



Full wwPDB EM Validation Report ⓘ

Sep 15, 2026 – 07:34 pm BST

PDB ID : 9SM8 / pdb_00009sm8
EMDB ID : EMD-55028
Title : Zuzalysin zymogen pentamer E439A
Authors : Rodriguez-Banqueri, A.; Madej, M.; Eckhard, U.; Potempa, J.; Gomis Ruth, F.X.
Deposited on : 2025-09-05
Resolution : 3.59 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:

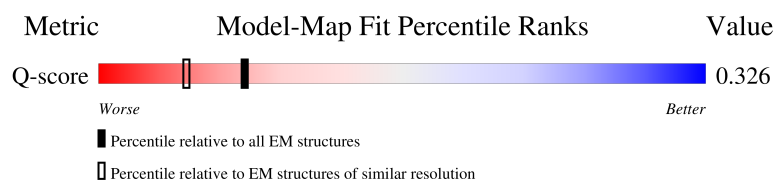
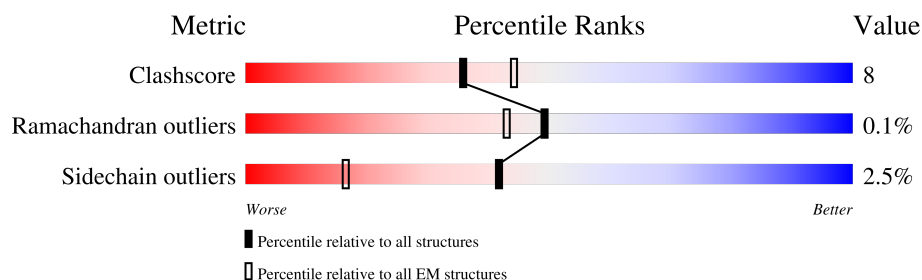
EMDB validation analysis : 0.0.1.dev133
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDb archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

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 3.59 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	12565 (3.09 - 4.09)

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	852	
1	B	852	
1	C	852	
1	D	852	

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Mol	Chain	Length	Quality of chain
1	E	852	74% 20%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 32820 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 Zinc-dependent metalloprotease.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	818	Total	C	N	O	S	0	0
			6562	4166	1139	1226	31		
1	B	818	Total	C	N	O	S	0	0
			6562	4166	1139	1226	31		
1	C	818	Total	C	N	O	S	0	0
			6562	4166	1139	1226	31		
1	D	818	Total	C	N	O	S	0	0
			6562	4166	1139	1226	31		
1	E	818	Total	C	N	O	S	0	0
			6562	4166	1139	1226	31		

There are 115 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	14	MET	-	initiating methionine	UNP A0AAF0BD41
A	15	ALA	-	expression tag	UNP A0AAF0BD41
A	16	SER	-	expression tag	UNP A0AAF0BD41
A	17	MET	-	expression tag	UNP A0AAF0BD41
A	18	THR	-	expression tag	UNP A0AAF0BD41
A	19	GLY	-	expression tag	UNP A0AAF0BD41
A	20	GLY	-	expression tag	UNP A0AAF0BD41
A	21	GLN	-	expression tag	UNP A0AAF0BD41
A	22	MET	-	expression tag	UNP A0AAF0BD41
A	23	GLY	-	expression tag	UNP A0AAF0BD41
A	197	MET	VAL	conflict	UNP A0AAF0BD41
A	298	PRO	LEU	conflict	UNP A0AAF0BD41
A	306	VAL	ILE	conflict	UNP A0AAF0BD41
A	439	ALA	GLU	conflict	UNP A0AAF0BD41
A	751	HIS	TYR	conflict	UNP A0AAF0BD41
A	774	HIS	TYR	conflict	UNP A0AAF0BD41
A	805	ALA	SER	conflict	UNP A0AAF0BD41
A	901	HIS	-	expression tag	UNP A0AAF0BD41
A	902	HIS	-	expression tag	UNP A0AAF0BD41
A	903	HIS	-	expression tag	UNP A0AAF0BD41

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Chain	Residue	Modelled	Actual	Comment	Reference
A	904	HIS	-	expression tag	UNP A0AAF0BD41
A	905	HIS	-	expression tag	UNP A0AAF0BD41
A	906	HIS	-	expression tag	UNP A0AAF0BD41
B	14	MET	-	initiating methionine	UNP A0AAF0BD41
B	15	ALA	-	expression tag	UNP A0AAF0BD41
B	16	SER	-	expression tag	UNP A0AAF0BD41
B	17	MET	-	expression tag	UNP A0AAF0BD41
B	18	THR	-	expression tag	UNP A0AAF0BD41
B	19	GLY	-	expression tag	UNP A0AAF0BD41
B	20	GLY	-	expression tag	UNP A0AAF0BD41
B	21	GLN	-	expression tag	UNP A0AAF0BD41
B	22	MET	-	expression tag	UNP A0AAF0BD41
B	23	GLY	-	expression tag	UNP A0AAF0BD41
B	197	MET	VAL	conflict	UNP A0AAF0BD41
B	298	PRO	LEU	conflict	UNP A0AAF0BD41
B	306	VAL	ILE	conflict	UNP A0AAF0BD41
B	439	ALA	GLU	conflict	UNP A0AAF0BD41
B	751	HIS	TYR	conflict	UNP A0AAF0BD41
B	774	HIS	TYR	conflict	UNP A0AAF0BD41
B	805	ALA	SER	conflict	UNP A0AAF0BD41
B	901	HIS	-	expression tag	UNP A0AAF0BD41
B	902	HIS	-	expression tag	UNP A0AAF0BD41
B	903	HIS	-	expression tag	UNP A0AAF0BD41
B	904	HIS	-	expression tag	UNP A0AAF0BD41
B	905	HIS	-	expression tag	UNP A0AAF0BD41
B	906	HIS	-	expression tag	UNP A0AAF0BD41
C	14	MET	-	initiating methionine	UNP A0AAF0BD41
C	15	ALA	-	expression tag	UNP A0AAF0BD41
C	16	SER	-	expression tag	UNP A0AAF0BD41
C	17	MET	-	expression tag	UNP A0AAF0BD41
C	18	THR	-	expression tag	UNP A0AAF0BD41
C	19	GLY	-	expression tag	UNP A0AAF0BD41
C	20	GLY	-	expression tag	UNP A0AAF0BD41
C	21	GLN	-	expression tag	UNP A0AAF0BD41
C	22	MET	-	expression tag	UNP A0AAF0BD41
C	23	GLY	-	expression tag	UNP A0AAF0BD41
C	197	MET	VAL	conflict	UNP A0AAF0BD41
C	298	PRO	LEU	conflict	UNP A0AAF0BD41
C	306	VAL	ILE	conflict	UNP A0AAF0BD41
C	439	ALA	GLU	conflict	UNP A0AAF0BD41
C	751	HIS	TYR	conflict	UNP A0AAF0BD41
C	774	HIS	TYR	conflict	UNP A0AAF0BD41

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Chain	Residue	Modelled	Actual	Comment	Reference
C	805	ALA	SER	conflict	UNP A0AAF0BD41
C	901	HIS	-	expression tag	UNP A0AAF0BD41
C	902	HIS	-	expression tag	UNP A0AAF0BD41
C	903	HIS	-	expression tag	UNP A0AAF0BD41
C	904	HIS	-	expression tag	UNP A0AAF0BD41
C	905	HIS	-	expression tag	UNP A0AAF0BD41
C	906	HIS	-	expression tag	UNP A0AAF0BD41
D	14	MET	-	initiating methionine	UNP A0AAF0BD41
D	15	ALA	-	expression tag	UNP A0AAF0BD41
D	16	SER	-	expression tag	UNP A0AAF0BD41
D	17	MET	-	expression tag	UNP A0AAF0BD41
D	18	THR	-	expression tag	UNP A0AAF0BD41
D	19	GLY	-	expression tag	UNP A0AAF0BD41
D	20	GLY	-	expression tag	UNP A0AAF0BD41
D	21	GLN	-	expression tag	UNP A0AAF0BD41
D	22	MET	-	expression tag	UNP A0AAF0BD41
D	23	GLY	-	expression tag	UNP A0AAF0BD41
D	197	MET	VAL	conflict	UNP A0AAF0BD41
D	298	PRO	LEU	conflict	UNP A0AAF0BD41
D	306	VAL	ILE	conflict	UNP A0AAF0BD41
D	439	ALA	GLU	conflict	UNP A0AAF0BD41
D	751	HIS	TYR	conflict	UNP A0AAF0BD41
D	774	HIS	TYR	conflict	UNP A0AAF0BD41
D	805	ALA	SER	conflict	UNP A0AAF0BD41
D	901	HIS	-	expression tag	UNP A0AAF0BD41
D	902	HIS	-	expression tag	UNP A0AAF0BD41
D	903	HIS	-	expression tag	UNP A0AAF0BD41
D	904	HIS	-	expression tag	UNP A0AAF0BD41
D	905	HIS	-	expression tag	UNP A0AAF0BD41
D	906	HIS	-	expression tag	UNP A0AAF0BD41
E	14	MET	-	initiating methionine	UNP A0AAF0BD41
E	15	ALA	-	expression tag	UNP A0AAF0BD41
E	16	SER	-	expression tag	UNP A0AAF0BD41
E	17	MET	-	expression tag	UNP A0AAF0BD41
E	18	THR	-	expression tag	UNP A0AAF0BD41
E	19	GLY	-	expression tag	UNP A0AAF0BD41
E	20	GLY	-	expression tag	UNP A0AAF0BD41
E	21	GLN	-	expression tag	UNP A0AAF0BD41
E	22	MET	-	expression tag	UNP A0AAF0BD41
E	23	GLY	-	expression tag	UNP A0AAF0BD41
E	197	MET	VAL	conflict	UNP A0AAF0BD41
E	298	PRO	LEU	conflict	UNP A0AAF0BD41

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Chain	Residue	Modelled	Actual	Comment	Reference
E	306	VAL	ILE	conflict	UNP A0AAF0BD41
E	439	ALA	GLU	conflict	UNP A0AAF0BD41
E	751	HIS	TYR	conflict	UNP A0AAF0BD41
E	774	HIS	TYR	conflict	UNP A0AAF0BD41
E	805	ALA	SER	conflict	UNP A0AAF0BD41
E	901	HIS	-	expression tag	UNP A0AAF0BD41
E	902	HIS	-	expression tag	UNP A0AAF0BD41
E	903	HIS	-	expression tag	UNP A0AAF0BD41
E	904	HIS	-	expression tag	UNP A0AAF0BD41
E	905	HIS	-	expression tag	UNP A0AAF0BD41
E	906	HIS	-	expression tag	UNP A0AAF0BD41

- Molecule 2 is CALCIUM ION (CCD ID: CA) (formula: Ca) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	AltConf
2	A	1	Total Ca 1 1	0
2	B	1	Total Ca 1 1	0
2	C	1	Total Ca 1 1	0
2	D	1	Total Ca 1 1	0
2	E	1	Total Ca 1 1	0

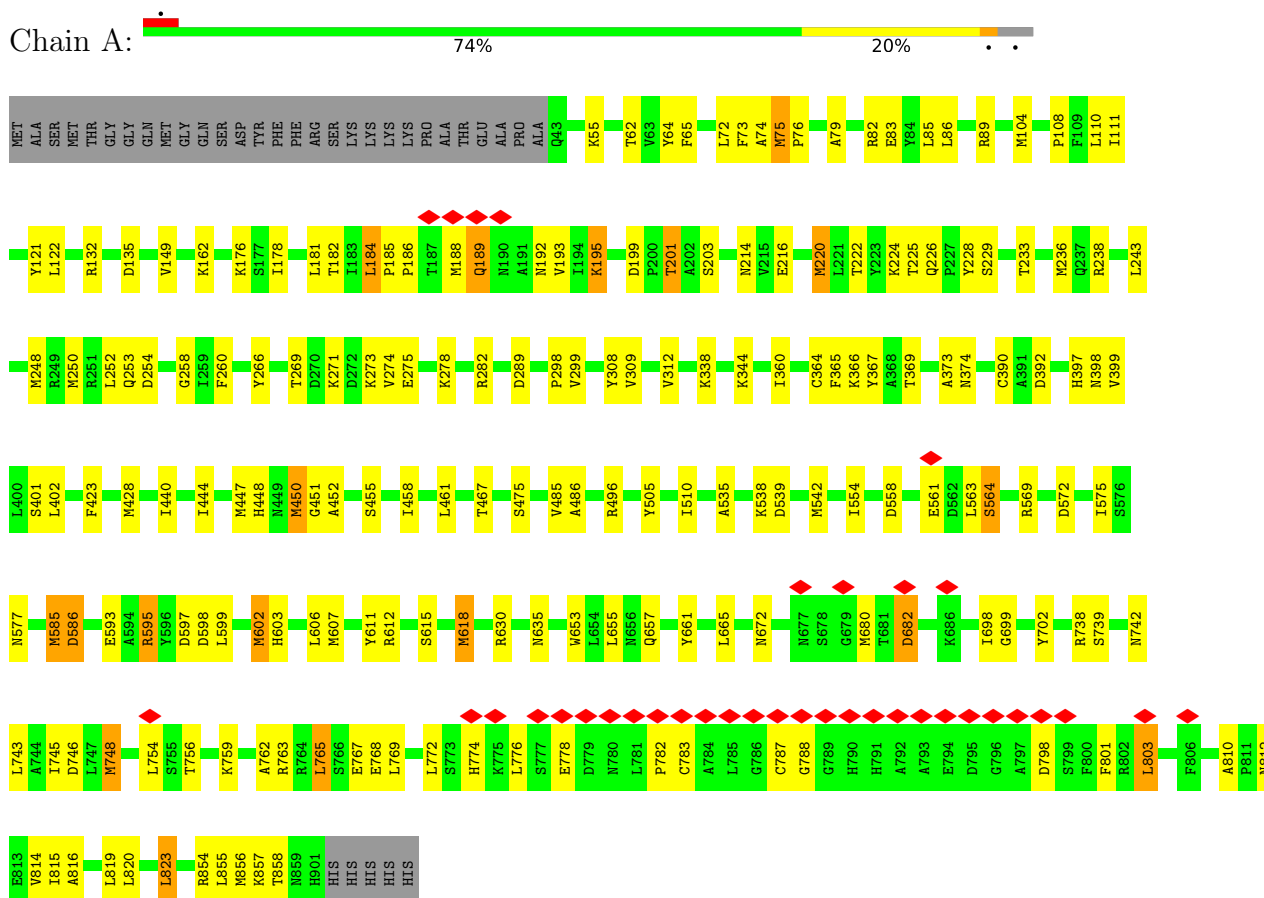
- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

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

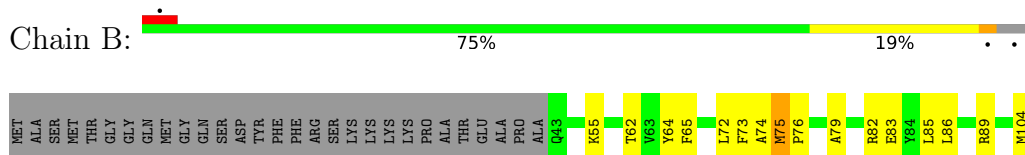
3 Residue-property plots

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

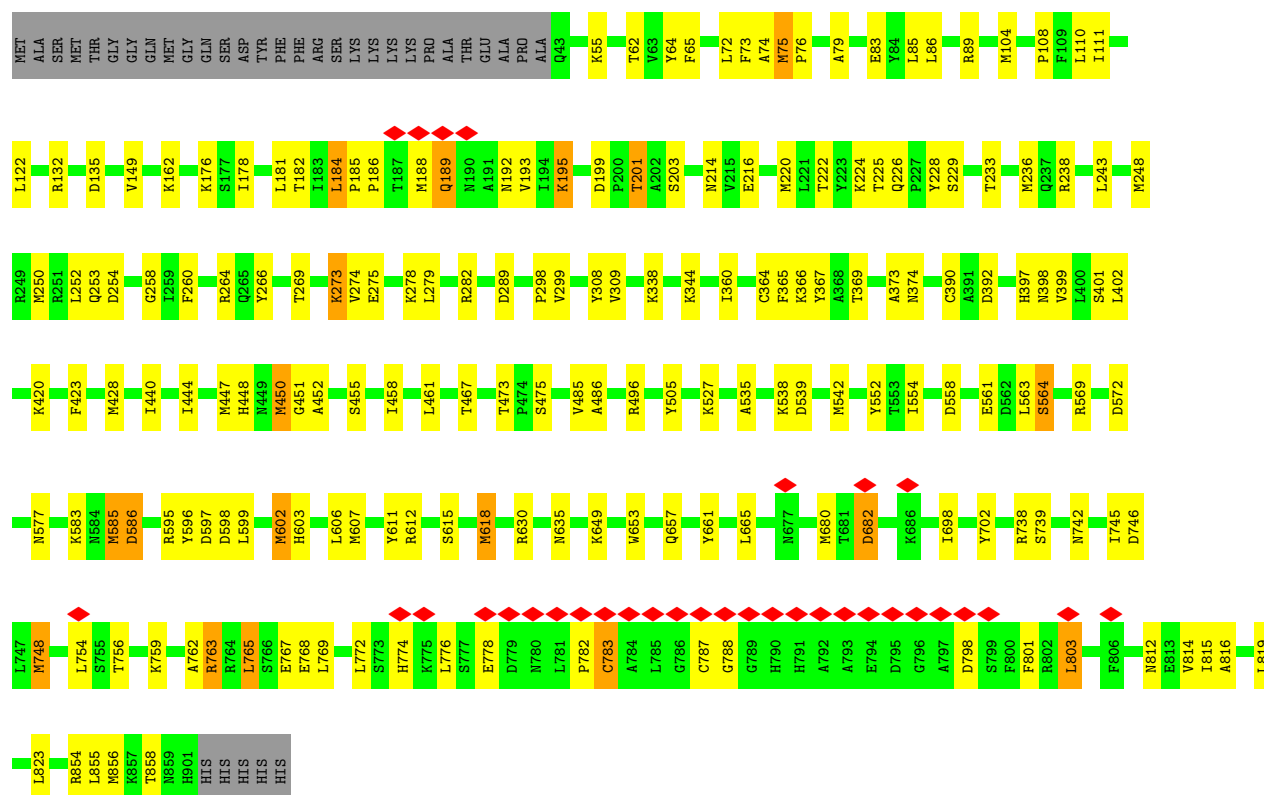
• Molecule 1: Zinc-dependent metalloprotease



• Molecule 1: Zinc-dependent metalloprotease

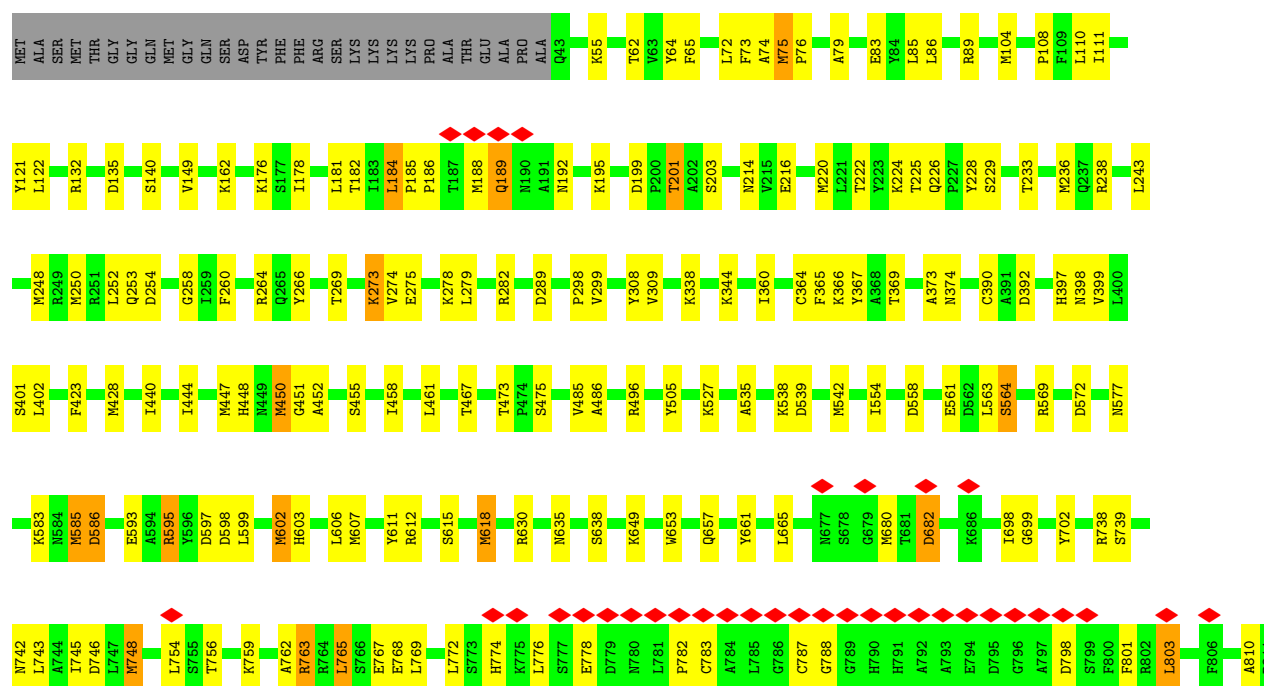


Chain D:  74% 20%



• Molecule 1: Zinc-dependent metalloprotease

Chain E:  74% 20%



V812	E813	V814	I815	A816	L819	L823	R854	L855	M856	K857	T858	N859	H901	HIS	HIS	HIS	HIS	HIS
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4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	212348	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS GLACIOS	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	38.58	Depositor
Minimum defocus (nm)	1700	Depositor
Maximum defocus (nm)	2700	Depositor
Magnification	Not provided	
Image detector	TFS FALCON 4i (4k x 4k)	Depositor
Maximum map value	0.204	Depositor
Minimum map value	-0.037	Depositor
Average map value	0.011	Depositor
Map value standard deviation	0.025	Depositor
Recommended contour level	0.062	Depositor
Map size (Å)	186.0, 186.0, 186.0	wwPDB
Map dimensions	200, 200, 200	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.93, 0.93, 0.93	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CA, ZN

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	0.39	0/6717	0.96	36/9094 (0.4%)
1	B	0.39	0/6717	0.96	36/9094 (0.4%)
1	C	0.39	0/6717	0.96	36/9094 (0.4%)
1	D	0.39	0/6717	0.96	36/9094 (0.4%)
1	E	0.39	0/6717	0.96	36/9094 (0.4%)
All	All	0.39	0/33585	0.96	180/45470 (0.4%)

There are no bond length outliers.

All (180) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	189	GLN	CA-CB-CG	9.15	132.39	114.10
1	D	189	GLN	CA-CB-CG	9.15	132.39	114.10
1	B	189	GLN	CA-CB-CG	9.13	132.36	114.10
1	E	189	GLN	CA-CB-CG	9.13	132.36	114.10
1	A	189	GLN	CA-CB-CG	9.12	132.34	114.10
1	B	273	LYS	CA-CB-CG	8.49	131.08	114.10
1	A	273	LYS	CA-CB-CG	8.47	131.04	114.10
1	D	273	LYS	CA-CB-CG	8.46	131.03	114.10
1	C	273	LYS	CA-CB-CG	8.46	131.02	114.10
1	E	273	LYS	CA-CB-CG	8.46	131.01	114.10
1	A	767	GLU	CA-CB-CG	7.44	128.98	114.10
1	E	767	GLU	CA-CB-CG	7.43	128.95	114.10
1	C	767	GLU	CA-CB-CG	7.40	128.89	114.10
1	B	767	GLU	CA-CB-CG	7.39	128.88	114.10
1	D	767	GLU	CA-CB-CG	7.38	128.87	114.10
1	C	273	LYS	CB-CG-CD	7.16	127.77	111.30
1	A	273	LYS	CB-CG-CD	7.16	127.77	111.30
1	E	273	LYS	CB-CG-CD	7.16	127.76	111.30
1	D	273	LYS	CB-CG-CD	7.16	127.76	111.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	273	LYS	CB-CG-CD	7.15	127.73	111.30
1	B	823	LEU	CA-CB-CG	7.02	140.86	116.30
1	C	823	LEU	CA-CB-CG	7.01	140.83	116.30
1	E	823	LEU	CA-CB-CG	7.01	140.82	116.30
1	D	823	LEU	CA-CB-CG	7.00	140.80	116.30
1	A	823	LEU	CA-CB-CG	7.00	140.79	116.30
1	A	768	GLU	CA-CB-CG	6.87	127.84	114.10
1	B	768	GLU	CA-CB-CG	6.87	127.83	114.10
1	E	768	GLU	CA-CB-CG	6.85	127.80	114.10
1	C	768	GLU	CA-CB-CG	6.83	127.77	114.10
1	D	768	GLU	CA-CB-CG	6.82	127.73	114.10
1	B	75	MET	CA-CB-CG	6.64	127.38	114.10
1	D	75	MET	CA-CB-CG	6.62	127.35	114.10
1	A	75	MET	CA-CB-CG	6.62	127.33	114.10
1	E	75	MET	CA-CB-CG	6.61	127.32	114.10
1	C	75	MET	CA-CB-CG	6.60	127.30	114.10
1	C	104	MET	CB-CG-SD	6.40	131.91	112.70
1	D	104	MET	CB-CG-SD	6.40	131.90	112.70
1	A	104	MET	CB-CG-SD	6.39	131.87	112.70
1	B	104	MET	CB-CG-SD	6.39	131.86	112.70
1	E	104	MET	CB-CG-SD	6.38	131.85	112.70
1	B	188	MET	CA-CB-CG	6.19	126.48	114.10
1	A	188	MET	CA-CB-CG	6.19	126.47	114.10
1	E	188	MET	CA-CB-CG	6.18	126.45	114.10
1	D	188	MET	CA-CB-CG	6.17	126.44	114.10
1	C	188	MET	CA-CB-CG	6.15	126.41	114.10
1	A	236	MET	CB-CG-SD	6.01	130.72	112.70
1	C	236	MET	CB-CG-SD	6.00	130.70	112.70
1	E	236	MET	CB-CG-SD	5.99	130.67	112.70
1	D	236	MET	CB-CG-SD	5.99	130.66	112.70
1	B	236	MET	CB-CG-SD	5.98	130.65	112.70
1	D	746	ASP	N-CA-CB	5.96	118.98	110.16
1	A	746	ASP	N-CA-CB	5.94	118.96	110.16
1	B	746	ASP	N-CA-CB	5.94	118.95	110.16
1	B	763	ARG	CA-CB-CG	5.93	125.97	114.10
1	C	554	ILE	N-CA-CB	-5.93	105.69	112.21
1	E	746	ASP	N-CA-CB	5.93	118.93	110.16
1	C	274	VAL	N-CA-C	-5.92	101.89	109.30
1	E	554	ILE	N-CA-CB	-5.92	105.69	112.21
1	E	763	ARG	CA-CB-CG	5.92	125.93	114.10
1	A	763	ARG	CA-CB-CG	5.91	125.92	114.10
1	C	746	ASP	N-CA-CB	5.91	118.90	110.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	274	VAL	N-CA-C	-5.90	101.92	109.30
1	D	274	VAL	N-CA-C	-5.90	101.92	109.30
1	C	763	ARG	CA-CB-CG	5.90	125.90	114.10
1	D	763	ARG	CA-CB-CG	5.90	125.90	114.10
1	E	274	VAL	N-CA-C	-5.90	101.93	109.30
1	A	274	VAL	CA-C-N	-5.89	114.35	122.30
1	A	274	VAL	C-N-CA	-5.89	114.35	122.30
1	E	274	VAL	CA-C-N	-5.88	114.36	122.30
1	E	274	VAL	C-N-CA	-5.88	114.36	122.30
1	A	554	ILE	N-CA-CB	-5.88	105.74	112.21
1	B	274	VAL	N-CA-C	-5.88	101.95	109.30
1	B	554	ILE	N-CA-CB	-5.87	105.75	112.21
1	C	274	VAL	CA-C-N	-5.86	114.39	122.30
1	C	274	VAL	C-N-CA	-5.86	114.39	122.30
1	D	554	ILE	N-CA-CB	-5.85	105.78	112.21
1	B	274	VAL	CA-C-N	-5.84	114.41	122.30
1	B	274	VAL	C-N-CA	-5.84	114.41	122.30
1	D	274	VAL	CA-C-N	-5.82	114.44	122.30
1	D	274	VAL	C-N-CA	-5.82	114.44	122.30
1	A	602	MET	CA-CB-CG	5.72	125.54	114.10
1	B	602	MET	CA-CB-CG	5.71	125.52	114.10
1	D	602	MET	CA-CB-CG	5.71	125.52	114.10
1	C	602	MET	CA-CB-CG	5.70	125.50	114.10
1	E	602	MET	CA-CB-CG	5.70	125.49	114.10
1	D	201	THR	N-CA-C	5.69	117.28	111.14
1	A	585	MET	N-CA-CB	5.69	119.09	110.28
1	B	201	THR	N-CA-C	5.68	117.27	111.14
1	C	585	MET	N-CA-CB	5.68	119.08	110.28
1	B	585	MET	N-CA-CB	5.67	119.08	110.28
1	C	201	THR	N-CA-C	5.67	117.27	111.14
1	E	585	MET	N-CA-CB	5.67	119.07	110.28
1	E	201	THR	N-CA-C	5.67	117.27	111.14
1	D	585	MET	N-CA-CB	5.67	119.07	110.28
1	E	595	ARG	CA-CB-CG	5.64	125.38	114.10
1	C	450	MET	CB-CG-SD	5.64	129.62	112.70
1	A	450	MET	CB-CG-SD	5.64	129.61	112.70
1	D	450	MET	CB-CG-SD	5.64	129.61	112.70
1	A	595	ARG	CA-CB-CG	5.63	125.36	114.10
1	C	595	ARG	CA-CB-CG	5.63	125.36	114.10
1	D	595	ARG	CA-CB-CG	5.63	125.36	114.10
1	A	201	THR	N-CA-C	5.63	117.22	111.14
1	B	450	MET	CB-CG-SD	5.62	129.57	112.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	450	MET	CB-CG-SD	5.62	129.56	112.70
1	B	595	ARG	CA-CB-CG	5.61	125.31	114.10
1	C	618	MET	CA-CB-CG	5.58	125.26	114.10
1	E	618	MET	CA-CB-CG	5.57	125.24	114.10
1	B	618	MET	CA-CB-CG	5.57	125.24	114.10
1	A	618	MET	CA-CB-CG	5.56	125.22	114.10
1	D	618	MET	CA-CB-CG	5.55	125.20	114.10
1	B	184	LEU	CA-CB-CG	5.46	135.41	116.30
1	D	184	LEU	CA-CB-CG	5.46	135.39	116.30
1	A	195	LYS	CB-CG-CD	5.45	123.84	111.30
1	C	184	LEU	CA-CB-CG	5.45	135.38	116.30
1	A	184	LEU	CA-CB-CG	5.45	135.38	116.30
1	E	184	LEU	CA-CB-CG	5.45	135.36	116.30
1	D	195	LYS	CB-CG-CD	5.44	123.81	111.30
1	C	195	LYS	CB-CG-CD	5.43	123.79	111.30
1	B	195	LYS	CB-CG-CD	5.42	123.78	111.30
1	D	226	GLN	CA-CB-CG	5.42	124.94	114.10
1	E	195	LYS	CB-CG-CD	5.42	123.77	111.30
1	B	226	GLN	CA-CB-CG	5.42	124.94	114.10
1	E	226	GLN	CA-CB-CG	5.40	124.90	114.10
1	C	226	GLN	CA-CB-CG	5.40	124.89	114.10
1	A	226	GLN	CA-CB-CG	5.39	124.89	114.10
1	B	801	PHE	N-CA-CB	-5.35	101.93	111.08
1	C	801	PHE	N-CA-CB	-5.34	101.95	111.08
1	E	801	PHE	N-CA-CB	-5.34	101.95	111.08
1	A	801	PHE	N-CA-CB	-5.33	101.96	111.08
1	D	801	PHE	N-CA-CB	-5.33	101.96	111.08
1	D	192	ASN	CA-CB-CG	5.33	117.93	112.60
1	E	192	ASN	CA-CB-CG	5.31	117.91	112.60
1	B	192	ASN	CA-CB-CG	5.29	117.89	112.60
1	C	192	ASN	CA-CB-CG	5.29	117.89	112.60
1	A	192	ASN	CA-CB-CG	5.28	117.88	112.60
1	A	585	MET	CA-CB-CG	5.28	124.65	114.10
1	B	680	MET	CB-CG-SD	5.27	128.50	112.70
1	B	585	MET	CA-CB-CG	5.26	124.63	114.10
1	C	680	MET	CB-CG-SD	5.26	128.49	112.70
1	E	680	MET	CB-CG-SD	5.26	128.49	112.70
1	D	680	MET	CB-CG-SD	5.26	128.48	112.70
1	D	585	MET	CA-CB-CG	5.26	124.62	114.10
1	E	585	MET	CA-CB-CG	5.26	124.62	114.10
1	A	680	MET	CB-CG-SD	5.26	128.47	112.70
1	C	585	MET	CA-CB-CG	5.24	124.58	114.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	192	ASN	CB-CA-C	5.24	119.45	110.81
1	D	192	ASN	CB-CA-C	5.23	119.43	110.81
1	B	192	ASN	CB-CA-C	5.22	119.42	110.81
1	C	192	ASN	CB-CA-C	5.21	119.41	110.81
1	B	195	LYS	CA-CB-CG	5.21	124.51	114.10
1	D	195	LYS	CA-CB-CG	5.21	124.51	114.10
1	E	192	ASN	CB-CA-C	5.20	119.39	110.81
1	E	195	LYS	CA-CB-CG	5.20	124.50	114.10
1	C	195	LYS	CA-CB-CG	5.19	124.49	114.10
1	C	776	LEU	CA-CB-CG	5.19	134.47	116.30
1	C	104	MET	CA-CB-CG	-5.19	103.72	114.10
1	A	104	MET	CA-CB-CG	-5.19	103.72	114.10
1	A	189	GLN	CB-CA-C	-5.19	99.46	110.31
1	E	776	LEU	CA-CB-CG	5.19	134.46	116.30
1	A	776	LEU	CA-CB-CG	5.19	134.45	116.30
1	B	104	MET	CA-CB-CG	-5.18	103.73	114.10
1	B	189	GLN	CB-CA-C	-5.18	99.48	110.31
1	E	104	MET	CA-CB-CG	-5.18	103.73	114.10
1	E	189	GLN	CB-CA-C	-5.18	99.49	110.31
1	B	776	LEU	CA-CB-CG	5.17	134.41	116.30
1	D	104	MET	CA-CB-CG	-5.17	103.75	114.10
1	D	776	LEU	CA-CB-CG	5.17	134.41	116.30
1	A	195	LYS	CA-CB-CG	5.17	124.44	114.10
1	D	189	GLN	CB-CA-C	-5.13	99.50	110.32
1	C	189	GLN	CB-CA-C	-5.12	99.52	110.32
1	A	765	LEU	CA-CB-CG	5.06	134.00	116.30
1	D	765	LEU	CA-CB-CG	5.05	133.99	116.30
1	C	765	LEU	CA-CB-CG	5.05	133.97	116.30
1	E	765	LEU	CA-CB-CG	5.04	133.94	116.30
1	B	765	LEU	CA-CB-CG	5.04	133.92	116.30
1	B	748	MET	CA-CB-CG	5.03	124.16	114.10
1	C	748	MET	CA-CB-CG	5.03	124.15	114.10
1	D	748	MET	CA-CB-CG	5.02	124.14	114.10
1	A	748	MET	CA-CB-CG	5.02	124.14	114.10
1	E	748	MET	CA-CB-CG	5.02	124.14	114.10

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	6562	0	6480	110	0
1	B	6562	0	6480	101	0
1	C	6562	0	6480	113	0
1	D	6562	0	6480	105	0
1	E	6562	0	6480	111	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
All	All	32820	0	32400	506	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

All (506) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:774:HIS:O	1:A:778:GLU:HB2	1.76	0.86
1:C:774:HIS:O	1:C:778:GLU:HB2	1.76	0.85
1:D:774:HIS:O	1:D:778:GLU:HB2	1.76	0.85
1:E:774:HIS:O	1:E:778:GLU:HB2	1.76	0.84
1:B:774:HIS:O	1:B:778:GLU:HB2	1.76	0.84
1:A:854:ARG:NH2	1:E:856:MET:O	2.15	0.80
1:A:233:THR:HG21	1:E:149:VAL:H	1.50	0.76
1:B:856:MET:O	1:C:854:ARG:NH2	2.21	0.73
1:A:184:LEU:HD11	1:A:189:GLN:HA	1.71	0.72
1:C:86:LEU:O	1:C:108:PRO:HA	1.89	0.72
1:B:86:LEU:O	1:B:108:PRO:HA	1.89	0.72
1:D:86:LEU:O	1:D:108:PRO:HA	1.89	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:86:LEU:O	1:E:108:PRO:HA	1.89	0.72
1:A:86:LEU:O	1:A:108:PRO:HA	1.89	0.71
1:C:184:LEU:HD11	1:C:189:GLN:HA	1.71	0.71
1:D:184:LEU:HD11	1:D:189:GLN:HA	1.71	0.70
1:E:184:LEU:HD11	1:E:189:GLN:HA	1.71	0.70
1:B:184:LEU:HD11	1:B:189:GLN:HA	1.71	0.70
1:E:83:GLU:HB3	1:E:110:LEU:HD11	1.75	0.69
1:B:83:GLU:HB3	1:B:110:LEU:HD11	1.75	0.69
1:A:83:GLU:HB3	1:A:110:LEU:HD11	1.75	0.69
1:B:225:THR:O	1:B:229:SER:HA	1.93	0.69
1:C:856:MET:O	1:D:854:ARG:NH2	2.26	0.68
1:C:149:VAL:H	1:D:233:THR:HG21	1.58	0.68
1:E:225:THR:O	1:E:229:SER:HA	1.93	0.68
1:A:225:THR:O	1:A:229:SER:HA	1.94	0.68
1:B:561:GLU:HG3	1:B:612:ARG:HD3	1.76	0.68
1:D:561:GLU:HG3	1:D:612:ARG:HD3	1.76	0.68
1:C:83:GLU:HB3	1:C:110:LEU:HD11	1.75	0.68
1:C:225:THR:O	1:C:229:SER:HA	1.93	0.68
1:D:83:GLU:HB3	1:D:110:LEU:HD11	1.75	0.68
1:B:62:THR:HB	1:B:74:ALA:HB3	1.76	0.67
1:A:62:THR:HB	1:A:74:ALA:HB3	1.76	0.67
1:E:561:GLU:HG3	1:E:612:ARG:HD3	1.76	0.67
1:B:224:LYS:HG3	1:B:229:SER:HB3	1.77	0.67
1:D:224:LYS:HG3	1:D:229:SER:HB3	1.77	0.67
1:E:756:THR:HA	1:E:759:LYS:HD2	1.77	0.67
1:C:224:LYS:HG3	1:C:229:SER:HB3	1.77	0.67
1:C:561:GLU:HG3	1:C:612:ARG:HD3	1.76	0.67
1:E:62:THR:HB	1:E:74:ALA:HB3	1.76	0.67
1:E:224:LYS:HG3	1:E:229:SER:HB3	1.77	0.67
1:D:225:THR:O	1:D:229:SER:HA	1.94	0.67
1:A:224:LYS:HG3	1:A:229:SER:HB3	1.77	0.66
1:D:149:VAL:H	1:E:233:THR:HG21	1.59	0.66
1:A:756:THR:HA	1:A:759:LYS:HD2	1.77	0.66
1:C:62:THR:HB	1:C:74:ALA:HB3	1.76	0.66
1:A:561:GLU:HG3	1:A:612:ARG:HD3	1.76	0.66
1:C:756:THR:HA	1:C:759:LYS:HD2	1.77	0.66
1:B:399:VAL:O	1:B:402:LEU:HB3	1.96	0.66
1:A:475:SER:HB2	1:A:505:TYR:HB3	1.78	0.66
1:B:756:THR:HA	1:B:759:LYS:HD2	1.77	0.66
1:A:149:VAL:H	1:B:233:THR:HG21	1.60	0.66
1:C:399:VAL:O	1:C:402:LEU:HB3	1.96	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:228:TYR:HE2	1:E:185:PRO:HG3	1.61	0.66
1:A:399:VAL:O	1:A:402:LEU:HB3	1.96	0.66
1:D:399:VAL:O	1:D:402:LEU:HB3	1.96	0.65
1:D:475:SER:HB2	1:D:505:TYR:HB3	1.78	0.65
1:D:62:THR:HB	1:D:74:ALA:HB3	1.76	0.65
1:E:475:SER:HB2	1:E:505:TYR:HB3	1.78	0.65
1:B:64:TYR:HB2	1:B:72:LEU:HB2	1.79	0.65
1:A:64:TYR:HB2	1:A:72:LEU:HB2	1.79	0.65
1:B:475:SER:HB2	1:B:505:TYR:HB3	1.78	0.65
1:D:756:THR:HA	1:D:759:LYS:HD2	1.77	0.65
1:C:64:TYR:HB2	1:C:72:LEU:HB2	1.79	0.65
1:E:64:TYR:HB2	1:E:72:LEU:HB2	1.79	0.65
1:A:856:MET:O	1:B:854:ARG:NH2	2.29	0.64
1:B:682:ASP:OD1	1:B:682:ASP:N	2.30	0.64
1:C:254:ASP:OD1	1:C:630:ARG:NH2	2.31	0.64
1:C:475:SER:HB2	1:C:505:TYR:HB3	1.78	0.64
1:D:64:TYR:HB2	1:D:72:LEU:HB2	1.79	0.64
1:E:399:VAL:O	1:E:402:LEU:HB3	1.96	0.64
1:E:682:ASP:OD1	1:E:682:ASP:N	2.30	0.64
1:D:682:ASP:OD1	1:D:682:ASP:N	2.30	0.64
1:A:738:ARG:O	1:A:742:ASN:ND2	2.31	0.64
1:A:254:ASP:OD1	1:A:630:ARG:NH2	2.31	0.63
1:E:738:ARG:O	1:E:742:ASN:ND2	2.31	0.63
1:D:132:ARG:HB3	1:D:135:ASP:HB2	1.81	0.63
1:E:132:ARG:HB3	1:E:135:ASP:HB2	1.80	0.63
1:B:738:ARG:O	1:B:742:ASN:ND2	2.31	0.63
1:C:738:ARG:O	1:C:742:ASN:ND2	2.31	0.63
1:B:250:MET:HE1	1:B:252:LEU:HD23	1.81	0.63
1:C:250:MET:HE1	1:C:252:LEU:HD23	1.81	0.63
1:D:738:ARG:O	1:D:742:ASN:ND2	2.31	0.63
1:C:132:ARG:HB3	1:C:135:ASP:HB2	1.81	0.62
1:E:250:MET:HE1	1:E:252:LEU:HD23	1.81	0.62
1:A:229:SER:HB2	1:E:176:LYS:HE2	1.82	0.62
1:B:149:VAL:H	1:C:233:THR:HG21	1.64	0.62
1:A:132:ARG:HB3	1:A:135:ASP:HB2	1.81	0.62
1:A:250:MET:HE1	1:A:252:LEU:HD23	1.81	0.62
1:E:254:ASP:OD1	1:E:630:ARG:NH2	2.31	0.62
1:B:254:ASP:OD1	1:B:630:ARG:NH2	2.31	0.61
1:B:132:ARG:HB3	1:B:135:ASP:HB2	1.81	0.61
1:C:308:TYR:HA	1:C:344:LYS:O	2.01	0.61
1:D:250:MET:HE1	1:D:252:LEU:HD23	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:308:TYR:HA	1:A:344:LYS:O	2.01	0.61
1:A:682:ASP:OD1	1:A:682:ASP:N	2.30	0.61
1:B:308:TYR:HA	1:B:344:LYS:O	2.01	0.61
1:D:308:TYR:HA	1:D:344:LYS:O	2.01	0.61
1:E:308:TYR:HA	1:E:344:LYS:O	2.01	0.61
1:A:193:VAL:HG22	1:A:195:LYS:HZ2	1.66	0.60
1:D:254:ASP:OD1	1:D:630:ARG:NH2	2.31	0.60
1:B:214:ASN:HD22	1:B:360:ILE:HG22	1.67	0.60
1:C:214:ASN:HD22	1:C:360:ILE:HG22	1.67	0.60
1:D:214:ASN:HD22	1:D:360:ILE:HG22	1.67	0.60
1:E:214:ASN:HD22	1:E:360:ILE:HG22	1.67	0.60
1:D:856:MET:O	1:E:854:ARG:NH2	2.35	0.59
1:A:214:ASN:HD22	1:A:360:ILE:HG22	1.67	0.58
1:A:222:THR:HG22	1:A:233:THR:HG22	1.85	0.58
1:D:193:VAL:HG22	1:D:195:LYS:HZ2	1.67	0.58
1:C:682:ASP:OD1	1:C:682:ASP:N	2.30	0.58
1:E:222:THR:HG22	1:E:233:THR:HG22	1.85	0.58
1:B:222:THR:HG22	1:B:233:THR:HG22	1.85	0.58
1:D:73:PHE:HB3	1:D:75:MET:HE3	1.87	0.57
1:A:199:ASP:OD1	1:A:222:THR:OG1	2.22	0.57
1:B:631:GLN:HG2	1:C:596:TYR:CZ	2.39	0.57
1:C:73:PHE:HB3	1:C:75:MET:HE3	1.87	0.57
1:A:73:PHE:HB3	1:A:75:MET:HE3	1.87	0.57
1:B:73:PHE:HB3	1:B:75:MET:HE3	1.87	0.57
1:D:222:THR:HG22	1:D:233:THR:HG22	1.85	0.57
1:C:222:THR:HG22	1:C:233:THR:HG22	1.85	0.57
1:E:73:PHE:HB3	1:E:75:MET:HE3	1.87	0.56
1:C:193:VAL:HG22	1:C:195:LYS:HZ2	1.69	0.56
1:B:199:ASP:OD1	1:B:222:THR:OG1	2.22	0.56
1:A:452:ALA:O	1:A:455:SER:OG	2.24	0.55
1:D:185:PRO:HG3	1:E:228:TYR:HE2	1.71	0.55
1:D:452:ALA:O	1:D:455:SER:OG	2.24	0.55
1:A:367:TYR:OH	1:A:397:HIS:ND1	2.36	0.55
1:D:458:ILE:HG21	1:D:569:ARG:HE	1.72	0.54
1:E:748:MET:HG2	1:E:819:LEU:HD22	1.90	0.54
1:C:199:ASP:OD1	1:C:222:THR:OG1	2.22	0.54
1:C:225:THR:O	1:C:229:SER:CA	2.56	0.54
1:C:458:ILE:HG21	1:C:569:ARG:HE	1.73	0.54
1:A:458:ILE:HG21	1:A:569:ARG:HE	1.73	0.54
1:A:593:GLU:O	1:E:527:LYS:NZ	2.41	0.54
1:A:748:MET:HG2	1:A:819:LEU:HD22	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:748:MET:HG2	1:C:819:LEU:HD22	1.90	0.54
1:D:199:ASP:OD1	1:D:222:THR:OG1	2.22	0.54
1:D:748:MET:HG2	1:D:819:LEU:HD22	1.90	0.54
1:B:458:ILE:HG21	1:B:569:ARG:HE	1.72	0.53
1:E:398:ASN:O	1:E:401:SER:OG	2.26	0.53
1:C:798:ASP:HB3	1:C:803:LEU:HD11	1.91	0.53
1:B:748:MET:HG2	1:B:819:LEU:HD22	1.90	0.53
1:D:798:ASP:HB3	1:D:803:LEU:HD11	1.91	0.53
1:A:185:PRO:HG3	1:B:228:TYR:HE2	1.73	0.53
1:C:452:ALA:O	1:C:455:SER:OG	2.24	0.53
1:E:458:ILE:HG21	1:E:569:ARG:HE	1.72	0.53
1:A:203:SER:HA	1:A:220:MET:O	2.09	0.53
1:B:798:ASP:HB3	1:B:803:LEU:HD11	1.91	0.53
1:C:76:PRO:HD2	1:C:79:ALA:HB2	1.91	0.53
1:C:203:SER:HA	1:C:220:MET:O	2.09	0.53
1:C:423:PHE:HB2	1:C:428:MET:HE2	1.91	0.53
1:E:423:PHE:HB2	1:E:428:MET:HE2	1.91	0.53
1:E:798:ASP:HB3	1:E:803:LEU:HD11	1.91	0.53
1:B:225:THR:O	1:B:229:SER:CA	2.56	0.53
1:D:225:THR:O	1:D:229:SER:CA	2.56	0.53
1:D:203:SER:HA	1:D:220:MET:O	2.09	0.52
1:E:225:THR:O	1:E:229:SER:CA	2.56	0.52
1:E:452:ALA:O	1:E:455:SER:OG	2.24	0.52
1:A:798:ASP:HB3	1:A:803:LEU:HD11	1.91	0.52
1:B:76:PRO:HD2	1:B:79:ALA:HB2	1.91	0.52
1:A:423:PHE:HB2	1:A:428:MET:HE2	1.91	0.52
1:B:203:SER:HA	1:B:220:MET:O	2.09	0.52
1:D:423:PHE:HB2	1:D:428:MET:HE2	1.91	0.52
1:E:203:SER:HA	1:E:220:MET:O	2.09	0.52
1:C:373:ALA:HB1	1:C:402:LEU:HB2	1.92	0.52
1:C:185:PRO:HG3	1:D:228:TYR:HE2	1.73	0.52
1:E:289:ASP:H	1:E:299:VAL:HG11	1.75	0.52
1:E:373:ALA:HB1	1:E:402:LEU:HB2	1.92	0.52
1:C:289:ASP:H	1:C:299:VAL:HG11	1.75	0.52
1:A:186:PRO:HA	1:A:189:GLN:NE2	2.25	0.52
1:A:225:THR:O	1:A:229:SER:CA	2.56	0.52
1:D:266:TYR:HB3	1:D:275:GLU:HB2	1.92	0.52
1:D:76:PRO:HD2	1:D:79:ALA:HB2	1.91	0.51
1:D:186:PRO:HA	1:D:189:GLN:NE2	2.25	0.51
1:C:186:PRO:HA	1:C:189:GLN:NE2	2.26	0.51
1:C:486:ALA:O	1:C:577:ASN:ND2	2.41	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:450:MET:H	1:D:450:MET:HE2	1.76	0.51
1:B:452:ALA:O	1:B:455:SER:OG	2.24	0.51
1:D:289:ASP:H	1:D:299:VAL:HG11	1.75	0.51
1:B:373:ALA:HB1	1:B:402:LEU:HB2	1.92	0.51
1:A:289:ASP:H	1:A:299:VAL:HG11	1.75	0.51
1:B:186:PRO:HA	1:B:189:GLN:NE2	2.25	0.51
1:C:132:ARG:NH2	1:C:135:ASP:OD1	2.44	0.51
1:D:615:SER:HA	1:D:618:MET:HG2	1.93	0.51
1:A:76:PRO:HD2	1:A:79:ALA:HB2	1.91	0.51
1:A:132:ARG:NH2	1:A:135:ASP:OD1	2.44	0.51
1:B:289:ASP:H	1:B:299:VAL:HG11	1.75	0.51
1:B:423:PHE:HB2	1:B:428:MET:HE2	1.91	0.51
1:C:450:MET:HE2	1:C:450:MET:H	1.75	0.51
1:D:486:ALA:O	1:D:577:ASN:ND2	2.41	0.51
1:D:373:ALA:HB1	1:D:402:LEU:HB2	1.92	0.51
1:E:186:PRO:HA	1:E:189:GLN:NE2	2.25	0.51
1:B:132:ARG:NH2	1:B:135:ASP:OD1	2.44	0.51
1:E:199:ASP:OD1	1:E:222:THR:OG1	2.22	0.50
1:A:312:VAL:HG21	1:E:140:SER:HB2	1.93	0.50
1:A:373:ALA:HB1	1:A:402:LEU:HB2	1.92	0.50
1:A:535:ALA:HA	1:A:538:LYS:HG2	1.94	0.50
1:A:615:SER:HA	1:A:618:MET:HG2	1.93	0.50
1:E:76:PRO:HD2	1:E:79:ALA:HB2	1.91	0.50
1:E:367:TYR:OH	1:E:397:HIS:ND1	2.36	0.50
1:B:615:SER:HA	1:B:618:MET:HG2	1.93	0.50
1:E:266:TYR:HB3	1:E:275:GLU:HB2	1.92	0.50
1:E:615:SER:HA	1:E:618:MET:HG2	1.93	0.50
1:A:266:TYR:HB3	1:A:275:GLU:HB2	1.92	0.50
1:D:132:ARG:NH2	1:D:135:ASP:OD1	2.44	0.50
1:D:535:ALA:HA	1:D:538:LYS:HG2	1.94	0.50
1:E:535:ALA:HA	1:E:538:LYS:HG2	1.94	0.50
1:B:266:TYR:HB3	1:B:275:GLU:HB2	1.92	0.50
1:B:535:ALA:HA	1:B:538:LYS:HG2	1.94	0.50
1:C:75:MET:O	1:C:162:LYS:HA	2.12	0.50
1:A:450:MET:HE2	1:A:450:MET:H	1.75	0.49
1:B:450:MET:HE2	1:B:450:MET:H	1.76	0.49
1:C:535:ALA:HA	1:C:538:LYS:HG2	1.94	0.49
1:C:615:SER:HA	1:C:618:MET:HG2	1.93	0.49
1:B:75:MET:O	1:B:162:LYS:HA	2.12	0.49
1:E:132:ARG:NH2	1:E:135:ASP:OD1	2.44	0.49
1:A:599:LEU:HA	1:A:602:MET:HG3	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:266:TYR:HB3	1:C:275:GLU:HB2	1.92	0.49
1:E:599:LEU:HA	1:E:602:MET:HG3	1.95	0.49
1:E:75:MET:O	1:E:162:LYS:HA	2.12	0.49
1:B:598:ASP:OD2	1:B:599:LEU:N	2.46	0.49
1:E:450:MET:HE2	1:E:450:MET:H	1.76	0.49
1:D:598:ASP:OD2	1:D:599:LEU:N	2.46	0.49
1:B:486:ALA:O	1:B:577:ASN:ND2	2.41	0.49
1:D:599:LEU:HA	1:D:602:MET:HG3	1.95	0.49
1:E:55:LYS:HG2	1:E:65:PHE:HB3	1.95	0.49
1:E:598:ASP:OD2	1:E:599:LEU:N	2.46	0.49
1:A:672:ASN:O	1:E:638:SER:OG	2.23	0.49
1:B:812:ASN:O	1:B:816:ALA:HB3	2.13	0.49
1:C:298:PRO:HB2	1:C:338:LYS:HD3	1.95	0.49
1:C:598:ASP:OD2	1:C:599:LEU:N	2.46	0.49
1:D:812:ASN:O	1:D:816:ALA:HB3	2.13	0.49
1:A:75:MET:O	1:A:162:LYS:HA	2.12	0.49
1:A:812:ASN:O	1:A:816:ALA:HB3	2.13	0.49
1:B:298:PRO:HB2	1:B:338:LYS:HD3	1.95	0.49
1:C:812:ASN:O	1:C:816:ALA:HB3	2.13	0.49
1:D:75:MET:O	1:D:162:LYS:HA	2.12	0.49
1:A:586:ASP:OD1	1:A:586:ASP:N	2.38	0.48
1:A:743:LEU:HD12	1:A:743:LEU:HA	1.69	0.48
1:E:812:ASN:O	1:E:816:ALA:HB3	2.13	0.48
1:A:598:ASP:OD2	1:A:599:LEU:N	2.46	0.48
1:B:55:LYS:HG2	1:B:65:PHE:HB3	1.95	0.48
1:C:367:TYR:OH	1:C:397:HIS:ND1	2.36	0.48
1:D:55:LYS:HG2	1:D:65:PHE:HB3	1.95	0.48
1:E:298:PRO:HB2	1:E:338:LYS:HD3	1.95	0.48
1:D:367:TYR:OH	1:D:397:HIS:ND1	2.36	0.48
1:B:599:LEU:HA	1:B:602:MET:HG3	1.95	0.48
1:C:599:LEU:HA	1:C:602:MET:HG3	1.95	0.48
1:E:486:ALA:O	1:E:577:ASN:ND2	2.41	0.48
1:A:298:PRO:HB2	1:A:338:LYS:HD3	1.95	0.48
1:D:762:ALA:HA	1:D:765:LEU:HG	1.96	0.48
1:A:611:TYR:O	1:A:615:SER:N	2.44	0.47
1:A:854:ARG:NH2	1:E:857:LYS:HB3	2.29	0.47
1:B:762:ALA:HA	1:B:765:LEU:HG	1.96	0.47
1:D:611:TYR:O	1:D:615:SER:N	2.44	0.47
1:D:298:PRO:HB2	1:D:338:LYS:HD3	1.95	0.47
1:C:55:LYS:HG2	1:C:65:PHE:HB3	1.95	0.47
1:C:611:TYR:O	1:C:615:SER:N	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:539:ASP:OD1	1:C:539:ASP:N	2.47	0.47
1:E:762:ALA:HA	1:E:765:LEU:HG	1.96	0.47
1:A:55:LYS:HG2	1:A:65:PHE:HB3	1.95	0.47
1:A:787:CYS:SG	1:A:788:GLY:N	2.88	0.47
1:E:597:ASP:OD1	1:E:598:ASP:N	2.48	0.47
1:E:611:TYR:O	1:E:615:SER:N	2.44	0.47
1:E:787:CYS:SG	1:E:788:GLY:N	2.88	0.47
1:B:597:ASP:OD1	1:B:598:ASP:N	2.48	0.47
1:B:485:VAL:HG23	1:B:563:LEU:HD12	1.97	0.47
1:B:586:ASP:OD1	1:B:586:ASP:N	2.38	0.47
1:B:787:CYS:SG	1:B:788:GLY:N	2.88	0.47
1:C:762:ALA:HA	1:C:765:LEU:HG	1.96	0.47
1:D:539:ASP:OD1	1:D:539:ASP:N	2.47	0.47
1:D:787:CYS:SG	1:D:788:GLY:N	2.88	0.47
1:A:597:ASP:OD1	1:A:598:ASP:N	2.48	0.46
1:A:486:ALA:O	1:A:577:ASN:ND2	2.41	0.46
1:C:597:ASP:OD1	1:C:598:ASP:N	2.48	0.46
1:E:539:ASP:N	1:E:539:ASP:OD1	2.47	0.46
1:A:485:VAL:HG23	1:A:563:LEU:HD12	1.97	0.46
1:B:661:TYR:O	1:B:665:LEU:HB2	2.16	0.46
1:C:787:CYS:SG	1:C:788:GLY:N	2.88	0.46
1:B:185:PRO:HG3	1:C:228:TYR:HE2	1.81	0.46
1:A:762:ALA:HA	1:A:765:LEU:HG	1.96	0.46
1:C:572:ASP:OD1	1:C:653:TRP:NE1	2.43	0.46
1:D:597:ASP:OD1	1:D:598:ASP:N	2.48	0.46
1:B:367:TYR:OH	1:B:397:HIS:ND1	2.36	0.46
1:C:485:VAL:HG23	1:C:563:LEU:HD12	1.97	0.46
1:D:485:VAL:HG23	1:D:563:LEU:HD12	1.97	0.46
1:A:661:TYR:O	1:A:665:LEU:HB2	2.16	0.46
1:E:661:TYR:O	1:E:665:LEU:HB2	2.16	0.46
1:A:467:THR:HB	1:A:496:ARG:HB3	1.98	0.46
1:E:485:VAL:HG23	1:E:563:LEU:HD12	1.97	0.46
1:D:467:THR:HB	1:D:496:ARG:HB3	1.98	0.45
1:D:661:TYR:O	1:D:665:LEU:HB2	2.16	0.45
1:E:258:GLY:C	1:E:447:MET:HG2	2.42	0.45
1:A:258:GLY:C	1:A:447:MET:HG2	2.42	0.45
1:B:214:ASN:ND2	1:B:216:GLU:OE2	2.50	0.45
1:B:539:ASP:N	1:B:539:ASP:OD1	2.47	0.45
1:C:214:ASN:ND2	1:C:216:GLU:OE2	2.50	0.45
1:C:260:PHE:CD1	1:C:447:MET:HE1	2.52	0.45
1:E:467:THR:HB	1:E:496:ARG:HB3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:661:TYR:O	1:C:665:LEU:HB2	2.16	0.45
1:D:258:GLY:C	1:D:447:MET:HG2	2.42	0.45
1:C:178:ILE:HD12	1:C:238:ARG:HG2	1.99	0.45
1:C:258:GLY:C	1:C:447:MET:HG2	2.42	0.45
1:C:448:HIS:HB3	1:C:450:MET:SD	2.57	0.45
1:B:467:THR:HB	1:B:496:ARG:HB3	1.99	0.45
1:D:178:ILE:HD12	1:D:238:ARG:HG2	1.99	0.45
1:A:448:HIS:HB3	1:A:450:MET:SD	2.57	0.45
1:C:176:LYS:HE2	1:D:229:SER:HB2	1.99	0.45
1:C:467:THR:HB	1:C:496:ARG:HB3	1.98	0.45
1:E:178:ILE:HD12	1:E:238:ARG:HG2	1.99	0.45
1:E:260:PHE:CD1	1:E:447:MET:HE1	2.52	0.45
1:E:448:HIS:HB3	1:E:450:MET:SD	2.57	0.45
1:E:698:ILE:HG21	1:E:815:ILE:HD13	1.98	0.45
1:B:258:GLY:C	1:B:447:MET:HG2	2.42	0.45
1:D:248:MET:HE1	1:D:282:ARG:HE	1.82	0.45
1:A:82:ARG:NH2	1:A:243:LEU:O	2.37	0.45
1:A:214:ASN:ND2	1:A:216:GLU:OE2	2.50	0.45
1:A:260:PHE:CD1	1:A:447:MET:HE1	2.52	0.45
1:C:631:GLN:HG2	1:D:596:TYR:CZ	2.52	0.45
1:D:448:HIS:HB3	1:D:450:MET:SD	2.57	0.45
1:E:248:MET:HE1	1:E:282:ARG:HE	1.82	0.45
1:B:448:HIS:HB3	1:B:450:MET:SD	2.57	0.44
1:A:539:ASP:OD1	1:A:539:ASP:N	2.47	0.44
1:B:698:ILE:HG21	1:B:815:ILE:HD13	1.98	0.44
1:D:473:THR:OG1	1:D:475:SER:O	2.34	0.44
1:B:260:PHE:CD1	1:B:447:MET:HE1	2.52	0.44
1:B:373:ALA:HB2	1:B:398:ASN:HB3	2.00	0.44
1:C:373:ALA:HB2	1:C:398:ASN:HB3	2.00	0.44
1:C:698:ILE:HG21	1:C:815:ILE:HD13	1.98	0.44
1:D:649:LYS:HA	1:D:649:LYS:HD3	1.80	0.44
1:D:698:ILE:HG21	1:D:815:ILE:HD13	1.99	0.44
1:C:369:THR:HA	1:C:397:HIS:HB2	2.00	0.44
1:D:260:PHE:CD1	1:D:447:MET:HE1	2.52	0.44
1:E:473:THR:OG1	1:E:475:SER:O	2.34	0.44
1:B:178:ILE:HD12	1:B:238:ARG:HG2	1.99	0.44
1:E:214:ASN:ND2	1:E:216:GLU:OE2	2.50	0.44
1:A:698:ILE:HG21	1:A:815:ILE:HD13	1.98	0.44
1:D:214:ASN:ND2	1:D:216:GLU:OE2	2.50	0.44
1:A:373:ALA:HB2	1:A:398:ASN:HB3	2.00	0.44
1:A:657:GLN:O	1:A:661:TYR:HB3	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:248:MET:HE1	1:C:282:ARG:HE	1.82	0.44
1:D:369:THR:HA	1:D:397:HIS:HB2	2.00	0.44
1:D:373:ALA:HB2	1:D:398:ASN:HB3	2.00	0.44
1:D:273:LYS:HE3	1:E:401:SER:HB2	2.00	0.44
1:E:743:LEU:HD12	1:E:743:LEU:HA	1.69	0.44
1:B:82:ARG:NH2	1:B:243:LEU:O	2.37	0.43
1:E:702:TYR:CD1	1:E:814:VAL:HG11	2.53	0.43
1:A:178:ILE:HD12	1:A:238:ARG:HG2	1.99	0.43
1:A:248:MET:HE1	1:A:282:ARG:HE	1.82	0.43
1:A:401:SER:HB2	1:E:273:LYS:HE3	2.00	0.43
1:B:248:MET:HE1	1:B:282:ARG:HE	1.82	0.43
1:B:309:VAL:HA	1:B:365:PHE:HB3	2.01	0.43
1:B:657:GLN:O	1:B:661:TYR:HB3	2.18	0.43
1:B:702:TYR:CD1	1:B:814:VAL:HG11	2.53	0.43
1:D:754:LEU:HD21	1:D:856:MET:HA	2.01	0.43
1:A:754:LEU:HD21	1:A:856:MET:HA	2.01	0.43
1:E:657:GLN:O	1:E:661:TYR:HB3	2.18	0.43
1:A:309:VAL:HA	1:A:365:PHE:HB3	2.01	0.43
1:E:369:THR:HA	1:E:397:HIS:HB2	2.00	0.43
1:E:665:LEU:HD23	1:E:665:LEU:HA	1.80	0.43
1:C:364:CYS:HB2	1:C:366:LYS:HE2	2.01	0.43
1:C:586:ASP:OD1	1:C:586:ASP:N	2.38	0.43
1:D:702:TYR:CD1	1:D:814:VAL:HG11	2.54	0.43
1:E:309:VAL:HA	1:E:365:PHE:HB3	2.01	0.43
1:A:702:TYR:CD1	1:A:814:VAL:HG11	2.53	0.43
1:C:309:VAL:HA	1:C:365:PHE:HB3	2.01	0.43
1:C:657:GLN:O	1:C:661:TYR:HB3	2.18	0.43
1:C:743:LEU:HD12	1:C:743:LEU:HA	1.69	0.43
1:D:364:CYS:HB2	1:D:366:LYS:HE2	2.01	0.43
1:D:527:LYS:NZ	1:E:593:GLU:O	2.51	0.43
1:B:253:GLN:HB3	1:B:278:LYS:HB2	2.01	0.43
1:D:572:ASP:OD1	1:D:653:TRP:NE1	2.43	0.43
1:E:607:MET:HE1	1:E:665:LEU:HB3	2.01	0.43
1:C:82:ARG:NH2	1:C:243:LEU:O	2.37	0.43
1:A:253:GLN:HB3	1:A:278:LYS:HB2	2.01	0.43
1:D:583:LYS:HA	1:D:583:LYS:HD3	1.89	0.43
1:D:657:GLN:O	1:D:661:TYR:HB3	2.18	0.43
1:D:856:MET:HG3	1:D:858:THR:HG23	2.01	0.43
1:E:373:ALA:HB2	1:E:398:ASN:HB3	2.00	0.43
1:A:369:THR:HA	1:A:397:HIS:HB2	2.00	0.43
1:B:85:LEU:HG	1:B:243:LEU:HD11	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:271:LYS:HD2	1:B:271:LYS:HA	1.82	0.43
1:B:856:MET:HG3	1:B:858:THR:HG23	2.01	0.43
1:C:85:LEU:HD23	1:C:85:LEU:HA	1.87	0.43
1:C:702:TYR:CD1	1:C:814:VAL:HG11	2.53	0.43
1:D:739:SER:HA	1:D:742:ASN:HD21	1.84	0.43
1:E:364:CYS:HB2	1:E:366:LYS:HE2	2.01	0.43
1:A:595:ARG:HH22	1:E:630:ARG:NH1	2.16	0.42
1:E:253:GLN:HB3	1:E:278:LYS:HB2	2.01	0.42
1:A:856:MET:HG3	1:A:858:THR:HG23	2.01	0.42
1:B:369:THR:HA	1:B:397:HIS:HB2	2.00	0.42
1:B:754:LEU:HD21	1:B:856:MET:HA	2.01	0.42
1:C:739:SER:HA	1:C:742:ASN:HD21	1.84	0.42
1:D:85:LEU:HG	1:D:243:LEU:HD11	2.01	0.42
1:D:253:GLN:HB3	1:D:278:LYS:HB2	2.01	0.42
1:D:607:MET:HE1	1:D:665:LEU:HB3	2.01	0.42
1:B:754:LEU:HD11	1:C:854:ARG:HH21	1.84	0.42
1:C:85:LEU:HG	1:C:243:LEU:HD11	2.01	0.42
1:D:309:VAL:HA	1:D:365:PHE:HB3	2.01	0.42
1:E:856:MET:HG3	1:E:858:THR:HG23	2.01	0.42
1:B:603:HIS:O	1:B:606:LEU:HB3	2.19	0.42
1:C:253:GLN:HB3	1:C:278:LYS:HB2	2.01	0.42
1:C:607:MET:HE1	1:C:665:LEU:HB3	2.01	0.42
1:A:607:MET:HE1	1:A:665:LEU:HB3	2.01	0.42
1:B:607:MET:HE1	1:B:665:LEU:HB3	2.01	0.42
1:C:473:THR:OG1	1:C:475:SER:O	2.34	0.42
1:D:176:LYS:HE2	1:E:229:SER:HB2	2.02	0.42
1:E:754:LEU:HD21	1:E:856:MET:HA	2.01	0.42
1:A:85:LEU:HG	1:A:243:LEU:HD11	2.01	0.42
1:B:572:ASP:OD1	1:B:653:TRP:NE1	2.43	0.42
1:C:603:HIS:O	1:C:606:LEU:HB3	2.19	0.42
1:D:603:HIS:O	1:D:606:LEU:HB3	2.19	0.42
1:C:649:LYS:HA	1:C:649:LYS:HD3	1.80	0.42
1:C:856:MET:HG3	1:C:858:THR:HG23	2.01	0.42
1:D:440:ILE:O	1:D:444:ILE:HG12	2.20	0.42
1:E:603:HIS:O	1:E:606:LEU:HB3	2.19	0.42
1:A:739:SER:HA	1:A:742:ASN:HD21	1.84	0.42
1:B:364:CYS:HB2	1:B:366:LYS:HE2	2.01	0.42
1:B:455:SER:HB2	1:B:542:MET:HG2	2.02	0.42
1:C:455:SER:HB2	1:C:542:MET:HG2	2.02	0.42
1:E:572:ASP:OD1	1:E:653:TRP:NE1	2.43	0.42
1:E:649:LYS:HD3	1:E:649:LYS:HA	1.80	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:739:SER:HA	1:E:742:ASN:HD21	1.84	0.42
1:A:857:LYS:HB3	1:B:854:ARG:NH2	2.34	0.42
1:B:611:TYR:O	1:B:615:SER:N	2.44	0.42
1:A:85:LEU:HD23	1:A:85:LEU:HA	1.87	0.42
1:A:364:CYS:HB2	1:A:366:LYS:HE2	2.01	0.41
1:B:440:ILE:O	1:B:444:ILE:HG12	2.20	0.41
1:A:374:ASN:CG	1:A:782:PRO:HD2	2.45	0.41
1:A:572:ASP:OD1	1:A:653:TRP:NE1	2.43	0.41
1:D:374:ASN:CG	1:D:782:PRO:HD2	2.46	0.41
1:D:586:ASP:OD1	1:D:586:ASP:N	2.38	0.41
1:E:455:SER:HB2	1:E:542:MET:HG2	2.02	0.41
1:A:440:ILE:O	1:A:444:ILE:HG12	2.20	0.41
1:A:510:ILE:HD13	1:A:510:ILE:HA	1.94	0.41
1:B:374:ASN:CG	1:B:782:PRO:HD2	2.46	0.41
1:C:374:ASN:CG	1:C:782:PRO:HD2	2.46	0.41
1:C:583:LYS:HA	1:C:583:LYS:HD3	1.88	0.41
1:C:754:LEU:HD21	1:C:856:MET:HA	2.01	0.41
1:E:89:ARG:NH2	1:E:390:CYS:SG	2.94	0.41
1:E:374:ASN:CG	1:E:782:PRO:HD2	2.46	0.41
1:E:440:ILE:O	1:E:444:ILE:HG12	2.20	0.41
1:A:603:HIS:O	1:A:606:LEU:HB3	2.19	0.41
1:B:739:SER:HA	1:B:742:ASN:HD21	1.84	0.41
1:C:184:LEU:HA	1:C:185:PRO:HD3	1.91	0.41
1:C:440:ILE:O	1:C:444:ILE:HG12	2.20	0.41
1:D:89:ARG:NH2	1:D:390:CYS:SG	2.94	0.41
1:D:461:LEU:HD12	1:D:564:SER:HB3	2.03	0.41
1:E:85:LEU:HG	1:E:243:LEU:HD11	2.02	0.41
1:A:176:LYS:HE2	1:B:229:SER:HB2	2.02	0.41
1:C:89:ARG:NH2	1:C:390:CYS:SG	2.94	0.41
1:C:820:LEU:HA	1:C:823:LEU:HG	2.03	0.41
1:D:630:ARG:NH1	1:E:595:ARG:HH22	2.18	0.41
1:A:89:ARG:NH2	1:A:390:CYS:SG	2.94	0.41
1:A:455:SER:HB2	1:A:542:MET:HG2	2.02	0.41
1:D:455:SER:HB2	1:D:542:MET:HG2	2.02	0.41
1:E:461:LEU:HD12	1:E:564:SER:HB3	2.03	0.41
1:A:398:ASN:O	1:A:401:SER:OG	2.26	0.41
1:D:85:LEU:HD23	1:D:85:LEU:HA	1.87	0.41
1:A:575:ILE:HD13	1:A:575:ILE:HA	1.91	0.41
1:B:83:GLU:O	1:B:243:LEU:HB2	2.21	0.41
1:B:176:LYS:HE2	1:C:229:SER:HB2	2.03	0.41
1:B:451:GLY:N	1:B:558:ASP:OD2	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:630:ARG:HA	1:C:630:ARG:HD3	1.96	0.41
1:D:83:GLU:O	1:D:243:LEU:HB2	2.21	0.41
1:A:451:GLY:N	1:A:558:ASP:OD2	2.54	0.41
1:B:89:ARG:NH2	1:B:390:CYS:SG	2.94	0.41
1:B:448:HIS:HE1	1:B:783:CYS:HB3	1.86	0.41
1:B:461:LEU:HD12	1:B:564:SER:HB3	2.03	0.41
1:C:83:GLU:O	1:C:243:LEU:HB2	2.21	0.41
1:C:461:LEU:HD12	1:C:564:SER:HB3	2.03	0.41
1:D:448:HIS:HE1	1:D:783:CYS:HB3	1.86	0.41
1:E:85:LEU:HD23	1:E:85:LEU:HA	1.87	0.41
1:E:586:ASP:OD1	1:E:586:ASP:N	2.38	0.41
1:A:121:TYR:HD1	1:A:149:VAL:HG11	1.86	0.41
1:B:763:ARG:NH1	1:B:763:ARG:HB2	2.36	0.41
1:C:398:ASN:O	1:C:401:SER:OG	2.26	0.41
1:C:451:GLY:N	1:C:558:ASP:OD2	2.54	0.41
1:E:121:TYR:HD1	1:E:149:VAL:HG11	1.86	0.41
1:E:451:GLY:N	1:E:558:ASP:OD2	2.54	0.41
1:E:583:LYS:HA	1:E:583:LYS:HD3	1.88	0.41
1:A:271:LYS:HA	1:A:271:LYS:HD2	1.82	0.40
1:A:655:LEU:HD23	1:A:655:LEU:HA	1.91	0.40
1:B:820:LEU:HA	1:B:823:LEU:HG	2.03	0.40
1:E:83:GLU:O	1:E:243:LEU:HB2	2.21	0.40
1:A:83:GLU:O	1:A:243:LEU:HB2	2.21	0.40
1:A:461:LEU:HD12	1:A:564:SER:HB3	2.03	0.40
1:C:471:GLY:HA3	1:C:500:PRO:HD3	2.03	0.40
1:D:763:ARG:NH1	1:D:763:ARG:HB2	2.36	0.40
1:A:820:LEU:HA	1:A:823:LEU:HG	2.03	0.40
1:C:346:TYR:HA	1:C:347:PRO:HD3	1.95	0.40
1:C:420:LYS:HE2	1:C:420:LYS:HB3	1.95	0.40
1:C:540:ASP:OD1	1:C:542:MET:HG3	2.22	0.40
1:B:121:TYR:HD1	1:B:149:VAL:HG11	1.86	0.40
1:B:540:ASP:OD1	1:B:542:MET:HG3	2.22	0.40
1:C:264:ARG:HG3	1:C:279:LEU:HD23	2.04	0.40
1:C:273:LYS:HE3	1:D:401:SER:HB2	2.04	0.40
1:C:400:LEU:O	1:C:403:VAL:HG22	2.22	0.40
1:D:420:LYS:HE2	1:D:420:LYS:HB3	1.95	0.40
1:D:451:GLY:N	1:D:558:ASP:OD2	2.54	0.40
1:E:763:ARG:NH1	1:E:763:ARG:HB2	2.36	0.40
1:A:699:GLY:HA2	1:A:810:ALA:HB2	2.04	0.40
1:C:121:TYR:HD1	1:C:149:VAL:HG11	1.86	0.40
1:D:264:ARG:HG3	1:D:279:LEU:HD23	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:264:ARG:HG3	1:E:279:LEU:HD23	2.04	0.40
1:E:699:GLY:HA2	1:E:810:ALA:HB2	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	A	816/852 (96%)	798 (98%)	17 (2%)	1 (0%)	48	79
1	B	816/852 (96%)	797 (98%)	18 (2%)	1 (0%)	48	79
1	C	816/852 (96%)	798 (98%)	17 (2%)	1 (0%)	48	79
1	D	816/852 (96%)	797 (98%)	18 (2%)	1 (0%)	48	79
1	E	816/852 (96%)	799 (98%)	16 (2%)	1 (0%)	48	79
All	All	4080/4260 (96%)	3989 (98%)	86 (2%)	5 (0%)	49	79

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	564	SER
1	A	564	SER
1	B	564	SER
1	C	564	SER
1	D	564	SER

5.3.2 Protein sidechains [i](#)

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	711/738 (96%)	693 (98%)	18 (2%)	42	63
1	B	711/738 (96%)	693 (98%)	18 (2%)	42	63
1	C	711/738 (96%)	693 (98%)	18 (2%)	42	63
1	D	711/738 (96%)	693 (98%)	18 (2%)	42	63
1	E	711/738 (96%)	694 (98%)	17 (2%)	43	63
All	All	3555/3690 (96%)	3466 (98%)	89 (2%)	42	63

All (89) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	111	ILE
1	A	122	LEU
1	A	181	LEU
1	A	182	THR
1	A	201	THR
1	A	220	MET
1	A	269	THR
1	A	392	ASP
1	A	585	MET
1	A	586	ASP
1	A	635	ASN
1	A	682	ASP
1	A	745	ILE
1	A	769	LEU
1	A	772	LEU
1	A	783	CYS
1	A	803	LEU
1	A	855	LEU
1	B	111	ILE
1	B	122	LEU
1	B	181	LEU
1	B	182	THR
1	B	201	THR
1	B	269	THR
1	B	392	ASP
1	B	552	TYR
1	B	585	MET
1	B	586	ASP

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Mol	Chain	Res	Type
1	B	635	ASN
1	B	682	ASP
1	B	745	ILE
1	B	769	LEU
1	B	772	LEU
1	B	783	CYS
1	B	803	LEU
1	B	855	LEU
1	C	111	ILE
1	C	122	LEU
1	C	181	LEU
1	C	182	THR
1	C	201	THR
1	C	269	THR
1	C	392	ASP
1	C	552	TYR
1	C	585	MET
1	C	586	ASP
1	C	635	ASN
1	C	682	ASP
1	C	745	ILE
1	C	769	LEU
1	C	772	LEU
1	C	783	CYS
1	C	803	LEU
1	C	855	LEU
1	D	111	ILE
1	D	122	LEU
1	D	181	LEU
1	D	182	THR
1	D	201	THR
1	D	269	THR
1	D	392	ASP
1	D	552	TYR
1	D	585	MET
1	D	586	ASP
1	D	635	ASN
1	D	682	ASP
1	D	745	ILE
1	D	769	LEU
1	D	772	LEU
1	D	783	CYS

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Mol	Chain	Res	Type
1	D	803	LEU
1	D	855	LEU
1	E	111	ILE
1	E	122	LEU
1	E	181	LEU
1	E	182	THR
1	E	201	THR
1	E	269	THR
1	E	392	ASP
1	E	585	MET
1	E	586	ASP
1	E	635	ASN
1	E	682	ASP
1	E	745	ILE
1	E	769	LEU
1	E	772	LEU
1	E	783	CYS
1	E	803	LEU
1	E	855	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (44) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	103	GLN
1	A	189	GLN
1	A	190	ASN
1	A	214	ASN
1	A	405	ASN
1	A	483	ASN
1	A	609	GLN
1	A	657	GLN
1	A	742	ASN
1	B	144	ASN
1	B	189	GLN
1	B	190	ASN
1	B	214	ASN
1	B	265	GLN
1	B	405	ASN
1	B	483	ASN
1	B	609	GLN
1	B	657	GLN
1	B	742	ASN

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Mol	Chain	Res	Type
1	C	144	ASN
1	C	190	ASN
1	C	214	ASN
1	C	405	ASN
1	C	483	ASN
1	C	609	GLN
1	C	657	GLN
1	C	742	ASN
1	D	144	ASN
1	D	189	GLN
1	D	190	ASN
1	D	214	ASN
1	D	405	ASN
1	D	483	ASN
1	D	609	GLN
1	D	742	ASN
1	E	144	ASN
1	E	189	GLN
1	E	190	ASN
1	E	214	ASN
1	E	405	ASN
1	E	483	ASN
1	E	609	GLN
1	E	657	GLN
1	E	742	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

Of 10 ligands modelled in this entry, 10 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

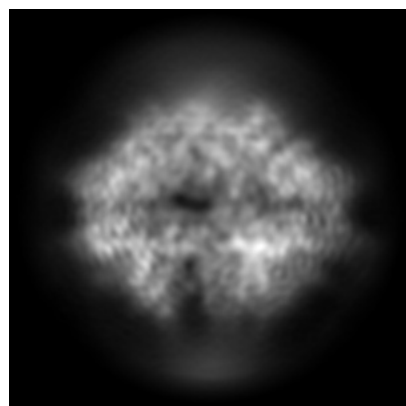
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-55028. These allow visual inspection of the internal detail of the map and identification of artifacts.

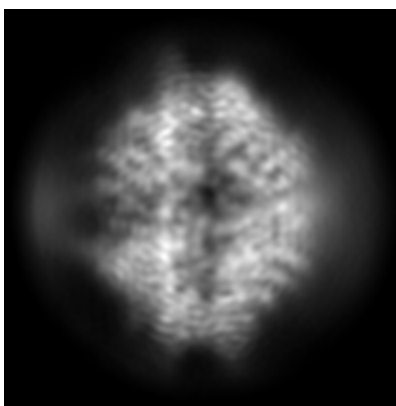
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

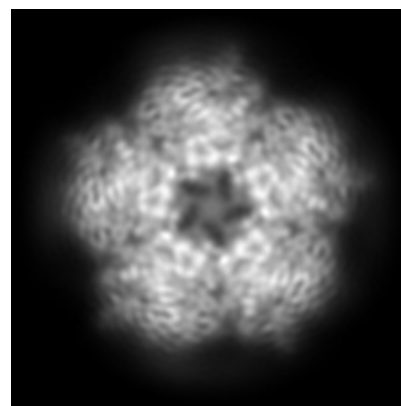
6.1.1 Primary map



X

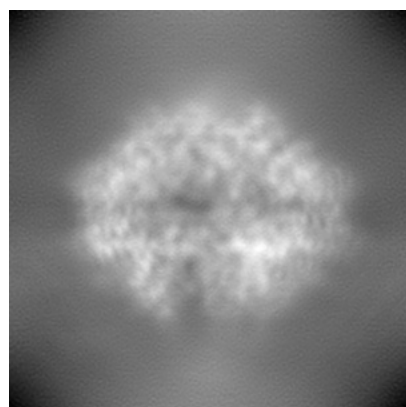


Y

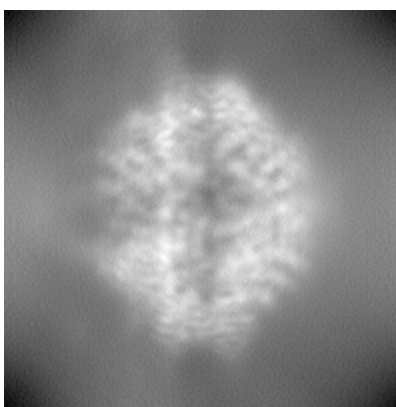


Z

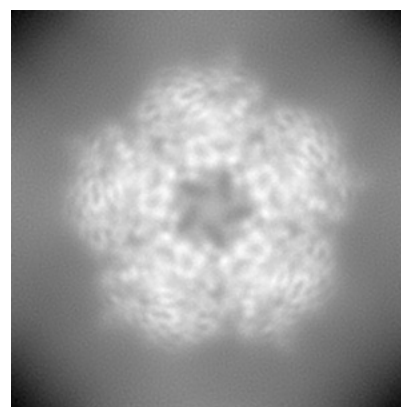
6.1.2 Raw map



X



Y

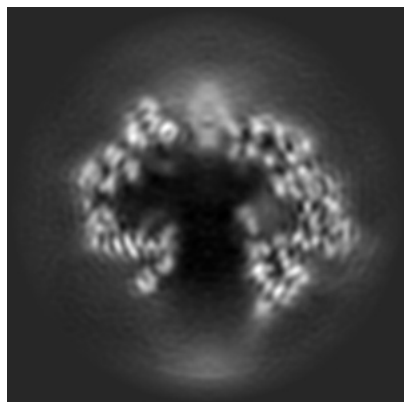


Z

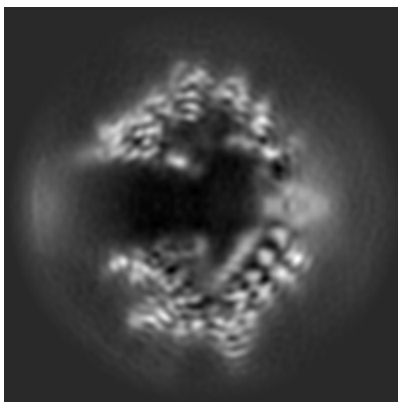
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

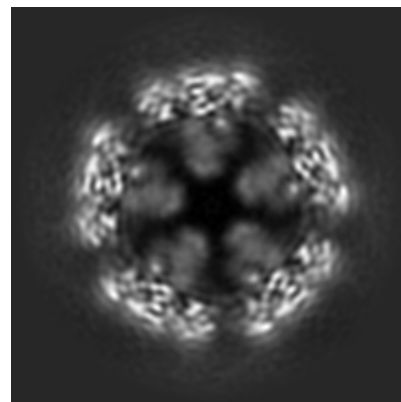
6.2.1 Primary map



X Index: 100

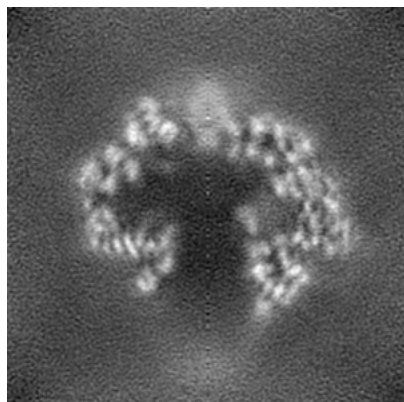


Y Index: 100

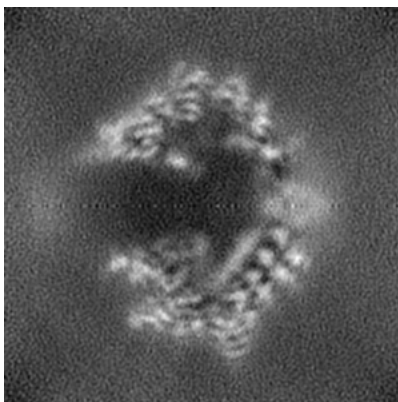


Z Index: 100

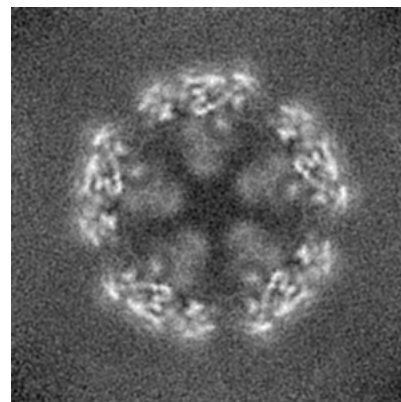
6.2.2 Raw map



X Index: 100



Y Index: 100

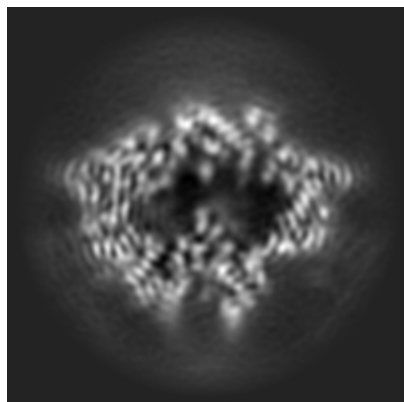


Z Index: 100

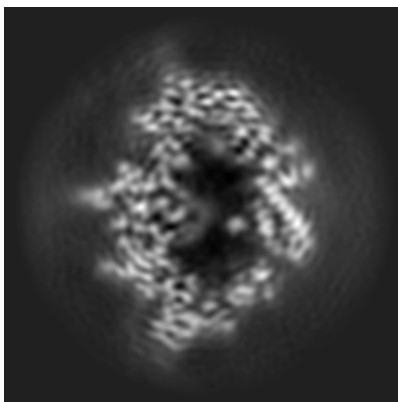
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

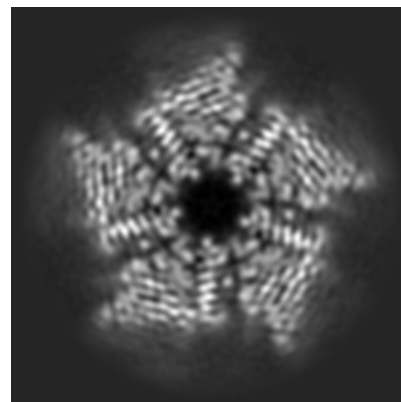
6.3.1 Primary map



X Index: 76

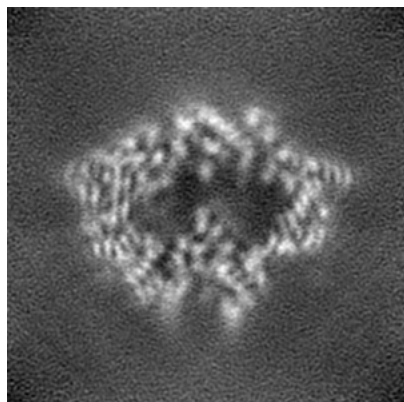


Y Index: 125

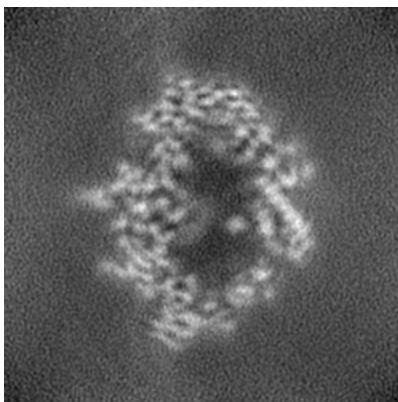


Z Index: 81

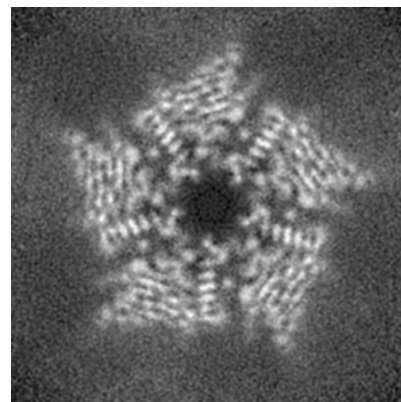
6.3.2 Raw map



X Index: 76



Y Index: 125

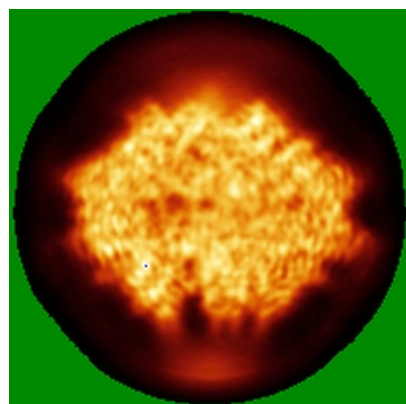


Z Index: 82

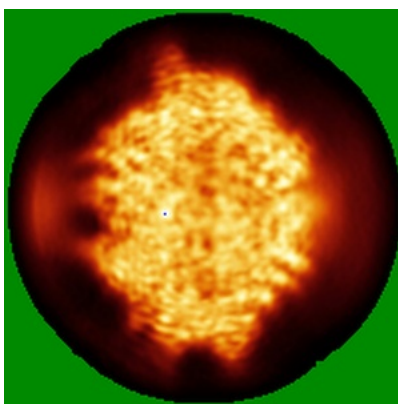
The images above show the largest variance slices of the map in three orthogonal directions.

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

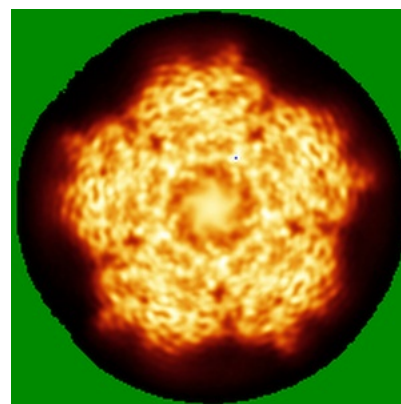
6.4.1 Primary map



X

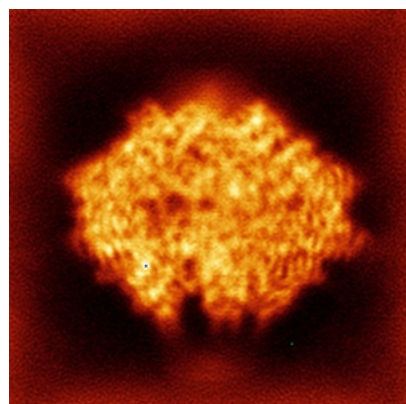


Y

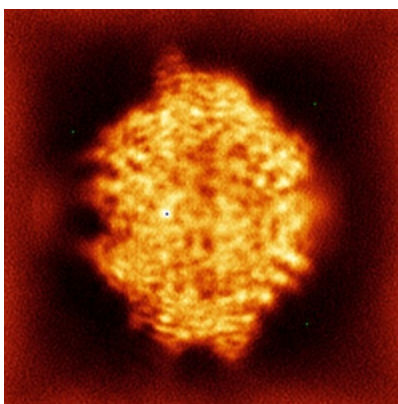


Z

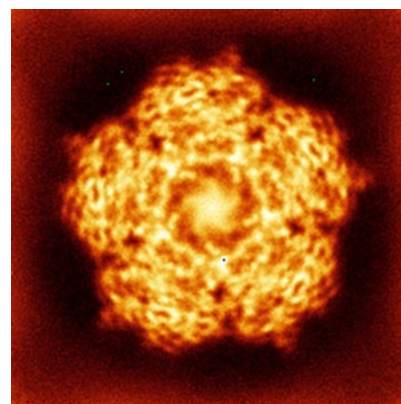
6.4.2 Raw map



X



Y

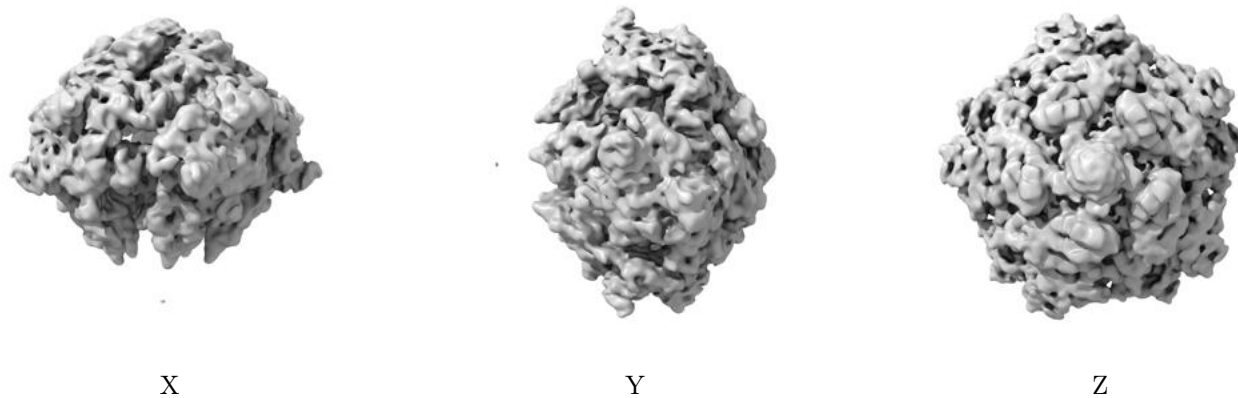


Z

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.

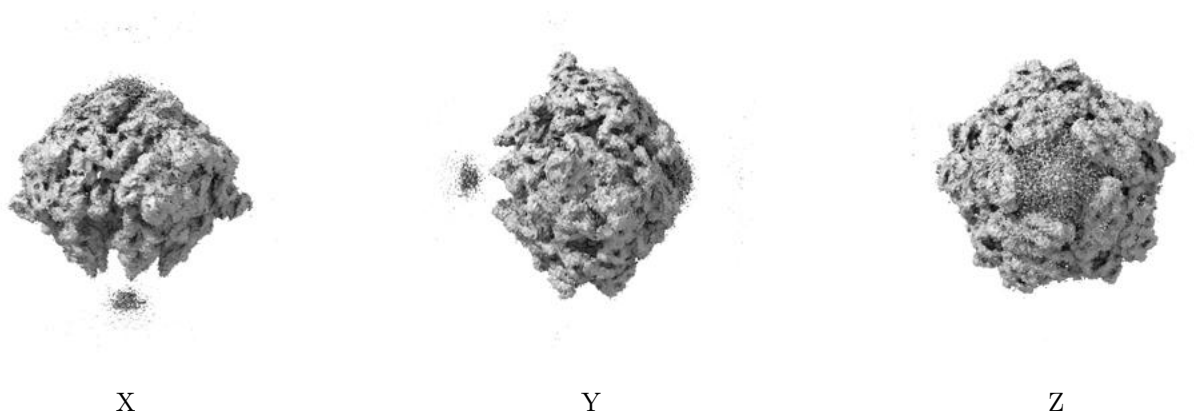
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.062. 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.

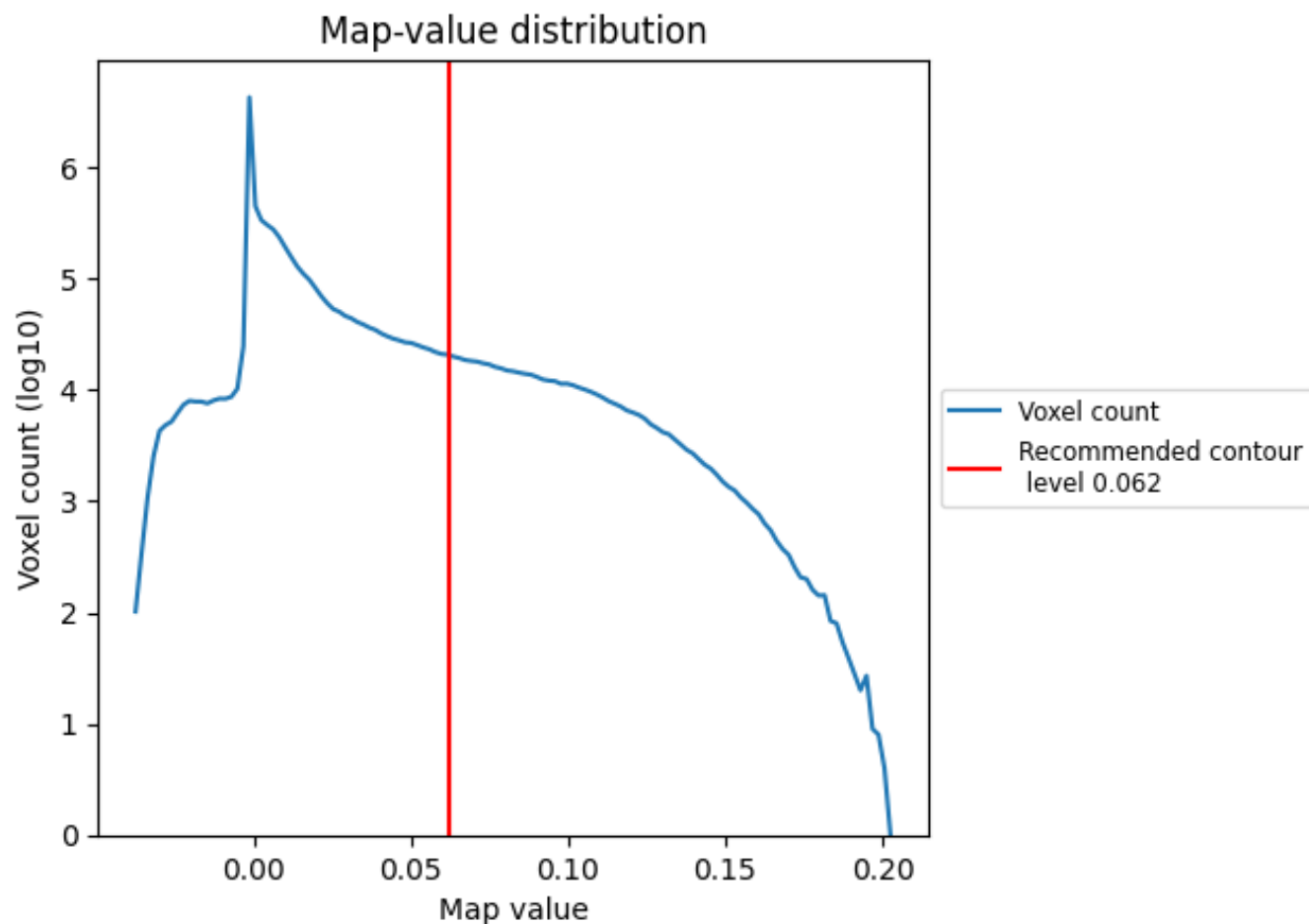
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

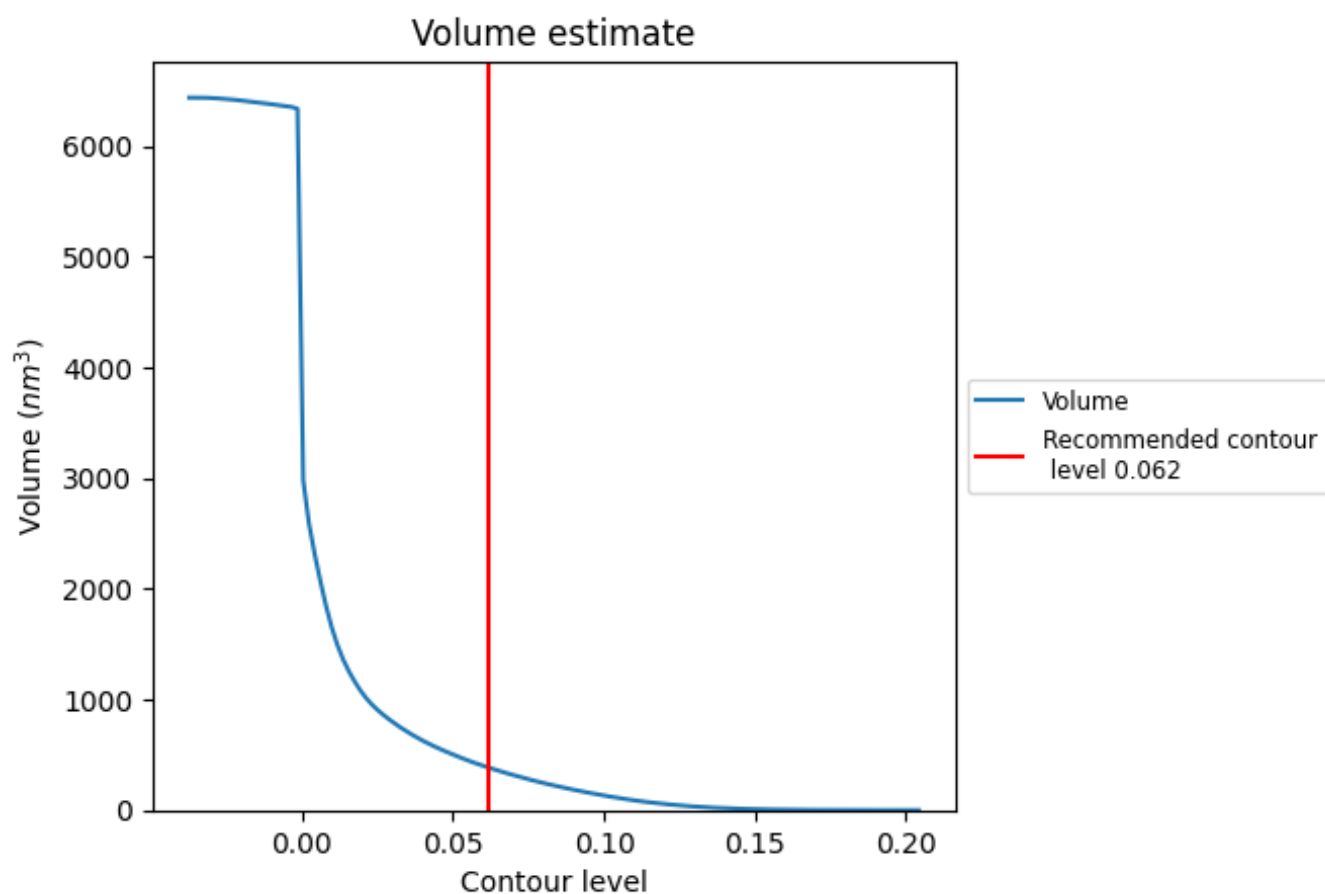
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

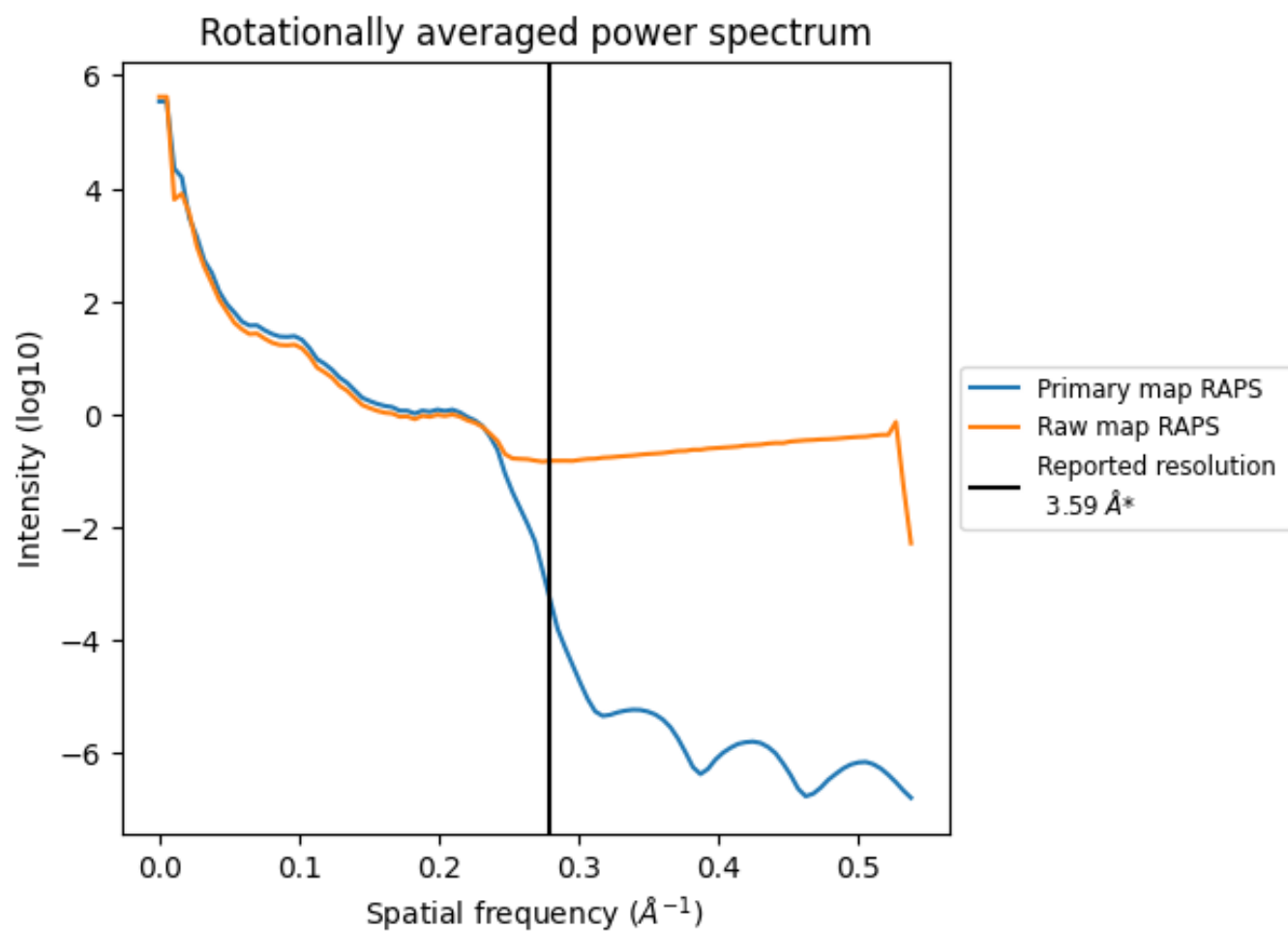
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 383 nm³; this corresponds to an approximate mass of 346 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 ⓘ

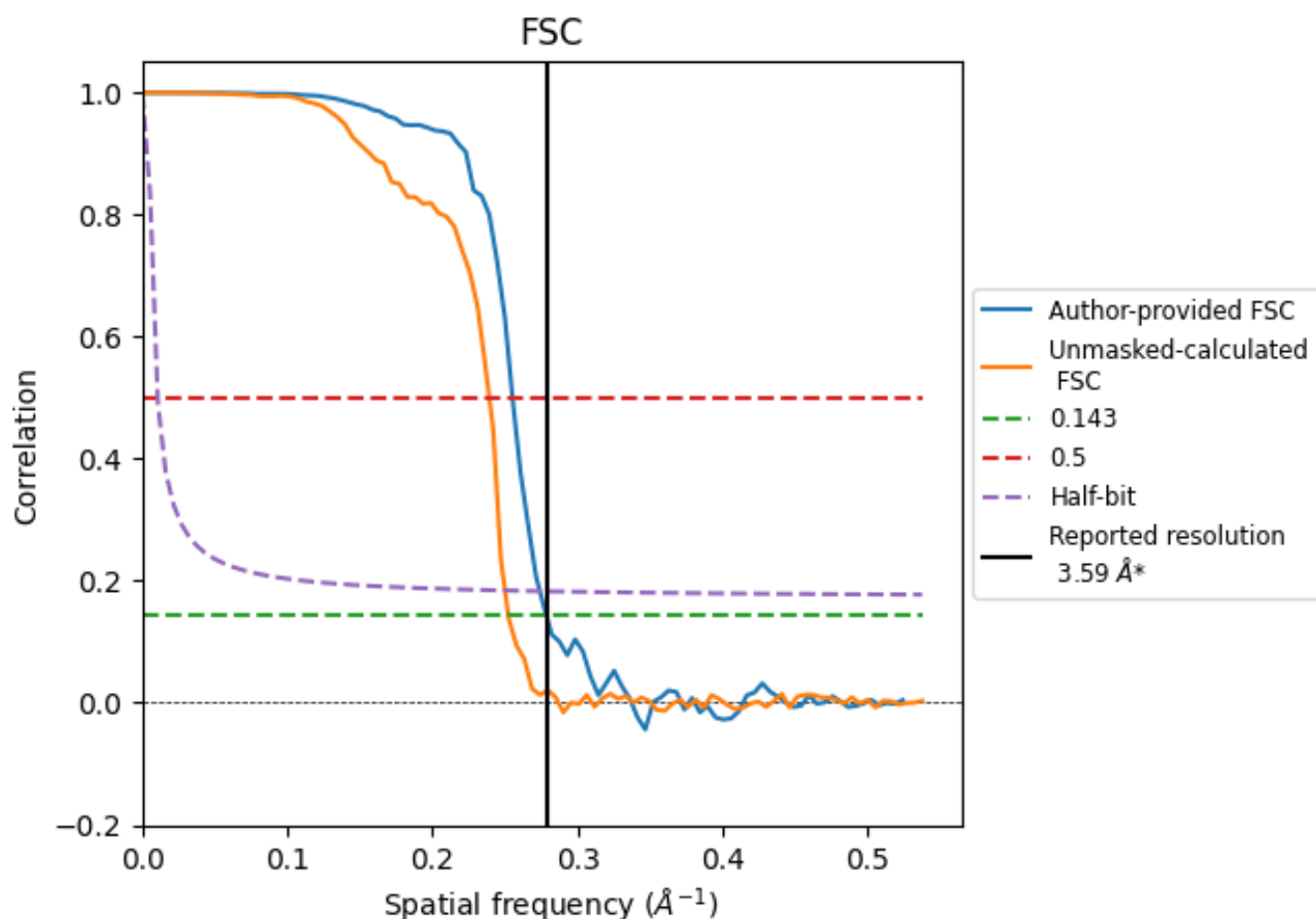


*Reported resolution corresponds to spatial frequency of 0.279 Å^{-1}

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 0.279 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

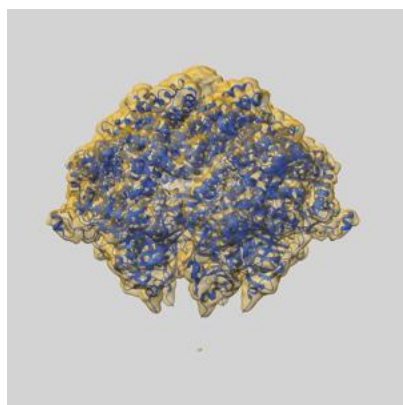
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.59	-	-
Author-provided FSC curve	3.59	3.92	3.65
Unmasked-calculated*	3.96	4.18	4.00

*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 3.96 differs from the reported value 3.59 by more than 10 %

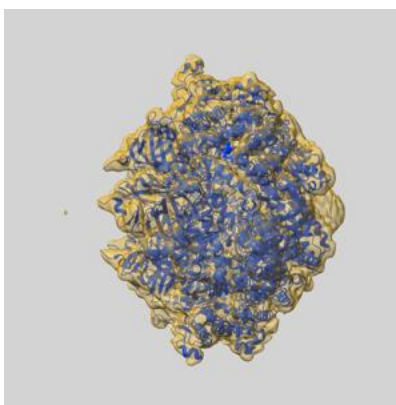
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-55028 and PDB model 9SM8. Per-residue inclusion information can be found in section [3](#) on page [8](#).

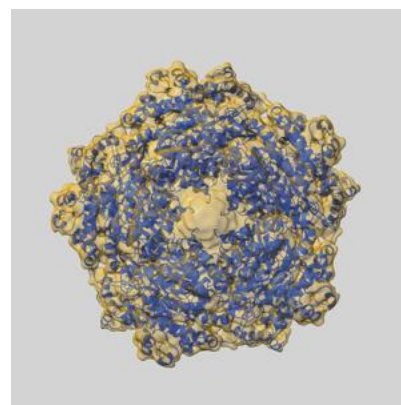
9.1 Map-model overlay [i](#)



X



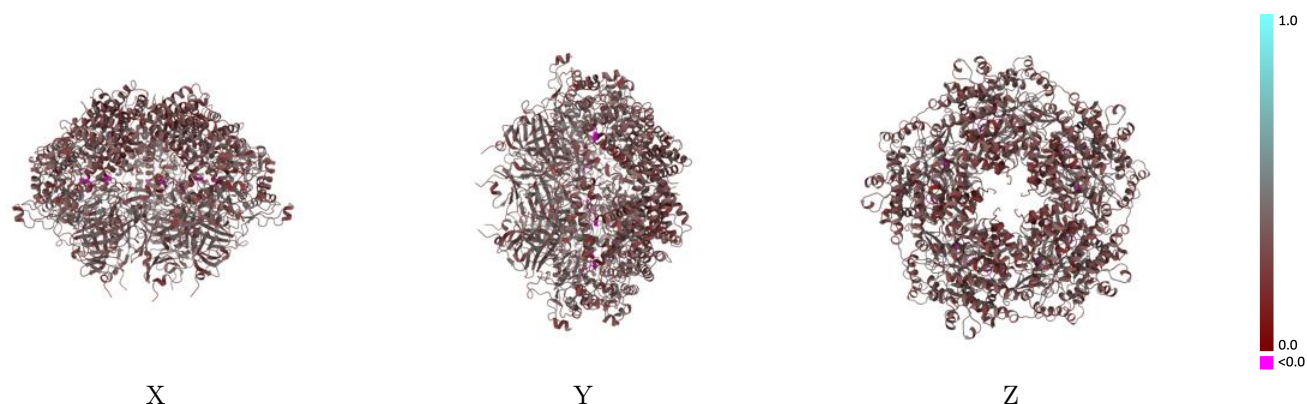
Y



Z

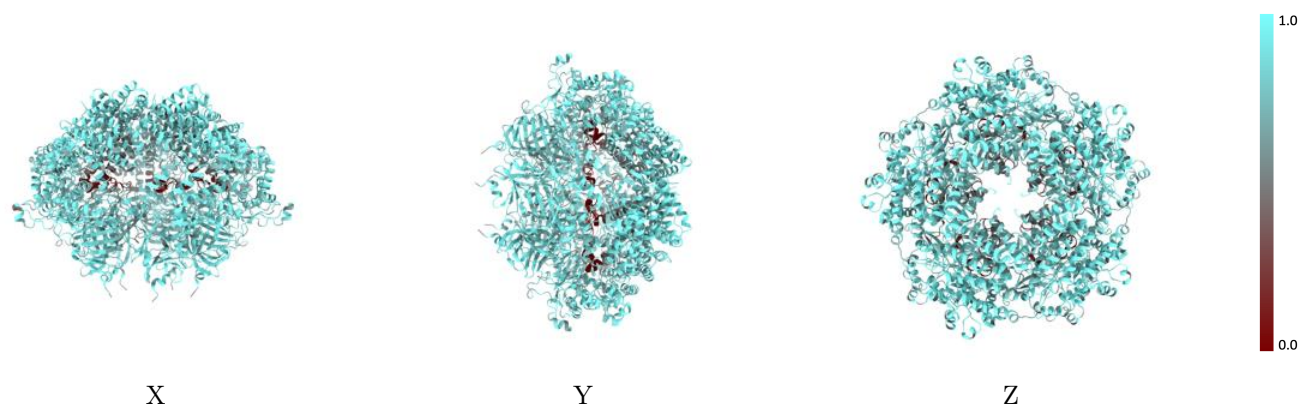
The images above show the 3D surface view of the map at the recommended contour level 0.062 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



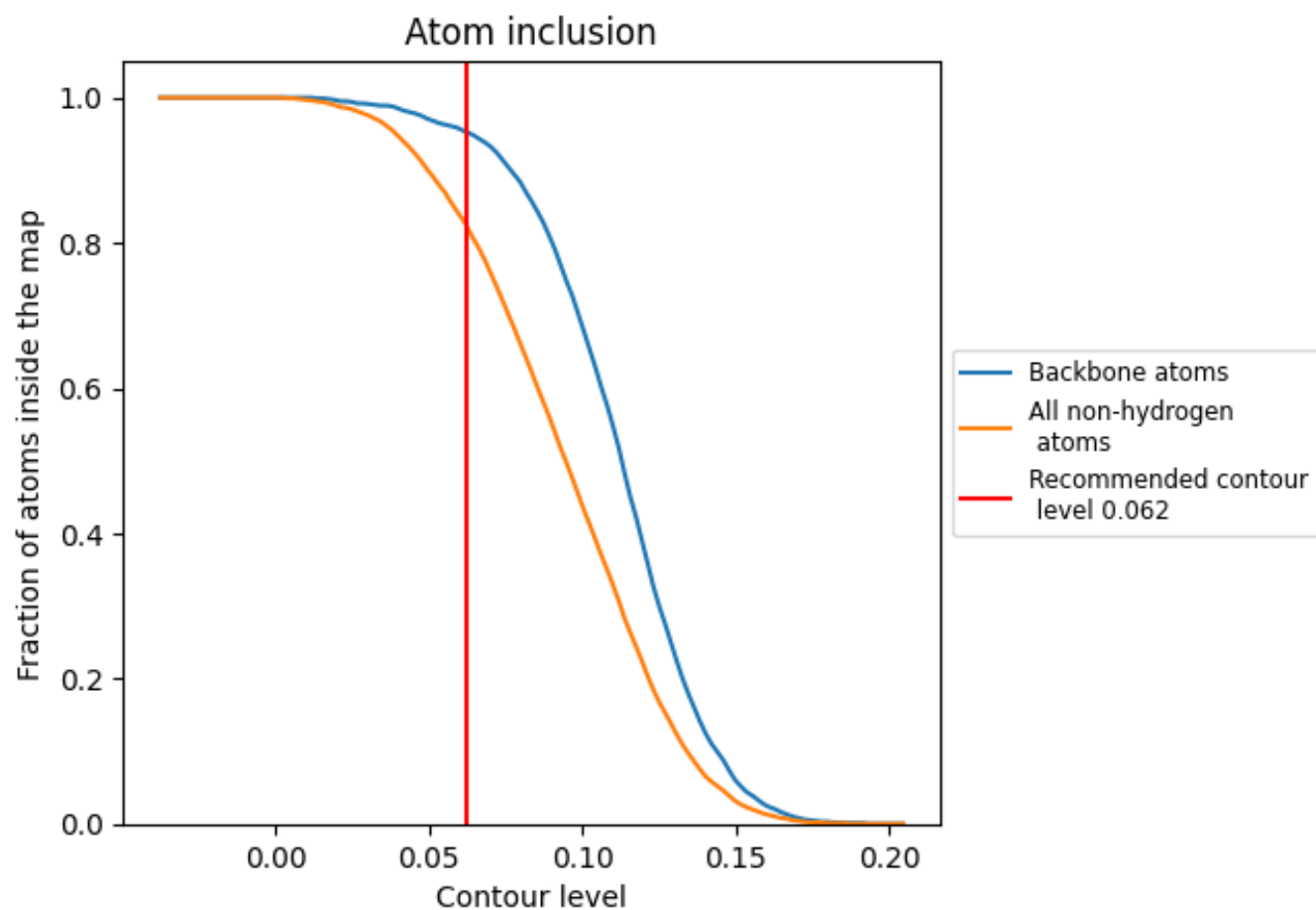
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.062).

9.4 Atom inclusion [i](#)



At the recommended contour level, 95% of all backbone atoms, 83% 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 (0.062) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8260	0.3260
A	0.8240	0.3280
B	0.8260	0.3240
C	0.8250	0.3230
D	0.8270	0.3270
E	0.8260	0.3270

