



Full wwPDB EM Validation Report ⓘ

Mar 6, 2026 – 03:43 AM UTC

PDB ID : 9MPV / pdb_00009mpv
EMDB ID : EMD-48506
Title : Cryo-EM structure of three VCPIP1 VCPIDs bound to VCP
Authors : Shah, B.; Hunkeler, M.; Buhrlage, S.J.; Fischer, E.F.
Deposited on : 2024-12-31
Resolution : 3.10 Å(reported)
Based on initial model : 5FTK

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:

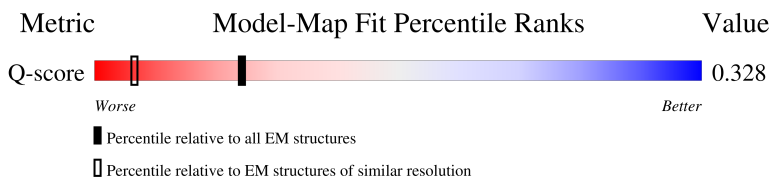
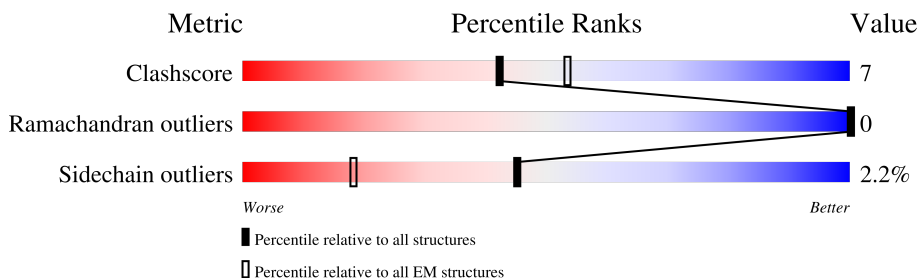
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDb archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & 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 3.10 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	14724 (2.60 - 3.60)

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	G	1250	6% . 92%
1	H	1250	. . 95%
1	I	1250	5% . 92%
2	A	832	57% 10% 32%

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Mol	Chain	Length	Quality of chain
2	B	832	59%9%32%
2	C	832	56%11%33%
2	D	832	56%11%32%
2	E	832	58%10%32%
2	F	832	56%12%32%

2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 56770 atoms, of which 28287 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 Deubiquitinating protein VCPIP1.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	G	94	Total	C	H	N	O	S	0	0
			1484	487	723	130	141	3		
1	H	66	Total	C	H	N	O	S	0	0
			1054	351	514	88	100	1		
1	I	98	Total	C	H	N	O	S	0	0
			1525	503	736	134	149	3		

There are 84 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	-27	MET	-	expression tag	UNP Q96JH7
G	-26	GLY	-	expression tag	UNP Q96JH7
G	-25	ASP	-	expression tag	UNP Q96JH7
G	-24	TRP	-	expression tag	UNP Q96JH7
G	-23	SER	-	expression tag	UNP Q96JH7
G	-22	HIS	-	expression tag	UNP Q96JH7
G	-21	PRO	-	expression tag	UNP Q96JH7
G	-20	GLN	-	expression tag	UNP Q96JH7
G	-19	PHE	-	expression tag	UNP Q96JH7
G	-18	GLU	-	expression tag	UNP Q96JH7
G	-17	LYS	-	expression tag	UNP Q96JH7
G	-16	SER	-	expression tag	UNP Q96JH7
G	-15	GLY	-	expression tag	UNP Q96JH7
G	-14	GLY	-	expression tag	UNP Q96JH7
G	-13	GLY	-	expression tag	UNP Q96JH7
G	-12	SER	-	expression tag	UNP Q96JH7
G	-11	GLY	-	expression tag	UNP Q96JH7
G	-10	GLY	-	expression tag	UNP Q96JH7
G	-9	LEU	-	expression tag	UNP Q96JH7
G	-8	GLU	-	expression tag	UNP Q96JH7
G	-7	VAL	-	expression tag	UNP Q96JH7
G	-6	LEU	-	expression tag	UNP Q96JH7
G	-5	PHE	-	expression tag	UNP Q96JH7
G	-4	GLN	-	expression tag	UNP Q96JH7

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Chain	Residue	Modelled	Actual	Comment	Reference
G	-3	GLY	-	expression tag	UNP Q96JH7
G	-2	PRO	-	expression tag	UNP Q96JH7
G	-1	GLY	-	expression tag	UNP Q96JH7
G	0	SER	-	expression tag	UNP Q96JH7
H	-27	MET	-	expression tag	UNP Q96JH7
H	-26	GLY	-	expression tag	UNP Q96JH7
H	-25	ASP	-	expression tag	UNP Q96JH7
H	-24	TRP	-	expression tag	UNP Q96JH7
H	-23	SER	-	expression tag	UNP Q96JH7
H	-22	HIS	-	expression tag	UNP Q96JH7
H	-21	PRO	-	expression tag	UNP Q96JH7
H	-20	GLN	-	expression tag	UNP Q96JH7
H	-19	PHE	-	expression tag	UNP Q96JH7
H	-18	GLU	-	expression tag	UNP Q96JH7
H	-17	LYS	-	expression tag	UNP Q96JH7
H	-16	SER	-	expression tag	UNP Q96JH7
H	-15	GLY	-	expression tag	UNP Q96JH7
H	-14	GLY	-	expression tag	UNP Q96JH7
H	-13	GLY	-	expression tag	UNP Q96JH7
H	-12	SER	-	expression tag	UNP Q96JH7
H	-11	GLY	-	expression tag	UNP Q96JH7
H	-10	GLY	-	expression tag	UNP Q96JH7
H	-9	LEU	-	expression tag	UNP Q96JH7
H	-8	GLU	-	expression tag	UNP Q96JH7
H	-7	VAL	-	expression tag	UNP Q96JH7
H	-6	LEU	-	expression tag	UNP Q96JH7
H	-5	PHE	-	expression tag	UNP Q96JH7
H	-4	GLN	-	expression tag	UNP Q96JH7
H	-3	GLY	-	expression tag	UNP Q96JH7
H	-2	PRO	-	expression tag	UNP Q96JH7
H	-1	GLY	-	expression tag	UNP Q96JH7
H	0	SER	-	expression tag	UNP Q96JH7
I	-27	MET	-	expression tag	UNP Q96JH7
I	-26	GLY	-	expression tag	UNP Q96JH7
I	-25	ASP	-	expression tag	UNP Q96JH7
I	-24	TRP	-	expression tag	UNP Q96JH7
I	-23	SER	-	expression tag	UNP Q96JH7
I	-22	HIS	-	expression tag	UNP Q96JH7
I	-21	PRO	-	expression tag	UNP Q96JH7
I	-20	GLN	-	expression tag	UNP Q96JH7
I	-19	PHE	-	expression tag	UNP Q96JH7
I	-18	GLU	-	expression tag	UNP Q96JH7

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Chain	Residue	Modelled	Actual	Comment	Reference
I	-17	LYS	-	expression tag	UNP Q96JH7
I	-16	SER	-	expression tag	UNP Q96JH7
I	-15	GLY	-	expression tag	UNP Q96JH7
I	-14	GLY	-	expression tag	UNP Q96JH7
I	-13	GLY	-	expression tag	UNP Q96JH7
I	-12	SER	-	expression tag	UNP Q96JH7
I	-11	GLY	-	expression tag	UNP Q96JH7
I	-10	GLY	-	expression tag	UNP Q96JH7
I	-9	LEU	-	expression tag	UNP Q96JH7
I	-8	GLU	-	expression tag	UNP Q96JH7
I	-7	VAL	-	expression tag	UNP Q96JH7
I	-6	LEU	-	expression tag	UNP Q96JH7
I	-5	PHE	-	expression tag	UNP Q96JH7
I	-4	GLN	-	expression tag	UNP Q96JH7
I	-3	GLY	-	expression tag	UNP Q96JH7
I	-2	PRO	-	expression tag	UNP Q96JH7
I	-1	GLY	-	expression tag	UNP Q96JH7
I	0	SER	-	expression tag	UNP Q96JH7

- Molecule 2 is a protein called Transitional endoplasmic reticulum ATPase.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	A	565	Total	C	H	N	O	S	0	0
			8808	2770	4400	785	831	22		
2	B	564	Total	C	H	N	O	S	0	0
			8782	2766	4382	783	829	22		
2	C	559	Total	C	H	N	O	S	0	0
			8699	2741	4338	778	821	21		
2	D	563	Total	C	H	N	O	S	0	0
			8779	2762	4387	781	827	22		
2	E	566	Total	C	H	N	O	S	0	0
			8813	2776	4397	786	832	22		
2	F	566	Total	C	H	N	O	S	0	0
			8826	2776	4410	786	832	22		

There are 156 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-25	MET	-	expression tag	UNP P55072
A	-24	GLY	-	expression tag	UNP P55072
A	-23	ASP	-	expression tag	UNP P55072
A	-22	TYR	-	expression tag	UNP P55072

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-21	LYS	-	expression tag	UNP P55072
A	-20	ASP	-	expression tag	UNP P55072
A	-19	ASP	-	expression tag	UNP P55072
A	-18	ASP	-	expression tag	UNP P55072
A	-17	ASP	-	expression tag	UNP P55072
A	-16	LYS	-	expression tag	UNP P55072
A	-15	GLY	-	expression tag	UNP P55072
A	-14	GLY	-	expression tag	UNP P55072
A	-13	GLY	-	expression tag	UNP P55072
A	-12	SER	-	expression tag	UNP P55072
A	-11	GLY	-	expression tag	UNP P55072
A	-10	GLY	-	expression tag	UNP P55072
A	-9	LEU	-	expression tag	UNP P55072
A	-8	GLU	-	expression tag	UNP P55072
A	-7	VAL	-	expression tag	UNP P55072
A	-6	LEU	-	expression tag	UNP P55072
A	-5	PHE	-	expression tag	UNP P55072
A	-4	GLN	-	expression tag	UNP P55072
A	-3	GLY	-	expression tag	UNP P55072
A	-2	PRO	-	expression tag	UNP P55072
A	-1	GLY	-	expression tag	UNP P55072
A	0	SER	-	expression tag	UNP P55072
B	-25	MET	-	expression tag	UNP P55072
B	-24	GLY	-	expression tag	UNP P55072
B	-23	ASP	-	expression tag	UNP P55072
B	-22	TYR	-	expression tag	UNP P55072
B	-21	LYS	-	expression tag	UNP P55072
B	-20	ASP	-	expression tag	UNP P55072
B	-19	ASP	-	expression tag	UNP P55072
B	-18	ASP	-	expression tag	UNP P55072
B	-17	ASP	-	expression tag	UNP P55072
B	-16	LYS	-	expression tag	UNP P55072
B	-15	GLY	-	expression tag	UNP P55072
B	-14	GLY	-	expression tag	UNP P55072
B	-13	GLY	-	expression tag	UNP P55072
B	-12	SER	-	expression tag	UNP P55072
B	-11	GLY	-	expression tag	UNP P55072
B	-10	GLY	-	expression tag	UNP P55072
B	-9	LEU	-	expression tag	UNP P55072
B	-8	GLU	-	expression tag	UNP P55072
B	-7	VAL	-	expression tag	UNP P55072
B	-6	LEU	-	expression tag	UNP P55072

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-5	PHE	-	expression tag	UNP P55072
B	-4	GLN	-	expression tag	UNP P55072
B	-3	GLY	-	expression tag	UNP P55072
B	-2	PRO	-	expression tag	UNP P55072
B	-1	GLY	-	expression tag	UNP P55072
B	0	SER	-	expression tag	UNP P55072
C	-25	MET	-	expression tag	UNP P55072
C	-24	GLY	-	expression tag	UNP P55072
C	-23	ASP	-	expression tag	UNP P55072
C	-22	TYR	-	expression tag	UNP P55072
C	-21	LYS	-	expression tag	UNP P55072
C	-20	ASP	-	expression tag	UNP P55072
C	-19	ASP	-	expression tag	UNP P55072
C	-18	ASP	-	expression tag	UNP P55072
C	-17	ASP	-	expression tag	UNP P55072
C	-16	LYS	-	expression tag	UNP P55072
C	-15	GLY	-	expression tag	UNP P55072
C	-14	GLY	-	expression tag	UNP P55072
C	-13	GLY	-	expression tag	UNP P55072
C	-12	SER	-	expression tag	UNP P55072
C	-11	GLY	-	expression tag	UNP P55072
C	-10	GLY	-	expression tag	UNP P55072
C	-9	LEU	-	expression tag	UNP P55072
C	-8	GLU	-	expression tag	UNP P55072
C	-7	VAL	-	expression tag	UNP P55072
C	-6	LEU	-	expression tag	UNP P55072
C	-5	PHE	-	expression tag	UNP P55072
C	-4	GLN	-	expression tag	UNP P55072
C	-3	GLY	-	expression tag	UNP P55072
C	-2	PRO	-	expression tag	UNP P55072
C	-1	GLY	-	expression tag	UNP P55072
C	0	SER	-	expression tag	UNP P55072
D	-25	MET	-	expression tag	UNP P55072
D	-24	GLY	-	expression tag	UNP P55072
D	-23	ASP	-	expression tag	UNP P55072
D	-22	TYR	-	expression tag	UNP P55072
D	-21	LYS	-	expression tag	UNP P55072
D	-20	ASP	-	expression tag	UNP P55072
D	-19	ASP	-	expression tag	UNP P55072
D	-18	ASP	-	expression tag	UNP P55072
D	-17	ASP	-	expression tag	UNP P55072
D	-16	LYS	-	expression tag	UNP P55072

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-15	GLY	-	expression tag	UNP P55072
D	-14	GLY	-	expression tag	UNP P55072
D	-13	GLY	-	expression tag	UNP P55072
D	-12	SER	-	expression tag	UNP P55072
D	-11	GLY	-	expression tag	UNP P55072
D	-10	GLY	-	expression tag	UNP P55072
D	-9	LEU	-	expression tag	UNP P55072
D	-8	GLU	-	expression tag	UNP P55072
D	-7	VAL	-	expression tag	UNP P55072
D	-6	LEU	-	expression tag	UNP P55072
D	-5	PHE	-	expression tag	UNP P55072
D	-4	GLN	-	expression tag	UNP P55072
D	-3	GLY	-	expression tag	UNP P55072
D	-2	PRO	-	expression tag	UNP P55072
D	-1	GLY	-	expression tag	UNP P55072
D	0	SER	-	expression tag	UNP P55072
E	-25	MET	-	expression tag	UNP P55072
E	-24	GLY	-	expression tag	UNP P55072
E	-23	ASP	-	expression tag	UNP P55072
E	-22	TYR	-	expression tag	UNP P55072
E	-21	LYS	-	expression tag	UNP P55072
E	-20	ASP	-	expression tag	UNP P55072
E	-19	ASP	-	expression tag	UNP P55072
E	-18	ASP	-	expression tag	UNP P55072
E	-17	ASP	-	expression tag	UNP P55072
E	-16	LYS	-	expression tag	UNP P55072
E	-15	GLY	-	expression tag	UNP P55072
E	-14	GLY	-	expression tag	UNP P55072
E	-13	GLY	-	expression tag	UNP P55072
E	-12	SER	-	expression tag	UNP P55072
E	-11	GLY	-	expression tag	UNP P55072
E	-10	GLY	-	expression tag	UNP P55072
E	-9	LEU	-	expression tag	UNP P55072
E	-8	GLU	-	expression tag	UNP P55072
E	-7	VAL	-	expression tag	UNP P55072
E	-6	LEU	-	expression tag	UNP P55072
E	-5	PHE	-	expression tag	UNP P55072
E	-4	GLN	-	expression tag	UNP P55072
E	-3	GLY	-	expression tag	UNP P55072
E	-2	PRO	-	expression tag	UNP P55072
E	-1	GLY	-	expression tag	UNP P55072
E	0	SER	-	expression tag	UNP P55072

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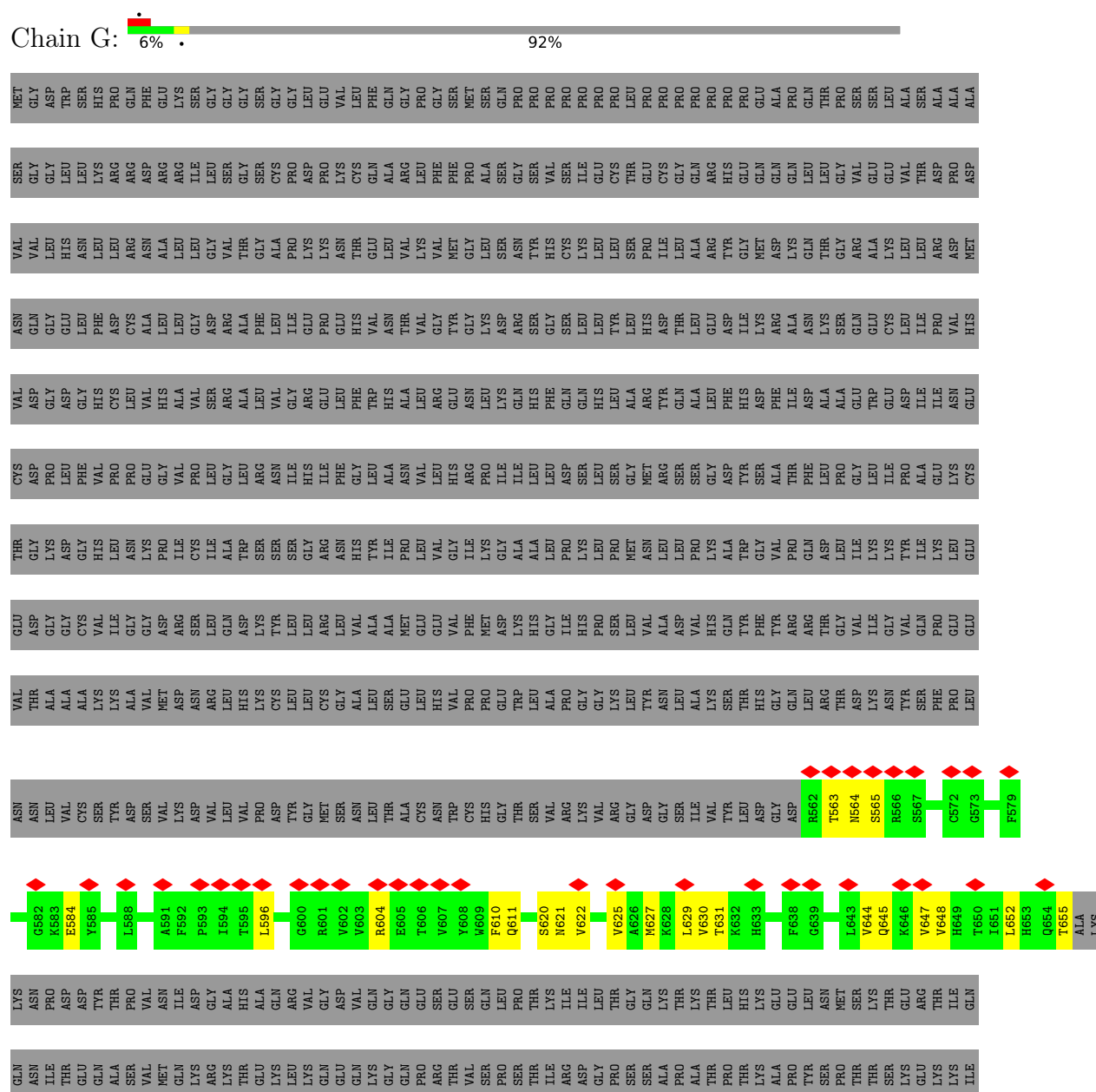
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Chain	Residue	Modelled	Actual	Comment	Reference
F	-25	MET	-	expression tag	UNP P55072
F	-24	GLY	-	expression tag	UNP P55072
F	-23	ASP	-	expression tag	UNP P55072
F	-22	TYR	-	expression tag	UNP P55072
F	-21	LYS	-	expression tag	UNP P55072
F	-20	ASP	-	expression tag	UNP P55072
F	-19	ASP	-	expression tag	UNP P55072
F	-18	ASP	-	expression tag	UNP P55072
F	-17	ASP	-	expression tag	UNP P55072
F	-16	LYS	-	expression tag	UNP P55072
F	-15	GLY	-	expression tag	UNP P55072
F	-14	GLY	-	expression tag	UNP P55072
F	-13	GLY	-	expression tag	UNP P55072
F	-12	SER	-	expression tag	UNP P55072
F	-11	GLY	-	expression tag	UNP P55072
F	-10	GLY	-	expression tag	UNP P55072
F	-9	LEU	-	expression tag	UNP P55072
F	-8	GLU	-	expression tag	UNP P55072
F	-7	VAL	-	expression tag	UNP P55072
F	-6	LEU	-	expression tag	UNP P55072
F	-5	PHE	-	expression tag	UNP P55072
F	-4	GLN	-	expression tag	UNP P55072
F	-3	GLY	-	expression tag	UNP P55072
F	-2	PRO	-	expression tag	UNP P55072
F	-1	GLY	-	expression tag	UNP P55072
F	0	SER	-	expression tag	UNP P55072

3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Deubiquitinating protein VCP1P1



[illegible]

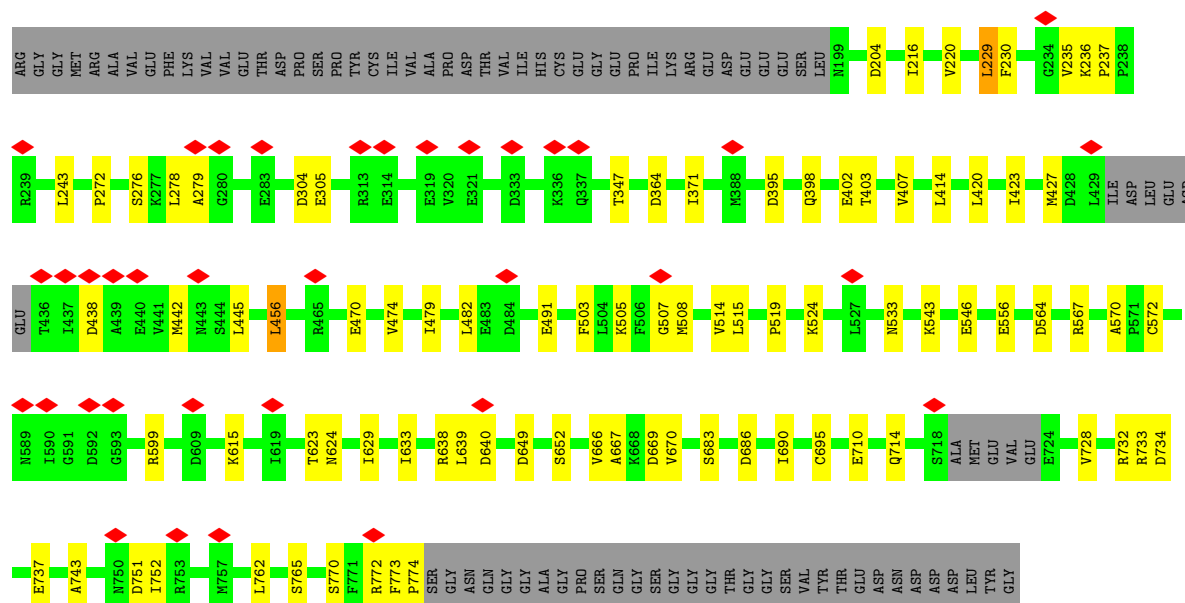
- Molecule 1: Deubiquitinating protein VCIPI1

Chain H:

[illegible]

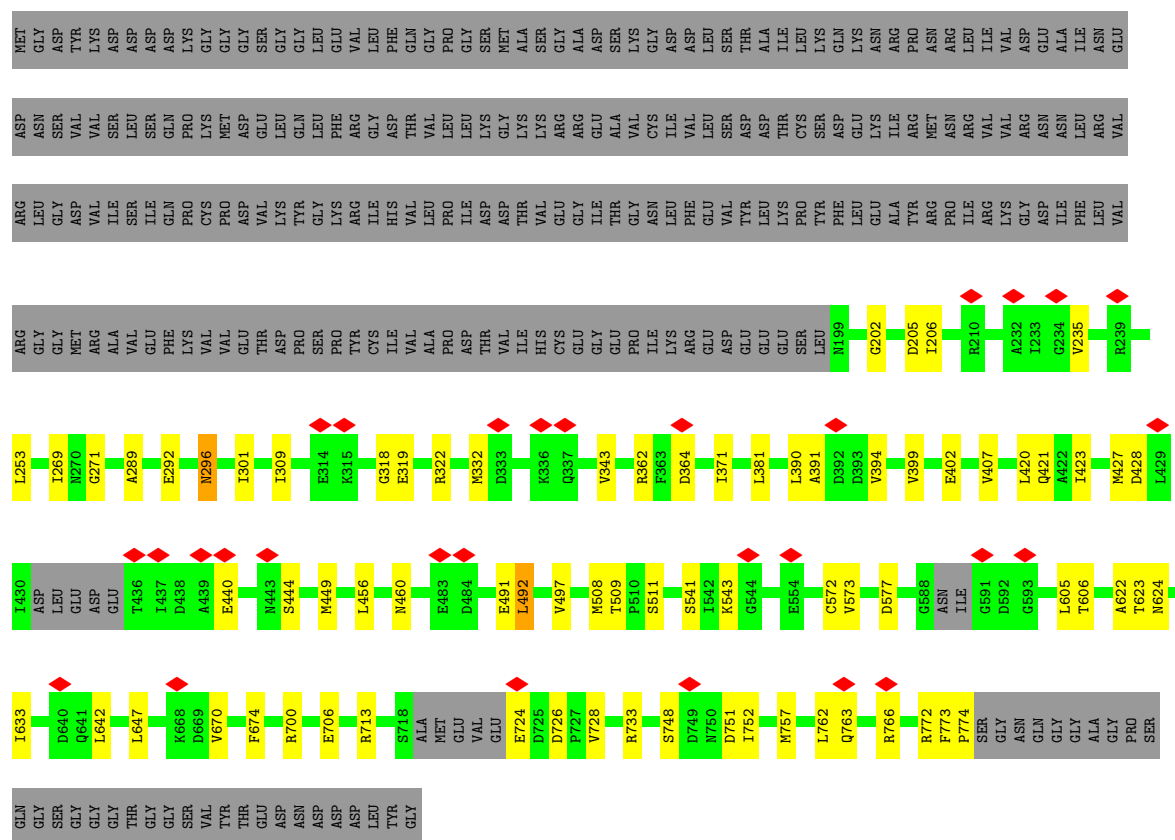


WORLDWIDE
PDB
PROTEIN DATA BANK



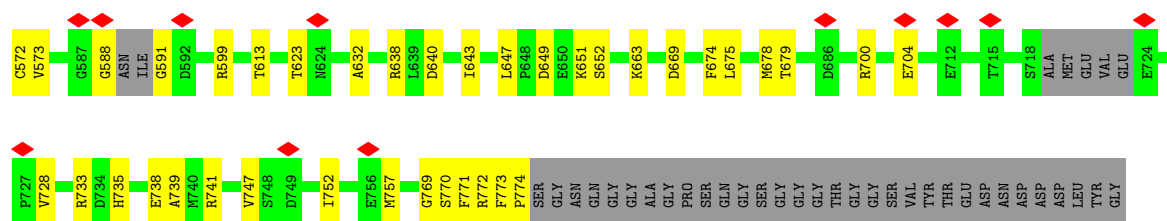
• Molecule 2: Transitional endoplasmic reticulum ATPase

Chain B: 59% 9% 32%



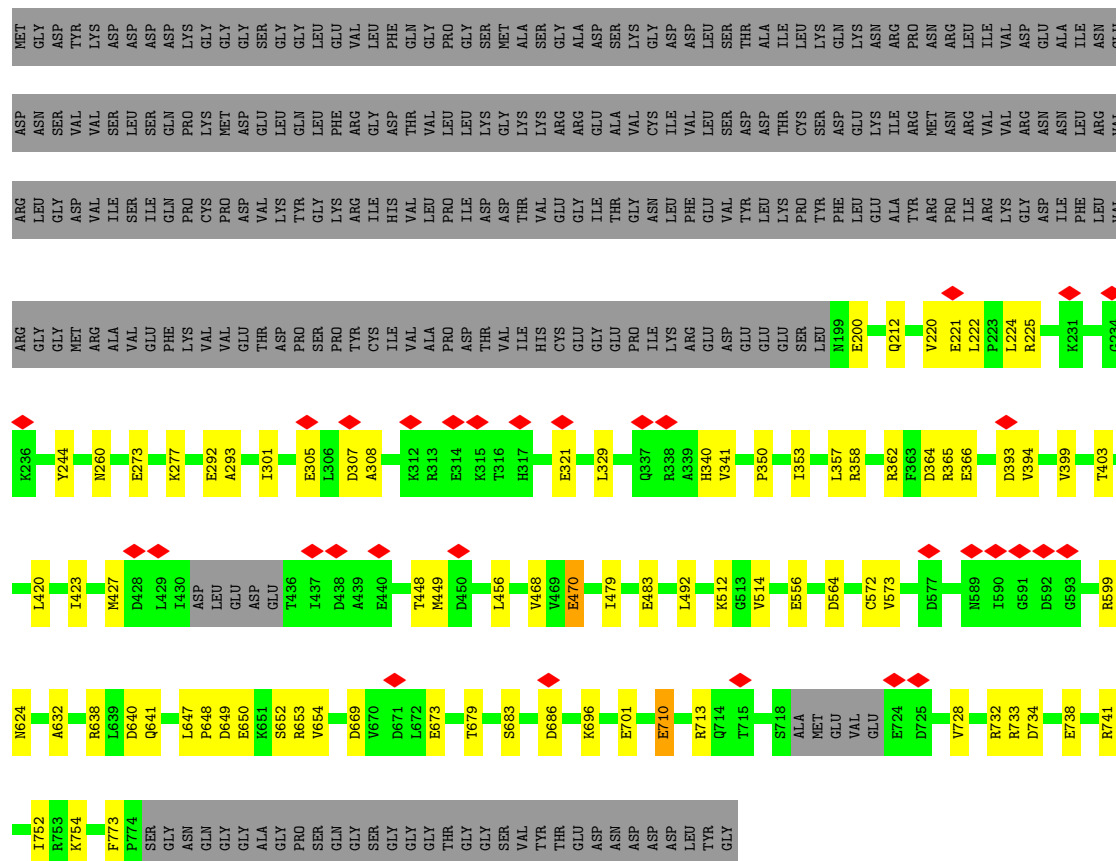
• Molecule 2: Transitional endoplasmic reticulum ATPase

Chain C: 56% 11% 33%



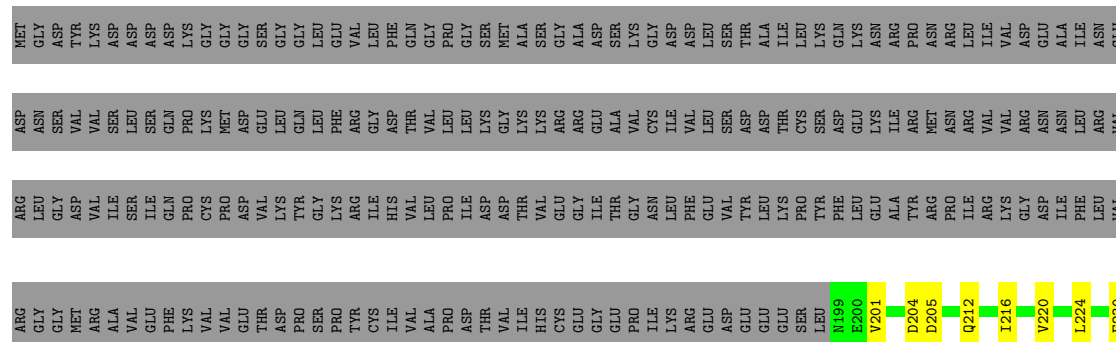
• Molecule 2: Transitional endoplasmic reticulum ATPase

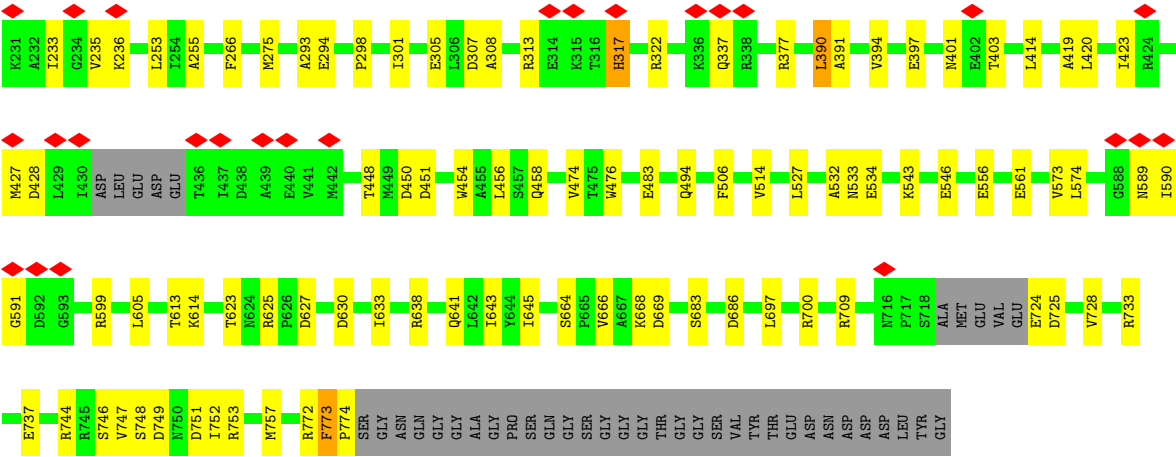
Chain E:



• Molecule 2: Transitional endoplasmic reticulum ATPase

Chain F:





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	77321	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	49.22	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	165000	Depositor
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	0.637	Depositor
Minimum map value	-0.309	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	0.020	Depositor
Recommended contour level	0.0906	Depositor
Map size (Å)	352.0, 352.0, 352.0	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.1, 1.1, 1.1	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	G	0.09	0/783	0.26	0/1060
1	H	0.08	0/555	0.23	0/755
1	I	0.10	0/811	0.25	0/1098
2	A	0.12	0/4482	0.24	0/6045
2	B	0.11	0/4473	0.24	0/6031
2	C	0.11	0/4434	0.28	2/5978 (0.0%)
2	D	0.12	0/4465	0.25	0/6020
2	E	0.11	0/4490	0.23	0/6056
2	F	0.11	0/4490	0.22	0/6056
All	All	0.11	0/28983	0.24	2/39099 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	739	ALA	CA-C-N	7.17	132.07	120.60
2	C	739	ALA	C-N-CA	7.17	132.07	120.60

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	G	761	723	722	14	0
1	H	540	514	522	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	I	789	736	744	22	0
2	A	4408	4400	4442	62	0
2	B	4400	4382	4435	56	0
2	C	4361	4338	4393	71	0
2	D	4392	4387	4429	72	0
2	E	4416	4397	4453	61	0
2	F	4416	4410	4453	74	0
All	All	28483	28287	28593	384	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

All (384) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:414:LEU:HD11	2:A:456:LEU:HD22	1.55	0.89
2:C:235:VAL:HG11	2:D:420:LEU:HD23	1.59	0.84
1:H:638:PHE:HA	2:C:754:LYS:HE3	1.59	0.83
2:F:666:VAL:O	2:F:668:LYS:NZ	2.12	0.82
2:A:564:ASP:OD1	2:A:567:ARG:NH2	2.13	0.81
2:E:710:GLU:OE1	2:E:713:ARG:NH2	2.12	0.81
2:A:737:GLU:OE2	2:F:773:PHE:HB2	1.82	0.79
2:A:710:GLU:OE2	2:A:714:GLN:NE2	2.17	0.78
2:F:216:ILE:O	2:F:220:VAL:HG12	1.83	0.78
1:G:645:GLN:NE2	2:F:627:ASP:O	2.15	0.78
2:A:543:LYS:N	2:A:546:GLU:OE1	2.17	0.77
2:B:772:ARG:HA	2:C:737:GLU:OE1	1.85	0.77
2:B:773:PHE:HB2	2:C:733:ARG:CZ	2.15	0.76
2:E:244:TYR:OH	2:E:366:GLU:OE1	2.04	0.75
2:F:483:GLU:OE1	2:F:483:GLU:N	2.19	0.75
2:F:419:ALA:O	2:F:423:ILE:HG23	1.86	0.74
2:C:281:GLU:N	2:C:281:GLU:OE1	2.19	0.73
2:B:202:GLY:N	2:B:205:ASP:OD2	2.22	0.73
2:D:281:GLU:N	2:D:281:GLU:OE2	2.19	0.73
2:F:556:GLU:OE1	2:F:599:ARG:NE	2.21	0.73
2:C:648:PRO:O	2:C:653:ARG:NH1	2.23	0.71
2:F:561:GLU:N	2:F:561:GLU:OE1	2.23	0.71
2:A:774:PRO:HD2	2:B:674:PHE:CE2	2.26	0.71
2:D:669:ASP:OD1	2:D:733:ARG:NH2	2.24	0.71
2:C:366:GLU:OE1	2:C:366:GLU:N	2.24	0.70
2:F:423:ILE:O	2:F:427:MET:N	2.25	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:332:MET:HE1	2:B:343:VAL:HG21	1.73	0.69
2:B:391:ALA:O	2:B:394:VAL:HG22	1.93	0.69
2:F:397:GLU:O	2:F:401:ASN:ND2	2.25	0.69
2:A:728:VAL:HG23	2:A:728:VAL:O	1.94	0.67
2:F:448:THR:OG1	2:F:450:ASP:OD1	2.13	0.67
2:A:669:ASP:OD2	2:A:733:ARG:NE	2.27	0.67
2:A:762:LEU:O	2:A:765:SER:OG	2.13	0.67
2:D:470:GLU:N	2:D:470:GLU:OE1	2.27	0.67
2:F:589:ASN:OD1	2:F:625:ARG:NH2	2.28	0.66
2:E:653:ARG:NE	2:E:679:THR:O	2.29	0.66
2:B:713:ARG:NH2	2:B:724:GLU:OE2	2.29	0.66
1:I:638:PHE:CD1	2:E:754:LYS:HD2	2.31	0.66
2:F:669:ASP:OD1	2:F:733:ARG:NE	2.29	0.65
2:A:420:LEU:CD2	2:F:235:VAL:HG21	2.26	0.65
2:A:403:THR:HG22	2:A:456:LEU:HD11	1.78	0.65
2:B:762:LEU:HD23	2:B:763:GLN:HB2	1.79	0.65
2:D:556:GLU:OE1	2:D:599:ARG:NE	2.27	0.65
2:F:709:ARG:NH1	2:F:724:GLU:OE1	2.30	0.65
2:C:541:SER:OG	2:C:543:LYS:NZ	2.29	0.64
1:H:607:VAL:HG22	1:H:629:LEU:HD21	1.78	0.64
2:C:624:ASN:OD1	2:C:755:TYR:OH	2.13	0.64
1:H:595:THR:OG1	1:H:604:ARG:NH2	2.30	0.64
2:A:474:VAL:O	2:A:533:ASN:ND2	2.30	0.64
2:F:454:TRP:NE1	2:F:458:GLN:OE1	2.30	0.64
2:C:442:MET:C	2:C:442:MET:HE2	2.23	0.63
2:B:318:GLY:O	2:B:322:ARG:NH1	2.30	0.63
2:E:738:GLU:OE2	2:E:741:ARG:NH1	2.32	0.63
2:F:224:LEU:HD22	2:F:298:PRO:HB2	1.80	0.62
2:B:402:GLU:OE1	2:B:456:LEU:HD11	1.99	0.62
2:F:686:ASP:OD1	2:F:746:SER:OG	2.18	0.61
2:B:423:ILE:O	2:B:427:MET:N	2.33	0.61
2:E:647:LEU:HD11	2:E:747:VAL:HG21	1.81	0.61
2:B:292:GLU:OE2	2:B:296:ASN:ND2	2.34	0.61
2:C:313:ARG:O	2:C:316:THR:OG1	2.17	0.60
2:A:420:LEU:HD23	2:F:235:VAL:HG21	1.82	0.60
2:B:235:VAL:HG11	2:C:420:LEU:HD21	1.83	0.60
1:I:640:SER:O	1:I:644:VAL:HG23	2.01	0.60
1:G:627:MET:CE	1:G:644:VAL:HG11	2.31	0.60
2:E:221:GLU:OE1	2:E:225:ARG:NH2	2.35	0.60
2:D:588:GLY:O	2:D:591:GLY:N	2.35	0.60
2:A:774:PRO:HD2	2:B:674:PHE:CZ	2.37	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:669:ASP:OD2	2:E:733:ARG:NE	2.34	0.60
2:A:773:PHE:HD1	2:A:773:PHE:O	1.85	0.60
1:H:641:GLU:N	1:H:641:GLU:OE1	2.35	0.59
2:E:220:VAL:HG12	2:E:224:LEU:HD12	1.84	0.59
2:E:673:GLU:N	2:E:673:GLU:OE1	2.35	0.59
2:A:235:VAL:HG11	2:B:420:LEU:CD2	2.31	0.59
2:B:235:VAL:HG21	2:C:420:LEU:HD23	1.84	0.59
2:E:394:VAL:HG12	2:E:449:MET:N	2.17	0.59
2:F:514:VAL:HG23	2:F:641:GLN:HB2	1.84	0.59
1:I:570:GLY:O	1:I:587:ASN:ND2	2.34	0.59
2:C:321:GLU:N	2:C:321:GLU:OE1	2.36	0.58
2:D:484:ASP:OD1	2:D:484:ASP:N	2.34	0.58
2:B:491:GLU:OE2	2:C:700:ARG:NE	2.34	0.58
2:C:607:GLU:OE2	2:D:465:ARG:NH2	2.36	0.58
2:F:201:VAL:HG11	2:F:253:LEU:CD1	2.34	0.58
2:F:725:ASP:OD1	2:F:725:ASP:N	2.36	0.58
2:C:482:LEU:HD21	2:C:646:PRO:HD2	1.86	0.58
2:D:632:ALA:O	2:D:638:ARG:NH1	2.33	0.58
2:F:476:TRP:NE1	2:F:534:GLU:OE1	2.35	0.58
2:A:649:ASP:N	2:A:652:SER:OG	2.37	0.57
1:I:615:ASP:OD1	1:I:617:SER:N	2.37	0.57
2:C:235:VAL:HG11	2:D:420:LEU:CD2	2.34	0.57
2:A:770:SER:O	2:A:772:ARG:HD2	2.05	0.57
2:D:297:ALA:HB1	2:D:298:PRO:HD2	1.86	0.57
2:F:201:VAL:HG11	2:F:253:LEU:HD12	1.87	0.57
2:A:470:GLU:OE1	2:A:470:GLU:N	2.38	0.57
2:E:329:LEU:HD11	2:E:357:LEU:HG	1.86	0.57
2:D:728:VAL:HG13	2:D:728:VAL:O	2.05	0.57
2:E:200:GLU:OE1	2:E:260:ASN:ND2	2.38	0.56
2:F:377:ARG:NE	2:F:403:THR:O	2.38	0.56
1:I:610:PHE:N	1:I:620:SER:OG	2.36	0.56
2:D:391:ALA:O	2:D:394:VAL:HG22	2.06	0.56
2:F:204:ASP:OD1	2:F:205:ASP:N	2.37	0.56
2:D:769:GLY:O	2:D:770:SER:OG	2.23	0.56
2:E:773:PHE:N	2:F:737:GLU:OE2	2.37	0.56
2:D:349:ARG:NH1	2:D:351:ASN:OD1	2.39	0.56
2:E:649:ASP:N	2:E:652:SER:OG	2.39	0.56
2:B:332:MET:HE1	2:B:343:VAL:HG11	1.88	0.55
2:E:732:ARG:NE	2:E:734:ASP:OD1	2.39	0.55
2:D:773:PHE:HB3	2:D:774:PRO:HD2	1.88	0.55
2:E:640:ASP:OD1	2:E:640:ASP:N	2.40	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:605:LEU:HD23	2:F:633:ILE:HD12	1.87	0.55
2:C:221:GLU:OE1	2:C:222:LEU:N	2.40	0.55
2:B:206:ILE:HG22	2:B:253:LEU:HD23	1.88	0.55
2:E:632:ALA:O	2:E:638:ARG:NH1	2.38	0.55
1:I:638:PHE:CG	2:E:754:LYS:HD2	2.41	0.55
1:I:622:VAL:HG22	2:D:757:MET:SD	2.47	0.54
1:G:564:ASN:OD1	1:G:565:SER:N	2.40	0.54
2:E:399:VAL:O	2:E:403:THR:HG22	2.08	0.54
2:D:235:VAL:HG11	2:E:420:LEU:CD2	2.38	0.54
2:A:556:GLU:OE2	2:A:599:ARG:NH2	2.41	0.54
2:F:590:ILE:HD12	2:F:591:GLY:O	2.07	0.54
2:A:503:PHE:O	2:A:507:GLY:N	2.41	0.53
2:B:774:PRO:HD3	2:C:674:PHE:CE2	2.43	0.53
2:A:278:LEU:HD23	2:A:279:ALA:O	2.09	0.53
2:C:567:ARG:NH1	2:D:460:ASN:OD1	2.41	0.53
2:A:420:LEU:HD11	2:F:230:PHE:CZ	2.44	0.53
2:D:770:SER:O	2:D:772:ARG:HD3	2.08	0.53
2:B:728:VAL:HG13	2:B:728:VAL:O	2.09	0.53
2:D:675:LEU:O	2:D:679:THR:OG1	2.13	0.53
2:F:390:LEU:HB3	2:F:394:VAL:HG11	1.91	0.53
1:G:622:VAL:HG22	2:F:757:MET:SD	2.49	0.52
2:E:572:CYS:SG	2:E:573:VAL:N	2.81	0.52
2:F:494:GLN:NE2	2:F:534:GLU:OE2	2.41	0.52
2:A:427:MET:SD	2:A:427:MET:C	2.92	0.52
2:B:757:MET:N	2:B:757:MET:SD	2.82	0.52
2:F:294:GLU:OE2	2:F:337:GLN:NE2	2.41	0.52
2:A:229:LEU:HD23	2:A:230:PHE:N	2.23	0.52
1:I:578:HIS:N	1:I:585:TYR:O	2.42	0.52
2:A:773:PHE:CE1	2:B:733:ARG:HD3	2.44	0.52
1:I:595:THR:O	1:I:646:LYS:NZ	2.42	0.52
2:A:235:VAL:HG11	2:B:420:LEU:HD23	1.91	0.52
2:A:479:ILE:HG23	2:A:479:ILE:O	2.10	0.52
2:E:222:LEU:HD21	2:F:423:ILE:HD11	1.91	0.52
2:F:317:HIS:O	2:F:322:ARG:NH1	2.42	0.52
2:C:377:ARG:NE	2:C:403:THR:O	2.43	0.52
2:F:450:ASP:OD1	2:F:451:ASP:N	2.43	0.52
2:D:663:LYS:HD2	2:D:663:LYS:O	2.10	0.51
2:D:336:LYS:HE2	2:D:336:LYS:HA	1.91	0.51
2:F:630:ASP:O	2:F:633:ILE:HG22	2.10	0.51
2:A:773:PHE:O	2:A:773:PHE:CD1	2.62	0.51
2:B:642:LEU:HD13	2:B:762:LEU:HD21	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:647:LEU:HD11	2:D:752:ILE:HD13	1.92	0.51
2:E:648:PRO:O	2:E:653:ARG:NH1	2.44	0.51
2:D:771:PHE:C	2:D:772:ARG:HD3	2.36	0.51
2:A:272:PRO:O	2:A:276:SER:OG	2.28	0.51
2:E:728:VAL:HG23	2:E:728:VAL:O	2.10	0.51
2:D:293:ALA:CB	2:D:301:ILE:HD11	2.41	0.51
2:D:390:LEU:HB2	2:D:394:VAL:HG21	1.93	0.50
2:F:556:GLU:OE2	2:F:599:ARG:NH2	2.43	0.50
2:F:664:SER:O	2:F:666:VAL:HG23	2.11	0.50
2:C:556:GLU:OE2	2:C:599:ARG:NH2	2.44	0.50
2:F:428:ASP:OD1	2:F:428:ASP:N	2.43	0.50
2:B:748:SER:N	2:B:751:ASP:OD2	2.40	0.50
2:E:362:ARG:NH2	2:F:305:GLU:OE2	2.42	0.50
2:E:364:ASP:OD1	2:E:365:ARG:N	2.42	0.50
2:C:200:GLU:OE1	2:C:260:ASN:ND2	2.45	0.50
1:I:563:THR:OG1	1:I:584:GLU:OE2	2.27	0.50
2:B:362:ARG:O	2:B:364:ASP:N	2.45	0.50
2:C:233:ILE:CG2	2:C:235:VAL:HG23	2.42	0.50
2:D:700:ARG:NH1	2:D:704:GLU:OE2	2.40	0.50
2:B:541:SER:OG	2:B:543:LYS:NZ	2.44	0.49
2:C:485:VAL:HG22	2:C:643:ILE:CG2	2.43	0.49
2:F:543:LYS:N	2:F:546:GLU:OE1	2.44	0.49
2:F:573:VAL:O	2:F:574:LEU:C	2.54	0.49
2:D:300:ILE:HG23	2:D:344:MET:HE3	1.95	0.49
2:E:212:GLN:OE1	2:E:212:GLN:N	2.43	0.49
2:B:235:VAL:HG21	2:C:420:LEU:CD2	2.43	0.49
2:C:442:MET:HE2	2:C:442:MET:O	2.12	0.49
2:D:212:GLN:O	2:D:216:ILE:HG13	2.13	0.49
2:F:728:VAL:O	2:F:728:VAL:HG13	2.13	0.49
2:E:307:ASP:OD1	2:E:308:ALA:N	2.45	0.49
2:D:362:ARG:NH2	2:E:305:GLU:OE2	2.46	0.49
2:F:605:LEU:HD22	2:F:638:ARG:HH11	1.76	0.49
2:F:514:VAL:HG21	2:F:643:ILE:CD1	2.43	0.49
1:G:630:VAL:HG21	1:G:644:VAL:HG22	1.95	0.48
1:H:650:THR:O	1:H:654:GLN:NE2	2.45	0.48
1:I:637:GLU:C	2:E:754:LYS:HD3	2.38	0.48
2:C:233:ILE:HG22	2:C:235:VAL:HG23	1.95	0.48
2:C:235:VAL:HG13	2:D:416:SER:CB	2.42	0.48
2:D:490:GLN:NE2	2:D:534:GLU:OE2	2.46	0.48
1:I:585:TYR:CD2	1:I:618:LEU:HD23	2.48	0.48
2:A:666:VAL:CG2	2:A:670:VAL:HG11	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:508:MET:SD	2:B:509:THR:N	2.86	0.48
2:C:293:ALA:CB	2:C:301:ILE:HD11	2.43	0.48
2:E:362:ARG:O	2:E:364:ASP:N	2.47	0.48
2:F:307:ASP:OD1	2:F:307:ASP:N	2.44	0.48
2:B:394:VAL:HA	2:B:449:MET:HE2	1.96	0.48
2:D:466:GLU:OE1	2:D:466:GLU:HA	2.13	0.48
2:F:275:MET:HE2	2:F:308:ALA:O	2.14	0.48
2:F:230:PHE:HA	2:F:233:ILE:HG22	1.96	0.48
2:C:317:HIS:O	2:C:322:ARG:NH2	2.45	0.48
2:C:638:ARG:O	2:C:640:ASP:N	2.46	0.48
2:D:322:ARG:NE	2:E:321:GLU:OE2	2.46	0.48
2:F:669:ASP:O	2:F:733:ARG:NH2	2.45	0.48
2:C:592:ASP:N	2:C:592:ASP:OD1	2.46	0.47
2:C:598:ASP:OD1	2:C:599:ARG:N	2.47	0.47
2:E:556:GLU:OE2	2:E:599:ARG:NH2	2.46	0.47
1:I:580:TRP:O	1:I:583:LYS:N	2.45	0.47
2:A:235:VAL:HG11	2:B:420:LEU:HD21	1.94	0.47
2:A:732:ARG:NH2	2:A:734:ASP:OD2	2.47	0.47
2:C:296:ASN:OD1	2:C:296:ASN:N	2.47	0.47
2:E:456:LEU:O	2:E:456:LEU:HD23	2.15	0.47
1:G:652:LEU:O	2:F:753:ARG:NH2	2.47	0.47
1:I:622:VAL:HB	1:I:648:VAL:HG23	1.96	0.47
2:E:483:GLU:N	2:E:483:GLU:OE1	2.47	0.47
1:H:594:ILE:HD12	1:H:607:VAL:HG21	1.97	0.47
1:I:637:GLU:O	2:E:754:LYS:HD3	2.14	0.47
2:A:623:THR:HG21	2:A:629:ILE:HD11	1.96	0.47
2:B:497:VAL:O	2:B:497:VAL:HG22	2.15	0.47
2:C:356:ALA:O	2:C:362:ARG:NH1	2.48	0.47
1:I:638:PHE:HA	2:E:754:LYS:CD	2.45	0.47
2:A:229:LEU:HD23	2:A:229:LEU:C	2.40	0.47
2:C:398:GLN:O	2:C:402:GLU:HG3	2.14	0.47
1:I:588:LEU:HD23	1:I:588:LEU:H	1.80	0.47
2:A:236:LYS:HD2	2:A:237:PRO:HD2	1.96	0.47
2:A:204:ASP:OD1	2:A:204:ASP:N	2.48	0.46
2:B:773:PHE:HA	2:C:674:PHE:CE1	2.50	0.46
2:C:391:ALA:O	2:C:394:VAL:HG22	2.15	0.46
2:D:538:ASN:ND2	2:D:569:ALA:O	2.47	0.46
2:B:440:GLU:O	2:B:444:SER:N	2.44	0.46
2:A:638:ARG:O	2:A:639:LEU:C	2.59	0.46
2:C:235:VAL:HG21	2:D:419:ALA:HB3	1.96	0.46
2:C:693:ARG:O	2:C:694:ALA:HB3	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:394:VAL:HA	2:E:449:MET:HE2	1.96	0.46
2:D:514:VAL:HG21	2:D:643:ILE:HD12	1.98	0.46
2:D:647:LEU:HD21	2:D:747:VAL:HG21	1.98	0.46
2:B:371:ILE:CD1	2:B:407:VAL:HG12	2.46	0.46
2:C:572:CYS:SG	2:C:573:VAL:N	2.88	0.46
2:F:224:LEU:HD22	2:F:298:PRO:CB	2.46	0.46
1:H:637:GLU:C	2:C:754:LYS:HZ1	2.24	0.46
2:A:423:ILE:HG13	2:A:445:LEU:HD21	1.97	0.46
2:F:212:GLN:OE1	2:F:212:GLN:N	2.45	0.46
2:B:605:LEU:HD23	2:B:633:ILE:HD12	1.98	0.46
2:C:550:MET:HE2	2:C:558:ASN:HB2	1.98	0.46
2:E:353:ILE:HD12	2:E:357:LEU:HD13	1.96	0.46
2:A:567:ARG:NH1	2:B:460:ASN:OD1	2.48	0.46
2:C:726:ASP:OD1	2:C:726:ASP:N	2.49	0.46
2:D:514:VAL:HG22	2:D:515:LEU:N	2.31	0.45
2:D:773:PHE:HD1	2:D:774:PRO:HD2	1.81	0.45
2:B:577:ASP:O	2:B:622:ALA:HB3	2.16	0.45
2:E:683:SER:OG	2:E:686:ASP:OD2	2.34	0.45
2:A:395:ASP:OD2	2:A:398:GLN:NE2	2.43	0.45
2:D:649:ASP:OD1	2:D:649:ASP:N	2.50	0.45
2:D:773:PHE:CB	2:D:774:PRO:HD2	2.46	0.45
1:I:624:ASP:OD1	1:I:624:ASP:C	2.58	0.45
2:A:364:ASP:OD1	2:A:364:ASP:N	2.50	0.45
2:C:770:SER:O	2:C:770:SER:OG	2.30	0.45
2:E:350:PRO:O	2:E:358:ARG:NH1	2.48	0.45
1:H:637:GLU:O	1:H:640:SER:OG	2.30	0.45
2:A:773:PHE:CD1	2:A:773:PHE:C	2.95	0.45
2:D:235:VAL:HG11	2:E:420:LEU:HD21	1.99	0.45
2:C:712:GLU:O	2:C:716:ASN:N	2.41	0.45
2:D:320:VAL:O	2:D:324:ILE:HD12	2.17	0.45
2:E:273:GLU:O	2:E:277:LYS:NZ	2.49	0.45
2:B:766:ARG:HH11	2:C:745:ARG:HG3	1.82	0.45
2:D:735:HIS:O	2:D:739:ALA:N	2.47	0.45
2:C:319:GLU:OE2	2:C:323:ARG:NH1	2.49	0.45
2:C:602:ASN:HA	2:C:605:LEU:HD12	1.98	0.45
2:D:332:MET:HE3	2:D:363:PHE:CE2	2.52	0.45
2:B:763:GLN:CD	2:B:763:GLN:O	2.60	0.44
2:D:320:VAL:HG22	2:D:324:ILE:HD11	1.99	0.44
2:E:468:VAL:HG22	2:E:470:GLU:HG2	1.98	0.44
2:C:479:ILE:HB	2:C:526:LEU:HD22	1.99	0.44
2:C:728:VAL:O	2:C:728:VAL:HG22	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:572:CYS:SG	2:D:573:VAL:N	2.90	0.44
1:H:638:PHE:CA	2:C:754:LYS:HE3	2.38	0.44
2:A:519:PRO:O	2:A:524:LYS:NZ	2.50	0.44
2:D:738:GLU:OE1	2:D:741:ARG:NH2	2.50	0.44
2:C:773:PHE:HB3	2:D:733:ARG:NH1	2.32	0.44
2:D:244:TYR:OH	2:D:366:GLU:OE1	2.33	0.44
2:D:556:GLU:OE2	2:D:599:ARG:NH2	2.51	0.44
2:D:773:PHE:CD1	2:D:774:PRO:HD2	2.52	0.44
2:A:371:ILE:HG22	2:A:407:VAL:HG12	2.00	0.44
2:D:674:PHE:CE1	2:D:678:MET:HE3	2.52	0.44
2:F:613:THR:HG23	2:F:614:LYS:HD2	1.99	0.44
2:D:229:LEU:O	2:D:233:ILE:HG22	2.18	0.44
2:C:390:LEU:HB3	2:C:394:VAL:HG11	1.99	0.44
2:F:293:ALA:CB	2:F:301:ILE:HD11	2.48	0.44
2:D:638:ARG:O	2:D:640:ASP:N	2.50	0.44
2:B:269:ILE:HD11	2:B:289:ALA:HB1	1.99	0.43
2:C:335:LEU:HD22	2:C:341:VAL:CG2	2.48	0.43
2:D:297:ALA:HB1	2:D:298:PRO:CD	2.48	0.43
2:B:624:ASN:OD1	2:B:624:ASN:N	2.51	0.43
1:I:654:GLN:CD	1:I:654:GLN:C	2.86	0.43
2:F:235:VAL:HG22	2:F:236:LYS:H	1.83	0.43
2:A:304:ASP:OD1	2:A:305:GLU:N	2.52	0.43
2:A:773:PHE:HZ	2:B:670:VAL:HA	1.84	0.43
2:D:649:ASP:N	2:D:652:SER:OG	2.52	0.43
2:E:293:ALA:CB	2:E:301:ILE:HD11	2.49	0.43
2:E:647:LEU:CD1	2:E:752:ILE:HD11	2.49	0.43
2:A:216:ILE:O	2:A:220:VAL:HG22	2.18	0.43
2:A:420:LEU:HD21	2:F:235:VAL:HG11	2.00	0.43
2:D:440:GLU:OE2	2:D:443:ASN:ND2	2.51	0.43
2:A:666:VAL:HG22	2:A:670:VAL:HG11	2.01	0.43
1:G:563:THR:OG1	1:G:584:GLU:OE2	2.33	0.43
1:I:654:GLN:OE1	1:I:655:THR:N	2.51	0.43
2:A:398:GLN:O	2:A:402:GLU:HG2	2.19	0.43
2:A:442:MET:N	2:A:442:MET:SD	2.91	0.43
2:B:428:ASP:N	2:B:428:ASP:OD1	2.49	0.43
2:C:231:LYS:HA	2:C:231:LYS:HE2	2.01	0.43
2:E:341:VAL:O	2:E:341:VAL:HG12	2.17	0.43
2:F:474:VAL:O	2:F:533:ASN:ND2	2.52	0.42
2:A:690:ILE:HD12	2:A:743:ALA:HB2	2.02	0.42
2:E:701:GLU:OE2	2:E:732:ARG:NH2	2.48	0.42
1:G:627:MET:HE1	1:G:644:VAL:HG11	1.99	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:512:LYS:NZ	2:E:611:MET:O	2.47	0.42
1:I:630:VAL:HG22	1:I:643:LEU:HD23	2.02	0.42
2:B:492:LEU:HD12	2:B:511:SER:HB3	2.02	0.42
2:F:391:ALA:O	2:F:394:VAL:HG12	2.20	0.42
2:F:414:LEU:HD11	2:F:456:LEU:HD23	2.00	0.42
2:B:381:LEU:HD13	2:B:399:VAL:HG23	2.01	0.42
2:D:394:VAL:HG12	2:D:449:MET:HA	2.01	0.42
2:E:220:VAL:CG1	2:E:224:LEU:HD12	2.49	0.42
2:F:527:LEU:CD1	2:F:645:ILE:HD12	2.50	0.42
2:F:749:ASP:HA	2:F:752:ILE:CG2	2.49	0.42
2:A:491:GLU:OE2	2:B:700:ARG:NE	2.52	0.42
2:C:233:ILE:CD1	2:D:423:ILE:HD11	2.48	0.42
1:G:622:VAL:HG21	1:G:648:VAL:HG13	2.01	0.42
1:I:645:GLN:O	1:I:648:VAL:HG12	2.20	0.42
2:C:633:ILE:HG23	2:C:634:LEU:HD23	2.02	0.42
2:D:292:GLU:OE1	2:D:292:GLU:HA	2.20	0.42
2:D:297:ALA:O	2:D:298:PRO:C	2.63	0.42
2:E:393:ASP:OD2	2:E:448:THR:OG1	2.35	0.42
2:E:564:ASP:OD2	2:E:564:ASP:C	2.62	0.42
2:F:233:ILE:HG23	2:F:235:VAL:H	1.84	0.42
2:A:514:VAL:HG22	2:A:515:LEU:N	2.34	0.42
2:B:269:ILE:HD12	2:B:301:ILE:CG2	2.50	0.42
2:B:766:ARG:CZ	2:C:744:ARG:HA	2.50	0.42
1:G:627:MET:O	1:G:631:THR:HG23	2.20	0.41
2:C:527:LEU:CD1	2:C:645:ILE:HD12	2.49	0.41
2:C:747:VAL:HG23	2:C:747:VAL:O	2.20	0.41
2:F:697:LEU:HD23	2:F:700:ARG:NH2	2.35	0.41
2:F:772:ARG:H	2:F:772:ARG:HG2	1.69	0.41
2:A:773:PHE:HA	2:B:674:PHE:CE1	2.55	0.41
2:C:605:LEU:CD2	2:C:633:ILE:HD12	2.51	0.41
2:C:442:MET:SD	2:C:443:ASN:N	2.93	0.41
2:D:747:VAL:O	2:D:747:VAL:HG23	2.20	0.41
2:E:650:GLU:O	2:E:654:VAL:HG23	2.19	0.41
2:C:439:ALA:O	2:C:442:MET:SD	2.79	0.41
2:D:508:MET:HE2	2:E:696:LYS:HG3	2.03	0.41
2:D:674:PHE:HE1	2:D:678:MET:HE3	1.86	0.41
2:C:514:VAL:HG12	2:C:515:LEU:N	2.35	0.41
1:G:610:PHE:O	1:G:620:SER:OG	2.39	0.41
2:F:532:ALA:HB2	2:F:573:VAL:HG21	2.02	0.41
2:F:573:VAL:O	2:F:573:VAL:HG12	2.20	0.41
2:F:748:SER:N	2:F:751:ASP:OD2	2.45	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:271:GLY:HA2	2:B:309:ILE:HD11	2.03	0.41
2:B:319:GLU:OE1	2:B:319:GLU:HA	2.20	0.41
2:C:235:VAL:HG13	2:D:416:SER:HB3	2.03	0.41
2:A:695:CYS:SG	2:F:506:PHE:HB3	2.61	0.41
2:C:691:CYS:O	2:C:693:ARG:O	2.39	0.41
2:D:533:ASN:O	2:D:536:GLN:NE2	2.54	0.41
2:D:649:ASP:N	2:D:652:SER:HG	2.19	0.41
2:E:235:VAL:HG11	2:F:420:LEU:HD21	2.02	0.41
2:E:514:VAL:HG23	2:E:641:GLN:HB3	2.03	0.41
2:F:255:ALA:HB1	2:F:266:PHE:HE1	1.85	0.41
2:A:686:ASP:O	2:A:690:ILE:HG12	2.22	0.41
2:E:423:ILE:O	2:E:427:MET:N	2.45	0.41
2:A:505:LYS:NZ	2:B:726:ASP:OD2	2.46	0.40
2:C:426:LYS:NZ	2:C:444:SER:OG	2.49	0.40
2:D:338:ARG:HB3	2:D:341:VAL:HG21	2.04	0.40
2:F:313:ARG:HD2	2:F:313:ARG:O	2.21	0.40
1:G:604:ARG:HD2	1:G:604:ARG:N	2.37	0.40
2:A:640:ASP:OD1	2:A:640:ASP:C	2.63	0.40
2:B:572:CYS:SG	2:B:573:VAL:N	2.94	0.40
2:D:329:LEU:HD23	2:D:357:LEU:HD23	2.03	0.40
2:E:407:VAL:HG22	2:E:410:ASP:OD2	2.21	0.40
2:F:772:ARG:NH1	2:F:774:PRO:HG3	2.35	0.40
1:G:596:LEU:HD21	1:G:629:LEU:HD21	2.04	0.40
2:A:570:ALA:HB1	2:A:615:LYS:O	2.21	0.40
2:B:647:LEU:CD1	2:B:752:ILE:HD11	2.51	0.40
2:C:366:GLU:OE2	2:C:568:GLN:NE2	2.51	0.40
2:E:292:GLU:OE2	2:E:292:GLU:HA	2.22	0.40
1:G:621:ASN:O	1:G:625:VAL:HG22	2.22	0.40
2:A:666:VAL:HG22	2:A:667:ALA:N	2.37	0.40
2:E:293:ALA:HB3	2:E:301:ILE:HD11	2.04	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	G	92/1250 (7%)	91 (99%)	1 (1%)	0	100	100
1	H	64/1250 (5%)	63 (98%)	1 (2%)	0	100	100
1	I	96/1250 (8%)	95 (99%)	1 (1%)	0	100	100
2	A	559/832 (67%)	539 (96%)	20 (4%)	0	100	100
2	B	556/832 (67%)	532 (96%)	24 (4%)	0	100	100
2	C	551/832 (66%)	536 (97%)	15 (3%)	0	100	100
2	D	555/832 (67%)	537 (97%)	18 (3%)	0	100	100
2	E	560/832 (67%)	539 (96%)	21 (4%)	0	100	100
2	F	560/832 (67%)	546 (98%)	14 (2%)	0	100	100
All	All	3593/8742 (41%)	3478 (97%)	115 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	G	83/1065 (8%)	80 (96%)	3 (4%)	31	62
1	H	60/1065 (6%)	56 (93%)	4 (7%)	15	43
1	I	86/1065 (8%)	84 (98%)	2 (2%)	44	70
2	A	470/696 (68%)	457 (97%)	13 (3%)	38	66
2	B	469/696 (67%)	462 (98%)	7 (2%)	57	75
2	C	464/696 (67%)	450 (97%)	14 (3%)	36	65
2	D	468/696 (67%)	458 (98%)	10 (2%)	47	71
2	E	471/696 (68%)	464 (98%)	7 (2%)	57	75
2	F	471/696 (68%)	464 (98%)	7 (2%)	57	75
All	All	3042/7371 (41%)	2975 (98%)	67 (2%)	45	71

All (67) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	611	GLN
1	G	647	VAL
1	G	655	THR
1	H	592	PHE
1	H	595	THR
1	H	629	LEU
1	H	654	GLN
1	I	602	VAL
1	I	631	THR
2	A	229	LEU
2	A	243	LEU
2	A	347	THR
2	A	438	ASP
2	A	456	LEU
2	A	482	LEU
2	A	508	MET
2	A	572	CYS
2	A	624	ASN
2	A	633	ILE
2	A	683	SER
2	A	751	ASP
2	A	752	ILE
2	B	296	ASN
2	B	390	LEU
2	B	421	GLN
2	B	492	LEU
2	B	606	THR
2	B	623	THR
2	B	706	GLU
2	C	221	GLU
2	C	229	LEU
2	C	282	SER
2	C	296	ASN
2	C	323	ARG
2	C	362	ARG
2	C	474	VAL
2	C	522	CYS
2	C	606	THR
2	C	695	CYS
2	C	726	ASP
2	C	728	VAL
2	C	740	MET

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Mol	Chain	Res	Type
2	C	771	PHE
2	D	218	GLU
2	D	244	TYR
2	D	341	VAL
2	D	353	ILE
2	D	420	LEU
2	D	425	LYS
2	D	508	MET
2	D	613	THR
2	D	623	THR
2	D	651	LYS
2	E	340	HIS
2	E	470	GLU
2	E	479	ILE
2	E	492	LEU
2	E	623	THR
2	E	624	ASN
2	E	710	GLU
2	F	317	HIS
2	F	390	LEU
2	F	623	THR
2	F	683	SER
2	F	744	ARG
2	F	747	VAL
2	F	773	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	H	633	HIS
2	A	285	ASN
2	A	340	HIS
2	A	406	HIS
2	A	499	HIS
2	A	602	ASN
2	A	680	ASN
2	A	692	GLN
2	B	215	GLN
2	B	494	GLN
2	B	680	ASN
2	C	348	ASN
2	C	602	ASN

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Mol	Chain	Res	Type
2	C	764	GLN
2	D	340	HIS
2	D	421	GLN
2	D	443	ASN
2	E	317	HIS
2	E	602	ASN
2	E	660	ASN
2	E	735	HIS
2	F	215	GLN
2	F	602	ASN
2	F	750	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.

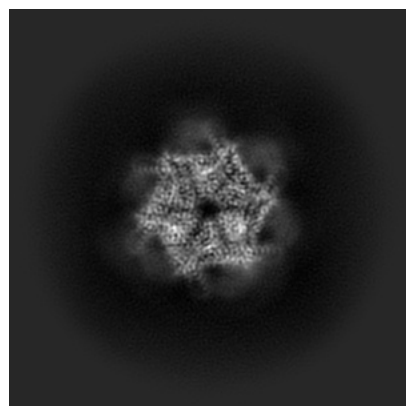
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-48506. These allow visual inspection of the internal detail of the map and identification of artifacts.

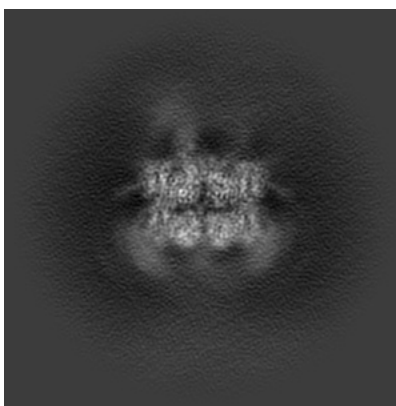
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

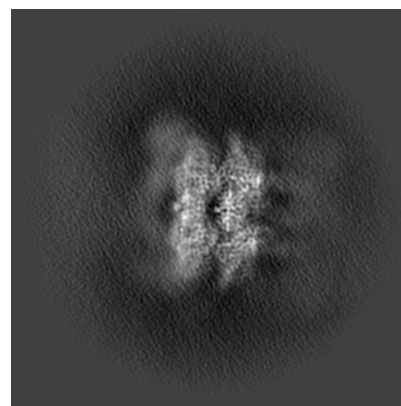
6.1.1 Primary map



X

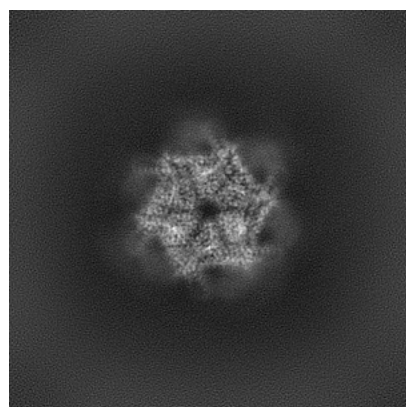


Y

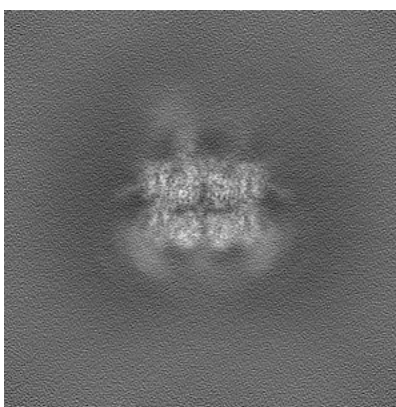


Z

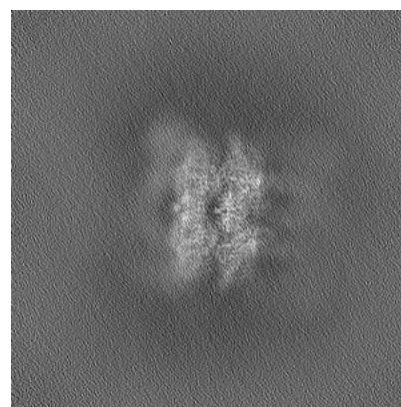
6.1.2 Raw map



X



Y

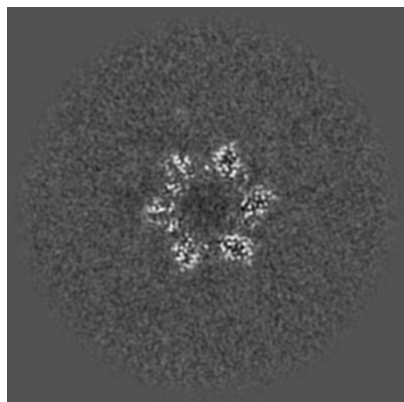


Z

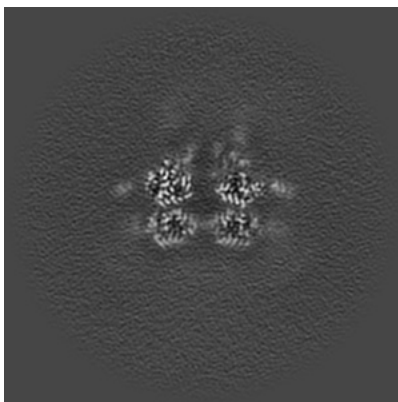
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

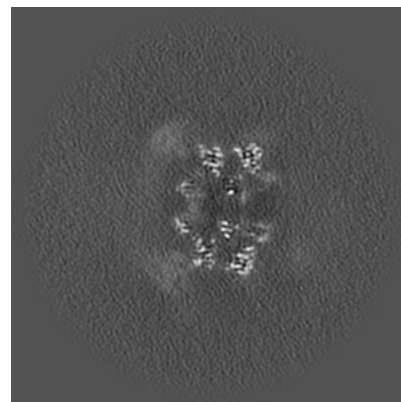
6.2.1 Primary map



X Index: 160

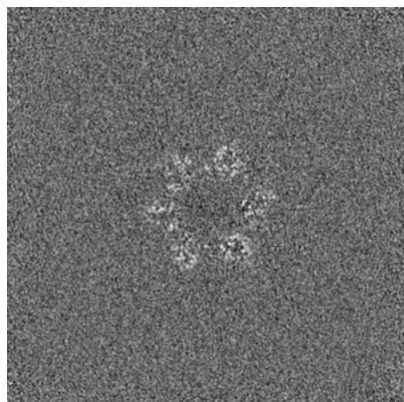


Y Index: 160

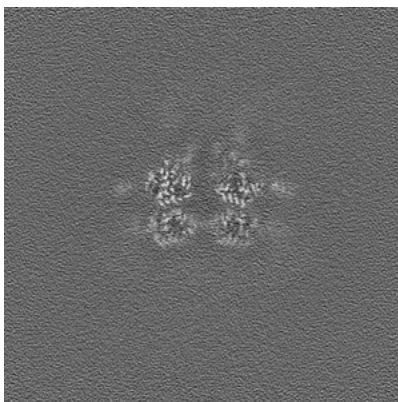


Z Index: 160

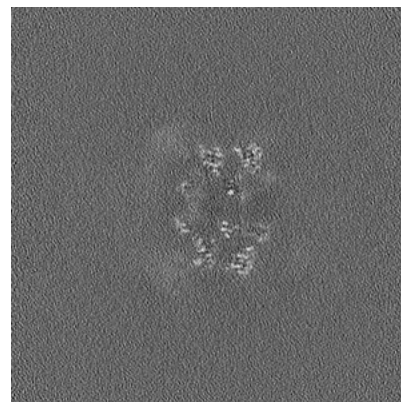
6.2.2 Raw map



X Index: 160



Y Index: 160

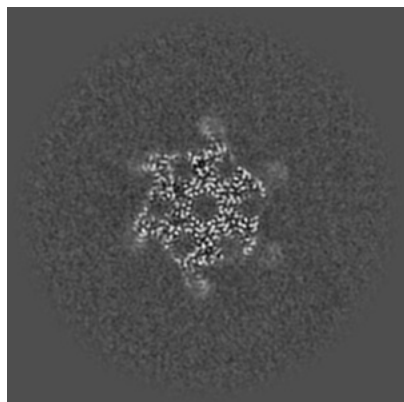


Z Index: 160

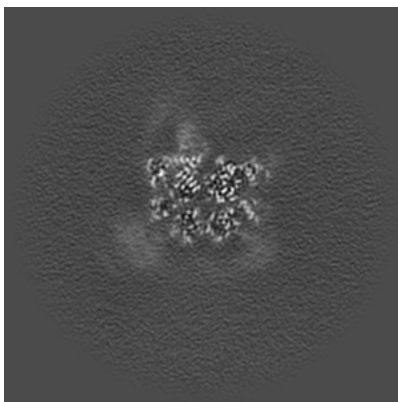
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

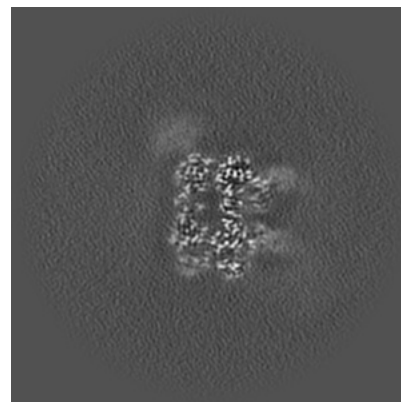
6.3.1 Primary map



X Index: 174

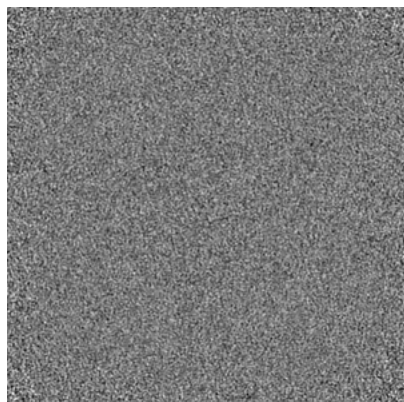


Y Index: 183

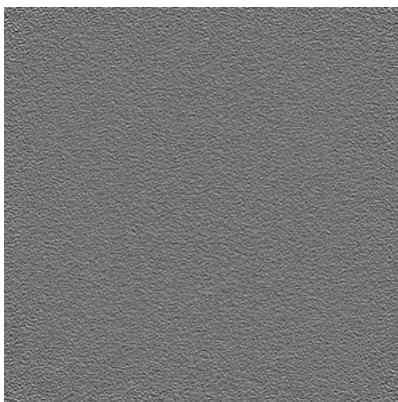


Z Index: 145

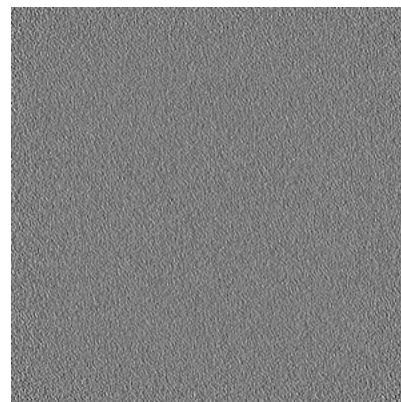
6.3.2 Raw map



X Index: 0



Y Index: 0

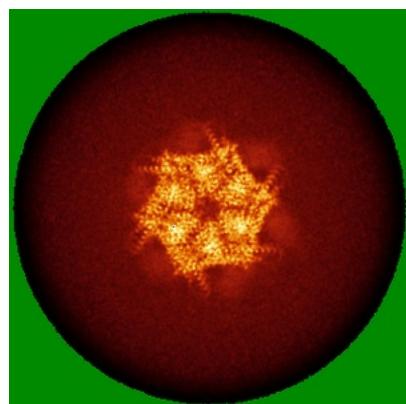


Z Index: 0

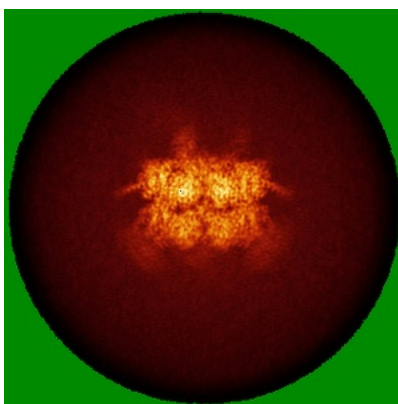
The images above show the largest variance slices of the map in three orthogonal directions.

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

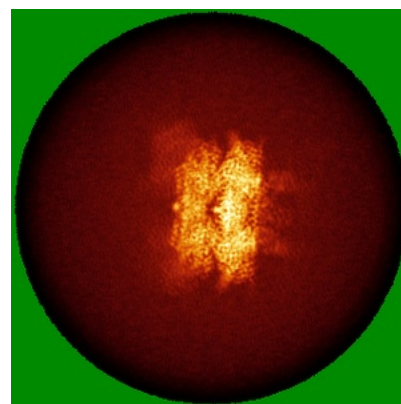
6.4.1 Primary map



X

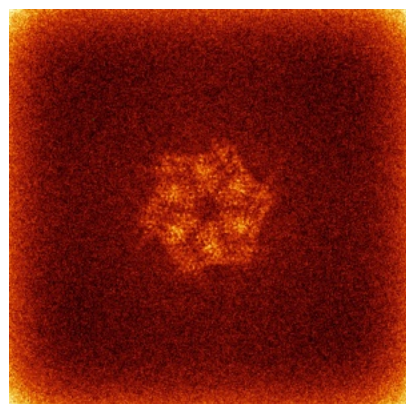


Y

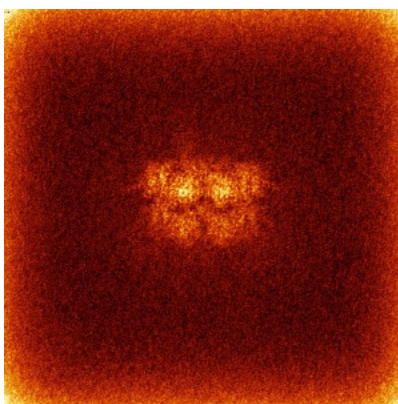


Z

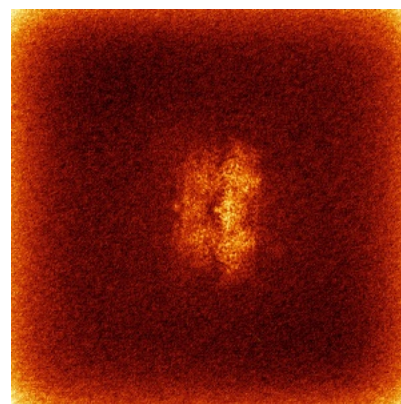
6.4.2 Raw map



X



Y

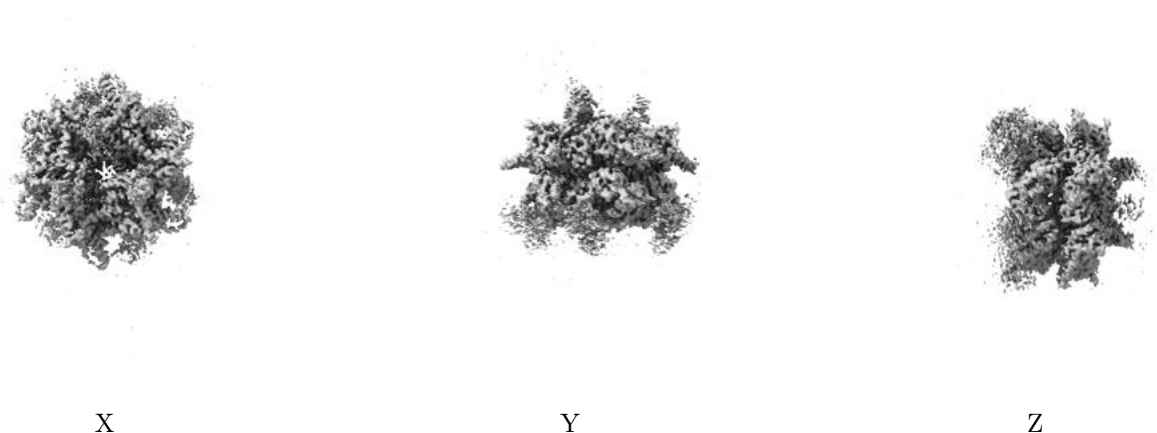


Z

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.

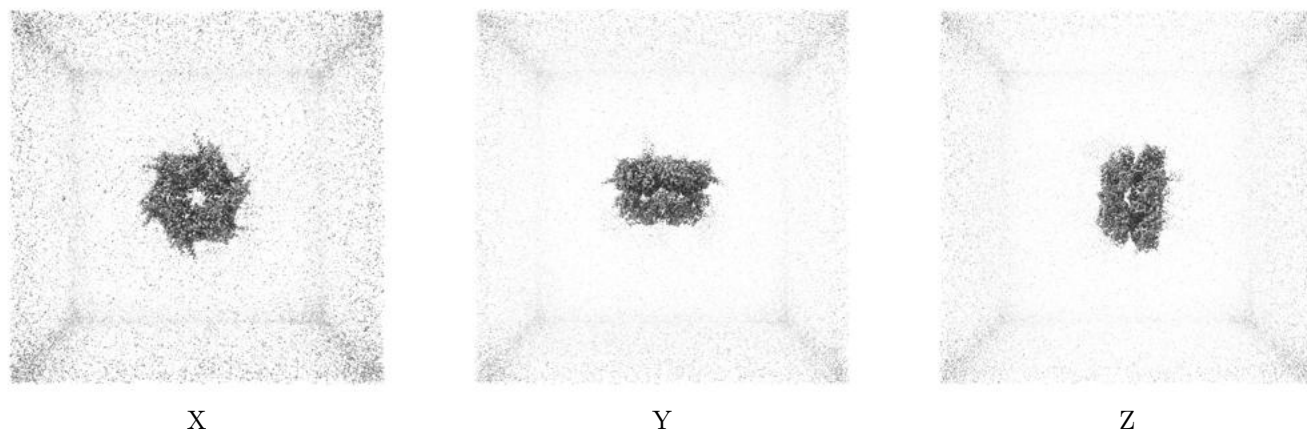
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0906. 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.

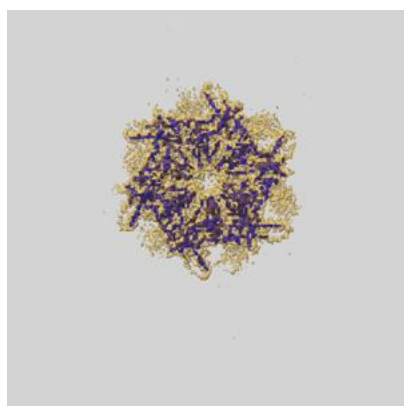
6.6 Mask visualisation [i](#)

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

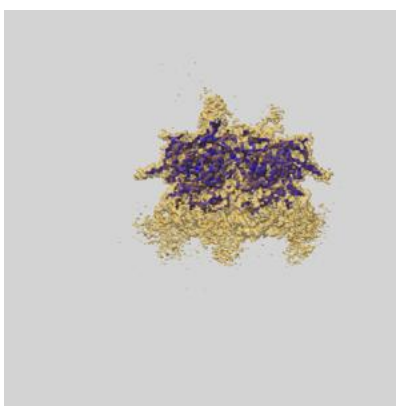
A mask typically either:

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

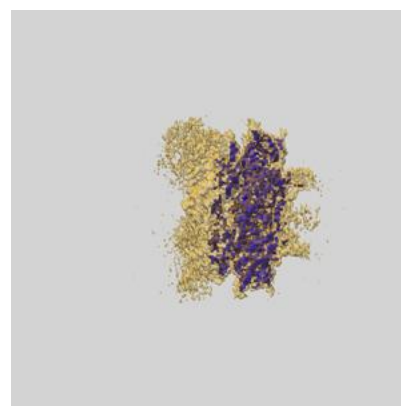
6.6.1 emd_48506_msk_2.map [i](#)



X

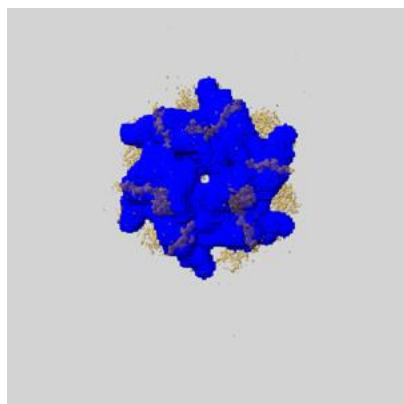


Y

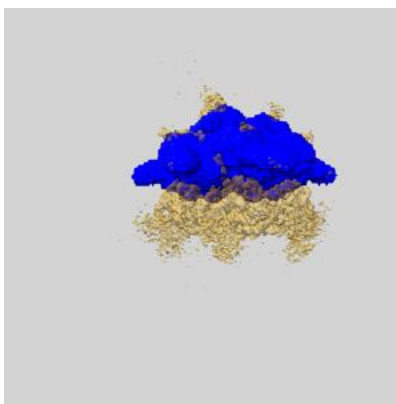


Z

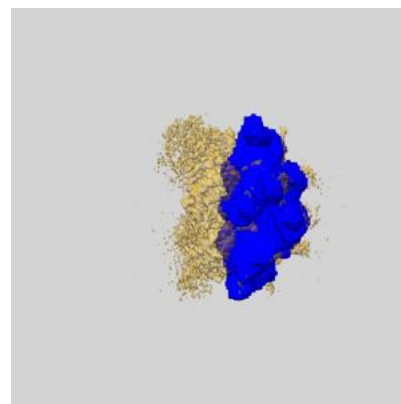
6.6.2 emd_48506_msk_1.map [i](#)



X



Y

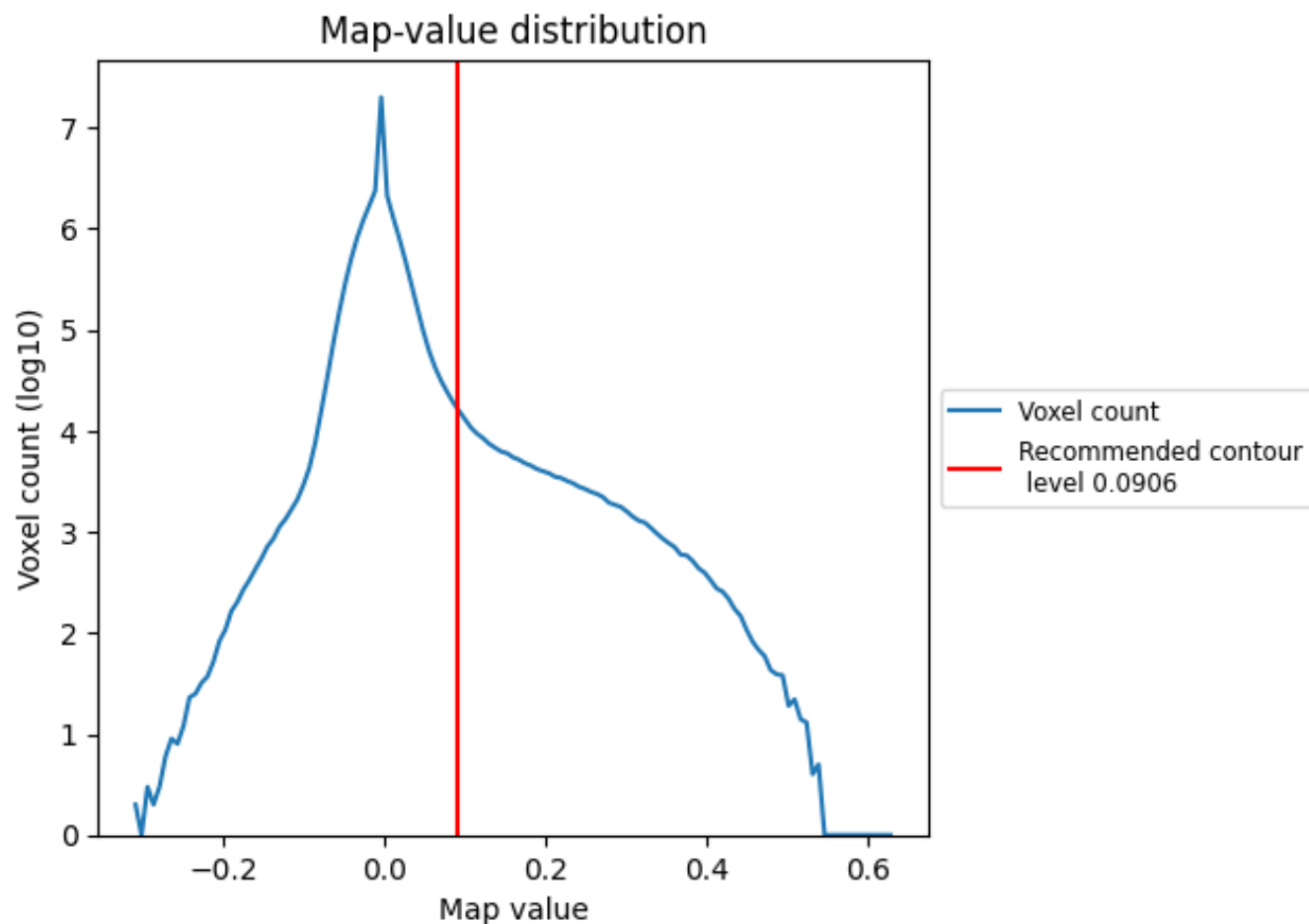


Z

7 Map analysis [i](#)

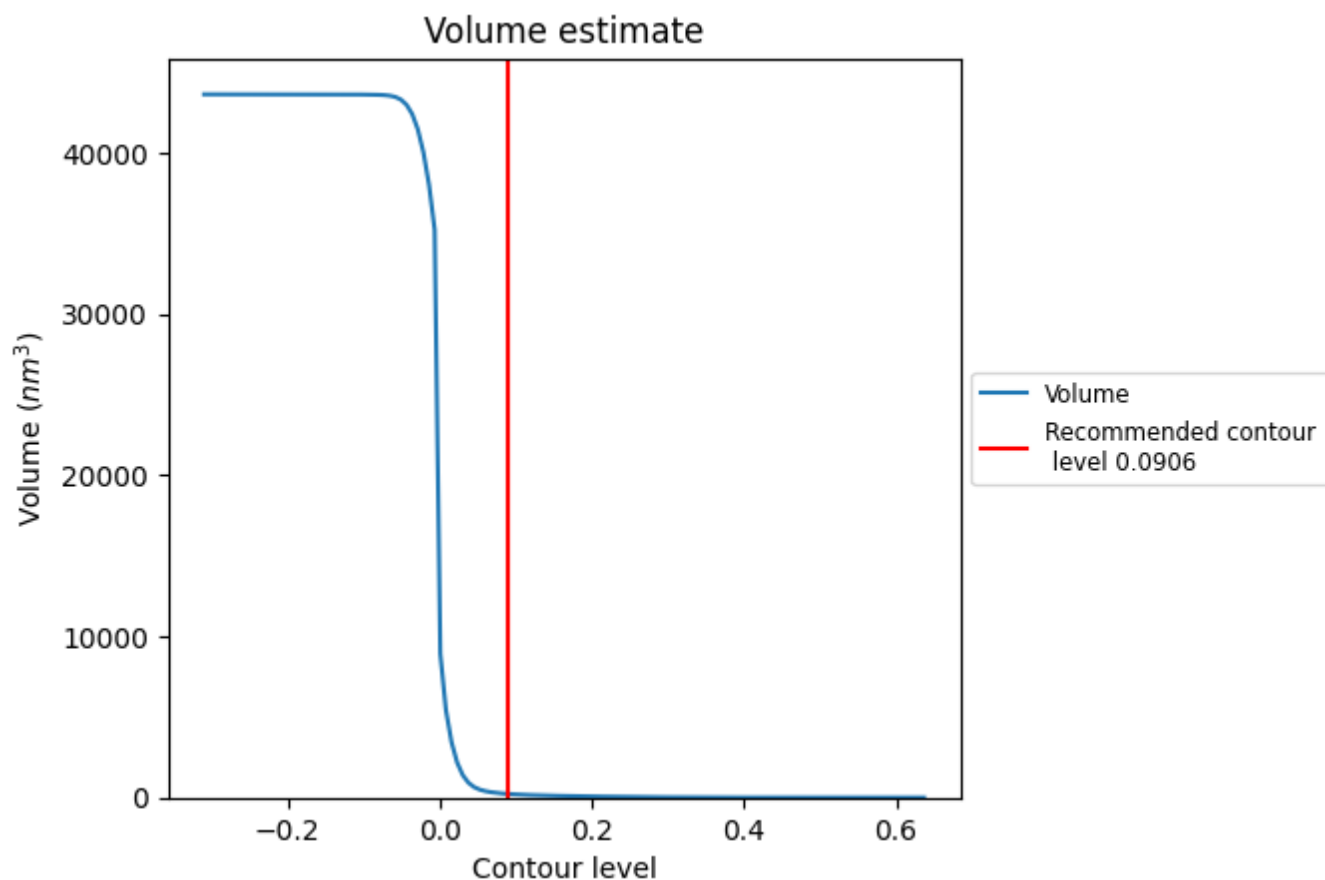
This section contains the results of statistical analysis of the map.

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.

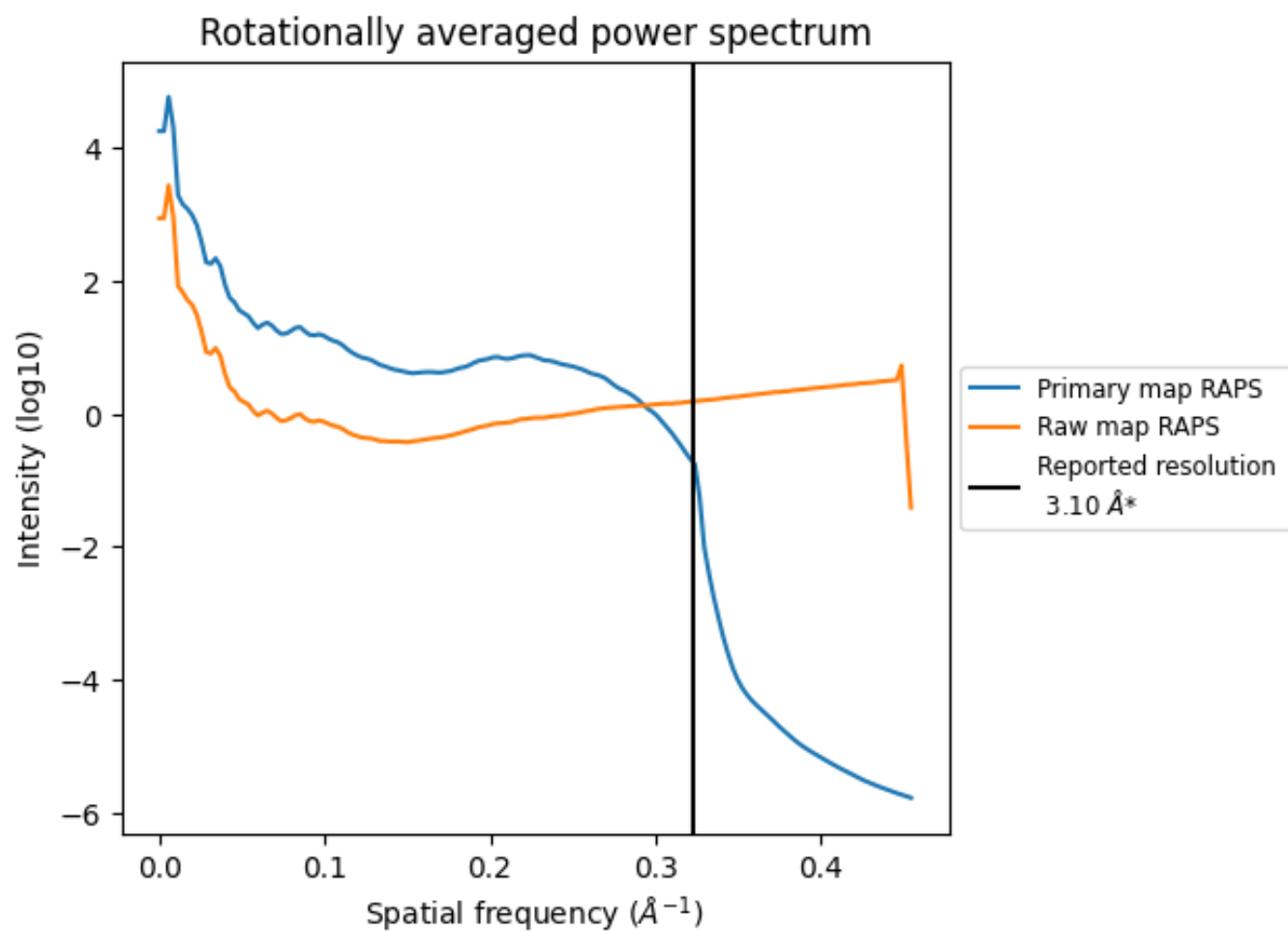
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 222 nm³; this corresponds to an approximate mass of 201 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 [i](#)

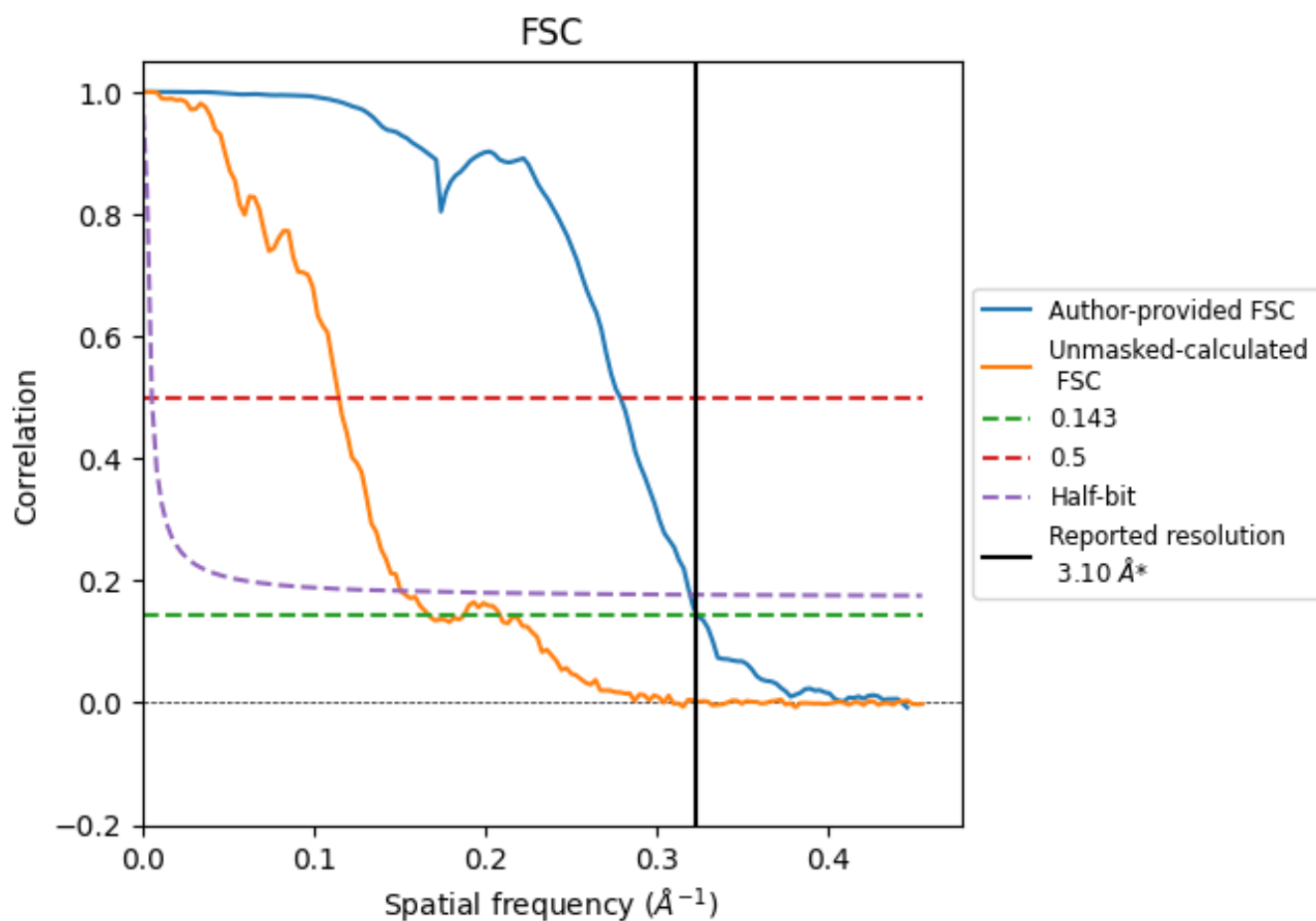


*Reported resolution corresponds to spatial frequency of 0.323 Å⁻¹

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 0.323 Å⁻¹

8.2 Resolution estimates [i](#)

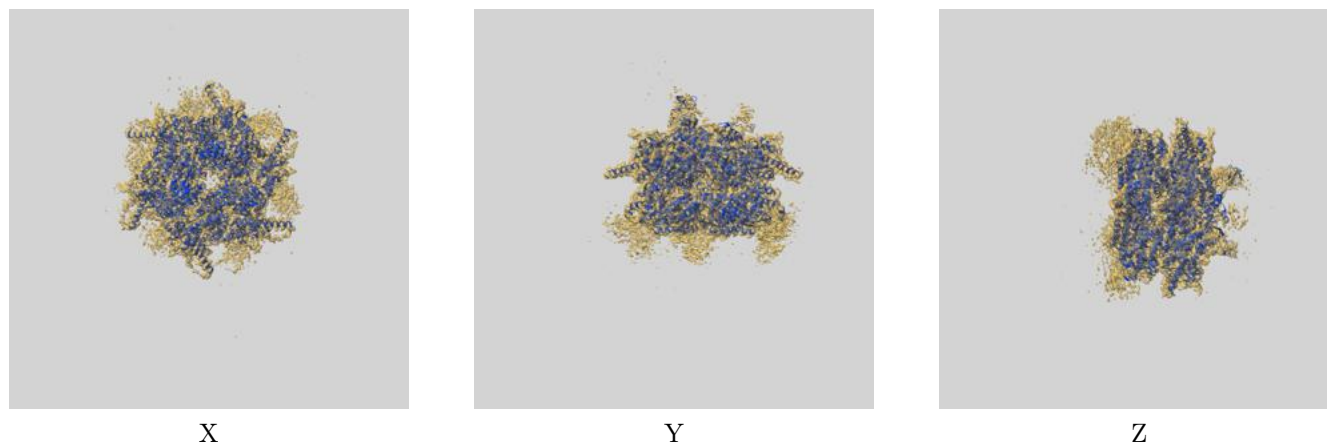
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.10	-	-
Author-provided FSC curve	3.09	3.59	3.13
Unmasked-calculated*	5.99	8.73	6.64

*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 5.99 differs from the reported value 3.1 by more than 10 %

9 Map-model fit [i](#)

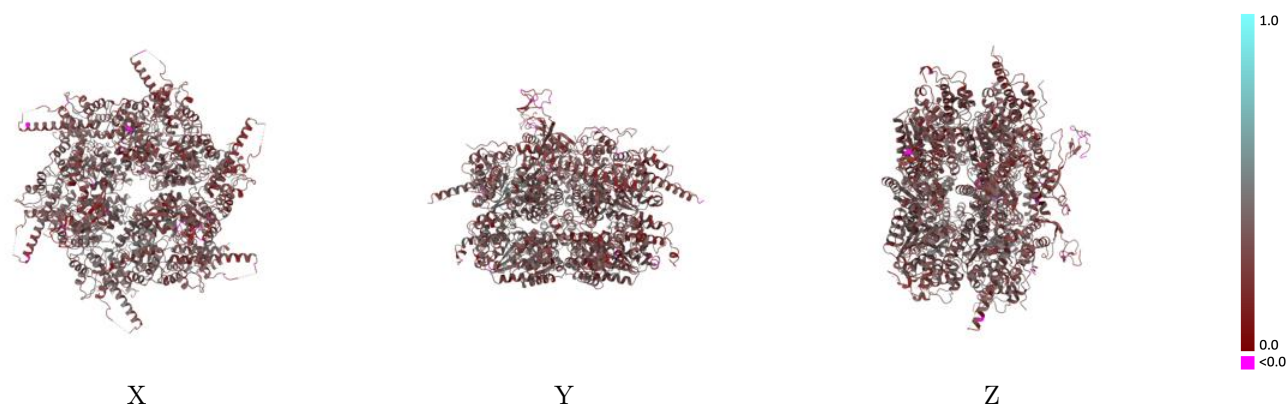
This section contains information regarding the fit between EMDB map EMD-48506 and PDB model 9MPV. Per-residue inclusion information can be found in [section 3](#) on [page 11](#).

9.1 Map-model overlay [i](#)



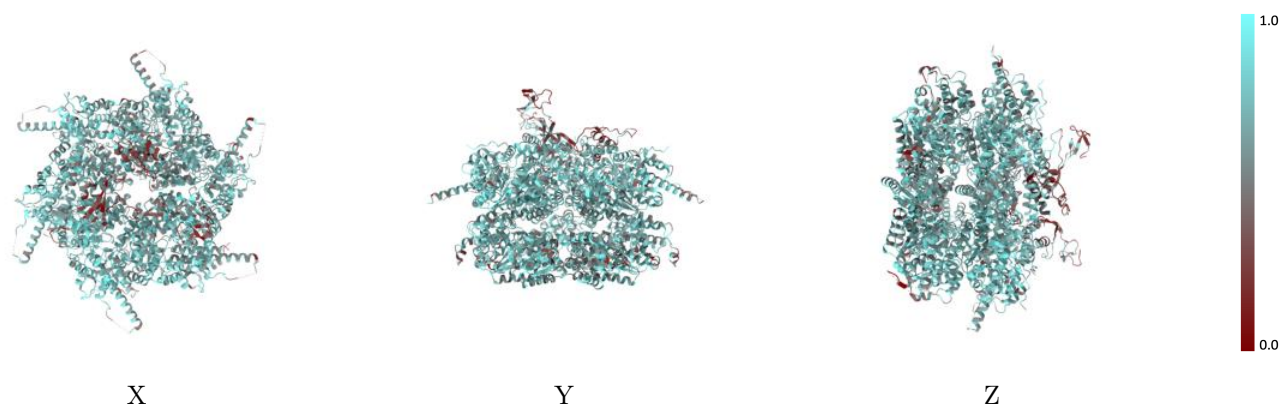
The images above show the 3D surface view of the map at the recommended contour level 0.0906 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



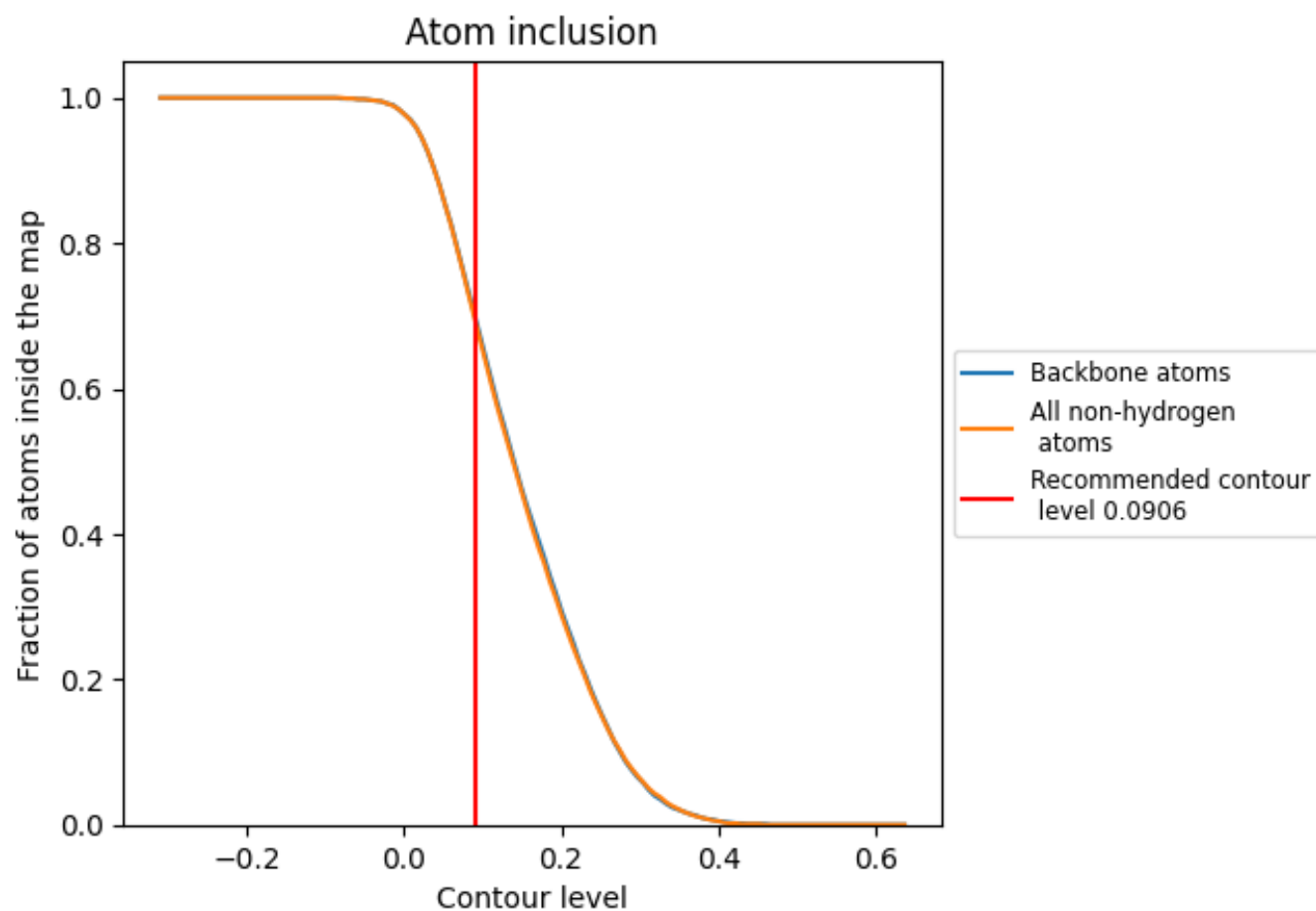
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0906).

9.4 Atom inclusion [i](#)



At the recommended contour level, 70% of all backbone atoms, 69% 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 (0.0906) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6940	0.3280
A	0.7240	0.3410
B	0.7140	0.3140
C	0.6960	0.3050
D	0.7180	0.3220
E	0.7320	0.3540
F	0.7590	0.3660
G	0.4850	0.2530
H	0.3320	0.2600
I	0.5440	0.2410

1.0

0.0

<0.0