



Full wwPDB EM Validation Report ⓘ

Aug 11, 2026 – 03:02 PM JST

PDB ID : 25VJ / pdb_000025vj
EMDB ID : EMD-80404
Title : tail fiber of F2-pyocin
Authors : Gu, Z.W.; Xie, Y.F.; Wang, J.W.
Deposited on : 2026-04-19
Resolution : 3.26 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

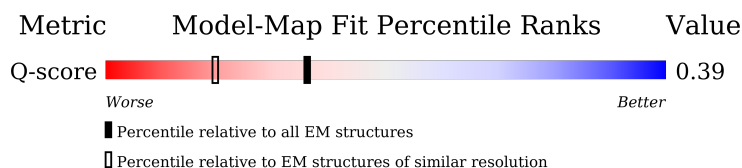
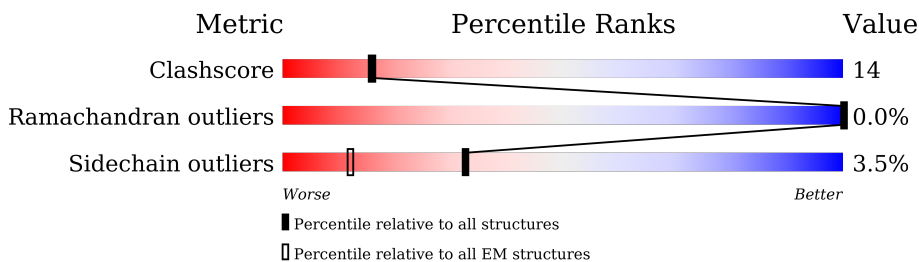
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.26 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.



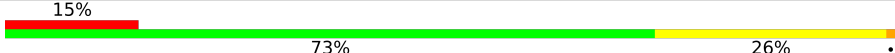
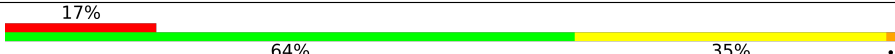
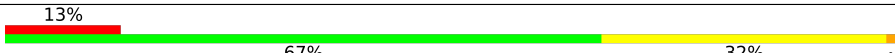
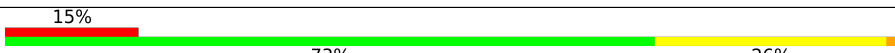
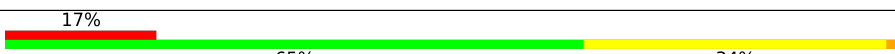
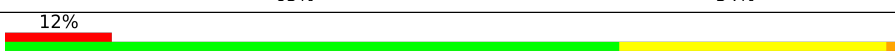
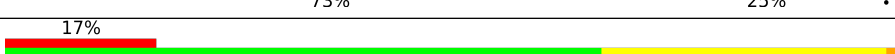
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	14557 (2.76 - 3.76)

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	D	1204	7% . 91%
1	E	1204	7% . 91%
1	I	1204	7% . 91%
2	A	363	12% 69% 29% .

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Mol	Chain	Length	Quality of chain
2	B	363	
2	C	363	
2	F	363	
2	G	363	
2	H	363	
2	J	363	
2	K	363	
2	L	363	

2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 26916 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 tail fiber protein of F2-pyocin.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	D	110	Total	C	N	O	S	0	0
			809	477	156	175	1		
1	E	110	Total	C	N	O	S	0	0
			809	477	156	175	1		
1	I	110	Total	C	N	O	S	0	0
			809	477	156	175	1		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	945	LEU	GLN	conflict	UNP A0A5E5R453
E	945	LEU	GLN	conflict	UNP A0A5E5R453
I	945	LEU	GLN	conflict	UNP A0A5E5R453

- Molecule 2 is a protein called F2-pyocin side fiber.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A	362	Total	C	N	O	S	0	0
			2721	1711	477	521	12		
2	B	362	Total	C	N	O	S	0	0
			2721	1711	477	521	12		
2	C	362	Total	C	N	O	S	0	0
			2721	1711	477	521	12		
2	F	362	Total	C	N	O	S	0	0
			2721	1711	477	521	12		
2	G	362	Total	C	N	O	S	0	0
			2721	1711	477	521	12		
2	H	362	Total	C	N	O	S	0	0
			2721	1711	477	521	12		
2	J	362	Total	C	N	O	S	0	0
			2721	1711	477	521	12		
2	K	362	Total	C	N	O	S	0	0
			2721	1711	477	521	12		

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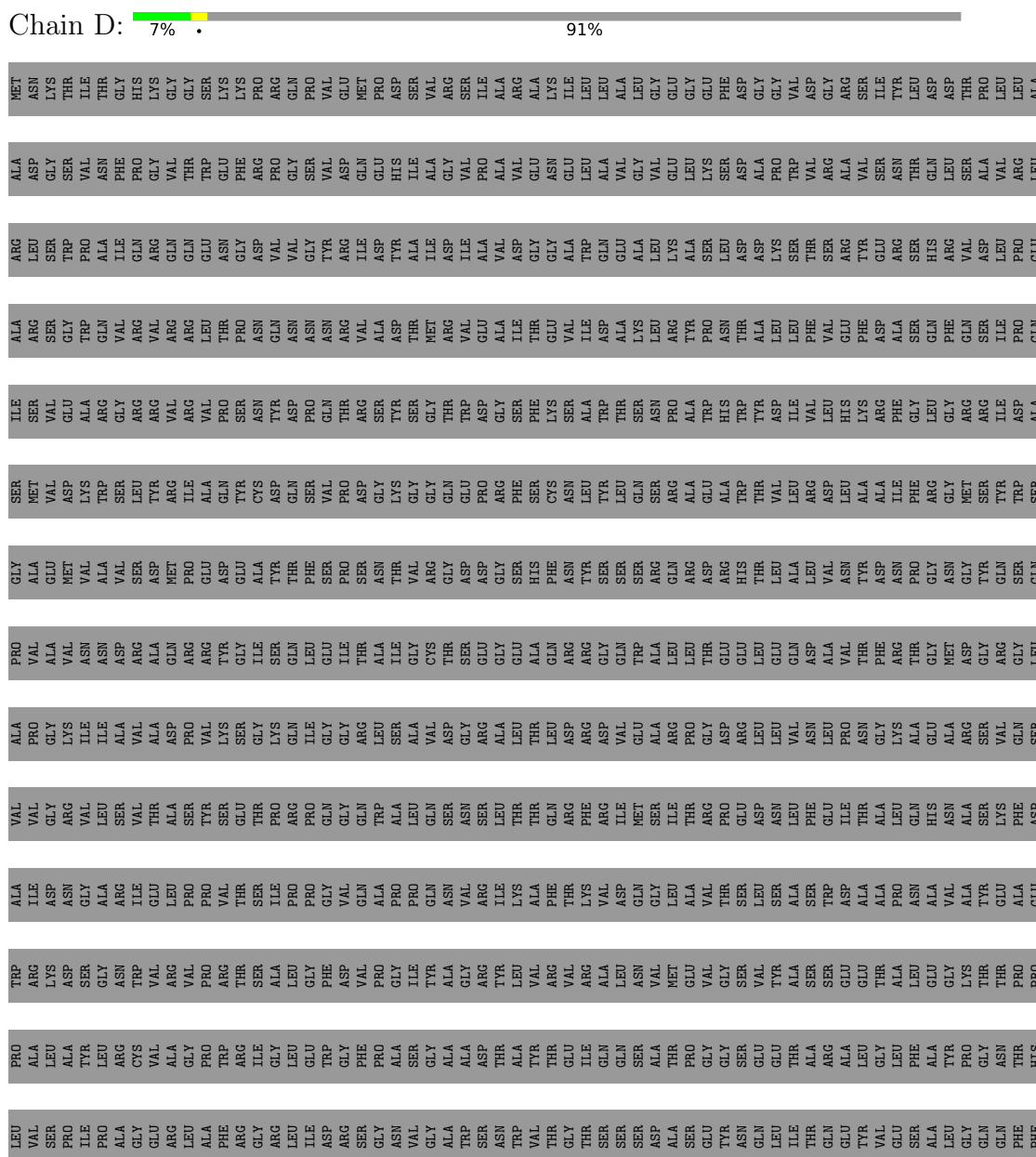
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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	L	362	2721	1711	477	521	12	0	0

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: tail fiber protein of F2-pyocin



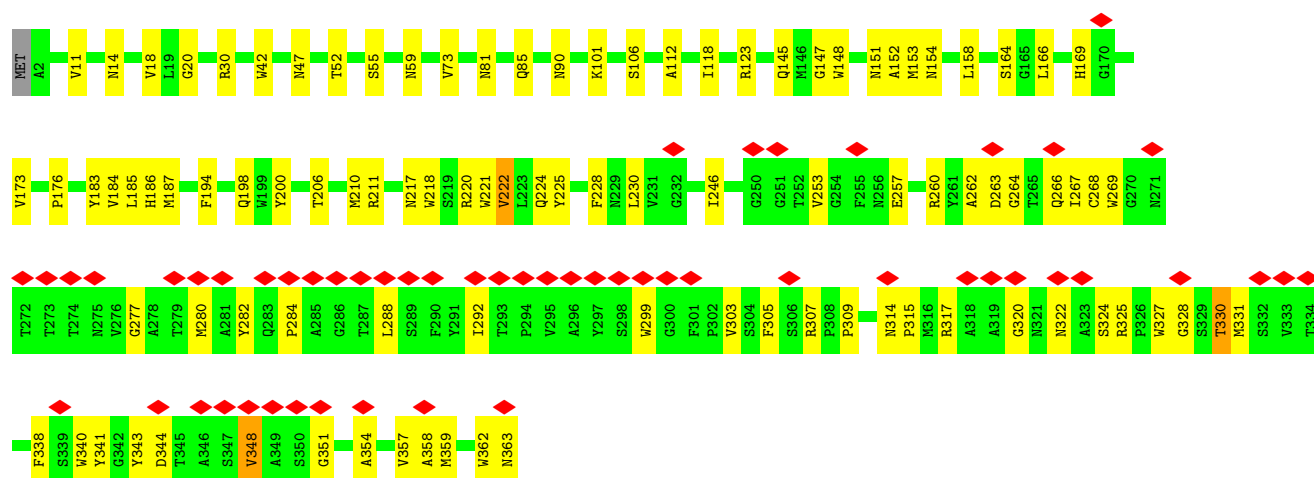


NET	ILE	ASP	Q1016	ALA	SER	LEU	PRO
		GLY	A1017	TYR	ASP	VAL	ALA
SER	PHE	MET	R1021	ILE	MET	ALA	ARG
		GLN	L1022	ILE	GLN	ALA	ARG
SER	ILE	TYR	L1025	GLN	VAL	GLY	CYS
		TYR	L1028	SER	ASP	VAL	VAL
SER	ASN	VAL	ILE	LEU	GLY	LEU	GLY
		VAL	THR	THR	GLY	LEU	PRO
SER	ILE	GLN	GLY	ALA	LEU	PHE	TRP
		ALA	THR	ASN	GLN	ARG	ARG
SER	ASP	HIS	ALA	GLY	LYS	ILE	ILE
		ALA	ALA	LEU	GLN	ARG	GLY
SER	ALA	ASN	SER	ALA	VAL	VAL	SER
		GLY	LEU	GLN	GLY	GLY	GLU
SER	ASP	GLN	GLN	Q919	ASP	ASP	TRP
		LYS	SER	GLY	LEU	ARG	GLY
SER	ALA	TYR	GLU	S922	ALA	SER	PHE
		ALA	GLN	GLN	ASP	GLY	PRO
SER	ILE	GLY	THR	E926	VAL	ASN	ALA
		GLY	ALA	I927	LEU	VAL	SER
SER	ASN	TRP	ARG	D931	TYR	ALA	ALA
		GLN	ALA	G932	ASP	TRP	ALA
SER	GLN	GLY	ALA	S939	ALA	ASN	GLN
		PHE	ASP	R940	LYS	SER	GLN
SER	ASN	ASP	SER	L941	VAL	TRP	ALA
		SER	ALA	G942	VAL	VAL	TYR
SER	SER	THR	LEU	V943	ALA	GLY	GLU
		ASN	GLN	L944	LYS	THR	ILE
SER	ASN	VAL	ARG	L945	ASN	SER	GLN
		GLY	ILE	D950	ASP	SER	SER
SER	MET	THR	ASP	THR	MET	SER	SER
		PRO	THR	D954	VAL	ASP	ALA
SER	ILE	ALA	VAL	G955	ARG	ALA	THR
		THR	GLN	GLY	GLN	SER	PRO
SER	ARG	GLN	ALA	M959	GLN	TYR	GLY
		ALA	SER	A960	ARG	ASN	SER
SER	LYS	ASP	THR	D961	LEU	GLN	GLY
		PHE	THR	A962	TYR	ILE	GLU
SER	GLY	ILE	ASN	E976	GLN	THR	ALA
		THR	SER	ALA	LEU	THR	ALA
SER	THR	PHE	ALA	R979	LYS	GLU	ARG
		ASP	ALA	E982	ALA	TYR	ALA
SER	VAL	SER	GLN	THR	VAL	VAL	GLY
		ASP	THR	R1003	PRO	GLY	LEU
SER	ALA	THR	SER	I1004	LYS	SER	PHE
		ALA	GLN	E1008	THR	ALA	ALA
SER	GLN	VAL	VAL	S1013	PRO	GLN	PRO
		ARG	THR	D1014	ASN	GLN	GLY
SER	GLN	VAL	SER	R1015	ALA	PHE	THR
		THR	THR		ALA	THR	THR

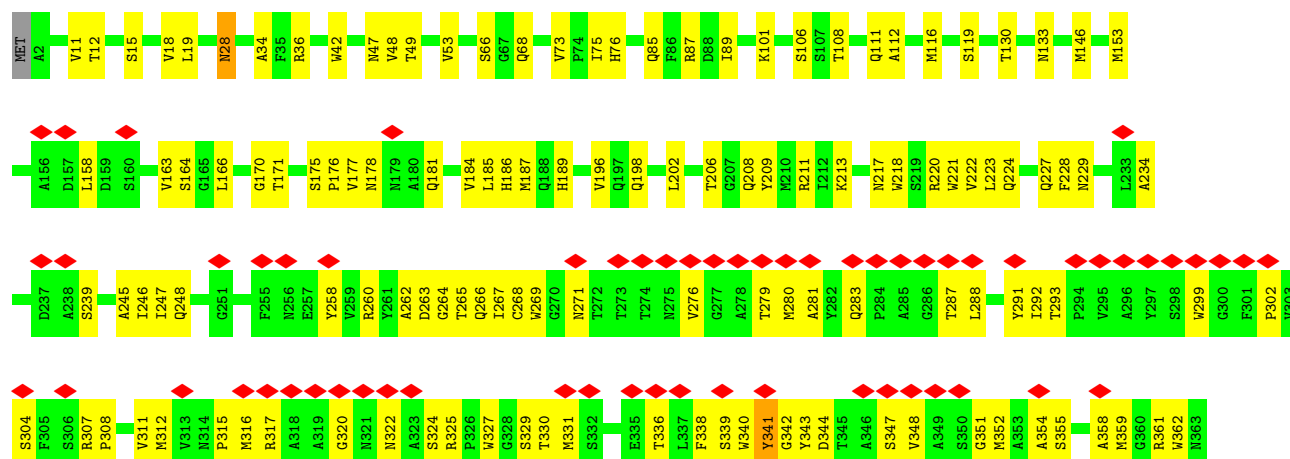
- Molecule 1: tail fiber protein of F2-pyocin

Chain I: 7% . 91%

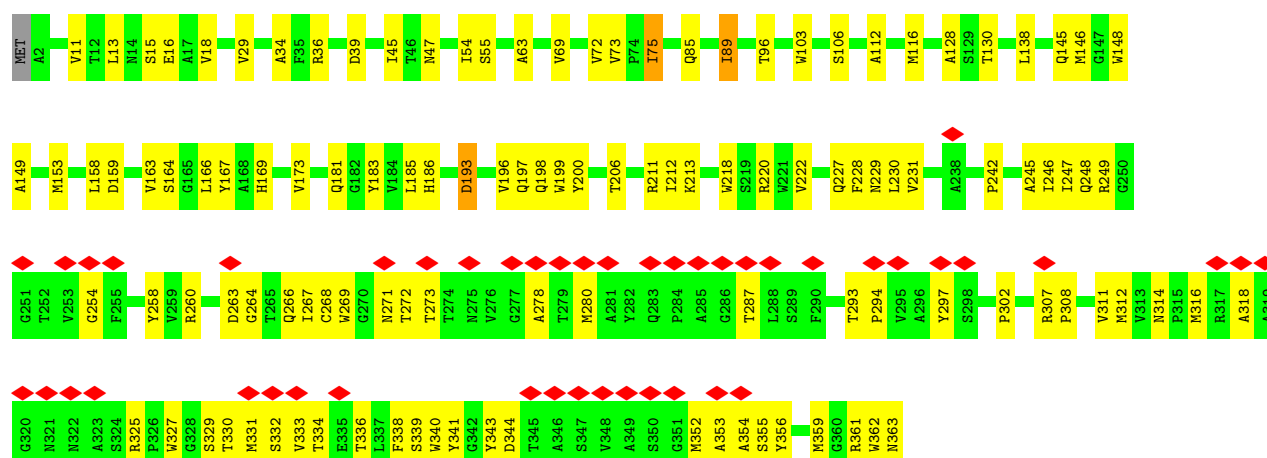
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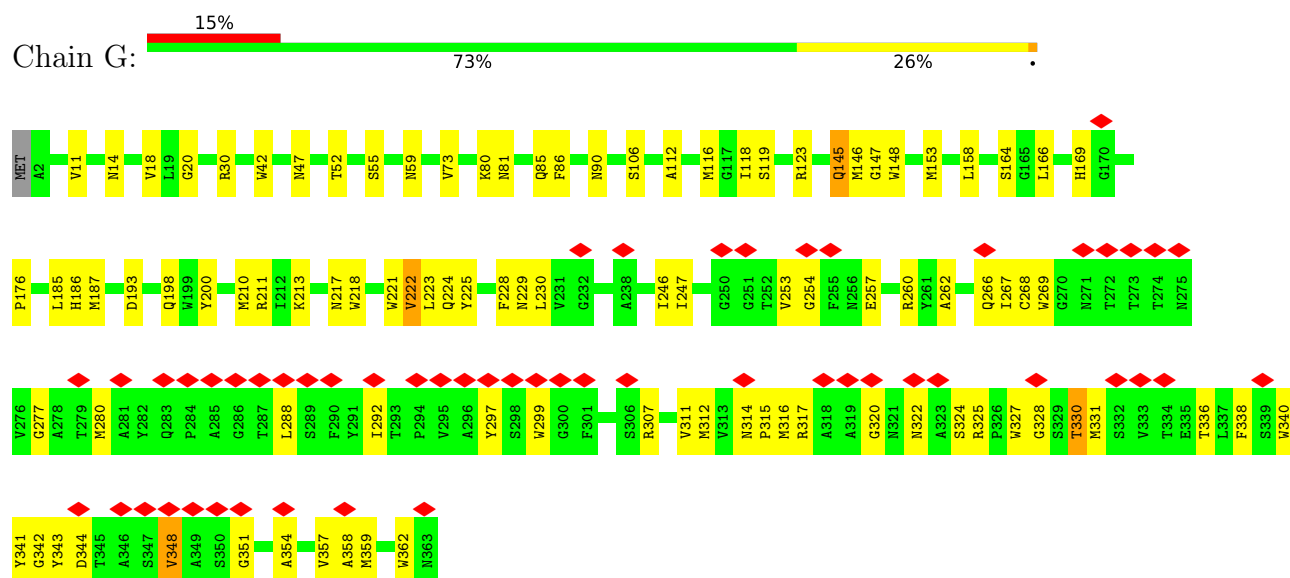
• Molecule 2: F2-pyocin side fiber



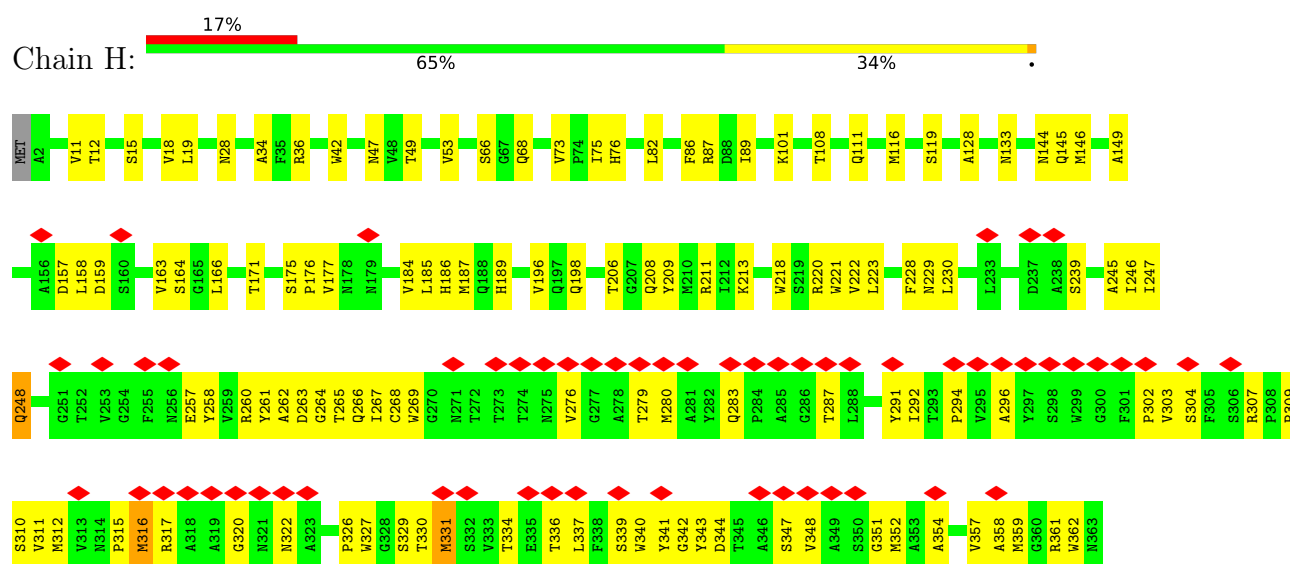
• Molecule 2: F2-pyocin side fiber



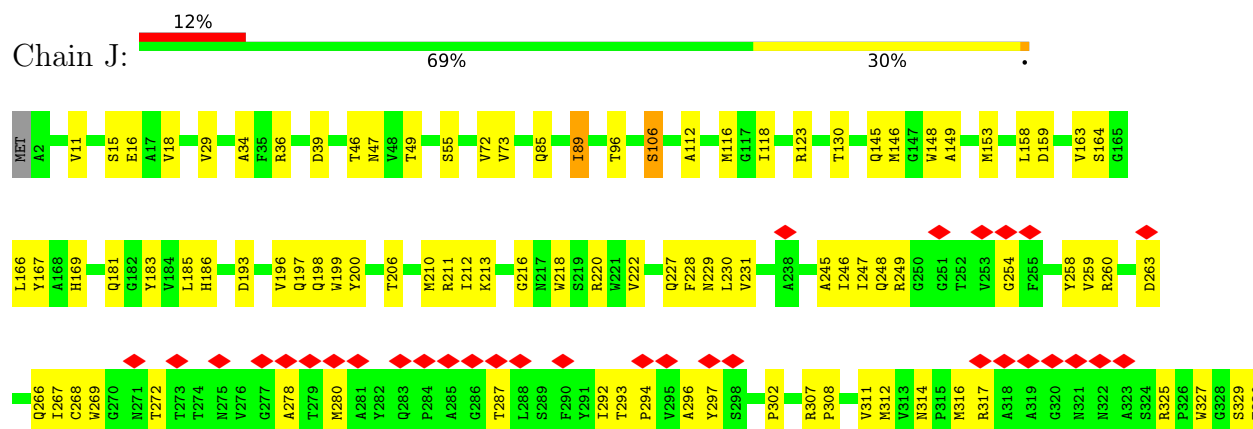
- Molecule 2: F2-pyocin side fiber



- Molecule 2: F2-pyocin side fiber

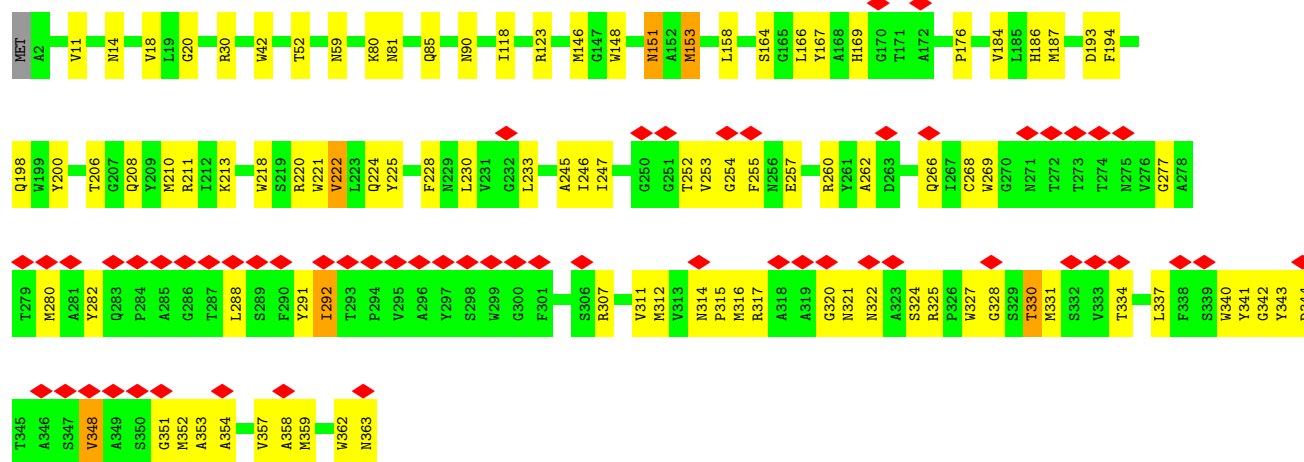
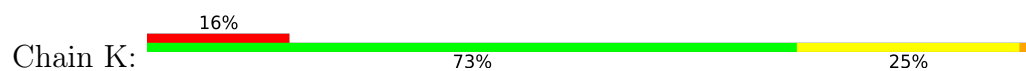


- Molecule 2: F2-pyocin side fiber

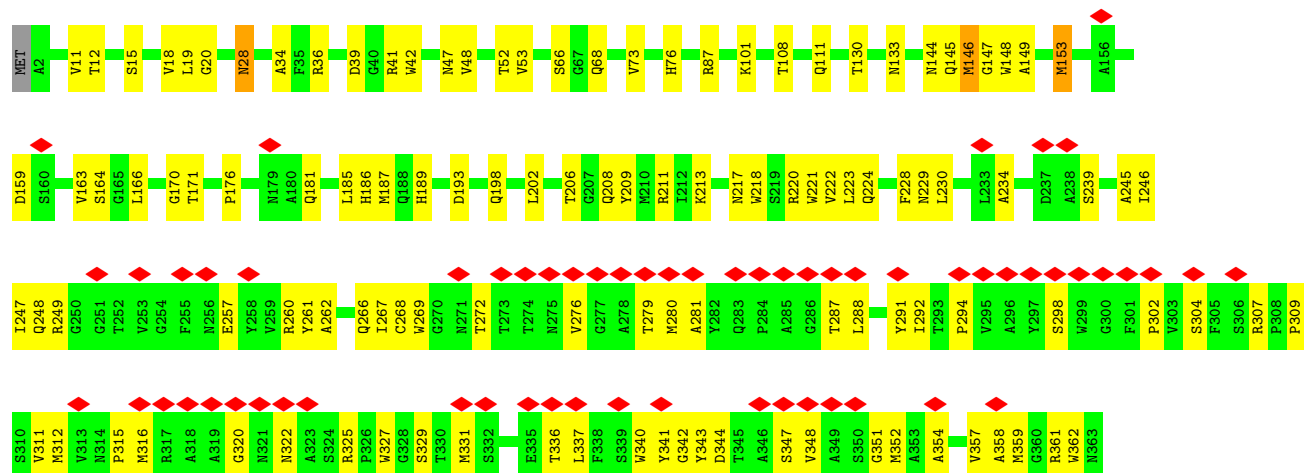




• Molecule 2: F2-pyocin side fiber



• Molecule 2: F2-pyocin side fiber



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	20186	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	49.91	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	1.940	Depositor
Minimum map value	-1.037	Depositor
Average map value	-0.002	Depositor
Map value standard deviation	0.037	Depositor
Recommended contour level	0.233	Depositor
Map size (Å)	474.112, 474.112, 474.112	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.926, 0.926, 0.926	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	D	0.16	0/811	0.33	0/1099
1	E	0.17	0/811	0.35	0/1099
1	I	0.16	0/811	0.34	0/1099
2	A	0.15	0/2797	0.32	0/3826
2	B	0.15	0/2797	0.31	0/3826
2	C	0.18	0/2797	0.36	0/3826
2	F	0.15	0/2797	0.33	0/3826
2	G	0.15	0/2797	0.30	0/3826
2	H	0.17	0/2797	0.37	0/3826
2	J	0.15	0/2797	0.33	0/3826
2	K	0.15	0/2797	0.31	0/3826
2	L	0.17	0/2797	0.36	0/3826
All	All	0.16	0/27606	0.33	0/37731

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	809	0	789	22	0
1	E	809	0	789	30	0
1	I	809	0	789	27	0
2	A	2721	0	2570	91	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	2721	0	2570	87	0
2	C	2721	0	2570	119	0
2	F	2721	0	2570	92	0
2	G	2721	0	2570	83	0
2	H	2721	0	2570	109	0
2	J	2721	0	2570	93	0
2	K	2721	0	2570	87	0
2	L	2721	0	2570	112	0
All	All	26916	0	25497	757	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 14.

All (757) 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:K:146:MET:HB2	2:L:149:ALA:HB2	1.57	0.86
2:J:149:ALA:HB2	2:L:146:MET:HB2	1.59	0.84
2:J:292:ILE:HG13	2:J:343:TYR:HD1	1.43	0.83
2:K:317:ARG:HH22	2:K:322:ASN:HA	1.45	0.82
2:C:266:GLN:HB2	2:C:362:TRP:HD1	1.46	0.79
2:J:331:MET:HB2	2:K:317:ARG:HD3	1.65	0.79
2:C:246:ILE:HG13	2:C:247:ILE:HG13	1.64	0.79
2:F:246:ILE:HG22	2:F:247:ILE:HG23	1.65	0.79
2:A:312:MET:HE2	2:B:357:VAL:HG22	1.64	0.78
2:F:331:MET:HB2	2:G:317:ARG:HD3	1.65	0.78
2:F:149:ALA:HB2	2:H:146:MET:HB2	1.64	0.77
2:A:246:ILE:HG22	2:A:247:ILE:HG23	1.66	0.77
2:H:279:THR:HG22	2:H:347:SER:HB2	1.66	0.77
2:J:246:ILE:HG22	2:J:247:ILE:HG23	1.66	0.76
1:D:941:LEU:HD21	1:I:940:ARG:HG2	1.67	0.76
2:C:279:THR:HG22	2:C:347:SER:HB2	1.68	0.75
2:L:279:THR:HG22	2:L:347:SER:HB2	1.68	0.75
2:C:342:GLY:HA3	2:C:352:MET:HE1	1.68	0.74
1:E:940:ARG:HG2	1:I:941:LEU:HD21	1.67	0.74
2:A:314:ASN:HD21	2:C:330:THR:HB	1.53	0.73
2:A:206:THR:HG22	2:A:228:PHE:HB3	1.70	0.73
2:C:307:ARG:HH21	2:C:361:ARG:HG2	1.53	0.73
2:J:206:THR:HG22	2:J:228:PHE:HB3	1.70	0.73
2:G:148:TRP:HZ3	2:G:166:LEU:HB2	1.53	0.73
2:C:246:ILE:HA	2:C:262:ALA:HB2	1.71	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:220:ARG:HE	2:K:228:PHE:HE1	1.37	0.73
2:L:342:GLY:HA3	2:L:352:MET:HE1	1.71	0.73
2:A:146:MET:HG3	2:B:148:TRP:HB3	1.70	0.72
2:G:30:ARG:NH1	2:L:47:ASN:OD1	2.23	0.72
2:F:206:THR:HG22	2:F:228:PHE:HB3	1.72	0.71
2:G:280:MET:HE2	2:G:292:ILE:H	1.55	0.71
2:A:149:ALA:HB2	2:C:146:MET:HB2	1.72	0.71
2:L:331:MET:HE1	2:L:340:TRP:HA	1.72	0.71
2:K:317:ARG:NH2	2:K:322:ASN:HA	2.05	0.71
2:B:148:TRP:HZ3	2:B:166:LEU:HB2	1.56	0.70
2:C:47:ASN:OD1	2:K:30:ARG:NH1	2.25	0.70
2:F:185:LEU:HD11	2:H:187:MET:HE3	1.74	0.70
2:L:164:SER:HA	2:L:186:HIS:O	1.90	0.70
2:C:260:ARG:HG2	2:C:362:TRP:CD1	2.27	0.70
2:B:206:THR:HG22	2:B:228:PHE:HB3	1.73	0.70
2:H:280:MET:SD	2:H:280:MET:N	2.65	0.69
2:K:148:TRP:HZ3	2:K:166:LEU:HB2	1.57	0.69
2:K:206:THR:HG22	2:K:228:PHE:HB3	1.74	0.69
2:B:230:LEU:HD12	2:B:246:ILE:HD13	1.76	0.68
2:F:206:THR:O	2:F:229:ASN:ND2	2.26	0.68
2:H:316:MET:HA	2:H:316:MET:HE3	1.75	0.68
1:E:1004:ILE:HG13	1:I:1004:ILE:HD12	1.76	0.68
1:E:961:ASP:OD2	2:L:87:ARG:NH1	2.28	0.66
2:K:330:THR:HA	2:K:340:TRP:HA	1.77	0.66
2:A:185:LEU:HD11	2:C:187:MET:HE3	1.78	0.66
2:B:30:ARG:NH1	2:H:47:ASN:OD1	2.29	0.66
2:F:146:MET:HG3	2:G:148:TRP:HB3	1.77	0.66
2:A:164:SER:HA	2:A:186:HIS:O	1.96	0.66
2:A:314:ASN:OD1	2:C:329:SER:OG	2.14	0.65
2:A:293:THR:O	2:B:325:ARG:NH2	2.30	0.65
1:D:940:ARG:HG2	1:E:941:LEU:HD21	1.77	0.65
2:J:206:THR:O	2:J:229:ASN:ND2	2.30	0.65
2:J:266:GLN:NE2	2:J:268:CYS:SG	2.67	0.65
2:F:85:GLN:OE1	2:G:90:ASN:ND2	2.30	0.65
2:F:312:MET:HE2	2:G:357:VAL:HG22	1.79	0.65
2:A:266:GLN:NE2	2:A:268:CYS:SG	2.69	0.64
2:A:325:ARG:HD3	2:C:343:TYR:HE1	1.62	0.64
2:F:266:GLN:NE2	2:F:268:CYS:SG	2.70	0.64
2:H:267:ILE:HG23	2:H:359:MET:HB3	1.79	0.64
2:B:211:ARG:HD2	2:B:218:TRP:HB3	1.79	0.64
2:J:85:GLN:OE1	2:K:90:ASN:ND2	2.30	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:961:ASP:OD1	2:C:87:ARG:NH1	2.30	0.64
2:A:85:GLN:OE1	2:B:90:ASN:ND2	2.31	0.64
2:H:342:GLY:HA3	2:H:352:MET:HE1	1.78	0.64
2:C:158:LEU:HD11	2:C:184:VAL:HG21	1.80	0.64
2:G:330:THR:HA	2:G:340:TRP:HA	1.79	0.64
2:A:269:TRP:CE2	2:C:359:MET:HE1	2.33	0.63
2:H:206:THR:HG22	2:H:228:PHE:HB3	1.80	0.63
2:C:206:THR:O	2:C:229:ASN:ND2	2.29	0.63
2:G:317:ARG:NH2	2:G:322:ASN:HA	2.13	0.63
2:K:211:ARG:HD2	2:K:218:TRP:HB3	1.80	0.63
2:B:280:MET:HE2	2:B:292:ILE:H	1.63	0.63
2:H:331:MET:HE1	2:H:340:TRP:HA	1.81	0.63
2:A:206:THR:O	2:A:229:ASN:ND2	2.31	0.63
2:K:225:TYR:CG	2:K:246:ILE:HD11	2.34	0.63
2:C:206:THR:HG22	2:C:228:PHE:HB3	1.81	0.62
2:J:293:THR:O	2:K:325:ARG:NH2	2.32	0.62
1:E:1014:ASP:HB2	1:I:1015:ARG:NH1	2.13	0.62
2:K:315:PRO:HA	2:K:354:ALA:HA	1.81	0.62
2:A:334:THR:HG23	2:A:336:THR:H	1.65	0.62
2:K:164:SER:HA	2:K:186:HIS:O	2.00	0.62
2:L:266:GLN:HB2	2:L:362:TRP:HD1	1.65	0.62
2:C:266:GLN:HB2	2:C:362:TRP:CD1	2.33	0.62
2:G:277:GLY:HA2	2:G:351:GLY:HA3	1.82	0.62
2:B:277:GLY:HA2	2:B:351:GLY:HA3	1.80	0.61
2:F:164:SER:HA	2:F:186:HIS:O	2.00	0.61
2:A:220:ARG:HE	2:B:228:PHE:HE1	1.48	0.61
2:J:213:LYS:HE3	2:J:216:GLY:HA2	1.83	0.61
2:H:206:THR:O	2:H:229:ASN:ND2	2.31	0.61
2:J:334:THR:HG23	2:J:336:THR:H	1.66	0.61
2:F:334:THR:HG23	2:F:336:THR:H	1.65	0.61
2:L:130:THR:OG1	2:L:133:ASN:OD1	2.19	0.61
2:F:293:THR:O	2:G:325:ARG:NH2	2.33	0.60
2:B:260:ARG:NE	2:B:266:GLN:OE1	2.26	0.60
2:G:176:PRO:HG3	2:G:221:TRP:CG	2.35	0.60
2:C:267:ILE:HG23	2:C:359:MET:HB3	1.82	0.60
1:E:1021:ARG:HE	1:I:1022:LEU:HD22	1.67	0.60
2:F:34:ALA:HB3	2:F:73:VAL:HB	1.84	0.60
2:B:330:THR:HA	2:B:340:TRP:HA	1.82	0.60
2:C:130:THR:OG1	2:C:133:ASN:OD1	2.19	0.60
2:L:246:ILE:HA	2:L:262:ALA:HB2	1.82	0.60
2:L:267:ILE:HG23	2:L:359:MET:HB3	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:14:ASN:HA	2:G:59:ASN:HB3	1.83	0.59
2:A:213:LYS:HB2	2:A:218:TRP:CE3	2.38	0.59
2:G:164:SER:HA	2:G:186:HIS:O	2.02	0.59
2:L:211:ARG:HB3	2:L:221:TRP:CE3	2.38	0.59
2:C:316:MET:HA	2:C:316:MET:HE3	1.84	0.59
2:H:260:ARG:HG2	2:H:362:TRP:CD1	2.38	0.59
1:D:1014:ASP:HB2	1:E:1015:ARG:CZ	2.33	0.59
2:B:176:PRO:HG3	2:B:221:TRP:CG	2.38	0.59
2:C:28:ASN:N	2:C:28:ASN:OD1	2.35	0.59
2:C:87:ARG:HD2	1:I:961:ASP:HB2	1.84	0.59
1:D:954:ASP:HA	1:D:956:ASN:H	1.68	0.59
2:H:246:ILE:HA	2:H:262:ALA:HB2	1.83	0.59
2:J:361:ARG:NE	2:K:257:GLU:OE1	2.35	0.59
2:L:28:ASN:OD1	2:L:28:ASN:N	2.35	0.59
2:F:220:ARG:HE	2:G:228:PHE:HE2	1.51	0.59
2:K:176:PRO:HG3	2:K:221:TRP:CG	2.38	0.59
2:L:276:VAL:O	2:L:352:MET:N	2.36	0.59
2:G:146:MET:HB2	2:H:149:ALA:HB2	1.85	0.58
2:L:311:VAL:C	2:L:312:MET:HE2	2.28	0.58
2:C:108:THR:HG23	2:C:111:GLN:H	1.68	0.58
2:G:348:VAL:HG13	2:G:351:GLY:HA2	1.85	0.58
2:K:14:ASN:HA	2:K:59:ASN:HB3	1.84	0.58
2:A:213:LYS:HE3	2:A:216:GLY:HA2	1.85	0.58
2:K:20:GLY:N	2:K:52:THR:O	2.36	0.58
2:A:34:ALA:HB3	2:A:73:VAL:HB	1.86	0.58
2:C:211:ARG:HB3	2:C:221:TRP:CE3	2.39	0.58
2:J:352:MET:N	2:J:352:MET:SD	2.77	0.58
2:A:249:ARG:HB2	2:C:361:ARG:HH22	1.69	0.58
2:G:20:GLY:N	2:G:52:THR:O	2.36	0.58
2:H:144:ASN:OD1	2:H:145:GLN:N	2.36	0.58
2:F:213:LYS:HB2	2:F:218:TRP:CD2	2.39	0.57
2:B:20:GLY:N	2:B:52:THR:O	2.37	0.57
2:H:211:ARG:HB3	2:H:221:TRP:CE3	2.39	0.57
2:H:239:SER:O	2:H:239:SER:OG	2.23	0.57
2:B:194:PHE:HB3	2:C:202:LEU:HD21	1.84	0.57
2:C:276:VAL:O	2:C:352:MET:N	2.37	0.57
2:C:280:MET:SD	2:C:280:MET:N	2.78	0.57
2:L:213:LYS:HB2	2:L:218:TRP:CD2	2.40	0.57
2:J:312:MET:HE2	2:K:357:VAL:HG22	1.87	0.57
2:B:348:VAL:HG13	2:B:351:GLY:HA2	1.86	0.57
2:G:211:ARG:HD2	2:G:218:TRP:HB3	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:258:TYR:HE2	2:H:260:ARG:HE	1.53	0.57
2:G:320:GLY:O	2:G:322:ASN:ND2	2.37	0.57
1:I:954:ASP:HA	1:I:956:ASN:H	1.69	0.57
2:J:34:ALA:HB3	2:J:73:VAL:HB	1.87	0.57
2:J:292:ILE:HG13	2:J:343:TYR:CD1	2.34	0.57
2:K:277:GLY:HA2	2:K:351:GLY:HA3	1.86	0.56
2:K:348:VAL:HG13	2:K:351:GLY:HA2	1.86	0.56
1:D:1013:SER:HA	1:D:1016:GLN:HE22	1.70	0.56
2:A:193:ASP:HA	2:A:213:LYS:HE2	1.86	0.56
2:A:352:MET:SD	2:A:352:MET:N	2.78	0.56
2:K:280:MET:HE1	2:K:282:TYR:HB2	1.86	0.56
2:K:316:MET:SD	2:K:316:MET:N	2.78	0.56
2:B:359:MET:HE1	2:C:269:TRP:CE3	2.40	0.56
2:A:11:VAL:HG12	2:A:18:VAL:HG22	1.88	0.56
2:J:331:MET:CB	2:K:317:ARG:HD3	2.34	0.56
2:K:187:MET:HG2	2:L:166:LEU:HD13	1.88	0.56
2:L:108:THR:HG23	2:L:111:GLN:H	1.70	0.56
2:J:331:MET:HA	2:K:316:MET:HB3	1.88	0.56
2:L:206:THR:O	2:L:229:ASN:ND2	2.33	0.56
2:B:348:VAL:HG22	2:B:351:GLY:H	1.71	0.56
2:K:317:ARG:NH1	2:K:324:SER:H	2.03	0.56
2:A:325:ARG:HD2	2:C:292:ILE:HD12	1.88	0.55
2:F:29:VAL:HG22	2:F:72:VAL:HG11	1.87	0.55
2:G:198:GLN:NE2	2:G:200:TYR:OH	2.37	0.55
2:F:267:ILE:HD11	2:F:359:MET:HE2	1.89	0.55
2:F:325:ARG:HD3	2:H:343:TYR:HE1	1.70	0.55
2:G:153:MET:SD	2:G:153:MET:N	2.79	0.55
2:G:225:TYR:CE2	2:H:230:LEU:HD13	2.41	0.55
2:J:329:SER:HA	2:K:314:ASN:HD21	1.70	0.55
2:B:153:MET:SD	2:B:153:MET:N	2.77	0.55
2:L:266:GLN:HB2	2:L:362:TRP:CD1	2.41	0.55
2:B:280:MET:HE1	2:B:282:TYR:HB2	1.87	0.55
2:B:307:ARG:HH22	2:C:269:TRP:HE1	1.55	0.55
2:H:331:MET:SD	2:H:331:MET:N	2.80	0.55
2:G:145:GLN:O	2:G:147:GLY:N	2.38	0.55
2:J:11:VAL:HG12	2:J:18:VAL:HG22	1.88	0.55
2:J:344:ASP:OD1	2:J:344:ASP:N	2.40	0.55
2:K:210:MET:HG3	2:K:222:VAL:HG22	1.89	0.55
2:L:291:TYR:O	2:L:344:ASP:N	2.31	0.55
2:K:348:VAL:HG22	2:K:351:GLY:H	1.72	0.55
2:A:318:ALA:HB2	2:A:353:ALA:HB2	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:225:TYR:CG	2:B:246:ILE:HD11	2.42	0.55
2:B:151:ASN:OD1	2:B:151:ASN:N	2.40	0.55
2:F:213:LYS:HB2	2:F:218:TRP:CE3	2.42	0.55
2:G:210:MET:HG3	2:G:222:VAL:HG22	1.88	0.55
2:K:359:MET:HE1	2:L:269:TRP:CE3	2.42	0.55
1:D:961:ASP:HB2	2:H:87:ARG:HD2	1.90	0.54
2:A:344:ASP:OD1	2:A:344:ASP:N	2.40	0.54
2:F:11:VAL:HG12	2:F:18:VAL:HG22	1.88	0.54
2:G:257:GLU:HB2	2:G:269:TRP:CE2	2.42	0.54
2:J:159:ASP:OD1	2:J:211:ARG:NH2	2.41	0.54
2:A:112:ALA:O	2:A:116:MET:HG3	2.06	0.54
2:C:176:PRO:HG3	2:C:221:TRP:CD2	2.42	0.54
2:L:340:TRP:CH2	2:L:352:MET:HE3	2.42	0.54
2:L:176:PRO:HG3	2:L:221:TRP:CD2	2.42	0.54
2:B:220:ARG:HH11	2:C:228:PHE:HE1	1.55	0.54
2:B:266:GLN:NE2	2:B:303:VAL:HG13	2.22	0.54
2:F:352:MET:SD	2:F:352:MET:N	2.81	0.54
2:G:223:LEU:HD11	2:G:229:ASN:HD22	1.72	0.54
2:H:176:PRO:HG3	2:H:221:TRP:CD2	2.43	0.54
2:J:249:ARG:HB2	2:L:361:ARG:HH22	1.73	0.54
2:A:29:VAL:HG22	2:A:72:VAL:HG11	1.90	0.54
2:G:327:TRP:HE1	2:H:327:TRP:CD1	2.26	0.54
2:H:276:VAL:O	2:H:352:MET:N	2.33	0.54
2:H:291:TYR:O	2:H:344:ASP:N	2.33	0.54
2:B:14:ASN:HA	2:B:59:ASN:HB3	1.90	0.54
2:F:318:ALA:HB2	2:F:353:ALA:HB2	1.90	0.54
1:I:1004:ILE:O	1:I:1008:GLU:HG3	2.08	0.54
2:K:151:ASN:OD1	2:K:151:ASN:N	2.40	0.54
2:L:316:MET:HE3	2:L:316:MET:HA	1.90	0.54
2:F:246:ILE:HG12	2:G:230:LEU:HD21	1.89	0.53
2:J:267:ILE:HD11	2:J:359:MET:HE2	1.89	0.53
2:L:144:ASN:OD1	2:L:145:GLN:N	2.41	0.53
2:B:320:GLY:O	2:B:322:ASN:ND2	2.37	0.53
2:B:359:MET:HE1	2:C:269:TRP:CD2	2.43	0.53
2:J:164:SER:HA	2:J:186:HIS:O	2.08	0.53
2:H:280:MET:CE	2:H:294:PRO:HG3	2.37	0.53
2:B:327:TRP:HE1	2:C:327:TRP:CD1	2.27	0.53
2:C:164:SER:HA	2:C:186:HIS:O	2.09	0.53
2:F:278:ALA:HA	2:F:294:PRO:HD3	1.91	0.53
2:A:278:ALA:HA	2:A:294:PRO:HD3	1.89	0.53
2:J:278:ALA:HA	2:J:294:PRO:HD3	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:225:TYR:HE2	2:L:230:LEU:HD13	1.73	0.53
2:B:210:MET:HG3	2:B:222:VAL:HG22	1.90	0.53
2:K:280:MET:HE2	2:K:292:ILE:H	1.73	0.53
2:K:328:GLY:HA3	2:K:342:GLY:HA2	1.90	0.53
2:C:19:LEU:HD13	2:C:53:VAL:HG22	1.91	0.52
2:F:47:ASN:HB3	2:F:55:SER:HB2	1.91	0.52
2:J:327:TRP:NE1	2:L:327:TRP:HE1	2.08	0.52
2:A:227:GLN:OE1	2:C:220:ARG:NH2	2.38	0.52
2:A:327:TRP:NE1	2:C:327:TRP:HE1	2.07	0.52
2:C:268:CYS:HB3	2:C:302:PRO:HD2	1.92	0.52
2:H:158:LEU:HD11	2:H:184:VAL:HG21	1.90	0.52
2:J:29:VAL:HG22	2:J:72:VAL:HG11	1.91	0.52
2:J:331:MET:SD	2:J:339:SER:HB2	2.49	0.52
2:F:159:ASP:OD1	2:F:211:ARG:NH2	2.43	0.52
2:B:315:PRO:HA	2:B:354:ALA:HA	1.91	0.52
2:F:128:ALA:O	2:H:119:SER:OG	2.21	0.52
2:F:158:LEU:HD21	2:F:169:HIS:HB3	1.92	0.52
2:G:225:TYR:CG	2:G:246:ILE:HD11	2.44	0.52
2:K:359:MET:HE1	2:L:269:TRP:CD2	2.44	0.52
2:A:39:ASP:OD1	2:A:39:ASP:N	2.42	0.52
2:F:327:TRP:NE1	2:H:327:TRP:HE1	2.07	0.52
2:J:158:LEU:HD21	2:J:169:HIS:HB3	1.91	0.52
1:E:950:ASP:OD2	2:G:30:ARG:NH2	2.43	0.52
2:F:331:MET:SD	2:F:339:SER:HB2	2.50	0.52
2:F:361:ARG:NE	2:G:257:GLU:OE1	2.41	0.52
2:H:331:MET:HE1	2:H:340:TRP:CA	2.40	0.52
2:L:268:CYS:HB3	2:L:302:PRO:HD2	1.91	0.52
2:L:320:GLY:O	2:L:322:ASN:ND2	2.40	0.52
2:B:317:ARG:NH2	2:B:322:ASN:HA	2.24	0.52
2:H:213:LYS:HB2	2:H:218:TRP:CD2	2.44	0.52
2:A:159:ASP:OD1	2:A:211:ARG:NH2	2.42	0.52
2:F:331:MET:HA	2:G:316:MET:HB3	1.92	0.52
2:G:348:VAL:HG22	2:G:351:GLY:H	1.74	0.52
2:H:19:LEU:HD13	2:H:53:VAL:HG22	1.91	0.52
2:L:34:ALA:HB3	2:L:73:VAL:HB	1.91	0.52
2:H:108:THR:HG23	2:H:111:GLN:H	1.75	0.52
2:A:361:ARG:NE	2:B:257:GLU:OE1	2.38	0.51
2:C:213:LYS:HB2	2:C:218:TRP:CD2	2.44	0.51
2:L:327:TRP:CE2	2:L:343:TYR:HD2	2.29	0.51
2:F:112:ALA:O	2:F:116:MET:HG3	2.10	0.51
2:L:331:MET:HE2	2:L:341:TYR:CD2	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:979:ARG:NH2	1:E:976:GLU:O	2.43	0.51
2:A:311:VAL:HG23	2:A:330:THR:HG21	1.93	0.51
2:G:47:ASN:HB3	2:G:55:SER:HB2	1.91	0.51
2:G:118:ILE:O	2:G:123:ARG:NH1	2.43	0.51
2:H:327:TRP:CE2	2:H:343:TYR:HD2	2.28	0.51
1:I:976:GLU:HG3	1:I:977:THR:N	2.25	0.51
2:A:158:LEU:HD21	2:A:169:HIS:HB3	1.91	0.51
2:J:106:SER:O	2:L:101:LYS:HE2	2.10	0.51
2:L:331:MET:HE1	2:L:340:TRP:CA	2.39	0.51
1:D:922:SER:O	1:D:926:GLU:HG2	2.10	0.51
2:C:307:ARG:HG2	2:C:308:PRO:HD2	1.93	0.51
1:E:1014:ASP:HB2	1:I:1015:ARG:CZ	2.41	0.51
2:F:344:ASP:OD1	2:F:344:ASP:N	2.42	0.51
2:H:315:PRO:HB2	2:H:352:MET:HG2	1.92	0.51
2:K:220:ARG:HH11	2:L:228:PHE:HE1	1.57	0.51
2:C:329:SER:HB3	2:C:341:TYR:HE1	1.76	0.51
2:C:331:MET:HE1	2:C:340:TRP:HA	1.92	0.51
2:J:112:ALA:O	2:J:116:MET:HG3	2.11	0.51
2:A:331:MET:HB2	2:B:317:ARG:HD3	1.92	0.50
2:L:331:MET:SD	2:L:331:MET:N	2.82	0.50
2:C:112:ALA:O	2:C:116:MET:HG3	2.12	0.50
2:F:39:ASP:OD1	2:F:39:ASP:N	2.44	0.50
2:F:148:TRP:HZ2	2:H:185:LEU:HD11	1.75	0.50
2:J:148:TRP:HZ2	2:L:185:LEU:HD11	1.76	0.50
2:G:225:TYR:HE2	2:H:230:LEU:HD13	1.75	0.50
2:G:230:LEU:HD22	2:G:246:ILE:HD13	1.93	0.50
2:G:317:ARG:HH22	2:G:322:ASN:HA	1.76	0.50
1:I:922:SER:O	1:I:926:GLU:HG2	2.10	0.50
2:K:307:ARG:NH2	2:L:257:GLU:OE2	2.44	0.50
2:F:230:LEU:HD13	2:H:246:ILE:HG21	1.94	0.50
2:G:341:TYR:OH	2:H:326:PRO:O	2.26	0.50
2:K:334:THR:OG1	2:K:337:LEU:HD23	2.11	0.50
2:J:213:LYS:HB2	2:J:218:TRP:CE3	2.46	0.50
2:F:198:GLN:OE1	2:F:199:TRP:N	2.44	0.50
2:A:259:VAL:HG21	2:C:265:THR:HG21	1.92	0.50
2:C:291:TYR:O	2:C:344:ASP:N	2.29	0.50
2:F:249:ARG:HD2	2:H:263:ASP:HB2	1.93	0.50
2:G:148:TRP:CZ3	2:G:166:LEU:HB2	2.41	0.50
2:J:47:ASN:HB3	2:J:55:SER:HB2	1.94	0.50
2:K:292:ILE:HG21	2:L:325:ARG:HD2	1.94	0.50
2:C:331:MET:SD	2:C:331:MET:N	2.85	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:316:MET:HB3	2:L:331:MET:O	2.12	0.50
2:K:198:GLN:NE2	2:K:200:TYR:OH	2.38	0.50
1:D:1004:ILE:O	1:D:1008:GLU:HG3	2.12	0.49
2:A:312:MET:HB3	2:C:312:MET:SD	2.52	0.49
2:B:198:GLN:NE2	2:B:200:TYR:OH	2.38	0.49
2:H:261:TYR:HD2	2:H:265:THR:HB	1.77	0.49
2:H:320:GLY:O	2:H:322:ASN:ND2	2.40	0.49
2:J:340:TRP:CZ2	2:J:354:ALA:HB2	2.47	0.49
2:B:268:CYS:SG	2:B:358:ALA:HB3	2.52	0.49
2:B:299:TRP:HB3	2:B:338:PHE:CE1	2.48	0.49
2:G:307:ARG:NH2	2:H:257:GLU:OE2	2.46	0.49
2:H:340:TRP:CZ2	2:H:354:ALA:HB2	2.47	0.49
2:A:106:SER:O	2:C:101:LYS:HE2	2.13	0.49
2:A:314:ASN:ND2	2:C:330:THR:HB	2.24	0.49
2:C:292:ILE:HA	2:C:343:TYR:HA	1.93	0.49
2:F:263:ASP:HB3	2:G:247:ILE:HD13	1.94	0.49
2:G:316:MET:SD	2:G:316:MET:N	2.85	0.49
2:A:269:TRP:CD2	2:C:359:MET:HE1	2.48	0.49
2:C:11:VAL:HG12	2:C:18:VAL:HG22	1.94	0.49
1:E:1013:SER:HA	1:E:1016:GLN:HE22	1.77	0.49
1:E:1013:SER:HA	1:E:1016:GLN:NE2	2.27	0.49
2:F:254:GLY:HA2	2:H:307:ARG:NH1	2.28	0.49
2:H:304:SER:HB2	2:H:336:THR:HG22	1.94	0.49
2:J:325:ARG:HD3	2:L:343:TYR:HE1	1.78	0.49
2:J:331:MET:N	2:J:331:MET:HE3	2.27	0.49
1:D:976:GLU:O	1:I:979:ARG:NH2	2.45	0.49
2:K:257:GLU:HB2	2:K:269:TRP:CE2	2.47	0.49
2:C:320:GLY:O	2:C:322:ASN:ND2	2.42	0.49
2:F:148:TRP:HZ3	2:F:166:LEU:HB2	1.78	0.49
2:K:307:ARG:HH22	2:L:269:TRP:HE1	1.61	0.49
2:L:340:TRP:CZ2	2:L:354:ALA:HB2	2.47	0.49
2:H:260:ARG:HH22	2:H:303:VAL:HG21	1.78	0.49
2:L:280:MET:HE1	2:L:294:PRO:HG3	1.95	0.49
2:B:145:GLN:O	2:B:147:GLY:N	2.44	0.49
2:B:266:GLN:HB2	2:B:362:TRP:CD1	2.48	0.49
2:C:340:TRP:CH2	2:C:352:MET:HE3	2.48	0.49
2:A:47:ASN:HB3	2:A:55:SER:HB2	1.95	0.48
2:B:81:ASN:O	2:B:85:GLN:NE2	2.46	0.48
2:F:227:GLN:OE1	2:H:220:ARG:NH2	2.38	0.48
2:F:311:VAL:HG23	2:F:330:THR:HG21	1.93	0.48
2:F:331:MET:HE3	2:F:331:MET:N	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:210:MET:SD	2:K:208:GLN:NE2	2.86	0.48
2:B:101:LYS:NZ	2:C:106:SER:O	2.37	0.48
2:B:118:ILE:O	2:B:123:ARG:NH1	2.46	0.48
1:E:979:ARG:NH2	1:I:976:GLU:O	2.46	0.48
2:H:268:CYS:HB3	2:H:302:PRO:HD2	1.95	0.48
2:K:327:TRP:HE1	2:L:327:TRP:CD1	2.30	0.48
2:C:234:ALA:N	2:C:248:GLN:OE1	2.47	0.48
2:C:239:SER:O	2:C:239:SER:OG	2.22	0.48
2:G:359:MET:HE1	2:H:269:TRP:CE3	2.48	0.48
2:H:157:ASP:OD2	2:H:157:ASP:N	2.47	0.48
2:A:200:TYR:OH	2:C:198:GLN:OE1	2.20	0.48
2:K:11:VAL:HG12	2:K:18:VAL:HG22	1.95	0.48
2:B:11:VAL:HG12	2:B:18:VAL:HG22	1.94	0.48
2:F:254:GLY:HA2	2:H:307:ARG:HH11	1.79	0.48
2:A:287:THR:HG21	2:C:287:THR:HG21	1.95	0.48
2:B:164:SER:HA	2:B:186:HIS:O	2.13	0.48
2:J:146:MET:HG2	2:K:148:TRP:HD1	1.78	0.48
2:K:331:MET:C	2:L:316:MET:HE1	2.39	0.48
2:A:330:THR:HA	2:A:340:TRP:HA	1.94	0.48
1:E:922:SER:O	1:E:926:GLU:HG2	2.13	0.48
2:F:329:SER:HA	2:G:314:ASN:HD21	1.79	0.48
2:J:230:LEU:HD13	2:L:246:ILE:HG21	1.94	0.48
2:L:206:THR:HG22	2:L:228:PHE:HB3	1.95	0.48
2:L:260:ARG:HG2	2:L:362:TRP:CD1	2.49	0.48
2:A:272:THR:HB	2:A:354:ALA:HB3	1.96	0.48
2:K:225:TYR:CE2	2:L:230:LEU:HD13	2.48	0.48
2:F:85:GLN:O	2:F:89:ILE:HD13	2.14	0.47
2:K:148:TRP:CZ3	2:K:166:LEU:HB2	2.42	0.47
2:L:12:THR:HB	2:L:15:SER:HB3	1.95	0.47
2:B:267:ILE:CD1	2:B:359:MET:HG2	2.43	0.47
2:C:170:GLY:HA2	2:C:181:GLN:HG2	1.96	0.47
2:F:75:ILE:HD12	2:F:75:ILE:HA	1.73	0.47
2:G:11:VAL:HG12	2:G:18:VAL:HG22	1.95	0.47
2:J:311:VAL:HG23	2:J:330:THR:HG21	1.96	0.47
2:L:292:ILE:HA	2:L:343:TYR:HA	1.95	0.47
2:C:330:THR:HG23	2:C:339:SER:O	2.14	0.47
2:F:196:VAL:HG22	2:F:212:ILE:HD13	1.96	0.47
2:F:340:TRP:CZ2	2:F:354:ALA:HB2	2.50	0.47
2:J:185:LEU:HD11	2:L:187:MET:HE3	1.96	0.47
2:J:287:THR:HG21	2:L:287:THR:HG21	1.96	0.47
2:A:280:MET:C	2:A:280:MET:HE2	2.39	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:331:MET:SD	2:F:332:SER:N	2.87	0.47
2:H:209:TYR:CZ	2:H:223:LEU:HD12	2.49	0.47
2:J:280:MET:HE2	2:J:280:MET:C	2.40	0.47
2:H:329:SER:HB3	2:H:341:TYR:HE1	1.80	0.47
2:F:316:MET:HE1	2:F:355:SER:HB2	1.95	0.47
2:A:248:GLN:OE1	2:A:258:TYR:OH	2.33	0.47
1:E:1003:ARG:HE	1:I:1004:ILE:HD13	1.78	0.47
2:F:106:SER:O	2:H:101:LYS:HE2	2.13	0.47
2:H:12:THR:HB	2:H:15:SER:HB3	1.97	0.47
2:J:39:ASP:OD1	2:J:39:ASP:N	2.42	0.47
2:J:148:TRP:HZ3	2:J:166:LEU:HB2	1.79	0.47
2:K:254:GLY:H	2:K:257:GLU:CD	2.23	0.47
2:K:320:GLY:O	2:K:322:ASN:ND2	2.40	0.47
2:A:148:TRP:HZ2	2:C:185:LEU:HD11	1.80	0.47
2:B:305:PHE:CD1	2:B:309:PRO:HB3	2.50	0.47
2:C:12:THR:HB	2:C:15:SER:HB3	1.97	0.47
2:C:175:SER:OG	2:C:177:VAL:O	2.28	0.47
2:C:327:TRP:CE2	2:C:343:TYR:HD2	2.32	0.47
1:E:1004:ILE:O	1:E:1008:GLU:HG3	2.15	0.47
2:G:315:PRO:HA	2:G:354:ALA:HA	1.96	0.47
2:H:230:LEU:HD11	2:H:246:ILE:HD11	1.97	0.47
2:J:36:ARG:NE	2:K:42:TRP:O	2.47	0.47
2:J:227:GLN:OE1	2:L:220:ARG:NH2	2.39	0.47
2:C:48:VAL:H	2:K:30:ARG:HH12	1.63	0.47
2:F:248:GLN:OE1	2:F:258:TYR:OH	2.32	0.47
2:F:316:MET:HB3	2:H:331:MET:O	2.14	0.47
2:L:36:ARG:HB2	2:L:42:TRP:CE3	2.49	0.47
2:A:198:GLN:OE1	2:A:199:TRP:N	2.47	0.47
2:B:341:TYR:HB2	2:C:325:ARG:HH12	1.80	0.47
1:E:1021:ARG:NE	1:I:1022:LEU:HD22	2.28	0.47
2:F:287:THR:HG21	2:H:287:THR:HG21	1.96	0.47
2:H:164:SER:HA	2:H:186:HIS:O	2.15	0.47
2:H:292:ILE:HA	2:H:343:TYR:HA	1.97	0.47
2:L:234:ALA:N	2:L:248:GLN:OE1	2.48	0.46
2:J:316:MET:SD	2:J:316:MET:N	2.88	0.46
2:L:147:GLY:N	2:L:153:MET:SD	2.88	0.46
2:A:213:LYS:HB2	2:A:218:TRP:CD2	2.50	0.46
2:K:81:ASN:O	2:K:85:GLN:NE2	2.48	0.46
2:K:363:ASN:OD1	2:K:363:ASN:N	2.48	0.46
2:G:328:GLY:HA2	2:G:343:TYR:CD1	2.50	0.46
2:K:224:GLN:OE1	2:L:208:GLN:NE2	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:304:SER:HB2	2:L:336:THR:HG22	1.97	0.46
2:A:148:TRP:HZ3	2:A:166:LEU:HB2	1.80	0.46
2:C:36:ARG:HB2	2:C:42:TRP:CE3	2.50	0.46
2:L:315:PRO:HB2	2:L:352:MET:HG2	1.96	0.46
2:A:230:LEU:HD13	2:C:246:ILE:HG21	1.98	0.46
2:G:297:TYR:HB2	2:G:340:TRP:CD1	2.51	0.46
2:H:307:ARG:CZ	2:H:309:PRO:HA	2.46	0.46
2:A:87:ARG:HB2	2:C:85:GLN:OE1	2.16	0.46
2:A:87:ARG:HD3	2:C:85:GLN:HE22	1.81	0.46
2:B:331:MET:C	2:C:316:MET:HE1	2.41	0.46
2:C:245:ALA:HB3	2:C:248:GLN:HE22	1.79	0.46
1:E:1021:ARG:HH21	1:I:1022:LEU:HD22	1.81	0.46
2:H:36:ARG:HB2	2:H:42:TRP:CE3	2.51	0.46
2:H:175:SER:OG	2:H:177:VAL:O	2.28	0.46
2:K:230:LEU:HD22	2:K:246:ILE:HD13	1.97	0.46
2:K:268:CYS:SG	2:K:358:ALA:HB3	2.56	0.46
2:L:348:VAL:HG12	2:L:351:GLY:H	1.81	0.46
2:A:316:MET:HB3	2:C:331:MET:O	2.16	0.46
2:B:328:GLY:HA2	2:B:343:TYR:CD1	2.50	0.46
2:C:315:PRO:HB2	2:C:352:MET:HG2	1.97	0.46
2:F:272:THR:HB	2:F:354:ALA:HB3	1.98	0.46
2:H:280:MET:HE2	2:H:294:PRO:HG3	1.97	0.46
2:A:340:TRP:CZ2	2:A:354:ALA:HB2	2.51	0.46
2:G:268:CYS:SG	2:G:358:ALA:HB3	2.56	0.46
2:G:80:LYS:HE3	2:G:80:LYS:HB3	1.63	0.46
2:G:331:MET:HB2	2:G:341:TYR:HD1	1.80	0.46
2:A:230:LEU:O	2:A:245:ALA:HB1	2.16	0.45
2:F:307:ARG:HG2	2:F:308:PRO:HD2	1.98	0.45
2:K:317:ARG:HH11	2:K:317:ARG:HG2	1.81	0.45
2:J:145:GLN:HA	2:J:153:MET:HE1	1.99	0.45
2:J:254:GLY:HA2	2:L:307:ARG:NH1	2.31	0.45
2:J:307:ARG:HG2	2:J:308:PRO:HD2	1.99	0.45
2:K:327:TRP:O	2:K:343:TYR:N	2.41	0.45
2:J:200:TYR:OH	2:L:198:GLN:OE1	2.19	0.45
2:J:327:TRP:N	2:J:343:TYR:O	2.41	0.45
2:L:311:VAL:HG22	2:L:358:ALA:HB1	1.99	0.45
2:A:85:GLN:O	2:A:89:ILE:HD13	2.17	0.45
2:A:316:MET:N	2:A:316:MET:SD	2.90	0.45
2:B:154:ASN:N	2:B:154:ASN:OD1	2.49	0.45
2:C:348:VAL:HG12	2:C:351:GLY:H	1.82	0.45
2:F:273:THR:O	2:F:273:THR:OG1	2.33	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:266:GLN:HB2	2:G:362:TRP:CD1	2.52	0.45
2:H:266:GLN:HB2	2:H:362:TRP:CD1	2.52	0.45
2:K:246:ILE:HA	2:K:262:ALA:HB2	1.97	0.45
1:D:939:SER:O	1:D:943:VAL:HG23	2.17	0.45
2:F:280:MET:C	2:F:280:MET:HE2	2.42	0.45
2:C:146:MET:O	2:C:146:MET:HG2	2.15	0.45
2:C:263:ASP:OD1	2:C:264:GLY:N	2.50	0.45
2:H:28:ASN:OD1	2:H:28:ASN:N	2.49	0.45
2:H:327:TRP:CZ3	2:H:343:TYR:HB2	2.52	0.45
2:J:85:GLN:O	2:J:89:ILE:HD13	2.17	0.45
2:G:224:GLN:OE1	2:H:208:GLN:NE2	2.49	0.45
2:J:325:ARG:HB3	2:L:343:TYR:OH	2.16	0.45
2:A:118:ILE:O	2:A:123:ARG:NH1	2.50	0.44
2:A:297:TYR:O	2:A:340:TRP:HD1	2.00	0.44
2:A:313:VAL:HG12	2:A:356:TYR:HB2	1.98	0.44
2:B:169:HIS:HD1	2:B:173:VAL:HB	1.82	0.44
2:B:187:MET:HG2	2:C:166:LEU:HD12	1.98	0.44
2:C:34:ALA:HB3	2:C:73:VAL:HB	1.99	0.44
2:G:81:ASN:O	2:G:85:GLN:NE2	2.50	0.44
2:J:272:THR:HB	2:J:354:ALA:HB3	1.99	0.44
2:L:239:SER:O	2:L:239:SER:OG	2.22	0.44
2:A:36:ARG:NE	2:B:42:TRP:O	2.48	0.44
2:H:246:ILE:O	2:H:261:TYR:HA	2.17	0.44
1:I:973:ALA:O	1:I:977:THR:HG23	2.17	0.44
2:K:316:MET:O	2:K:353:ALA:N	2.32	0.44
2:A:316:MET:HE1	2:A:355:SER:HB2	1.99	0.44
1:I:941:LEU:O	1:I:945:LEU:HD23	2.16	0.44
2:J:196:VAL:HG22	2:J:212:ILE:HD13	2.00	0.44
2:B:224:GLN:OE1	2:C:208:GLN:NE2	2.51	0.44
2:G:73:VAL:HG11	2:H:75:ILE:HD13	1.98	0.44
2:J:198:GLN:OE1	2:J:199:TRP:N	2.51	0.44
2:J:230:LEU:O	2:J:245:ALA:HB1	2.17	0.44
2:L:246:ILE:HG13	2:L:247:ILE:HG13	1.99	0.44
2:C:133:ASN:OD1	2:C:133:ASN:N	2.50	0.44
2:F:138:LEU:HD23	2:F:138:LEU:HA	1.84	0.44
2:F:314:ASN:CG	2:H:329:SER:HG	2.24	0.44
2:H:246:ILE:HG13	2:H:247:ILE:HG13	1.99	0.44
2:L:307:ARG:HG2	2:L:361:ARG:HB2	1.98	0.44
2:L:329:SER:HB3	2:L:341:TYR:HE1	1.81	0.44
2:C:264:GLY:HA2	2:C:362:TRP:CE2	2.53	0.44
2:C:340:TRP:CZ2	2:C:354:ALA:HB2	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:200:TYR:OH	2:H:198:GLN:OE1	2.18	0.44
2:F:302:PRO:HD3	2:F:356:TYR:OH	2.18	0.44
2:L:66:SER:O	2:L:68:GLN:NE2	2.45	0.44
2:L:198:GLN:HE22	2:L:224:GLN:HE22	1.66	0.44
1:D:949:ARG:HH21	2:B:30:ARG:HB2	1.81	0.44
2:F:103:TRP:HA	2:F:106:SER:OG	2.17	0.44
2:G:119:SER:OG	2:H:128:ALA:O	2.27	0.44
2:G:213:LYS:HB2	2:G:218:TRP:CD2	2.52	0.44
2:J:302:PRO:HD3	2:J:356:TYR:OH	2.18	0.44
2:A:49:THR:HB	2:A:53:VAL:HG13	1.98	0.44
2:B:264:GLY:HA3	2:B:363:ASN:ND2	2.32	0.44
2:C:209:TYR:CZ	2:C:223:LEU:HD12	2.53	0.44
2:C:327:TRP:CZ3	2:C:343:TYR:HB2	2.53	0.44
2:K:80:LYS:HB3	2:K:80:LYS:HE3	1.81	0.44
2:K:260:ARG:HG2	2:K:362:TRP:CD1	2.53	0.44
2:L:36:ARG:HB2	2:L:42:TRP:CZ3	2.53	0.44
2:A:307:ARG:HG2	2:A:308:PRO:HD2	2.00	0.44
2:B:158:LEU:HD21	2:B:169:HIS:HB3	2.00	0.44
2:C:178:ASN:N	2:C:178:ASN:OD1	2.50	0.44
1:E:954:ASP:OD1	1:E:955:GLY:N	2.51	0.44
2:K:158:LEU:HD21	2:K:169:HIS:HB3	2.00	0.44
2:K:266:GLN:HB2	2:K:362:TRP:CD1	2.53	0.44
2:L:19:LEU:HD13	2:L:53:VAL:HG22	1.99	0.44
2:A:145:GLN:HA	2:A:153:MET:HE1	2.00	0.43
2:A:297:TYR:HB2	2:A:340:TRP:NE1	2.33	0.43
2:G:185:LEU:HD23	2:G:185:LEU:HA	1.81	0.43
2:H:260:ARG:NH2	2:H:303:VAL:HG21	2.33	0.43
2:H:331:MET:HE2	2:H:341:TYR:CD2	2.53	0.43
2:J:15:SER:OG	2:J:16:GLU:N	2.51	0.43
2:K:312:MET:HE2	2:L:357:VAL:HG22	2.00	0.43
2:L:170:GLY:HA2	2:L:181:GLN:NE2	2.33	0.43
2:A:128:ALA:O	2:C:119:SER:OG	2.24	0.43
2:A:213:LYS:HG3	2:A:218:TRP:CE2	2.53	0.43
2:A:302:PRO:HD3	2:A:356:TYR:OH	2.17	0.43
2:C:66:SER:O	2:C:68:GLN:NE2	2.44	0.43
2:C:293:THR:N	2:C:342:GLY:O	2.47	0.43
2:F:169:HIS:HD1	2:F:173:VAL:HB	1.82	0.43
2:J:333:VAL:HG22	2:J:338:PHE:HB2	2.00	0.43
2:B:106:SER:OG	2:B:112:ALA:HB2	2.18	0.43
2:F:325:ARG:HD2	2:H:292:ILE:HD12	2.00	0.43
2:H:11:VAL:HG12	2:H:18:VAL:HG22	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:246:ILE:HG12	2:K:230:LEU:HD21	1.99	0.43
1:D:1021:ARG:HH12	1:E:1022:LEU:HD22	1.82	0.43
2:A:208:GLN:OE1	2:C:224:GLN:NE2	2.36	0.43
2:A:317:ARG:HG3	2:C:331:MET:HB2	1.99	0.43
2:L:133:ASN:OD1	2:L:133:ASN:N	2.50	0.43
2:B:185:LEU:HD23	2:B:185:LEU:HA	1.86	0.43
2:G:213:LYS:HB2	2:G:218:TRP:CE3	2.54	0.43
2:J:158:LEU:O	2:J:197:GLN:NE2	2.40	0.43
2:B:153:MET:H	2:B:153:MET:CE	2.31	0.43
2:G:280:MET:CE	2:G:292:ILE:H	2.26	0.43
2:J:269:TRP:HB3	2:L:359:MET:HE1	2.00	0.43
2:K:42:TRP:HE1	2:L:42:TRP:NE1	2.17	0.43
2:K:213:LYS:HB2	2:K:218:TRP:CD2	2.53	0.43
2:K:331:MET:HB2	2:K:341:TYR:HD1	1.83	0.43
2:L:209:TYR:CZ	2:L:223:LEU:HD12	2.54	0.43
2:J:325:ARG:HD2	2:L:292:ILE:HD12	2.00	0.43
2:K:311:VAL:HG23	2:K:330:THR:HG21	2.00	0.43
2:A:75:ILE:HD12	2:A:75:ILE:HA	1.75	0.43
2:A:183:TYR:OH	2:C:189:HIS:HB2	2.19	0.43
2:F:13:LEU:HD12	2:F:63:ALA:HA	2.00	0.43
2:F:145:GLN:HA	2:F:153:MET:HE1	2.01	0.43
2:G:30:ARG:HH12	2:L:48:VAL:H	1.66	0.43
2:K:252:THR:OG1	2:K:255:PHE:HB3	2.18	0.43
2:G:158:LEU:HD21	2:G:169:HIS:HB3	2.00	0.43
2:J:314:ASN:OD1	2:L:329:SER:OG	2.30	0.43
2:J:314:ASN:CG	2:L:329:SER:HG	2.23	0.43
1:D:1021:ARG:NH2	1:D:1024:GLN:OE1	2.49	0.43
2:A:269:TRP:HE1	2:C:307:ARG:NH2	2.17	0.43
1:E:962:ALA:HB1	2:H:86:PHE:CD2	2.54	0.43
1:E:1004:ILE:CG1	1:I:1004:ILE:HD12	2.46	0.43
2:H:310:SER:HB3	2:H:312:MET:HE1	1.99	0.43
2:B:47:ASN:HB3	2:B:55:SER:HB2	2.01	0.42
2:B:158:LEU:HD22	2:B:184:VAL:HG21	2.00	0.42
2:C:311:VAL:HG22	2:C:358:ALA:HB1	2.01	0.42
2:F:36:ARG:NE	2:G:42:TRP:O	2.50	0.42
2:F:269:TRP:CD2	2:H:359:MET:HE1	2.54	0.42
2:G:328:GLY:HA3	2:G:342:GLY:HA2	2.00	0.42
2:H:66:SER:O	2:H:68:GLN:NE2	2.46	0.42
2:K:233:LEU:O	2:K:245:ALA:N	2.50	0.42
2:F:242:PRO:HG2	2:G:230:LEU:HB3	2.00	0.42
2:J:118:ILE:O	2:J:123:ARG:NH1	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:297:TYR:O	2:J:340:TRP:HD1	2.02	0.42
2:A:329:SER:HA	2:B:314:ASN:HD21	1.84	0.42
2:F:230:LEU:O	2:F:245:ALA:HB1	2.18	0.42
2:H:36:ARG:HB2	2:H:42:TRP:CZ3	2.54	0.42
2:K:328:GLY:HA2	2:K:343:TYR:CD1	2.55	0.42
2:L:11:VAL:HG12	2:L:18:VAL:HG22	2.01	0.42
2:C:361:ARG:HA	2:C:361:ARG:HD3	1.72	0.42
2:J:213:LYS:HB2	2:J:218:TRP:CD2	2.54	0.42
2:L:20:GLY:N	2:L:52:THR:O	2.32	0.42
2:B:340:TRP:CZ2	2:B:354:ALA:HB2	2.54	0.42
1:E:931:ASP:OD1	1:E:932:GLY:N	2.53	0.42
2:L:246:ILE:O	2:L:261:TYR:HA	2.19	0.42
2:J:327:TRP:NE1	2:J:343:TYR:HD2	2.17	0.42
2:L:246:ILE:HG13	2:L:247:ILE:N	2.34	0.42
1:D:994:GLU:OE2	1:I:996:ARG:NH1	2.52	0.42
2:A:189:HIS:HB2	2:B:183:TYR:OH	2.20	0.42
2:B:187:MET:HG2	2:C:166:LEU:CD1	2.50	0.42
2:G:185:LEU:HB3	2:G:187:MET:HE3	2.02	0.42
2:H:34:ALA:HB3	2:H:73:VAL:HB	2.02	0.42
2:H:263:ASP:OD1	2:H:264:GLY:N	2.53	0.42
2:H:329:SER:HG	2:H:330:THR:H	1.66	0.42
2:H:334:THR:OG1	2:H:337:LEU:O	2.35	0.42
2:A:103:TRP:HA	2:A:106:SER:OG	2.20	0.42
2:B:225:TYR:OH	2:C:227:GLN:HA	2.20	0.42
2:B:280:MET:HE1	2:B:282:TYR:CB	2.50	0.42
2:B:324:SER:HB2	2:B:344:ASP:OD1	2.20	0.42
2:C:187:MET:HB2	2:C:196:VAL:HG13	2.00	0.42
2:C:281:ALA:HB1	2:C:288:LEU:HD13	2.02	0.42
2:F:260:ARG:HG2	2:F:362:TRP:CD1	2.55	0.42
2:G:254:GLY:H	2:G:257:GLU:CD	2.27	0.42
2:K:317:ARG:HH12	2:K:324:SER:H	1.67	0.42
2:A:340:TRP:CH2	2:A:354:ALA:HB2	2.54	0.42
1:E:1021:ARG:HH21	1:I:1022:LEU:HB3	1.85	0.42
2:F:15:SER:OG	2:F:16:GLU:N	2.52	0.42
2:F:340:TRP:CH2	2:F:354:ALA:HB2	2.55	0.42
2:H:176:PRO:HG3	2:H:221:TRP:CG	2.55	0.42
2:H:311:VAL:HG22	2:H:358:ALA:HB1	2.02	0.42
2:J:263:ASP:HB3	2:K:247:ILE:HD13	2.01	0.42
2:J:331:MET:HE2	2:J:341:TYR:CE1	2.55	0.42
2:K:291:TYR:O	2:K:344:ASP:N	2.51	0.42
2:L:272:THR:N	2:L:354:ALA:O	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:331:MET:HB2	2:B:341:TYR:HD1	1.84	0.42
2:F:116:MET:SD	2:H:116:MET:HE1	2.60	0.42
2:F:314:ASN:OD1	2:H:329:SER:OG	2.29	0.42
1:I:1013:SER:HA	1:I:1016:GLN:HE22	1.84	0.42
2:K:118:ILE:O	2:K:123:ARG:NH1	2.53	0.42
2:B:217:ASN:OD1	2:B:217:ASN:N	2.53	0.41
2:B:266:GLN:O	2:B:267:ILE:HD13	2.20	0.41
2:F:158:LEU:O	2:F:197:GLN:NE2	2.35	0.41
2:G:42:TRP:HE1	2:H:42:TRP:NE1	2.18	0.41
2:G:340:TRP:CZ2	2:G:354:ALA:HB2	2.55	0.41
2:J:163:VAL:HG23	2:J:167:TYR:OH	2.20	0.41
2:J:248:GLN:OE1	2:J:258:TYR:OH	2.34	0.41
2:B:73:VAL:HG11	2:C:75:ILE:HD13	2.01	0.41
2:C:176:PRO:HG3	2:C:221:TRP:CG	2.55	0.41
1:E:939:SER:O	1:E:943:VAL:HG23	2.20	0.41
2:F:297:TYR:O	2:F:340:TRP:HD1	2.03	0.41
2:F:333:VAL:HG22	2:F:338:PHE:HB2	2.01	0.41
2:L:280:MET:CE	2:L:294:PRO:HG3	2.51	0.41
1:D:931:ASP:OD1	1:D:932:GLY:N	2.52	0.41
2:B:42:TRP:HE1	2:C:42:TRP:NE1	2.17	0.41
2:C:87:ARG:CD	1:I:961:ASP:HB2	2.48	0.41
2:L:298:SER:HB3	2:L:337:LEU:HD21	2.02	0.41
2:C:36:ARG:HB2	2:C:42:TRP:CZ3	2.55	0.41
2:F:163:VAL:HG23	2:F:167:TYR:OH	2.20	0.41
2:F:271:ASN:OD1	2:F:355:SER:OG	2.33	0.41
2:G:106:SER:OG	2:G:112:ALA:HB2	2.21	0.41
2:H:187:MET:HB2	2:H:196:VAL:HG13	2.01	0.41
2:J:316:MET:HE1	2:J:355:SER:HB2	2.02	0.41
2:K:153:MET:HE2	2:K:167:TYR:CE2	2.55	0.41
2:L:176:PRO:HG3	2:L:221:TRP:CG	2.55	0.41
2:L:340:TRP:CE2	2:L:354:ALA:HB2	2.55	0.41
2:A:13:LEU:HD12	2:A:63:ALA:HA	2.02	0.41
2:A:176:PRO:HG3	2:A:221:TRP:CD2	2.56	0.41
2:C:153:MET:H	2:C:153:MET:HG2	1.71	0.41
2:F:45:ILE:HG23	2:F:54:ILE:HG23	2.02	0.41
2:L:245:ALA:HB3	2:L:248:GLN:HE22	1.85	0.41
2:B:260:ARG:HG2	2:B:362:TRP:CD1	2.56	0.41
2:G:266:GLN:O	2:G:267:ILE:HD13	2.20	0.41
2:G:312:MET:HE2	2:H:357:VAL:HG22	2.03	0.41
2:G:331:MET:HG2	2:H:317:ARG:HD2	2.02	0.41
2:H:348:VAL:HG12	2:H:351:GLY:H	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:931:ASP:OD1	1:I:932:GLY:N	2.53	0.41
2:J:183:TYR:OH	2:L:189:HIS:HB2	2.19	0.41
2:A:15:SER:OG	2:A:16:GLU:N	2.53	0.41
2:B:263:ASP:OD1	2:B:264:GLY:N	2.53	0.41
2:C:258:TYR:CE2	2:C:260:ARG:HD2	2.55	0.41
2:C:271:ASN:HA	2:C:355:SER:HA	2.03	0.41
2:G:324:SER:HB2	2:G:344:ASP:OD1	2.21	0.41
2:J:213:LYS:HB2	2:J:218:TRP:CZ3	2.55	0.41
2:J:228:PHE:HE1	2:L:220:ARG:HH21	1.69	0.41
2:J:317:ARG:HG3	2:L:331:MET:HB2	2.01	0.41
2:K:158:LEU:HD22	2:K:184:VAL:HG21	2.02	0.41
2:K:363:ASN:HD21	2:L:249:ARG:NH1	2.18	0.41
2:L:230:LEU:HD11	2:L:246:ILE:HD11	2.02	0.41
1:D:933:SER:O	1:D:937:GLN:HG2	2.21	0.41
1:D:996:ARG:HE	1:D:996:ARG:HB3	1.77	0.41
2:A:260:ARG:HG2	2:A:362:TRP:CD1	2.55	0.41
2:B:246:ILE:HA	2:B:262:ALA:HB2	2.03	0.41
2:H:245:ALA:HB3	2:H:248:GLN:HE22	1.86	0.41
2:J:331:MET:SD	2:J:332:SER:N	2.93	0.41
2:K:246:ILE:H	2:K:246:ILE:HD12	1.86	0.41
2:L:39:ASP:OD2	2:L:41:ARG:NH1	2.53	0.41
1:D:944:LEU:HD22	1:D:944:LEU:HA	1.83	0.41
2:A:163:VAL:HG23	2:A:167:TYR:OH	2.21	0.41
2:B:148:TRP:CH2	2:B:185:LEU:HD21	2.56	0.41
2:B:220:ARG:NH1	2:C:227:GLN:OE1	2.54	0.41
2:B:257:GLU:HB2	2:B:269:TRP:CE2	2.55	0.41
2:B:282:TYR:CE2	2:B:284:PRO:HD3	2.56	0.41
2:C:299:TRP:HD1	2:C:338:PHE:HE1	1.69	0.41
2:F:193:ASP:HA	2:F:213:LYS:HE3	2.03	0.41
2:F:264:GLY:HA3	2:F:363:ASN:CG	2.46	0.41
2:G:311:VAL:HG23	2:G:330:THR:HG21	2.02	0.41
1:I:939:SER:O	1:I:943:VAL:HG23	2.21	0.41
2:J:47:ASN:OD1	2:J:49:THR:OG1	2.34	0.41
2:J:296:ALA:HB2	2:J:341:TYR:HE1	1.85	0.41
2:L:281:ALA:HB1	2:L:288:LEU:HD13	2.02	0.41
2:A:306:SER:OG	2:A:361:ARG:O	2.37	0.41
2:A:312:MET:HB3	2:C:312:MET:CE	2.51	0.41
2:B:328:GLY:HA2	2:B:343:TYR:HD1	1.86	0.41
2:G:116:MET:HE1	2:H:116:MET:CE	2.51	0.41
2:G:260:ARG:HG2	2:G:362:TRP:CD1	2.56	0.41
2:H:159:ASP:OD1	2:H:159:ASP:N	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:228:PHE:N	2:H:228:PHE:CD1	2.89	0.41
2:J:260:ARG:HG2	2:J:362:TRP:CD1	2.56	0.41
1:D:1018:THR:OG1	1:E:1015:ARG:NH2	2.54	0.40
2:C:304:SER:HB2	2:C:336:THR:HG22	2.02	0.40
2:C:331:MET:HE2	2:C:341:TYR:CD2	2.56	0.40
1:E:962:ALA:HB1	2:H:86:PHE:HD2	1.84	0.40
2:F:183:TYR:OH	2:H:189:HIS:HB2	2.21	0.40
2:F:249:ARG:HH21	2:H:361:ARG:HD2	1.86	0.40
2:K:194:PHE:HB3	2:L:202:LEU:HD21	2.02	0.40
2:L:144:ASN:OD1	2:L:144:ASN:C	2.64	0.40
2:A:331:MET:HB2	2:B:317:ARG:CD	2.51	0.40
1:E:927:ILE:HD11	1:I:927:ILE:HD11	2.02	0.40
1:E:959:MET:HB3	2:G:86:PHE:HE2	1.86	0.40
2:F:269:TRP:HB3	2:H:359:MET:HE1	2.03	0.40
1:I:989:ARG:HE	1:I:989:ARG:HB3	1.75	0.40
2:J:116:MET:HE2	2:J:116:MET:HB3	1.79	0.40
2:J:210:MET:HE1	2:J:212:ILE:HG12	2.03	0.40
1:D:927:ILE:HD11	1:E:927:ILE:HD11	2.03	0.40
2:C:331:MET:HE1	2:C:340:TRP:CA	2.51	0.40
2:F:331:MET:HG3	2:F:341:TYR:OH	2.21	0.40
2:G:299:TRP:HB3	2:G:338:PHE:CE1	2.56	0.40
2:H:296:ALA:HB1	2:H:339:SER:OG	2.21	0.40
2:J:249:ARG:HB2	2:L:361:ARG:NH2	2.37	0.40
2:L:159:ASP:N	2:L:159:ASP:OD1	2.54	0.40
2:L:307:ARG:CZ	2:L:309:PRO:HA	2.50	0.40
2:B:152:ALA:HB2	2:B:166:LEU:HG	2.04	0.40
2:B:176:PRO:HG3	2:B:221:TRP:CD2	2.56	0.40
2:G:246:ILE:HA	2:G:262:ALA:HB2	2.03	0.40
2:J:254:GLY:HA2	2:L:307:ARG:HH11	1.86	0.40
2:K:280:MET:HE1	2:K:282:TYR:CB	2.50	0.40
2:L:217:ASN:OD1	2:L:217:ASN:N	2.54	0.40
2:C:317:ARG:HH21	2:C:324:SER:H	1.69	0.40
2:G:217:ASN:N	2:G:217:ASN:OD1	2.53	0.40
2:H:340:TRP:CE2	2:H:354:ALA:HB2	2.56	0.40
2:H:361:ARG:HA	2:H:361:ARG:HD3	1.76	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	108/1204 (9%)	107 (99%)	1 (1%)	0	100	100
1	E	108/1204 (9%)	107 (99%)	1 (1%)	0	100	100
1	I	108/1204 (9%)	107 (99%)	1 (1%)	0	100	100
2	A	360/363 (99%)	342 (95%)	18 (5%)	0	100	100
2	B	360/363 (99%)	340 (94%)	20 (6%)	0	100	100
2	C	360/363 (99%)	339 (94%)	21 (6%)	0	100	100
2	F	360/363 (99%)	343 (95%)	17 (5%)	0	100	100
2	G	360/363 (99%)	343 (95%)	17 (5%)	0	100	100
2	H	360/363 (99%)	339 (94%)	21 (6%)	0	100	100
2	J	360/363 (99%)	342 (95%)	18 (5%)	0	100	100
2	K	360/363 (99%)	343 (95%)	16 (4%)	1 (0%)	36	66
2	L	360/363 (99%)	340 (94%)	20 (6%)	0	100	100
All	All	3564/6879 (52%)	3392 (95%)	171 (5%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	K	321	ASN

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	D	80/959 (8%)	76 (95%)	4 (5%)	22	49
1	E	80/959 (8%)	75 (94%)	5 (6%)	16	43
1	I	80/959 (8%)	79 (99%)	1 (1%)	61	73
2	A	277/278 (100%)	267 (96%)	10 (4%)	31	56
2	B	277/278 (100%)	272 (98%)	5 (2%)	51	69
2	C	277/278 (100%)	267 (96%)	10 (4%)	31	56
2	F	277/278 (100%)	267 (96%)	10 (4%)	31	56
2	G	277/278 (100%)	269 (97%)	8 (3%)	37	60
2	H	277/278 (100%)	264 (95%)	13 (5%)	23	51
2	J	277/278 (100%)	266 (96%)	11 (4%)	28	54
2	K	277/278 (100%)	267 (96%)	10 (4%)	31	56
2	L	277/278 (100%)	268 (97%)	9 (3%)	34	58
All	All	2733/5379 (51%)	2637 (96%)	96 (4%)	32	56

All (96) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	944	LEU
1	D	950	ASP
1	D	1018	THR
1	D	1025	LEU
2	A	75	ILE
2	A	89	ILE
2	A	96	THR
2	A	130	THR
2	A	181	GLN
2	A	193	ASP
2	A	222	VAL
2	A	231	VAL
2	A	259	VAL
2	A	343	TYR
2	B	222	VAL
2	B	253	VAL
2	B	288	LEU
2	B	330	THR
2	B	348	VAL
2	C	28	ASN
2	C	49	THR
2	C	76	HIS

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Mol	Chain	Res	Type
2	C	89	ILE
2	C	163	VAL
2	C	171	THR
2	C	217	ASN
2	C	222	VAL
2	C	283	GLN
2	C	341	TYR
1	E	945	LEU
1	E	950	ASP
1	E	982	GLU
1	E	1018	THR
1	E	1025	LEU
2	F	69	VAL
2	F	75	ILE
2	F	89	ILE
2	F	96	THR
2	F	130	THR
2	F	181	GLN
2	F	193	ASP
2	F	222	VAL
2	F	231	VAL
2	F	343	TYR
2	G	145	GLN
2	G	193	ASP
2	G	222	VAL
2	G	253	VAL
2	G	288	LEU
2	G	330	THR
2	G	336	THR
2	G	348	VAL
2	H	49	THR
2	H	76	HIS
2	H	82	LEU
2	H	89	ILE
2	H	133	ASN
2	H	163	VAL
2	H	166	LEU
2	H	171	THR
2	H	222	VAL
2	H	248	GLN
2	H	283	GLN
2	H	316	MET

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Mol	Chain	Res	Type
2	H	331	MET
1	I	1025	LEU
2	J	46	THR
2	J	89	ILE
2	J	96	THR
2	J	106	SER
2	J	130	THR
2	J	181	GLN
2	J	193	ASP
2	J	222	VAL
2	J	231	VAL
2	J	259	VAL
2	J	343	TYR
2	K	151	ASN
2	K	153	MET
2	K	193	ASP
2	K	222	VAL
2	K	253	VAL
2	K	288	LEU
2	K	292	ILE
2	K	330	THR
2	K	348	VAL
2	K	352	MET
2	L	28	ASN
2	L	76	HIS
2	L	146	MET
2	L	148	TRP
2	L	153	MET
2	L	163	VAL
2	L	171	THR
2	L	193	ASP
2	L	222	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (39) such sidechains are listed below:

Mol	Chain	Res	Type
2	A	85	GLN
2	A	188	GLN
2	A	224	GLN
2	B	90	ASN
2	B	111	GLN
2	B	197	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	201	GLN
2	C	14	ASN
2	C	76	HIS
2	C	85	GLN
2	C	113	GLN
2	C	145	GLN
2	C	241	ASN
2	C	248	GLN
2	C	266	GLN
2	C	275	ASN
2	F	85	GLN
2	F	188	GLN
2	F	224	GLN
2	G	59	ASN
2	G	90	ASN
2	G	197	GLN
2	H	14	ASN
2	H	113	GLN
2	H	224	GLN
1	I	937	GLN
2	J	85	GLN
2	J	188	GLN
2	J	224	GLN
2	K	14	ASN
2	K	59	ASN
2	K	90	ASN
2	K	197	GLN
2	K	241	ASN
2	L	14	ASN
2	L	145	GLN
2	L	191	ASN
2	L	224	GLN
2	L	248	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [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.

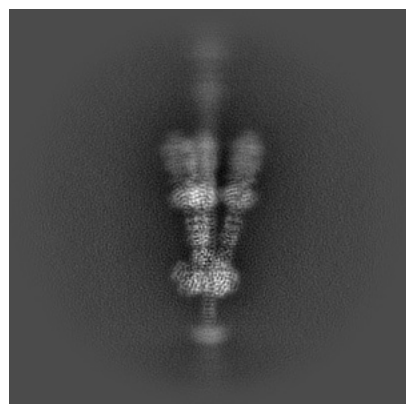
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-80404. These allow visual inspection of the internal detail of the map and identification of artifacts.

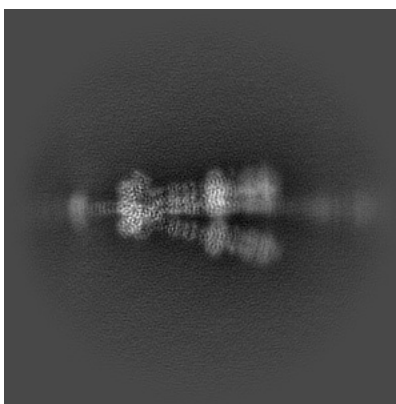
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

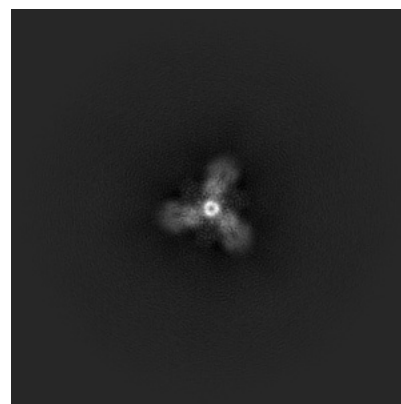
6.1.1 Primary map



X

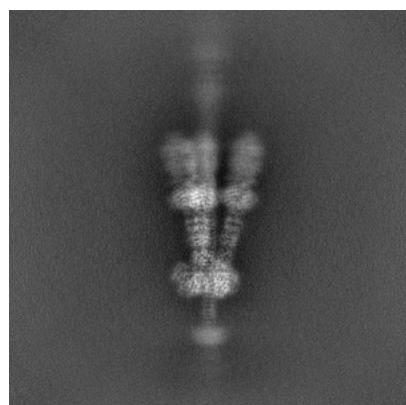


Y

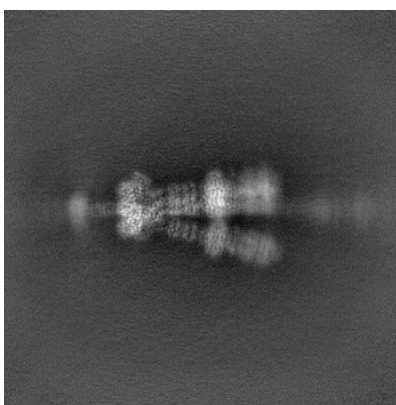


Z

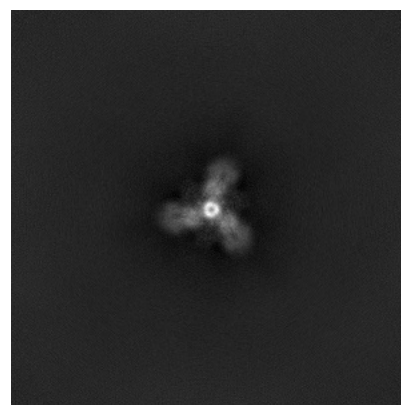
6.1.2 Raw map



X



Y

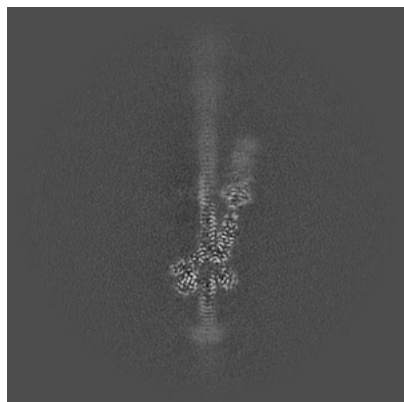


Z

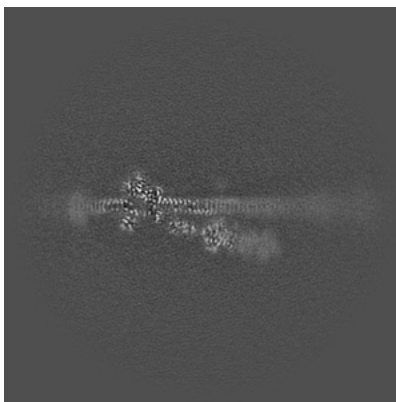
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

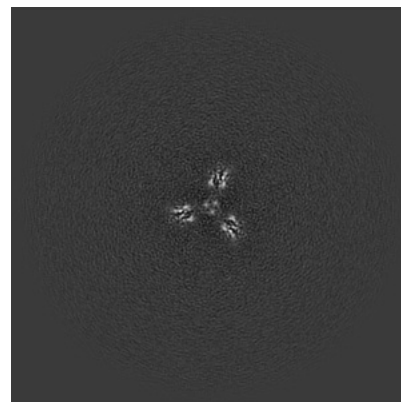
6.2.1 Primary map



X Index: 256

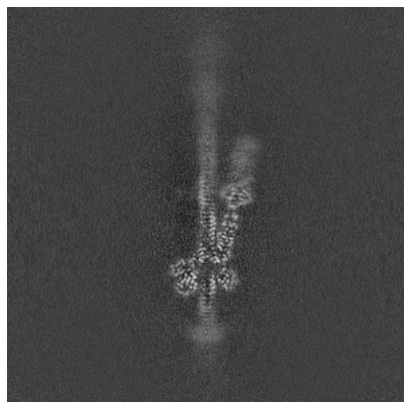


Y Index: 256

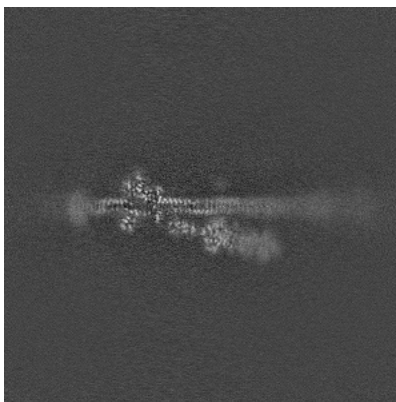


Z Index: 256

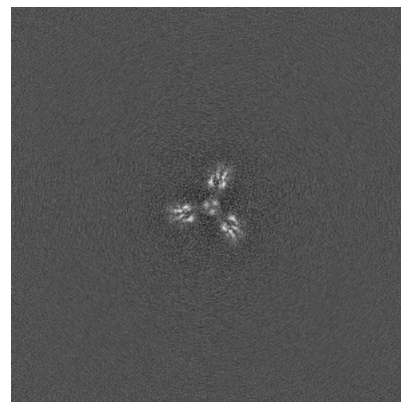
6.2.2 Raw map



X Index: 256



Y Index: 256

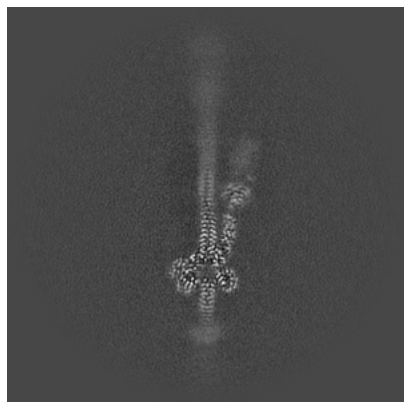


Z Index: 256

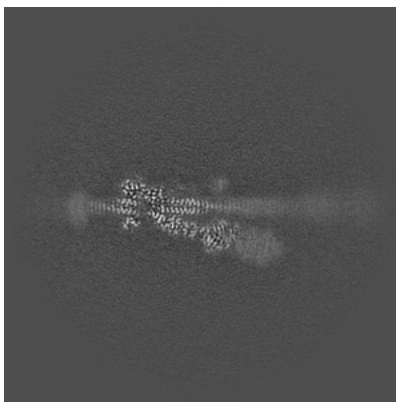
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

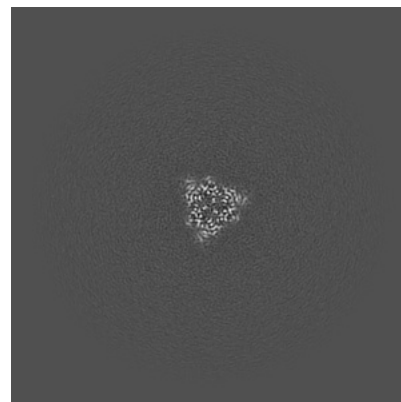
6.3.1 Primary map



X Index: 253

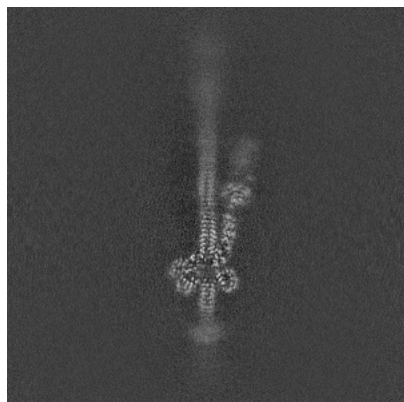


Y Index: 252

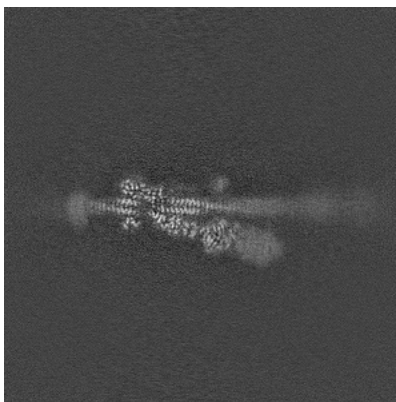


Z Index: 164

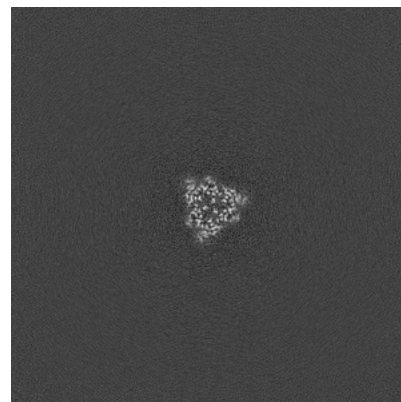
6.3.2 Raw map



X Index: 253



Y Index: 252

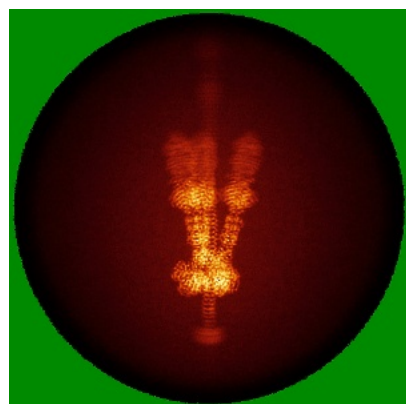


Z Index: 164

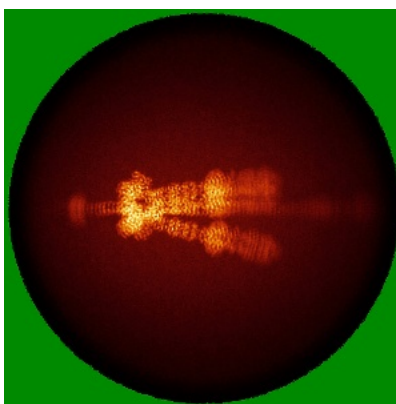
The images above show the largest variance slices of the map in three orthogonal directions.

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

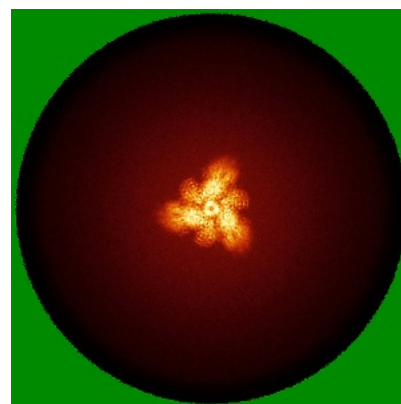
6.4.1 Primary map



X

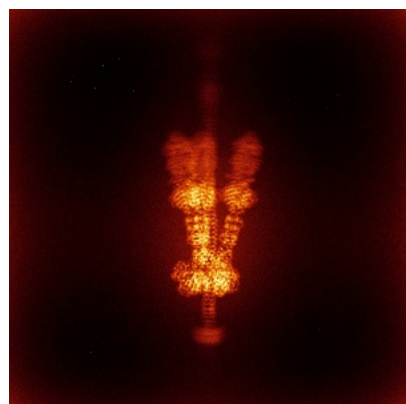


Y

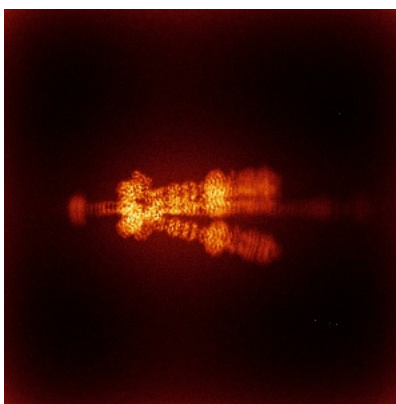


Z

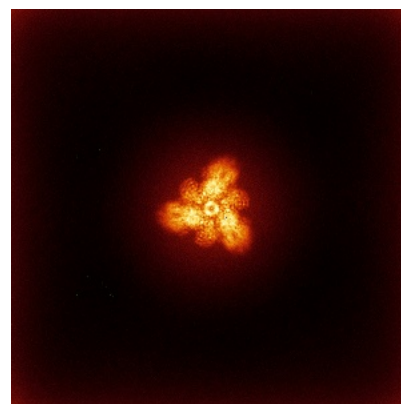
6.4.2 Raw map



X



Y

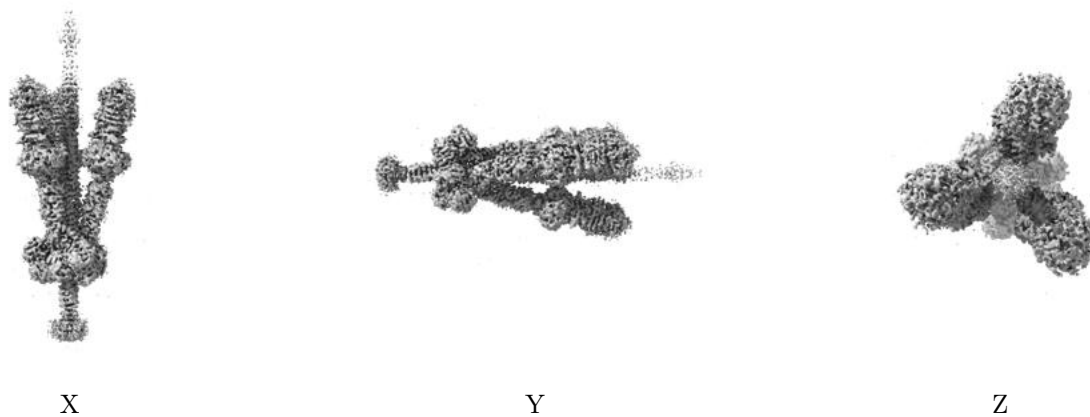


Z

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.

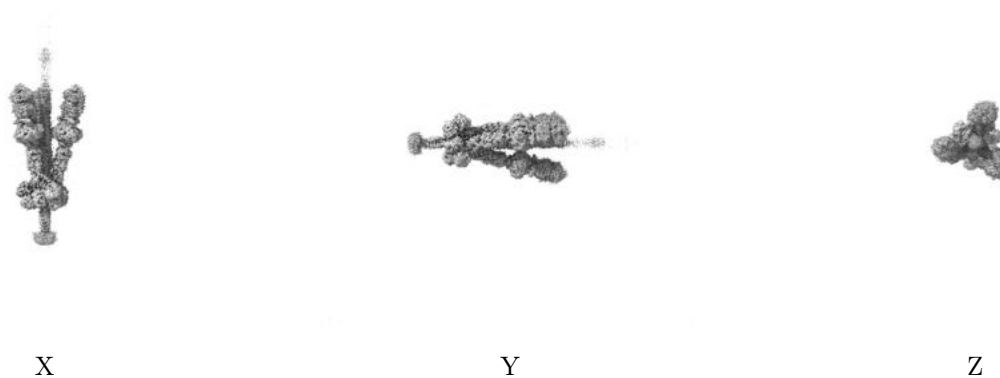
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.233. 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.

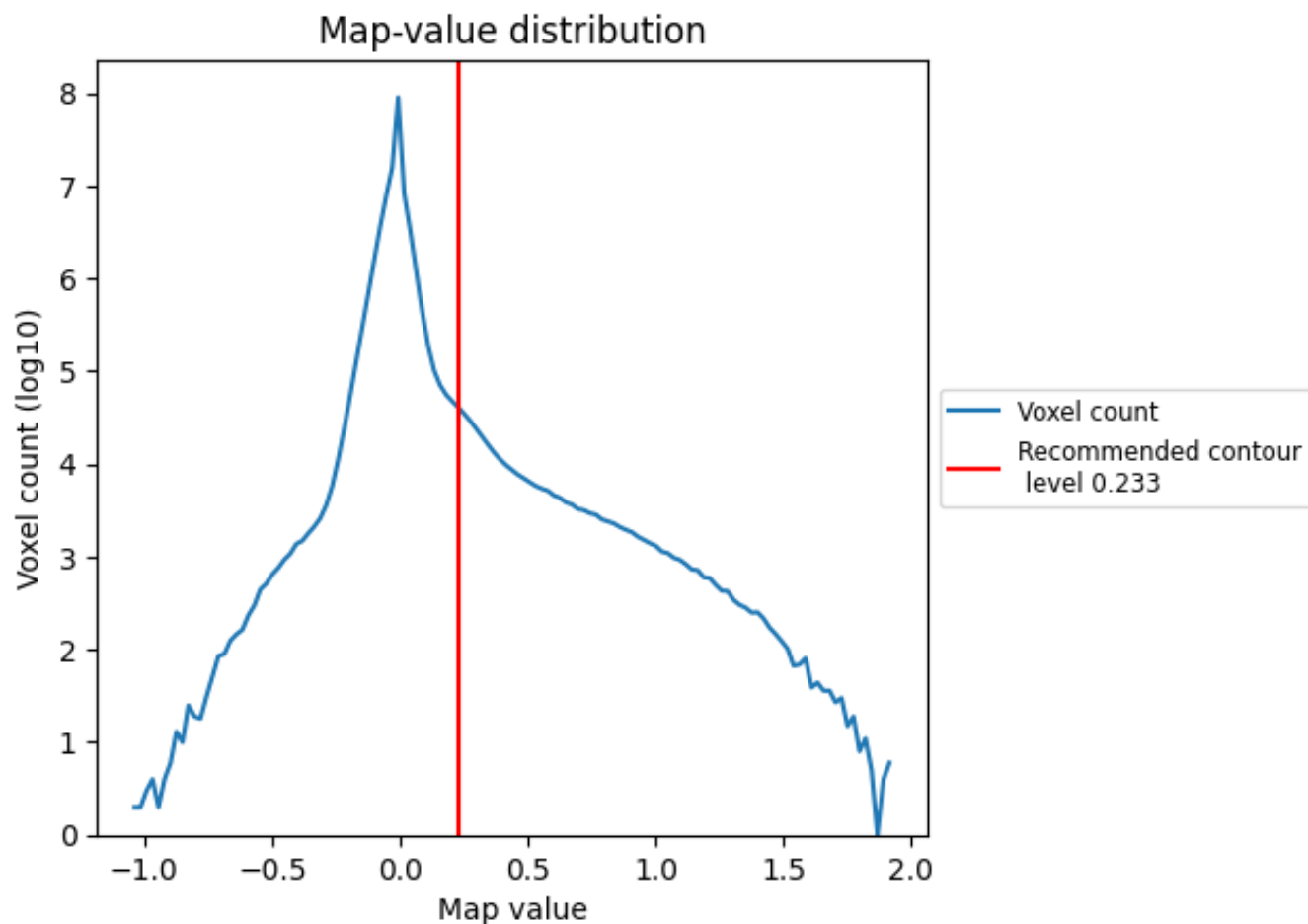
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

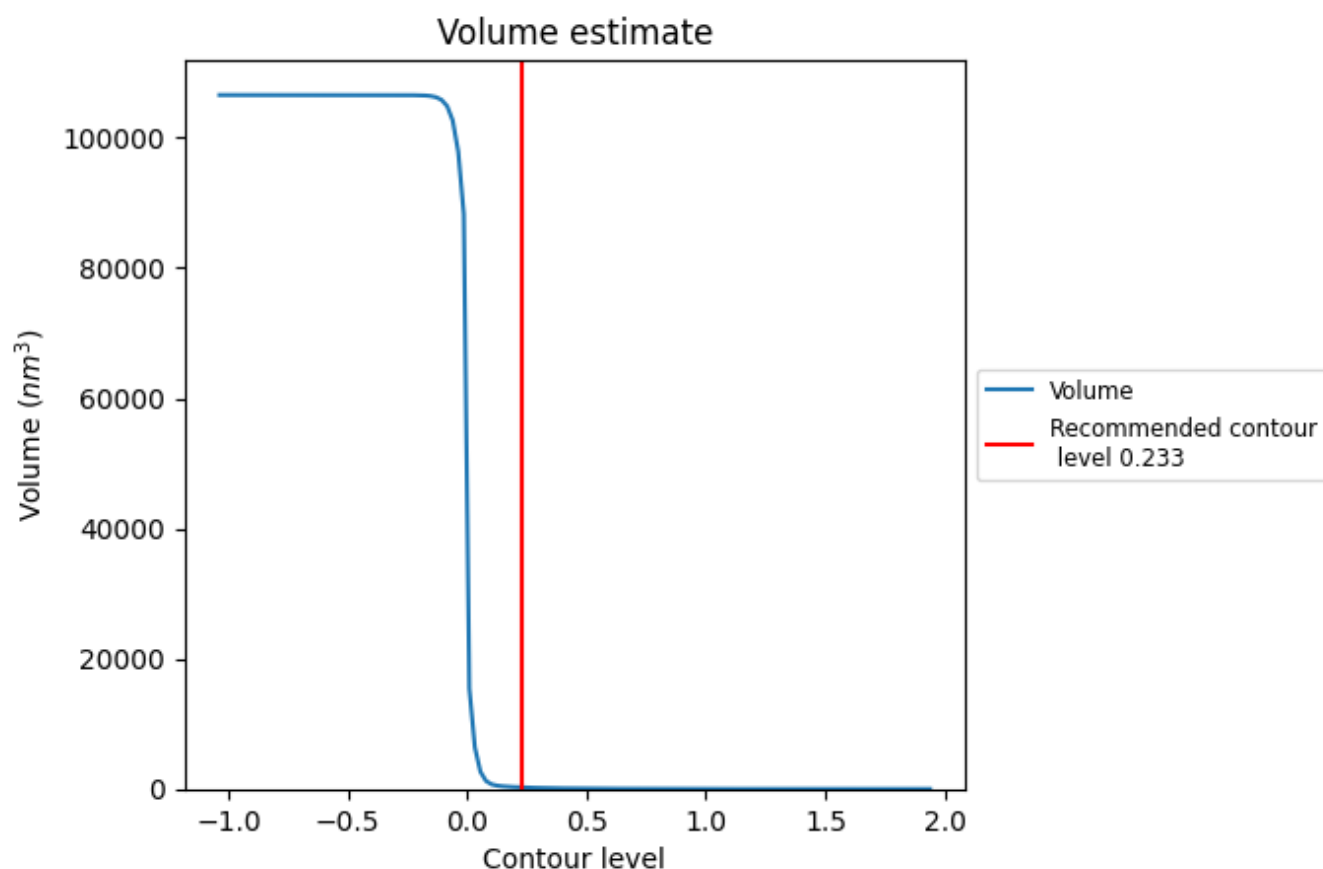
This section contains the results of statistical analysis of the map.

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.

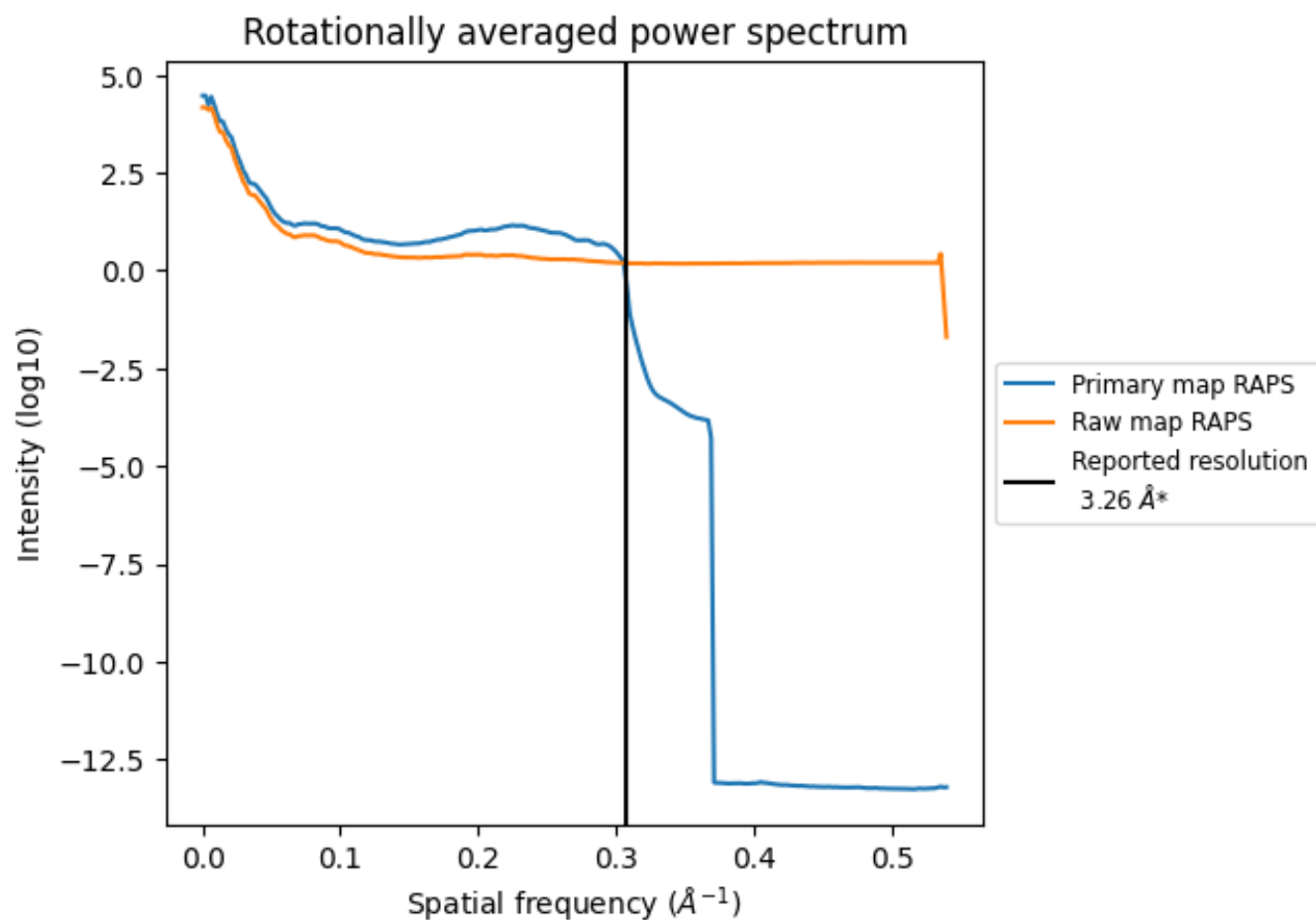
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 237 nm³; this corresponds to an approximate mass of 214 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 ⓘ

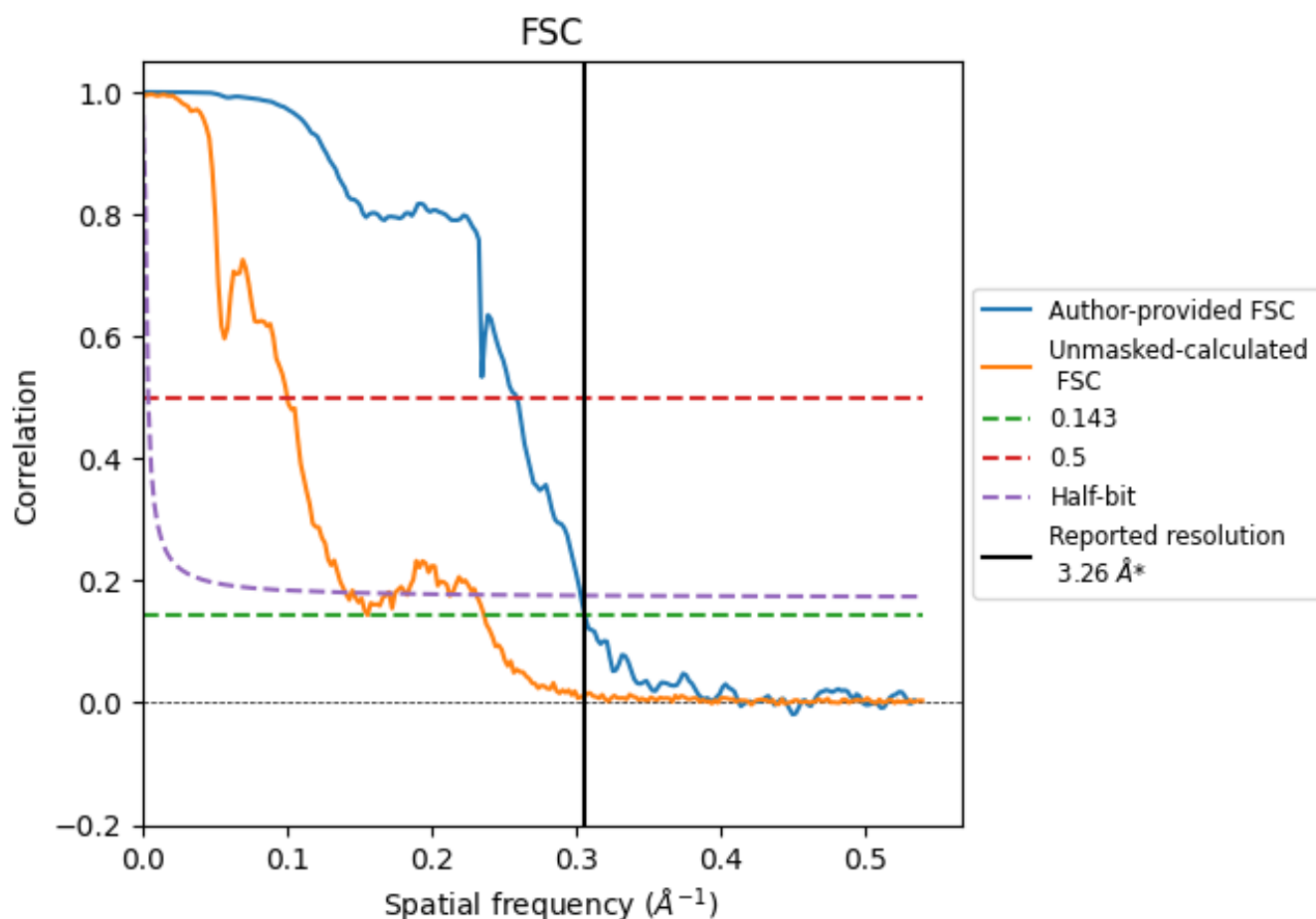


*Reported resolution corresponds to spatial frequency of 0.307 Å⁻¹

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 0.307 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

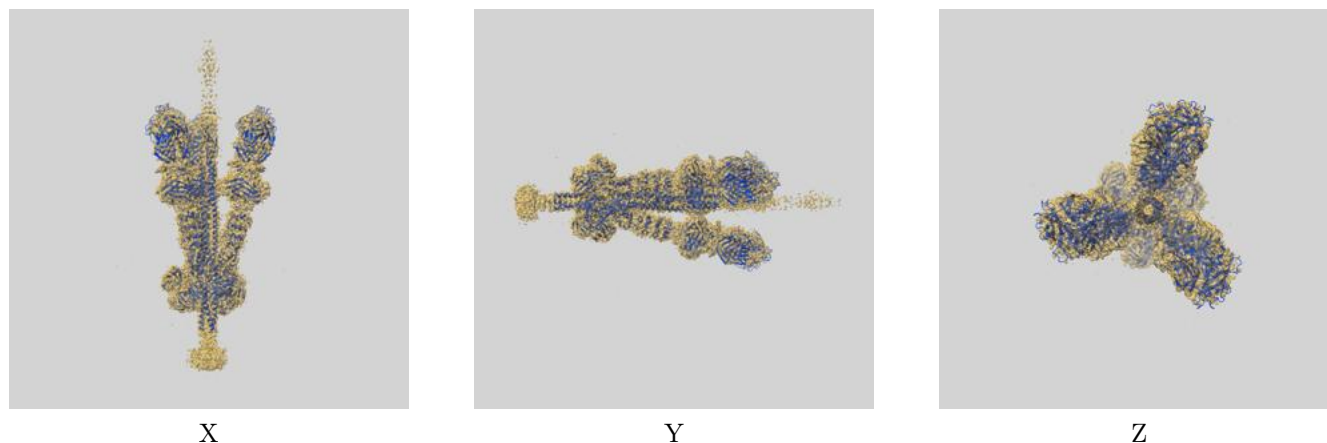
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.26	-	-
Author-provided FSC curve	3.26	3.86	3.29
Unmasked-calculated*	4.22	9.95	7.10

*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 4.22 differs from the reported value 3.26 by more than 10 %

9 Map-model fit [i](#)

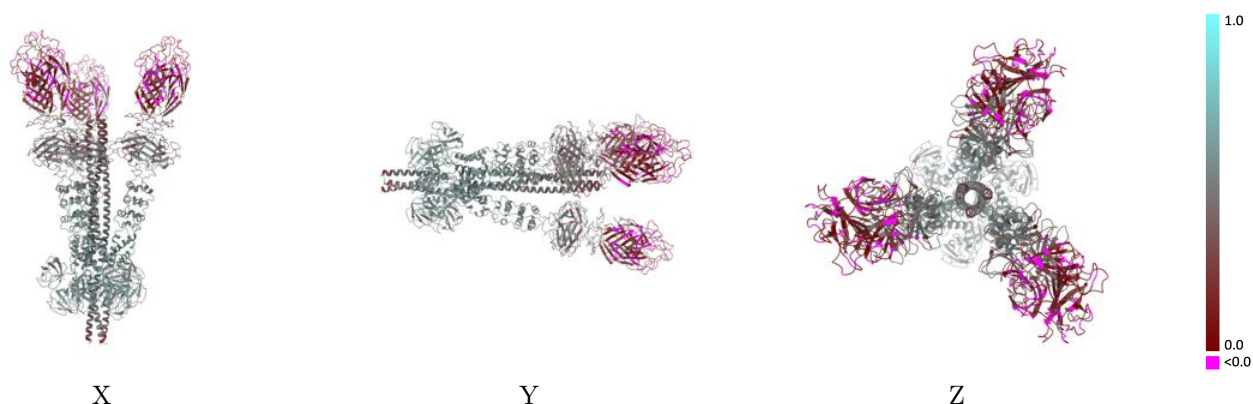
This section contains information regarding the fit between EMDB map EMD-80404 and PDB model 25VJ. Per-residue inclusion information can be found in [section 3](#) on [page 6](#).

9.1 Map-model overlay [i](#)



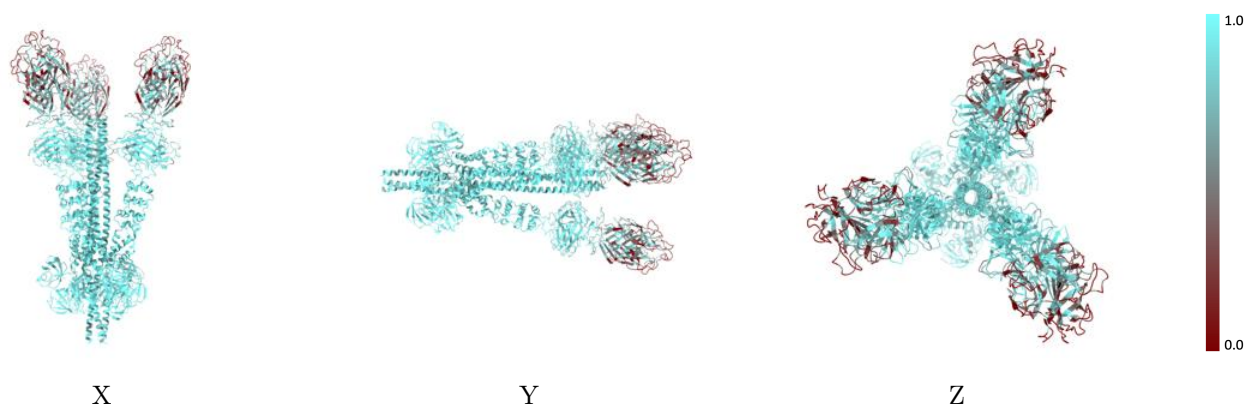
The images above show the 3D surface view of the map at the recommended contour level 0.233 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



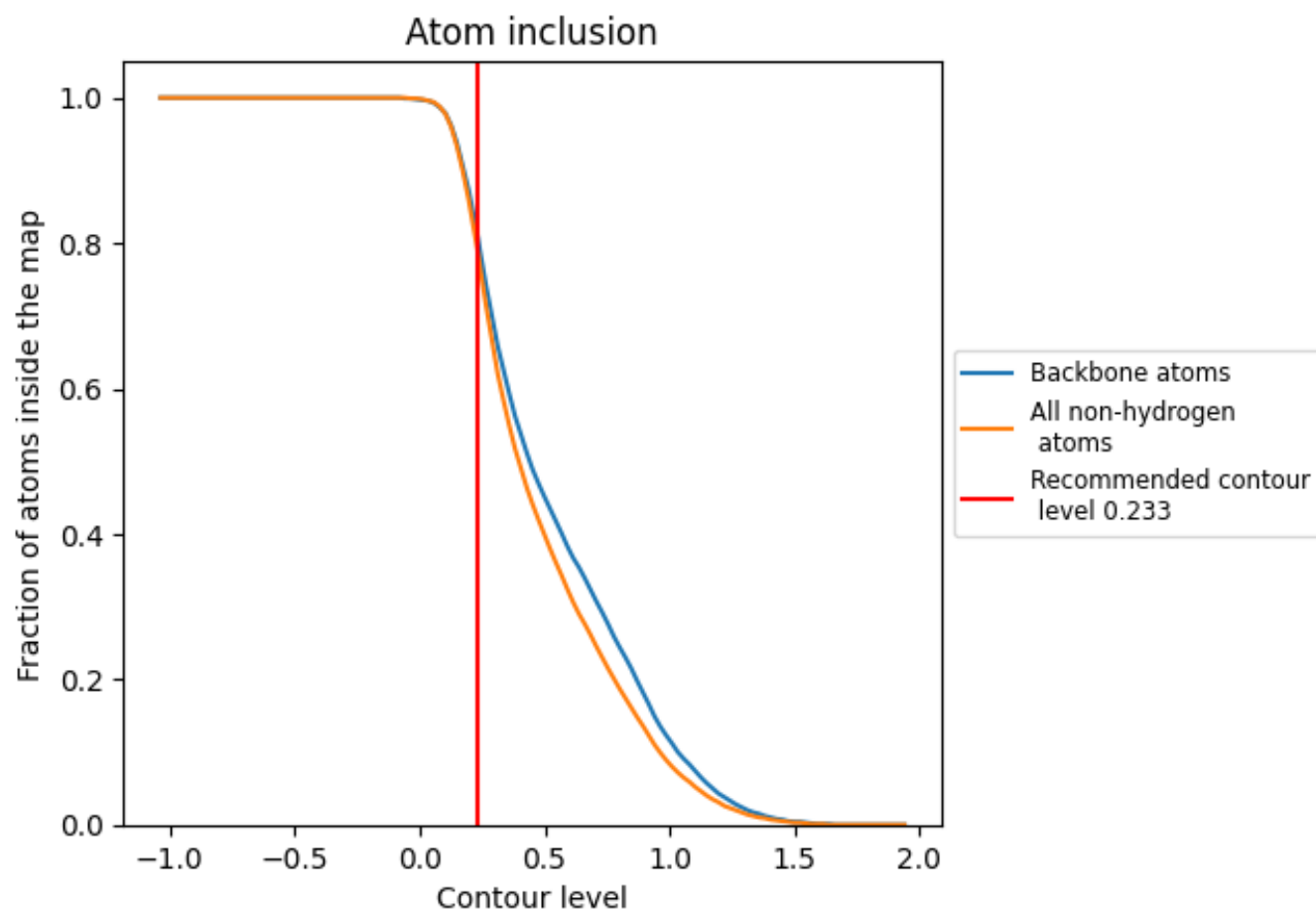
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.233).

9.4 Atom inclusion [i](#)



At the recommended contour level, 81% of all backbone atoms, 79% 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 (0.233) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7870	0.3900
A	0.7990	0.3770
B	0.7710	0.3880
C	0.7540	0.3830
D	0.9080	0.4660
E	0.9100	0.4680
F	0.7940	0.3770
G	0.7730	0.3860
H	0.7560	0.3830
I	0.9080	0.4690
J	0.7970	0.3770
K	0.7690	0.3880
L	0.7570	0.3850

