Full wwPDB EM Validation Report ⓘ

Nov 19, 2024 – 12:52 PM EST

PDB ID	:	9BAX
EMDB ID	:	EMD-44413
Title	:	PI4KA complex bound to C-terminus of EFR3A
Authors	:	Shaw, A.L.; Suresh, S.; Yip, C.K.; Burke, J.E.
Deposited on	:	2024-04-04
Resolution	:	3.65 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:

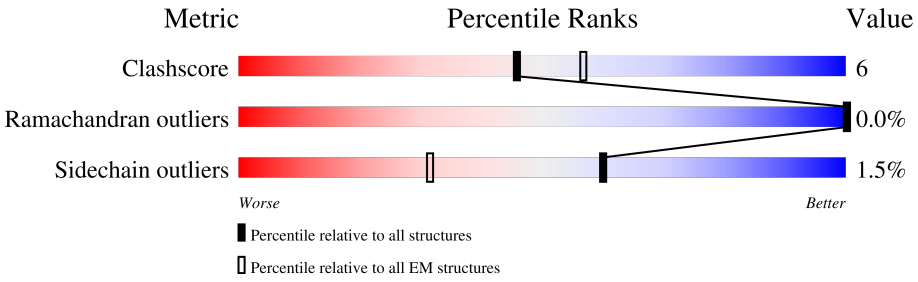
EMDB validation analysis	:	0.0.1.dev113
MolProbity	:	4.02b-467
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

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 3.65 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)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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 <=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	C	130	16% 36% 13% 51%
1	H	130	16% 35% 14% 51%
2	A	2102	69% 13% 18%
2	B	2102	69% 13% 18%
3	D	843	60% 10% 30%
3	F	843	59% 11% 30%
4	E	308	66% 15% 18%
4	G	308	66% 15% 18%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 42100 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 Protein EFR3 homolog A.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	C	64	Total	C	N	O	S	0	0
			522	328	90	102	2		
1	H	64	Total	C	N	O	S	0	0
			522	328	90	102	2		

There are 118 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	662	MET	-	initiating methionine	UNP Q14156
C	663	ALA	-	expression tag	UNP Q14156
C	664	SER	-	expression tag	UNP Q14156
C	665	ALA	-	expression tag	UNP Q14156
C	666	TRP	-	expression tag	UNP Q14156
C	667	SER	-	expression tag	UNP Q14156
C	668	HIS	-	expression tag	UNP Q14156
C	669	PRO	-	expression tag	UNP Q14156
C	670	GLN	-	expression tag	UNP Q14156
C	671	PHE	-	expression tag	UNP Q14156
C	672	GLU	-	expression tag	UNP Q14156
C	673	LYS	-	expression tag	UNP Q14156
C	674	GLY	-	expression tag	UNP Q14156
C	675	GLY	-	expression tag	UNP Q14156
C	676	GLY	-	expression tag	UNP Q14156
C	677	SER	-	expression tag	UNP Q14156
C	678	GLY	-	expression tag	UNP Q14156
C	679	GLY	-	expression tag	UNP Q14156
C	680	GLY	-	expression tag	UNP Q14156
C	681	SER	-	expression tag	UNP Q14156
C	682	GLY	-	expression tag	UNP Q14156
C	683	GLY	-	expression tag	UNP Q14156
C	684	SER	-	expression tag	UNP Q14156
C	685	ALA	-	expression tag	UNP Q14156
C	686	TRP	-	expression tag	UNP Q14156
C	687	SER	-	expression tag	UNP Q14156

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Chain	Residue	Modelled	Actual	Comment	Reference
C	688	HIS	-	expression tag	UNP Q14156
C	689	PRO	-	expression tag	UNP Q14156
C	690	GLN	-	expression tag	UNP Q14156
C	691	PHE	-	expression tag	UNP Q14156
C	692	GLU	-	expression tag	UNP Q14156
C	693	LYS	-	expression tag	UNP Q14156
C	694	SER	-	expression tag	UNP Q14156
C	695	GLY	-	expression tag	UNP Q14156
C	696	MET	-	expression tag	UNP Q14156
C	697	HIS	-	expression tag	UNP Q14156
C	698	HIS	-	expression tag	UNP Q14156
C	699	HIS	-	expression tag	UNP Q14156
C	700	HIS	-	expression tag	UNP Q14156
C	701	HIS	-	expression tag	UNP Q14156
C	702	HIS	-	expression tag	UNP Q14156
C	703	HIS	-	expression tag	UNP Q14156
C	704	HIS	-	expression tag	UNP Q14156
C	705	HIS	-	expression tag	UNP Q14156
C	706	HIS	-	expression tag	UNP Q14156
C	707	GLY	-	expression tag	UNP Q14156
C	708	SER	-	expression tag	UNP Q14156
C	709	GLY	-	expression tag	UNP Q14156
C	710	GLY	-	expression tag	UNP Q14156
C	711	SER	-	expression tag	UNP Q14156
C	712	GLU	-	expression tag	UNP Q14156
C	713	ASN	-	expression tag	UNP Q14156
C	714	LEU	-	expression tag	UNP Q14156
C	715	TYR	-	expression tag	UNP Q14156
C	716	PHE	-	expression tag	UNP Q14156
C	717	GLN	-	expression tag	UNP Q14156
C	718	GLY	-	expression tag	UNP Q14156
C	719	ALA	-	expression tag	UNP Q14156
C	720	GLY	-	expression tag	UNP Q14156
H	662	MET	-	initiating methionine	UNP Q14156
H	663	ALA	-	expression tag	UNP Q14156
H	664	SER	-	expression tag	UNP Q14156
H	665	ALA	-	expression tag	UNP Q14156
H	666	TRP	-	expression tag	UNP Q14156
H	667	SER	-	expression tag	UNP Q14156
H	668	HIS	-	expression tag	UNP Q14156
H	669	PRO	-	expression tag	UNP Q14156
H	670	GLN	-	expression tag	UNP Q14156

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Chain	Residue	Modelled	Actual	Comment	Reference
H	671	PHE	-	expression tag	UNP Q14156
H	672	GLU	-	expression tag	UNP Q14156
H	673	LYS	-	expression tag	UNP Q14156
H	674	GLY	-	expression tag	UNP Q14156
H	675	GLY	-	expression tag	UNP Q14156
H	676	GLY	-	expression tag	UNP Q14156
H	677	SER	-	expression tag	UNP Q14156
H	678	GLY	-	expression tag	UNP Q14156
H	679	GLY	-	expression tag	UNP Q14156
H	680	GLY	-	expression tag	UNP Q14156
H	681	SER	-	expression tag	UNP Q14156
H	682	GLY	-	expression tag	UNP Q14156
H	683	GLY	-	expression tag	UNP Q14156
H	684	SER	-	expression tag	UNP Q14156
H	685	ALA	-	expression tag	UNP Q14156
H	686	TRP	-	expression tag	UNP Q14156
H	687	SER	-	expression tag	UNP Q14156
H	688	HIS	-	expression tag	UNP Q14156
H	689	PRO	-	expression tag	UNP Q14156
H	690	GLN	-	expression tag	UNP Q14156
H	691	PHE	-	expression tag	UNP Q14156
H	692	GLU	-	expression tag	UNP Q14156
H	693	LYS	-	expression tag	UNP Q14156
H	694	SER	-	expression tag	UNP Q14156
H	695	GLY	-	expression tag	UNP Q14156
H	696	MET	-	expression tag	UNP Q14156
H	697	HIS	-	expression tag	UNP Q14156
H	698	HIS	-	expression tag	UNP Q14156
H	699	HIS	-	expression tag	UNP Q14156
H	700	HIS	-	expression tag	UNP Q14156
H	701	HIS	-	expression tag	UNP Q14156
H	702	HIS	-	expression tag	UNP Q14156
H	703	HIS	-	expression tag	UNP Q14156
H	704	HIS	-	expression tag	UNP Q14156
H	705	HIS	-	expression tag	UNP Q14156
H	706	HIS	-	expression tag	UNP Q14156
H	707	GLY	-	expression tag	UNP Q14156
H	708	SER	-	expression tag	UNP Q14156
H	709	GLY	-	expression tag	UNP Q14156
H	710	GLY	-	expression tag	UNP Q14156
H	711	SER	-	expression tag	UNP Q14156
H	712	GLU	-	expression tag	UNP Q14156

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Chain	Residue	Modelled	Actual	Comment	Reference
H	713	ASN	-	expression tag	UNP Q14156
H	714	LEU	-	expression tag	UNP Q14156
H	715	TYR	-	expression tag	UNP Q14156
H	716	PHE	-	expression tag	UNP Q14156
H	717	GLN	-	expression tag	UNP Q14156
H	718	GLY	-	expression tag	UNP Q14156
H	719	ALA	-	expression tag	UNP Q14156
H	720	GLY	-	expression tag	UNP Q14156

- Molecule 2 is a protein called Phosphatidylinositol 4-kinase alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	1724	Total	C	N	O	S	0	0
			13842	8951	2305	2489	97		
2	A	1724	Total	C	N	O	S	0	0
			13842	8951	2305	2489	97		

- Molecule 3 is a protein called Tetratricopeptide repeat protein 7B.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	F	592	Total	C	N	O	S	0	0
			4676	2983	811	855	27		
3	D	592	Total	C	N	O	S	0	0
			4676	2983	811	855	27		

- Molecule 4 is a protein called Hyccin.

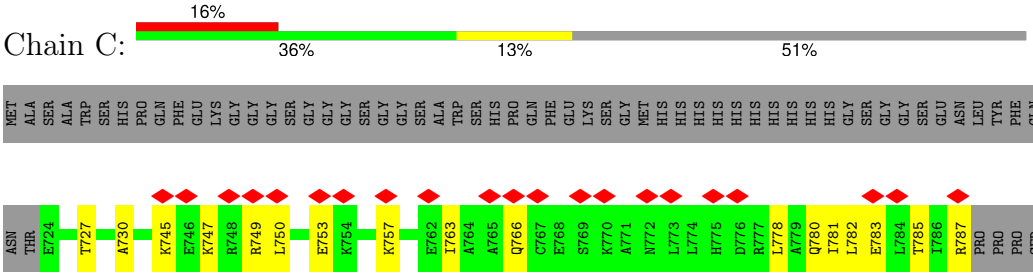
Mol	Chain	Residues	Atoms					AltConf	Trace
4	G	252	Total	C	N	O	S	0	0
			2010	1309	323	366	12		
4	E	252	Total	C	N	O	S	0	0
			2010	1309	323	366	12		

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.

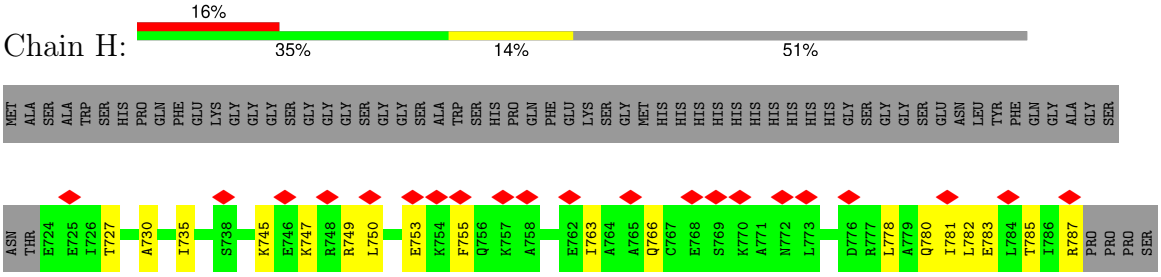
• Molecule 1: Protein EFR3 homolog A

Chain C:



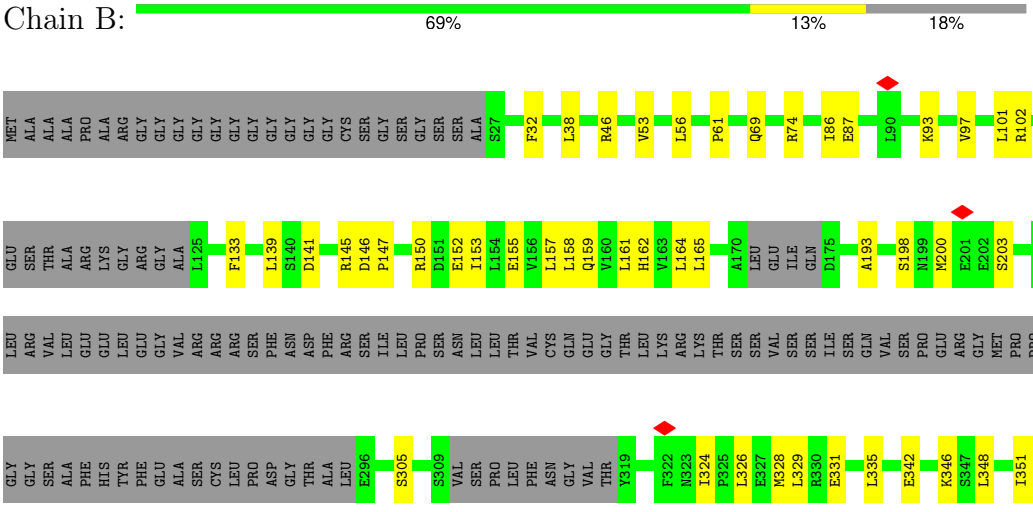
• Molecule 1: Protein EFR3 homolog A

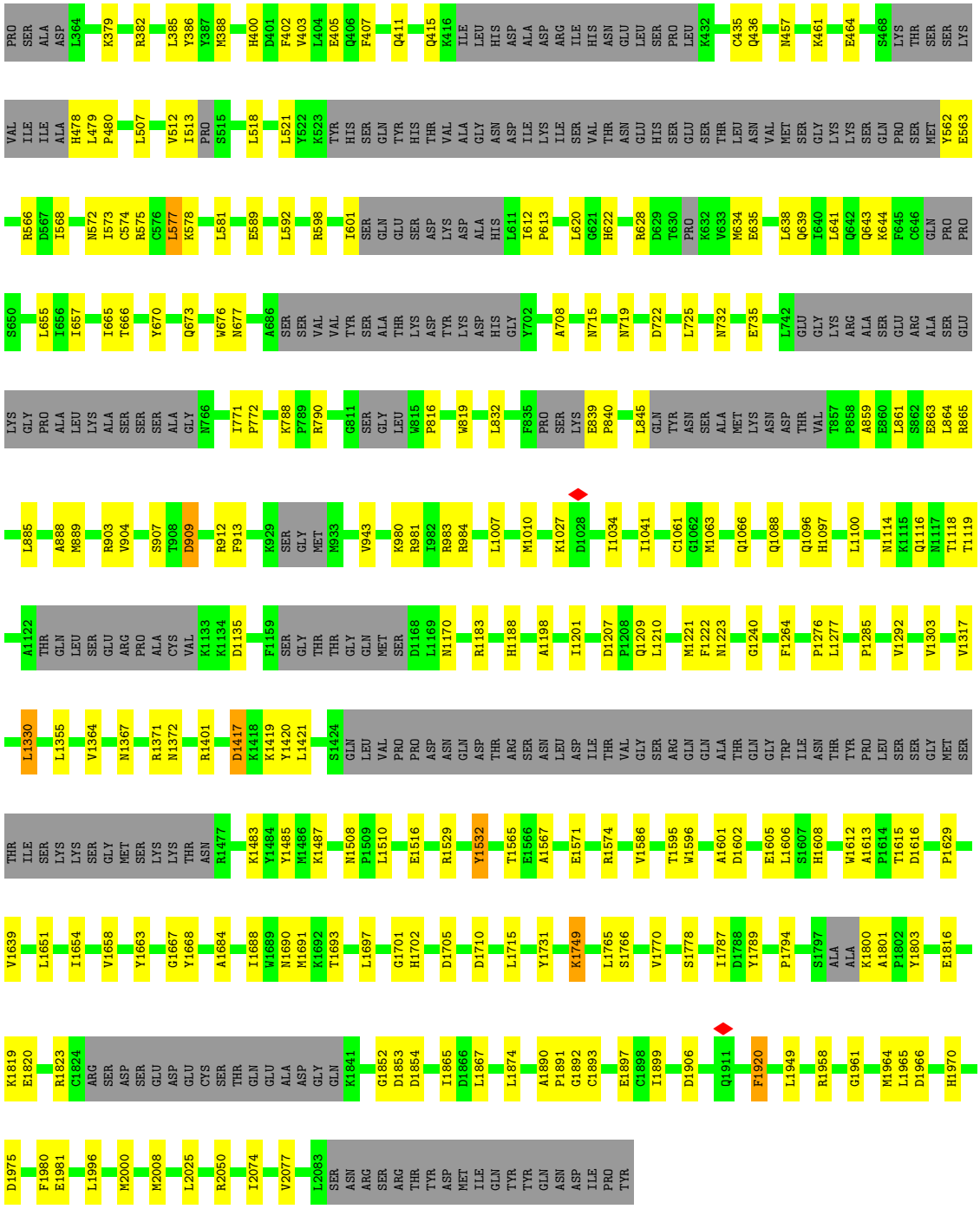
Chain H:



• Molecule 2: Phosphatidylinositol 4-kinase alpha

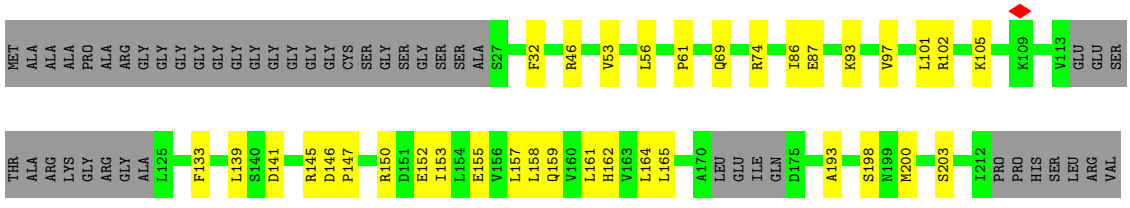
Chain B:

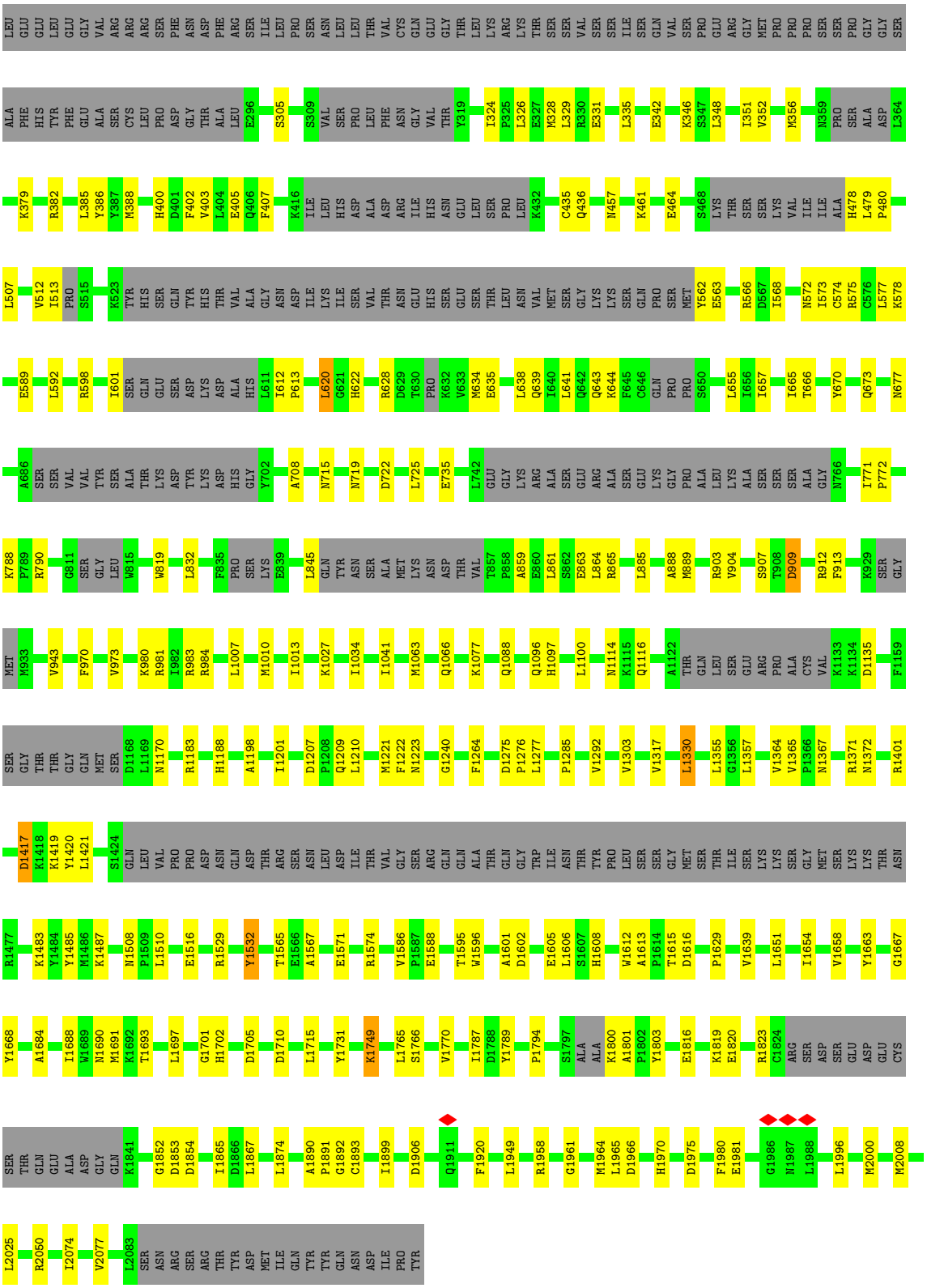




• Molecule 2: Phosphatidylinositol 4-kinase alpha

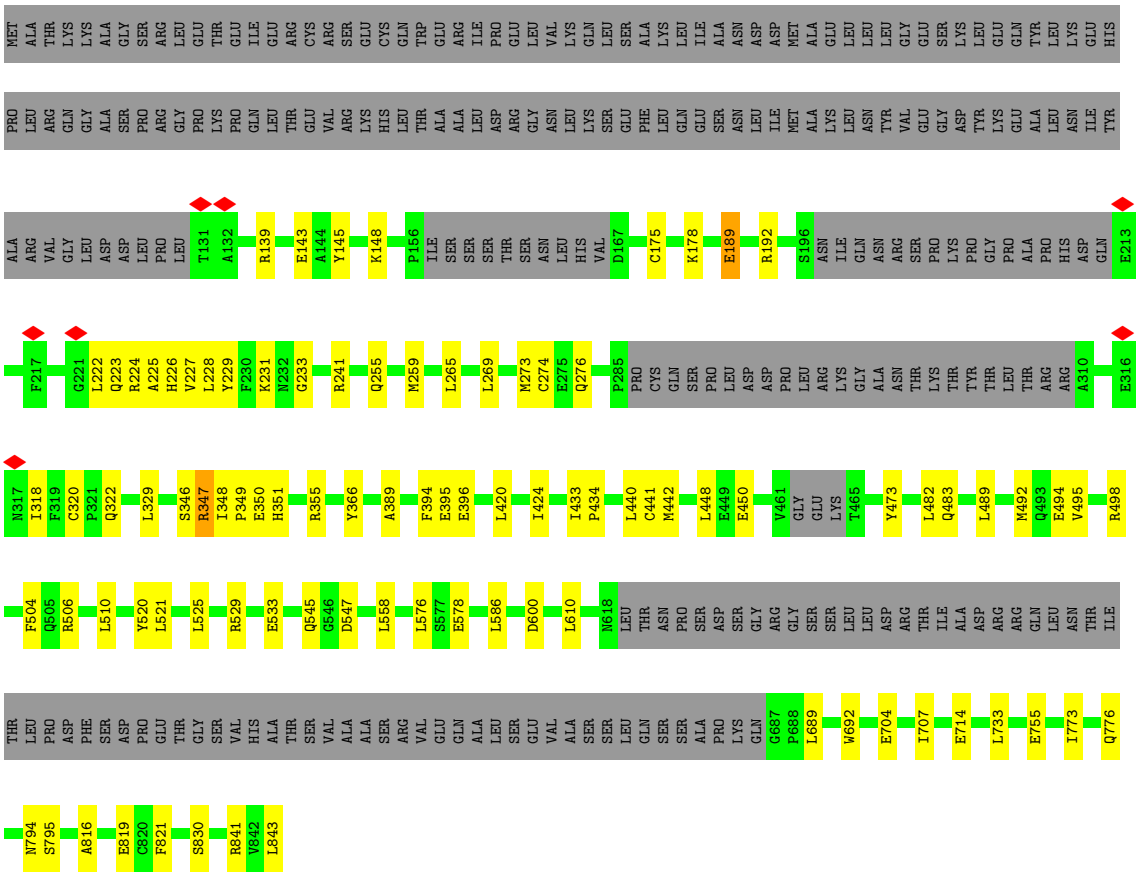
Chain A:





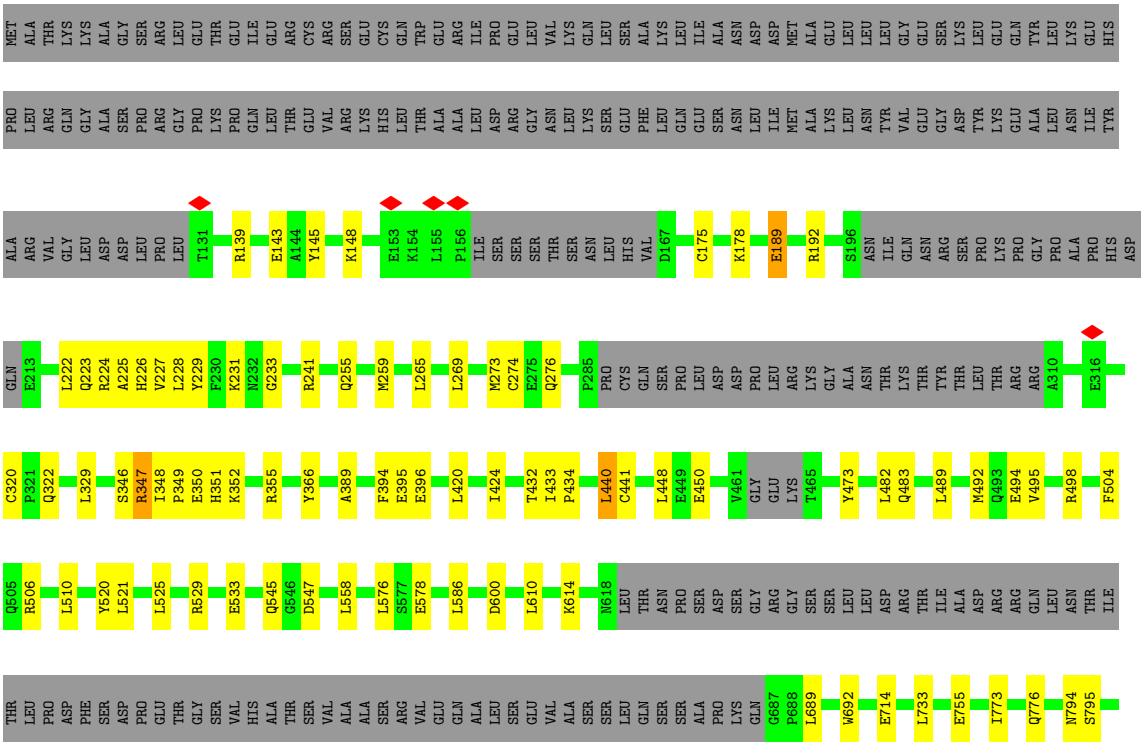
• Molecule 3: Tetratricopeptide repeat protein 7B

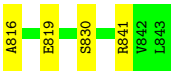
Chain F:



• Molecule 3: Tetratricopeptide repeat protein 7B

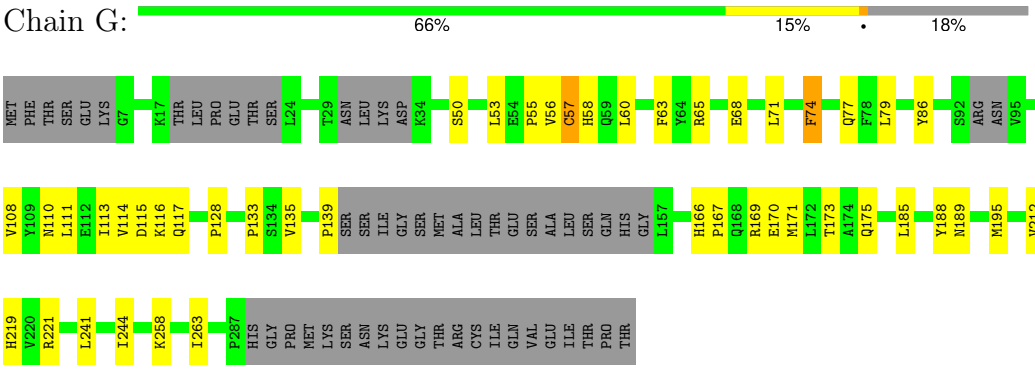
Chain D:





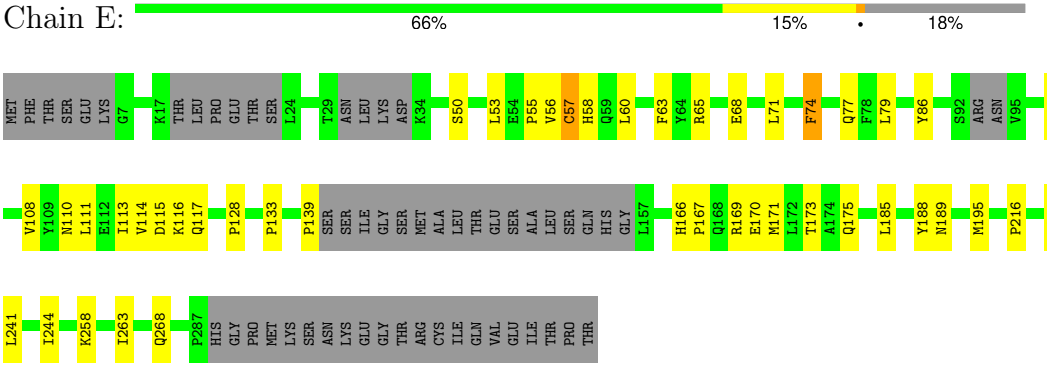
• Molecule 4: Hyccin

Chain G:



• Molecule 4: Hyccin

Chain E:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	135126	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 ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	165000	Depositor
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	0.208	Depositor
Minimum map value	-0.100	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.0284	Depositor
Map size (Å)	462.0, 462.0, 462.0	wwPDB
Map dimensions	600, 600, 600	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.77, 0.77, 0.77	Depositor

5 Model quality

5.1 Standard geometry

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	C	0.25	0/526	0.49	0/701
1	H	0.24	0/526	0.49	0/701
2	A	0.24	0/14149	0.45	0/19141
2	B	0.24	0/14149	0.45	0/19141
3	D	0.23	0/4762	0.46	0/6443
3	F	0.24	0/4762	0.46	0/6443
4	E	0.24	0/2058	0.46	0/2793
4	G	0.24	0/2058	0.46	0/2793
All	All	0.24	0/42990	0.45	0/58156

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

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	C	522	0	536	9	0
1	H	522	0	536	10	0
2	A	13842	0	13974	158	0
2	B	13842	0	13974	162	0
3	D	4676	0	4734	63	0
3	F	4676	0	4734	62	0
4	E	2010	0	2017	29	0
4	G	2010	0	2017	29	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	42100	0	42522	508	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 6.

All (508) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:1667:GLY:HA3	3:D:347:ARG:HH22	1.49	0.78
2:B:1667:GLY:HA3	3:F:347:ARG:HH22	1.50	0.77
3:D:222:LEU:O	3:D:241:ARG:NH2	2.21	0.74
3:F:222:LEU:O	3:F:241:ARG:NH2	2.21	0.73
2:B:1596:TRP:HE1	2:B:1602:ASP:H	1.37	0.73
2:A:1596:TRP:HE1	2:A:1602:ASP:H	1.37	0.73
4:E:86:TYR:OH	4:E:99:GLY:N	2.24	0.71
4:E:113:ILE:HG23	4:E:114:VAL:HG23	1.74	0.70
4:G:113:ILE:HG23	4:G:114:VAL:HG23	1.74	0.70
4:G:86:TYR:OH	4:G:99:GLY:N	2.24	0.69
4:E:167:PRO:HG2	4:E:169:ARG:HH12	1.57	0.69
2:B:1890:ALA:HB3	2:B:1893:CYS:HB2	1.75	0.68
4:G:167:PRO:HG2	4:G:169:ARG:HH12	1.58	0.68
2:A:1417:ASP:O	2:A:1419:LYS:N	2.27	0.68
2:A:1890:ALA:HB3	2:A:1893:CYS:HB2	1.75	0.68
2:B:1417:ASP:O	2:B:1419:LYS:N	2.27	0.67
2:A:980:LYS:HD2	2:A:983:ARG:HH21	1.59	0.67
2:B:980:LYS:HD2	2:B:983:ARG:HH21	1.60	0.67
2:B:507:LEU:HD13	2:B:573:ILE:HG12	1.76	0.67
2:A:507:LEU:HD13	2:A:573:ILE:HG12	1.76	0.67
2:A:1865:ILE:HG12	2:A:1949:LEU:HD11	1.77	0.66
2:B:1865:ILE:HG12	2:B:1949:LEU:HD11	1.77	0.66
2:A:735:GLU:OE2	2:A:790:ARG:NH2	2.28	0.65
2:B:1221:MET:O	2:B:1223:ASN:ND2	2.30	0.65
3:F:347:ARG:HG3	3:F:349:PRO:HD3	1.79	0.65
3:F:424:ILE:HD11	3:F:434:PRO:HD3	1.79	0.65
4:G:53:LEU:O	4:G:57:CYS:HB3	1.97	0.65
2:A:161:LEU:HD23	2:A:164:LEU:HD21	1.78	0.64
3:D:347:ARG:HG3	3:D:349:PRO:HD3	1.79	0.64
3:D:424:ILE:HD11	3:D:434:PRO:HD3	1.79	0.64
2:B:161:LEU:HD23	2:B:164:LEU:HD21	1.78	0.64
2:A:1221:MET:O	2:A:1223:ASN:ND2	2.30	0.64
4:E:53:LEU:O	4:E:57:CYS:HB3	1.97	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:771:ILE:HD11	2:A:819:TRP:HA	1.79	0.63
2:B:1483:LYS:HG2	2:B:1487:LYS:HE2	1.80	0.63
3:F:274:CYS:SG	3:F:276:GLN:NE2	2.72	0.63
2:A:1483:LYS:HG2	2:A:1487:LYS:HE2	1.80	0.62
2:B:771:ILE:HD11	2:B:819:TRP:HA	1.79	0.62
3:D:274:CYS:SG	3:D:276:GLN:NE2	2.72	0.62
2:B:348:LEU:HD13	2:B:351:ILE:HD11	1.82	0.62
2:B:628:ARG:HG2	2:B:666:THR:HG22	1.81	0.62
2:A:348:LEU:HD13	2:A:351:ILE:HD11	1.82	0.61
4:G:116:LYS:HG3	4:G:117:GLN:H	1.65	0.61
2:A:981:ARG:HG2	2:A:984:ARG:HH21	1.65	0.61
4:E:55:PRO:HA	4:E:58:HIS:CD2	2.35	0.61
2:A:634:MET:SD	2:A:634:MET:N	2.74	0.61
2:A:628:ARG:HG2	2:A:666:THR:HG22	1.81	0.61
2:A:1770:VAL:HG22	2:A:1787:ILE:HG12	1.82	0.61
2:B:634:MET:SD	2:B:634:MET:N	2.74	0.61
2:B:981:ARG:HG2	2:B:984:ARG:HH21	1.65	0.61
2:B:1770:VAL:HG22	2:B:1787:ILE:HG12	1.82	0.61
3:F:225:ALA:HB3	3:F:241:ARG:HH22	1.66	0.60
4:G:55:PRO:HA	4:G:58:HIS:CD2	2.35	0.60
2:B:735:GLU:OE2	2:B:790:ARG:NH2	2.28	0.60
3:F:329:LEU:HD22	4:G:128:PRO:HD2	1.82	0.60
2:A:93:LYS:NZ	2:A:146:ASP:OD2	2.35	0.60
4:E:116:LYS:HG3	4:E:117:GLN:H	1.65	0.60
3:D:225:ALA:HB3	3:D:241:ARG:HH22	1.66	0.60
2:B:1372:ASN:OD1	2:B:1485:TYR:OH	2.19	0.60
2:B:1639:VAL:HG21	2:B:1668:TYR:HB3	1.83	0.60
3:F:494:GLU:HB3	3:F:498:ARG:HH21	1.67	0.60
2:A:1639:VAL:HG21	2:A:1668:TYR:HB3	1.83	0.60
2:B:93:LYS:NZ	2:B:146:ASP:OD2	2.35	0.59
2:A:1170:ASN:HD22	2:A:1210:LEU:HD11	1.67	0.59
2:A:563:GLU:HB3	2:A:566:ARG:HH21	1.67	0.59
2:B:563:GLU:HB3	2:B:566:ARG:HH21	1.68	0.59
2:A:1372:ASN:OD1	2:A:1485:TYR:OH	2.19	0.59
2:B:1401:ARG:NH2	2:B:1516:GLU:O	2.36	0.59
2:A:1401:ARG:NH2	2:A:1516:GLU:O	2.36	0.59
3:D:494:GLU:HB3	3:D:498:ARG:HH21	1.67	0.59
2:A:1852:GLY:N	2:A:1892:GLY:O	2.36	0.59
2:B:46:ARG:NH2	2:B:87:GLU:O	2.35	0.58
3:F:492:MET:SD	3:F:492:MET:N	2.73	0.58
2:A:1596:TRP:NE1	2:A:1602:ASP:O	2.36	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1596:TRP:NE1	2:B:1602:ASP:O	2.36	0.58
2:A:46:ARG:NH2	2:A:87:GLU:O	2.35	0.58
2:A:1034:ILE:HD11	2:A:1041:ILE:HG12	1.85	0.58
2:B:1170:ASN:HD22	2:B:1210:LEU:HD11	1.68	0.58
2:B:832:LEU:HD23	2:B:903:ARG:HH22	1.69	0.58
2:B:1034:ILE:HD11	2:B:1041:ILE:HG12	1.85	0.57
2:A:832:LEU:HD23	2:A:903:ARG:HH22	1.69	0.57
4:G:241:LEU:HD21	4:G:263:ILE:HG21	1.86	0.57
2:B:388:MET:SD	2:B:388:MET:N	2.77	0.57
2:B:1852:GLY:N	2:B:1892:GLY:O	2.36	0.57
2:A:388:MET:SD	2:A:388:MET:N	2.77	0.57
3:D:773:ILE:O	3:D:776:GLN:NE2	2.36	0.57
3:F:773:ILE:O	3:F:776:GLN:NE2	2.36	0.57
3:D:492:MET:SD	3:D:492:MET:N	2.73	0.57
4:E:241:LEU:HD21	4:E:263:ILE:HG21	1.86	0.57
2:A:1207:ASP:OD1	2:A:1209:GLN:NE2	2.38	0.56
2:B:1207:ASP:OD1	2:B:1209:GLN:NE2	2.38	0.56
2:B:1303:VAL:HG22	2:B:1355:LEU:HD13	1.87	0.56
2:A:1303:VAL:HG22	2:A:1355:LEU:HD13	1.87	0.56
3:D:347:ARG:O	3:D:347:ARG:NE	2.34	0.56
2:A:1958:ARG:NH2	2:A:1975:ASP:O	2.39	0.56
2:B:1701:GLY:O	2:B:1702:HIS:ND1	2.39	0.56
2:B:903:ARG:O	2:B:907:SER:HB2	2.06	0.56
2:A:903:ARG:O	2:A:907:SER:HB2	2.06	0.56
2:A:1701:GLY:O	2:A:1702:HIS:ND1	2.39	0.56
2:B:1608:HIS:O	2:B:1608:HIS:ND1	2.39	0.56
3:F:347:ARG:O	3:F:347:ARG:NE	2.34	0.56
2:B:1958:ARG:NH2	2:B:1975:ASP:O	2.39	0.55
2:A:865:ARG:NH2	2:A:885:LEU:O	2.36	0.55
2:A:1201:ILE:HD11	2:A:1240:GLY:HA3	1.87	0.55
2:A:1608:HIS:O	2:A:1608:HIS:ND1	2.39	0.55
2:B:865:ARG:NH2	2:B:885:LEU:O	2.36	0.55
2:B:1201:ILE:HD11	2:B:1240:GLY:HA3	1.87	0.55
3:F:229:TYR:O	3:F:233:GLY:N	2.32	0.55
2:B:86:ILE:HG21	2:B:203:SER:HB2	1.88	0.55
3:F:228:LEU:HD13	3:F:231:LYS:HD2	1.88	0.55
2:A:86:ILE:HG21	2:A:203:SER:HB2	1.88	0.55
2:B:673:GLN:O	2:B:677:ASN:ND2	2.30	0.54
2:A:673:GLN:O	2:A:677:ASN:ND2	2.30	0.54
3:F:576:LEU:HD11	3:F:586:LEU:HG	1.89	0.54
3:D:576:LEU:HD11	3:D:586:LEU:HG	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:889:MET:SD	2:A:889:MET:N	2.81	0.54
3:D:228:LEU:HD13	3:D:231:LYS:HD2	1.88	0.54
2:B:889:MET:N	2:B:889:MET:SD	2.81	0.54
2:A:165:LEU:HD11	2:A:335:LEU:HD22	1.90	0.54
2:A:562:TYR:CD2	2:A:563:GLU:HG3	2.43	0.53
2:A:1667:GLY:CA	3:D:347:ARG:HH22	2.20	0.53
2:B:562:TYR:CD2	2:B:563:GLU:HG3	2.43	0.53
1:H:727:THR:HG23	1:H:730:ALA:H	1.72	0.53
2:B:512:VAL:HG23	2:B:513:ILE:HG13	1.90	0.53
1:C:727:THR:HG23	1:C:730:ALA:H	1.73	0.53
2:B:165:LEU:HD11	2:B:335:LEU:HD22	1.91	0.53
2:A:788:LYS:HG3	2:A:790:ARG:H	1.73	0.53
2:B:788:LYS:HG3	2:B:790:ARG:H	1.73	0.53
2:A:512:VAL:HG23	2:A:513:ILE:HG13	1.90	0.53
3:D:189:GLU:OE2	3:D:192:ARG:NH1	2.42	0.53
3:F:255:GLN:O	3:F:259:MET:HG3	2.09	0.53
2:B:352:VAL:O	2:B:356:MET:HG2	2.09	0.53
3:F:189:GLU:OE2	3:F:192:ARG:NH1	2.42	0.53
2:A:352:VAL:O	2:A:356:MET:HG2	2.09	0.53
2:A:1794:PRO:HA	2:A:1803:TYR:HA	1.90	0.52
2:A:305:SER:O	2:A:379:LYS:NZ	2.31	0.52
3:D:226:HIS:HA	3:D:229:TYR:HB2	1.92	0.52
3:F:226:HIS:HA	3:F:229:TYR:HB2	1.92	0.52
1:C:782:LEU:O	1:C:785:THR:OG1	2.27	0.52
2:B:612:ILE:N	2:B:613:PRO:HD2	2.24	0.52
3:D:255:GLN:O	3:D:259:MET:HG3	2.09	0.52
2:B:435:CYS:HG	2:B:478:HIS:N	2.07	0.52
3:F:600:ASP:OD1	3:F:600:ASP:N	2.43	0.52
1:H:782:LEU:O	1:H:785:THR:OG1	2.27	0.52
2:B:1601:ALA:HB2	2:B:1629:PRO:HG2	1.92	0.52
2:B:1794:PRO:HA	2:B:1803:TYR:HA	1.90	0.52
2:A:435:CYS:HG	2:A:478:HIS:N	2.07	0.52
2:A:436:GLN:OE1	2:A:436:GLN:N	2.42	0.52
2:A:612:ILE:N	2:A:613:PRO:HD2	2.24	0.52
4:G:241:LEU:HA	4:G:244:ILE:HG22	1.92	0.52
4:E:216:PRO:HA	4:E:219:HIS:HD2	1.75	0.52
2:A:342:GLU:O	2:A:346:LYS:HG2	2.09	0.52
2:A:1601:ALA:HB2	2:A:1629:PRO:HG2	1.92	0.52
2:A:1088:GLN:OE1	2:A:1088:GLN:N	2.41	0.51
3:D:396:GLU:N	3:D:396:GLU:OE1	2.43	0.51
2:B:305:SER:O	2:B:379:LYS:NZ	2.31	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:331:GLU:O	2:B:335:LEU:HG	2.10	0.51
3:F:396:GLU:N	3:F:396:GLU:OE1	2.43	0.51
2:B:1096:GLN:NE2	2:A:1114:ASN:OD1	2.43	0.51
3:D:432:THR:OG1	4:E:268:GLN:NE2	2.35	0.51
2:B:69:GLN:O	2:B:74:ARG:NH2	2.43	0.51
3:F:145:TYR:HD1	3:F:148:LYS:HZ1	1.56	0.51
2:A:69:GLN:O	2:A:74:ARG:NH2	2.43	0.51
2:A:331:GLU:O	2:A:335:LEU:HG	2.10	0.51
4:G:216:PRO:HA	4:G:219:HIS:HD2	1.75	0.51
3:D:145:TYR:HD1	3:D:148:LYS:HZ1	1.56	0.51
4:E:241:LEU:HA	4:E:244:ILE:HG22	1.92	0.51
3:D:394:PHE:N	3:D:396:GLU:OE1	2.44	0.51
2:B:342:GLU:O	2:B:346:LYS:HG2	2.09	0.51
4:G:50:SER:HB2	4:G:53:LEU:HG	1.93	0.51
4:E:170:GLU:HG2	4:E:171:MET:HG2	1.93	0.51
2:B:139:LEU:HD21	2:B:157:LEU:HD21	1.92	0.50
3:F:366:TYR:CZ	3:F:389:ALA:HB2	2.46	0.50
3:F:394:PHE:N	3:F:396:GLU:OE1	2.44	0.50
2:A:139:LEU:HD21	2:A:157:LEU:HD21	1.92	0.50
4:E:50:SER:HB2	4:E:53:LEU:HG	1.93	0.50
2:B:1899:ILE:HD11	2:B:1964:MET:HG2	1.92	0.50
4:G:221:ARG:HH12	4:G:258:LYS:HB2	1.76	0.50
2:A:1565:THR:HG22	2:A:1567:ALA:H	1.76	0.50
2:B:1114:ASN:OD1	2:A:1096:GLN:NE2	2.44	0.50
3:D:229:TYR:O	3:D:233:GLY:N	2.32	0.50
2:B:436:GLN:OE1	2:B:436:GLN:N	2.42	0.50
2:B:1565:THR:HG22	2:B:1567:ALA:H	1.76	0.50
2:A:1586:VAL:HG12	2:A:1612:TRP:HE3	1.77	0.50
2:B:1088:GLN:OE1	2:B:1088:GLN:N	2.41	0.50
3:F:223:GLN:HA	3:F:226:HIS:NE2	2.26	0.50
4:G:79:LEU:HD21	4:G:188:TYR:HB2	1.94	0.50
3:D:223:GLN:HA	3:D:226:HIS:NE2	2.26	0.50
3:D:366:TYR:CZ	3:D:389:ALA:HB2	2.46	0.50
4:E:221:ARG:HH12	4:E:258:LYS:HB2	1.76	0.50
2:A:1899:ILE:HD11	2:A:1964:MET:HG2	1.92	0.50
4:G:170:GLU:HG2	4:G:171:MET:HG2	1.93	0.50
2:B:639:GLN:O	2:B:643:GLN:NE2	2.44	0.49
3:D:504:PHE:HE2	3:D:520:TYR:HB3	1.77	0.49
2:B:152:GLU:O	2:B:155:GLU:HG2	2.13	0.49
3:F:504:PHE:HE2	3:F:520:TYR:HB3	1.77	0.49
2:A:639:GLN:O	2:A:643:GLN:NE2	2.44	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1586:VAL:HG12	2:B:1612:TRP:HE3	1.77	0.49
2:A:152:GLU:O	2:A:155:GLU:HG2	2.13	0.49
4:E:79:LEU:HD21	4:E:188:TYR:HB2	1.94	0.49
3:F:320:CYS:O	3:F:322:GLN:NE2	2.45	0.49
2:A:1966:ASP:OD1	2:A:1970:HIS:N	2.45	0.49
2:B:1508:ASN:ND2	2:B:1510:LEU:O	2.45	0.49
2:B:1765:LEU:HD22	2:B:1789:TYR:HA	1.95	0.49
3:D:320:CYS:O	3:D:322:GLN:NE2	2.45	0.49
3:D:600:ASP:OD1	3:D:600:ASP:N	2.43	0.49
2:B:1966:ASP:OD1	2:B:1970:HIS:N	2.46	0.49
2:B:1529:ARG:HA	2:B:1532:TYR:CD1	2.48	0.48
4:G:111:LEU:HA	4:G:115:ASP:HB3	1.94	0.48
2:A:1765:LEU:HD22	2:A:1789:TYR:HA	1.95	0.48
3:F:689:LEU:HA	3:F:692:TRP:HD1	1.77	0.48
4:G:185:LEU:O	4:G:189:ASN:ND2	2.31	0.48
2:A:1529:ARG:HA	2:A:1532:TYR:CD1	2.48	0.48
2:B:61:PRO:HB3	2:B:74:ARG:HE	1.78	0.48
2:B:61:PRO:HB3	2:B:74:ARG:NE	2.29	0.48
4:G:56:VAL:O	4:G:60:LEU:HG	2.14	0.48
3:D:348:ILE:HG22	3:D:355:ARG:NH1	2.28	0.48
3:D:689:LEU:HA	3:D:692:TRP:HD1	1.77	0.48
2:A:1508:ASN:ND2	2:A:1510:LEU:O	2.45	0.48
3:D:329:LEU:HD22	4:E:128:PRO:HD2	1.96	0.48
2:A:61:PRO:HB3	2:A:74:ARG:HE	1.79	0.48
4:E:173:THR:HG23	4:E:175:GLN:H	1.79	0.48
2:B:1710:ASP:N	2:B:1710:ASP:OD1	2.47	0.48
4:E:111:LEU:HA	4:E:115:ASP:HB3	1.94	0.48
4:E:116:LYS:HG3	4:E:117:GLN:N	2.28	0.48
3:F:175:CYS:HA	3:F:178:LYS:HE3	1.95	0.48
3:D:545:GLN:HE21	3:D:547:ASP:HB2	1.78	0.48
3:F:348:ILE:HG22	3:F:355:ARG:NH1	2.28	0.48
2:A:574:CYS:SG	2:A:622:HIS:ND1	2.82	0.48
4:E:56:VAL:O	4:E:60:LEU:HG	2.13	0.48
4:G:173:THR:HG23	4:G:175:GLN:H	1.79	0.47
2:A:1277:LEU:HD23	2:A:1867:LEU:HD11	1.96	0.47
2:A:1710:ASP:OD1	2:A:1710:ASP:N	2.47	0.47
3:F:545:GLN:HE21	3:F:547:ASP:HB2	1.77	0.47
2:A:589:GLU:O	2:A:592:LEU:HG	2.14	0.47
3:D:227:VAL:HG12	3:D:231:LYS:HE2	1.97	0.47
2:B:1277:LEU:HD23	2:B:1867:LEU:HD11	1.96	0.47
3:D:175:CYS:HA	3:D:178:LYS:HE3	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:589:GLU:O	2:B:592:LEU:HG	2.14	0.47
3:F:227:VAL:HG12	3:F:231:LYS:HE2	1.97	0.47
2:A:61:PRO:HB3	2:A:74:ARG:NE	2.29	0.47
2:A:1285:PRO:HB2	2:A:1874:LEU:HD13	1.97	0.47
2:B:479:LEU:HD12	2:B:479:LEU:H	1.80	0.47
2:B:1285:PRO:HB2	2:B:1874:LEU:HD13	1.97	0.47
1:H:778:LEU:O	1:H:781:ILE:HG13	2.14	0.47
4:E:185:LEU:O	4:E:189:ASN:ND2	2.31	0.47
1:C:778:LEU:O	1:C:781:ILE:HG13	2.14	0.47
2:B:1063:MET:O	2:B:1066:GLN:HG3	2.14	0.47
4:G:116:LYS:HG3	4:G:117:GLN:N	2.28	0.47
2:A:655:LEU:H	2:A:655:LEU:HD23	1.80	0.47
2:B:575:ARG:HA	2:B:578:LYS:HG2	1.97	0.47
3:F:714:GLU:OE1	3:F:714:GLU:N	2.41	0.47
2:A:1063:MET:O	2:A:1066:GLN:HG3	2.14	0.47
2:A:479:LEU:HD12	2:A:479:LEU:H	1.80	0.47
2:A:575:ARG:HA	2:A:578:LYS:HG2	1.97	0.46
3:D:350:GLU:OE2	3:D:351:HIS:ND1	2.43	0.46
3:F:350:GLU:OE2	3:F:351:HIS:ND1	2.43	0.46
2:B:655:LEU:HD23	2:B:655:LEU:H	1.80	0.46
2:B:1820:GLU:HG2	2:B:1823:ARG:HD3	1.97	0.46
2:A:638:LEU:HD21	2:A:670:TYR:HE2	1.81	0.46
3:D:504:PHE:CE2	3:D:520:TYR:HB3	2.51	0.46
3:D:482:LEU:HD23	3:D:841:ARG:HH21	1.81	0.46
2:B:324:ILE:HB	2:B:328:MET:HE2	1.96	0.46
2:A:1529:ARG:HA	2:A:1532:TYR:HD1	1.80	0.46
2:A:402:PHE:O	2:A:405:GLU:HG2	2.16	0.46
3:D:525:LEU:HD21	3:D:533:GLU:HB2	1.98	0.46
4:E:74:PHE:O	4:E:77:GLN:NE2	2.47	0.46
2:B:1330:LEU:HD23	2:B:1330:LEU:H	1.81	0.46
3:F:448:LEU:HD13	3:F:483:GLN:HG2	1.98	0.46
3:F:525:LEU:HD21	3:F:533:GLU:HB2	1.98	0.46
2:A:1330:LEU:HD23	2:A:1330:LEU:H	1.81	0.46
2:A:1697:LEU:HD21	2:A:1705:ASP:HB3	1.98	0.46
2:B:198:SER:HB2	2:B:200:MET:HG2	1.98	0.46
2:B:1007:LEU:O	2:B:1010:MET:HG3	2.15	0.46
2:A:198:SER:HB2	2:A:200:MET:HG2	1.98	0.46
2:B:1697:LEU:HD21	2:B:1705:ASP:HB3	1.98	0.46
2:A:859:ALA:O	2:A:863:GLU:HG2	2.16	0.46
3:D:448:LEU:HD13	3:D:483:GLN:HG2	1.98	0.46
2:B:577:LEU:HD13	2:B:577:LEU:HA	1.77	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:1820:GLU:HG2	2:A:1823:ARG:HD3	1.97	0.45
2:A:1007:LEU:O	2:A:1010:MET:HG3	2.16	0.45
2:A:1275:ASP:OD1	2:A:1275:ASP:N	2.48	0.45
2:B:1529:ARG:HA	2:B:1532:TYR:HD1	1.81	0.45
3:F:529:ARG:NH1	3:F:830:SER:O	2.50	0.45
3:D:489:LEU:HB2	3:D:492:MET:SD	2.55	0.45
4:E:113:ILE:HG12	4:E:166:HIS:HB2	1.98	0.45
1:C:780:GLN:O	1:C:783:GLU:HG3	2.17	0.45
2:B:1684:ALA:O	2:B:1688:ILE:HG22	2.17	0.45
3:F:504:PHE:CE2	3:F:520:TYR:HB3	2.51	0.45
1:H:763:ILE:O	1:H:766:GLN:HG3	2.16	0.45
2:A:845:LEU:HD23	2:A:888:ALA:HB1	1.99	0.45
2:A:1684:ALA:O	2:A:1688:ILE:HG22	2.17	0.45
3:D:529:ARG:NH1	3:D:830:SER:O	2.50	0.45
3:F:482:LEU:HD23	3:F:841:ARG:HH21	1.81	0.45
3:D:225:ALA:HB3	3:D:241:ARG:NH2	2.32	0.45
3:D:420:LEU:HD13	3:D:433:ILE:HG23	1.98	0.45
1:C:763:ILE:O	1:C:766:GLN:HG3	2.16	0.45
2:B:457:ASN:O	2:B:461:LYS:HG2	2.17	0.45
3:F:489:LEU:HB2	3:F:492:MET:SD	2.55	0.45
2:A:657:ILE:HD11	2:A:708:ALA:HB1	1.98	0.45
2:A:1114:ASN:ND2	2:A:1116:GLN:H	2.15	0.45
2:B:402:PHE:O	2:B:405:GLU:HG2	2.16	0.45
2:B:845:LEU:HD23	2:B:888:ALA:HB1	1.99	0.45
4:G:74:PHE:O	4:G:77:GLN:NE2	2.47	0.45
2:B:638:LEU:HD21	2:B:670:TYR:HE2	1.81	0.45
2:B:722:ASP:HB3	2:B:725:LEU:HB2	1.98	0.45
3:F:420:LEU:HD13	3:F:433:ILE:HG23	1.98	0.45
2:A:1816:GLU:HA	2:A:1819:LYS:HE3	1.99	0.45
3:D:273:MET:SD	3:D:273:MET:N	2.90	0.45
4:E:108:VAL:HA	4:E:111:LEU:HG	1.99	0.45
2:B:657:ILE:HD11	2:B:708:ALA:HB1	1.98	0.45
2:B:1586:VAL:HG11	2:B:1613:ALA:O	2.17	0.45
3:F:273:MET:SD	3:F:273:MET:N	2.90	0.45
2:A:133:PHE:CE2	2:A:193:ALA:HB2	2.52	0.45
2:A:722:ASP:HB3	2:A:725:LEU:HB2	1.98	0.45
3:D:576:LEU:HD13	3:D:576:LEU:HA	1.85	0.45
2:B:102:ARG:HA	2:B:105:LYS:HG2	1.99	0.44
2:B:861:LEU:HD12	2:B:864:LEU:HD11	1.99	0.44
2:B:1114:ASN:ND2	2:B:1116:GLN:H	2.15	0.44
3:F:139:ARG:NH1	3:F:143:GLU:OE2	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:G:113:ILE:HG12	4:G:166:HIS:HB2	1.98	0.44
1:H:780:GLN:O	1:H:783:GLU:HG3	2.17	0.44
2:A:152:GLU:OE1	2:A:152:GLU:N	2.46	0.44
2:A:382:ARG:O	2:A:386:TYR:HB2	2.17	0.44
3:D:139:ARG:NH1	3:D:143:GLU:OE2	2.50	0.44
2:B:859:ALA:O	2:B:863:GLU:HG2	2.16	0.44
2:A:102:ARG:HA	2:A:105:LYS:HG2	1.99	0.44
2:A:457:ASN:O	2:A:461:LYS:HG2	2.17	0.44
4:G:108:VAL:HA	4:G:111:LEU:HG	2.00	0.44
2:A:861:LEU:HD12	2:A:864:LEU:HD11	1.99	0.44
2:A:1586:VAL:HG11	2:A:1613:ALA:O	2.17	0.44
2:A:1996:LEU:HA	2:A:2000:MET:SD	2.58	0.44
2:B:1749:LYS:HE2	2:B:1801:ALA:HB2	2.00	0.44
2:A:324:ILE:HB	2:A:328:MET:HE2	1.99	0.44
2:B:1778:SER:OG	2:B:1897:GLU:OE2	2.29	0.44
2:A:568:ILE:O	2:A:572:ASN:ND2	2.34	0.44
2:A:1749:LYS:HE2	2:A:1801:ALA:HB2	1.99	0.44
3:D:733:LEU:HD13	3:D:755:GLU:HG3	1.99	0.44
2:B:382:ARG:O	2:B:386:TYR:HB2	2.17	0.44
2:B:1816:GLU:HA	2:B:1819:LYS:HE3	1.99	0.44
2:B:133:PHE:CE2	2:B:193:ALA:HB2	2.52	0.44
2:B:1996:LEU:HA	2:B:2000:MET:SD	2.58	0.44
2:A:1800:LYS:HE2	2:A:1800:LYS:HB2	1.86	0.44
1:C:750:LEU:O	1:C:753:GLU:HG2	2.17	0.44
2:B:411:GLN:O	2:B:415:GLN:NE2	2.39	0.44
1:H:755:PHE:HZ	4:E:103:ALA:O	2.01	0.44
2:B:1651:LEU:HA	2:B:1654:ILE:HG12	2.00	0.44
3:F:733:LEU:HD13	3:F:755:GLU:HG3	1.99	0.44
2:B:715:ASN:O	2:B:719:ASN:ND2	2.48	0.43
1:H:750:LEU:O	1:H:753:GLU:HG2	2.17	0.43
2:B:1317:VAL:HG11	2:B:1364:VAL:HG11	2.00	0.43
2:B:1981:GLU:HB3	2:B:2050:ARG:HE	1.84	0.43
2:A:1317:VAL:HG11	2:A:1364:VAL:HG11	2.00	0.43
2:A:1981:GLU:HB3	2:A:2050:ARG:HE	1.84	0.43
2:B:568:ILE:O	2:B:572:ASN:ND2	2.34	0.43
2:A:628:ARG:HH22	2:A:665:ILE:HG22	1.83	0.43
2:A:1651:LEU:HA	2:A:1654:ILE:HG12	2.00	0.43
2:B:152:GLU:OE1	2:B:152:GLU:N	2.46	0.43
2:B:155:GLU:O	2:B:159:GLN:HG2	2.19	0.43
1:H:747:LYS:O	1:H:750:LEU:HG	2.18	0.43
2:B:1691:MET:SD	2:B:1715:LEU:HD22	2.59	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:265:LEU:O	3:F:269:LEU:HB2	2.19	0.43
4:G:167:PRO:O	4:G:169:ARG:NH1	2.52	0.43
2:A:620:LEU:HD12	2:A:620:LEU:HA	1.91	0.43
3:D:224:ARG:HA	3:D:227:VAL:HB	2.01	0.43
3:D:265:LEU:O	3:D:269:LEU:HB2	2.19	0.43
2:A:635:GLU:O	2:A:639:GLN:NE2	2.52	0.43
2:B:628:ARG:HH22	2:B:665:ILE:HG22	1.83	0.43
2:B:771:ILE:HG13	2:B:772:PRO:HD3	2.00	0.43
3:F:794:ASN:OD1	3:F:795:SER:N	2.51	0.43
4:G:110:ASN:HA	4:G:113:ILE:HG22	2.00	0.43
2:A:1693:THR:HG23	2:A:1891:PRO:HA	2.01	0.43
3:D:441:CYS:SG	3:D:450:GLU:HB2	2.59	0.43
4:E:167:PRO:O	4:E:169:ARG:NH1	2.52	0.43
2:B:635:GLU:O	2:B:639:GLN:NE2	2.51	0.43
2:B:1183:ARG:HH22	2:B:1188:HIS:CE1	2.37	0.43
3:F:224:ARG:HA	3:F:227:VAL:HB	2.01	0.43
2:A:479:LEU:HB2	2:A:480:PRO:HD3	2.01	0.43
2:B:1276:PRO:HD3	2:B:1874:LEU:HD22	2.00	0.42
3:F:441:CYS:SG	3:F:450:GLU:HB2	2.59	0.42
1:C:747:LYS:O	1:C:750:LEU:HG	2.18	0.42
2:B:38:LEU:HD13	3:F:821:PHE:HB2	2.00	0.42
2:B:574:CYS:HG	2:B:622:HIS:CE1	2.37	0.42
2:B:1693:THR:HG23	2:B:1891:PRO:HA	2.01	0.42
4:G:68:GLU:HG3	4:G:71:LEU:HD13	2.01	0.42
2:A:385:LEU:HA	2:A:388:MET:HG2	2.00	0.42
3:D:794:ASN:OD1	3:D:795:SER:N	2.51	0.42
4:E:110:ASN:HA	4:E:113:ILE:HG22	2.00	0.42
2:B:385:LEU:HA	2:B:388:MET:HG2	2.00	0.42
2:B:479:LEU:HB2	2:B:480:PRO:HD3	2.01	0.42
2:B:1800:LYS:HE2	2:B:1800:LYS:HB2	1.86	0.42
2:B:1920:PHE:HD2	2:B:1920:PHE:HA	1.71	0.42
4:G:102:GLU:OE1	4:G:102:GLU:N	2.40	0.42
2:A:155:GLU:O	2:A:159:GLN:HG2	2.19	0.42
2:A:715:ASN:O	2:A:719:ASN:ND2	2.48	0.42
2:A:2074:ILE:HA	2:A:2077:VAL:HG12	2.00	0.42
2:B:153:ILE:O	2:B:157:LEU:HG	2.20	0.42
2:B:400:HIS:HA	2:B:403:VAL:HG22	2.01	0.42
2:A:771:ILE:HG13	2:A:772:PRO:HD3	2.00	0.42
1:C:745:LYS:O	1:C:749:ARG:HG2	2.20	0.42
2:A:141:ASP:O	2:A:145:ARG:HG2	2.20	0.42
2:B:1198:ALA:O	2:B:1201:ILE:HG22	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:1198:ALA:O	2:A:1201:ILE:HG22	2.20	0.42
2:A:1691:MET:SD	2:A:1715:LEU:HD22	2.59	0.42
2:B:2074:ILE:HA	2:B:2077:VAL:HG12	2.00	0.42
2:A:97:VAL:O	2:A:101:LEU:HG	2.20	0.42
2:A:641:LEU:HA	2:A:644:LYS:HG2	2.02	0.42
4:E:68:GLU:HG3	4:E:71:LEU:HD13	2.01	0.42
2:B:572:ASN:OD1	2:B:575:ARG:NH2	2.53	0.42
2:B:1605:GLU:O	2:B:1606:LEU:HG	2.19	0.42
2:A:400:HIS:HA	2:A:403:VAL:HG22	2.01	0.42
1:C:757:LYS:HE2	1:C:757:LYS:HB3	1.88	0.42
2:B:641:LEU:HA	2:B:644:LYS:HG2	2.02	0.42
2:B:1367:ASN:O	2:B:1371:ARG:NH1	2.53	0.42
2:A:572:ASN:OD1	2:A:575:ARG:NH2	2.53	0.42
2:A:1276:PRO:HD3	2:A:1874:LEU:HD22	2.00	0.42
2:A:1605:GLU:O	2:A:1606:LEU:HG	2.19	0.42
3:D:816:ALA:HA	3:D:819:GLU:HG2	2.02	0.42
2:B:1097:HIS:HD2	2:B:1100:LEU:HD22	1.85	0.42
3:F:395:GLU:N	3:F:396:GLU:OE1	2.53	0.42
2:A:1097:HIS:HD2	2:A:1100:LEU:HD22	1.85	0.42
2:A:1367:ASN:O	2:A:1371:ARG:NH1	2.52	0.42
2:A:1571:GLU:OE2	2:A:1574:ARG:NH1	2.53	0.42
2:A:1816:GLU:HA	2:A:1819:LYS:HG2	2.02	0.42
2:B:326:LEU:HD13	2:B:329:LEU:HD12	2.02	0.41
2:B:2008:MET:SD	2:B:2008:MET:N	2.93	0.41
2:A:147:PRO:HA	2:A:150:ARG:HG3	2.02	0.41
3:D:440:LEU:HA	3:D:440:LEU:HD23	1.78	0.41
2:B:1114:ASN:N	2:B:1135:ASP:OD2	2.53	0.41
2:A:326:LEU:HD13	2:A:329:LEU:HD12	2.02	0.41
2:A:1853:ASP:OD1	2:A:1854:ASP:N	2.54	0.41
3:D:395:GLU:N	3:D:396:GLU:OE1	2.53	0.41
3:D:714:GLU:OE1	3:D:714:GLU:N	2.41	0.41
2:B:97:VAL:O	2:B:101:LEU:HG	2.20	0.41
2:B:904:VAL:HG11	2:B:943:VAL:HG23	2.02	0.41
2:B:1816:GLU:HA	2:B:1819:LYS:HG2	2.02	0.41
4:G:133:PRO:HG3	4:G:139:PRO:HD2	2.02	0.41
2:A:1183:ARG:HH22	2:A:1188:HIS:CE1	2.37	0.41
2:A:1658:VAL:HG21	2:A:1690:ASN:HD21	1.85	0.41
4:E:133:PRO:HG3	4:E:139:PRO:HD2	2.02	0.41
2:B:1571:GLU:OE2	2:B:1574:ARG:NH1	2.53	0.41
2:B:1906:ASP:HB2	2:B:1961:GLY:HA2	2.03	0.41
2:A:904:VAL:HG11	2:A:943:VAL:HG23	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:1420:TYR:O	2:A:1421:LEU:HB2	2.20	0.41
2:B:141:ASP:O	2:B:145:ARG:HG2	2.20	0.41
2:B:1420:TYR:O	2:B:1421:LEU:HB2	2.20	0.41
3:F:225:ALA:HB3	3:F:241:ARG:NH2	2.32	0.41
3:F:576:LEU:HD13	3:F:576:LEU:HA	1.86	0.41
3:F:816:ALA:HA	3:F:819:GLU:HG2	2.02	0.41
2:A:1114:ASN:N	2:A:1135:ASP:OD2	2.53	0.41
2:A:1906:ASP:HB2	2:A:1961:GLY:HA2	2.03	0.41
3:D:175:CYS:HA	3:D:178:LYS:HG2	2.01	0.41
3:D:346:SER:HA	3:D:355:ARG:HG3	2.02	0.41
3:D:424:ILE:HD13	3:D:424:ILE:HA	1.93	0.41
2:B:816:PRO:HD2	2:B:819:TRP:CD2	2.56	0.41
2:B:839:GLU:HA	2:B:840:PRO:HD3	1.98	0.41
2:B:909:ASP:O	2:B:912:ARG:HG3	2.21	0.41
2:B:1853:ASP:OD1	2:B:1854:ASP:N	2.54	0.41
3:F:318:ILE:HD12	4:G:135:VAL:HB	2.02	0.41
3:F:704:GLU:O	3:F:707:ILE:HG22	2.21	0.41
2:A:1615:THR:OG1	2:A:1616:ASP:N	2.54	0.41
2:B:147:PRO:HA	2:B:150:ARG:HG3	2.02	0.41
2:A:2008:MET:SD	2:A:2008:MET:N	2.93	0.41
2:B:1135:ASP:OD1	2:A:1096:GLN:NE2	2.54	0.41
2:B:1658:VAL:HG21	2:B:1690:ASN:HD21	1.85	0.41
2:B:1981:GLU:HG3	2:B:2050:ARG:HG2	2.02	0.41
2:A:909:ASP:O	2:A:912:ARG:HG3	2.21	0.41
2:A:1077:LYS:HE3	2:A:1077:LYS:HB2	1.92	0.41
2:B:1667:GLY:CA	3:F:347:ARG:HH22	2.28	0.41
2:B:1766:SER:HA	2:B:1789:TYR:CD1	2.56	0.41
3:F:226:HIS:HB3	3:F:241:ARG:NE	2.36	0.41
3:F:424:ILE:HD13	3:F:424:ILE:HA	1.93	0.41
3:F:495:VAL:O	3:F:498:ARG:HG2	2.20	0.41
3:F:506:ARG:HH22	3:F:510:LEU:HD21	1.85	0.41
2:A:53:VAL:O	2:A:56:LEU:HG	2.21	0.41
2:A:153:ILE:O	2:A:157:LEU:HG	2.20	0.41
2:A:1010:MET:HA	2:A:1013:ILE:HG12	2.02	0.41
3:D:269:LEU:HD12	3:D:269:LEU:HA	1.83	0.41
3:D:506:ARG:HH22	3:D:510:LEU:HD21	1.85	0.41
2:B:676:TRP:CE2	2:B:732:ASN:HB3	2.56	0.41
3:F:346:SER:HA	3:F:355:ARG:HG3	2.02	0.41
3:F:442:MET:HE1	3:F:843:LEU:HB3	2.03	0.41
2:A:1357:LEU:HD23	2:A:1357:LEU:HA	1.95	0.41
2:A:1588:GLU:OE2	2:A:1588:GLU:N	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:1766:SER:HA	2:A:1789:TYR:CD1	2.56	0.41
2:B:598:ARG:HA	2:B:601:ILE:HG12	2.03	0.40
4:G:212:VAL:HG13	4:G:218:GLN:HB3	2.03	0.40
1:H:745:LYS:O	1:H:749:ARG:HG2	2.20	0.40
2:A:1749:LYS:HB2	2:A:1801:ALA:HB2	2.03	0.40
2:B:158:LEU:HG	2:B:162:HIS:CE1	2.57	0.40
2:B:578:LYS:HA	2:B:581:LEU:HG	2.03	0.40
2:B:1615:THR:OG1	2:B:1616:ASP:N	2.54	0.40
1:H:735:ILE:O	3:D:614:LYS:HE3	2.20	0.40
2:A:598:ARG:HA	2:A:601:ILE:HG12	2.03	0.40
3:D:352:LYS:HG2	3:D:355:ARG:HH12	1.86	0.40
2:B:53:VAL:O	2:B:56:LEU:HG	2.21	0.40
3:F:175:CYS:HA	3:F:178:LYS:HG2	2.01	0.40
3:F:504:PHE:HB3	3:F:521:LEU:HD13	2.02	0.40
2:A:1981:GLU:HG3	2:A:2050:ARG:HG2	2.02	0.40
3:D:226:HIS:HB3	3:D:241:ARG:NE	2.36	0.40
2:B:518:LEU:HD12	2:B:521:LEU:HD22	2.03	0.40
2:B:1010:MET:HE1	2:B:1061:CYS:HA	2.02	0.40
2:A:970:PHE:O	2:A:973:VAL:HG12	2.21	0.40
3:D:495:VAL:O	3:D:498:ARG:HG2	2.20	0.40
4:E:102:GLU:OE1	4:E:102:GLU:N	2.40	0.40
2:B:1118:THR:HG23	2:B:1119:THR:HG23	2.03	0.40
2:A:158:LEU:HG	2:A:162:HIS:CE1	2.57	0.40
3:D:504:PHE:HB3	3:D:521:LEU:HD13	2.02	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	C	62/130 (48%)	61 (98%)	1 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	H	62/130 (48%)	61 (98%)	1 (2%)	0	100	100
2	A	1676/2102 (80%)	1596 (95%)	79 (5%)	1 (0%)	48	78
2	B	1676/2102 (80%)	1596 (95%)	79 (5%)	1 (0%)	48	78
3	D	580/843 (69%)	567 (98%)	13 (2%)	0	100	100
3	F	580/843 (69%)	567 (98%)	13 (2%)	0	100	100
4	E	242/308 (79%)	234 (97%)	8 (3%)	0	100	100
4	G	242/308 (79%)	234 (97%)	8 (3%)	0	100	100
All	All	5120/6766 (76%)	4916 (96%)	202 (4%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	1980	PHE
2	A	1980	PHE

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	C	56/104 (54%)	55 (98%)	1 (2%)	54	71
1	H	56/104 (54%)	55 (98%)	1 (2%)	54	71
2	A	1527/1841 (83%)	1505 (99%)	22 (1%)	62	77
2	B	1527/1841 (83%)	1506 (99%)	21 (1%)	62	77
3	D	494/712 (69%)	487 (99%)	7 (1%)	62	77
3	F	494/712 (69%)	487 (99%)	7 (1%)	62	77
4	E	227/277 (82%)	222 (98%)	5 (2%)	47	65
4	G	227/277 (82%)	222 (98%)	5 (2%)	47	65
All	All	4608/5868 (78%)	4539 (98%)	69 (2%)	60	75

All (69) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	787	ARG
2	B	32	PHE
2	B	407	PHE
2	B	464	GLU
2	B	577	LEU
2	B	620	LEU
2	B	909	ASP
2	B	913	PHE
2	B	1027	LYS
2	B	1222	PHE
2	B	1264	PHE
2	B	1292	VAL
2	B	1330	LEU
2	B	1417	ASP
2	B	1532	TYR
2	B	1595	THR
2	B	1663	TYR
2	B	1731	TYR
2	B	1749	LYS
2	B	1920	PHE
2	B	1965	LEU
2	B	2025	LEU
3	F	189	GLU
3	F	347	ARG
3	F	440	LEU
3	F	473	TYR
3	F	558	LEU
3	F	578	GLU
3	F	610	LEU
4	G	57	CYS
4	G	63	PHE
4	G	65	ARG
4	G	74	PHE
4	G	195	MET
1	H	787	ARG
2	A	32	PHE
2	A	407	PHE
2	A	464	GLU
2	A	577	LEU
2	A	620	LEU
2	A	909	ASP
2	A	913	PHE
2	A	1027	LYS

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Mol	Chain	Res	Type
2	A	1222	PHE
2	A	1264	PHE
2	A	1292	VAL
2	A	1330	LEU
2	A	1365	VAL
2	A	1417	ASP
2	A	1532	TYR
2	A	1595	THR
2	A	1663	TYR
2	A	1731	TYR
2	A	1749	LYS
2	A	1920	PHE
2	A	1965	LEU
2	A	2025	LEU
3	D	189	GLU
3	D	347	ARG
3	D	440	LEU
3	D	473	TYR
3	D	558	LEU
3	D	578	GLU
3	D	610	LEU
4	E	57	CYS
4	E	63	PHE
4	E	65	ARG
4	E	74	PHE
4	E	195	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (40) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	91	GLN
2	B	639	GLN
2	B	643	GLN
2	B	766	ASN
2	B	969	GLN
2	B	1170	ASN
2	B	1304	GLN
2	B	1631	HIS
2	B	1685	HIS
2	B	1690	ASN
2	B	1694	ASN
3	F	188	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	F	276	GLN
3	F	524	GLN
3	F	545	GLN
3	F	611	GLN
4	G	49	GLN
4	G	70	GLN
4	G	218	GLN
4	G	219	HIS
2	A	91	GLN
2	A	639	GLN
2	A	643	GLN
2	A	766	ASN
2	A	969	GLN
2	A	1170	ASN
2	A	1304	GLN
2	A	1685	HIS
2	A	1690	ASN
2	A	1694	ASN
3	D	188	GLN
3	D	276	GLN
3	D	515	HIS
3	D	524	GLN
3	D	545	GLN
3	D	611	GLN
4	E	49	GLN
4	E	70	GLN
4	E	218	GLN
4	E	219	HIS

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

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.

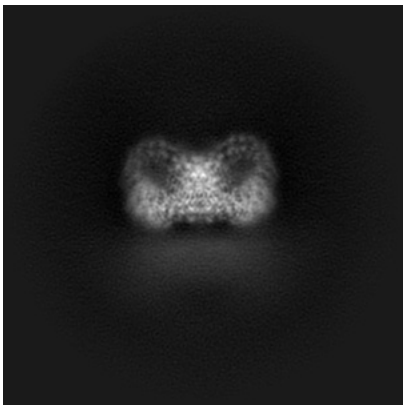
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-44413. These allow visual inspection of the internal detail of the map and identification of artifacts.

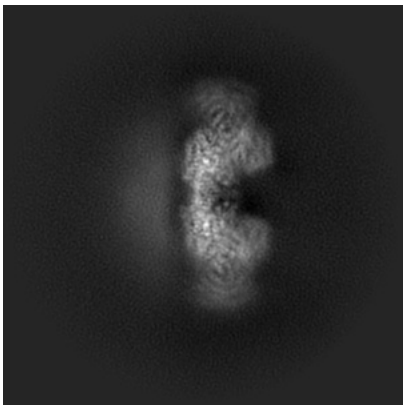
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

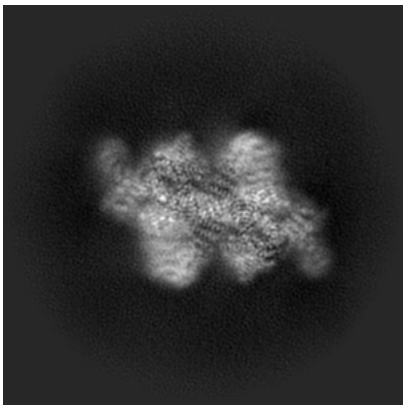
6.1.1 Primary map



X

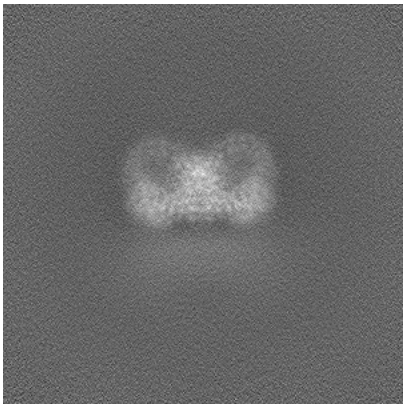


Y

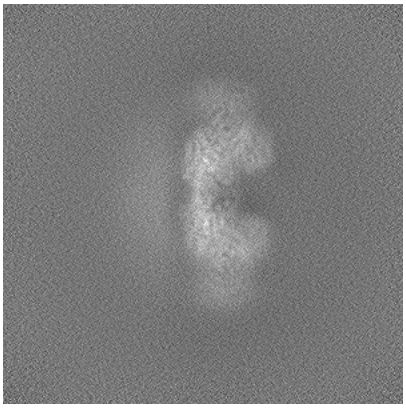


Z

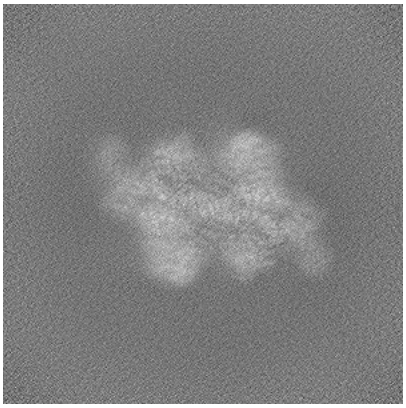
6.1.2 Raw map



X



Y

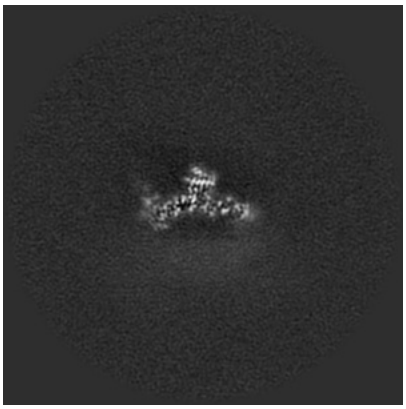


Z

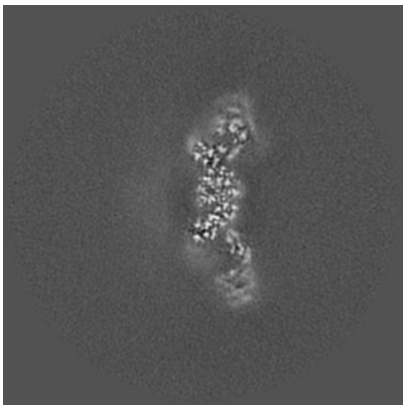
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

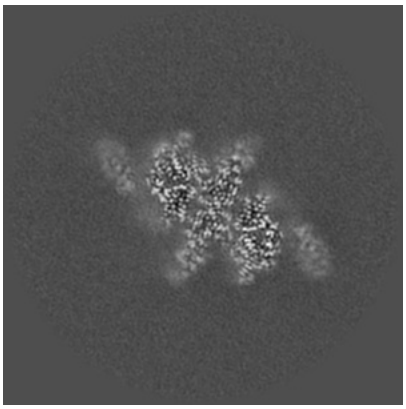
6.2.1 Primary map



X Index: 300

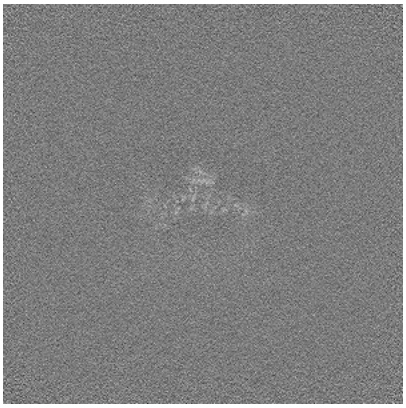


Y Index: 300

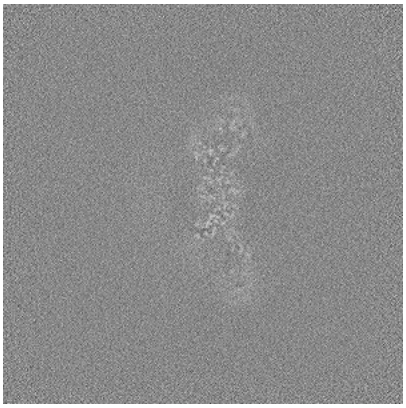


Z Index: 300

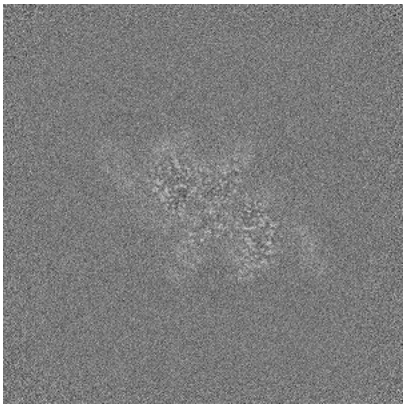
6.2.2 Raw map



X Index: 300



Y Index: 300

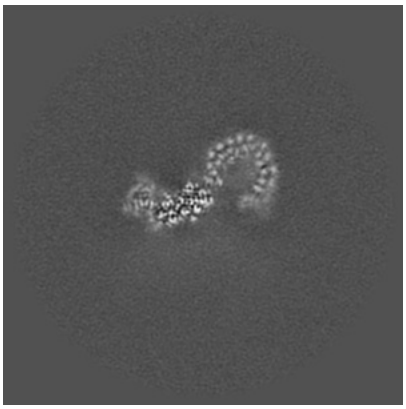


Z Index: 300

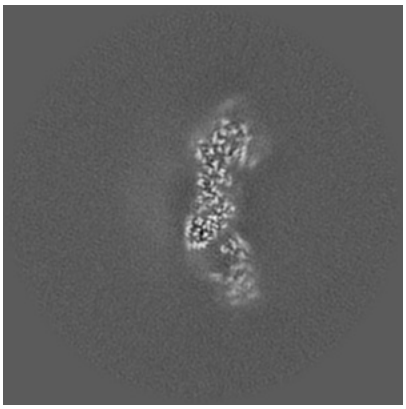
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

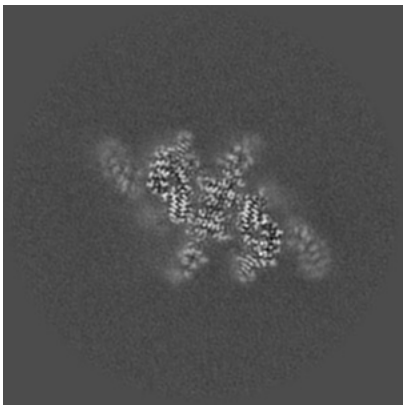
6.3.1 Primary map



X Index: 366

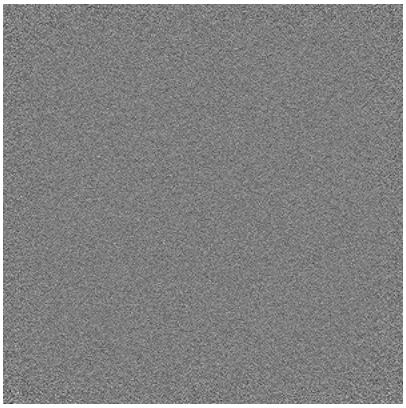


Y Index: 308

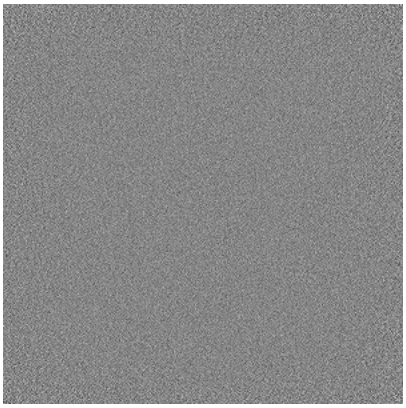


Z Index: 305

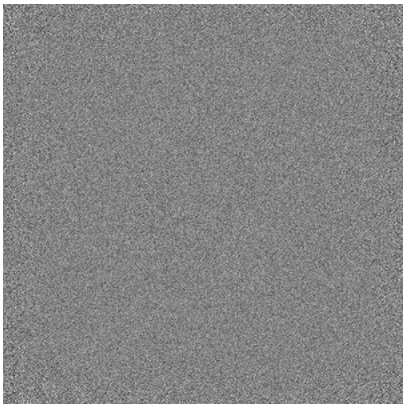
6.3.2 Raw map



X Index: 0



Y Index: 0

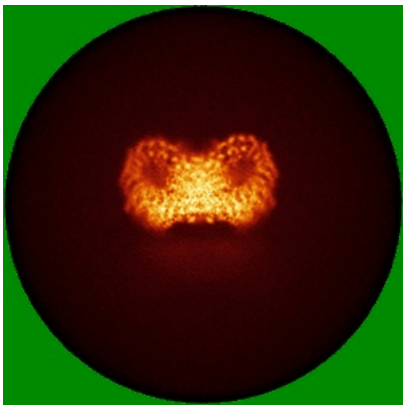


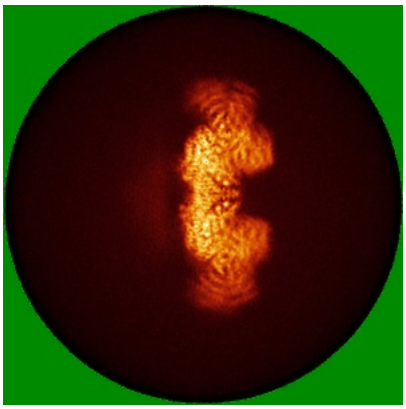
Z Index: 0

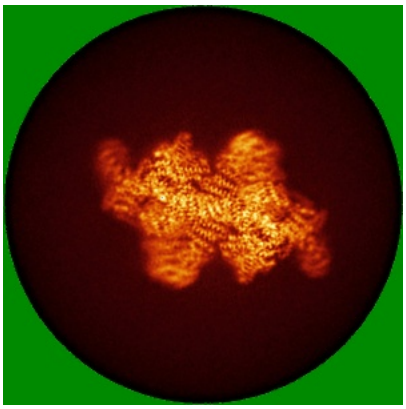
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

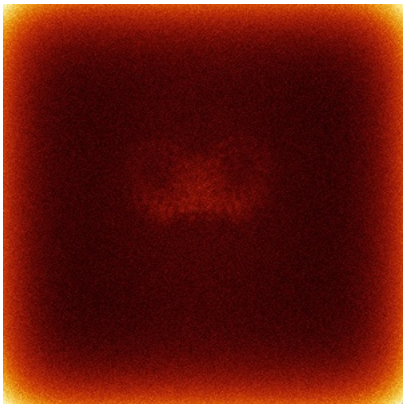
6.4.1 Primary map

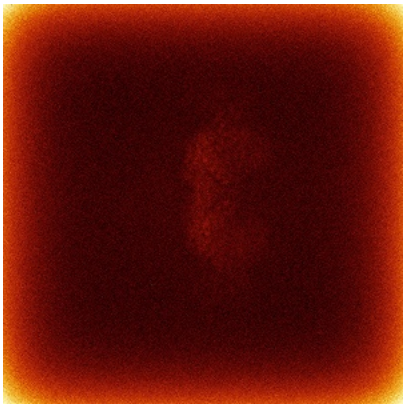

X

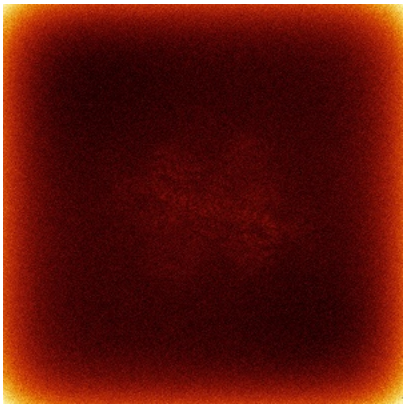

Y


Z

6.4.2 Raw map


X


Y


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

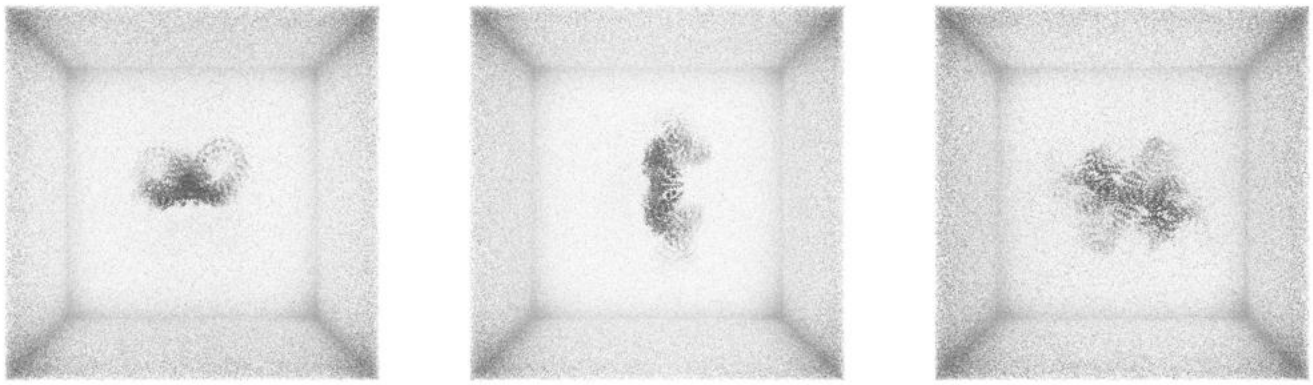
6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.0284. 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



X Y Z

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.

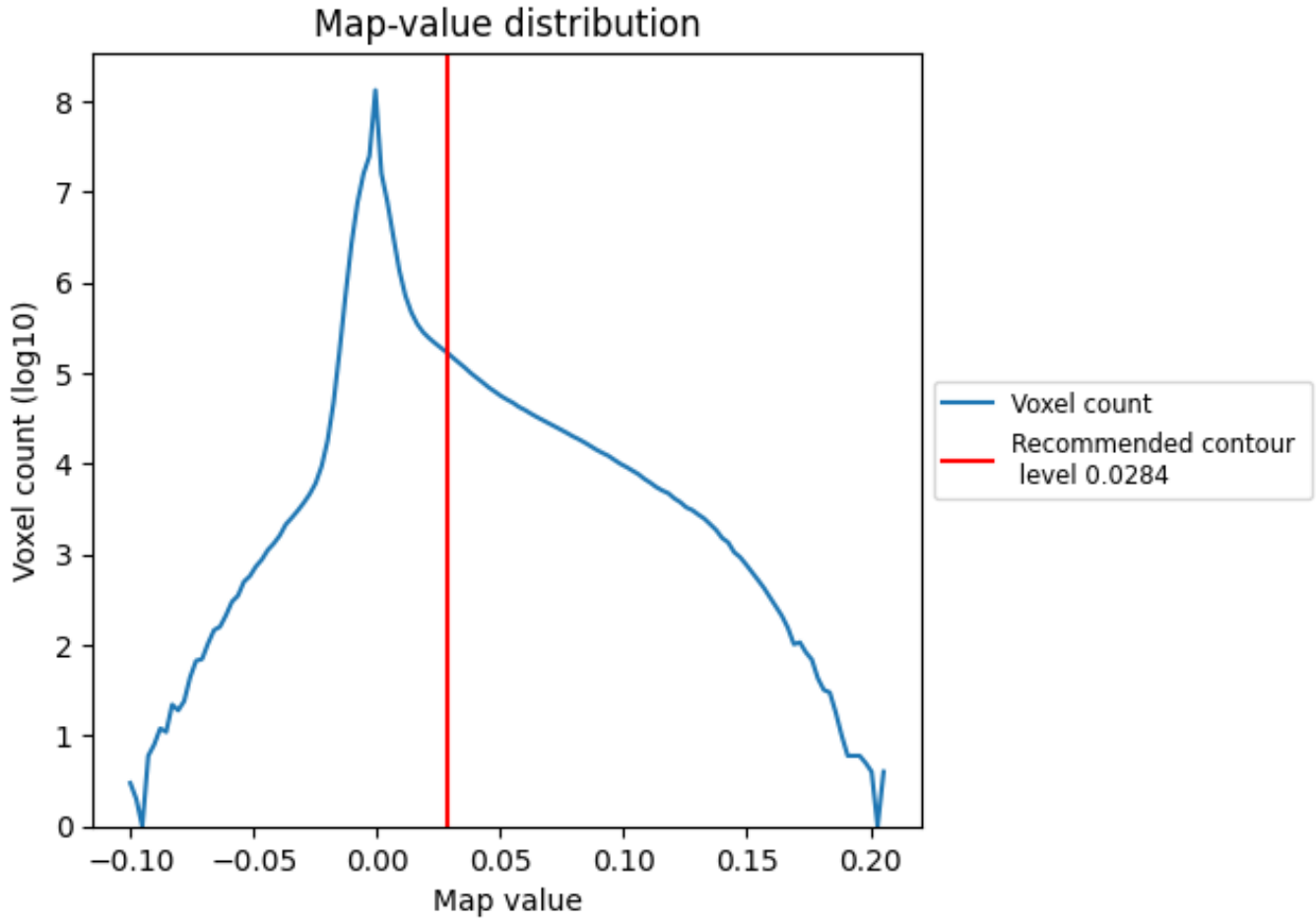
6.6 Mask visualisation (i)

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

7 Map analysis

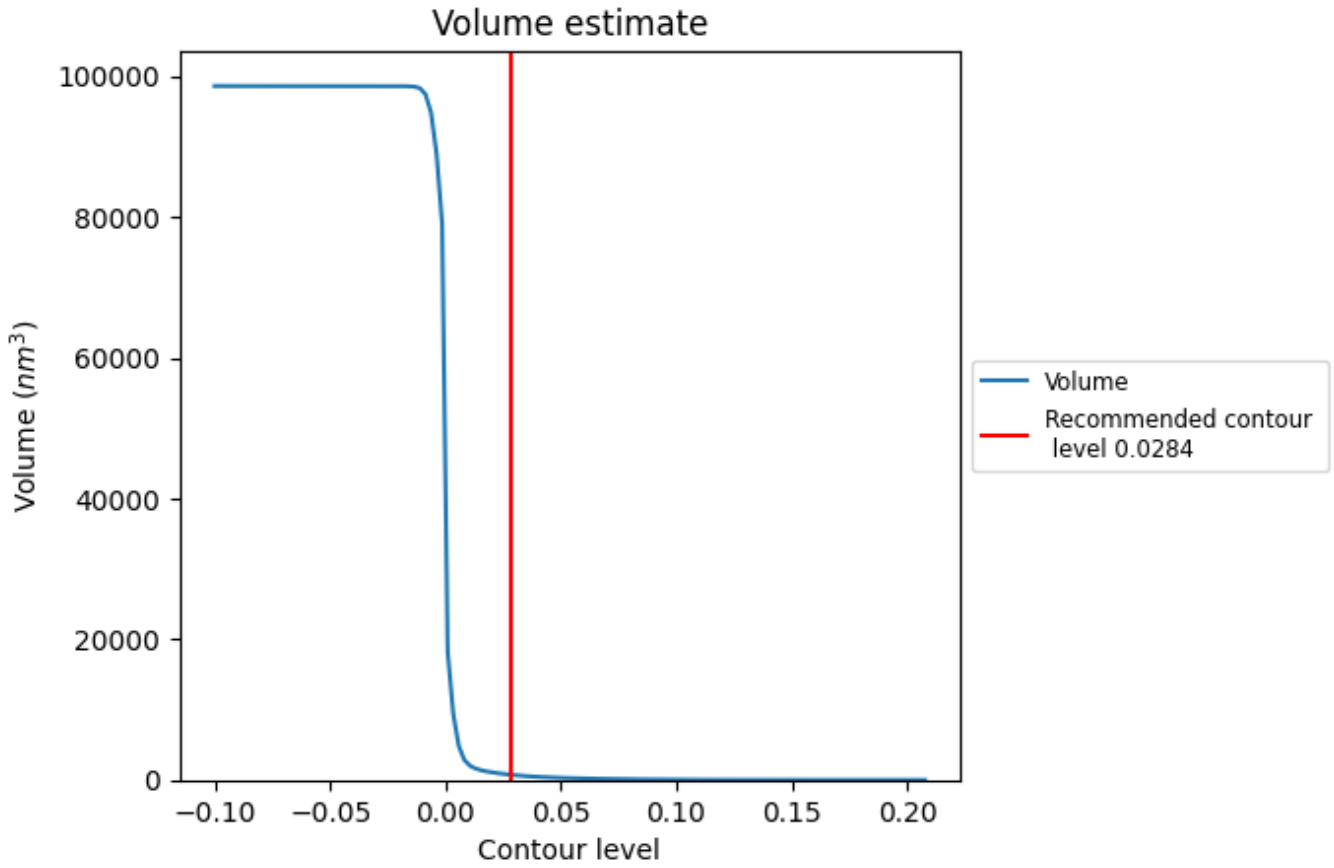
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

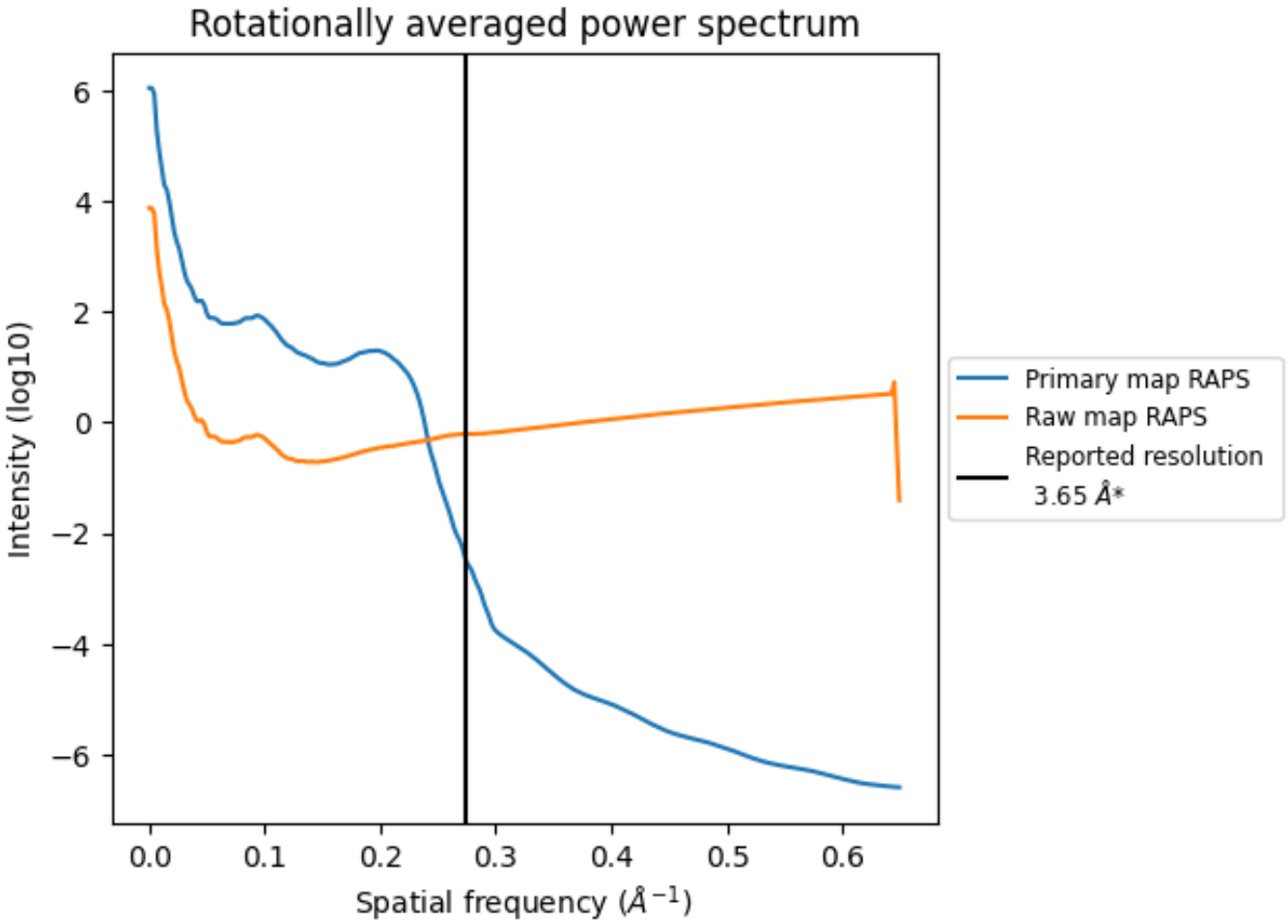
7.2 Volume estimate



The volume at the recommended contour level is 736 nm^3; this corresponds to an approximate mass of 665 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)

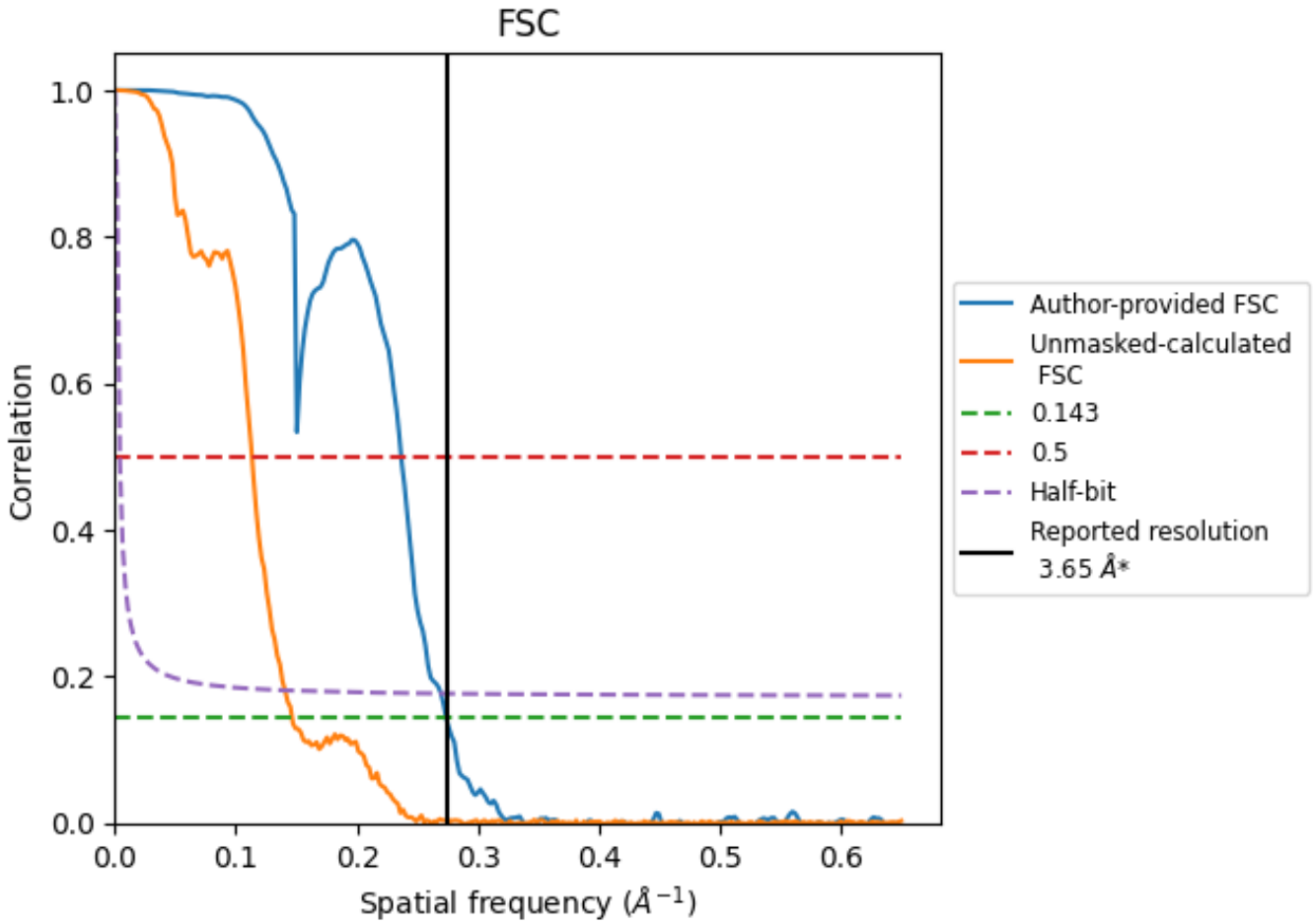


*Reported resolution corresponds to spatial frequency of 0.274 Å^{-1}

8 Fourier-Shell correlation

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



*Reported resolution corresponds to spatial frequency of 0.274 Å^{-1}

8.2 Resolution estimates (i)

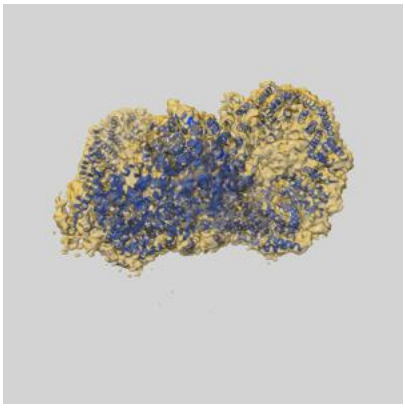
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.65	-	-
Author-provided FSC curve	3.65	4.23	3.71
Unmasked-calculated*	6.83	8.83	7.11

*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 6.83 differs from the reported value 3.65 by more than 10 %

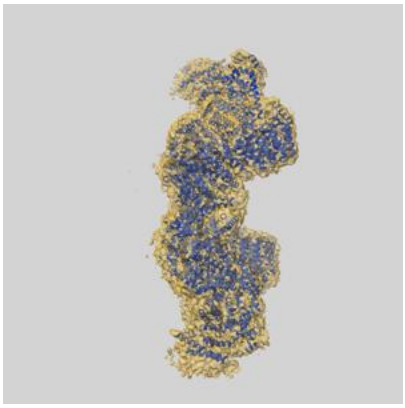
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-44413 and PDB model 9BAX. Per-residue inclusion information can be found in section 3 on page 7.

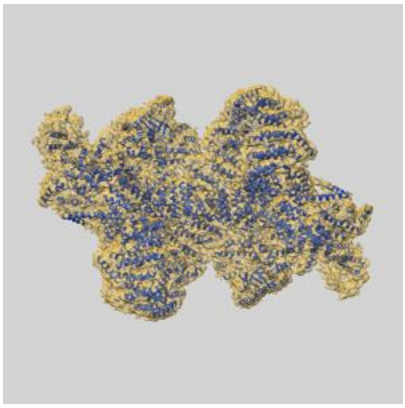
9.1 Map-model overlay



X



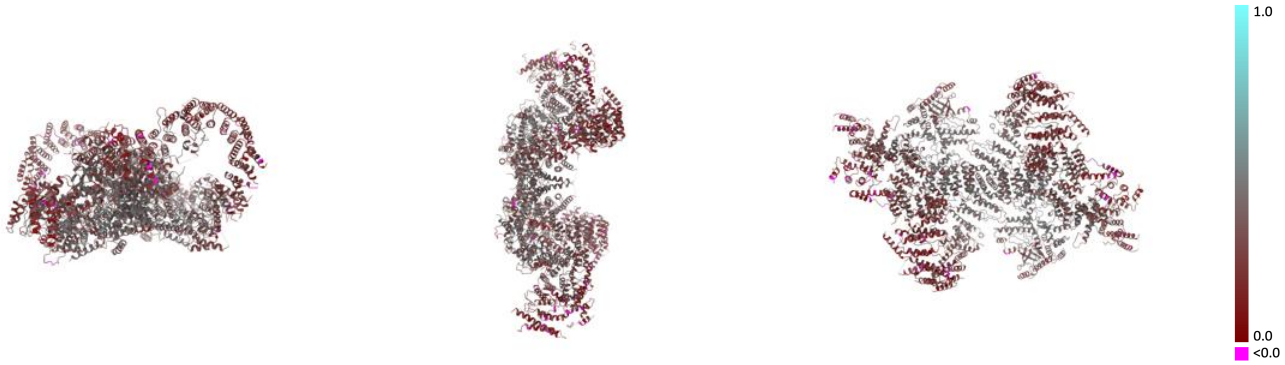
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0284 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.

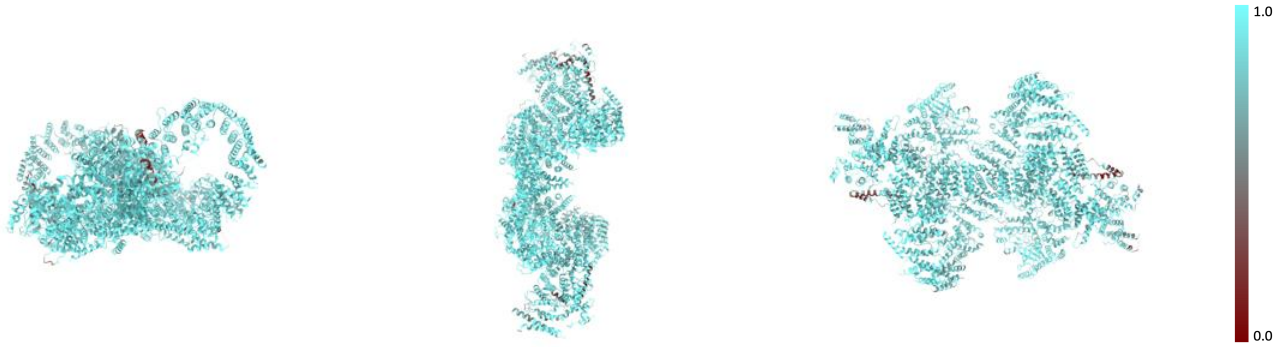
9.2 Q-score mapped to coordinate model



X Y Z

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

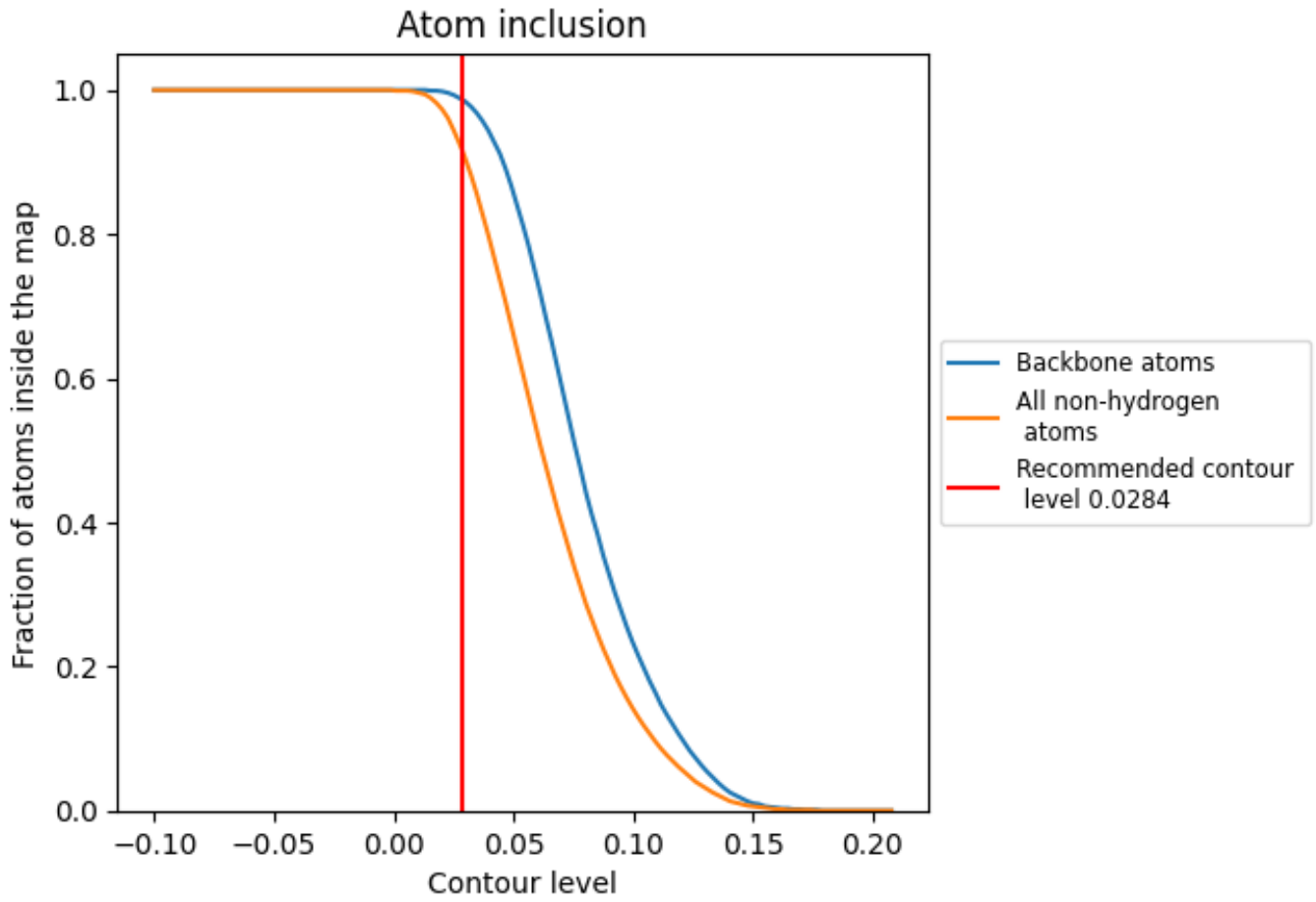
9.3 Atom inclusion mapped to coordinate model



X Y Z

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 (0.0284).

9.4 Atom inclusion (i)



At the recommended contour level, 99% of all backbone atoms, 92% 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 (0.0284) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9180	0.3270
A	0.9450	0.3530
B	0.9320	0.3360
C	0.6030	0.1460
D	0.9110	0.3320
E	0.8820	0.2860
F	0.8950	0.3070
G	0.9160	0.2500
H	0.5520	0.1770