



## Full wwPDB EM Validation Report ⓘ

May 30, 2026 – 01:06 PM EDT

PDB ID : 10FF / pdb\_000010ff  
EMDB ID : EMD-75129  
Title : SK5A-Matured glycine/glutamate in complex with GluN1-GluN2B, full refinement  
Authors : Kleeman, S.O.; Furukawa, H.F.  
Deposited on : 2026-01-15  
Resolution : 4.06 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

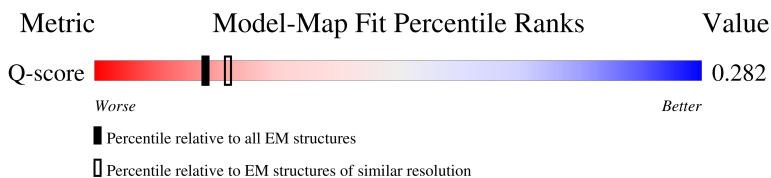
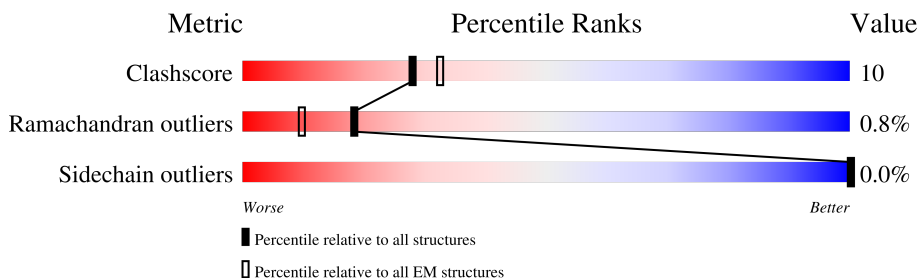
EMDB validation analysis : 0.0.1.dev132  
MolProbity : 4-5-2 with Phenix2.0  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:  
*ELECTRON MICROSCOPY*

The reported resolution of this entry is 4.06 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	6515 ( 3.56 - 4.56 )

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion  $< 40\%$ ). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	844	 5% 77% 17% 6%
1	C	844	 5% 73% 21% 6%
2	B	826	 9% 74% 17% 9%
2	D	826	 9% 76% 15% 9%

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Mol	Chain	Length	Quality of chain
3	E	107	
3	I	107	
4	F	116	
4	J	116	

## 2 Entry composition i

There are 4 unique types of molecules in this entry. The entry contains 26017 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 Glutamate receptor ionotropic, NMDA 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	795	5897	3780	1016	1073	28	0	0
1	C	795	5709	3648	991	1042	28	0	0

There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	5	HIS	ARG	conflict	UNP Q05586
A	9	PHE	LEU	conflict	UNP Q05586
A	17	PHE	VAL	conflict	UNP Q05586
A	22	SER	CYS	conflict	UNP Q05586
A	212	ARG	LYS	conflict	UNP Q05586
A	267	ILE	LEU	conflict	UNP Q05586
A	556	ASN	GLN	conflict	UNP Q05586
A	819	ILE	LEU	conflict	UNP Q05586
A	839	SER	-	expression tag	UNP Q05586
A	840	ARG	-	expression tag	UNP Q05586
A	841	ALA	-	expression tag	UNP Q05586
C	5	HIS	ARG	conflict	UNP Q05586
C	9	PHE	LEU	conflict	UNP Q05586
C	17	PHE	VAL	conflict	UNP Q05586
C	22	SER	CYS	conflict	UNP Q05586
C	212	ARG	LYS	conflict	UNP Q05586
C	267	ILE	LEU	conflict	UNP Q05586
C	556	ASN	GLN	conflict	UNP Q05586
C	819	ILE	LEU	conflict	UNP Q05586
C	839	SER	-	expression tag	UNP Q05586
C	840	ARG	-	expression tag	UNP Q05586
C	841	ALA	-	expression tag	UNP Q05586

- Molecule 2 is a protein called Glutamate receptor ionotropic, NMDA 2B.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	752	5565	3572	922	1037	34	0	0
2	D	749	5428	3480	896	1022	30	0	0

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	271	SER	ALA	conflict	UNP Q13224
B	437	GLU	GLN	conflict	UNP Q13224
B	588	SER	CYS	conflict	UNP Q13224
B	838	SER	CYS	conflict	UNP Q13224
B	849	SER	CYS	conflict	UNP Q13224
D	271	SER	ALA	conflict	UNP Q13224
D	437	GLU	GLN	conflict	UNP Q13224
D	588	SER	CYS	conflict	UNP Q13224
D	838	SER	CYS	conflict	UNP Q13224
D	849	SER	CYS	conflict	UNP Q13224

- Molecule 3 is a protein called Light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	E	107	816	508	133	172	3	0	0
3	I	107	816	508	133	172	3	0	0

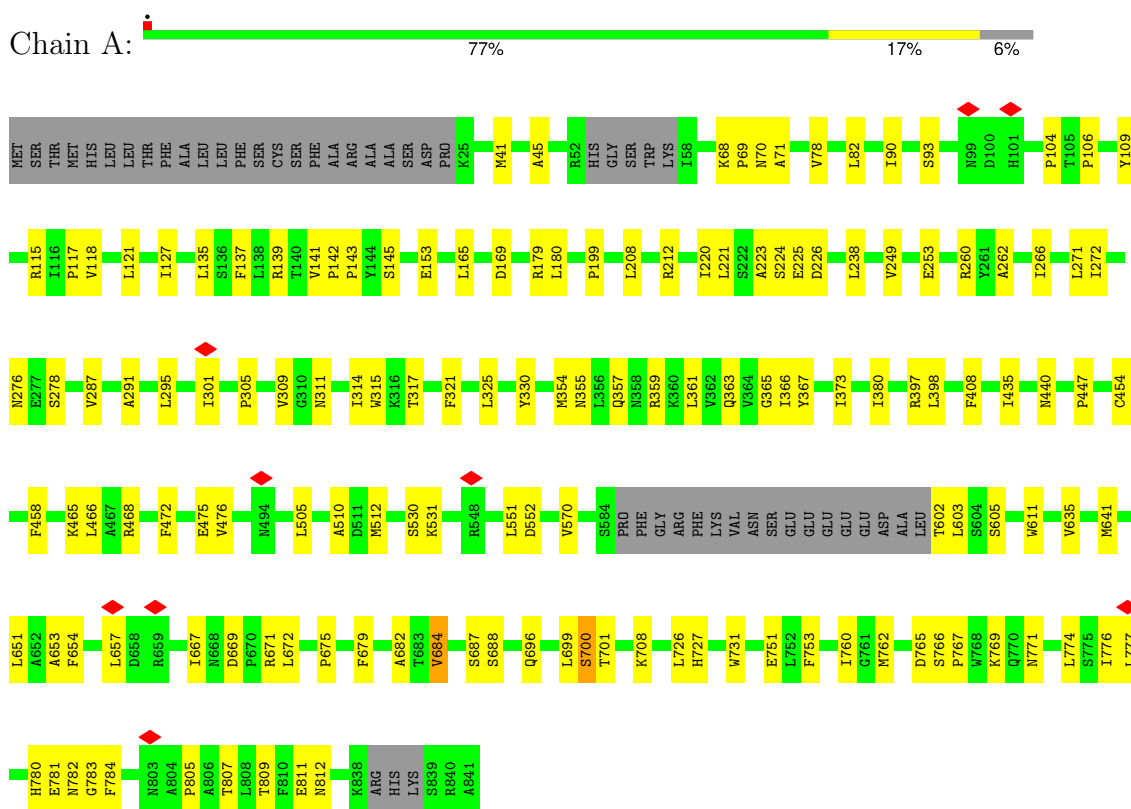
- Molecule 4 is a protein called Heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	F	116	893	563	150	178	2	0	0
4	J	116	893	563	150	178	2	0	0

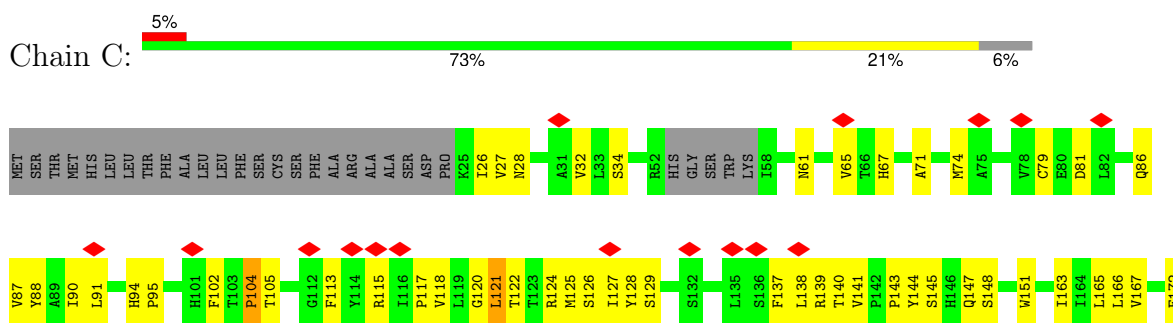
### 3 Residue-property plots [i](#)

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.

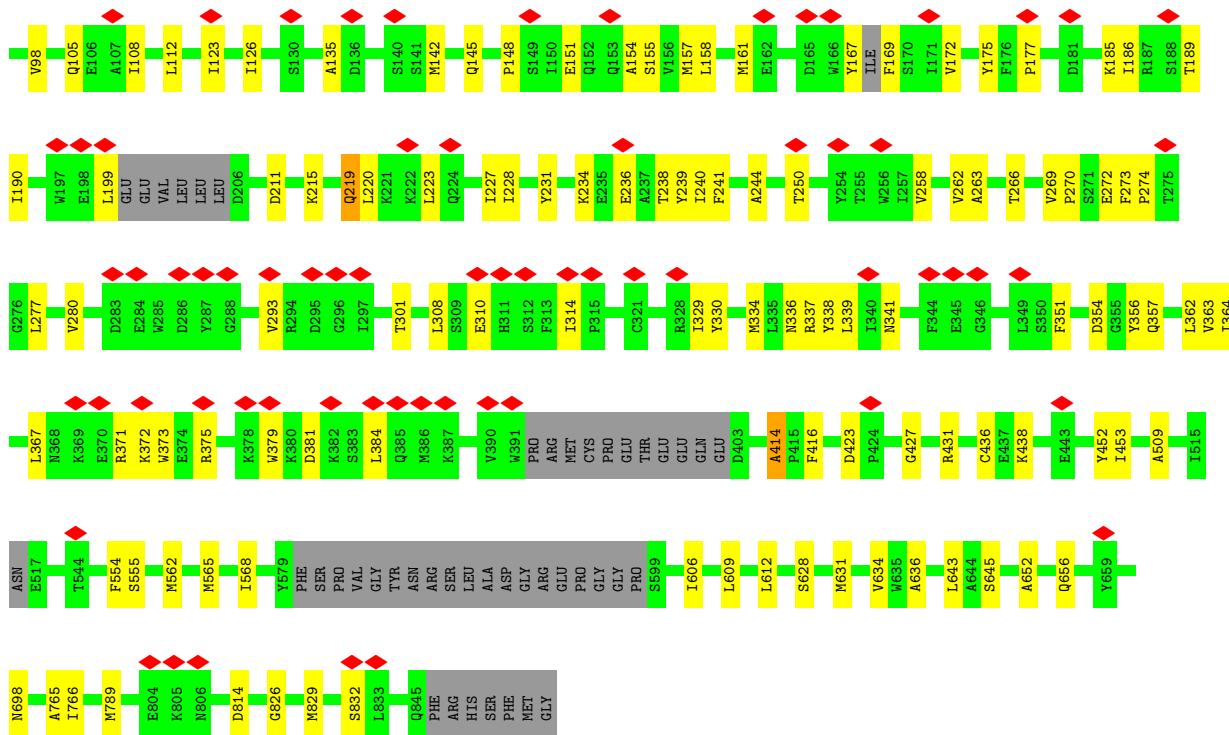
- Molecule 1: Glutamate receptor ionotropic, NMDA 1



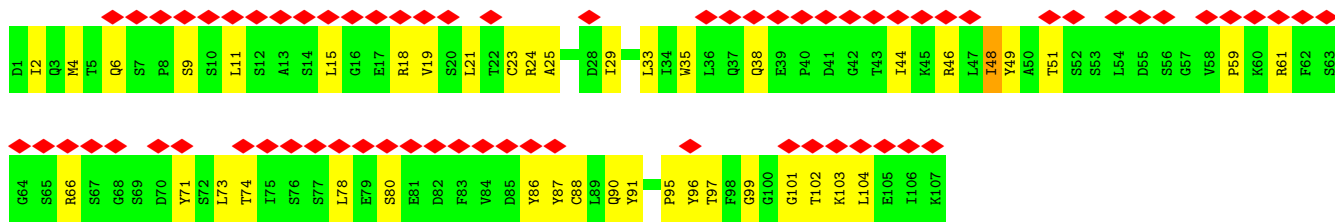
- Molecule 1: Glutamate receptor ionotropic, NMDA 1



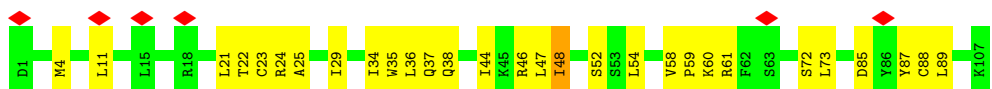




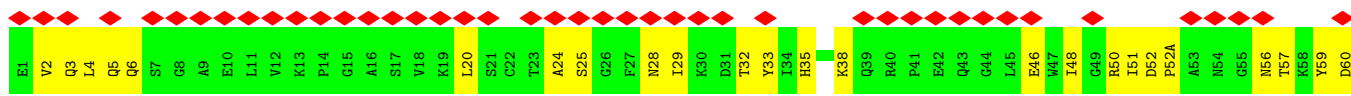
• Molecule 3: Light chain



• Molecule 3: Light chain



• Molecule 4: Heavy chain





- Molecule 4: Heavy chain



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	87672	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	71.7	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOCONTINUUM (6k x 4k)	Depositor
Maximum map value	0.511	Depositor
Minimum map value	-0.218	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.009	Depositor
Recommended contour level	0.05	Depositor
Map size ( $\text{\AA}$ )	400.0, 400.0, 400.0	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	1.0, 1.0, 1.0	Depositor

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.24	0/6030	0.60	0/8224
1	C	0.24	0/5836	0.62	4/7978 (0.1%)
2	B	0.24	0/5685	0.61	1/7734 (0.0%)
2	D	0.24	0/5543	0.65	1/7549 (0.0%)
3	E	0.28	0/830	0.78	0/1122
3	I	0.27	0/830	0.72	0/1122
4	F	0.29	0/914	0.72	0/1244
4	J	0.28	0/914	0.70	0/1244
All	All	0.25	0/26582	0.64	6/36217 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	C	0	1
2	B	0	1
2	D	0	1
All	All	0	4

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	86	GLN	CB-CG-CD	7.17	124.80	112.60
2	D	431	ARG	CB-CA-C	-5.53	110.21	116.63
1	C	86	GLN	CA-CB-CG	5.35	124.80	114.10
1	C	296	LEU	CB-CA-C	-5.20	110.56	116.54
2	B	678	SER	C-N-CD	-5.07	104.21	125.00
1	C	541	LEU	CA-CB-CG	5.02	133.86	116.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	767	PRO	Peptide
2	B	678	SER	Peptide
1	C	121	LEU	Peptide
2	D	436	CYS	Peptide

## 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5897	0	5623	93	0
1	C	5709	0	5256	117	0
2	B	5565	0	5201	90	0
2	D	5428	0	4956	83	0
3	E	816	0	794	35	0
3	I	816	0	794	21	0
4	F	893	0	857	31	0
4	J	893	0	857	38	0
All	All	26017	0	24338	482	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 10.

All (482) 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:653:ALA:O	1:A:657:LEU:HB3	1.82	0.80
1:A:641:MET:HE2	2:B:614:PHE:HA	1.65	0.78
1:A:408:PHE:HB3	1:A:458:PHE:HB3	1.67	0.76
2:B:308:LEU:HA	2:B:312:SER:HA	1.69	0.75
4:F:90:THR:HG23	4:F:113:VAL:H	1.54	0.73
3:E:4:MET:HB2	3:E:99:GLY:HA3	1.69	0.72
1:C:121:LEU:HD23	1:C:122:THR:H	1.55	0.71
3:I:58:VAL:HG12	3:I:60:LYS:H	1.56	0.71
1:A:305:PRO:HB3	1:A:311:ASN:HD22	1.56	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:310:GLU:OE2	2:B:311:HIS:CE1	2.44	0.70
2:B:275:THR:HA	2:B:367:LEU:HD23	1.73	0.69
1:A:169:ASP:HB2	1:A:199:PRO:HD3	1.73	0.69
3:I:46:ARG:NH2	4:J:101:SER:OG	2.26	0.68
1:A:466:LEU:HD22	1:A:769:LYS:HZ2	1.58	0.68
2:D:142:MET:HE2	2:D:336:ASN:HB2	1.76	0.67
1:A:366:ILE:HG23	1:A:373:ILE:HB	1.77	0.67
1:C:744:CYS:SG	1:C:745:ASP:N	2.68	0.67
1:C:355:ASN:ND2	1:C:357:GLN:OE1	2.28	0.66
4:J:72:ASP:HB3	4:J:78:ALA:HA	1.75	0.66
1:C:34:SER:HA	1:C:67:HIS:HB2	1.78	0.65
1:C:269:LEU:HD13	1:C:353:ILE:HG12	1.78	0.65
4:F:32:THR:HB	4:F:52(A):PRO:HD2	1.78	0.65
3:E:46:ARG:NH1	3:E:48:ILE:O	2.29	0.65
2:D:241:PHE:HB3	2:D:274:PRO:HD3	1.79	0.64
4:F:4:LEU:HD11	4:F:106:GLY:H	1.63	0.64
3:I:35:TRP:HA	3:I:88:CYS:HA	1.80	0.64
2:D:423:ASP:HB2	2:D:427:GLY:HA2	1.79	0.64
1:C:628:SER:HB3	2:D:832:SER:HB2	1.79	0.64
4:J:33:TYR:OH	4:J:50:ARG:NH1	2.31	0.64
3:I:38:GLN:HB3	3:I:85:ASP:HB2	1.79	0.64
3:I:36:LEU:HB3	3:I:87:TYR:HB2	1.80	0.63
1:C:266:ILE:HG22	1:C:356:LEU:HB2	1.81	0.63
4:F:48:ILE:HD11	4:F:66:LYS:HE3	1.81	0.63
4:J:35:HIS:HB2	4:J:96:ALA:HB3	1.80	0.63
2:B:367:LEU:HD21	2:B:371:ARG:HG3	1.80	0.63
3:I:35:TRP:HE1	3:I:48:ILE:HD12	1.64	0.62
1:C:235:ALA:HA	1:C:238:LEU:HD12	1.80	0.62
3:E:59:PRO:HG2	3:E:61:ARG:HD2	1.81	0.62
2:B:119:THR:O	2:B:328:ARG:NH2	2.33	0.62
4:F:82:LEU:HB3	4:F:85:LEU:HD21	1.82	0.62
3:E:49:TYR:O	3:E:91:TYR:OH	2.18	0.61
1:C:679:PHE:HA	1:C:727:HIS:HB2	1.81	0.61
2:D:250:THR:HG22	2:D:274:PRO:HG3	1.82	0.61
1:C:138:LEU:HG	1:C:322:LYS:HD2	1.83	0.61
2:D:234:LYS:HE2	2:D:263:ALA:HA	1.83	0.61
2:B:358:MET:O	2:B:382:LYS:NZ	2.33	0.61
4:J:50:ARG:O	4:J:57:THR:OG1	2.19	0.61
2:D:238:THR:HA	2:D:272:GLU:HA	1.82	0.61
3:E:46:ARG:HH12	3:E:49:TYR:HA	1.66	0.61
1:A:671:ARG:HG3	1:A:675:PRO:HB3	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:47:LEU:HD23	3:I:58:VAL:HG22	1.83	0.60
4:J:18:VAL:HB	4:J:79:TYR:HB2	1.82	0.60
2:B:214:SER:HA	2:B:218:ASN:HB2	1.82	0.60
2:D:158:LEU:HD13	2:D:161:MET:HG3	1.82	0.60
2:B:68:VAL:HG11	2:B:97:VAL:HA	1.84	0.60
1:C:167:VAL:HA	1:C:222:SER:HB3	1.84	0.60
1:A:287:VAL:HG23	1:A:330:TYR:HB3	1.84	0.60
1:C:339:GLU:HB2	1:C:347:LYS:H	1.67	0.59
4:J:4:LEU:HD13	4:J:104:TYR:HB3	1.83	0.59
1:C:641:MET:HE1	2:D:643:LEU:HG	1.83	0.59
1:C:562:LEU:HD11	2:D:814:ASP:HA	1.83	0.59
3:E:29:ILE:HD11	3:E:33:LEU:HB2	1.85	0.59
2:D:172:VAL:HG23	2:D:223:LEU:HD13	1.85	0.59
2:B:785:GLY:O	1:C:695:ARG:NH2	2.35	0.59
3:E:2:ILE:HG12	3:E:95:PRO:HG2	1.85	0.59
1:A:260:ARG:O	1:A:359:ARG:NH2	2.36	0.59
1:C:91:LEU:HD21	1:C:288:VAL:HG11	1.85	0.59
2:B:612:LEU:HD23	2:B:635:TRP:HD1	1.68	0.58
1:A:115:ARG:HH21	1:A:314:ILE:HD12	1.69	0.58
2:B:242:GLU:HB3	2:B:272:GLU:HG3	1.85	0.58
2:D:364:ILE:HG13	2:D:384:LEU:HD23	1.85	0.58
1:A:654:PHE:HA	1:A:657:LEU:HD22	1.84	0.58
2:D:169:PHE:HB2	2:D:199:LEU:HD23	1.85	0.58
1:C:262:ALA:O	1:C:359:ARG:NH1	2.36	0.58
2:D:151:GLU:HB3	2:D:185:LYS:HB2	1.85	0.58
2:B:90:SER:HB2	4:J:99:TYR:HB3	1.85	0.58
4:J:82:LEU:HB3	4:J:85:LEU:HD21	1.85	0.58
1:C:341:ASN:OD1	1:C:344:GLY:N	2.37	0.58
2:D:190:ILE:HD11	2:D:199:LEU:HB2	1.86	0.58
2:B:517:GLU:HG2	1:C:774:LEU:HD12	1.86	0.57
1:A:139:ARG:HH21	1:A:141:VAL:HG23	1.69	0.57
1:A:641:MET:HE1	2:B:643:LEU:HD11	1.86	0.57
2:B:613:VAL:HG23	2:B:614:PHE:HD1	1.70	0.57
1:A:115:ARG:HG2	1:A:135:LEU:HD11	1.86	0.57
2:D:135:ALA:HB2	2:D:177:PRO:HB2	1.86	0.57
3:E:38:GLN:HA	3:E:44:ILE:HG23	1.85	0.57
1:A:355:ASN:ND2	1:A:357:GLN:OE1	2.38	0.57
1:C:775:SER:HB2	1:C:780:HIS:CG	2.39	0.57
2:B:686:VAL:HG23	2:B:729:PHE:HZ	1.70	0.57
1:A:602:THR:N	1:A:605:SER:HG	2.02	0.57
1:C:147:GLN:NE2	1:C:251:GLU:OE1	2.38	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:J:97:ARG:N	4:J:102:PHE:O	2.33	0.57
4:F:50:ARG:NH1	4:F:56:ASN:O	2.38	0.57
3:E:86:TYR:HB2	3:E:102:THR:HB	1.87	0.57
1:C:567:GLY:O	1:C:571:HIS:ND1	2.38	0.56
2:B:386:MET:SD	2:B:387:LYS:N	2.74	0.56
1:C:163:ILE:HB	1:C:191:ALA:HB1	1.85	0.56
1:C:372:VAL:HG12	1:C:374:PRO:HD3	1.87	0.56
1:C:560:SER:HA	1:C:563:TRP:HD1	1.69	0.56
2:D:73:MET:SD	2:D:73:MET:N	2.78	0.56
4:F:92:VAL:HB	4:F:110:LEU:HD13	1.87	0.56
2:B:365:ILE:HD12	2:B:373:TRP:HB3	1.87	0.56
2:B:509:ALA:HB3	2:B:765:ALA:HB3	1.87	0.56
2:D:652:ALA:O	2:D:656:GLN:NE2	2.39	0.56
4:J:34:ILE:HG23	4:J:51:ILE:HB	1.88	0.56
1:C:216:ALA:HA	1:C:392:TYR:HA	1.86	0.56
4:J:60:ASP:HB2	4:J:63:PHE:HB2	1.87	0.56
1:A:762:MET:HE3	1:A:769:LYS:HG2	1.88	0.56
4:J:6:GLN:HE22	4:J:106:GLY:HA3	1.70	0.56
2:D:158:LEU:HA	2:D:161:MET:HB2	1.88	0.56
2:D:337:ARG:O	2:D:341:ASN:ND2	2.39	0.56
2:D:339:LEU:HD12	2:D:351:PHE:HE2	1.71	0.56
1:C:126:SER:O	1:C:128:TYR:N	2.39	0.56
4:J:60:ASP:OD2	4:J:62:LYS:NZ	2.39	0.56
1:A:440:ASN:HB3	1:A:447:PRO:HB3	1.87	0.55
2:D:363:VAL:HG22	2:D:379:TRP:H	1.71	0.55
3:E:9:SER:HA	3:E:102:THR:HA	1.87	0.55
3:I:54:LEU:HD12	3:I:58:VAL:HB	1.89	0.55
2:B:86:CYS:O	2:B:90:SER:N	2.39	0.55
1:C:140:THR:HA	1:C:345:ASP:HA	1.88	0.55
2:D:270:PRO:O	2:D:371:ARG:NH2	2.39	0.55
1:A:70:ASN:ND2	2:B:322:TYR:O	2.39	0.55
4:F:68:THR:O	4:F:81:HIS:N	2.39	0.55
1:A:505:LEU:HA	1:A:510:ALA:HB3	1.88	0.55
2:B:260:SER:HB3	2:B:281:SER:HA	1.89	0.55
2:D:280:VAL:HG22	2:D:362:LEU:HB3	1.89	0.55
3:I:24:ARG:HH11	3:I:25:ALA:H	1.54	0.55
2:D:308:LEU:HD12	2:D:314:ILE:HD11	1.88	0.55
3:I:37:GLN:NE2	3:I:85:ASP:O	2.40	0.55
2:B:494:TRP:HB3	2:B:499:GLY:HA2	1.89	0.55
1:C:148:SER:HB2	1:C:180:LEU:HB2	1.88	0.55
2:D:215:LYS:HB3	2:D:240:ILE:HG21	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:301:ILE:HG23	1:A:317:THR:HG21	1.88	0.54
2:D:145:GLN:HB2	2:D:356:TYR:H	1.71	0.54
4:J:35:HIS:N	4:J:96:ALA:O	2.37	0.54
1:C:121:LEU:HD11	1:C:281:ILE:HG12	1.88	0.54
2:D:258:VAL:HG13	2:D:277:LEU:HD11	1.88	0.54
1:A:751:GLU:N	1:A:751:GLU:OE2	2.40	0.54
3:E:6:GLN:HA	3:E:23:CYS:HA	1.90	0.54
3:E:35:TRP:HH2	3:E:86:TYR:HB3	1.73	0.54
1:A:165:LEU:HD11	1:A:180:LEU:HD22	1.90	0.54
1:A:669:ASP:HB2	1:A:672:LEU:HB2	1.90	0.54
1:C:405:GLN:HE21	1:C:735:VAL:HG21	1.73	0.54
1:C:208:LEU:HD13	1:C:238:LEU:HD11	1.90	0.54
1:C:380:ILE:HG12	1:C:386:THR:HG22	1.88	0.54
2:D:215:LYS:HA	2:D:219:GLN:HG2	1.89	0.54
1:A:68:LYS:NZ	1:A:69:PRO:O	2.39	0.54
2:D:351:PHE:HA	2:D:357:GLN:HA	1.90	0.54
2:D:628:SER:HA	2:D:631:MET:HE3	1.91	0.53
1:A:260:ARG:HB2	1:A:359:ARG:HH22	1.73	0.53
4:J:20:LEU:HD21	4:J:93:TYR:HD2	1.72	0.53
4:J:37:VAL:HA	4:J:48:ILE:H	1.74	0.53
2:B:537:MET:HE1	2:B:748:LEU:HD23	1.90	0.53
3:I:4:MET:HE3	3:I:89:LEU:HA	1.90	0.53
1:A:291:ALA:O	1:A:295:LEU:N	2.41	0.53
2:B:133:ILE:HD11	2:B:147:GLY:HA3	1.91	0.53
1:C:140:THR:HB	1:C:346:ARG:HG2	1.90	0.53
3:E:11:LEU:HB3	3:E:104:LEU:HA	1.91	0.52
4:J:37:VAL:HG12	4:J:47:TRP:HA	1.91	0.52
1:A:71:ALA:HB1	1:A:106:PRO:HG3	1.91	0.52
1:C:269:LEU:HD11	1:C:351:TYR:HB3	1.91	0.52
2:D:126:ILE:HD12	2:D:293:VAL:HG22	1.92	0.52
4:J:29:ILE:HD12	4:J:73:THR:HG21	1.90	0.52
1:A:354:MET:HB3	1:A:361:LEU:HD22	1.90	0.52
2:B:307:MET:HE2	2:B:313:PHE:HB2	1.92	0.52
1:A:687:SER:OG	1:A:688:SER:N	2.42	0.52
2:B:105:GLN:HG3	2:B:107:ALA:H	1.74	0.52
3:I:59:PRO:O	3:I:61:ARG:NH1	2.42	0.52
1:C:113:PHE:O	1:C:115:ARG:NH1	2.42	0.52
1:C:489:ARG:HA	1:C:496:LYS:HA	1.91	0.52
1:C:780:HIS:HB3	1:C:785:MET:N	2.25	0.52
2:D:826:GLY:HA2	2:D:829:MET:SD	2.50	0.52
1:C:350:ASN:HA	1:C:368:ASN:HA	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:220:ILE:HG22	1:C:248:LEU:HB3	1.90	0.52
3:E:44:ILE:HD12	4:F:94:TYR:HE1	1.75	0.52
1:C:88:TYR:HA	1:C:315:TRP:HH2	1.75	0.52
2:B:138:ASP:O	2:B:141:SER:OG	2.28	0.51
1:C:287:VAL:HB	1:C:330:TYR:HE1	1.75	0.51
1:C:403:ILE:HD12	1:C:479:VAL:HG11	1.92	0.51
2:D:68:VAL:HA	2:D:94:ILE:HB	1.91	0.51
3:E:18:ARG:HH22	3:E:74:THR:HB	1.76	0.51
1:C:766:SER:OG	1:C:768:TRP:O	2.25	0.51
2:D:373:TRP:O	2:D:375:ARG:NH1	2.42	0.51
1:A:118:VAL:HG13	1:A:137:PHE:HD1	1.75	0.51
2:B:408:ILE:HD13	2:B:465:LEU:HD11	1.91	0.51
3:E:21:LEU:HB3	3:E:73:LEU:HD21	1.91	0.51
2:B:241:PHE:CD2	2:B:273:PHE:HB3	2.45	0.51
1:C:137:PHE:HE1	1:C:139:ARG:HB2	1.75	0.51
1:C:240:MET:HG3	1:C:247:TRP:HZ2	1.76	0.51
1:A:145:SER:O	1:A:179:ARG:NH1	2.44	0.51
1:A:212:ARG:NH2	1:A:238:LEU:O	2.44	0.51
1:C:32:VAL:HA	1:C:65:VAL:HB	1.92	0.51
4:J:33:TYR:CE2	4:J:99:TYR:HA	2.46	0.51
2:B:282:TYR:HE2	2:B:292:ARG:HH22	1.59	0.51
2:D:270:PRO:HG2	2:D:272:GLU:HG3	1.92	0.51
2:B:68:VAL:HG12	2:B:98:VAL:HG22	1.92	0.51
1:C:120:GLY:HA3	1:C:139:ARG:HG3	1.91	0.51
2:D:155:SER:HA	2:D:158:LEU:HB2	1.92	0.50
1:A:570:VAL:HG11	1:A:611:TRP:HZ3	1.77	0.50
1:C:27:VAL:HG21	1:C:292:VAL:HG21	1.92	0.50
2:D:85:ILE:O	2:D:89:MET:N	2.45	0.50
3:E:90:GLN:HE22	3:E:95:PRO:HB2	1.76	0.50
1:C:290:GLN:HG3	1:C:330:TYR:HB3	1.93	0.50
3:E:24:ARG:NH1	3:E:25:ALA:O	2.45	0.50
1:A:805:PRO:HG3	2:D:656:GLN:HE21	1.77	0.50
1:C:184:LEU:HD13	1:C:190:LYS:HA	1.92	0.50
1:C:28:ASN:HB3	1:C:87:VAL:HA	1.93	0.50
4:J:69:VAL:HG21	4:J:78:ALA:HB1	1.92	0.50
4:F:6:GLN:H	4:F:107:GLN:HE21	1.60	0.50
4:J:19:LYS:O	4:J:80:LEU:N	2.45	0.50
1:C:166:LEU:HG	1:C:195:LEU:HB2	1.94	0.49
2:B:224:GLN:CD	2:B:225:SER:H	2.21	0.49
3:E:15:LEU:HD13	3:E:80:SER:HA	1.93	0.49
4:F:20:LEU:HD12	4:F:111:VAL:HG21	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:682:ALA:HB2	1:A:726:LEU:HD21	1.94	0.49
2:B:195:VAL:HG22	2:B:432:ASN:H	1.77	0.49
2:D:509:ALA:H	2:D:765:ALA:HB3	1.77	0.49
4:J:1:GLU:HG2	4:J:2:VAL:HG23	1.93	0.49
4:J:38:LYS:HZ1	4:J:91:ALA:N	2.10	0.49
1:C:163:ILE:HG12	1:C:218:VAL:HG11	1.94	0.49
2:D:175:TYR:N	2:D:231:TYR:O	2.43	0.49
3:E:19:VAL:HG21	3:E:78:LEU:HD22	1.94	0.49
4:J:14:PRO:HA	4:J:85:LEU:HB2	1.94	0.49
1:A:93:SER:HA	1:A:121:LEU:HB3	1.93	0.49
1:C:365:GLY:HA2	1:C:374:PRO:HA	1.94	0.49
1:C:441:ASP:O	1:C:446:SER:OG	2.23	0.49
3:E:61:ARG:NH1	3:E:80:SER:O	2.34	0.49
4:F:51:ILE:HD13	4:F:69:VAL:HG12	1.95	0.49
1:A:317:THR:HG22	1:A:321:PHE:HB2	1.94	0.49
2:D:244:ALA:O	2:D:250:THR:OG1	2.24	0.49
4:F:60:ASP:HB3	4:F:63:PHE:HB2	1.95	0.49
1:A:117:PRO:HG2	1:A:321:PHE:HD1	1.78	0.49
2:B:488:LYS:HD3	2:B:688:ASN:HA	1.95	0.49
3:I:21:LEU:HD23	3:I:73:LEU:HD21	1.94	0.49
4:J:10:GLU:HB2	4:J:111:VAL:HG22	1.95	0.49
2:B:170:SER:HA	2:B:199:LEU:HD22	1.94	0.48
2:B:477:ASP:OD1	2:B:477:ASP:N	2.46	0.48
4:F:28:ASN:OD1	4:F:29:ILE:N	2.45	0.48
1:C:165:LEU:HA	1:C:220:ILE:HG12	1.94	0.48
1:C:218:VAL:HA	1:C:246:VAL:HB	1.96	0.48
2:B:79:LYS:NZ	3:I:52:SER:HB2	2.29	0.48
2:B:172:VAL:HG21	2:B:223:LEU:HD22	1.95	0.48
1:C:124:ARG:HH12	1:C:144:TYR:HA	1.78	0.48
2:D:269:VAL:HG12	2:D:273:PHE:HZ	1.78	0.48
3:E:38:GLN:HG2	3:E:44:ILE:HG23	1.96	0.48
2:B:108:ILE:HD11	2:B:129:GLY:HA3	1.95	0.48
2:D:310:GLU:OE1	2:D:338:TYR:OH	2.30	0.48
1:C:172:GLU:HG2	1:C:252:ARG:HH21	1.78	0.48
2:D:211:ASP:HA	2:D:215:LYS:HB2	1.94	0.48
1:C:202:LYS:NZ	1:C:203:ASN:O	2.46	0.48
3:E:90:GLN:HE21	3:E:97:THR:HG22	1.79	0.48
1:A:398:LEU:HD12	1:A:512:MET:HE2	1.96	0.48
1:A:602:THR:N	1:A:605:SER:OG	2.47	0.48
2:B:85:ILE:HG21	2:B:115:ILE:HD13	1.96	0.48
1:A:696:GLN:HB2	1:A:699:LEU:HD23	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:59:TYR:HB2	4:F:64:GLN:HA	1.96	0.48
1:A:262:ALA:HB1	1:A:266:ILE:HG13	1.96	0.48
2:B:554:PHE:O	2:B:559:TRP:NE1	2.40	0.48
1:C:102:PHE:O	1:C:105:THR:OG1	2.30	0.48
1:C:775:SER:HB2	1:C:780:HIS:CD2	2.49	0.48
4:F:3:GLN:HG3	4:F:5:GLN:H	1.79	0.48
1:A:271:LEU:HG	1:A:272:ILE:H	1.79	0.47
1:A:684:VAL:HG21	1:A:731:TRP:HZ3	1.79	0.47
1:C:263:PRO:HD2	1:C:266:ILE:HD13	1.96	0.47
1:A:221:LEU:HB3	1:A:249:VAL:HG12	1.95	0.47
1:A:651:LEU:HD21	2:D:645:SER:HA	1.96	0.47
1:A:777:LEU:O	1:A:782:ASN:ND2	2.48	0.47
2:B:613:VAL:HG23	2:B:614:PHE:CD1	2.50	0.47
4:J:47:TRP:CZ2	4:J:50:ARG:HB2	2.49	0.47
1:A:700:SER:OG	1:A:701:THR:N	2.46	0.47
1:A:212:ARG:HH22	1:A:238:LEU:HB3	1.80	0.47
1:C:541:LEU:HB2	1:C:742:GLN:NE2	2.29	0.47
2:D:158:LEU:HG	2:D:189:THR:HG21	1.97	0.47
1:A:776:ILE:HG22	1:A:780:HIS:HB3	1.97	0.47
1:C:124:ARG:HH21	1:C:351:TYR:HE1	1.63	0.47
1:C:515:ALA:O	1:C:517:LEU:N	2.48	0.47
2:D:70:LEU:HD21	2:D:98:VAL:HB	1.97	0.47
1:A:363:GLN:NE2	1:A:365:GLY:O	2.48	0.47
2:B:64:VAL:HG12	2:B:66:PRO:HD3	1.97	0.47
2:D:239:TYR:HD2	2:D:240:ILE:HG23	1.79	0.47
1:A:208:LEU:HD23	1:A:238:LEU:HD12	1.96	0.47
1:A:641:MET:HE1	2:B:643:LEU:HD21	1.97	0.47
2:B:538:VAL:HG12	2:B:728:ALA:HB2	1.95	0.47
4:J:33:TYR:CZ	4:J:50:ARG:HD2	2.50	0.46
1:C:388:LYS:O	1:C:390:ARG:NH1	2.42	0.46
2:B:112:LEU:HB3	2:B:123:ILE:HD13	1.96	0.46
2:B:334:MET:HG3	2:B:337:ARG:HH12	1.81	0.46
1:C:541:LEU:HD23	1:C:736:LEU:HD13	1.97	0.46
2:D:239:TYR:CD2	2:D:240:ILE:HG23	2.50	0.46
1:C:124:ARG:HA	1:C:141:VAL:HG12	1.97	0.46
1:C:224:SER:OG	1:C:225:GLU:N	2.48	0.46
1:C:226:ASP:OD1	1:C:226:ASP:N	2.49	0.46
1:C:232:TYR:HE2	1:C:258:ALA:HB1	1.80	0.46
2:D:789:MET:HE2	2:D:789:MET:HB2	1.83	0.46
4:J:18:VAL:HG12	4:J:81:HIS:HB2	1.98	0.46
1:A:465:LYS:HE2	1:A:468:ARG:HH12	1.79	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:438:LYS:HB3	2:D:452:TYR:HA	1.97	0.46
3:I:38:GLN:HG2	3:I:44:ILE:HG23	1.97	0.46
4:J:93:TYR:N	4:J:109:THR:O	2.34	0.46
1:C:357:GLN:N	1:C:360:LYS:O	2.42	0.46
2:B:233:THR:O	2:B:237:ALA:N	2.48	0.46
1:C:403:ILE:HG22	1:C:515:ALA:HB1	1.96	0.46
1:C:737:GLU:HG2	1:C:738:PHE:H	1.81	0.46
2:D:339:LEU:HB3	2:D:351:PHE:HD2	1.80	0.46
2:B:280:VAL:HG22	2:B:362:LEU:HD12	1.98	0.45
1:A:635:VAL:HG11	2:B:828:ALA:HB1	1.97	0.45
2:B:516:ASN:OD1	2:B:517:GLU:N	2.48	0.45
4:F:24:ALA:HB2	4:F:97:ARG:HH22	1.81	0.45
4:J:38:LYS:HE3	4:J:40:ARG:HB2	1.97	0.45
1:C:126:SER:HB3	1:C:143:PRO:HD3	1.98	0.45
2:D:154:ALA:HB1	2:D:157:MET:HE3	1.99	0.45
2:D:379:TRP:CE2	2:D:381:ASP:HA	2.52	0.45
2:D:562:MET:HA	2:D:565:MET:HG2	1.99	0.45
1:A:679:PHE:HB3	1:A:726:LEU:HA	1.99	0.45
1:A:776:ILE:O	1:A:781:GLU:HG3	2.17	0.45
1:A:807:THR:OG1	2:D:554:PHE:N	2.49	0.45
4:F:33:TYR:HA	4:F:52:ASP:HA	1.98	0.45
1:A:530:SER:OG	1:A:760:ILE:O	2.31	0.45
1:C:438:GLY:HA3	1:C:478:LEU:HB2	1.99	0.45
2:D:329:ILE:HG23	2:D:330:TYR:HD1	1.82	0.45
1:A:153:GLU:OE1	1:A:367:TYR:OH	2.29	0.45
1:A:357:GLN:HE22	1:A:380:ILE:HG13	1.81	0.45
2:B:85:ILE:HD11	2:B:97:VAL:HG11	1.97	0.45
3:E:51:THR:HB	3:E:66:ARG:HH21	1.82	0.45
1:C:247:TRP:H	1:C:382:PRO:HG3	1.82	0.45
4:F:33:TYR:CD1	4:F:99:TYR:HA	2.52	0.45
2:B:572:VAL:HG21	1:C:824:ILE:HG12	1.99	0.45
1:C:353:ILE:H	1:C:363:GLN:HE22	1.65	0.45
4:J:67:ALA:HB1	4:J:80:LEU:HD23	1.98	0.45
1:A:142:PRO:HA	1:A:143:PRO:HD3	1.87	0.44
2:D:65:VAL:HG22	2:D:301:THR:HG21	1.99	0.44
1:A:781:GLU:OE1	2:D:698:ASN:ND2	2.50	0.44
1:C:145:SER:HA	1:C:176:ALA:HB2	1.98	0.44
2:D:112:LEU:HD22	2:D:123:ILE:HD13	2.00	0.44
2:D:238:THR:HA	2:D:272:GLU:HG2	1.99	0.44
2:D:367:LEU:HD13	2:D:373:TRP:CE2	2.52	0.44
3:E:46:ARG:HB3	4:F:105:TRP:CH2	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:223:ALA:N	1:A:253:GLU:OE2	2.37	0.44
4:J:38:LYS:HZ1	4:J:91:ALA:H	1.65	0.44
1:A:78:VAL:HA	1:A:82:LEU:HD12	1.98	0.44
1:C:212:ARG:HD3	1:C:240:MET:HE2	2.00	0.44
2:D:266:THR:OG1	2:D:372:LYS:O	2.31	0.44
4:J:59:TYR:HE2	4:J:68:THR:HG22	1.82	0.44
3:E:4:MET:HE3	3:E:90:GLN:HG2	2.00	0.44
3:I:22:THR:HA	3:I:72:SER:HA	1.99	0.44
1:A:309:VAL:HG12	2:B:79:LYS:HE2	1.98	0.44
4:F:38:LYS:N	4:F:46:GLU:O	2.45	0.44
3:I:34:ILE:HB	3:I:46:ARG:HD3	1.98	0.44
1:A:142:PRO:HD2	1:A:271:LEU:HD21	1.99	0.44
2:B:273:PHE:HA	2:B:274:PRO:HD3	1.89	0.44
2:B:256:TRP:HE3	2:B:277:LEU:HD11	1.83	0.44
2:B:604:LYS:HD2	2:B:621:GLN:HB3	2.00	0.44
4:J:49:GLY:HA3	4:J:59:TYR:HA	2.00	0.44
1:C:520:ASN:OD1	1:C:521:ASN:N	2.49	0.44
1:C:602:THR:HG23	1:C:625:ARG:HH21	1.83	0.44
2:D:354:ASP:HB2	2:D:356:TYR:HE1	1.83	0.44
4:F:51:ILE:HG21	4:F:69:VAL:HG12	1.99	0.44
1:A:41:MET:O	1:A:45:ALA:N	2.50	0.43
1:C:333:GLY:HA3	1:C:346:ARG:HH22	1.83	0.43
4:J:40:ARG:HE	4:J:43:GLN:CD	2.26	0.43
1:A:276:ASN:OD1	1:A:278:SER:OG	2.36	0.43
2:B:795:LEU:HG	2:B:796:TRP:CD1	2.52	0.43
1:C:264:ASP:HA	1:C:356:LEU:HD23	2.00	0.43
1:C:821:ALA:HA	1:C:824:ILE:HD12	1.99	0.43
2:D:258:VAL:HB	2:D:262:VAL:HG21	2.01	0.43
1:A:90:ILE:HG23	1:A:118:VAL:HG23	1.99	0.43
2:B:707:GLY:O	2:B:709:PHE:N	2.52	0.43
1:A:397:ARG:HH21	1:A:475:GLU:HB3	1.84	0.43
2:B:125:GLY:N	2:B:144:PHE:O	2.51	0.43
4:F:102:PHE:HB2	4:F:105:TRP:CH2	2.54	0.43
2:B:197:TRP:HB3	2:B:198:GLU:H	1.59	0.43
2:B:318:LYS:H	2:B:328:ARG:NH1	2.17	0.43
2:D:334:MET:SD	2:D:337:ARG:NE	2.82	0.43
4:F:35:HIS:HB2	4:F:96:ALA:HB3	2.00	0.43
4:J:40:ARG:HB3	4:J:43:GLN:HG2	2.00	0.43
1:A:165:LEU:HD23	1:A:220:ILE:HB	2.00	0.43
1:A:226:ASP:OD1	1:A:226:ASP:N	2.50	0.43
2:B:279:SER:HB2	2:B:365:ILE:HD11	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:95:PRO:HG2	1:C:102:PHE:HD2	1.83	0.43
1:A:398:LEU:HD21	1:A:472:PHE:CD2	2.53	0.43
1:A:531:LYS:HG3	1:A:774:LEU:HD12	2.00	0.43
2:B:310:GLU:CD	2:B:311:HIS:CE1	2.96	0.43
2:B:362:LEU:HB2	2:B:379:TRP:CD1	2.53	0.43
1:C:125:MET:HA	1:C:143:PRO:HB3	2.00	0.43
1:C:217:ARG:HA	1:C:217:ARG:HD3	1.85	0.43
1:A:435:ILE:HD13	1:A:454:CYS:HA	2.00	0.43
2:B:273:PHE:HB2	2:B:277:LEU:HD22	2.00	0.43
1:C:81:ASP:HB3	3:E:71:TYR:HE1	1.84	0.43
3:I:54:LEU:HB2	3:I:58:VAL:HG21	2.00	0.43
1:C:126:SER:HB2	1:C:129:SER:HB2	2.01	0.42
1:A:603:LEU:HD12	1:A:603:LEU:HA	1.93	0.42
1:A:726:LEU:HD12	1:A:727:HIS:H	1.84	0.42
1:C:443:SER:O	1:C:446:SER:OG	2.37	0.42
1:C:768:TRP:CD1	1:C:769:LYS:H	2.38	0.42
2:D:565:MET:HA	2:D:568:ILE:HD12	2.01	0.42
1:A:315:TRP:CE2	1:A:317:THR:HB	2.55	0.42
1:A:551:LEU:HB3	1:A:552:ASP:H	1.61	0.42
1:C:731:TRP:HB3	1:C:736:LEU:HD11	2.01	0.42
2:B:142:MET:SD	2:B:142:MET:N	2.92	0.42
2:D:148:PRO:HG3	2:D:362:LEU:HD21	2.00	0.42
2:D:220:LEU:HG	2:D:228:ILE:HD12	2.01	0.42
4:F:32:THR:OG1	4:F:52:ASP:OD1	2.32	0.42
4:F:50:ARG:H	4:F:59:TYR:HA	1.85	0.42
2:B:498:ILE:HD13	2:B:498:ILE:HA	1.89	0.42
1:C:354:MET:HB3	1:C:361:LEU:HB3	2.01	0.42
1:C:217:ARG:NE	1:C:393:GLN:OE1	2.50	0.42
1:C:614:LEU:HD23	1:C:615:LEU:HD22	2.01	0.42
2:B:557:ASP:OD1	2:B:557:ASP:N	2.52	0.42
1:C:126:SER:H	1:C:143:PRO:HB3	1.84	0.42
1:C:295:LEU:HD11	1:C:324:VAL:HG21	2.02	0.42
3:I:23:CYS:HB2	3:I:88:CYS:HB2	1.92	0.42
1:A:208:LEU:HD12	1:A:208:LEU:HA	1.92	0.42
1:C:26:ILE:HB	1:C:61:ASN:HB2	2.01	0.42
1:C:438:GLY:HA3	1:C:478:LEU:H	1.85	0.42
2:D:167:TYR:HE2	2:D:227:ILE:HD11	1.84	0.42
2:D:606:ILE:HA	2:D:609:LEU:HG	2.01	0.42
2:B:98:VAL:HG23	2:B:99:PHE:H	1.85	0.42
2:B:220:LEU:HD13	2:B:223:LEU:HD21	2.00	0.42
1:C:231:VAL:O	1:C:235:ALA:N	2.45	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:35:TRP:CE3	3:E:88:CYS:HB3	2.55	0.42
1:A:769:LYS:N	1:A:771:ASN:OD1	2.53	0.42
2:B:266:THR:HG21	2:B:285:TRP:HZ2	1.84	0.42
2:D:236:GLU:HA	2:D:239:TYR:CE1	2.55	0.42
4:F:51:ILE:HG13	4:F:57:THR:HB	2.01	0.42
2:B:817:ASN:OD1	2:B:818:MET:N	2.53	0.41
3:E:96:TYR:CD2	4:F:50:ARG:HG3	2.55	0.41
3:E:11:LEU:HG	3:E:104:LEU:HD13	2.02	0.41
1:A:811:GLU:CD	1:A:812:ASN:H	2.28	0.41
2:B:166:TRP:HB3	2:B:167:TYR:H	1.51	0.41
1:C:90:ILE:O	1:C:118:VAL:HA	2.20	0.41
1:C:192:GLU:HB3	1:C:193:LYS:H	1.76	0.41
2:D:186:ILE:HG23	2:D:199:LEU:HD13	2.01	0.41
3:E:9:SER:O	3:E:103:LYS:N	2.53	0.41
1:C:124:ARG:CZ	1:C:147:GLN:HE22	2.32	0.41
2:D:161:MET:HE1	2:D:227:ILE:HD12	2.02	0.41
3:E:2:ILE:HB	3:E:90:GLN:NE2	2.36	0.41
4:F:2:VAL:HA	4:F:25:SER:HB2	2.02	0.41
1:A:224:SER:OG	1:A:225:GLU:N	2.52	0.41
2:B:604:LYS:HB3	2:B:604:LYS:HE2	1.83	0.41
2:D:73:MET:HA	2:D:84:ARG:HH22	1.86	0.41
3:E:25:ALA:HB2	3:E:33:LEU:HD12	2.02	0.41
3:I:11:LEU:HD21	3:I:21:LEU:HD13	2.02	0.41
3:I:38:GLN:HA	3:I:44:ILE:HG23	2.02	0.41
1:A:667:ILE:HD11	1:A:753:PHE:CZ	2.56	0.41
2:B:118:GLN:HG2	2:B:327:LYS:HZ3	1.86	0.41
1:C:71:ALA:HA	1:C:74:MET:HE2	2.02	0.41
1:C:94:HIS:CD2	1:C:104:PRO:HD2	2.56	0.41
2:D:414:ALA:HB3	2:D:416:PHE:HD1	1.85	0.41
3:E:87:TYR:CZ	3:E:101:GLY:HA3	2.56	0.41
3:E:90:GLN:NE2	3:E:97:THR:H	2.19	0.41
1:A:109:TYR:CE2	2:B:114:PHE:HB2	2.56	0.41
2:B:230:LEU:HB3	2:B:258:VAL:HG12	2.02	0.41
2:B:337:ARG:NH2	2:B:338:TYR:OH	2.54	0.41
4:F:38:LYS:HB3	4:F:48:ILE:HB	2.03	0.41
1:A:765:ASP:OD2	1:A:766:SER:N	2.54	0.41
1:C:505:LEU:HD22	1:C:513:ILE:HG13	2.02	0.41
2:D:105:GLN:HG3	2:D:108:ILE:H	1.86	0.41
1:A:708:LYS:HE3	1:A:708:LYS:HB3	1.91	0.41
2:B:489:LYS:HD3	2:B:494:TRP:CD2	2.56	0.41
1:C:151:TRP:CD1	1:C:248:LEU:HD11	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:305:PRO:HG2	1:C:311:ASN:HD22	1.86	0.41
1:C:638:GLY:O	1:C:642:ILE:HG12	2.20	0.41
4:F:4:LEU:HD23	4:F:4:LEU:H	1.86	0.41
4:J:4:LEU:HA	4:J:24:ALA:HA	2.02	0.41
1:A:321:PHE:O	1:A:325:LEU:HD23	2.20	0.40
1:A:781:GLU:O	1:A:783:GLY:N	2.54	0.40
2:B:164:TYR:HE1	2:B:391:TRP:HB2	1.85	0.40
2:B:195:VAL:HG21	2:B:430:MET:HA	2.03	0.40
2:B:307:MET:HE2	2:B:313:PHE:H	1.86	0.40
2:D:79:LYS:HA	2:D:82:ILE:HG22	2.02	0.40
2:B:223:LEU:HD13	2:B:228:ILE:HG12	2.02	0.40
2:B:643:LEU:HA	2:B:643:LEU:HD13	1.88	0.40
2:B:171:ILE:HD12	2:B:229:LEU:HB2	2.02	0.40
2:B:237:ALA:HB1	2:B:241:PHE:CE2	2.56	0.40
1:C:421:LYS:HE3	1:C:421:LYS:HB2	1.86	0.40
2:D:631:MET:HA	2:D:634:VAL:HB	2.04	0.40
1:A:809:THR:HA	2:D:555:SER:HB3	2.03	0.40
2:B:537:MET:HA	2:B:750:THR:HA	2.02	0.40
1:C:79:CYS:HB3	2:D:79:LYS:HZ1	1.87	0.40
1:C:117:PRO:HB3	1:C:322:LYS:HB2	2.03	0.40
1:C:354:MET:SD	1:C:354:MET:N	2.94	0.40
2:D:612:LEU:HD23	2:D:636:ALA:HB2	2.03	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	789/844 (94%)	715 (91%)	68 (9%)	6 (1%)	16	52
1	C	789/844 (94%)	714 (90%)	70 (9%)	5 (1%)	21	58
2	B	744/826 (90%)	667 (90%)	69 (9%)	8 (1%)	11	44

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	D	739/826 (90%)	644 (87%)	91 (12%)	4 (0%)	24	61
3	E	105/107 (98%)	91 (87%)	13 (12%)	1 (1%)	12	46
3	I	105/107 (98%)	89 (85%)	14 (13%)	2 (2%)	6	34
4	F	114/116 (98%)	98 (86%)	15 (13%)	1 (1%)	14	49
4	J	114/116 (98%)	96 (84%)	18 (16%)	0	100	100
All	All	3499/3786 (92%)	3114 (89%)	358 (10%)	27 (1%)	18	52

All (27) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	104	PRO
1	A	476	VAL
2	B	329	ILE
2	B	679	PRO
1	C	104	PRO
2	D	219	GLN
2	D	766	ILE
3	E	48	ILE
1	A	684	VAL
1	A	700	SER
2	B	227	ILE
2	B	708	LYS
1	A	127	ILE
2	B	71	VAL
2	D	414	ALA
3	I	48	ILE
1	A	784	PHE
2	B	815	ILE
1	C	541	LEU
2	B	816	ASP
4	F	98	SER
1	C	527	ILE
2	B	414	ALA
1	C	127	ILE
3	I	29	ILE
1	C	680	ILE
2	D	453	ILE

### 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	586/727 (81%)	586 (100%)	0	100	100
1	C	535/727 (74%)	535 (100%)	0	100	100
2	B	550/722 (76%)	549 (100%)	1 (0%)	87	87
2	D	518/722 (72%)	518 (100%)	0	100	100
3	E	94/94 (100%)	94 (100%)	0	100	100
3	I	94/94 (100%)	94 (100%)	0	100	100
4	F	95/95 (100%)	95 (100%)	0	100	100
4	J	95/95 (100%)	95 (100%)	0	100	100
All	All	2567/3276 (78%)	2566 (100%)	1 (0%)	100	100

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	311	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	67	HIS
1	A	73	GLN
1	A	311	ASN
1	A	350	ASN
1	A	355	ASN
1	A	357	GLN
2	B	105	GLN
2	B	110	GLN
2	B	153	GLN
2	B	432	ASN
1	C	239	ASN
1	C	311	ASN
1	C	368	ASN

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Mol	Chain	Res	Type
1	C	405	GLN
2	D	61	HIS
2	D	219	GLN
2	D	245	ASN
2	D	341	ASN
2	D	486	HIS
2	D	649	ASN
2	D	656	GLN
3	E	90	GLN
4	F	107	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

### 5.7 Other polymers [i](#)

There are no such residues in this entry.

### 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

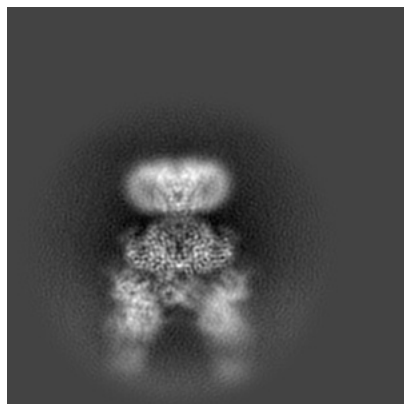
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-75129. These allow visual inspection of the internal detail of the map and identification of artifacts.

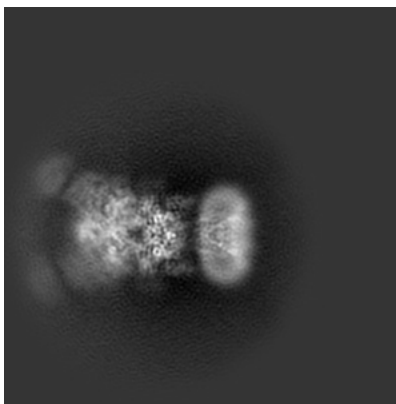
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

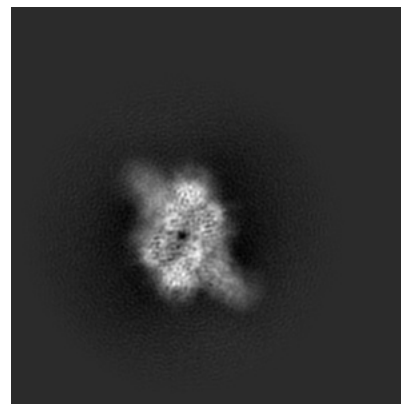
#### 6.1.1 Primary map



X

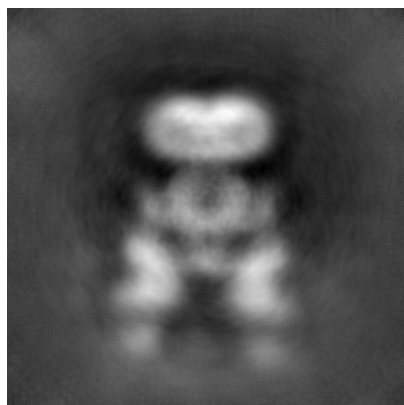


Y

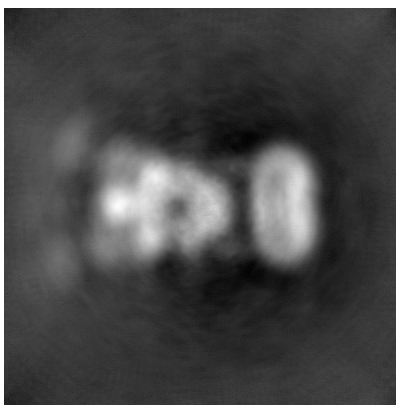


Z

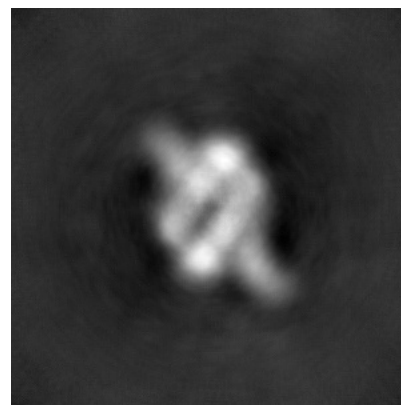
#### 6.1.2 Raw map



X



Y

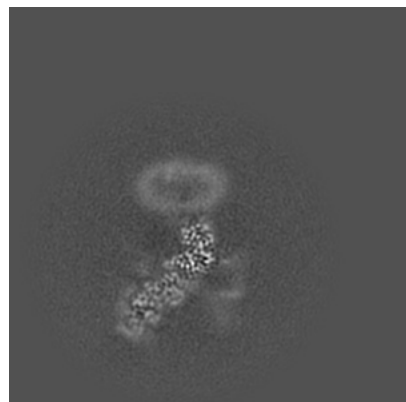


Z

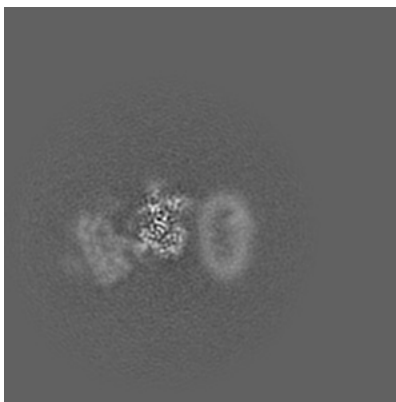
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

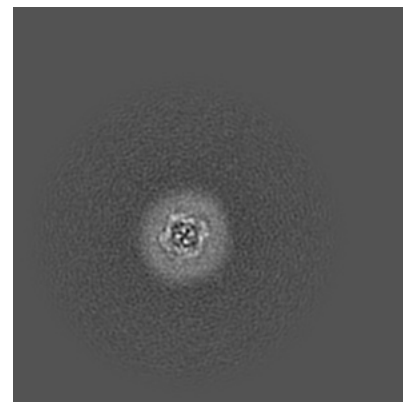
### 6.2.1 Primary map



X Index: 200

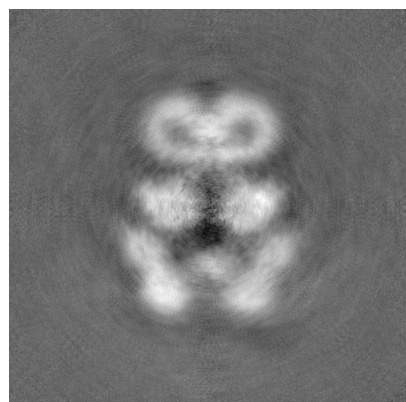


Y Index: 200

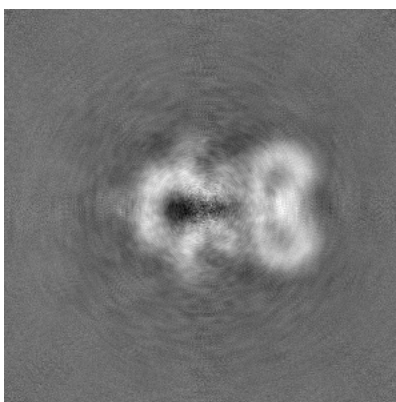


Z Index: 200

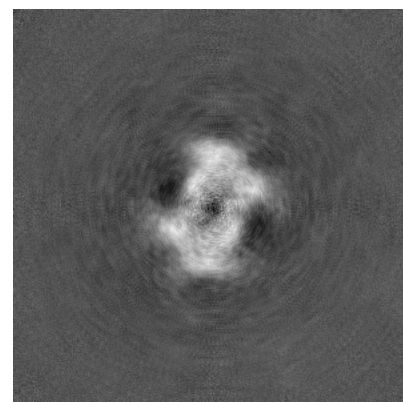
### 6.2.2 Raw map



X Index: 200



Y Index: 200

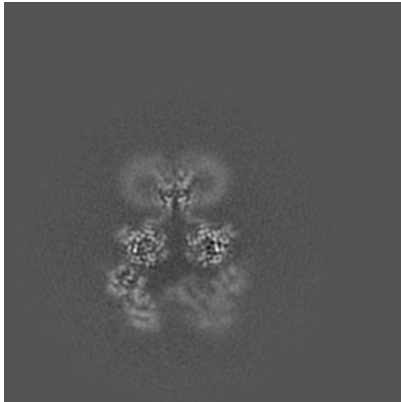


Z Index: 200

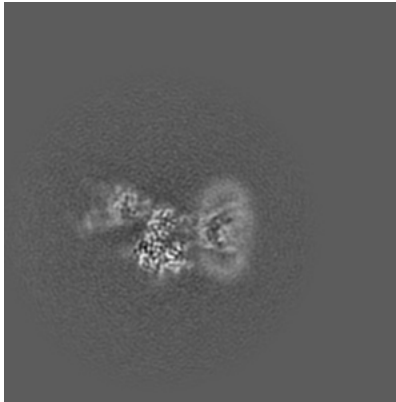
The images above show central slices of the map in three orthogonal directions.

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

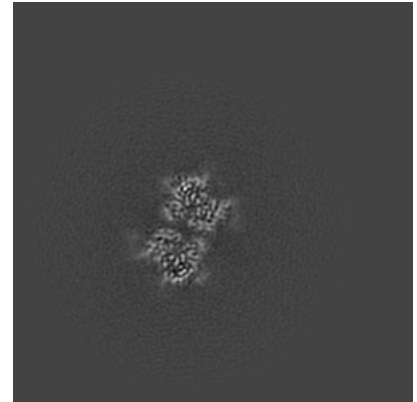
### 6.3.1 Primary map



X Index: 171

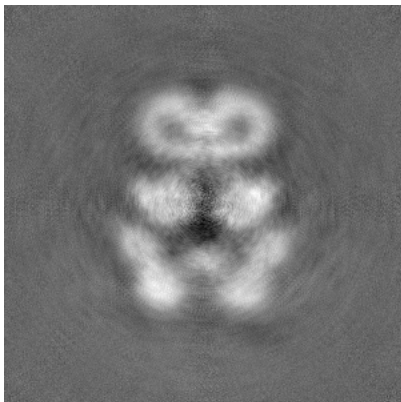


Y Index: 156

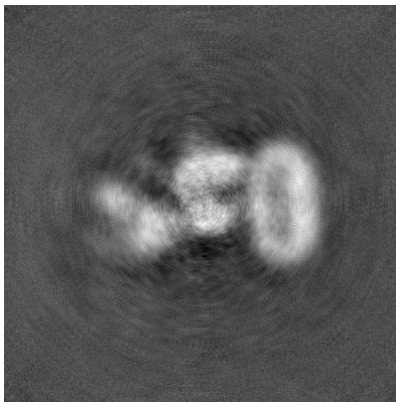


Z Index: 152

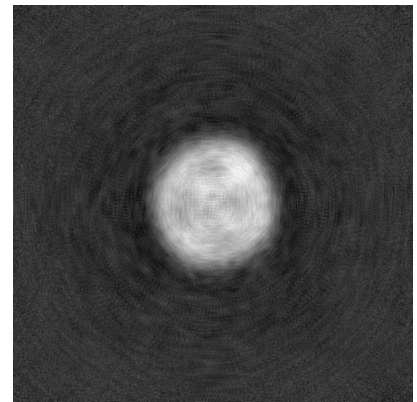
### 6.3.2 Raw map



X Index: 201



Y Index: 223

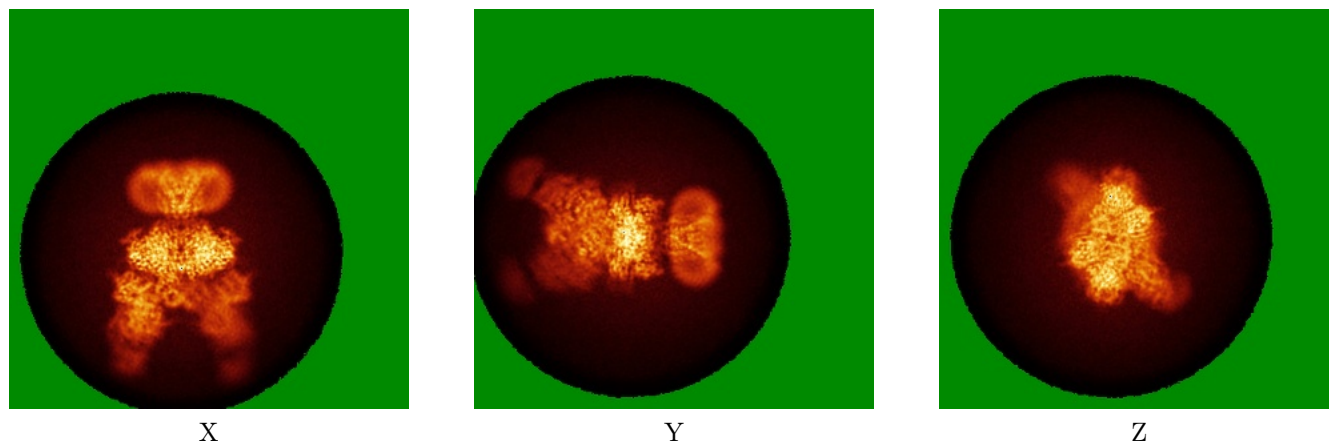


Z Index: 292

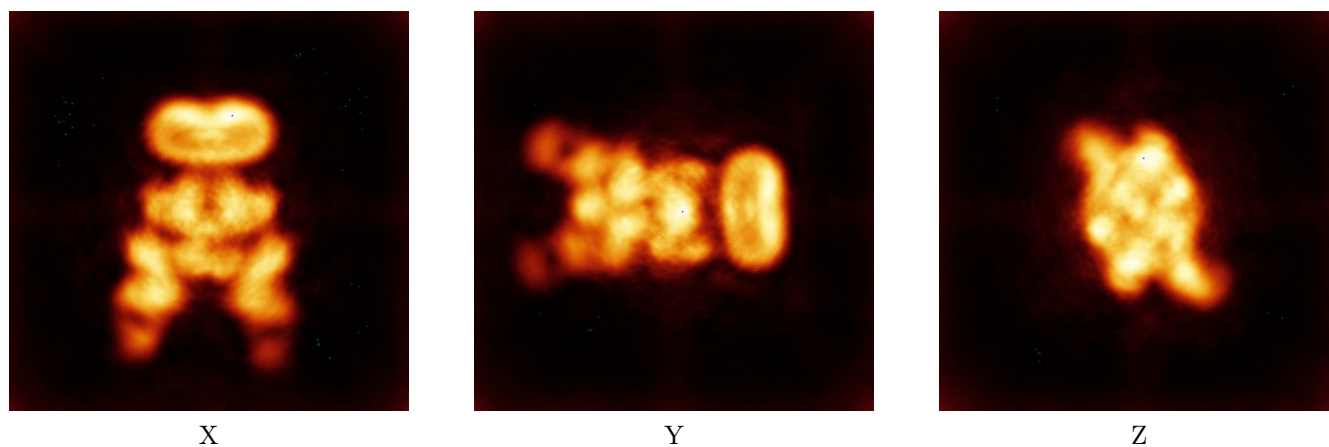
The images above show the largest variance slices of the map in three orthogonal directions.

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

### 6.4.1 Primary map



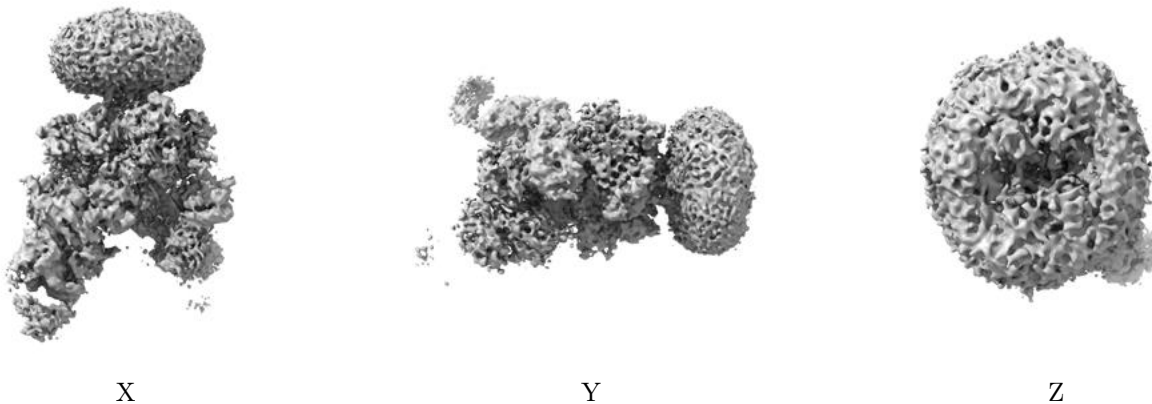
### 6.4.2 Raw map



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.

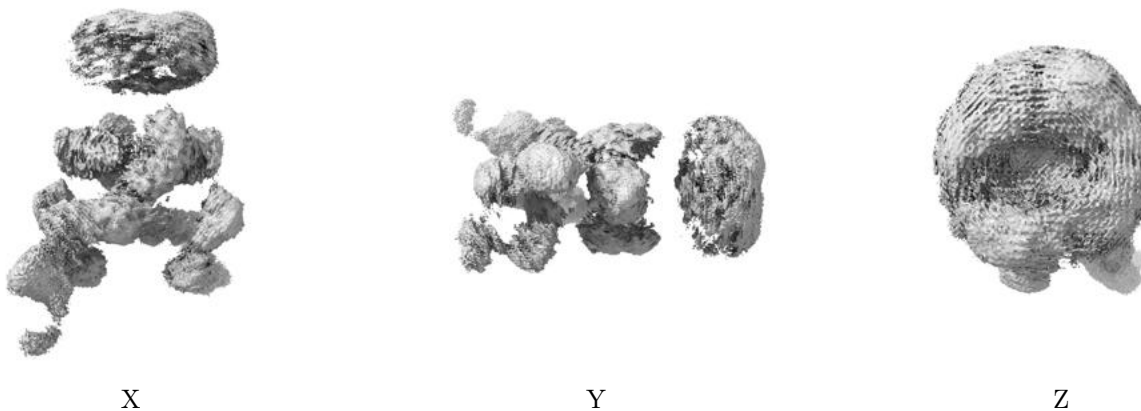
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.05. 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.

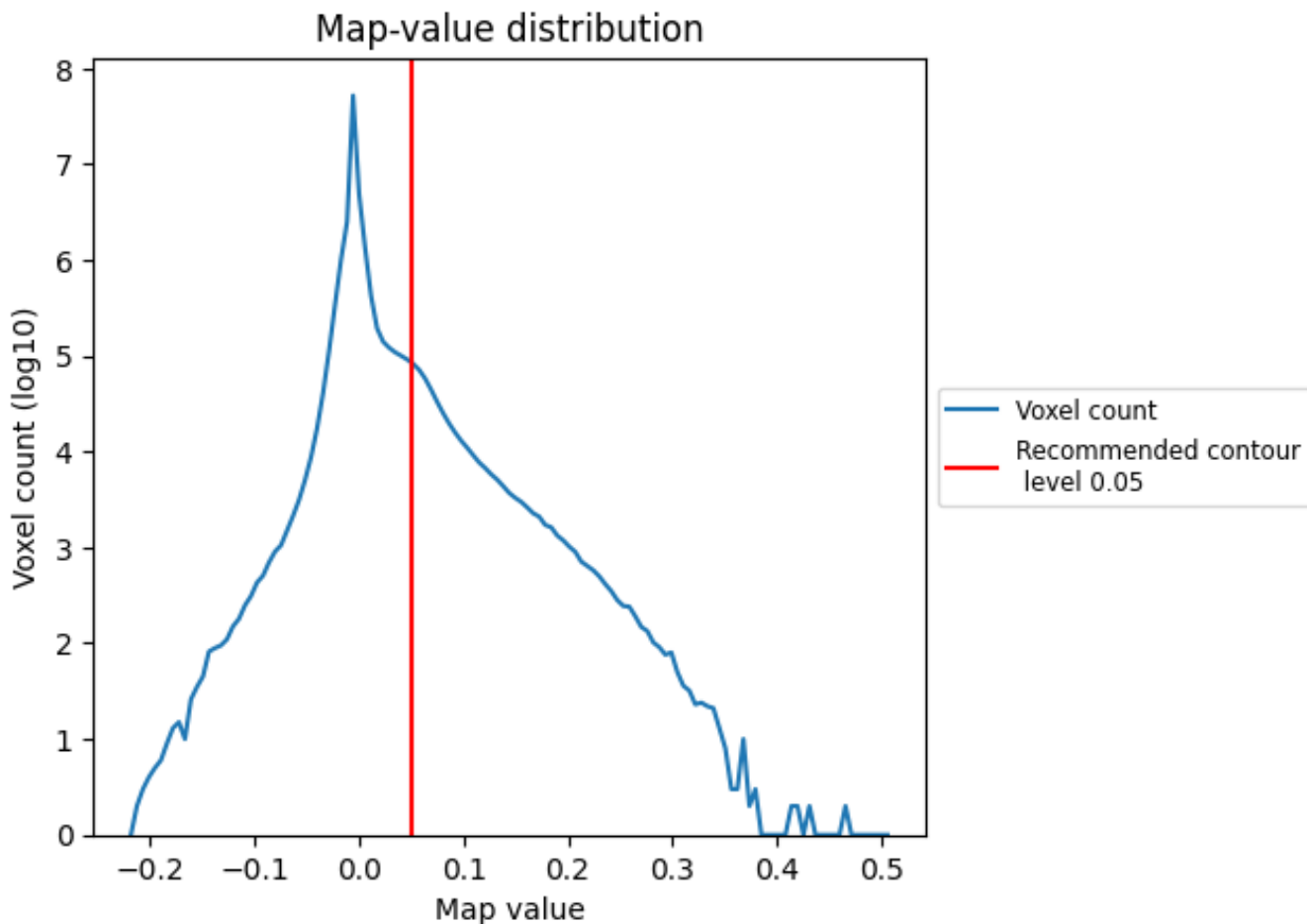
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

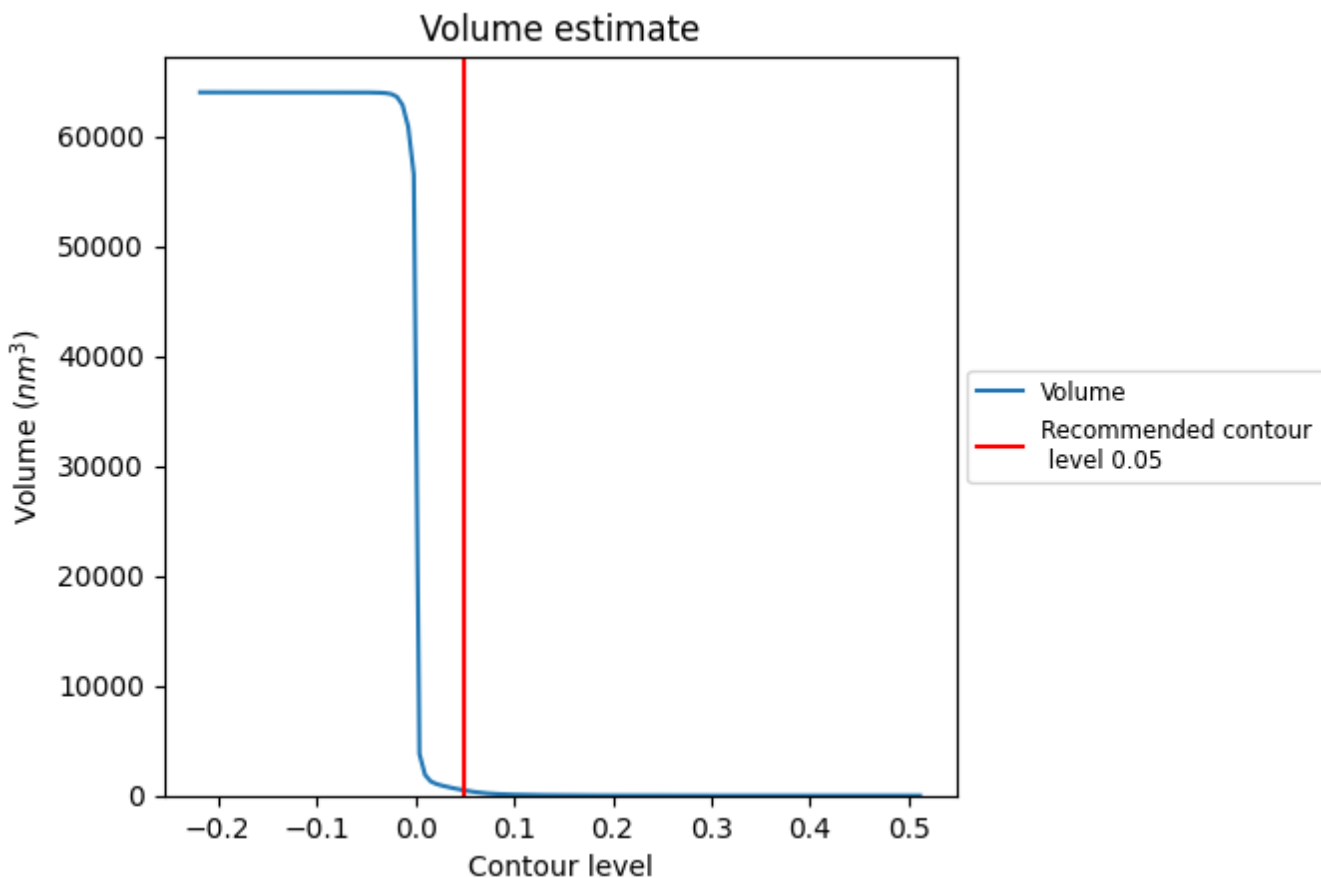
This section contains the results of statistical analysis of the map.

### 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.

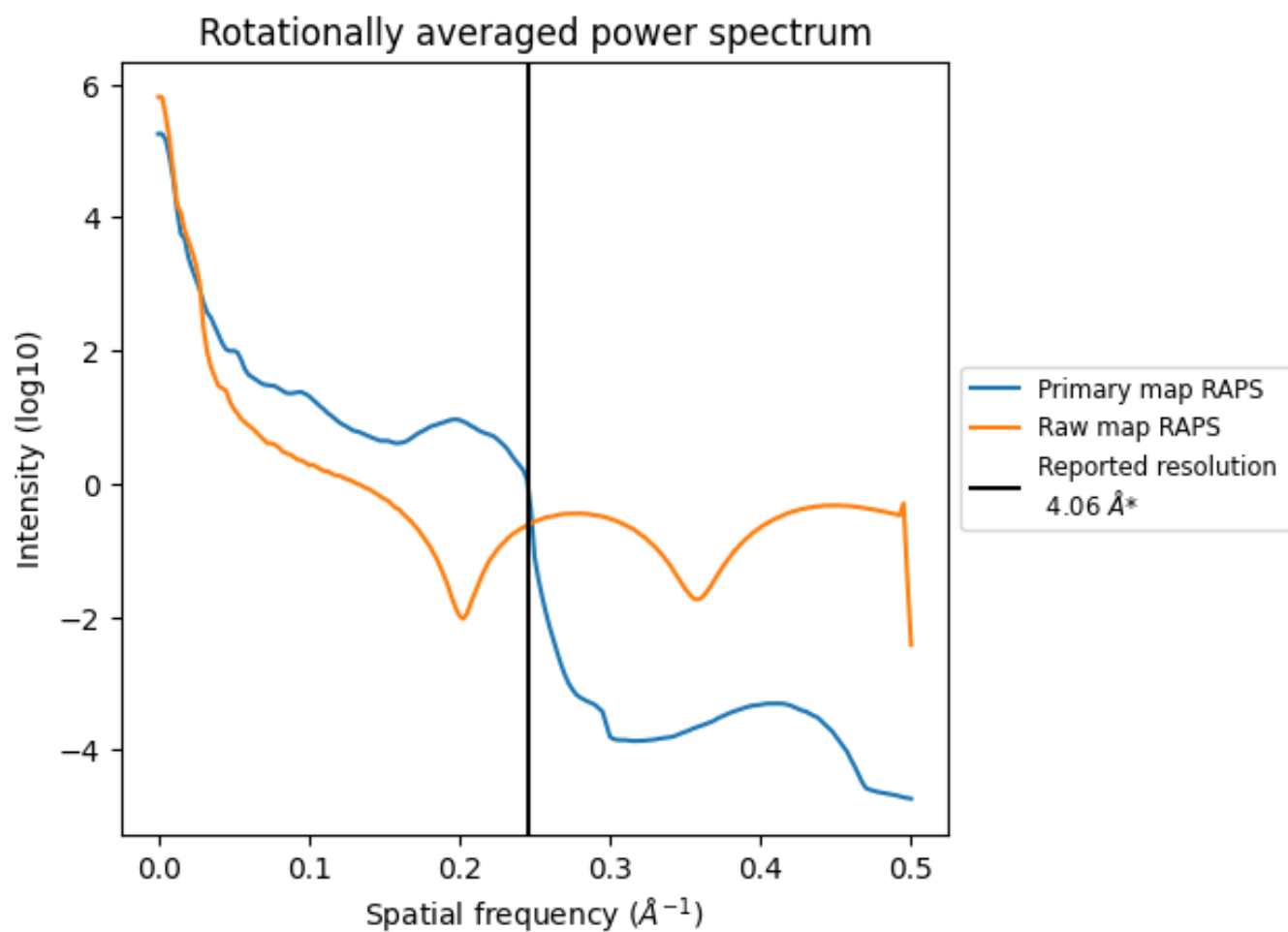
## 7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 472 nm<sup>3</sup>; this corresponds to an approximate mass of 426 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

### 7.3 Rotationally averaged power spectrum [i](#)

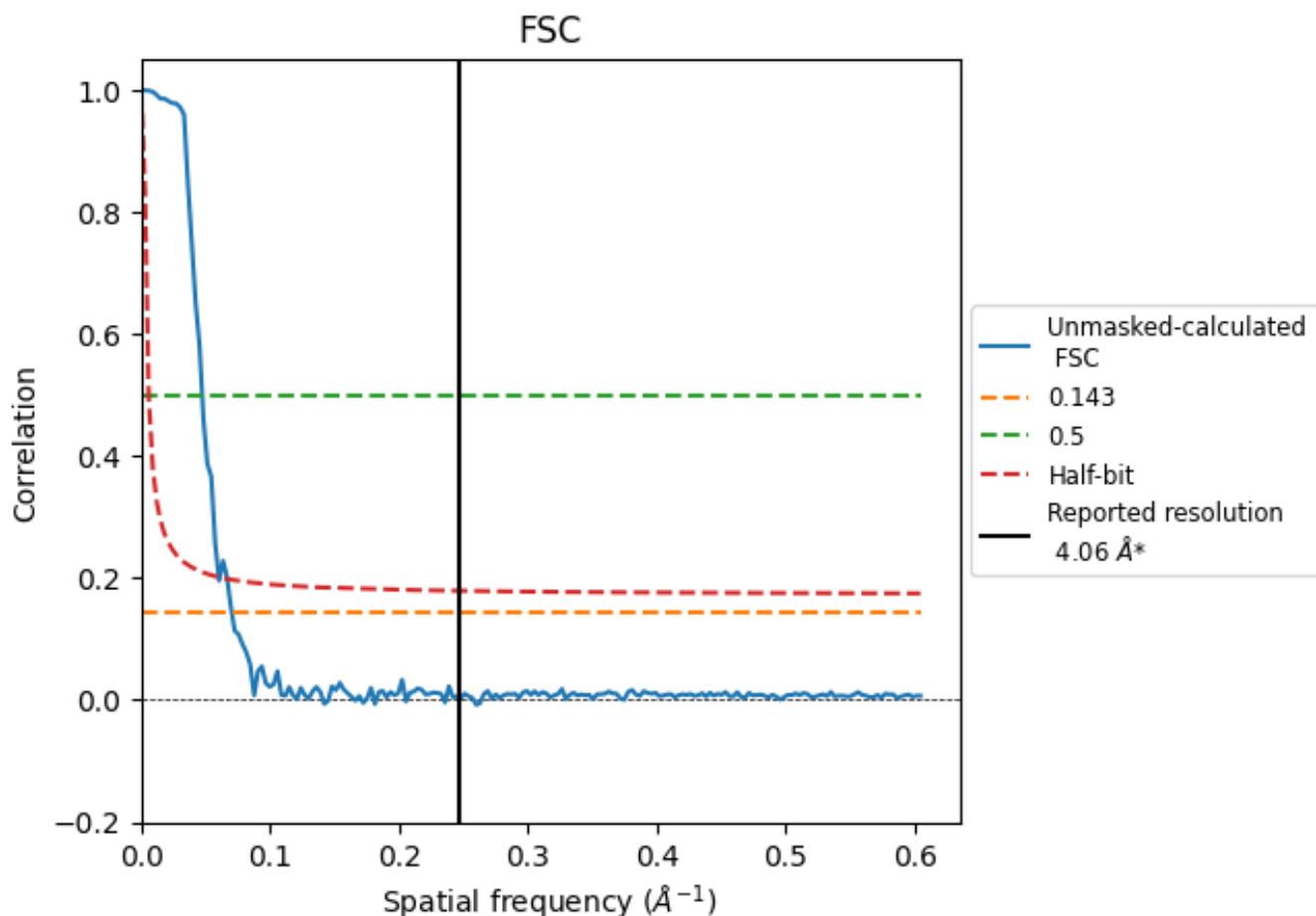


\*Reported resolution corresponds to spatial frequency of 0.246 Å<sup>-1</sup>

## 8 Fourier-Shell correlation [i](#)

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

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of 0.246 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

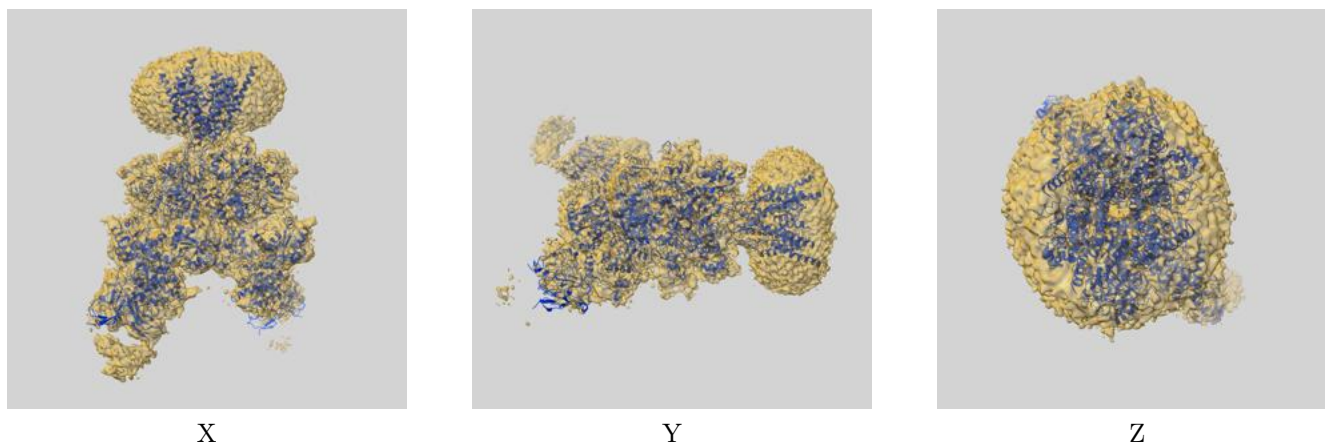
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.06	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	14.20	21.14	16.61

\*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 14.20 differs from the reported value 4.06 by more than 10 %

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

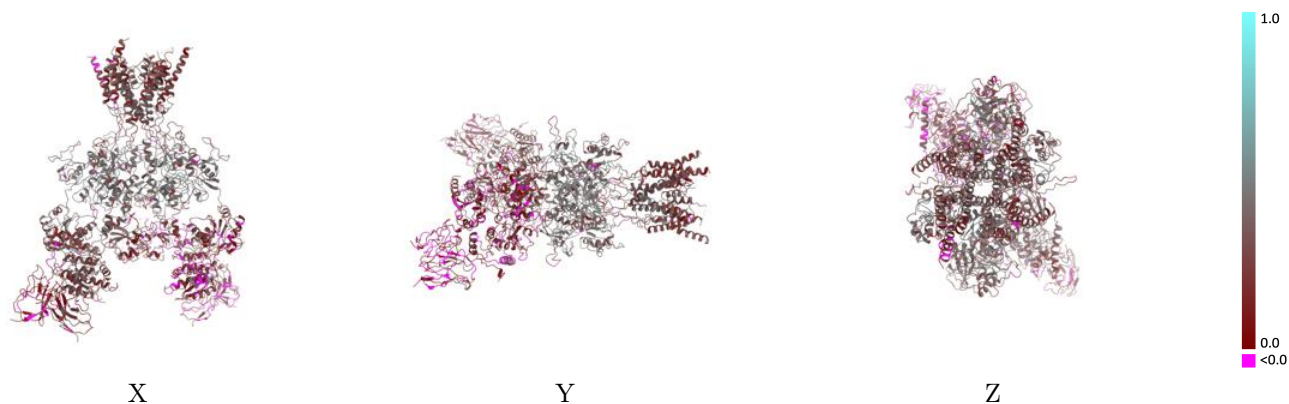
This section contains information regarding the fit between EMDB map EMD-75129 and PDB model 10FF. Per-residue inclusion information can be found in section 3 on page 6.

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



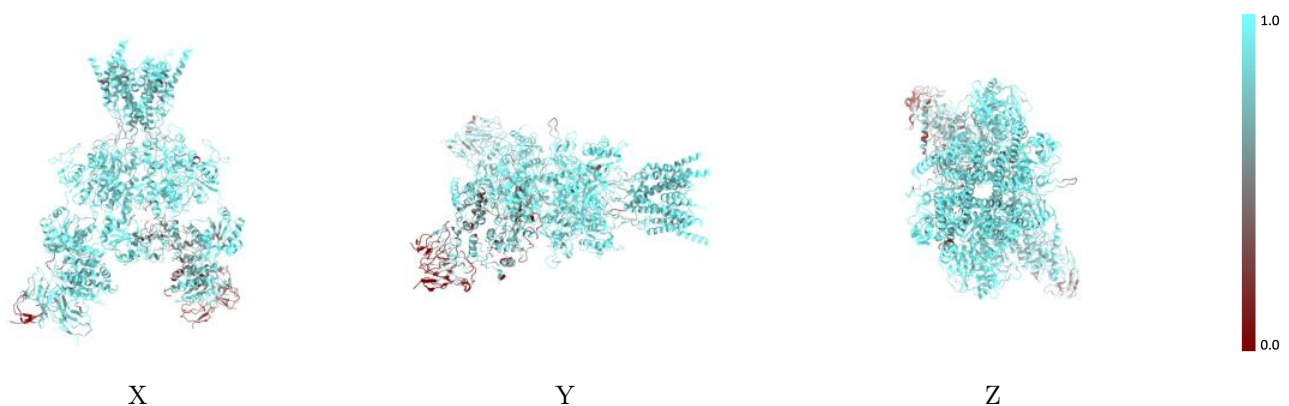
The images above show the 3D surface view of the map at the recommended contour level 0.05 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



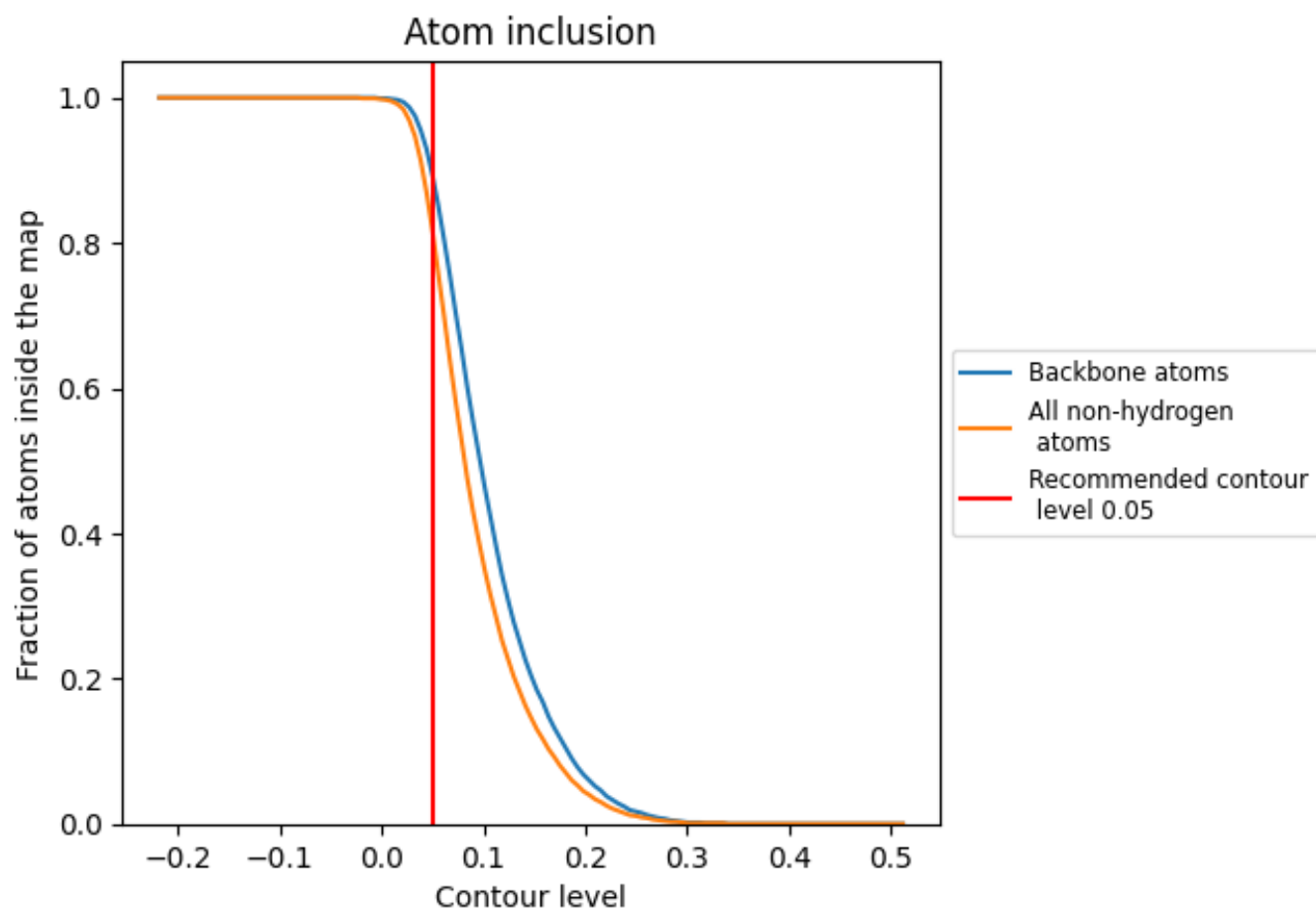
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.05).



















## 9.4 Atom inclusion [i](#)



At the recommended contour level, 89% of all backbone atoms, 82% 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 (0.05) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8150	 0.2820
A	 0.9060	 0.3390
B	 0.8880	 0.3460
C	 0.8550	 0.2730
D	 0.7930	 0.2600
E	 0.3050	 0.0710
F	 0.2820	 0.0960
I	 0.8080	 0.2200
J	 0.6240	 0.1390

