



## Full wwPDB EM Validation Report ⓘ

Oct 12, 2024 – 11:11 pm BST

PDB ID : 8AVE  
EMDB ID : EMD-15680  
Title : Human leptin in complex with the human LEP-R ectodomain fused to a C-terminal trimeric isoleucine GCN4 zipper (2:2 model)  
Authors : Verstraete, K.; Savvides, S.N.; Verschueren, K.G.; Tsirigotaki, A.  
Deposited on : 2022-08-26  
Resolution : 5.62 Å (reported)  
Based on initial models : 7Z3Q, 7Z3R

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.dev113  
MolProbity : 4.02b-467  
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

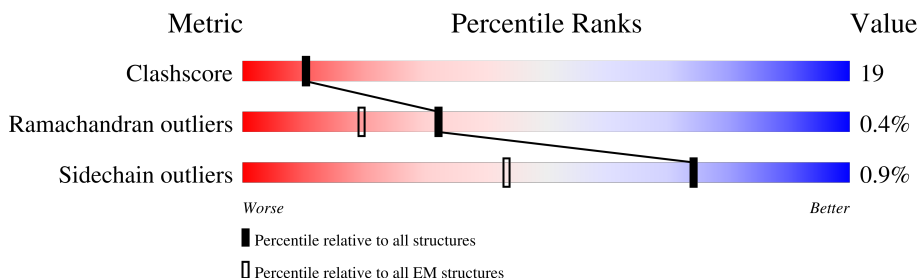
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 5.62 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	171	<div> <div>19%</div> <div>40%</div> <div>43%</div> <div>15%</div> </div>
1	C	171	<div> <div>6%</div> <div>38%</div> <div>45%</div> <div>15%</div> </div>
2	B	868	<div> <div>11%</div> <div>49%</div> <div>19%</div> <div>31%</div> </div>
2	D	868	<div> <div>27%</div> <div>48%</div> <div>20%</div> <div>31%</div> </div>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 11874 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 Leptin.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	146	Total	C	N	O	S	0	0
			1124	709	190	220	5		
1	C	146	Total	C	N	O	S	0	0
			1124	709	190	220	5		

There are 50 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	ALA	-	expression tag	UNP P41159
A	-2	HIS	-	expression tag	UNP P41159
A	-1	HIS	-	expression tag	UNP P41159
A	0	HIS	-	expression tag	UNP P41159
A	1	HIS	-	expression tag	UNP P41159
A	2	HIS	-	expression tag	UNP P41159
A	3	HIS	-	expression tag	UNP P41159
A	4	PRO	-	expression tag	UNP P41159
A	5	GLY	-	expression tag	UNP P41159
A	6	GLY	-	expression tag	UNP P41159
A	7	PRO	-	expression tag	UNP P41159
A	8	GLY	-	expression tag	UNP P41159
A	9	SER	-	expression tag	UNP P41159
A	10	GLU	-	expression tag	UNP P41159
A	11	ASN	-	expression tag	UNP P41159
A	12	LEU	-	expression tag	UNP P41159
A	13	TYR	-	expression tag	UNP P41159
A	14	PHE	-	expression tag	UNP P41159
A	15	GLN	-	expression tag	UNP P41159
A	16	GLY	-	expression tag	UNP P41159
A	17	GLY	-	expression tag	UNP P41159
A	18	SER	-	expression tag	UNP P41159
A	19	THR	-	expression tag	UNP P41159
A	20	GLY	-	expression tag	UNP P41159
A	21	GLY	-	expression tag	UNP P41159
C	-3	ALA	-	expression tag	UNP P41159

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-2	HIS	-	expression tag	UNP P41159
C	-1	HIS	-	expression tag	UNP P41159
C	0	HIS	-	expression tag	UNP P41159
C	1	HIS	-	expression tag	UNP P41159
C	2	HIS	-	expression tag	UNP P41159
C	3	HIS	-	expression tag	UNP P41159
C	4	PRO	-	expression tag	UNP P41159
C	5	GLY	-	expression tag	UNP P41159
C	6	GLY	-	expression tag	UNP P41159
C	7	PRO	-	expression tag	UNP P41159
C	8	GLY	-	expression tag	UNP P41159
C	9	SER	-	expression tag	UNP P41159
C	10	GLU	-	expression tag	UNP P41159
C	11	ASN	-	expression tag	UNP P41159
C	12	LEU	-	expression tag	UNP P41159
C	13	TYR	-	expression tag	UNP P41159
C	14	PHE	-	expression tag	UNP P41159
C	15	GLN	-	expression tag	UNP P41159
C	16	GLY	-	expression tag	UNP P41159
C	17	GLY	-	expression tag	UNP P41159
C	18	SER	-	expression tag	UNP P41159
C	19	THR	-	expression tag	UNP P41159
C	20	GLY	-	expression tag	UNP P41159
C	21	GLY	-	expression tag	UNP P41159

- Molecule 2 is a protein called Leptin receptor.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	596	Total	C	N	O	S	0	0
			4813	3113	786	887	27		
2	D	596	Total	C	N	O	S	0	0
			4813	3113	786	887	27		

There are 100 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	840	SER	-	expression tag	UNP P48357
B	841	THR	-	expression tag	UNP P48357
B	842	GLY	-	expression tag	UNP P48357
B	843	GLY	-	expression tag	UNP P48357
B	844	SER	-	expression tag	UNP P48357
B	845	GLY	-	expression tag	UNP P48357

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Chain	Residue	Modelled	Actual	Comment	Reference
B	846	GLY	-	expression tag	UNP P48357
B	847	SER	-	expression tag	UNP P48357
B	848	GLY	-	expression tag	UNP P48357
B	849	GLY	-	expression tag	UNP P48357
B	850	SER	-	expression tag	UNP P48357
B	851	GLY	-	expression tag	UNP P48357
B	852	GLY	-	expression tag	UNP P48357
B	853	SER	-	expression tag	UNP P48357
B	854	GLY	-	expression tag	UNP P48357
B	855	GLY	-	expression tag	UNP P48357
B	856	SER	-	expression tag	UNP P48357
B	857	ARG	-	expression tag	UNP P48357
B	858	MET	-	expression tag	UNP P48357
B	859	LYS	-	expression tag	UNP P48357
B	860	GLN	-	expression tag	UNP P48357
B	861	ILE	-	expression tag	UNP P48357
B	862	GLU	-	expression tag	UNP P48357
B	863	ASP	-	expression tag	UNP P48357
B	864	LYS	-	expression tag	UNP P48357
B	865	ILE	-	expression tag	UNP P48357
B	866	GLU	-	expression tag	UNP P48357
B	867	GLU	-	expression tag	UNP P48357
B	868	ILE	-	expression tag	UNP P48357
B	869	LEU	-	expression tag	UNP P48357
B	870	SER	-	expression tag	UNP P48357
B	871	LYS	-	expression tag	UNP P48357
B	872	ILE	-	expression tag	UNP P48357
B	873	TYR	-	expression tag	UNP P48357
B	874	HIS	-	expression tag	UNP P48357
B	875	ILE	-	expression tag	UNP P48357
B	876	GLU	-	expression tag	UNP P48357
B	877	ASN	-	expression tag	UNP P48357
B	878	GLU	-	expression tag	UNP P48357
B	879	ILE	-	expression tag	UNP P48357
B	880	ALA	-	expression tag	UNP P48357
B	881	ARG	-	expression tag	UNP P48357
B	882	ILE	-	expression tag	UNP P48357
B	883	LYS	-	expression tag	UNP P48357
B	884	LYS	-	expression tag	UNP P48357
B	885	LEU	-	expression tag	UNP P48357
B	886	ILE	-	expression tag	UNP P48357
B	887	GLY	-	expression tag	UNP P48357

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Chain	Residue	Modelled	Actual	Comment	Reference
B	888	GLU	-	expression tag	UNP P48357
B	889	ARG	-	expression tag	UNP P48357
D	840	SER	-	expression tag	UNP P48357
D	841	THR	-	expression tag	UNP P48357
D	842	GLY	-	expression tag	UNP P48357
D	843	GLY	-	expression tag	UNP P48357
D	844	SER	-	expression tag	UNP P48357
D	845	GLY	-	expression tag	UNP P48357
D	846	GLY	-	expression tag	UNP P48357
D	847	SER	-	expression tag	UNP P48357
D	848	GLY	-	expression tag	UNP P48357
D	849	GLY	-	expression tag	UNP P48357
D	850	SER	-	expression tag	UNP P48357
D	851	GLY	-	expression tag	UNP P48357
D	852	GLY	-	expression tag	UNP P48357
D	853	SER	-	expression tag	UNP P48357
D	854	GLY	-	expression tag	UNP P48357
D	855	GLY	-	expression tag	UNP P48357
D	856	SER	-	expression tag	UNP P48357
D	857	ARG	-	expression tag	UNP P48357
D	858	MET	-	expression tag	UNP P48357
D	859	LYS	-	expression tag	UNP P48357
D	860	GLN	-	expression tag	UNP P48357
D	861	ILE	-	expression tag	UNP P48357
D	862	GLU	-	expression tag	UNP P48357
D	863	ASP	-	expression tag	UNP P48357
D	864	LYS	-	expression tag	UNP P48357
D	865	ILE	-	expression tag	UNP P48357
D	866	GLU	-	expression tag	UNP P48357
D	867	GLU	-	expression tag	UNP P48357
D	868	ILE	-	expression tag	UNP P48357
D	869	LEU	-	expression tag	UNP P48357
D	870	SER	-	expression tag	UNP P48357
D	871	LYS	-	expression tag	UNP P48357
D	872	ILE	-	expression tag	UNP P48357
D	873	TYR	-	expression tag	UNP P48357
D	874	HIS	-	expression tag	UNP P48357
D	875	ILE	-	expression tag	UNP P48357
D	876	GLU	-	expression tag	UNP P48357
D	877	ASN	-	expression tag	UNP P48357
D	878	GLU	-	expression tag	UNP P48357
D	879	ILE	-	expression tag	UNP P48357

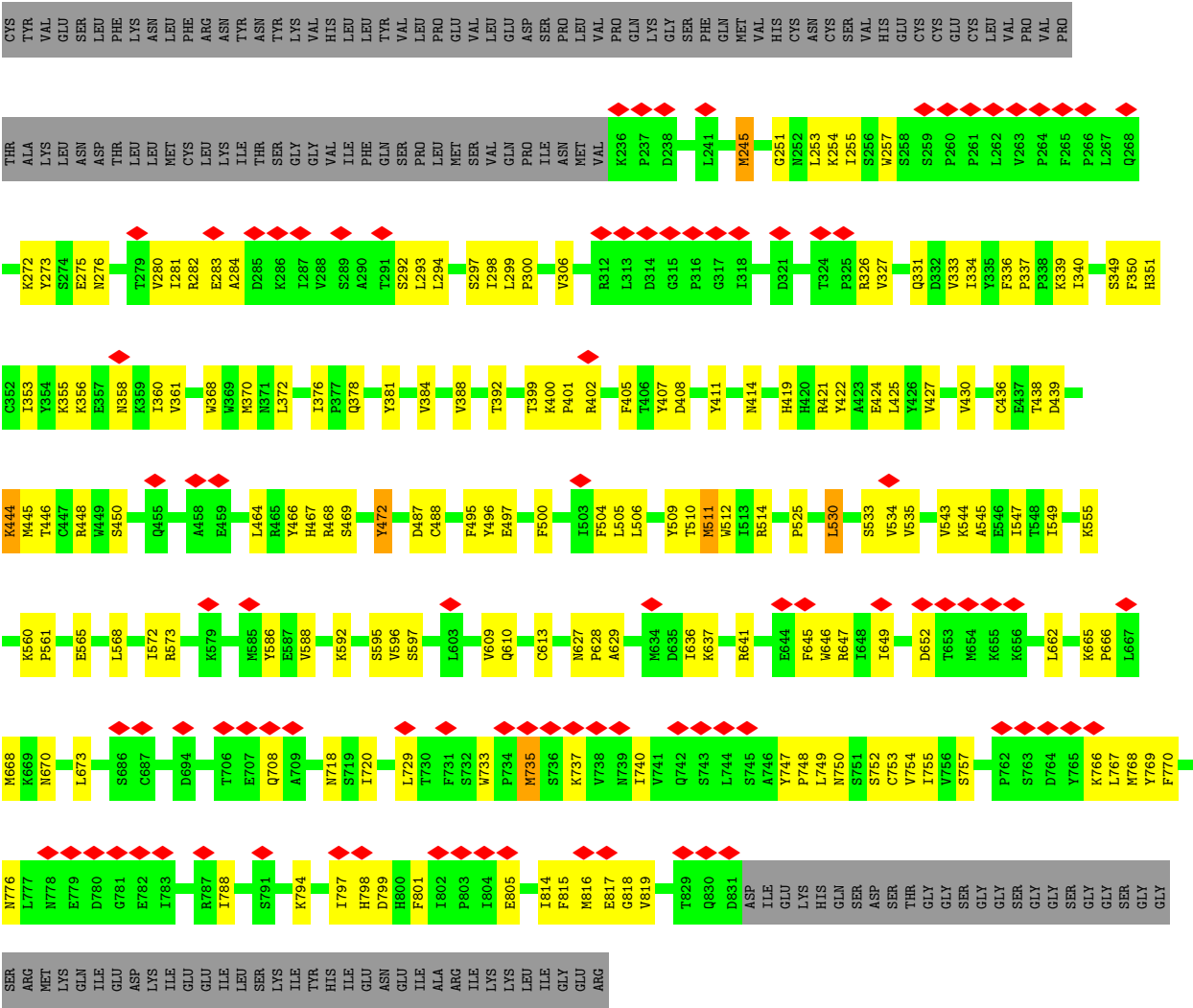
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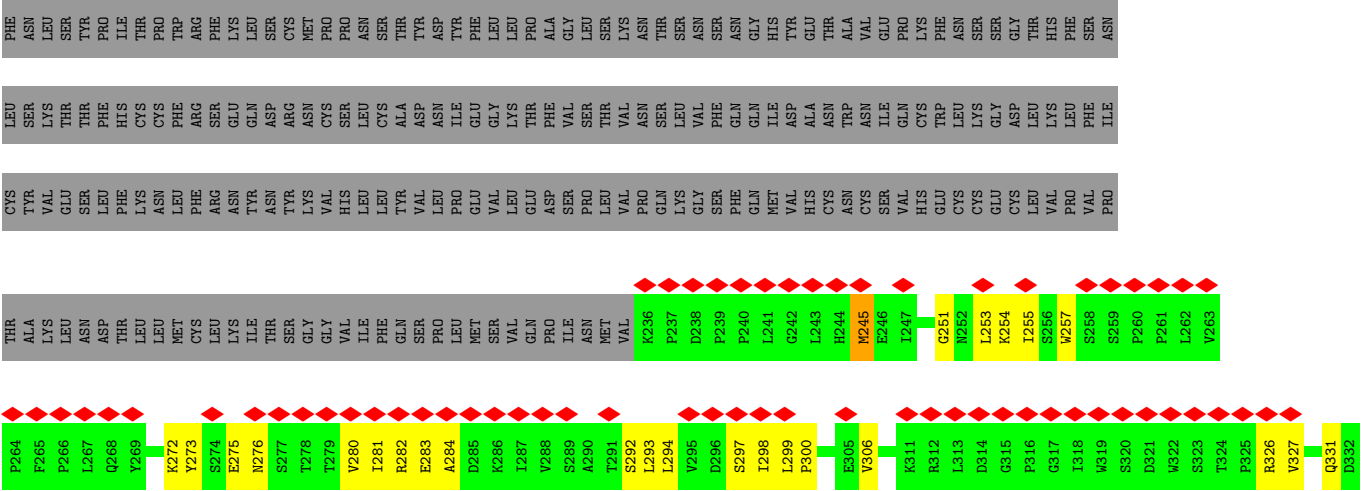
Chain	Residue	Modelled	Actual	Comment	Reference
D	880	ALA	-	expression tag	UNP P48357
D	881	ARG	-	expression tag	UNP P48357
D	882	ILE	-	expression tag	UNP P48357
D	883	LYS	-	expression tag	UNP P48357
D	884	LYS	-	expression tag	UNP P48357
D	885	LEU	-	expression tag	UNP P48357
D	886	ILE	-	expression tag	UNP P48357
D	887	GLY	-	expression tag	UNP P48357
D	888	GLU	-	expression tag	UNP P48357
D	889	ARG	-	expression tag	UNP P48357







● Molecule 2: Leptin receptor





## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	91899	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	JEOL CRYO ARM 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	62.4	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	2.772	Depositor
Minimum map value	-1.337	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.052	Depositor
Recommended contour level	0.55	Depositor
Map size (Å)	425.6, 425.6, 425.6	wwPDB
Map dimensions	280, 280, 280	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.52, 1.52, 1.52	Depositor

## 5 Model quality

### 5.1 Standard geometry

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	0.40	0/1141	0.87	4/1550 (0.3%)
1	C	0.41	0/1141	0.88	4/1550 (0.3%)
2	B	0.30	0/4956	0.64	4/6756 (0.1%)
2	D	0.30	0/4956	0.64	4/6756 (0.1%)
All	All	0.32	0/12194	0.69	16/16612 (0.1%)

There are no bond length outliers.

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	96	GLN	CB-CG-CD	-8.76	88.82	111.60
1	C	96	GLN	CB-CG-CD	-8.74	88.87	111.60
2	B	511	MET	CA-CB-CG	7.21	125.55	113.30
2	D	511	MET	CA-CB-CG	7.18	125.51	113.30
2	D	530	LEU	CA-CB-CG	6.15	129.44	115.30
2	B	530	LEU	CA-CB-CG	6.14	129.43	115.30
1	C	128	LEU	CB-CG-CD1	-5.99	100.82	111.00
1	A	128	LEU	CB-CG-CD1	-5.98	100.83	111.00
2	D	488	CYS	CA-CB-SG	-5.88	103.42	114.00
2	B	488	CYS	CA-CB-SG	-5.88	103.43	114.00
1	C	135	LEU	CA-CB-CG	5.85	128.75	115.30
1	A	135	LEU	CA-CB-CG	5.85	128.75	115.30
2	D	735	MET	CG-SD-CE	-5.77	90.97	100.20
2	B	735	MET	CG-SD-CE	-5.76	90.99	100.20
1	A	86	LEU	CB-CG-CD1	5.05	119.59	111.00
1	C	86	LEU	CB-CG-CD1	5.05	119.58	111.00

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	1124	0	1152	88	0
1	C	1124	0	1152	100	0
2	B	4813	0	4747	144	0
2	D	4813	0	4747	145	0
All	All	11874	0	11798	439	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 19.

All (439) 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:96:GLN:OE1	2:D:503:ILE:O	1.56	1.20
1:C:36:LYS:HD3	2:D:565:GLU:HB2	1.52	0.92
1:C:34:LEU:HD11	2:D:506:LEU:HG	1.53	0.91
1:C:96:GLN:O	1:C:99:ASN:HB2	1.72	0.90
1:A:96:GLN:O	1:A:99:ASN:HB2	1.72	0.89
2:B:794:LYS:HE3	2:D:802:ILE:HG21	1.57	0.86
1:C:70:LEU:H	1:C:74:LYS:HE3	1.40	0.86
1:A:70:LEU:H	1:A:74:LYS:HE3	1.40	0.83
2:D:439:ASP:HB3	2:D:444:LYS:HE3	1.64	0.80
2:B:439:ASP:HB3	2:B:444:LYS:HE3	1.64	0.79
2:D:333:VAL:HB	2:D:421:ARG:HD3	1.66	0.78
1:C:64:PRO:HG2	1:C:81:VAL:HG21	1.65	0.78
2:B:333:VAL:HB	2:B:421:ARG:HD3	1.66	0.77
1:A:160:GLN:HA	1:A:163:LEU:HD13	1.67	0.77
2:B:372:LEU:HD13	1:C:144:VAL:HG21	1.67	0.77
1:A:64:PRO:HG2	1:A:81:VAL:HG21	1.65	0.76
1:C:160:GLN:HA	1:C:163:LEU:HD13	1.67	0.75
2:B:411:TYR:CE1	2:B:422:TYR:HB3	2.22	0.75
1:A:60:LEU:HD21	1:A:142:THR:HG22	1.69	0.74
2:D:411:TYR:CE1	2:D:422:TYR:HB3	2.22	0.74
1:C:41:ARG:HH22	2:D:442:LEU:HB3	1.52	0.74
1:A:33:THR:O	1:A:37:THR:HG23	1.88	0.74
2:B:245:MET:SD	2:B:245:MET:N	2.61	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:99:ASN:O	1:A:102:GLU:HG3	1.89	0.73
1:C:33:THR:O	1:C:37:THR:HG23	1.88	0.73
1:A:70:LEU:N	1:A:74:LYS:HE3	2.04	0.73
1:C:60:LEU:HD21	1:C:142:THR:HG22	1.69	0.73
2:D:245:MET:SD	2:D:245:MET:N	2.61	0.73
2:D:419:HIS:HD2	2:D:421:ARG:HG2	1.53	0.73
1:C:99:ASN:O	1:C:102:GLU:HG3	1.89	0.73
1:A:63:ILE:HB	1:A:149:ARG:HH22	1.54	0.73
1:C:70:LEU:N	1:C:74:LYS:HE3	2.04	0.72
2:B:419:HIS:HD2	2:B:421:ARG:HG2	1.53	0.72
2:B:254:LYS:HD2	2:B:292:SER:HB2	1.71	0.72
2:D:768:MET:HG2	2:D:769:TYR:CD1	2.25	0.72
2:B:768:MET:HG2	2:B:769:TYR:CD1	2.25	0.72
2:D:445:MET:HB3	2:D:500:PHE:HB2	1.72	0.72
1:C:63:ILE:HB	1:C:149:ARG:HH22	1.54	0.71
2:D:665:LYS:HD2	2:D:666:PRO:O	1.91	0.71
1:A:62:PHE:HE2	1:A:131:LEU:HD12	1.55	0.71
1:C:62:PHE:HE2	1:C:131:LEU:HD12	1.55	0.71
2:B:445:MET:HB3	2:B:500:PHE:HB2	1.72	0.70
2:D:254:LYS:HD2	2:D:292:SER:HB2	1.71	0.70
2:D:337:PRO:HG2	2:D:340:ILE:HD11	1.73	0.70
2:B:665:LYS:HD2	2:B:666:PRO:O	1.91	0.70
1:C:99:ASN:HB3	2:D:504:PHE:HA	1.74	0.70
2:B:337:PRO:HG2	2:B:340:ILE:HD11	1.73	0.68
2:B:444:LYS:NZ	2:B:446:THR:OG1	2.20	0.68
2:B:749:LEU:O	2:D:751:SER:OG	2.11	0.68
2:B:560:LYS:NZ	2:B:561:PRO:O	2.26	0.68
2:D:560:LYS:NZ	2:D:561:PRO:O	2.26	0.67
2:D:755:ILE:HG21	2:D:794:LYS:HE2	1.76	0.67
1:C:81:VAL:O	1:C:84:GLN:HG3	1.94	0.67
2:B:755:ILE:HG21	2:B:794:LYS:HE2	1.76	0.66
1:A:81:VAL:O	1:A:84:GLN:HG3	1.94	0.66
2:D:300:PRO:HG2	2:D:355:LYS:HD2	1.78	0.66
2:B:300:PRO:HG2	2:B:355:LYS:HD2	1.78	0.66
1:A:85:ILE:HD13	1:A:131:LEU:HD11	1.77	0.65
2:D:370:MET:CE	2:D:408:ASP:HB3	2.27	0.65
2:B:399:THR:HG23	2:B:427:VAL:HB	1.78	0.65
2:D:399:THR:HG23	2:D:427:VAL:HB	1.78	0.65
2:B:370:MET:CE	2:B:408:ASP:HB3	2.27	0.65
1:C:41:ARG:HH12	2:D:442:LEU:HB2	1.62	0.65
2:D:444:LYS:NZ	2:D:446:THR:OG1	2.20	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:351:HIS:HE1	2:D:384:VAL:HG11	1.63	0.64
1:C:85:ILE:HD13	1:C:131:LEU:HD11	1.77	0.64
2:B:351:HIS:HE1	2:B:384:VAL:HG11	1.63	0.64
2:D:280:VAL:HB	2:D:282:ARG:HH11	1.62	0.64
2:D:509:TYR:HB3	2:D:511:MET:HE3	1.80	0.64
2:B:280:VAL:HB	2:B:282:ARG:NH1	2.13	0.64
1:A:96:GLN:NE2	1:A:100:ASP:OD2	2.30	0.64
1:C:96:GLN:NE2	1:C:100:ASP:OD2	2.30	0.64
2:B:280:VAL:HB	2:B:282:ARG:HH11	1.62	0.63
2:B:668:MET:SD	2:B:670:ASN:HB2	2.39	0.63
2:D:280:VAL:HB	2:D:282:ARG:NH1	2.13	0.63
1:A:36:LYS:CE	2:B:565:GLU:HB2	2.29	0.63
1:A:151:GLN:HG2	1:A:155:GLN:HE22	1.64	0.62
2:D:555:LYS:HE2	2:D:597:SER:HB3	1.81	0.62
1:A:157:MET:O	1:A:161:LEU:HG	1.98	0.62
1:C:151:GLN:HG2	1:C:155:GLN:HE22	1.64	0.62
1:C:157:MET:O	1:C:161:LEU:HG	1.98	0.62
2:B:549:ILE:HD11	2:B:720:ILE:HD11	1.82	0.62
2:B:509:TYR:HB3	2:B:511:MET:HE3	1.81	0.62
2:D:668:MET:SD	2:D:670:ASN:HB2	2.39	0.62
1:C:84:GLN:OE1	1:C:128:LEU:HD11	2.00	0.62
1:A:24:ILE:O	1:A:27:VAL:HG12	2.00	0.61
2:B:438:THR:HB	2:B:535:VAL:HA	1.81	0.61
1:A:84:GLN:OE1	1:A:128:LEU:HD11	2.00	0.61
2:D:438:THR:HB	2:D:535:VAL:HA	1.81	0.61
2:D:549:ILE:HD11	2:D:720:ILE:HD11	1.82	0.61
2:D:368:TRP:HB2	2:D:381:TYR:HE1	1.66	0.61
2:D:255:ILE:HG12	2:D:306:VAL:HG11	1.83	0.61
2:D:588:VAL:HG21	2:D:596:VAL:HG21	1.83	0.61
1:C:24:ILE:O	1:C:27:VAL:HG12	2.00	0.61
2:B:555:LYS:HE2	2:B:597:SER:HB3	1.81	0.60
1:C:95:ILE:O	1:C:98:SER:OG	2.12	0.60
1:C:151:GLN:O	1:C:155:GLN:NE2	2.35	0.60
1:A:151:GLN:O	1:A:155:GLN:NE2	2.35	0.60
2:B:588:VAL:HG21	2:B:596:VAL:HG21	1.83	0.60
2:D:573:ARG:NH2	2:D:610:GLN:OE1	2.30	0.59
1:C:33:THR:O	1:C:36:LYS:HG3	2.02	0.59
1:C:143:GLU:O	1:C:147:LEU:HG	2.02	0.59
2:B:368:TRP:HB2	2:B:381:TYR:HE1	1.66	0.59
2:B:255:ILE:HG12	2:B:306:VAL:HG11	1.83	0.59
1:A:36:LYS:HD3	2:B:565:GLU:HB2	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:143:GLU:O	1:A:147:LEU:HG	2.02	0.58
2:B:573:ARG:NH2	2:B:610:GLN:OE1	2.30	0.58
2:B:384:VAL:HG23	2:B:388:VAL:HG13	1.84	0.58
2:D:384:VAL:HG23	2:D:388:VAL:HG13	1.84	0.58
2:B:378:GLN:HA	2:B:381:TYR:CD2	2.39	0.58
2:D:748:PRO:HA	2:D:754:VAL:HG22	1.86	0.58
1:A:33:THR:O	1:A:36:LYS:HG3	2.03	0.58
2:B:748:PRO:HA	2:B:754:VAL:HG22	1.86	0.58
2:D:378:GLN:HA	2:D:381:TYR:CD2	2.39	0.58
2:D:400:LYS:HD2	2:D:401:PRO:HD2	1.85	0.58
1:A:36:LYS:HZ1	2:B:565:GLU:H	1.52	0.58
2:B:555:LYS:HD2	2:B:595:SER:OG	2.04	0.57
2:B:254:LYS:NZ	2:B:294:LEU:HG	2.20	0.57
2:D:334:ILE:HD11	2:D:353:ILE:HD12	1.86	0.57
2:D:555:LYS:HD2	2:D:595:SER:OG	2.04	0.57
2:B:400:LYS:HD2	2:B:401:PRO:HD2	1.85	0.57
2:B:421:ARG:HA	1:C:138:SER:OG	2.03	0.57
2:D:254:LYS:NZ	2:D:294:LEU:HG	2.20	0.57
2:B:334:ILE:HD11	2:B:353:ILE:HD12	1.87	0.57
2:B:419:HIS:HA	1:C:58:THR:OG1	2.05	0.57
1:C:63:ILE:HB	1:C:149:ARG:NH2	2.20	0.56
1:A:70:LEU:O	1:A:160:GLN:NE2	2.38	0.56
2:D:436:CYS:HB3	2:D:445:MET:HE3	1.87	0.56
1:A:108:LEU:HD23	1:A:111:LEU:HD21	1.88	0.56
2:B:407:TYR:CE2	2:B:424:GLU:HG2	2.41	0.56
1:A:33:THR:HG23	1:A:36:LYS:HE3	1.88	0.56
1:C:70:LEU:O	1:C:160:GLN:NE2	2.38	0.56
1:C:145:VAL:HG12	1:C:149:ARG:HE	1.71	0.56
2:B:472:TYR:HD1	2:B:530:LEU:HD11	1.71	0.56
2:D:407:TYR:CE2	2:D:424:GLU:HG2	2.41	0.56
1:C:108:LEU:HD23	1:C:111:LEU:HD21	1.88	0.55
2:B:766:LYS:HB3	2:B:816:MET:HE1	1.87	0.55
1:A:36:LYS:NZ	2:B:565:GLU:H	2.04	0.55
1:C:33:THR:HG23	1:C:36:LYS:HE3	1.88	0.55
2:B:794:LYS:NZ	2:D:802:ILE:HD13	2.22	0.55
1:C:65:GLY:HA3	1:C:149:ARG:HD2	1.89	0.55
2:B:272:LYS:HG3	2:B:283:GLU:OE2	2.07	0.55
2:D:766:LYS:HB3	2:D:816:MET:HE1	1.88	0.55
1:A:145:VAL:HG12	1:A:149:ARG:HE	1.71	0.54
2:B:757:SER:OG	2:D:804:ILE:HD13	2.06	0.54
1:C:99:ASN:ND2	2:D:504:PHE:CD2	2.73	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:125:LEU:O	1:C:128:LEU:HD23	2.07	0.54
2:D:272:LYS:HG3	2:D:283:GLU:OE2	2.07	0.54
1:A:63:ILE:HB	1:A:149:ARG:NH2	2.20	0.54
1:C:74:LYS:O	1:C:78:THR:HG23	2.07	0.54
2:D:472:TYR:HD1	2:D:530:LEU:HD11	1.71	0.54
2:D:446:THR:HG23	2:D:497:GLU:OE2	2.08	0.54
1:A:74:LYS:O	1:A:78:THR:HG23	2.07	0.54
1:A:95:ILE:O	1:A:98:SER:OG	2.12	0.54
1:A:132:GLY:O	1:A:135:LEU:HG	2.08	0.54
1:A:125:LEU:O	1:A:128:LEU:HD23	2.07	0.54
2:B:436:CYS:HB3	2:B:445:MET:HE3	1.90	0.54
1:A:65:GLY:HA3	1:A:149:ARG:HD2	1.89	0.53
1:A:71:THR:HG22	1:A:74:LYS:HE2	1.90	0.53
1:C:30:ASP:CG	2:D:472:TYR:OH	2.46	0.53
1:C:71:THR:HG22	1:C:74:LYS:HE2	1.90	0.53
1:C:132:GLY:O	1:C:135:LEU:HG	2.08	0.53
2:B:446:THR:HG23	2:B:497:GLU:OE2	2.08	0.53
2:D:645:PHE:HD2	2:D:662:LEU:HD12	1.73	0.53
1:A:82:TYR:CG	1:A:150:LEU:HD13	2.43	0.53
1:C:82:TYR:CG	1:C:150:LEU:HD13	2.43	0.53
1:C:32:LYS:HD3	1:C:161:LEU:HD12	1.91	0.53
2:B:326:ARG:NH1	2:B:327:VAL:O	2.42	0.53
2:D:448:ARG:HA	2:D:496:TYR:O	2.09	0.53
1:A:108:LEU:HA	1:A:111:LEU:HG	1.91	0.53
2:B:331:GLN:HG3	2:B:421:ARG:NH2	2.24	0.53
1:C:108:LEU:HA	1:C:111:LEU:HG	1.91	0.53
2:D:326:ARG:NH1	2:D:327:VAL:O	2.42	0.52
2:B:448:ARG:HA	2:B:496:TYR:O	2.09	0.52
2:D:509:TYR:HB3	2:D:511:MET:CE	2.40	0.52
2:B:645:PHE:HD2	2:B:662:LEU:HD12	1.73	0.52
2:D:331:GLN:HG3	2:D:421:ARG:NH2	2.24	0.52
1:A:32:LYS:HD3	1:A:161:LEU:HD12	1.91	0.52
1:C:72:LEU:HA	1:C:75:MET:CG	2.40	0.52
1:A:69:ILE:HG23	1:A:74:LYS:HG3	1.92	0.52
2:B:368:TRP:HB2	2:B:381:TYR:CE1	2.45	0.52
2:B:464:LEU:HD12	2:B:512:TRP:O	2.10	0.52
1:C:37:THR:HG21	2:D:505:LEU:CD2	2.39	0.51
1:C:69:ILE:HG23	1:C:74:LYS:HG3	1.92	0.51
2:D:464:LEU:HD12	2:D:512:TRP:O	2.10	0.51
2:B:509:TYR:HB3	2:B:511:MET:CE	2.39	0.51
2:B:568:LEU:HD12	2:B:613:CYS:HB2	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:735:MET:HE3	2:B:818:GLY:C	2.30	0.51
2:B:438:THR:OG1	2:B:445:MET:SD	2.58	0.51
2:B:645:PHE:CD2	2:B:662:LEU:HD12	2.46	0.51
2:B:505:LEU:HG	2:B:506:LEU:HD22	1.93	0.51
1:C:102:GLU:HG2	2:D:504:PHE:HE1	1.76	0.51
2:D:467:HIS:HB3	2:D:510:THR:OG1	2.11	0.51
1:A:63:ILE:O	1:A:149:ARG:NH1	2.42	0.51
1:A:72:LEU:HA	1:A:75:MET:CG	2.40	0.51
2:B:543:VAL:O	2:B:544:LYS:HD3	2.10	0.51
2:D:645:PHE:CD2	2:D:662:LEU:HD12	2.46	0.51
2:B:253:LEU:HB2	2:B:298:ILE:HG12	1.93	0.50
2:D:543:VAL:O	2:D:544:LYS:HD3	2.10	0.50
2:B:355:LYS:HG2	2:B:360:ILE:HD13	1.94	0.50
2:B:467:HIS:HB3	2:B:510:THR:OG1	2.11	0.50
2:D:735:MET:HE3	2:D:818:GLY:C	2.31	0.50
1:C:83:GLN:O	1:C:87:THR:HG23	2.12	0.50
2:D:568:LEU:HD12	2:D:613:CYS:HB2	1.92	0.50
2:B:572:ILE:CG2	2:B:586:TYR:HB3	2.42	0.50
1:C:37:THR:O	1:C:41:ARG:HG2	2.12	0.50
1:A:83:GLN:O	1:A:87:THR:HG23	2.12	0.50
1:A:37:THR:O	1:A:41:ARG:HG2	2.12	0.50
1:C:85:ILE:CD1	1:C:131:LEU:HD11	2.42	0.50
2:D:253:LEU:HB2	2:D:298:ILE:HG12	1.93	0.50
2:D:368:TRP:HB2	2:D:381:TYR:CE1	2.45	0.49
2:D:505:LEU:HG	2:D:506:LEU:HD22	1.93	0.49
1:C:139:GLY:O	1:C:143:GLU:OE1	2.30	0.49
2:D:572:ILE:CG2	2:D:586:TYR:HB3	2.42	0.49
1:C:153:SER:O	1:C:157:MET:HG2	2.12	0.49
1:A:36:LYS:NZ	2:B:565:GLU:HB2	2.27	0.49
1:A:132:GLY:O	1:A:136:GLU:OE1	2.31	0.49
1:A:140:TYR:O	1:A:144:VAL:HG22	2.13	0.49
1:C:162:ASP:OD1	1:C:163:LEU:HD12	2.12	0.49
1:A:153:SER:O	1:A:157:MET:HG2	2.12	0.49
2:B:339:LYS:HG2	2:B:424:GLU:HB2	1.94	0.49
2:B:754:VAL:O	2:B:797:ILE:HG22	2.13	0.49
1:C:140:TYR:O	1:C:144:VAL:HG22	2.13	0.49
2:D:592:LYS:O	2:D:592:LYS:HG3	2.13	0.49
1:C:63:ILE:O	1:C:149:ARG:NH1	2.42	0.49
1:C:74:LYS:O	1:C:77:GLN:HG3	2.12	0.49
2:D:336:PHE:HA	2:D:337:PRO:HA	1.46	0.49
2:D:547:ILE:HG21	2:D:636:ILE:HD13	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:627:ASN:OD1	2:D:628:PRO:HD2	2.13	0.49
1:A:74:LYS:O	1:A:77:GLN:HG3	2.12	0.48
1:A:139:GLY:O	1:A:143:GLU:OE1	2.30	0.48
1:A:145:VAL:CG1	1:A:149:ARG:HE	2.26	0.48
1:C:35:ILE:HD12	1:C:161:LEU:HD11	1.96	0.48
1:C:107:LEU:HA	2:D:471:LEU:HD11	1.93	0.48
1:C:132:GLY:O	1:C:136:GLU:OE1	2.31	0.48
1:C:145:VAL:CG1	1:C:149:ARG:HE	2.26	0.48
2:B:251:GLY:O	2:B:298:ILE:HG13	2.13	0.48
2:B:794:LYS:HZ1	2:D:802:ILE:HD13	1.77	0.48
2:D:251:GLY:O	2:D:298:ILE:HG13	2.13	0.48
2:D:370:MET:HB2	2:D:376:ILE:HD11	1.95	0.48
2:B:755:ILE:HD13	2:D:802:ILE:HG23	1.95	0.48
1:A:162:ASP:OD1	1:A:163:LEU:HD12	2.12	0.48
2:D:769:TYR:HB2	2:D:788:ILE:O	2.13	0.48
2:B:547:ILE:HG21	2:B:636:ILE:HD13	1.94	0.48
1:C:35:ILE:O	1:C:39:VAL:HG23	2.14	0.48
2:D:487:ASP:N	2:D:487:ASP:OD1	2.45	0.48
2:D:339:LYS:HG2	2:D:424:GLU:HB2	1.94	0.48
2:D:355:LYS:HG2	2:D:360:ILE:HD13	1.94	0.48
2:D:436:CYS:HA	2:D:446:THR:O	2.14	0.48
2:D:754:VAL:O	2:D:797:ILE:HG22	2.13	0.48
1:A:31:THR:OG1	1:A:107:LEU:HD21	2.13	0.48
2:B:769:TYR:HB2	2:B:788:ILE:O	2.13	0.48
1:A:36:LYS:CD	2:B:565:GLU:HB2	2.43	0.48
1:A:72:LEU:HA	1:A:75:MET:HG2	1.95	0.48
1:A:92:ARG:HG3	1:A:93:ASN:N	2.29	0.48
2:B:592:LYS:O	2:B:592:LYS:HG3	2.13	0.48
1:C:72:LEU:HA	1:C:75:MET:HG2	1.95	0.48
2:D:282:ARG:HH22	2:D:299:LEU:HD12	1.79	0.48
2:B:350:PHE:CE2	2:B:425:LEU:HD21	2.49	0.48
1:A:96:GLN:HA	1:A:99:ASN:OD1	2.14	0.47
2:B:336:PHE:HA	2:B:337:PRO:HA	1.46	0.47
1:C:107:LEU:HA	1:C:110:VAL:HG22	1.96	0.47
2:D:735:MET:SD	2:D:817:GLU:HB2	2.54	0.47
1:A:102:GLU:OE2	2:B:504:PHE:HD1	1.97	0.47
2:B:735:MET:SD	2:B:817:GLU:HB2	2.54	0.47
1:C:31:THR:OG1	1:C:107:LEU:HD21	2.13	0.47
2:D:350:PHE:CE2	2:D:425:LEU:HD21	2.49	0.47
2:D:652:ASP:N	2:D:652:ASP:OD1	2.47	0.47
1:A:78:THR:O	1:A:81:VAL:HG22	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:82:TYR:O	1:A:85:ILE:HG22	2.14	0.47
1:C:82:TYR:CD2	1:C:150:LEU:HD13	2.50	0.47
1:C:82:TYR:O	1:C:85:ILE:HG22	2.14	0.47
1:C:92:ARG:HG3	1:C:93:ASN:N	2.29	0.47
2:D:275:GLU:CD	2:D:282:ARG:HH21	2.18	0.47
2:D:767:LEU:HD12	2:D:814:ILE:O	2.14	0.47
1:A:35:ILE:HD12	1:A:161:LEU:HD11	1.96	0.47
1:A:107:LEU:HA	1:A:110:VAL:HG22	1.96	0.47
2:B:436:CYS:HA	2:B:446:THR:O	2.14	0.47
2:B:627:ASN:OD1	2:B:628:PRO:HD2	2.13	0.47
1:C:103:ASN:HD22	2:D:471:LEU:HD23	1.79	0.47
1:A:62:PHE:CE2	1:A:131:LEU:HD12	2.44	0.47
1:A:85:ILE:CD1	1:A:131:LEU:HD11	2.42	0.47
1:A:35:ILE:O	1:A:39:VAL:HG23	2.14	0.47
2:B:350:PHE:HE2	2:B:425:LEU:HD11	1.79	0.47
2:B:665:LYS:HG2	2:B:666:PRO:HD2	1.96	0.47
1:C:96:GLN:HA	1:C:99:ASN:OD1	2.14	0.47
2:D:349:SER:OG	2:D:392:THR:HG22	2.15	0.47
2:D:438:THR:OG1	2:D:445:MET:SD	2.58	0.47
2:D:665:LYS:HG2	2:D:666:PRO:HD2	1.96	0.47
2:B:282:ARG:HH22	2:B:299:LEU:HD12	1.79	0.47
2:B:370:MET:HB2	2:B:376:ILE:HD11	1.95	0.47
2:B:530:LEU:HB3	2:B:533:SER:OG	2.15	0.47
2:B:530:LEU:O	2:B:534:VAL:HG22	2.15	0.47
1:A:82:TYR:CD2	1:A:150:LEU:HD13	2.50	0.47
2:B:349:SER:OG	2:B:392:THR:HG22	2.15	0.47
2:D:350:PHE:HE2	2:D:425:LEU:HD11	1.79	0.46
1:C:78:THR:O	1:C:81:VAL:HG22	2.15	0.46
1:A:82:TYR:HA	1:A:85:ILE:HG22	1.97	0.46
2:D:282:ARG:NH2	2:D:299:LEU:HD12	2.30	0.46
2:D:530:LEU:O	2:D:534:VAL:HG22	2.15	0.46
2:B:282:ARG:NH2	2:B:299:LEU:HD12	2.30	0.46
2:B:487:ASP:N	2:B:487:ASP:OD1	2.45	0.46
1:C:82:TYR:HA	1:C:85:ILE:HG22	1.97	0.46
2:B:255:ILE:CG2	2:B:293:LEU:HB3	2.46	0.46
2:B:794:LYS:CE	2:D:802:ILE:HG21	2.36	0.46
2:D:411:TYR:CD1	2:D:422:TYR:HB3	2.50	0.46
2:D:530:LEU:HB3	2:D:533:SER:OG	2.15	0.46
2:B:543:VAL:HG23	2:B:629:ALA:HB2	1.98	0.46
2:B:652:ASP:N	2:B:652:ASP:OD1	2.47	0.46
2:D:334:ILE:CG1	2:D:353:ILE:HB	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:740:ILE:HD13	2:D:815:PHE:HZ	1.81	0.46
2:B:767:LEU:HD12	2:B:814:ILE:O	2.14	0.46
1:C:62:PHE:CE2	1:C:131:LEU:HD12	2.44	0.46
2:B:334:ILE:CG1	2:B:353:ILE:HB	2.46	0.46
2:D:543:VAL:HG23	2:D:629:ALA:HB2	1.98	0.46
2:D:750:ASN:OD1	2:D:753:CYS:N	2.49	0.46
1:C:131:LEU:O	1:C:134:VAL:HG22	2.16	0.46
2:B:749:LEU:HD22	2:D:751:SER:HB2	1.97	0.46
2:D:255:ILE:CG2	2:D:293:LEU:HB3	2.46	0.46
2:B:361:VAL:HG11	2:B:414:ASN:ND2	2.31	0.45
1:A:131:LEU:O	1:A:134:VAL:HG22	2.16	0.45
1:C:25:GLN:HA	1:C:28:GLN:NE2	2.32	0.45
2:D:361:VAL:HG11	2:D:414:ASN:ND2	2.31	0.45
2:B:370:MET:HE1	2:B:408:ASP:HB3	1.96	0.45
2:B:740:ILE:HD13	2:B:815:PHE:HZ	1.81	0.45
2:D:276:ASN:HA	2:D:281:ILE:HD13	1.98	0.45
1:A:47:HIS:HD2	1:A:144:VAL:HG12	1.81	0.45
2:B:255:ILE:HG23	2:B:257:TRP:HZ3	1.81	0.45
2:B:750:ASN:OD1	2:B:753:CYS:N	2.49	0.45
1:C:151:GLN:CG	1:C:155:GLN:HE22	2.29	0.45
1:C:35:ILE:HG23	1:C:154:LEU:HB3	1.99	0.45
2:B:275:GLU:CD	2:B:282:ARG:HH21	2.18	0.45
1:C:47:HIS:HD2	1:C:144:VAL:HG12	1.81	0.45
2:D:255:ILE:HG23	2:D:257:TRP:HZ3	1.81	0.45
2:D:300:PRO:HG2	2:D:355:LYS:CD	2.45	0.45
1:A:131:LEU:HD23	1:A:135:LEU:HD23	1.99	0.45
2:B:356:LYS:HD2	2:B:414:ASN:ND2	2.32	0.45
2:B:411:TYR:CD1	2:B:422:TYR:HB3	2.50	0.45
2:D:766:LYS:HB3	2:D:816:MET:CE	2.47	0.45
1:A:35:ILE:HG23	1:A:154:LEU:HB3	1.99	0.44
2:B:378:GLN:HA	2:B:381:TYR:CE2	2.52	0.44
1:A:25:GLN:HA	1:A:28:GLN:NE2	2.32	0.44
2:B:545:ALA:HB2	2:B:609:VAL:HG21	1.99	0.44
2:D:545:ALA:HB2	2:D:609:VAL:HG21	1.99	0.44
2:D:753:CYS:HA	2:D:797:ILE:O	2.18	0.44
2:B:300:PRO:HG2	2:B:355:LYS:CD	2.45	0.44
2:B:752:SER:O	2:B:798:HIS:HA	2.18	0.44
2:B:430:VAL:HG23	2:B:525:PRO:HD3	1.99	0.44
1:A:75:MET:HB2	1:A:157:MET:HE1	2.00	0.44
2:B:276:ASN:HA	2:B:281:ILE:HD13	1.98	0.44
2:B:747:TYR:CZ	2:D:803:PRO:HG2	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:25:GLN:HG2	1:A:26:LYS:N	2.32	0.44
1:C:42:ILE:HG21	1:C:151:GLN:HB2	2.00	0.44
2:B:753:CYS:HA	2:B:797:ILE:O	2.17	0.44
2:B:766:LYS:HB3	2:B:816:MET:CE	2.47	0.44
1:C:107:LEU:CA	2:D:471:LEU:HD11	2.48	0.44
2:D:752:SER:O	2:D:798:HIS:HA	2.18	0.44
1:C:25:GLN:HG2	1:C:26:LYS:N	2.32	0.43
1:C:131:LEU:HD23	1:C:135:LEU:HD23	1.99	0.43
1:C:56:LYS:NZ	1:C:61:ASP:OD1	2.46	0.43
2:D:430:VAL:HG23	2:D:525:PRO:HD3	1.99	0.43
2:B:757:SER:CB	2:D:804:ILE:HD13	2.48	0.43
2:D:378:GLN:HA	2:D:381:TYR:CE2	2.52	0.43
1:A:42:ILE:HG21	1:A:151:GLN:HB2	2.00	0.43
2:D:464:LEU:HD11	2:D:511:MET:HB3	2.00	0.43
2:D:645:PHE:CE2	2:D:729:LEU:HD12	2.54	0.43
2:B:645:PHE:CE2	2:B:729:LEU:HD12	2.54	0.43
1:C:25:GLN:HA	1:C:28:GLN:OE1	2.19	0.43
2:D:647:ARG:NH1	2:D:649:ILE:HD11	2.34	0.43
1:A:24:ILE:O	1:A:28:GLN:OE1	2.36	0.43
2:D:245:MET:HE1	2:D:326:ARG:HG2	2.01	0.43
2:D:350:PHE:CE2	2:D:425:LEU:HD11	2.53	0.43
2:D:356:LYS:HD2	2:D:414:ASN:ND2	2.32	0.43
1:A:151:GLN:CG	1:A:155:GLN:HE22	2.29	0.43
2:D:468:ARG:HD2	2:D:469:SER:O	2.19	0.43
1:A:56:LYS:NZ	1:A:61:ASP:OD1	2.46	0.43
1:A:82:TYR:CE2	1:A:150:LEU:HB2	2.53	0.43
2:D:466:TYR:HA	2:D:510:THR:O	2.19	0.43
1:A:33:THR:HG23	1:A:36:LYS:CE	2.48	0.43
2:B:814:ILE:HD12	2:B:819:VAL:HG22	2.00	0.43
1:C:24:ILE:O	1:C:28:GLN:OE1	2.36	0.43
1:C:82:TYR:CE2	1:C:150:LEU:HB2	2.53	0.43
2:D:814:ILE:HD12	2:D:819:VAL:HG22	2.00	0.43
2:B:647:ARG:NH1	2:B:649:ILE:HD11	2.34	0.42
1:A:25:GLN:HA	1:A:28:GLN:OE1	2.18	0.42
1:A:115:LYS:HE3	1:A:115:LYS:HB3	1.89	0.42
2:B:273:TYR:CZ	2:B:284:ALA:HB3	2.54	0.42
2:B:280:VAL:CB	2:B:282:ARG:HH11	2.31	0.42
2:B:466:TYR:HA	2:B:510:THR:O	2.19	0.42
1:C:75:MET:O	1:C:78:THR:OG1	2.27	0.42
1:C:102:GLU:HG2	2:D:504:PHE:CE1	2.54	0.42
2:D:361:VAL:HG21	2:D:414:ASN:HD22	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:735:MET:HB3	2:B:735:MET:HE2	1.74	0.42
1:C:38:ILE:HD13	1:C:101:LEU:HD23	2.00	0.42
2:B:464:LEU:HD11	2:B:511:MET:HB3	2.00	0.42
2:D:273:TYR:CZ	2:D:284:ALA:HB3	2.54	0.42
2:B:350:PHE:CE2	2:B:425:LEU:HD11	2.53	0.42
1:C:75:MET:HB2	1:C:157:MET:HE1	2.00	0.42
2:D:637:LYS:O	2:D:718:ASN:ND2	2.50	0.42
2:B:361:VAL:HG21	2:B:414:ASN:HD22	1.85	0.42
2:B:468:ARG:HD2	2:B:469:SER:O	2.19	0.42
1:A:38:ILE:HD13	1:A:101:LEU:HD23	2.00	0.42
1:A:81:VAL:HA	1:A:84:GLN:HG3	2.02	0.42
1:A:128:LEU:HD11	1:A:131:LEU:HD13	2.02	0.42
1:C:81:VAL:HA	1:C:84:GLN:HG3	2.02	0.42
2:D:776:ASN:ND2	2:D:805:GLU:OE1	2.52	0.42
1:C:154:LEU:HD23	1:C:154:LEU:HA	1.88	0.42
2:D:767:LEU:HD21	2:D:770:PHE:CZ	2.55	0.42
2:B:776:ASN:ND2	2:B:805:GLU:OE1	2.52	0.41
2:B:255:ILE:HG22	2:B:293:LEU:HB3	2.01	0.41
2:B:747:TYR:CE2	2:D:803:PRO:HG2	2.54	0.41
2:B:708:GLN:OE1	2:B:733:TRP:HB2	2.20	0.41
1:C:64:PRO:CG	1:C:81:VAL:HG21	2.44	0.41
2:D:512:TRP:HE1	2:D:514:ARG:NH2	2.19	0.41
1:A:36:LYS:HD3	2:B:565:GLU:CB	2.49	0.41
1:A:71:THR:OG1	1:A:166:GLY:O	2.25	0.41
2:D:360:ILE:HG21	2:D:387:HIS:HB2	2.02	0.41
1:A:71:THR:O	1:A:75:MET:HG2	2.20	0.41
2:B:512:TRP:HE1	2:B:514:ARG:NH2	2.19	0.41
2:D:799:ASP:HB3	2:D:801:PHE:CE2	2.56	0.41
2:B:450:SER:HB3	2:B:495:PHE:CE2	2.56	0.41
2:B:637:LYS:O	2:B:718:ASN:ND2	2.50	0.41
1:C:99:ASN:ND2	2:D:504:PHE:CE2	2.88	0.41
2:D:255:ILE:HG22	2:D:293:LEU:HB3	2.01	0.41
2:B:767:LEU:HD21	2:B:770:PHE:CZ	2.55	0.41
2:B:799:ASP:HB3	2:B:801:PHE:CE2	2.56	0.41
1:C:33:THR:HG23	1:C:36:LYS:CE	2.48	0.41
2:D:695:VAL:HG12	2:D:698:HIS:HB2	2.03	0.41
2:B:331:GLN:HG3	2:B:421:ARG:CZ	2.51	0.41
2:D:708:GLN:OE1	2:D:733:TRP:HB2	2.20	0.41
2:D:646:TRP:CG	2:D:647:ARG:N	2.89	0.40
1:C:71:THR:O	1:C:75:MET:HG2	2.20	0.40
2:B:405:PHE:CE1	1:C:140:TYR:CD2	3.09	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:65:GLY:HA3	1:C:149:ARG:HH11	1.86	0.40
1:C:128:LEU:HD11	1:C:131:LEU:HD13	2.02	0.40
2:D:450:SER:HB3	2:D:495:PHE:CE2	2.56	0.40
1:A:60:LEU:HD23	1:A:60:LEU:HA	1.92	0.40
2:B:402:ARG:NH2	2:B:408:ASP:OD1	2.55	0.40
2:B:646:TRP:CG	2:B:647:ARG:N	2.89	0.40

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	144/171 (84%)	134 (93%)	10 (7%)	0	100	100
1	C	144/171 (84%)	134 (93%)	10 (7%)	0	100	100
2	B	594/868 (68%)	578 (97%)	13 (2%)	3 (0%)	25	64
2	D	594/868 (68%)	578 (97%)	13 (2%)	3 (0%)	25	64
All	All	1476/2078 (71%)	1424 (96%)	46 (3%)	6 (0%)	32	68

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	472	TYR
2	B	673	LEU
2	D	472	TYR
2	D	673	LEU
2	B	297	SER
2	D	297	SER



### 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	133/150 (89%)	132 (99%)	1 (1%)	79	84
1	C	133/150 (89%)	132 (99%)	1 (1%)	79	84
2	B	555/802 (69%)	550 (99%)	5 (1%)	75	83
2	D	555/802 (69%)	550 (99%)	5 (1%)	75	83
All	All	1376/1904 (72%)	1364 (99%)	12 (1%)	74	83

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	36	LYS
2	B	245	MET
2	B	358	ASN
2	B	444	LYS
2	B	641	ARG
2	B	737	LYS
1	C	36	LYS
2	D	245	MET
2	D	358	ASN
2	D	444	LYS
2	D	641	ARG
2	D	737	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	96	GLN
1	A	155	GLN
2	B	351	HIS
2	B	414	ASN
1	C	103	ASN
1	C	155	GLN
2	D	351	HIS

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Mol	Chain	Res	Type
2	D	414	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

### 5.6 Ligand geometry ⓘ

There are no ligands in this entry.

### 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.

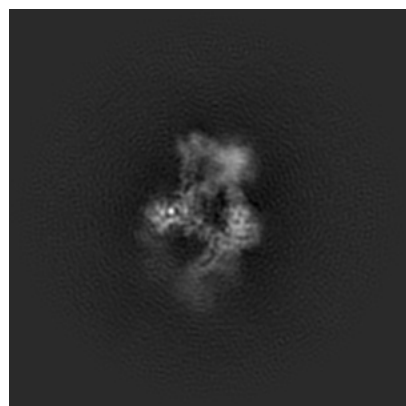
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-15680. These allow visual inspection of the internal detail of the map and identification of artifacts.

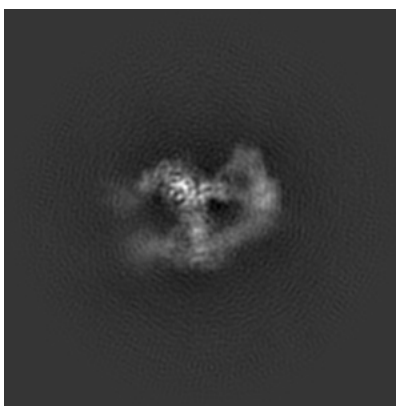
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

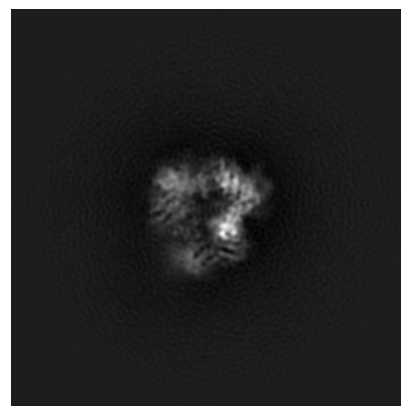
#### 6.1.1 Primary map



X

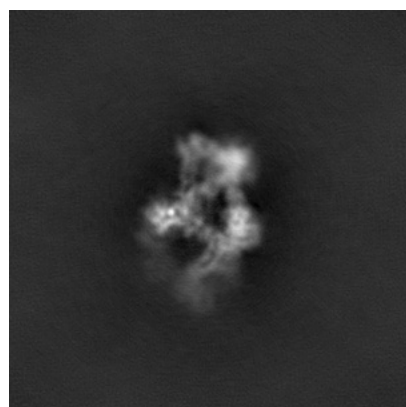


Y

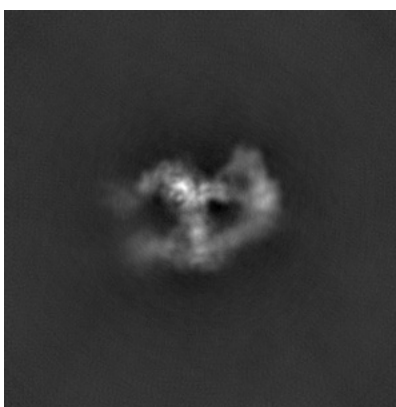


Z

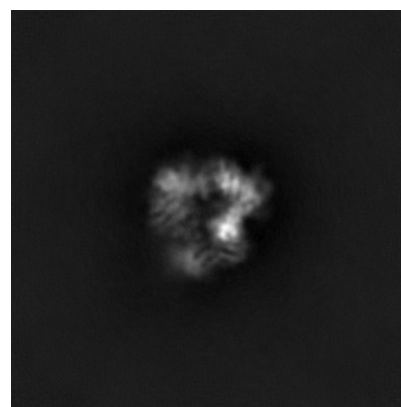
#### 6.1.2 Raw map



X



Y

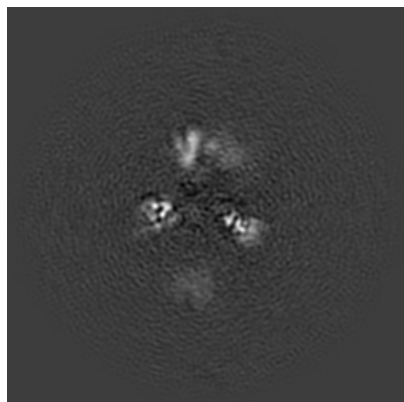


Z

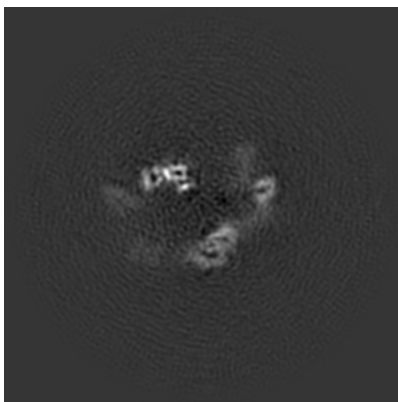
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

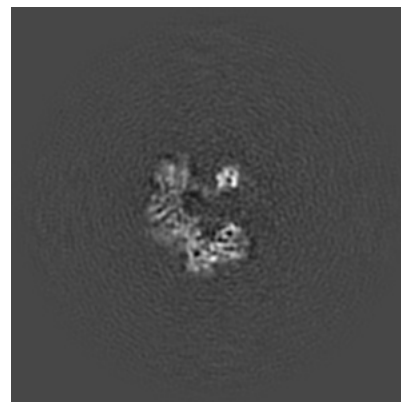
### 6.2.1 Primary map



X Index: 140

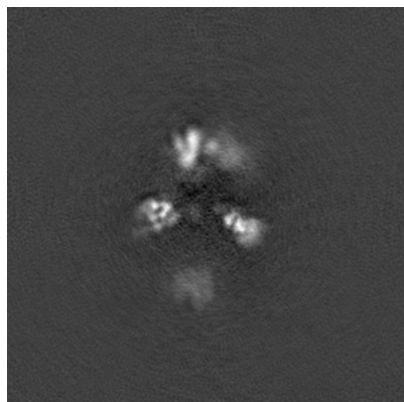


Y Index: 140

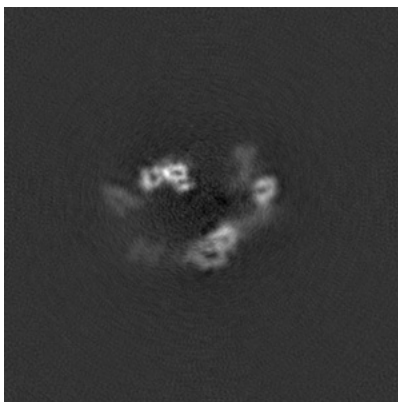


Z Index: 140

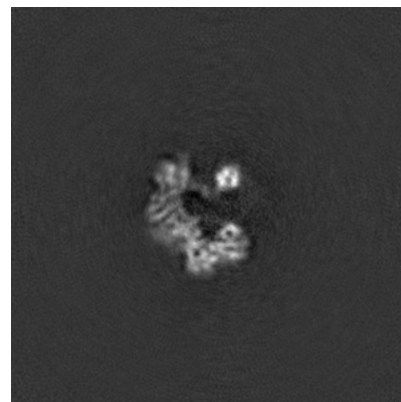
### 6.2.2 Raw map



X Index: 140



Y Index: 140

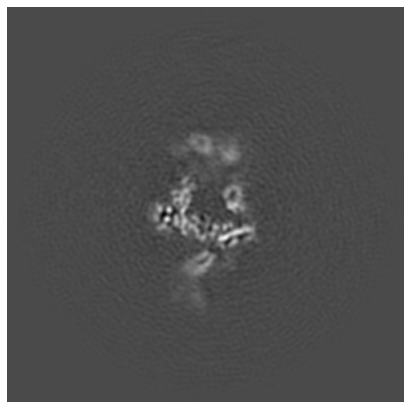


Z Index: 140

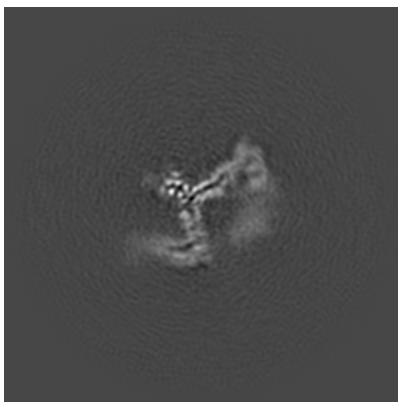
The images above show central slices of the map in three orthogonal directions.

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

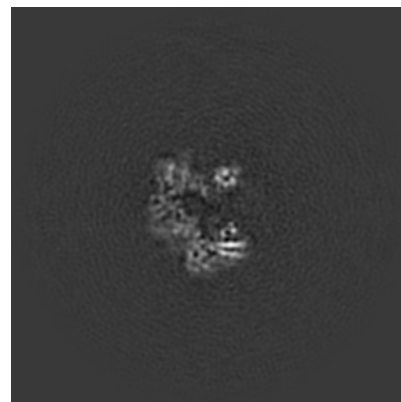
### 6.3.1 Primary map



X Index: 156

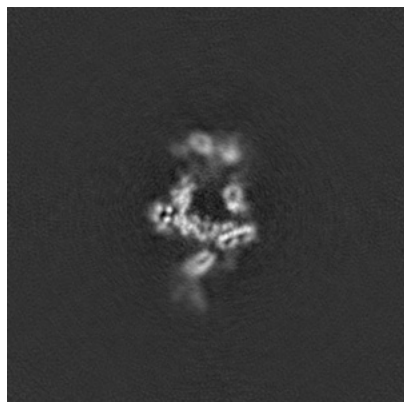


Y Index: 158

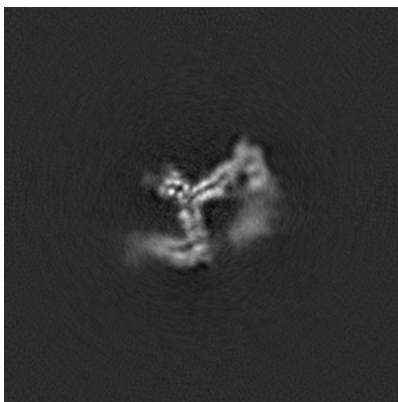


Z Index: 138

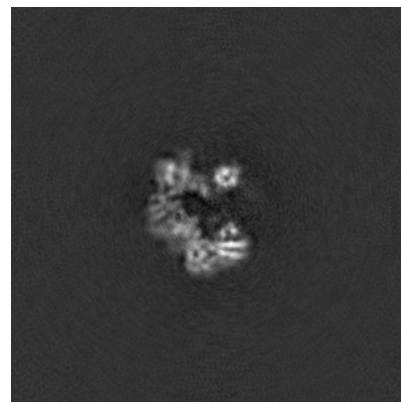
### 6.3.2 Raw map



X Index: 156



Y Index: 158

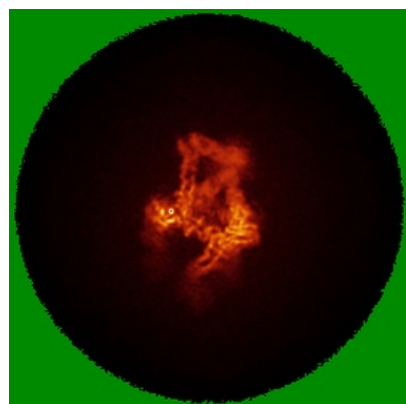


Z Index: 138

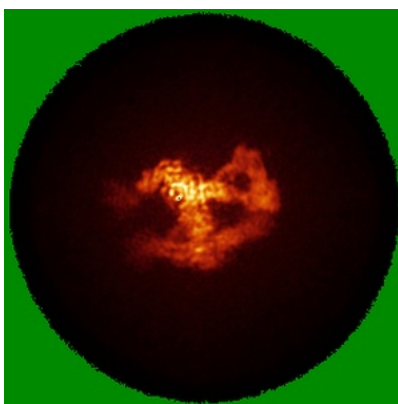
The images above show the largest variance slices of the map in three orthogonal directions.

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

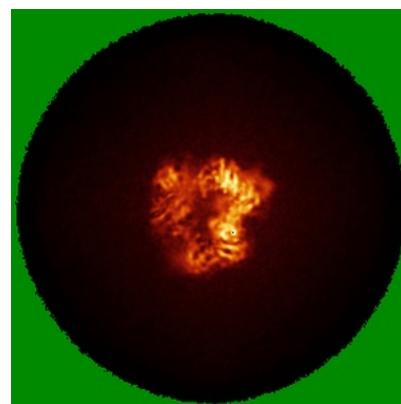
### 6.4.1 Primary map



X

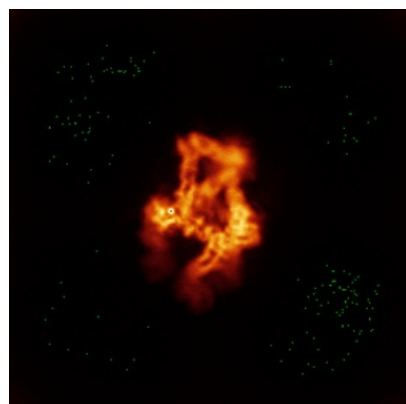


Y

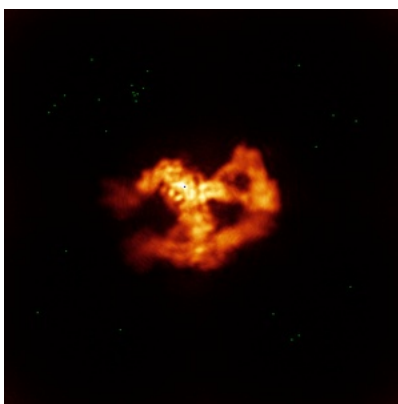


Z

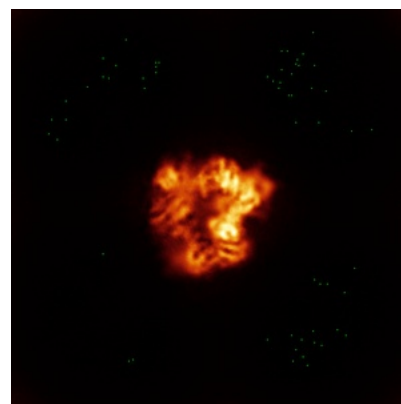
### 6.4.2 Raw map



X



Y

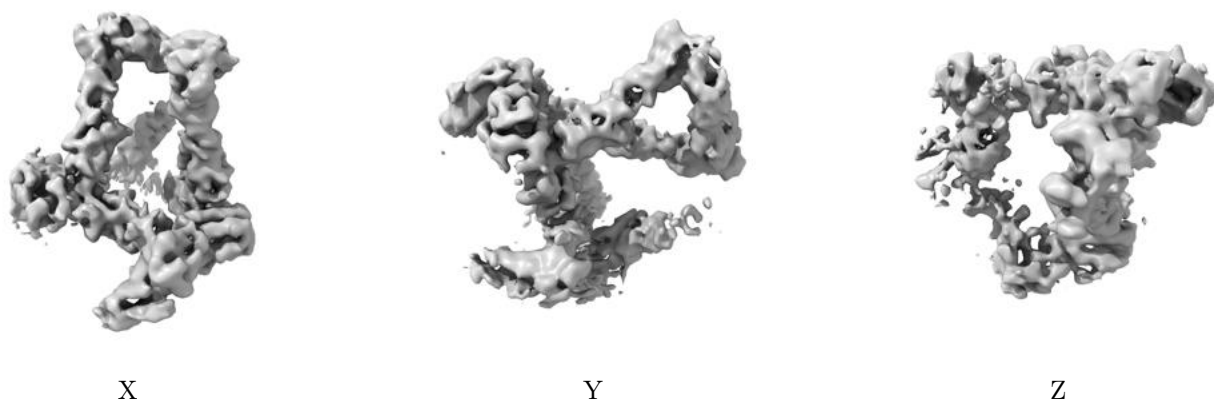


Z

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



The images above show the 3D surface view of the map at the recommended contour level 0.55. 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



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.



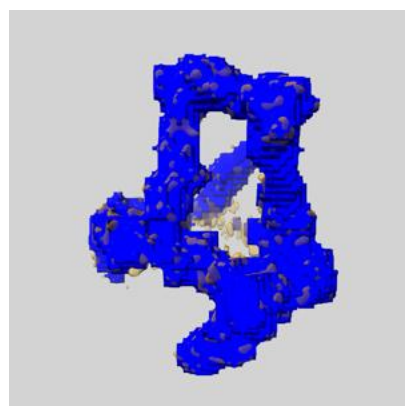
## 6.6 Mask visualisation [i](#)

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

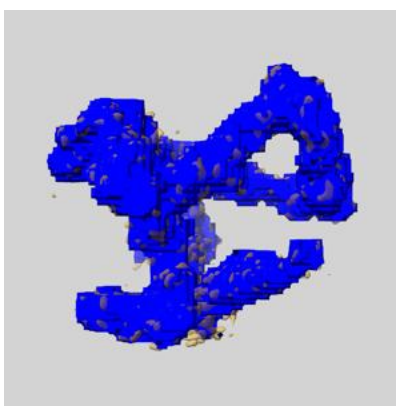
A mask typically either:

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

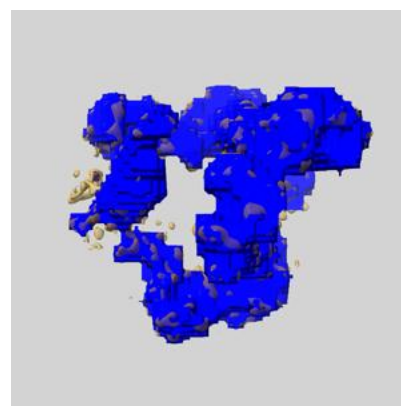
### 6.6.1 emd\_15680\_msk\_1.map [i](#)



X



Y



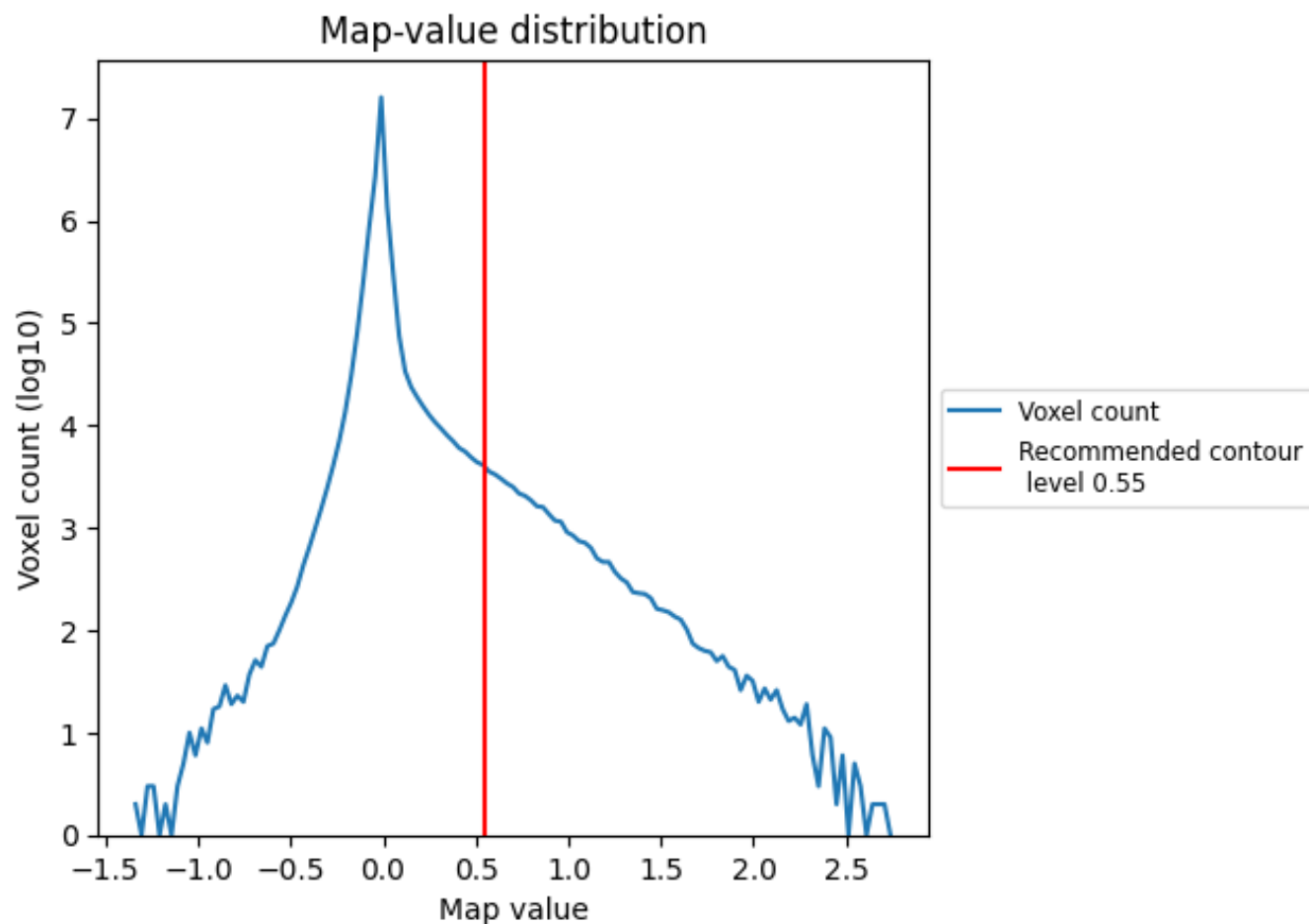
Z



## 7 Map analysis [i](#)

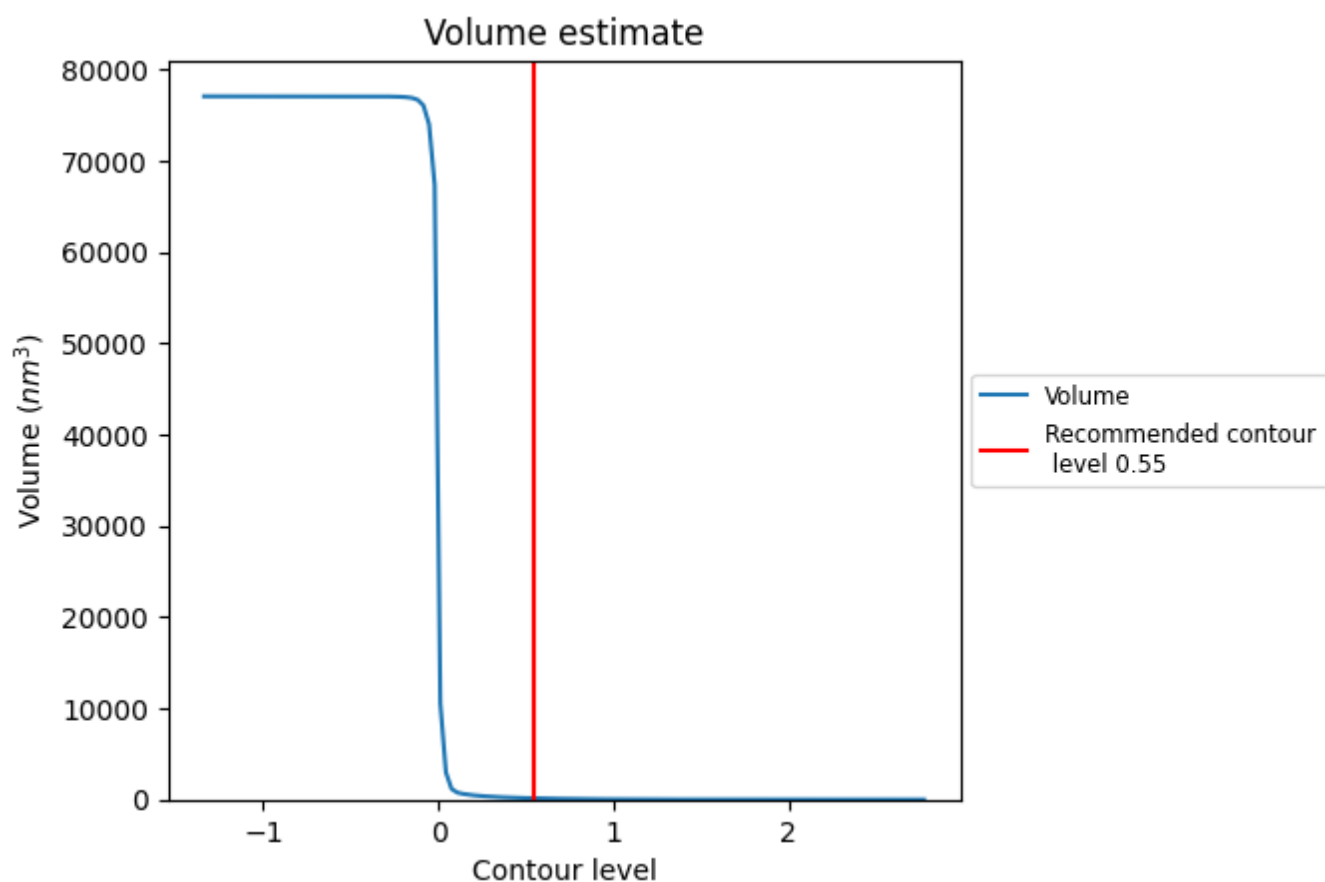
This section contains the results of statistical analysis of the map.

### 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.

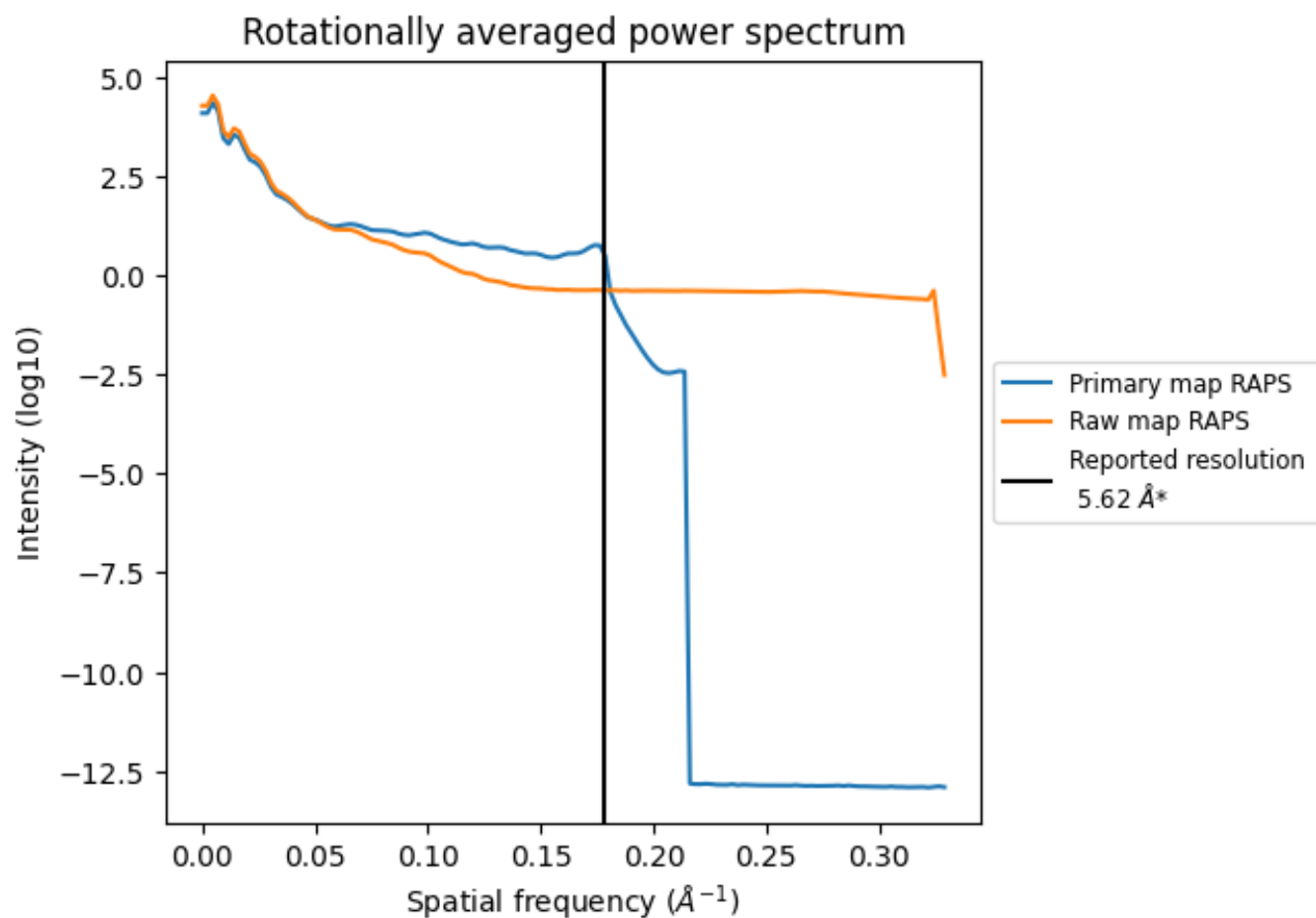
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 139 nm<sup>3</sup>; this corresponds to an approximate mass of 126 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 ⓘ

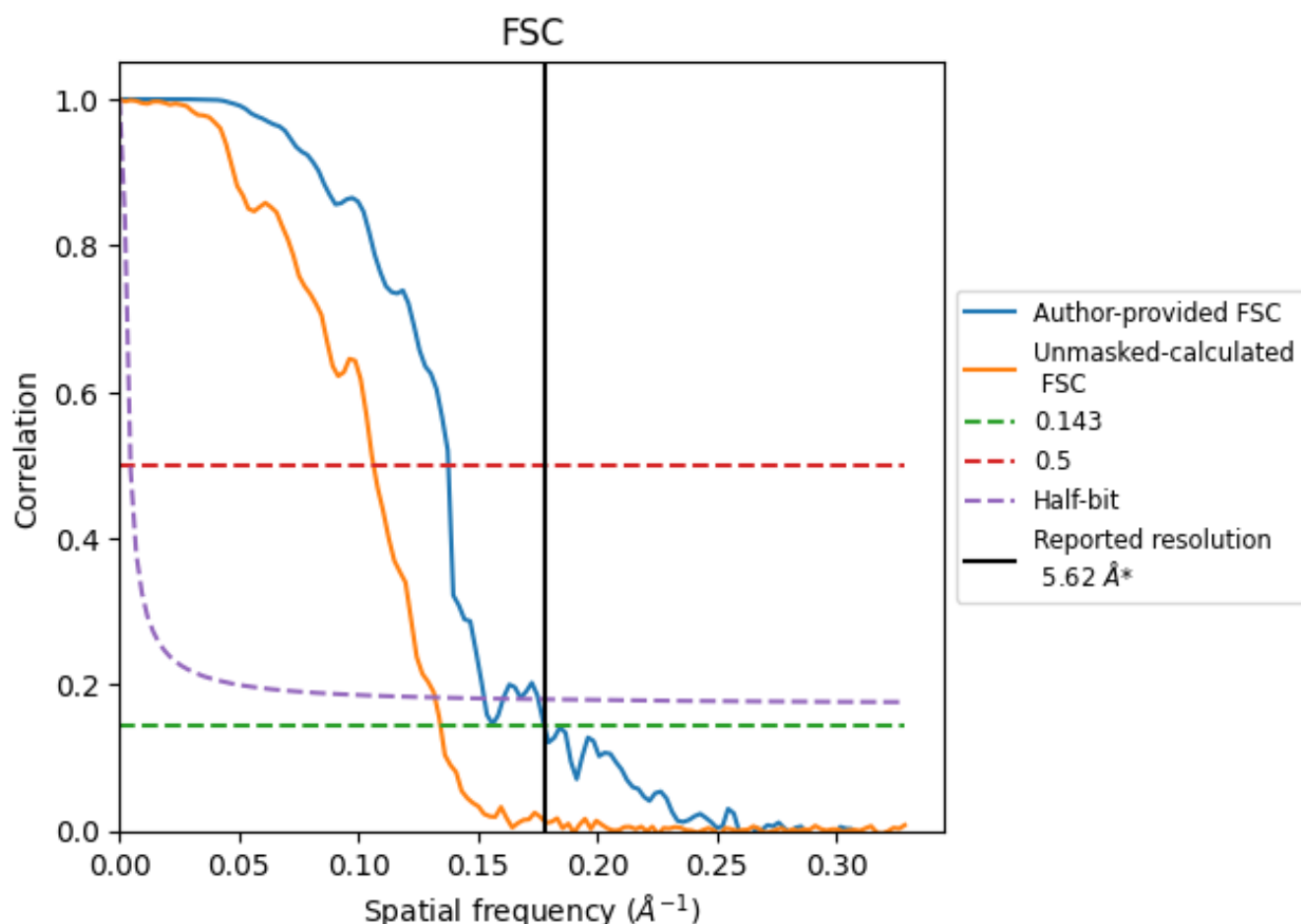


\*Reported resolution corresponds to spatial frequency of 0.178 Å<sup>-1</sup>

## 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 0.178 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

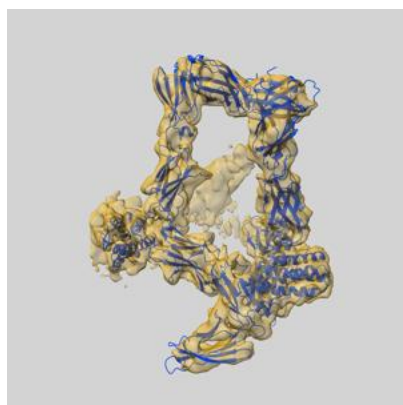
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	5.62	-	-
Author-provided FSC curve	5.62	7.26	6.54
Unmasked-calculated*	7.43	9.40	7.57

\*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 7.43 differs from the reported value 5.62 by more than 10 %

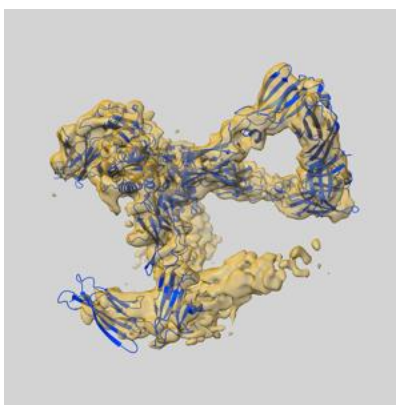
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-15680 and PDB model 8AVE. Per-residue inclusion information can be found in section 3 on page 8.

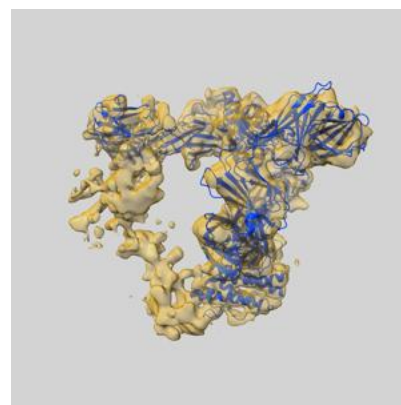
### 9.1 Map-model overlay [i](#)



X



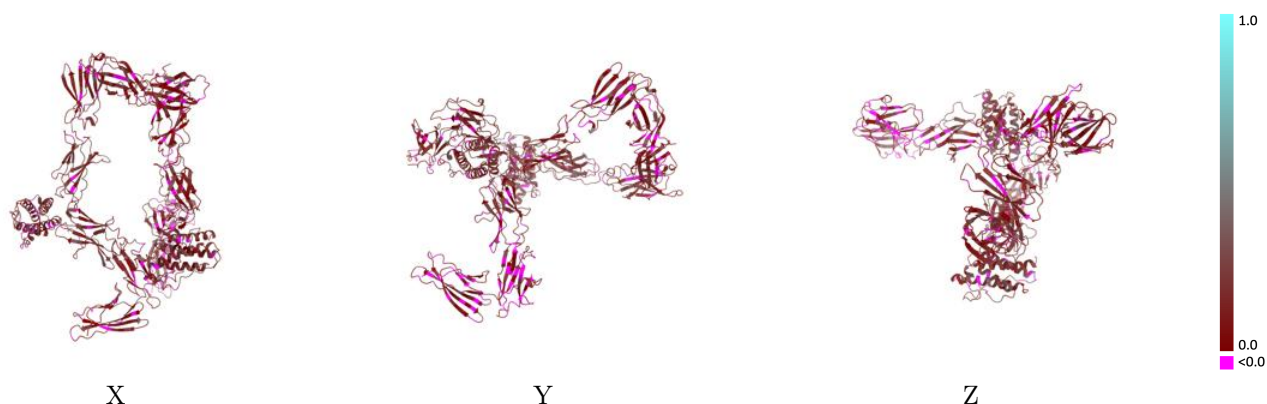
Y



Z

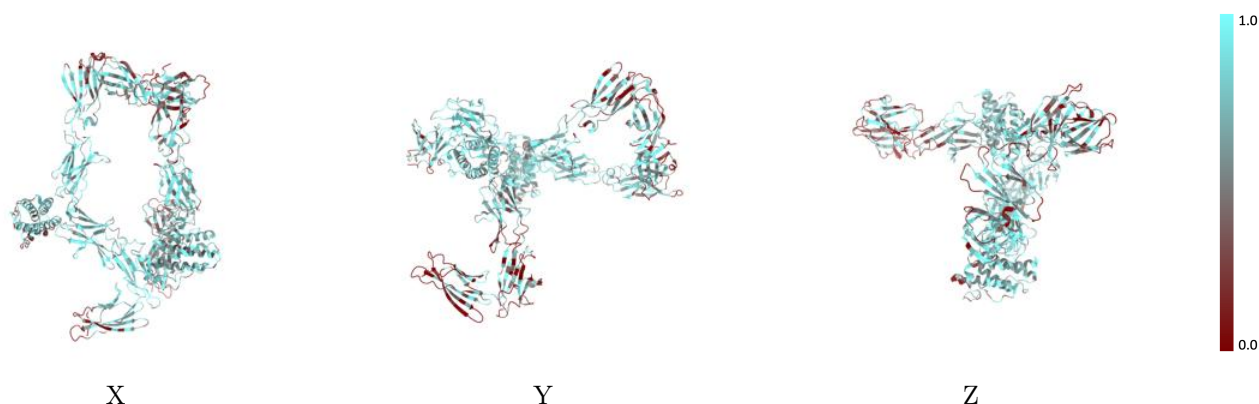
The images above show the 3D surface view of the map at the recommended contour level 0.55 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



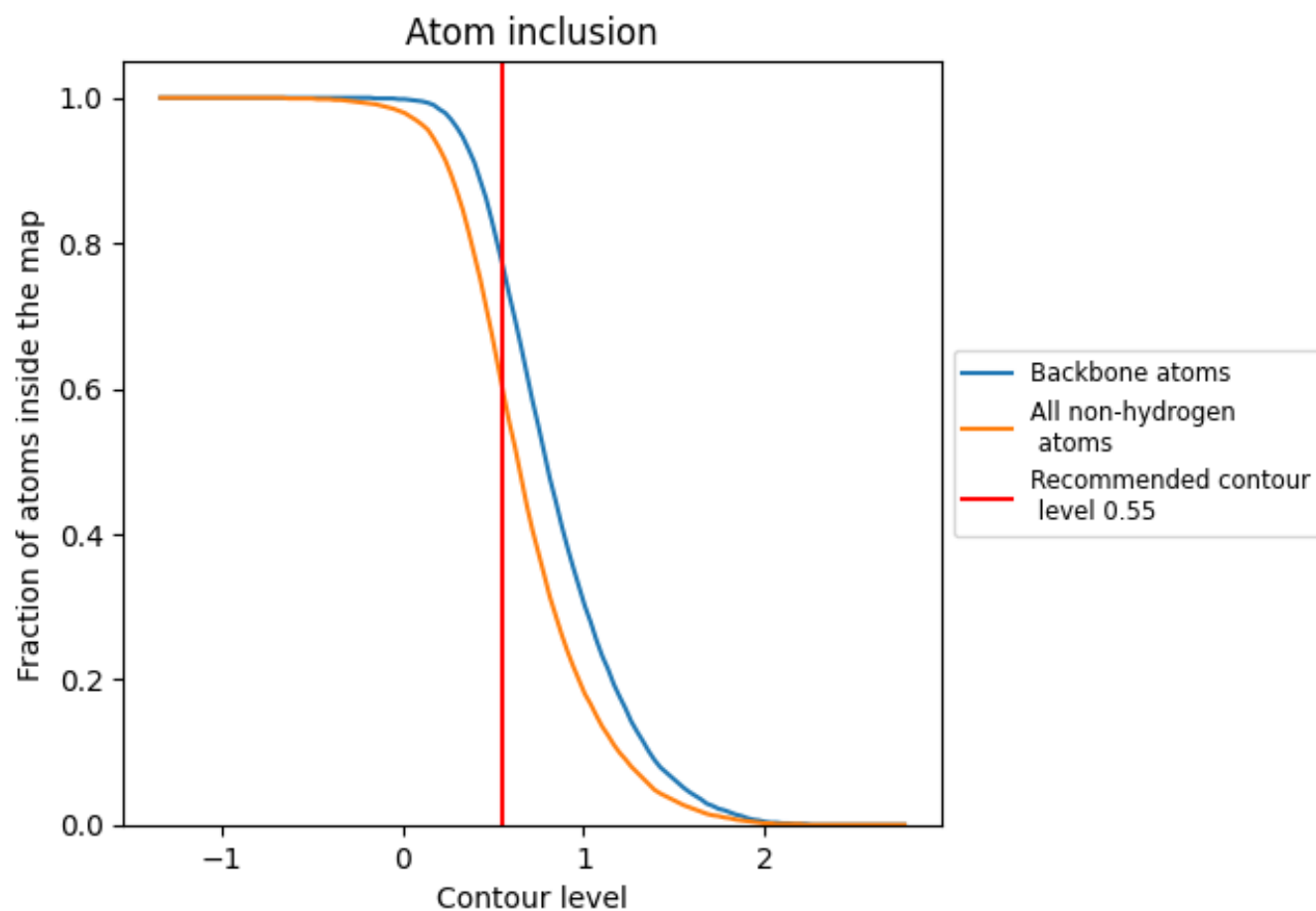
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.55).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 77% of all backbone atoms, 60% 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 (0.55) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.6010	<div></div> 0.1470
A	<div></div> 0.6050	<div></div> 0.1620
B	<div></div> 0.6720	<div></div> 0.1670
C	<div></div> 0.7000	<div></div> 0.1900
D	<div></div> 0.5060	<div></div> 0.1130

