



Full wwPDB EM Validation Report ⓘ

Mar 14, 2026 – 07:45 AM UTC

PDB ID : 6M04 / pdb_00006m04
EMDB ID : EMD-30029
Title : Structure of the human homo-hexameric LRRC8D channel at 4.36 Angstroms
Authors : Nakamura, R.; Kasuya, G.; Yokoyama, T.; Shirouzu, M.; Ishitani, R.; Nureki, O.
Deposited on : 2020-02-20
Resolution : 4.36 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

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:

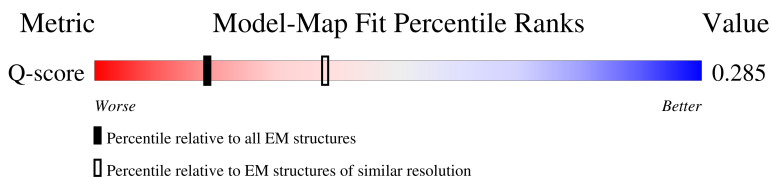
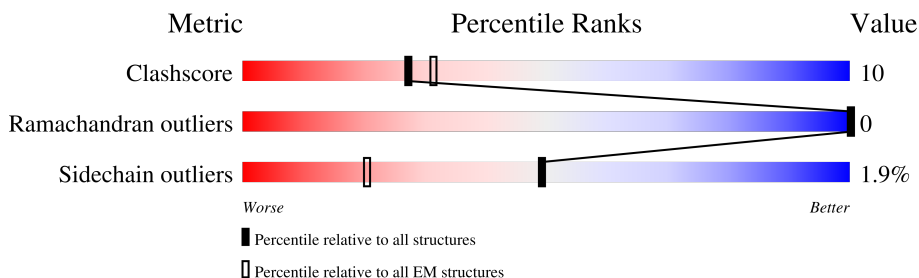
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & 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 4.36 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	3737 (3.87 - 4.86)

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	866	
1	B	866	
1	C	866	
1	D	866	

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Mol	Chain	Length	Quality of chain
1	E	866	5% 59% 22% 18%
1	F	866	9% 60% 21% 18%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 34666 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 Volume-regulated anion channel subunit LRRC8D.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	714	Total	C	N	O	S	0	0
			5780	3761	958	1026	35		
1	B	714	Total	C	N	O	S	0	0
			5780	3761	958	1026	35		
1	C	713	Total	C	N	O	S	0	0
			5773	3756	957	1025	35		
1	D	714	Total	C	N	O	S	0	0
			5780	3761	958	1026	35		
1	E	714	Total	C	N	O	S	0	0
			5780	3761	958	1026	35		
1	F	713	Total	C	N	O	S	0	0
			5773	3756	957	1025	35		

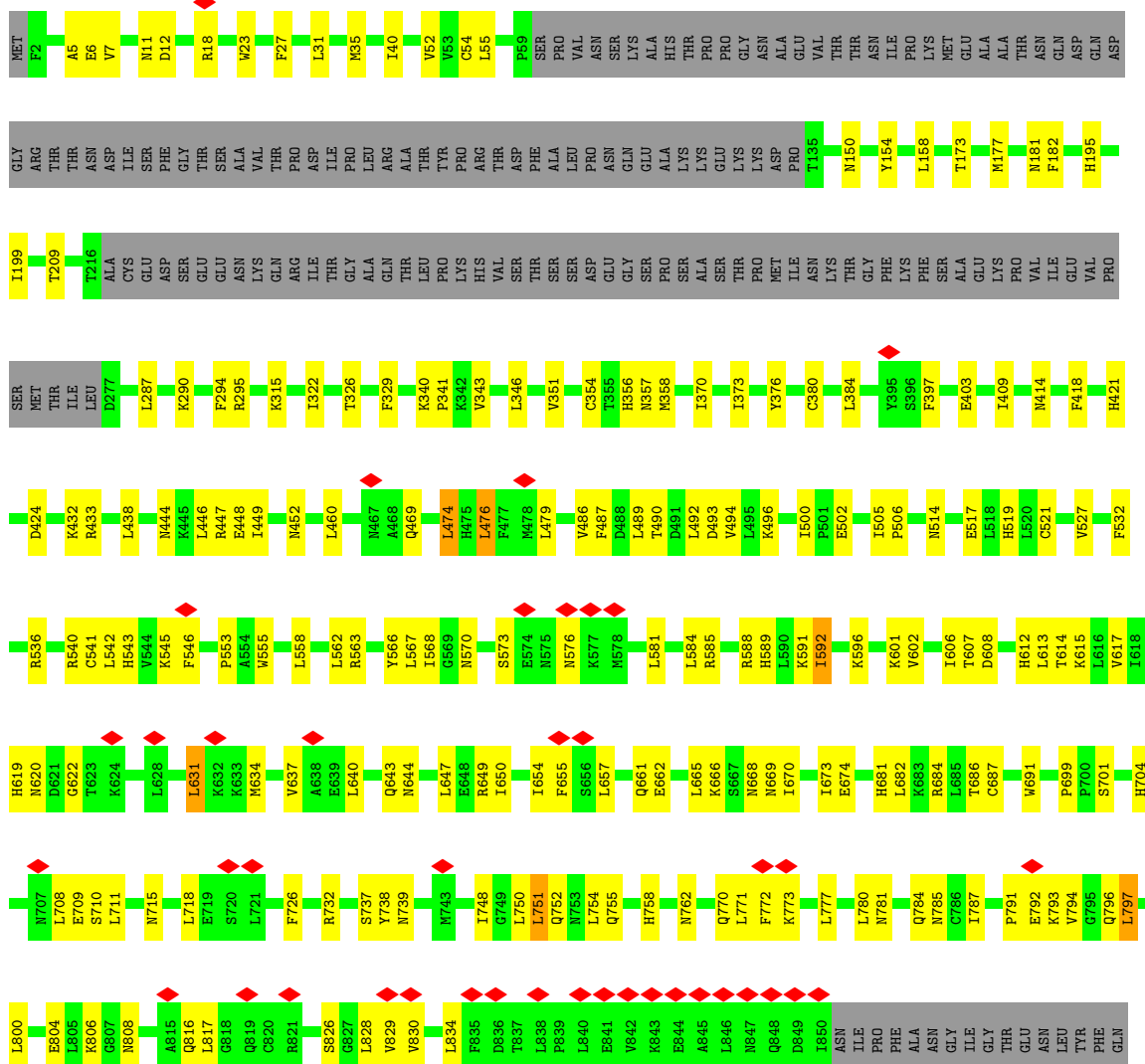
There are 54 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	810	PHE	LEU	engineered mutation	UNP Q7L1W4
A	859	GLY	-	expression tag	UNP Q7L1W4
A	860	THR	-	expression tag	UNP Q7L1W4
A	861	GLU	-	expression tag	UNP Q7L1W4
A	862	ASN	-	expression tag	UNP Q7L1W4
A	863	LEU	-	expression tag	UNP Q7L1W4
A	864	TYR	-	expression tag	UNP Q7L1W4
A	865	PHE	-	expression tag	UNP Q7L1W4
A	866	GLN	-	expression tag	UNP Q7L1W4
B	810	PHE	LEU	engineered mutation	UNP Q7L1W4
B	859	GLY	-	expression tag	UNP Q7L1W4
B	860	THR	-	expression tag	UNP Q7L1W4
B	861	GLU	-	expression tag	UNP Q7L1W4
B	862	ASN	-	expression tag	UNP Q7L1W4
B	863	LEU	-	expression tag	UNP Q7L1W4
B	864	TYR	-	expression tag	UNP Q7L1W4
B	865	PHE	-	expression tag	UNP Q7L1W4
B	866	GLN	-	expression tag	UNP Q7L1W4

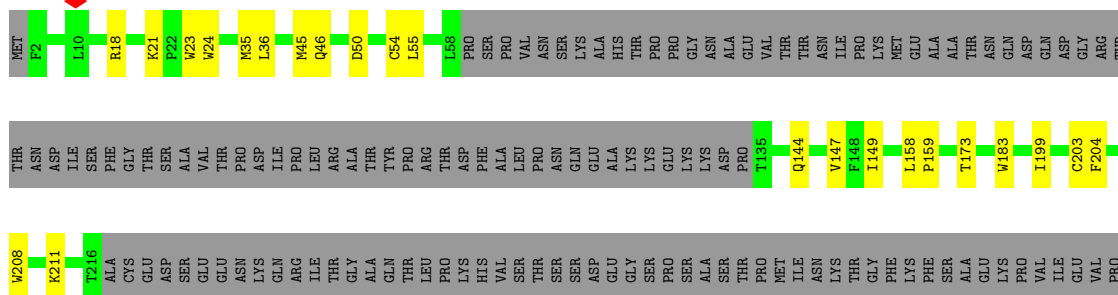
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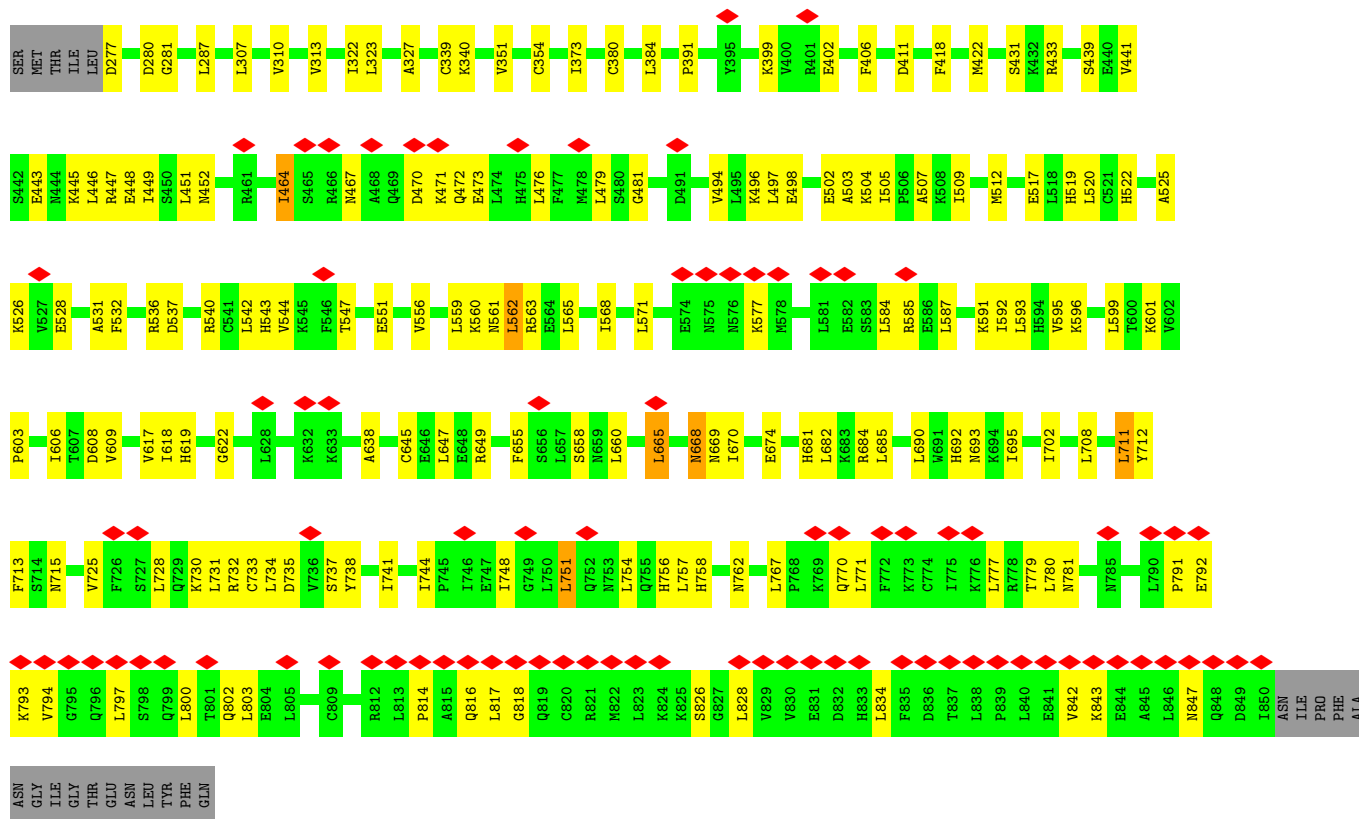
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Chain	Residue	Modelled	Actual	Comment	Reference
C	810	PHE	LEU	engineered mutation	UNP Q7L1W4
C	859	GLY	-	expression tag	UNP Q7L1W4
C	860	THR	-	expression tag	UNP Q7L1W4
C	861	GLU	-	expression tag	UNP Q7L1W4
C	862	ASN	-	expression tag	UNP Q7L1W4
C	863	LEU	-	expression tag	UNP Q7L1W4
C	864	TYR	-	expression tag	UNP Q7L1W4
C	865	PHE	-	expression tag	UNP Q7L1W4
C	866	GLN	-	expression tag	UNP Q7L1W4
D	810	PHE	LEU	engineered mutation	UNP Q7L1W4
D	859	GLY	-	expression tag	UNP Q7L1W4
D	860	THR	-	expression tag	UNP Q7L1W4
D	861	GLU	-	expression tag	UNP Q7L1W4
D	862	ASN	-	expression tag	UNP Q7L1W4
D	863	LEU	-	expression tag	UNP Q7L1W4
D	864	TYR	-	expression tag	UNP Q7L1W4
D	865	PHE	-	expression tag	UNP Q7L1W4
D	866	GLN	-	expression tag	UNP Q7L1W4
E	810	PHE	LEU	engineered mutation	UNP Q7L1W4
E	859	GLY	-	expression tag	UNP Q7L1W4
E	860	THR	-	expression tag	UNP Q7L1W4
E	861	GLU	-	expression tag	UNP Q7L1W4
E	862	ASN	-	expression tag	UNP Q7L1W4
E	863	LEU	-	expression tag	UNP Q7L1W4
E	864	TYR	-	expression tag	UNP Q7L1W4
E	865	PHE	-	expression tag	UNP Q7L1W4
E	866	GLN	-	expression tag	UNP Q7L1W4
F	810	PHE	LEU	engineered mutation	UNP Q7L1W4
F	859	GLY	-	expression tag	UNP Q7L1W4
F	860	THR	-	expression tag	UNP Q7L1W4
F	861	GLU	-	expression tag	UNP Q7L1W4
F	862	ASN	-	expression tag	UNP Q7L1W4
F	863	LEU	-	expression tag	UNP Q7L1W4
F	864	TYR	-	expression tag	UNP Q7L1W4
F	865	PHE	-	expression tag	UNP Q7L1W4
F	866	GLN	-	expression tag	UNP Q7L1W4

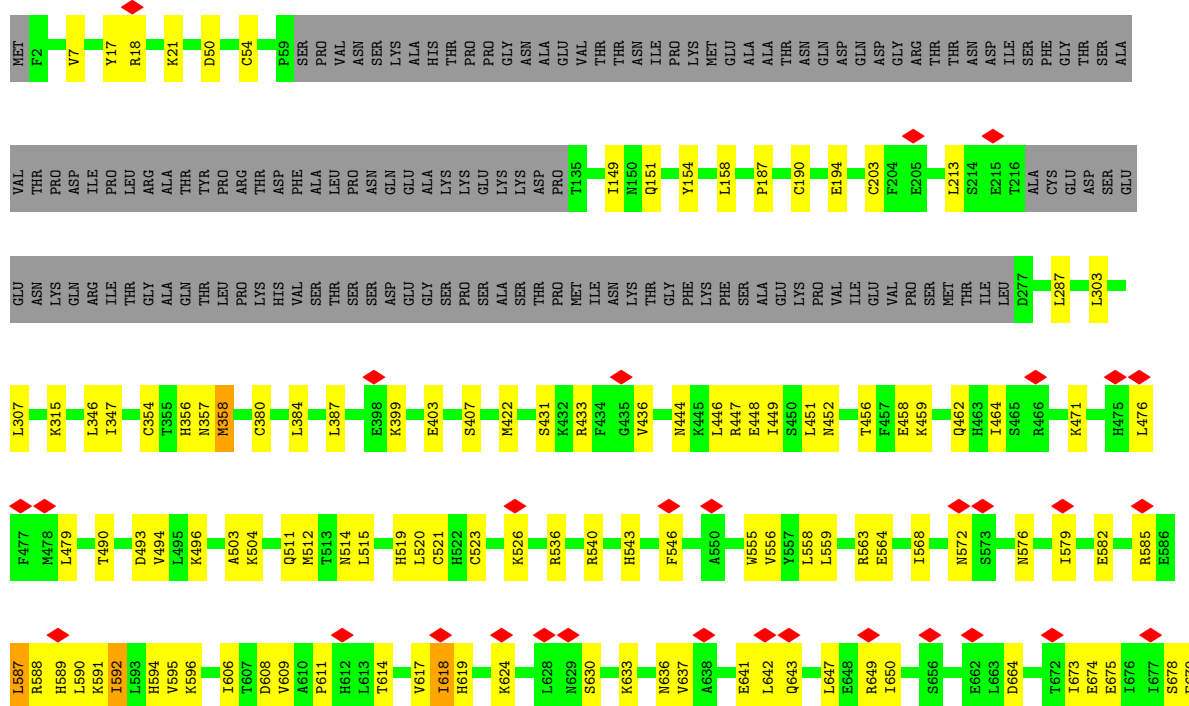


• Molecule 1: Volume-regulated anion channel subunit LRRC8D





• Molecule 1: Volume-regulated anion channel subunit LRRC8D







4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	247154	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50.0	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	23500	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.211	Depositor
Minimum map value	-0.092	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.0301	Depositor
Map size (Å)	357.6, 357.6, 357.6	wwPDB
Map dimensions	240, 240, 240	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.49, 1.49, 1.49	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	0.27	0/5908	0.70	0/8007
1	B	0.28	0/5908	0.71	0/8007
1	C	0.26	0/5900	0.66	0/7995
1	D	0.27	0/5908	0.69	0/8007
1	E	0.28	0/5908	0.71	0/8007
1	F	0.26	0/5900	0.66	0/7995
All	All	0.27	0/35432	0.69	0/48018

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3
1	B	0	1
1	C	0	1
1	D	0	3
1	E	0	1
1	F	0	1
All	All	0	10

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (10) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	358	MET	Peptide
1	A	464	ILE	Peptide
1	A	504	LYS	Peptide

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Mol	Chain	Res	Type	Group
1	B	182	PHE	Peptide
1	C	504	LYS	Peptide
1	D	358	MET	Peptide
1	D	464	ILE	Peptide
1	D	504	LYS	Peptide
1	E	182	PHE	Peptide
1	F	504	LYS	Peptide

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	5780	0	5895	113	0
1	B	5780	0	5895	123	0
1	C	5773	0	5888	119	0
1	D	5780	0	5895	109	0
1	E	5780	0	5895	123	0
1	F	5773	0	5888	119	0
All	All	34666	0	35356	683	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 10.

All (683) 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:D:403:GLU:O	1:D:407:SER:HB2	1.79	0.82
1:A:403:GLU:O	1:A:407:SER:HB2	1.79	0.82
1:C:203:CYS:SG	1:C:433:ARG:NH2	2.65	0.69
1:F:203:CYS:SG	1:F:433:ARG:NH2	2.65	0.69
1:B:326:THR:HA	1:B:329:PHE:HB3	1.74	0.68
1:E:326:THR:HA	1:E:329:PHE:HB3	1.74	0.68
1:F:503:ALA:HA	1:F:525:ALA:HA	1.75	0.67
1:B:771:LEU:HB3	1:B:793:LYS:HD2	1.77	0.67
1:E:771:LEU:HB3	1:E:793:LYS:HD2	1.77	0.67
1:C:503:ALA:HA	1:C:525:ALA:HA	1.75	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:791:PRO:HD2	1:D:793:LYS:HE3	1.77	0.67
1:A:755:GLN:HA	1:A:777:LEU:HA	1.76	0.67
1:A:791:PRO:HD2	1:A:793:LYS:HE3	1.77	0.66
1:D:187:PRO:HG2	1:E:23:TRP:HA	1.78	0.66
1:E:505:ILE:H	1:E:527:VAL:HG21	1.61	0.66
1:E:751:LEU:HB2	1:E:754:LEU:HD22	1.78	0.66
1:B:682:LEU:HA	1:B:684:ARG:HH11	1.61	0.65
1:E:682:LEU:HA	1:E:684:ARG:HH11	1.61	0.65
1:F:734:LEU:O	1:F:758:HIS:NE2	2.29	0.65
1:B:505:ILE:H	1:B:527:VAL:HG21	1.61	0.65
1:D:755:GLN:HA	1:D:777:LEU:HA	1.76	0.65
1:E:474:LEU:HD11	1:E:476:LEU:HD23	1.79	0.65
1:C:734:LEU:O	1:C:758:HIS:NE2	2.29	0.65
1:B:474:LEU:HD11	1:B:476:LEU:HD23	1.79	0.65
1:A:187:PRO:HG2	1:B:23:TRP:HA	1.78	0.64
1:B:806:LYS:HE2	1:C:563:ARG:HE	1.63	0.64
1:E:585:ARG:HA	1:E:607:THR:HG23	1.78	0.64
1:B:751:LEU:HB2	1:B:754:LEU:HD22	1.77	0.64
1:E:596:LYS:HA	1:E:619:HIS:HB3	1.79	0.64
1:B:596:LYS:HA	1:B:619:HIS:HB3	1.79	0.64
1:B:585:ARG:HA	1:B:607:THR:HG23	1.78	0.64
1:E:806:LYS:HE2	1:F:563:ARG:HE	1.63	0.64
1:A:18:ARG:HA	1:A:21:LYS:HE3	1.81	0.63
1:D:761:GLY:H	1:D:784:GLN:HE21	1.47	0.63
1:E:806:LYS:HD2	1:E:828:LEU:HB2	1.81	0.63
1:E:573:SER:H	1:E:576:ASN:HD22	1.47	0.63
1:A:832:ASP:HA	1:A:835:PHE:HB2	1.80	0.62
1:B:806:LYS:HD2	1:B:828:LEU:HB2	1.81	0.62
1:D:809:CYS:SG	1:E:661:GLN:NE2	2.72	0.62
1:A:761:GLY:H	1:A:784:GLN:HE21	1.47	0.62
1:F:380:CYS:O	1:F:384:LEU:HB2	1.99	0.62
1:A:809:CYS:SG	1:B:661:GLN:NE2	2.72	0.62
1:F:682:LEU:HB3	1:F:685:LEU:HD13	1.82	0.62
1:C:797:LEU:HD13	1:C:800:LEU:HD22	1.82	0.62
1:D:588:ARG:HD3	1:D:589:HIS:HB2	1.82	0.62
1:D:832:ASP:HA	1:D:835:PHE:HB2	1.80	0.62
1:F:711:LEU:H	1:F:733:CYS:HB2	1.64	0.62
1:C:711:LEU:H	1:C:733:CYS:HB2	1.64	0.62
1:D:681:HIS:O	1:D:684:ARG:NH1	2.31	0.62
1:B:421:HIS:O	1:B:424:ASP:HB3	2.00	0.61
1:C:380:CYS:O	1:C:384:LEU:HB2	1.99	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:421:HIS:O	1:E:424:ASP:HB3	2.00	0.61
1:B:573:SER:H	1:B:576:ASN:HD22	1.47	0.61
1:F:797:LEU:HD13	1:F:800:LEU:HD22	1.82	0.61
1:A:576:ASN:HA	1:A:579:ILE:HG22	1.81	0.61
1:A:681:HIS:O	1:A:684:ARG:NH1	2.31	0.61
1:A:380:CYS:O	1:A:384:LEU:HB2	2.01	0.61
1:C:682:LEU:HB3	1:C:685:LEU:HD13	1.82	0.61
1:A:588:ARG:HD3	1:A:589:HIS:HB2	1.82	0.61
1:D:380:CYS:O	1:D:384:LEU:HB2	2.01	0.61
1:D:18:ARG:HA	1:D:21:LYS:HE3	1.81	0.60
1:D:576:ASN:HA	1:D:579:ILE:HG22	1.81	0.60
1:F:682:LEU:HA	1:F:684:ARG:HH11	1.66	0.60
1:D:387:LEU:HD21	1:D:422:MET:HE1	1.84	0.60
1:B:737:SER:OG	1:B:758:HIS:ND1	2.33	0.60
1:C:682:LEU:HA	1:C:684:ARG:HH11	1.66	0.60
1:B:792:GLU:HA	1:B:816:GLN:HG2	1.84	0.60
1:D:585:ARG:HB2	1:D:606:ILE:HD11	1.84	0.60
1:B:12:ASP:OD1	1:B:181:ASN:ND2	2.30	0.60
1:C:601:LYS:HE3	1:C:622:GLY:HA3	1.85	0.59
1:D:503:ALA:HB1	1:D:526:LYS:H	1.67	0.59
1:F:737:SER:OG	1:F:758:HIS:ND1	2.32	0.59
1:F:792:GLU:HA	1:F:816:GLN:HG2	1.84	0.59
1:A:503:ALA:HB1	1:A:526:LYS:H	1.67	0.59
1:A:585:ARG:HB2	1:A:606:ILE:HD11	1.84	0.59
1:A:596:LYS:HG3	1:A:619:HIS:HD2	1.68	0.59
1:F:601:LYS:HE3	1:F:622:GLY:HA3	1.85	0.59
1:C:792:GLU:HA	1:C:816:GLN:HG2	1.84	0.59
1:E:792:GLU:HA	1:E:816:GLN:HG2	1.84	0.59
1:C:737:SER:OG	1:C:758:HIS:ND1	2.32	0.59
1:F:35:MET:HG3	1:F:373:ILE:HD11	1.85	0.59
1:B:715:ASN:H	1:B:738:TYR:HB2	1.68	0.58
1:D:596:LYS:HG3	1:D:619:HIS:HD2	1.68	0.58
1:A:387:LEU:HD21	1:A:422:MET:HE1	1.84	0.58
1:D:715:ASN:H	1:D:738:TYR:HB2	1.68	0.58
1:F:571:LEU:HG	1:F:599:LEU:HD22	1.86	0.58
1:E:12:ASP:OD1	1:E:181:ASN:ND2	2.30	0.58
1:E:715:ASN:H	1:E:738:TYR:HB2	1.68	0.58
1:F:794:VAL:HG11	1:F:817:LEU:HD22	1.86	0.58
1:C:571:LEU:HG	1:C:599:LEU:HD22	1.86	0.58
1:D:448:GLU:OE2	1:D:452:ASN:ND2	2.37	0.58
1:F:756:HIS:HB3	1:F:758:HIS:HD2	1.69	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:448:GLU:OE2	1:A:452:ASN:ND2	2.37	0.57
1:B:614:THR:HA	1:B:637:VAL:HA	1.85	0.57
1:A:315:LYS:NZ	1:A:380:CYS:SG	2.77	0.57
1:A:715:ASN:H	1:A:738:TYR:HB2	1.68	0.57
1:D:315:LYS:NZ	1:D:380:CYS:SG	2.77	0.57
1:A:611:PRO:O	1:A:636:ASN:ND2	2.37	0.57
1:E:380:CYS:O	1:E:384:LEU:HB2	2.05	0.57
1:D:190:CYS:SG	1:E:18:ARG:NH2	2.78	0.57
1:D:399:LYS:NZ	1:D:431:SER:OG	2.37	0.57
1:E:614:THR:HA	1:E:637:VAL:HA	1.85	0.57
1:A:190:CYS:SG	1:B:18:ARG:NH2	2.78	0.57
1:A:399:LYS:NZ	1:A:431:SER:OG	2.37	0.57
1:C:35:MET:HG3	1:C:373:ILE:HD11	1.85	0.57
1:B:380:CYS:O	1:B:384:LEU:HB2	2.05	0.57
1:E:726:PHE:HA	1:E:750:LEU:HD22	1.87	0.57
1:C:756:HIS:HB3	1:C:758:HIS:HD2	1.69	0.57
1:D:490:THR:O	1:D:514:ASN:ND2	2.36	0.57
1:C:537:ASP:O	1:C:561:ASN:ND2	2.38	0.56
1:B:726:PHE:HA	1:B:750:LEU:HD22	1.87	0.56
1:D:611:PRO:O	1:D:636:ASN:ND2	2.37	0.56
1:D:650:ILE:HB	1:D:674:GLU:HB2	1.88	0.56
1:F:537:ASP:O	1:F:561:ASN:ND2	2.38	0.56
1:A:496:LYS:HA	1:A:519:HIS:HB2	1.87	0.56
1:A:540:ARG:O	1:A:563:ARG:N	2.32	0.56
1:B:787:ILE:O	1:B:808:ASN:ND2	2.38	0.56
1:C:794:VAL:HG11	1:C:817:LEU:HD22	1.86	0.56
1:B:791:PRO:HD2	1:B:793:LYS:HE3	1.88	0.56
1:E:469:GLN:NE2	1:E:493:ASP:OD2	2.39	0.56
1:E:791:PRO:HD2	1:E:793:LYS:HE3	1.88	0.56
1:A:708:LEU:HD21	1:A:711:LEU:HD23	1.87	0.56
1:A:781:ASN:HA	1:A:804:GLU:HB3	1.88	0.56
1:E:563:ARG:O	1:E:591:LYS:N	2.39	0.56
1:A:614:THR:HA	1:A:637:VAL:HA	1.88	0.56
1:A:650:ILE:HB	1:A:674:GLU:HB2	1.87	0.56
1:B:490:THR:O	1:B:514:ASN:ND2	2.39	0.56
1:D:614:THR:HA	1:D:637:VAL:HA	1.88	0.56
1:A:490:THR:O	1:A:514:ASN:ND2	2.36	0.55
1:D:496:LYS:HA	1:D:519:HIS:HB2	1.87	0.55
1:E:490:THR:O	1:E:514:ASN:ND2	2.39	0.55
1:B:469:GLN:NE2	1:B:493:ASP:OD2	2.39	0.55
1:C:834:LEU:HD11	1:C:842:VAL:HG11	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:787:ILE:O	1:E:808:ASN:ND2	2.38	0.55
1:E:31:LEU:HD22	1:E:376:TYR:HD1	1.71	0.55
1:A:784:GLN:OE1	1:B:612:HIS:ND1	2.40	0.55
1:D:708:LEU:HD21	1:D:711:LEU:HD23	1.87	0.55
1:B:31:LEU:HD22	1:B:376:TYR:HD1	1.71	0.55
1:A:444:ASN:HA	1:A:447:ARG:HG2	1.89	0.55
1:A:737:SER:HG	1:A:758:HIS:HD1	1.52	0.55
1:F:834:LEU:HD11	1:F:842:VAL:HG11	1.88	0.55
1:B:563:ARG:O	1:B:591:LYS:N	2.39	0.55
1:B:448:GLU:OE2	1:B:452:ASN:ND2	2.40	0.55
1:F:577:LYS:NZ	1:F:603:PRO:O	2.40	0.55
1:B:829:VAL:HG12	1:B:834:LEU:HD22	1.90	0.54
1:E:647:LEU:HD23	1:E:649:ARG:HB2	1.89	0.54
1:A:7:VAL:HG11	1:B:6:GLU:HG2	1.89	0.54
1:A:837:THR:HG22	1:B:755:GLN:HE22	1.73	0.54
1:C:577:LYS:NZ	1:C:603:PRO:O	2.40	0.54
1:D:444:ASN:HA	1:D:447:ARG:HG2	1.89	0.54
1:D:769:LYS:HA	1:D:793:LYS:HD3	1.89	0.54
1:E:748:ILE:HG13	1:E:770:GLN:HB2	1.88	0.54
1:D:781:ASN:HA	1:D:804:GLU:HB3	1.88	0.54
1:D:784:GLN:OE1	1:E:612:HIS:ND1	2.40	0.54
1:D:837:THR:HG22	1:E:755:GLN:HE22	1.73	0.54
1:D:564:GLU:HB2	1:D:592:ILE:HG13	1.90	0.54
1:A:769:LYS:HA	1:A:793:LYS:HD3	1.89	0.54
1:E:829:VAL:HG12	1:E:834:LEU:HD22	1.90	0.54
1:A:403:GLU:O	1:A:407:SER:CB	2.54	0.54
1:A:734:LEU:O	1:A:758:HIS:NE2	2.41	0.54
1:A:786:CYS:HA	1:A:808:ASN:HA	1.89	0.54
1:B:209:THR:HG21	1:B:433:ARG:HH22	1.73	0.54
1:B:748:ILE:HG13	1:B:770:GLN:HB2	1.88	0.54
1:C:708:LEU:HB3	1:C:728:LEU:HD22	1.90	0.54
1:E:448:GLU:OE2	1:E:452:ASN:ND2	2.40	0.54
1:F:708:LEU:HB3	1:F:728:LEU:HD22	1.90	0.54
1:B:647:LEU:HD23	1:B:649:ARG:HB2	1.90	0.53
1:D:540:ARG:O	1:D:563:ARG:N	2.32	0.53
1:D:786:CYS:HA	1:D:808:ASN:HA	1.89	0.53
1:D:403:GLU:O	1:D:407:SER:CB	2.54	0.53
1:F:494:VAL:HG12	1:F:517:GLU:HG2	1.90	0.53
1:B:295:ARG:HD2	1:B:438:LEU:HD11	1.90	0.53
1:D:619:HIS:HB2	1:D:643:GLN:HE21	1.74	0.53
1:E:532:PHE:O	1:E:536:ARG:HB2	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:476:LEU:HA	1:B:479:LEU:HB2	1.91	0.53
1:B:666:LYS:HE3	1:B:691:TRP:HE1	1.73	0.53
1:E:209:THR:HG21	1:E:433:ARG:HH22	1.73	0.53
1:F:638:ALA:HA	1:F:660:LEU:HA	1.91	0.53
1:B:532:PHE:O	1:B:536:ARG:HB2	2.08	0.53
1:A:564:GLU:HB2	1:A:592:ILE:HG13	1.90	0.53
1:A:619:HIS:HB2	1:A:643:GLN:HE21	1.74	0.53
1:B:687:CYS:SG	1:B:710:SER:OG	2.60	0.53
1:B:718:LEU:HB2	1:B:739:ASN:HD22	1.74	0.53
1:C:658:SER:O	1:C:684:ARG:NE	2.42	0.53
1:C:771:LEU:HB3	1:C:793:LYS:HD2	1.91	0.53
1:D:649:ARG:NH2	1:D:673:ILE:O	2.41	0.53
1:C:638:ALA:HA	1:C:660:LEU:HA	1.91	0.53
1:A:679:PHE:HA	1:A:682:LEU:HB2	1.90	0.53
1:D:758:HIS:HA	1:D:781:ASN:HB3	1.90	0.53
1:F:441:VAL:O	1:F:445:LYS:NZ	2.41	0.53
1:C:46:GLN:NE2	1:C:50:ASP:OD1	2.42	0.53
1:F:560:LYS:HA	1:F:587:LEU:HB2	1.91	0.53
1:D:734:LEU:O	1:D:758:HIS:NE2	2.41	0.53
1:E:295:ARG:HD2	1:E:438:LEU:HD11	1.90	0.53
1:F:658:SER:O	1:F:684:ARG:NE	2.42	0.53
1:C:448:GLU:OE2	1:C:452:ASN:ND2	2.42	0.52
1:F:443:GLU:HG2	1:F:447:ARG:HH21	1.75	0.52
1:C:560:LYS:HA	1:C:587:LEU:HB2	1.91	0.52
1:F:505:ILE:HG12	1:F:528:GLU:HG2	1.91	0.52
1:F:771:LEU:HB3	1:F:793:LYS:HD2	1.91	0.52
1:C:494:VAL:HG12	1:C:517:GLU:HG2	1.90	0.52
1:E:521:CYS:HB2	1:E:546:PHE:HB2	1.92	0.52
1:A:758:HIS:HA	1:A:781:ASN:HB3	1.90	0.52
1:C:556:VAL:HA	1:C:559:LEU:HD22	1.91	0.52
1:E:666:LYS:HE3	1:E:691:TRP:HE1	1.73	0.52
1:F:46:GLN:NE2	1:F:50:ASP:OD1	2.42	0.52
1:C:281:GLY:HA2	1:C:446:LEU:HD13	1.91	0.52
1:C:441:VAL:O	1:C:445:LYS:NZ	2.41	0.52
1:C:803:LEU:O	1:C:826:SER:OG	2.25	0.52
1:D:679:PHE:HA	1:D:682:LEU:HB2	1.90	0.52
1:B:521:CYS:HB2	1:B:546:PHE:HB2	1.92	0.52
1:D:521:CYS:HB2	1:D:546:PHE:HB2	1.91	0.52
1:E:154:TYR:HA	1:E:158:LEU:HD23	1.92	0.52
1:E:718:LEU:HB2	1:E:739:ASN:HD22	1.74	0.52
1:C:443:GLU:HG2	1:C:447:ARG:HH21	1.75	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:803:LEU:O	1:F:826:SER:OG	2.25	0.52
1:C:411:ASP:HA	1:C:439:SER:HB2	1.92	0.52
1:C:748:ILE:HG13	1:C:770:GLN:HB2	1.91	0.52
1:E:476:LEU:HA	1:E:479:LEU:HB2	1.91	0.52
1:A:17:TYR:OH	1:A:194:GLU:OE1	2.28	0.52
1:A:521:CYS:HB2	1:A:546:PHE:HB2	1.91	0.52
1:B:154:TYR:HA	1:B:158:LEU:HD23	1.92	0.52
1:B:619:HIS:HB2	1:B:643:GLN:HE21	1.75	0.52
1:F:556:VAL:HA	1:F:559:LEU:HD22	1.91	0.52
1:C:744:ILE:HD11	1:C:767:LEU:HA	1.91	0.51
1:B:797:LEU:HD13	1:B:800:LEU:HD13	1.92	0.51
1:F:748:ILE:HG13	1:F:770:GLN:HB2	1.91	0.51
1:C:712:TYR:HA	1:C:735:ASP:HA	1.92	0.51
1:D:608:ASP:HB2	1:D:633:LYS:HB3	1.93	0.51
1:E:519:HIS:HA	1:E:543:HIS:HB2	1.92	0.51
1:D:17:TYR:OH	1:D:194:GLU:OE1	2.28	0.51
1:F:204:PHE:HD1	1:F:433:ARG:HE	1.59	0.51
1:F:712:TYR:HA	1:F:735:ASP:HA	1.92	0.51
1:B:647:LEU:O	1:B:668:ASN:ND2	2.43	0.51
1:C:505:ILE:HG12	1:C:528:GLU:HG2	1.91	0.51
1:F:281:GLY:HA2	1:F:446:LEU:HD13	1.91	0.51
1:C:732:ARG:HA	1:C:754:LEU:HA	1.92	0.51
1:C:751:LEU:HB2	1:C:754:LEU:HB3	1.92	0.51
1:F:751:LEU:HB2	1:F:754:LEU:HB3	1.92	0.51
1:A:641:GLU:HA	1:A:664:ASP:HB3	1.92	0.51
1:F:732:ARG:HA	1:F:754:LEU:HA	1.92	0.51
1:E:797:LEU:HD13	1:E:800:LEU:HD13	1.92	0.51
1:F:744:ILE:HD11	1:F:767:LEU:HA	1.91	0.51
1:D:585:ARG:HA	1:D:609:VAL:HG13	1.92	0.51
1:E:619:HIS:HB2	1:E:643:GLN:HE21	1.75	0.51
1:E:647:LEU:O	1:E:668:ASN:ND2	2.43	0.51
1:A:582:GLU:HA	1:A:606:ILE:HG12	1.94	0.50
1:D:641:GLU:HA	1:D:664:ASP:HB3	1.92	0.50
1:E:794:VAL:HG11	1:E:817:LEU:HD22	1.93	0.50
1:A:771:LEU:HG	1:A:793:LYS:HD2	1.94	0.50
1:A:585:ARG:HA	1:A:609:VAL:HG13	1.93	0.50
1:A:608:ASP:HB2	1:A:633:LYS:HB3	1.92	0.50
1:B:403:GLU:O	1:B:432:LYS:NZ	2.45	0.50
1:C:542:LEU:HD13	1:C:544:VAL:HG13	1.93	0.50
1:D:536:ARG:HA	1:D:559:LEU:HB2	1.93	0.50
1:A:213:LEU:HD21	1:A:436:VAL:HG21	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:624:LYS:HB3	1:D:647:LEU:HG	1.94	0.50
1:E:489:LEU:HB3	1:E:492:LEU:HD13	1.93	0.50
1:F:411:ASP:HA	1:F:439:SER:HB2	1.92	0.50
1:A:303:LEU:O	1:A:307:LEU:CB	2.60	0.50
1:C:204:PHE:HD1	1:C:433:ARG:HE	1.59	0.50
1:D:818:GLY:HA3	1:D:841:GLU:HB3	1.94	0.50
1:E:340:LYS:HG2	1:E:351:VAL:HG22	1.93	0.50
1:B:519:HIS:HA	1:B:543:HIS:HB2	1.92	0.50
1:C:183:TRP:HH2	1:C:422:MET:HE2	1.77	0.50
1:D:762:ASN:HD21	1:D:785:ASN:HD21	1.59	0.50
1:F:791:PRO:HD2	1:F:793:LYS:HE3	1.93	0.50
1:A:536:ARG:HA	1:A:559:LEU:HB2	1.93	0.50
1:B:340:LYS:HG2	1:B:351:VAL:HG22	1.93	0.50
1:B:489:LEU:HB3	1:B:492:LEU:HD13	1.93	0.50
1:F:779:THR:HG22	1:F:802:GLN:HE21	1.77	0.50
1:C:199:ILE:O	1:C:203:CYS:HB2	2.12	0.50
1:E:403:GLU:O	1:E:432:LYS:NZ	2.45	0.50
1:E:771:LEU:HD13	1:E:793:LYS:HZ3	1.77	0.50
1:F:183:TRP:HH2	1:F:422:MET:HE2	1.77	0.50
1:C:779:THR:HG22	1:C:802:GLN:HE21	1.77	0.49
1:F:448:GLU:OE2	1:F:452:ASN:ND2	2.42	0.49
1:B:794:VAL:HG11	1:B:817:LEU:HD22	1.93	0.49
1:E:494:VAL:HG12	1:E:517:GLU:HG3	1.94	0.49
1:C:473:GLU:HB2	1:C:496:LYS:HE3	1.94	0.49
1:D:213:LEU:HD21	1:D:436:VAL:HG21	1.94	0.49
1:E:35:MET:SD	1:E:173:THR:OG1	2.62	0.49
1:E:608:ASP:HB2	1:E:634:MET:HB2	1.94	0.49
1:F:199:ILE:O	1:F:203:CYS:HB2	2.12	0.49
1:C:310:VAL:HA	1:C:313:VAL:HG22	1.94	0.49
1:C:791:PRO:HD2	1:C:793:LYS:HE3	1.93	0.49
1:E:540:ARG:O	1:E:563:ARG:N	2.36	0.49
1:E:640:LEU:HB2	1:E:662:GLU:HG3	1.95	0.49
1:A:476:LEU:HA	1:A:479:LEU:HD23	1.95	0.49
1:A:818:GLY:HA3	1:A:841:GLU:HB3	1.94	0.49
1:D:476:LEU:HA	1:D:479:LEU:HD23	1.95	0.49
1:D:582:GLU:HA	1:D:606:ILE:HG12	1.94	0.49
1:D:771:LEU:HG	1:D:793:LYS:HD2	1.94	0.49
1:A:50:ASP:HA	1:A:358:MET:HE2	1.95	0.49
1:E:545:LYS:HB2	1:E:568:ILE:HG13	1.95	0.49
1:A:624:LYS:HB3	1:A:647:LEU:HG	1.94	0.49
1:B:585:ARG:HH12	1:B:606:ILE:HG13	1.78	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:585:ARG:HH12	1:E:606:ILE:HG13	1.78	0.49
1:F:322:ILE:HD11	1:F:373:ILE:HG21	1.95	0.49
1:F:476:LEU:HD22	1:F:498:GLU:H	1.77	0.49
1:A:563:ARG:O	1:A:591:LYS:N	2.46	0.48
1:A:649:ARG:NH2	1:A:673:ILE:O	2.41	0.48
1:B:762:ASN:HD21	1:B:785:ASN:HD21	1.61	0.48
1:C:307:LEU:HA	1:C:310:VAL:HG12	1.95	0.48
1:C:322:ILE:HD11	1:C:373:ILE:HG21	1.95	0.48
1:C:473:GLU:HA	1:C:496:LYS:HG2	1.95	0.48
1:D:50:ASP:HA	1:D:358:MET:HE2	1.95	0.48
1:A:762:ASN:HD21	1:A:785:ASN:HD21	1.59	0.48
1:B:5:ALA:HB2	1:B:40:ILE:HG21	1.95	0.48
1:B:608:ASP:HB2	1:B:634:MET:HB2	1.94	0.48
1:D:563:ARG:O	1:D:591:LYS:N	2.46	0.48
1:E:687:CYS:SG	1:E:710:SER:OG	2.60	0.48
1:B:588:ARG:HE	1:B:589:HIS:HB2	1.78	0.48
1:D:303:LEU:O	1:D:307:LEU:CB	2.60	0.48
1:F:307:LEU:HA	1:F:310:VAL:HG12	1.95	0.48
1:B:494:VAL:HG12	1:B:517:GLU:HG3	1.94	0.48
1:F:18:ARG:HA	1:F:21:LYS:HE3	1.95	0.48
1:A:687:CYS:SG	1:A:710:SER:OG	2.72	0.48
1:B:640:LEU:HB2	1:B:662:GLU:HG3	1.95	0.48
1:C:476:LEU:HD22	1:C:498:GLU:H	1.77	0.48
1:F:542:LEU:HD13	1:F:544:VAL:HG13	1.94	0.48
1:F:585:ARG:NH1	1:F:608:ASP:OD1	2.47	0.48
1:D:572:ASN:HA	1:D:576:ASN:HD22	1.78	0.48
1:D:831:GLU:HB2	1:D:833:HIS:CD2	2.49	0.48
1:E:762:ASN:HD21	1:E:785:ASN:HD21	1.61	0.48
1:A:831:GLU:HB2	1:A:833:HIS:CD2	2.49	0.48
1:E:7:VAL:O	1:E:11:ASN:HB2	2.14	0.48
1:E:592:ILE:HG22	1:E:615:LYS:HB3	1.96	0.48
1:E:681:HIS:O	1:E:684:ARG:NH1	2.47	0.48
1:F:310:VAL:HA	1:F:313:VAL:HG22	1.94	0.48
1:F:339:CYS:SG	1:F:340:LYS:N	2.87	0.48
1:F:681:HIS:O	1:F:684:ARG:NH1	2.47	0.48
1:B:35:MET:SD	1:B:173:THR:OG1	2.62	0.48
1:C:585:ARG:NH1	1:C:608:ASP:OD1	2.47	0.48
1:F:464:ILE:HD13	1:F:472:GLN:HA	1.96	0.48
1:B:545:LYS:HB2	1:B:568:ILE:HG13	1.95	0.48
1:C:211:LYS:NZ	1:C:277:ASP:OD2	2.47	0.48
1:B:195:HIS:O	1:B:199:ILE:HG13	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:339:CYS:SG	1:C:340:LYS:N	2.87	0.47
1:D:769:LYS:H	1:D:769:LYS:HD2	1.79	0.47
1:B:540:ARG:O	1:B:563:ARG:N	2.36	0.47
1:F:211:LYS:NZ	1:F:277:ASP:OD2	2.47	0.47
1:F:473:GLU:HA	1:F:496:LYS:HG2	1.95	0.47
1:F:473:GLU:HB2	1:F:496:LYS:HE3	1.94	0.47
1:C:471:LYS:HD2	1:C:473:GLU:HG2	1.97	0.47
1:E:737:SER:OG	1:E:758:HIS:ND1	2.33	0.47
1:F:399:LYS:NZ	1:F:431:SER:OG	2.47	0.47
1:A:520:LEU:HD13	1:A:523:CYS:HB2	1.96	0.47
1:A:572:ASN:HA	1:A:576:ASN:HD22	1.78	0.47
1:A:595:VAL:HB	1:A:618:ILE:HA	1.97	0.47
1:B:681:HIS:O	1:B:684:ARG:NH1	2.47	0.47
1:B:487:PHE:HE2	1:B:506:PRO:HD2	1.80	0.47
1:B:500:ILE:HG13	1:B:502:GLU:H	1.79	0.47
1:E:588:ARG:HE	1:E:589:HIS:HB2	1.78	0.47
1:A:769:LYS:H	1:A:769:LYS:HD2	1.80	0.47
1:C:399:LYS:NZ	1:C:431:SER:OG	2.47	0.47
1:C:681:HIS:O	1:C:684:ARG:NH1	2.47	0.47
1:D:149:ILE:HD13	1:D:347:ILE:HD13	1.96	0.47
1:D:587:LEU:HD12	1:D:590:LEU:HB2	1.97	0.47
1:D:798:SER:HB2	1:D:822:MET:HG2	1.96	0.47
1:E:195:HIS:O	1:E:199:ILE:HG13	2.14	0.47
1:E:487:PHE:HE2	1:E:506:PRO:HD2	1.80	0.47
1:F:23:TRP:HE3	1:F:24:TRP:HE3	1.62	0.47
1:F:668:ASN:HD22	1:F:669:ASN:H	1.63	0.47
1:F:702:ILE:HD11	1:F:725:VAL:HG12	1.96	0.47
1:B:592:ILE:HG22	1:B:615:LYS:HB3	1.96	0.47
1:B:781:ASN:HA	1:B:804:GLU:HB3	1.96	0.47
1:D:7:VAL:HG11	1:E:6:GLU:HG2	1.97	0.47
1:D:687:CYS:SG	1:D:710:SER:OG	2.72	0.47
1:E:650:ILE:H	1:E:674:GLU:HG3	1.80	0.47
1:E:673:ILE:HD11	1:E:699:PRO:HD2	1.97	0.47
1:E:732:ARG:NE	1:E:755:GLN:OE1	2.48	0.47
1:A:798:SER:HB2	1:A:822:MET:HG2	1.96	0.47
1:E:780:LEU:O	1:E:804:GLU:N	2.48	0.47
1:F:471:LYS:HD2	1:F:473:GLU:HG2	1.97	0.47
1:C:464:ILE:HD13	1:C:472:GLN:HA	1.96	0.47
1:E:500:ILE:HG13	1:E:502:GLU:H	1.79	0.47
1:A:732:ARG:HA	1:A:754:LEU:HA	1.97	0.46
1:C:668:ASN:HD22	1:C:669:ASN:H	1.63	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:509:ILE:HD12	1:F:512:MET:HB2	1.98	0.46
1:B:650:ILE:H	1:B:674:GLU:HG3	1.80	0.46
1:B:771:LEU:HD13	1:B:793:LYS:HZ3	1.80	0.46
1:E:27:PHE:O	1:E:31:LEU:HB2	2.15	0.46
1:E:346:LEU:HD23	1:F:55:LEU:HD11	1.97	0.46
1:C:522:HIS:H	1:C:547:THR:HG22	1.80	0.46
1:D:154:TYR:HA	1:D:158:LEU:HD23	1.97	0.46
1:D:451:LEU:HD22	1:D:479:LEU:HD13	1.97	0.46
1:D:520:LEU:HD13	1:D:523:CYS:HB2	1.96	0.46
1:D:732:ARG:HA	1:D:754:LEU:HA	1.97	0.46
1:E:781:ASN:HA	1:E:804:GLU:HB3	1.97	0.46
1:B:346:LEU:HD23	1:C:55:LEU:HD11	1.97	0.46
1:B:444:ASN:HA	1:B:447:ARG:HG2	1.96	0.46
1:E:326:THR:HG21	1:E:370:ILE:HD11	1.98	0.46
1:B:631:LEU:HB3	1:B:654:ILE:HD12	1.96	0.46
1:C:23:TRP:HE3	1:C:24:TRP:HE3	1.62	0.46
1:C:542:LEU:HG	1:C:562:LEU:HD11	1.97	0.46
1:D:595:VAL:HB	1:D:618:ILE:HA	1.97	0.46
1:E:620:ASN:H	1:E:644:ASN:HB3	1.80	0.46
1:E:631:LEU:HB3	1:E:654:ILE:HD12	1.96	0.46
1:F:323:LEU:O	1:F:327:ALA:HB2	2.16	0.46
1:A:596:LYS:HG3	1:A:619:HIS:CD2	2.50	0.46
1:C:532:PHE:O	1:C:536:ARG:N	2.45	0.46
1:C:702:ILE:HD11	1:C:725:VAL:HG12	1.96	0.46
1:D:596:LYS:HG3	1:D:619:HIS:CD2	2.50	0.46
1:E:444:ASN:HA	1:E:447:ARG:HG2	1.96	0.46
1:A:587:LEU:HD12	1:A:590:LEU:HB2	1.97	0.46
1:B:209:THR:OG1	1:B:433:ARG:NH1	2.49	0.46
1:E:601:LYS:HE3	1:E:622:GLY:H	1.81	0.46
1:B:655:PHE:HA	1:B:682:LEU:HD11	1.98	0.46
1:C:584:LEU:HB2	1:C:606:ILE:HG23	1.98	0.46
1:A:451:LEU:HD22	1:A:479:LEU:HD13	1.97	0.46
1:D:493:ASP:HA	1:D:515:LEU:HA	1.98	0.46
1:A:154:TYR:HA	1:A:158:LEU:HD23	1.97	0.46
1:C:323:LEU:O	1:C:327:ALA:HB2	2.16	0.46
1:C:509:ILE:HD12	1:C:512:MET:HB2	1.98	0.46
1:E:5:ALA:HB2	1:E:40:ILE:HG21	1.98	0.46
1:E:631:LEU:H	1:E:631:LEU:HG	1.60	0.46
1:E:655:PHE:HA	1:E:682:LEU:HD11	1.98	0.46
1:F:540:ARG:O	1:F:563:ARG:N	2.39	0.46
1:F:684:ARG:H	1:F:684:ARG:HD2	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:493:ASP:HA	1:A:515:LEU:HA	1.98	0.45
1:A:824:LYS:NZ	1:A:849:ASP:O	2.50	0.45
1:B:27:PHE:O	1:B:31:LEU:HB2	2.16	0.45
1:B:601:LYS:HE3	1:B:622:GLY:H	1.81	0.45
1:D:519:HIS:HD2	1:D:543:HIS:H	1.65	0.45
1:D:684:ARG:HA	1:D:707:ASN:HB2	1.98	0.45
1:E:54:CYS:HA	1:E:354:CYS:HA	1.98	0.45
1:A:519:HIS:HD2	1:A:543:HIS:H	1.65	0.45
1:B:826:SER:HB3	1:B:830:VAL:HG23	1.99	0.45
1:F:36:LEU:HB2	1:F:173:THR:HG21	1.98	0.45
1:F:730:LYS:HE2	1:F:732:ARG:HD2	1.98	0.45
1:A:149:ILE:HD13	1:A:347:ILE:HD13	1.96	0.45
1:A:750:LEU:O	1:A:752:GLN:NE2	2.50	0.45
1:A:760:THR:OG1	1:A:781:ASN:O	2.34	0.45
1:B:326:THR:HG21	1:B:370:ILE:HD11	1.98	0.45
1:F:496:LYS:HA	1:F:519:HIS:HB2	1.99	0.45
1:A:689:LYS:HB2	1:A:691:TRP:HZ3	1.82	0.45
1:B:620:ASN:H	1:B:644:ASN:HB3	1.79	0.45
1:B:673:ILE:HD11	1:B:699:PRO:HD2	1.97	0.45
1:D:760:THR:OG1	1:D:781:ASN:O	2.34	0.45
1:E:209:THR:OG1	1:E:433:ARG:NH1	2.48	0.45
1:E:647:LEU:HB3	1:E:649:ARG:H	1.81	0.45
1:A:568:ILE:HD13	1:A:596:LYS:HE3	1.98	0.45
1:B:52:VAL:HG23	1:B:150:ASN:HB2	1.98	0.45
1:B:322:ILE:HD11	1:B:373:ILE:HG21	1.99	0.45
1:C:692:HIS:HD2	1:C:715:ASN:HD22	1.65	0.45
1:C:758:HIS:HA	1:C:781:ASN:HB3	1.99	0.45
1:D:675:GLU:O	1:D:678:SER:OG	2.30	0.45
1:B:732:ARG:NE	1:B:755:GLN:OE1	2.48	0.45
1:C:18:ARG:HA	1:C:21:LYS:HE3	1.98	0.45
1:D:750:LEU:O	1:D:752:GLN:NE2	2.50	0.45
1:E:460:LEU:HD11	1:E:486:VAL:HG23	1.99	0.45
1:E:581:LEU:H	1:E:584:LEU:HD21	1.82	0.45
1:E:751:LEU:HD22	1:E:754:LEU:HD13	1.99	0.45
1:F:542:LEU:HG	1:F:562:LEU:HD11	1.97	0.45
1:B:7:VAL:O	1:B:11:ASN:HB2	2.17	0.45
1:D:730:LYS:HA	1:D:753:ASN:HD21	1.82	0.45
1:D:824:LYS:NZ	1:D:849:ASP:O	2.49	0.45
1:C:684:ARG:H	1:C:684:ARG:HD2	1.81	0.45
1:D:568:ILE:HD13	1:D:596:LYS:HE3	1.98	0.45
1:B:780:LEU:O	1:B:804:GLU:N	2.48	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:522:HIS:H	1:F:547:THR:HG22	1.81	0.45
1:B:581:LEU:H	1:B:584:LEU:HD21	1.82	0.44
1:B:751:LEU:HD22	1:B:754:LEU:HD13	1.99	0.44
1:C:596:LYS:HG3	1:C:619:HIS:CD2	2.52	0.44
1:F:584:LEU:HB2	1:F:606:ILE:HG23	1.98	0.44
1:F:741:ILE:HG22	1:F:762:ASN:HD22	1.82	0.44
1:C:741:ILE:HG22	1:C:762:ASN:HD22	1.82	0.44
1:D:303:LEU:O	1:D:307:LEU:HB3	2.17	0.44
1:A:303:LEU:O	1:A:307:LEU:HB3	2.17	0.44
1:A:684:ARG:HA	1:A:707:ASN:HB2	1.98	0.44
1:B:54:CYS:HA	1:B:354:CYS:HA	1.98	0.44
1:B:446:LEU:HD23	1:B:446:LEU:HA	1.82	0.44
1:E:52:VAL:HG23	1:E:150:ASN:HB2	1.98	0.44
1:E:826:SER:HB3	1:E:830:VAL:HG23	1.99	0.44
1:F:595:VAL:H	1:F:617:VAL:HG13	1.82	0.44
1:F:737:SER:HG	1:F:758:HIS:CE1	2.29	0.44
1:A:730:LYS:HA	1:A:753:ASN:HD21	1.82	0.44
1:B:460:LEU:HD11	1:B:486:VAL:HG23	1.99	0.44
1:C:149:ILE:HD12	1:C:149:ILE:HA	1.89	0.44
1:D:689:LYS:HB2	1:D:691:TRP:HZ3	1.81	0.44
1:B:647:LEU:HB3	1:B:649:ARG:H	1.82	0.44
1:C:730:LYS:HE2	1:C:732:ARG:HD2	1.98	0.44
1:C:843:LYS:O	1:C:847:ASN:HB2	2.17	0.44
1:E:322:ILE:HD11	1:E:373:ILE:HG21	1.99	0.44
1:E:517:GLU:HB3	1:E:541:CYS:SG	2.57	0.44
1:C:757:LEU:HB2	1:C:780:LEU:HA	2.00	0.44
1:E:12:ASP:HB2	1:E:177:MET:HE2	1.98	0.44
1:E:665:LEU:HG	1:E:670:ILE:HD11	1.99	0.44
1:F:757:LEU:HB2	1:F:780:LEU:HA	2.00	0.44
1:C:595:VAL:H	1:C:617:VAL:HG13	1.82	0.44
1:D:458:GLU:HG3	1:D:462:GLN:HE22	1.83	0.44
1:F:563:ARG:O	1:F:591:LYS:N	2.45	0.44
1:F:565:LEU:HB3	1:F:593:LEU:HA	2.00	0.44
1:B:665:LEU:HG	1:B:670:ILE:HD11	1.99	0.44
1:D:609:VAL:HA	1:D:633:LYS:HD2	2.00	0.44
1:F:532:PHE:O	1:F:536:ARG:N	2.45	0.44
1:F:665:LEU:HD11	1:F:690:LEU:HB2	2.00	0.44
1:F:692:HIS:HD2	1:F:715:ASN:HD22	1.65	0.44
1:F:758:HIS:HA	1:F:781:ASN:HB3	1.99	0.44
1:F:843:LYS:O	1:F:847:ASN:HB2	2.17	0.44
1:A:471:LYS:HB3	1:A:494:VAL:HG23	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:609:VAL:HA	1:A:633:LYS:HD2	2.00	0.44
1:B:496:LYS:HA	1:B:519:HIS:HB2	2.00	0.44
1:C:665:LEU:HD11	1:C:690:LEU:HB2	2.00	0.44
1:C:669:ASN:OD1	1:C:669:ASN:N	2.48	0.44
1:D:555:TRP:CD1	1:D:556:VAL:HG13	2.53	0.44
1:A:741:ILE:HG21	1:A:759:ILE:HD11	2.00	0.43
1:B:517:GLU:HB3	1:B:541:CYS:SG	2.57	0.43
1:B:709:GLU:O	1:B:732:ARG:N	2.51	0.43
1:D:787:ILE:O	1:D:808:ASN:ND2	2.50	0.43
1:A:772:PHE:HB3	1:A:793:LYS:HA	2.00	0.43
1:C:496:LYS:HA	1:C:519:HIS:HB2	1.99	0.43
1:D:568:ILE:HB	1:D:596:LYS:HB3	2.00	0.43
1:E:496:LYS:HA	1:E:519:HIS:HB2	2.00	0.43
1:E:709:GLU:O	1:E:732:ARG:N	2.51	0.43
1:E:755:GLN:HA	1:E:777:LEU:HA	1.99	0.43
1:A:563:ARG:HG3	1:A:564:GLU:HG3	2.00	0.43
1:B:12:ASP:HB2	1:B:177:MET:HE2	2.00	0.43
1:B:755:GLN:HA	1:B:777:LEU:HA	1.99	0.43
1:C:565:LEU:HB3	1:C:593:LEU:HA	2.00	0.43
1:D:741:ILE:HG21	1:D:759:ILE:HD11	2.00	0.43
1:E:668:ASN:HD22	1:E:669:ASN:N	2.16	0.43
1:A:555:TRP:CD1	1:A:556:VAL:HG13	2.53	0.43
1:B:290:LYS:HG3	1:B:294:PHE:CE2	2.54	0.43
1:B:568:ILE:HD13	1:B:596:LYS:HE3	2.00	0.43
1:C:540:ARG:O	1:C:563:ARG:N	2.39	0.43
1:C:645:CYS:HB3	1:C:647:LEU:HD13	2.01	0.43
1:A:594:HIS:HA	1:A:617:VAL:HG13	2.01	0.43
1:A:642:LEU:N	1:A:664:ASP:O	2.51	0.43
1:D:511:GLN:HG3	1:D:512:MET:HE2	2.00	0.43
1:D:721:LEU:HD12	1:D:745:PRO:HD3	2.00	0.43
1:E:290:LYS:HG3	1:E:294:PHE:CE2	2.54	0.43
1:F:585:ARG:HH11	1:F:609:VAL:HB	1.83	0.43
1:F:777:LEU:HG	1:F:800:LEU:HB2	2.01	0.43
1:B:35:MET:HE1	1:B:173:THR:HA	2.01	0.43
1:B:566:TYR:HD1	1:B:566:TYR:HA	1.78	0.43
1:C:464:ILE:HD13	1:C:472:GLN:HG3	2.01	0.43
1:C:507:ALA:HA	1:C:531:ALA:HB2	2.01	0.43
1:D:594:HIS:HA	1:D:617:VAL:HG13	2.01	0.43
1:D:772:PHE:HB3	1:D:793:LYS:HA	2.00	0.43
1:E:568:ILE:HD13	1:E:596:LYS:HE3	2.00	0.43
1:F:665:LEU:HD12	1:F:670:ILE:HG13	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:511:GLN:HG3	1:A:512:MET:HE2	2.00	0.43
1:E:567:LEU:HD13	1:E:570:ASN:HD22	1.83	0.43
1:F:149:ILE:HD12	1:F:149:ILE:HA	1.89	0.43
1:F:464:ILE:HD13	1:F:472:GLN:HG3	2.01	0.43
1:F:596:LYS:HG3	1:F:619:HIS:CD2	2.52	0.43
1:A:356:HIS:CD2	1:A:358:MET:H	2.37	0.43
1:A:568:ILE:HB	1:A:596:LYS:HB3	2.00	0.43
1:C:451:LEU:HD22	1:C:479:LEU:HD13	2.01	0.43
1:E:35:MET:HE1	1:E:173:THR:HA	2.01	0.43
1:E:686:THR:HA	1:E:708:LEU:HA	2.01	0.43
1:F:524:PRO:HA	1:F:526:LYS:HZ2	1.84	0.43
1:F:669:ASN:OD1	1:F:669:ASN:N	2.48	0.43
1:C:596:LYS:HA	1:C:619:HIS:HB3	2.01	0.42
1:A:458:GLU:HG3	1:A:462:GLN:HE22	1.83	0.42
1:A:674:GLU:HG3	1:A:675:GLU:H	1.84	0.42
1:B:668:ASN:HD22	1:B:669:ASN:N	2.17	0.42
1:C:585:ARG:HH11	1:C:609:VAL:HB	1.83	0.42
1:D:471:LYS:HB3	1:D:494:VAL:HG23	1.99	0.42
1:F:481:GLY:HA2	1:F:502:GLU:HB2	2.01	0.42
1:A:741:ILE:HG22	1:A:762:ASN:HB3	2.01	0.42
1:B:397:PHE:HA	1:B:414:ASN:H	1.85	0.42
1:B:567:LEU:HD13	1:B:570:ASN:HD22	1.83	0.42
1:C:144:GLN:HA	1:C:147:VAL:HG22	2.02	0.42
1:F:649:ARG:HH21	1:F:674:GLU:HA	1.85	0.42
1:A:35:MET:HE2	1:A:373:ILE:HD11	2.02	0.42
1:B:545:LYS:HD3	1:B:568:ILE:HD11	2.02	0.42
1:D:741:ILE:HG22	1:D:762:ASN:HB3	2.01	0.42
1:F:451:LEU:HD22	1:F:479:LEU:HD13	2.01	0.42
1:F:715:ASN:H	1:F:738:TYR:HB2	1.84	0.42
1:B:35:MET:HE2	1:B:373:ILE:HD11	2.02	0.42
1:C:665:LEU:HD12	1:C:670:ILE:HG13	2.00	0.42
1:D:356:HIS:CD2	1:D:358:MET:H	2.37	0.42
1:D:674:GLU:HG3	1:D:675:GLU:H	1.84	0.42
1:A:456:THR:H	1:A:459:LYS:HD3	1.84	0.42
1:D:563:ARG:HG3	1:D:564:GLU:HG3	2.00	0.42
1:F:402:GLU:HG3	1:F:406:PHE:HE1	1.84	0.42
1:A:787:ILE:O	1:A:808:ASN:ND2	2.50	0.42
1:C:715:ASN:H	1:C:738:TYR:HB2	1.84	0.42
1:E:35:MET:HE2	1:E:373:ILE:HD11	2.02	0.42
1:C:693:ASN:HB2	1:C:695:ILE:HG12	2.02	0.42
1:F:507:ALA:HA	1:F:531:ALA:HB2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:151:GLN:HE22	1:B:357:ASN:ND2	2.18	0.42
1:F:54:CYS:HA	1:F:354:CYS:HA	2.01	0.42
1:F:645:CYS:HB3	1:F:647:LEU:HD13	2.01	0.42
1:A:721:LEU:HD12	1:A:745:PRO:HD3	2.01	0.42
1:B:356:HIS:NE2	1:B:358:MET:HB2	2.35	0.42
1:D:456:THR:H	1:D:459:LYS:HD3	1.84	0.42
1:B:686:THR:HA	1:B:708:LEU:HA	2.01	0.41
1:C:777:LEU:HG	1:C:800:LEU:HB2	2.01	0.41
1:D:642:LEU:N	1:D:664:ASP:O	2.51	0.41
1:E:315:LYS:HE3	1:E:315:LYS:HB3	1.84	0.41
1:F:596:LYS:HA	1:F:619:HIS:HB3	2.01	0.41
1:A:54:CYS:HA	1:A:354:CYS:HA	2.02	0.41
1:B:661:GLN:N	1:B:662:GLU:OE1	2.53	0.41
1:B:701:SER:OG	1:B:704:HIS:ND1	2.50	0.41
1:C:208:TRP:HB2	1:C:280:ASP:HB2	2.02	0.41
1:C:391:PRO:HB2	1:C:418:PHE:HE1	1.84	0.41
1:C:497:LEU:HB2	1:C:520:LEU:HA	2.01	0.41
1:C:649:ARG:HH21	1:C:674:GLU:HA	1.84	0.41
1:A:737:SER:HG	1:A:758:HIS:CE1	2.37	0.41
1:C:45:MET:HE3	1:C:45:MET:HB3	1.78	0.41
1:C:402:GLU:HG3	1:C:406:PHE:HE1	1.84	0.41
1:C:526:LYS:NZ	1:C:551:GLU:OE2	2.54	0.41
1:E:397:PHE:HA	1:E:414:ASN:H	1.85	0.41
1:F:144:GLN:HA	1:F:147:VAL:HG22	2.02	0.41
1:F:713:PHE:CD2	1:F:735:ASP:HB2	2.56	0.41
1:D:650:ILE:HD12	1:D:674:GLU:H	1.86	0.41
1:F:391:PRO:HB2	1:F:418:PHE:HE1	1.84	0.41
1:F:497:LEU:HB2	1:F:520:LEU:HA	2.01	0.41
1:F:693:ASN:HB2	1:F:695:ILE:HG12	2.02	0.41
1:B:613:LEU:HD23	1:B:613:LEU:HA	1.93	0.41
1:C:470:ASP:OD1	1:C:470:ASP:N	2.51	0.41
1:E:446:LEU:HD23	1:E:446:LEU:HA	1.82	0.41
1:E:545:LYS:HD3	1:E:568:ILE:HD11	2.02	0.41
1:E:661:GLN:N	1:E:662:GLU:OE1	2.53	0.41
1:F:818:GLY:HA2	1:F:842:VAL:HG13	2.03	0.41
1:A:843:LYS:HD2	1:A:843:LYS:HA	1.92	0.41
1:C:481:GLY:HA2	1:C:502:GLU:HB2	2.02	0.41
1:D:608:ASP:HB3	1:D:630:SER:HA	2.03	0.41
1:F:526:LYS:NZ	1:F:551:GLU:OE2	2.53	0.41
1:C:713:PHE:CD2	1:C:735:ASP:HB2	2.56	0.41
1:C:751:LEU:HD22	1:C:754:LEU:HD13	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:356:HIS:NE2	1:E:358:MET:HB2	2.35	0.41
1:E:370:ILE:HD13	1:E:370:ILE:HA	1.81	0.41
1:F:655:PHE:HA	1:F:682:LEU:HD21	2.03	0.41
1:A:650:ILE:HD12	1:A:674:GLU:H	1.86	0.41
1:A:813:LEU:HD22	1:A:834:LEU:HD13	2.02	0.41
1:B:315:LYS:HE3	1:B:315:LYS:HB3	1.84	0.41
1:C:476:LEU:HD13	1:C:497:LEU:HA	2.03	0.41
1:C:814:PRO:HD2	1:C:817:LEU:HD23	2.03	0.41
1:D:446:LEU:HA	1:D:446:LEU:HD23	1.81	0.41
1:D:813:LEU:HD22	1:D:834:LEU:HD13	2.02	0.41
1:E:568:ILE:HB	1:E:596:LYS:HB3	2.03	0.41
1:E:772:PHE:O	1:E:796:GLN:NE2	2.54	0.41
1:F:470:ASP:OD1	1:F:470:ASP:N	2.51	0.41
1:A:186:TYR:HA	1:A:187:PRO:HD3	1.90	0.41
1:A:797:LEU:H	1:A:797:LEU:HG	1.66	0.41
1:C:36:LEU:HB2	1:C:173:THR:HG21	2.02	0.41
1:C:519:HIS:NE2	1:C:543:HIS:HD2	2.19	0.41
1:D:54:CYS:HA	1:D:354:CYS:HA	2.02	0.41
1:E:553:PRO:HB3	1:E:555:TRP:CH2	2.56	0.41
1:E:684:ARG:H	1:E:684:ARG:HD2	1.86	0.41
1:E:721:LEU:HD23	1:E:745:PRO:HB3	2.03	0.41
1:F:208:TRP:HB2	1:F:280:ASP:HB2	2.02	0.41
1:F:519:HIS:NE2	1:F:543:HIS:HD2	2.19	0.41
1:A:203:CYS:SG	1:A:433:ARG:NH2	2.94	0.41
1:A:310:VAL:HA	1:A:313:VAL:HG22	2.03	0.41
1:B:568:ILE:HB	1:B:596:LYS:HB3	2.03	0.41
1:C:617:VAL:HG22	1:C:619:HIS:H	1.86	0.41
1:D:151:GLN:HE22	1:E:357:ASN:ND2	2.18	0.41
1:B:341:PRO:HB2	1:B:343:VAL:HG22	2.03	0.40
1:B:553:PRO:HB3	1:B:555:TRP:CH2	2.56	0.40
1:B:784:GLN:HG3	1:C:591:LYS:HD2	2.04	0.40
1:C:158:LEU:HA	1:C:159:PRO:HD3	1.95	0.40
1:D:762:ASN:ND2	1:D:785:ASN:HD21	2.19	0.40
1:F:751:LEU:HD22	1:F:754:LEU:HD13	2.02	0.40
1:C:54:CYS:HA	1:C:354:CYS:HA	2.01	0.40
1:C:751:LEU:H	1:C:751:LEU:HG	1.54	0.40
1:F:751:LEU:H	1:F:751:LEU:HG	1.54	0.40
1:A:346:LEU:HD23	1:B:55:LEU:HD11	2.03	0.40
1:A:762:ASN:ND2	1:A:785:ASN:HD21	2.19	0.40
1:B:772:PHE:O	1:B:796:GLN:NE2	2.54	0.40
1:C:695:ILE:HG13	1:C:713:PHE:HE1	1.87	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:357:ASN:O	1:D:357:ASN:ND2	2.50	0.40
1:E:14:GLN:HG3	1:E:17:TYR:HB2	2.03	0.40
1:A:784:GLN:HA	1:B:612:HIS:CD2	2.57	0.40
1:B:684:ARG:HD2	1:B:684:ARG:H	1.86	0.40
1:C:655:PHE:HA	1:C:682:LEU:HD21	2.03	0.40
1:C:818:GLY:HA2	1:C:842:VAL:HG13	2.03	0.40
1:D:203:CYS:SG	1:D:433:ARG:NH2	2.94	0.40
1:D:346:LEU:HD23	1:E:55:LEU:HD11	2.03	0.40
1:E:427:ASP:HB3	1:E:429:LEU:H	1.87	0.40
1:E:784:GLN:HG3	1:F:591:LYS:HD2	2.04	0.40
1:F:617:VAL:HG22	1:F:619:HIS:H	1.87	0.40
1:F:814:PRO:HD2	1:F:817:LEU:HD23	2.03	0.40
1:B:752:GLN:HG3	1:B:773:LYS:HE3	2.02	0.40
1:C:731:LEU:HD23	1:C:751:LEU:HB3	2.04	0.40
1:E:341:PRO:HB2	1:E:343:VAL:HG22	2.04	0.40
1:F:476:LEU:HD13	1:F:497:LEU:HA	2.03	0.40
1:F:648:GLU:HG2	1:F:649:ARG:HG2	2.03	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	708/866 (82%)	610 (86%)	98 (14%)	0	100	100
1	B	708/866 (82%)	623 (88%)	85 (12%)	0	100	100
1	C	707/866 (82%)	625 (88%)	82 (12%)	0	100	100
1	D	708/866 (82%)	610 (86%)	98 (14%)	0	100	100
1	E	708/866 (82%)	623 (88%)	85 (12%)	0	100	100
1	F	707/866 (82%)	624 (88%)	83 (12%)	0	100	100
All	All	4246/5196 (82%)	3715 (88%)	531 (12%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	655/797 (82%)	648 (99%)	7 (1%)	65	74
1	B	655/797 (82%)	638 (97%)	17 (3%)	40	60
1	C	654/797 (82%)	640 (98%)	14 (2%)	47	65
1	D	655/797 (82%)	648 (99%)	7 (1%)	65	74
1	E	655/797 (82%)	638 (97%)	17 (3%)	40	60
1	F	654/797 (82%)	640 (98%)	14 (2%)	47	65
All	All	3928/4782 (82%)	3852 (98%)	76 (2%)	49	66

All (76) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	287	LEU
1	A	449	ILE
1	A	558	LEU
1	A	587	LEU
1	A	592	ILE
1	A	618	ILE
1	A	797	LEU
1	B	287	LEU
1	B	409	ILE
1	B	418	PHE
1	B	449	ILE
1	B	474	LEU
1	B	476	LEU
1	B	542	LEU
1	B	558	LEU
1	B	562	LEU
1	B	592	ILE
1	B	602	VAL
1	B	617	VAL

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Mol	Chain	Res	Type
1	B	631	LEU
1	B	657	LEU
1	B	711	LEU
1	B	751	LEU
1	B	797	LEU
1	C	287	LEU
1	C	351	VAL
1	C	449	ILE
1	C	464	ILE
1	C	467	ASN
1	C	562	LEU
1	C	568	ILE
1	C	592	ILE
1	C	618	ILE
1	C	665	LEU
1	C	668	ASN
1	C	711	LEU
1	C	751	LEU
1	C	828	LEU
1	D	287	LEU
1	D	449	ILE
1	D	558	LEU
1	D	587	LEU
1	D	592	ILE
1	D	618	ILE
1	D	797	LEU
1	E	287	LEU
1	E	409	ILE
1	E	418	PHE
1	E	449	ILE
1	E	474	LEU
1	E	476	LEU
1	E	542	LEU
1	E	558	LEU
1	E	562	LEU
1	E	592	ILE
1	E	602	VAL
1	E	617	VAL
1	E	631	LEU
1	E	657	LEU
1	E	711	LEU
1	E	751	LEU

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Mol	Chain	Res	Type
1	E	797	LEU
1	F	287	LEU
1	F	351	VAL
1	F	449	ILE
1	F	464	ILE
1	F	467	ASN
1	F	562	LEU
1	F	568	ILE
1	F	592	ILE
1	F	618	ILE
1	F	665	LEU
1	F	668	ASN
1	F	711	LEU
1	F	751	LEU
1	F	828	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (104) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	144	GLN
1	A	195	HIS
1	A	328	ASN
1	A	331	ASN
1	A	356	HIS
1	A	357	ASN
1	A	421	HIS
1	A	428	GLN
1	A	543	HIS
1	A	576	ASN
1	A	598	ASN
1	A	619	HIS
1	A	644	ASN
1	A	668	ASN
1	A	692	HIS
1	A	715	ASN
1	A	752	GLN
1	A	762	ASN
1	A	808	ASN
1	B	151	GLN
1	B	311	GLN
1	B	331	ASN
1	B	357	ASN

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Mol	Chain	Res	Type
1	B	428	GLN
1	B	453	HIS
1	B	469	GLN
1	B	472	GLN
1	B	519	HIS
1	B	529	GLN
1	B	543	HIS
1	B	576	ASN
1	B	643	GLN
1	B	661	GLN
1	B	668	ASN
1	B	755	GLN
1	B	785	ASN
1	B	796	GLN
1	B	808	ASN
1	C	331	ASN
1	C	357	ASN
1	C	421	HIS
1	C	428	GLN
1	C	453	HIS
1	C	467	ASN
1	C	543	HIS
1	C	598	ASN
1	C	680	GLN
1	C	692	HIS
1	C	715	ASN
1	C	752	GLN
1	C	796	GLN
1	C	802	GLN
1	C	808	ASN
1	D	144	GLN
1	D	195	HIS
1	D	328	ASN
1	D	331	ASN
1	D	356	HIS
1	D	357	ASN
1	D	421	HIS
1	D	428	GLN
1	D	543	HIS
1	D	576	ASN
1	D	598	ASN
1	D	619	HIS

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Mol	Chain	Res	Type
1	D	644	ASN
1	D	668	ASN
1	D	692	HIS
1	D	715	ASN
1	D	752	GLN
1	D	762	ASN
1	E	151	GLN
1	E	311	GLN
1	E	331	ASN
1	E	357	ASN
1	E	453	HIS
1	E	469	GLN
1	E	529	GLN
1	E	543	HIS
1	E	576	ASN
1	E	643	GLN
1	E	661	GLN
1	E	668	ASN
1	E	755	GLN
1	E	785	ASN
1	E	796	GLN
1	E	808	ASN
1	F	195	HIS
1	F	331	ASN
1	F	357	ASN
1	F	421	HIS
1	F	428	GLN
1	F	453	HIS
1	F	467	ASN
1	F	543	HIS
1	F	598	ASN
1	F	680	GLN
1	F	692	HIS
1	F	693	ASN
1	F	715	ASN
1	F	752	GLN
1	F	796	GLN
1	F	802	GLN
1	F	808	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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.

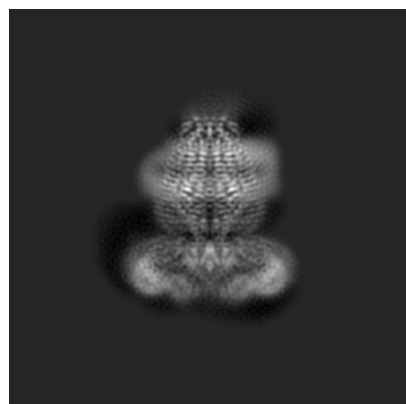
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-30029. These allow visual inspection of the internal detail of the map and identification of artifacts.

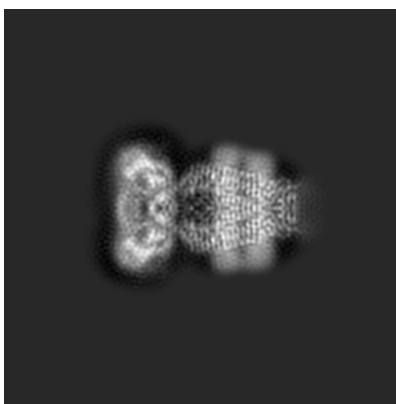
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

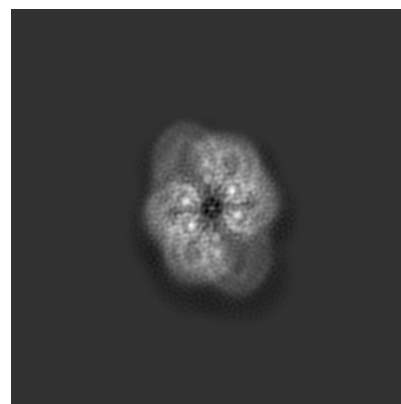
6.1.1 Primary map



X

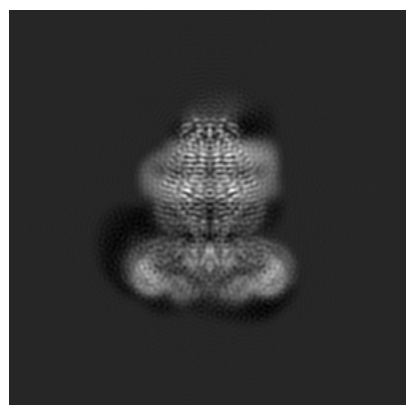


Y

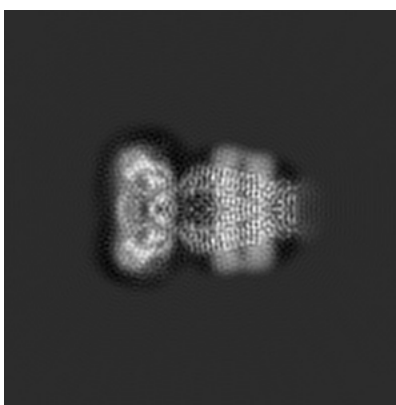


Z

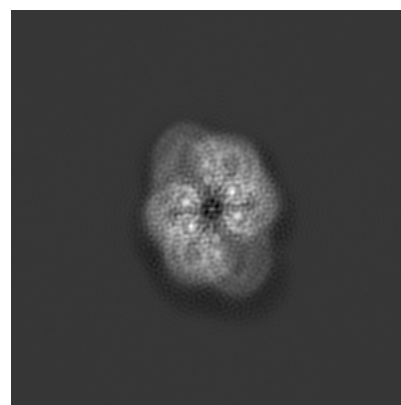
6.1.2 Raw map



X



Y

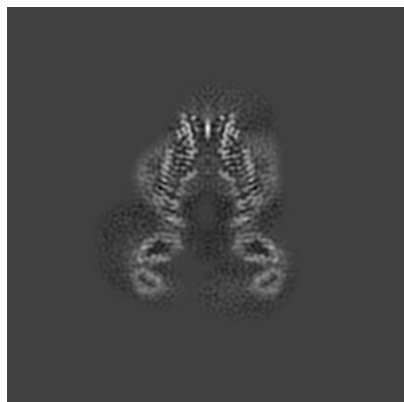


Z

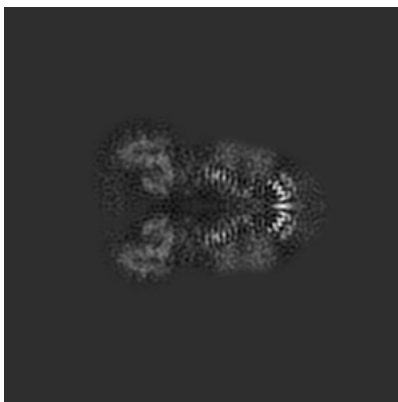
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

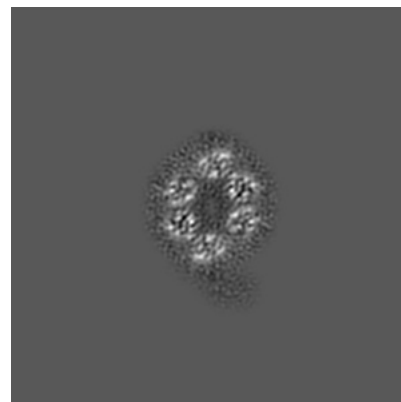
6.2.1 Primary map



X Index: 120

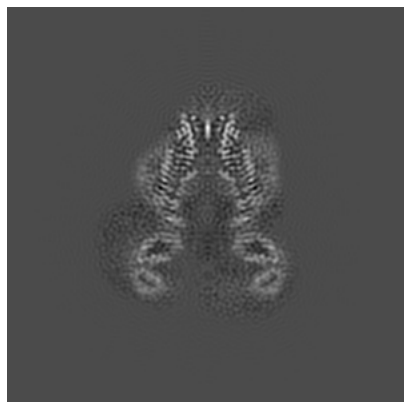


Y Index: 120

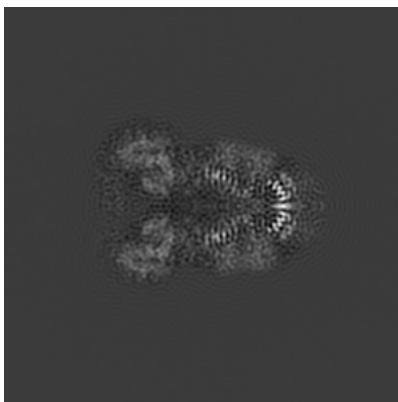


Z Index: 120

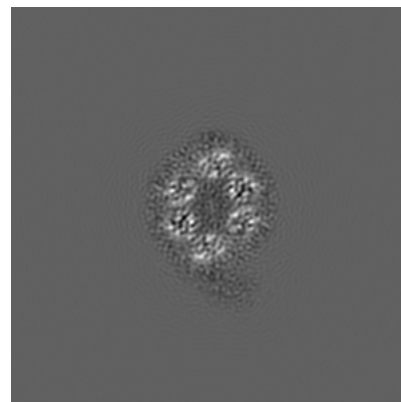
6.2.2 Raw map



X Index: 120



Y Index: 120

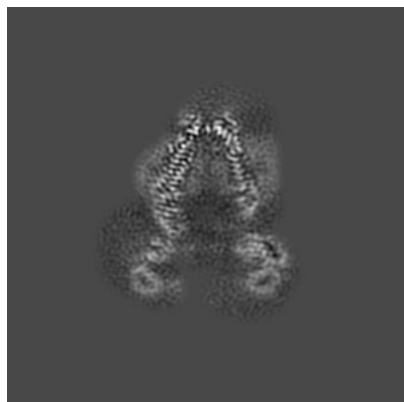


Z Index: 120

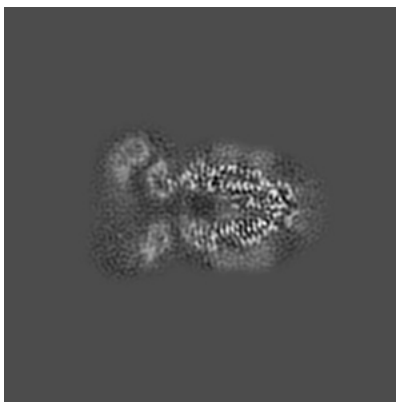
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

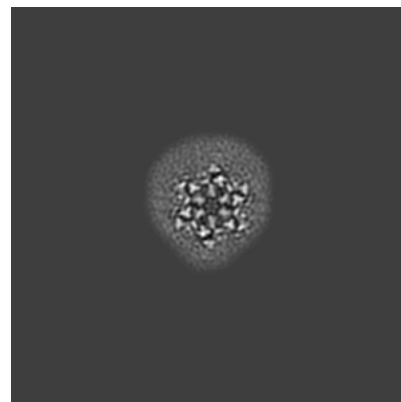
6.3.1 Primary map



X Index: 116

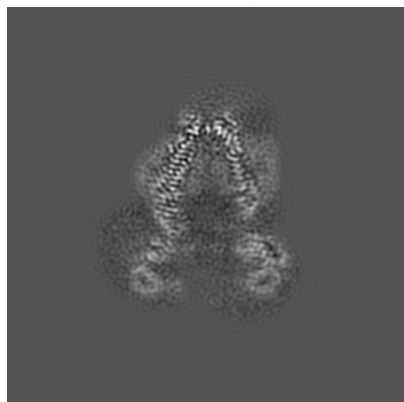


Y Index: 131

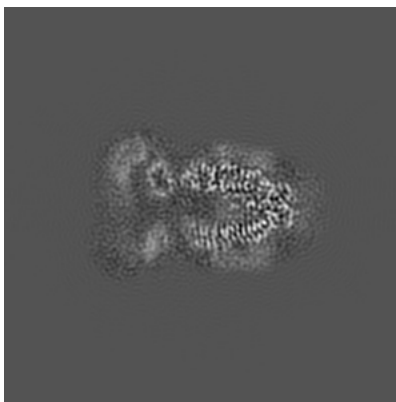


Z Index: 153

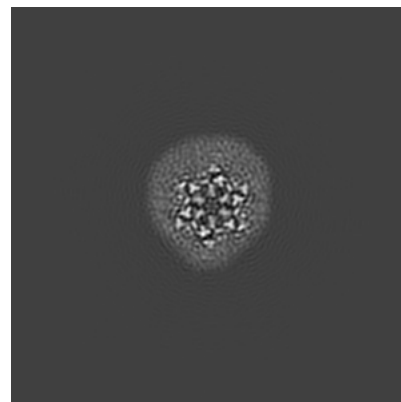
6.3.2 Raw map



X Index: 116



Y Index: 132

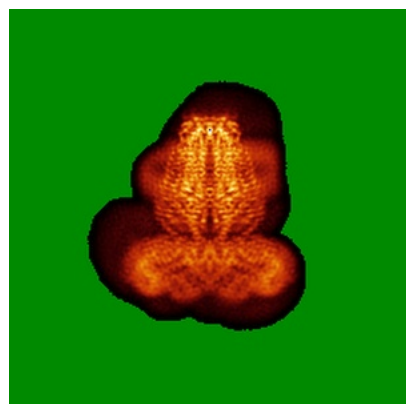


Z Index: 153

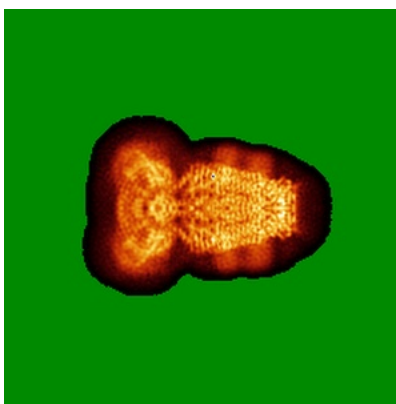
The images above show the largest variance slices of the map in three orthogonal directions.

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

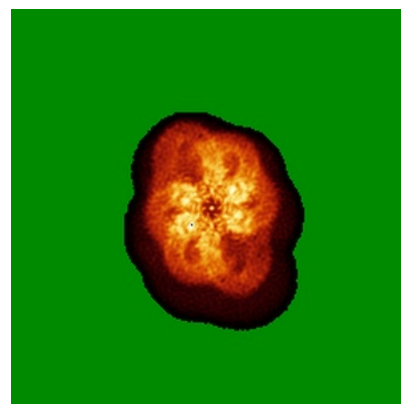
6.4.1 Primary map



X

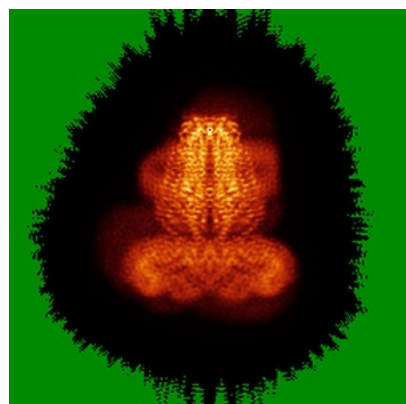


Y

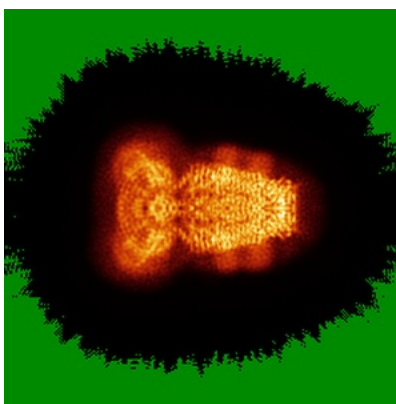


Z

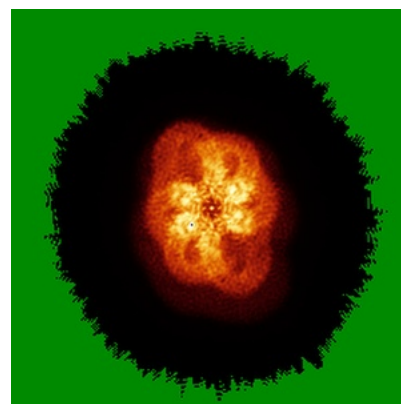
6.4.2 Raw map



X



Y

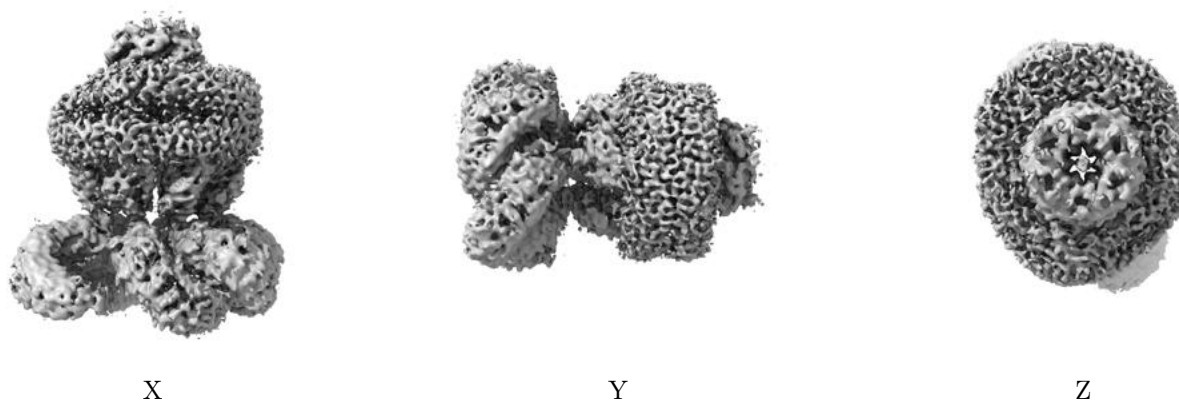


Z

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.

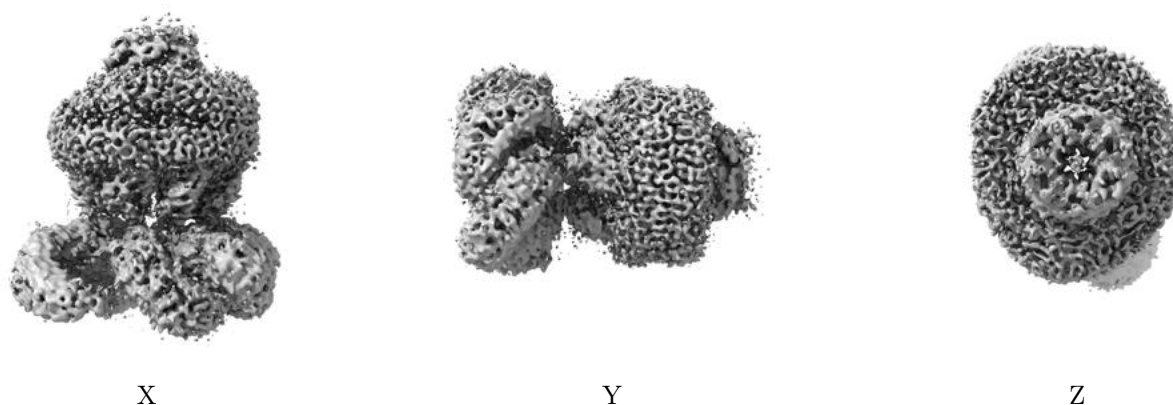
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0301. 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.

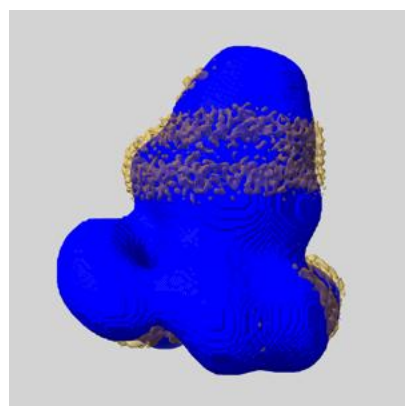
6.6 Mask visualisation [i](#)

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

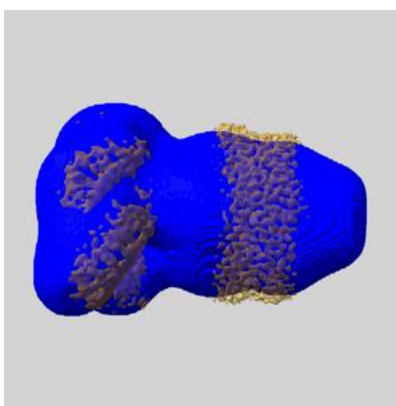
A mask typically either:

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

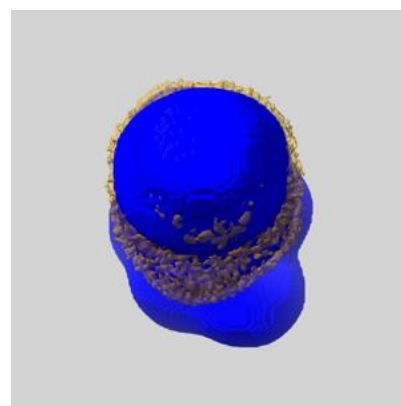
6.6.1 emd_30029_msk_1.map [i](#)



X



Y

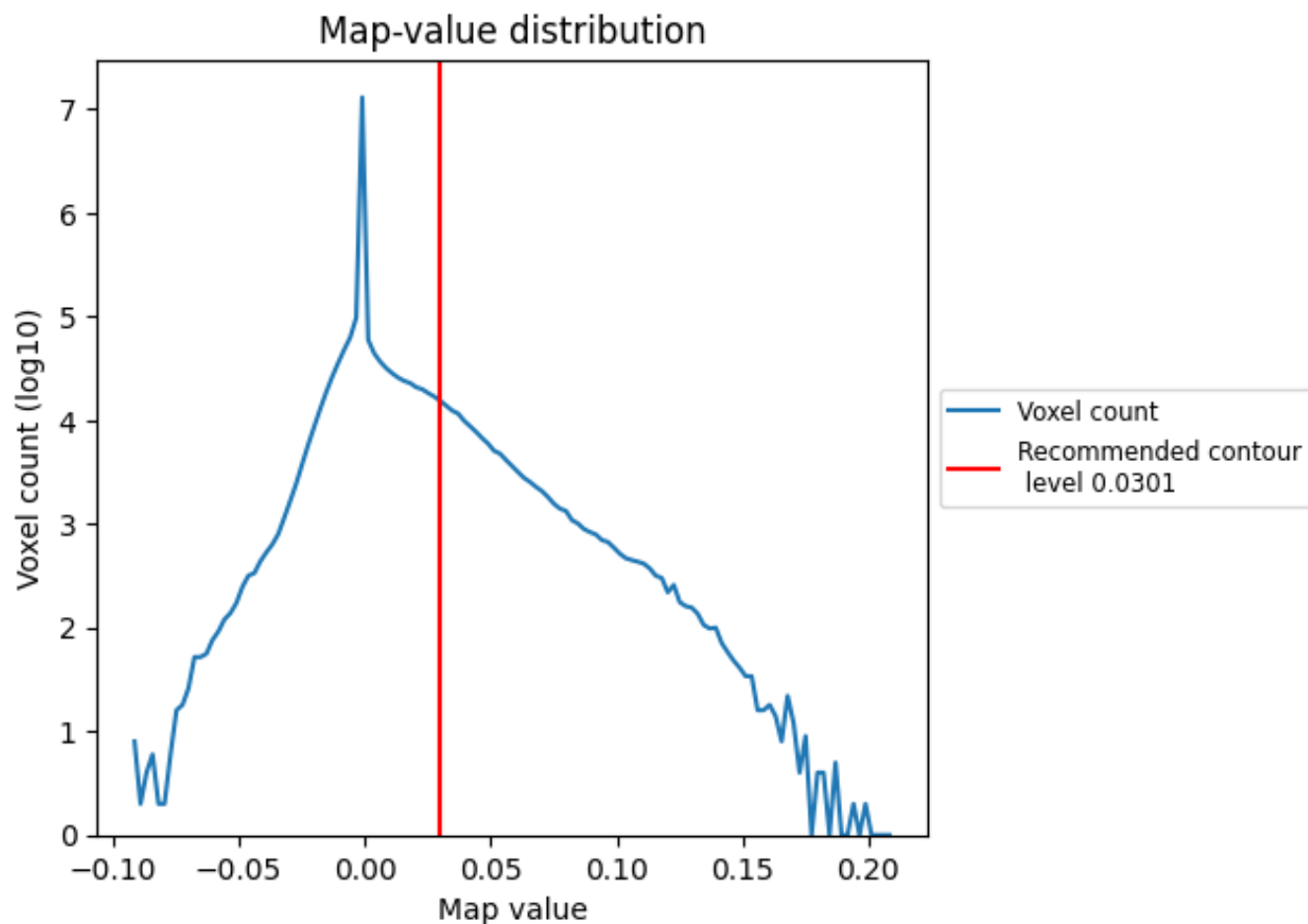


Z

7 Map analysis [i](#)

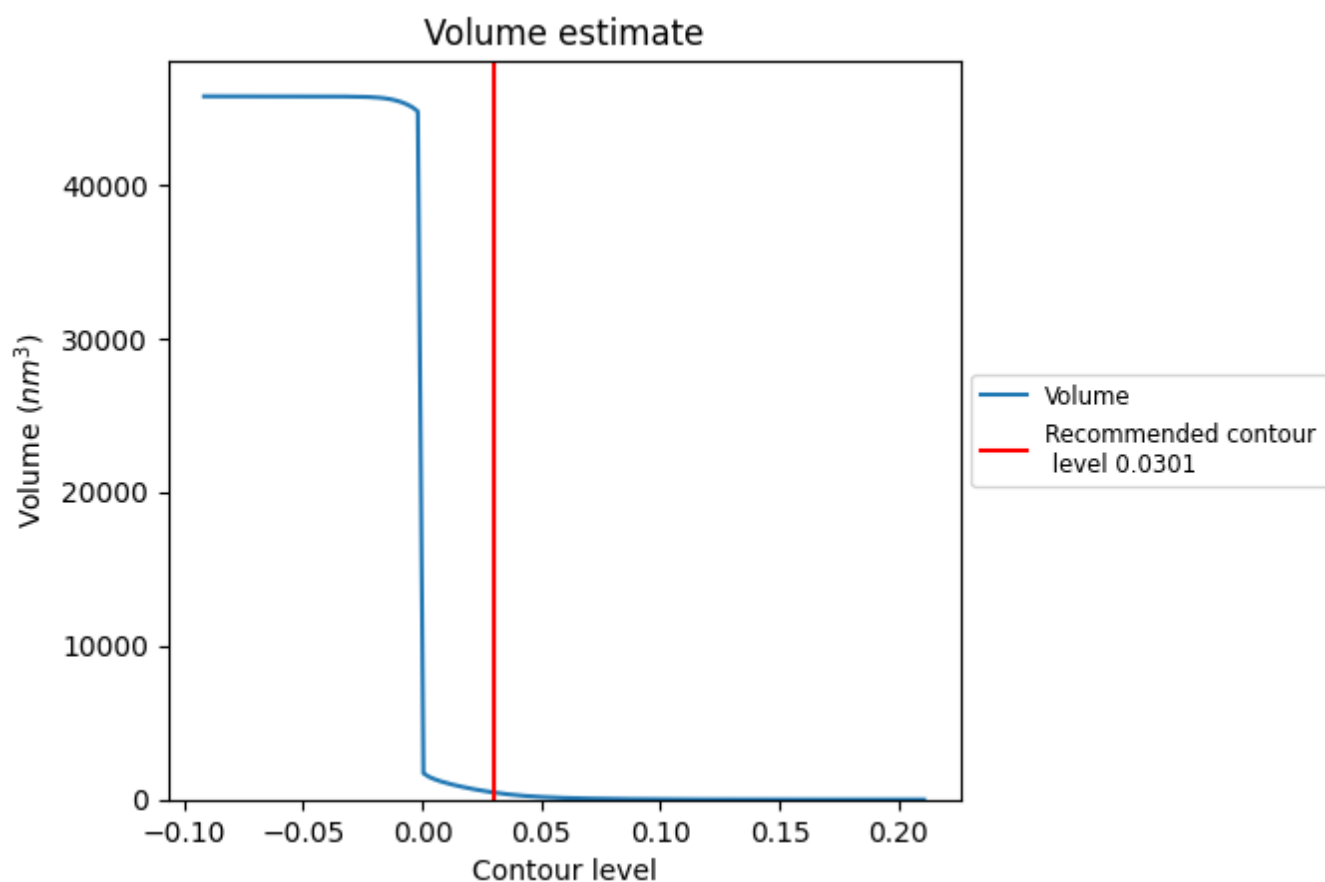
This section contains the results of statistical analysis of the map.

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.

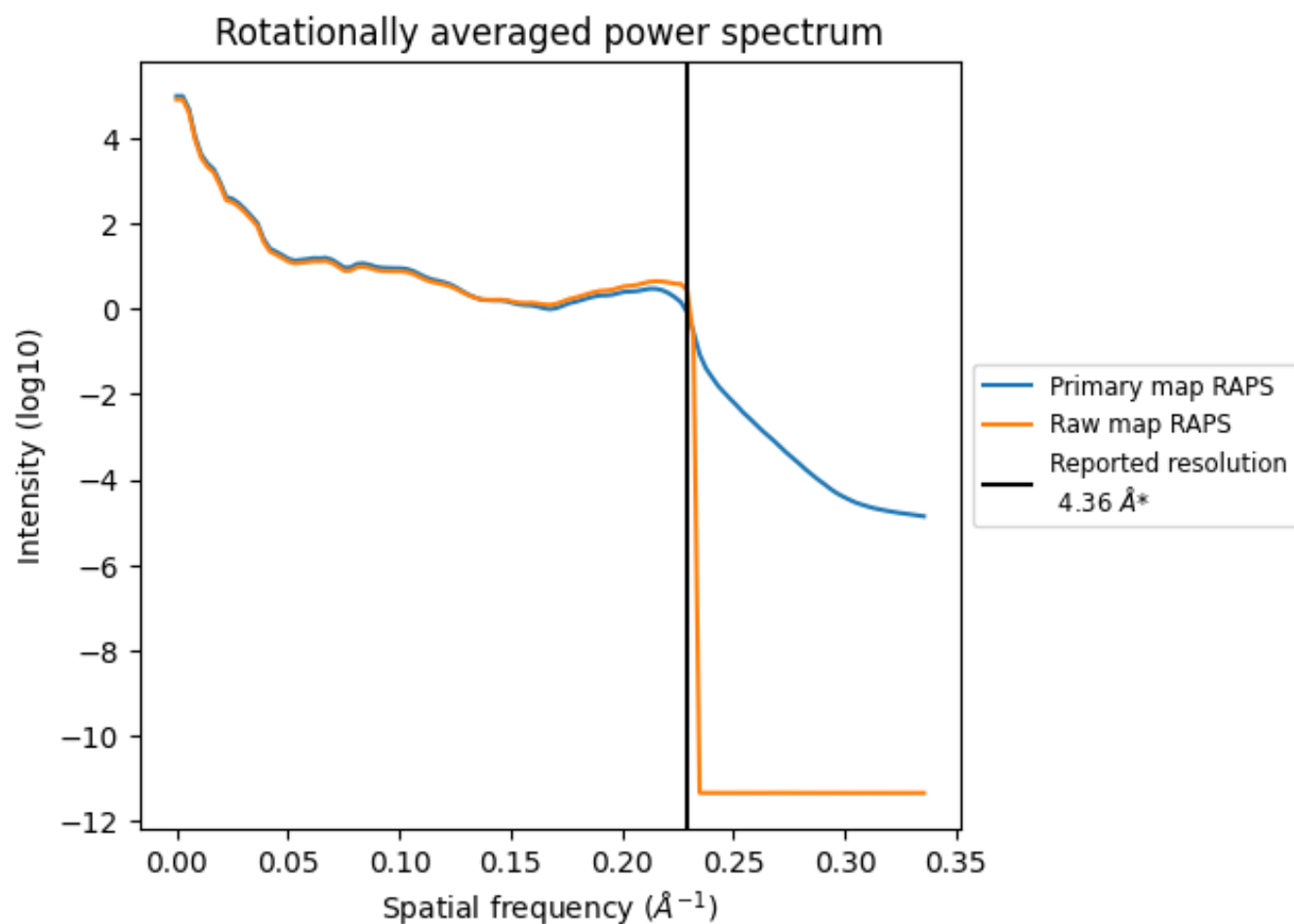
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 461 nm³; this corresponds to an approximate mass of 416 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 ⓘ

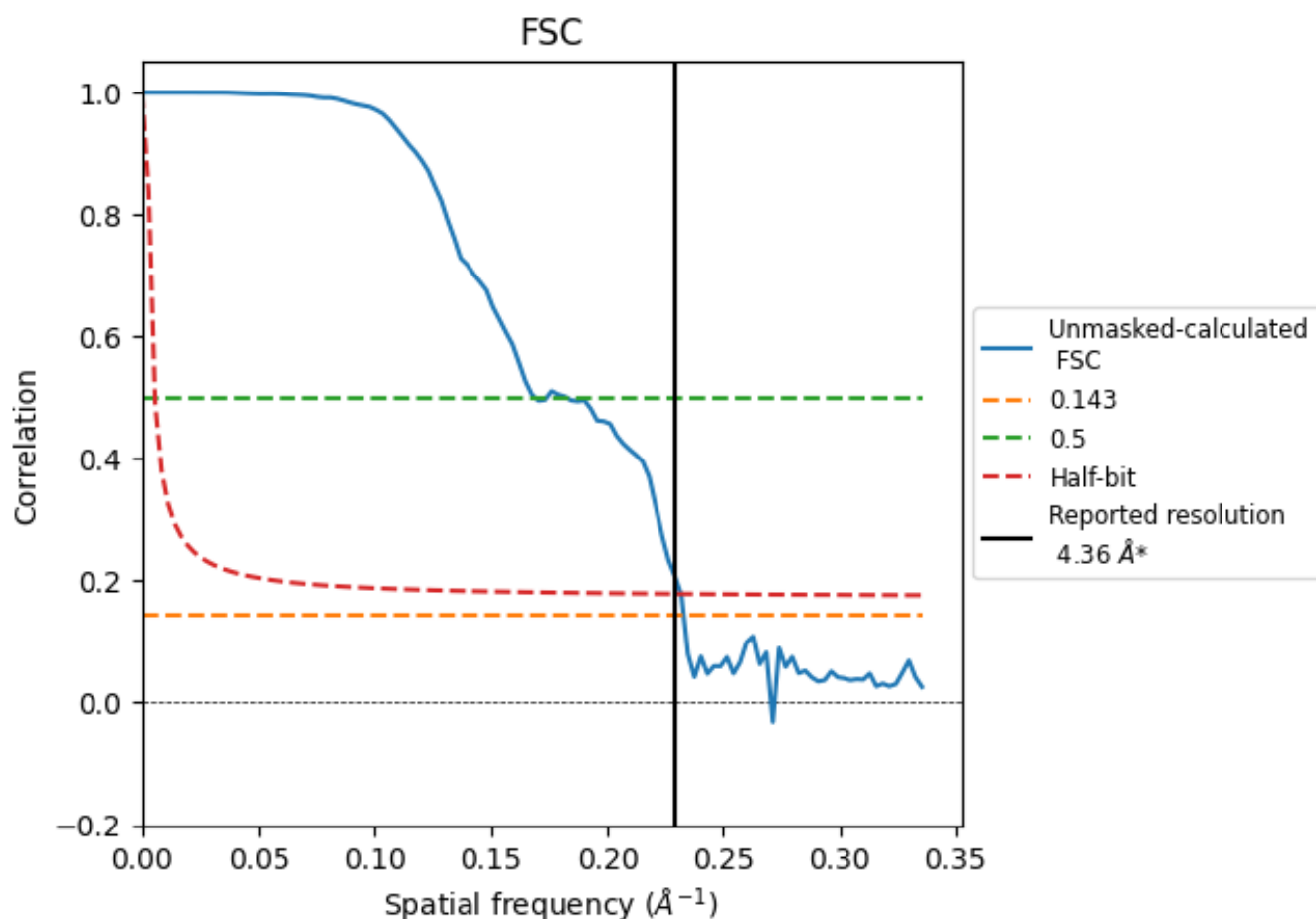


*Reported resolution corresponds to spatial frequency of 0.229 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of $0.229 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

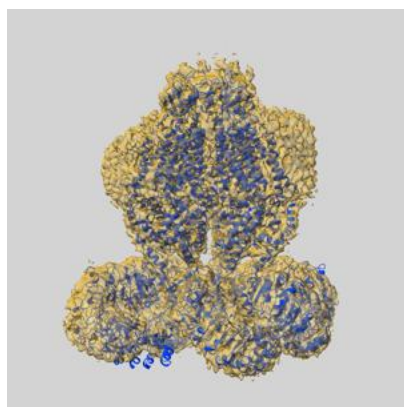
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.36	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.29	5.91	4.31

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

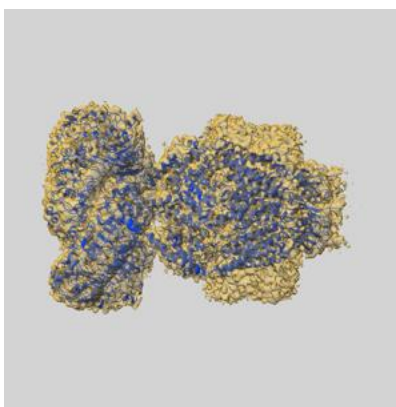
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-30029 and PDB model 6M04. Per-residue inclusion information can be found in section [3](#) on page [6](#).

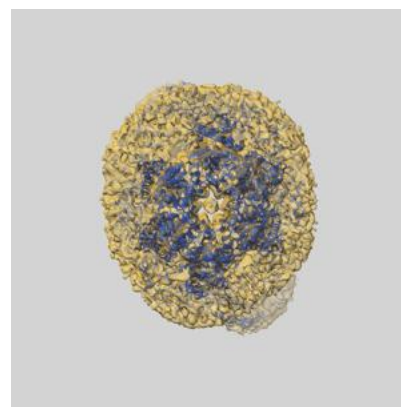
9.1 Map-model overlay [i](#)



X



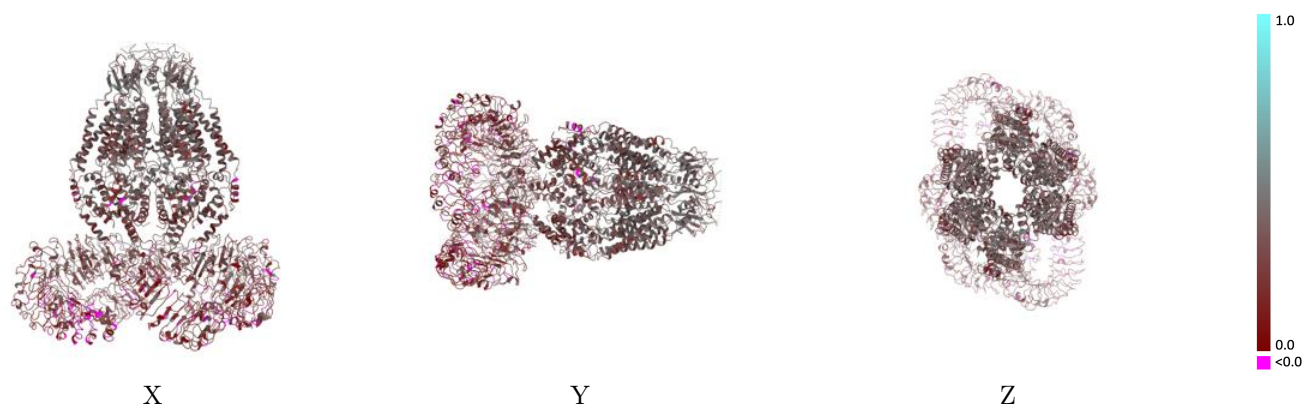
Y



Z

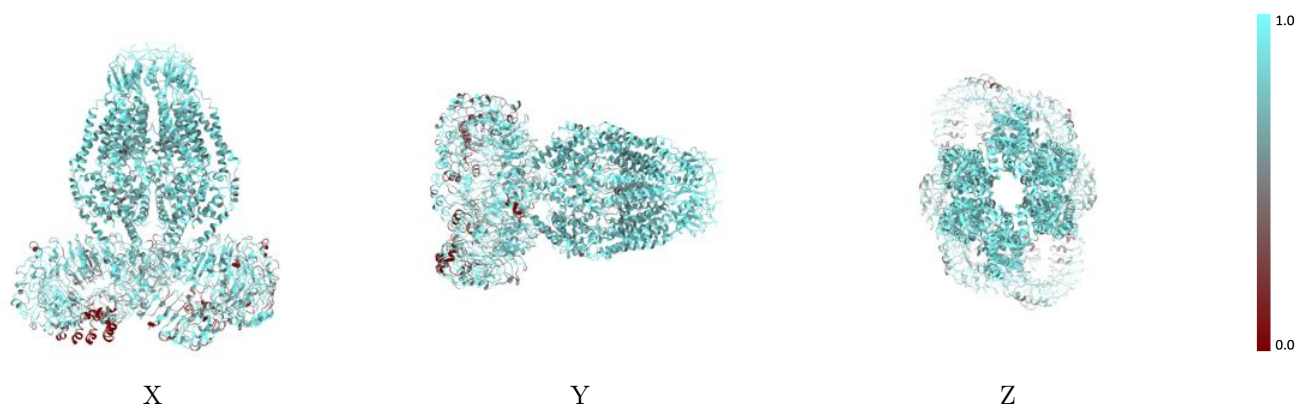
The images above show the 3D surface view of the map at the recommended contour level 0.0301 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



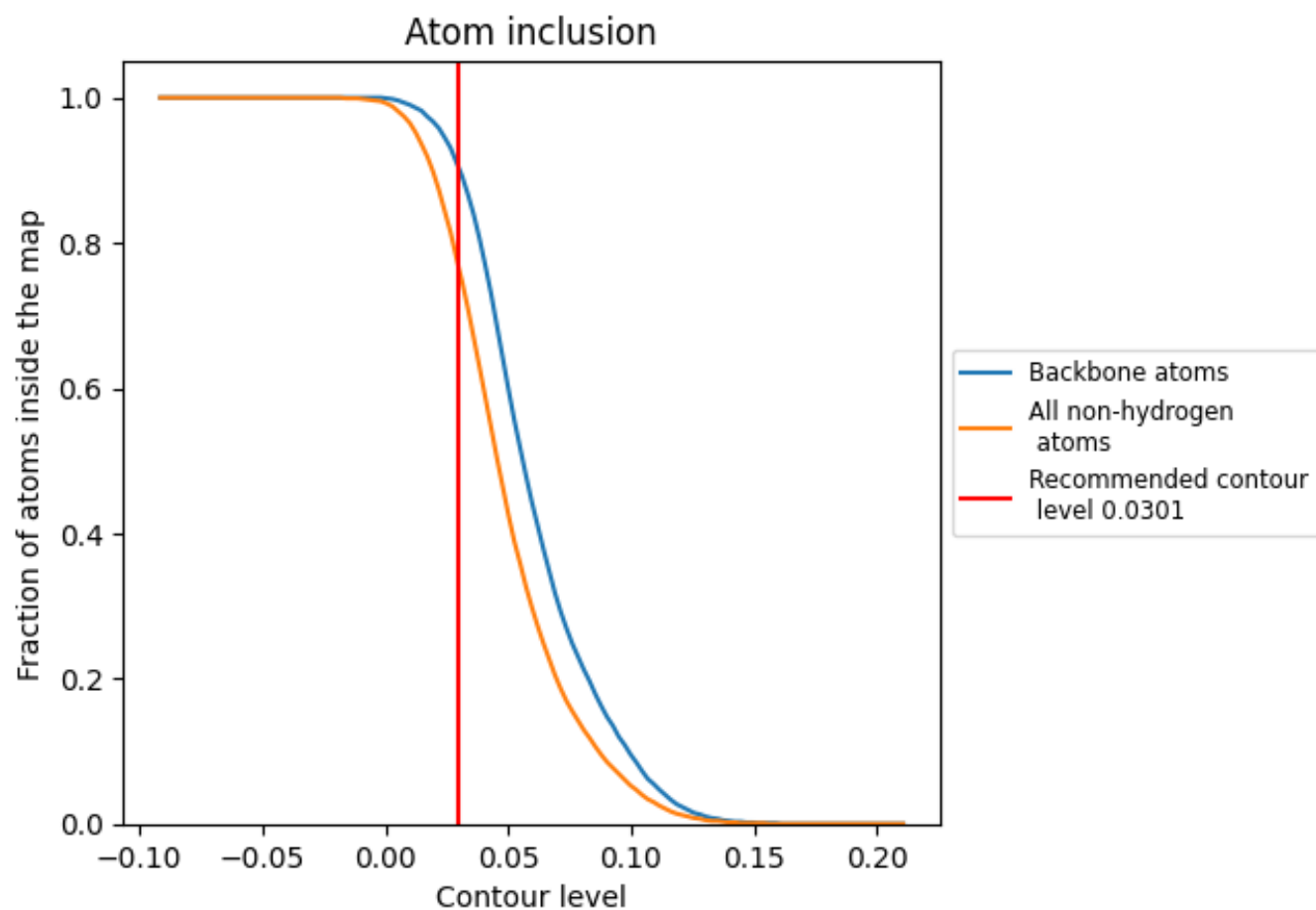
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0301).

9.4 Atom inclusion [i](#)



At the recommended contour level, 90% of all backbone atoms, 76% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.0301) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7630	0.2850
A	0.7540	0.2830
B	0.7860	0.2910
C	0.7440	0.2790
D	0.7590	0.2830
E	0.7870	0.2930
F	0.7500	0.2820

1.0

0.0

<0.0