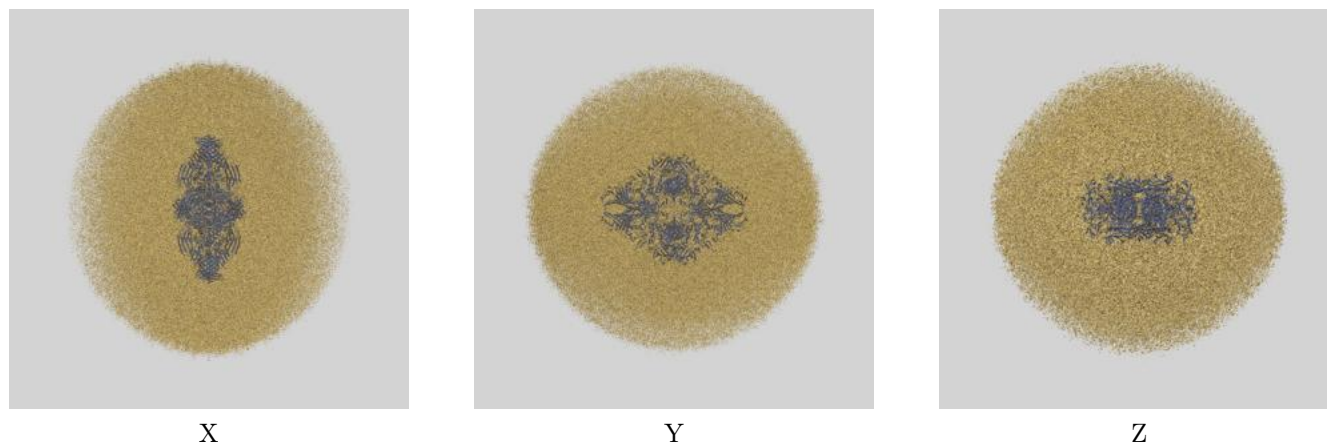
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.41	-	-
Author-provided FSC curve	2.41	2.71	2.44
Unmasked-calculated*	2.83	3.24	2.86

*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 2.83 differs from the reported value 2.41 by more than 10 %

9 Map-model fit [i](#)

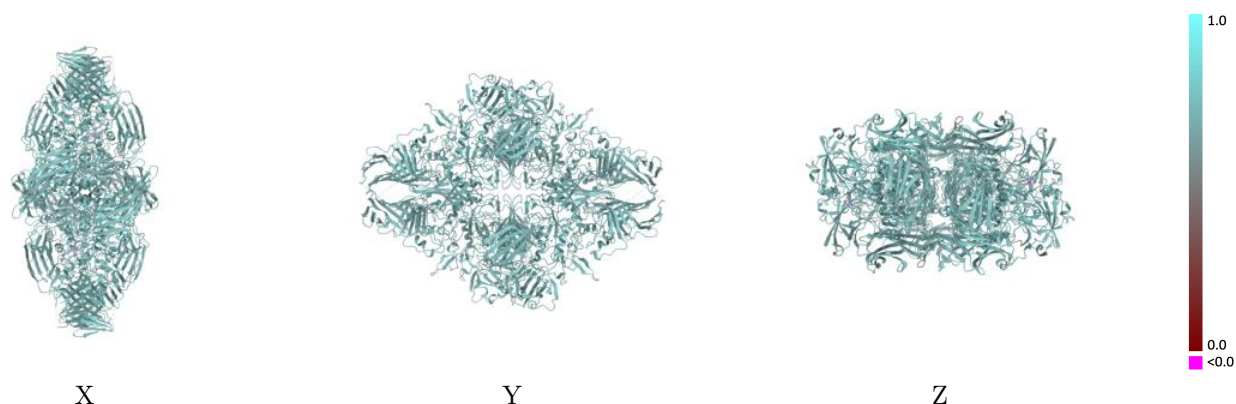
This section contains information regarding the fit between EMDB map EMD-72471 and PDB model 9Y45. Per-residue inclusion information can be found in [section 3](#) on [page 5](#).

9.1 Map-model overlay [i](#)



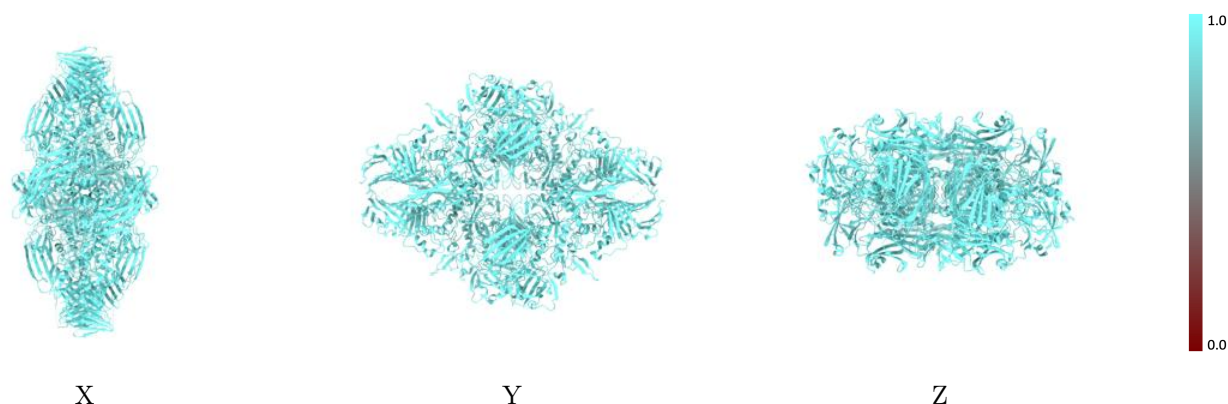
The images above show the 3D surface view of the map at the recommended contour level 0.1 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



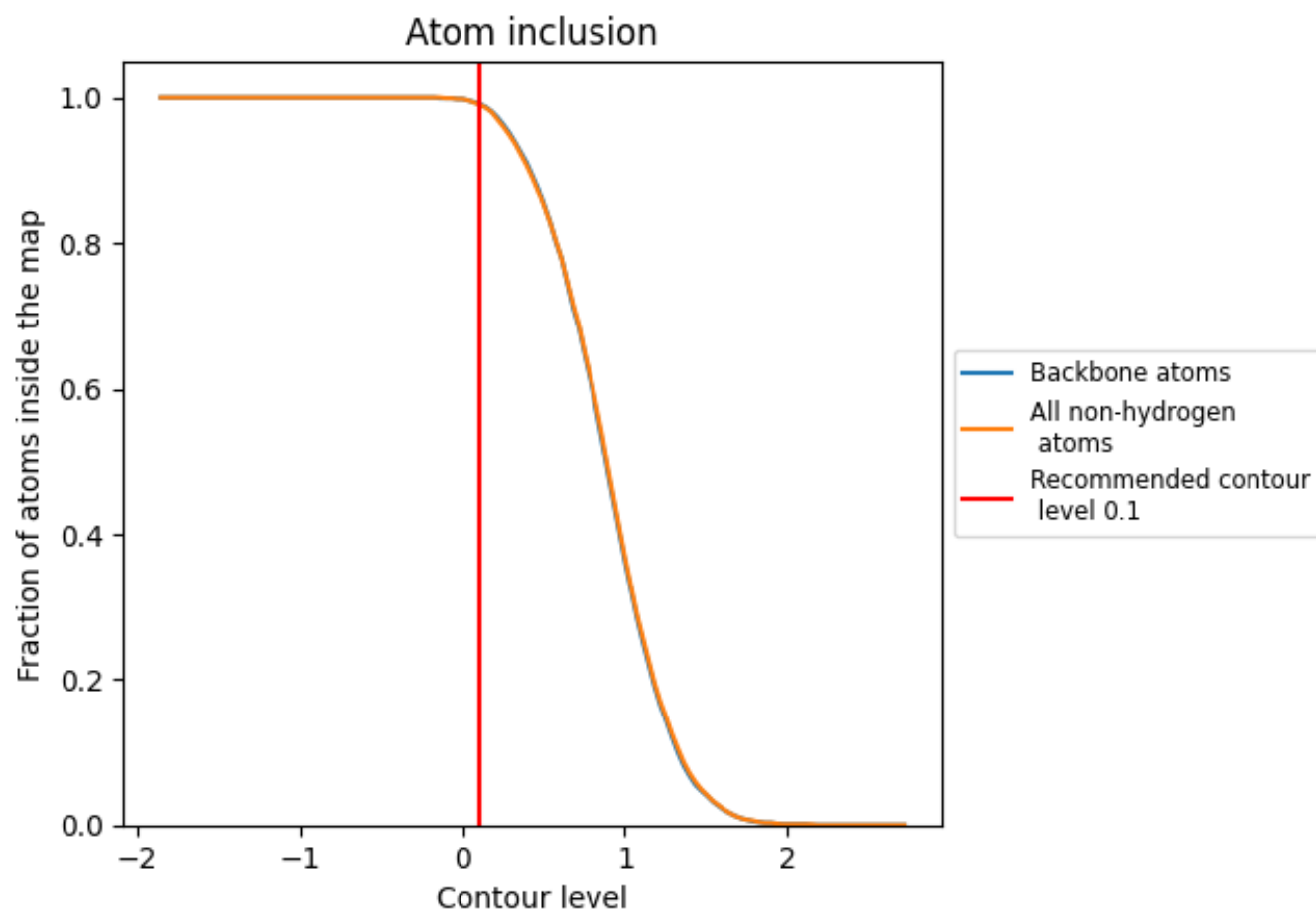
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.1).

9.4 Atom inclusion [i](#)



At the recommended contour level, 99% of all backbone atoms, 99% 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 (0.1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9910	0.6840
A	0.9920	0.6830
B	0.9920	0.6840
C	0.9920	0.6840
D	0.9920	0.6830

