



Full wwPDB EM Validation Report ⓘ

Nov 8, 2022 – 12:09 PM JST

PDB ID : 6A70
EMDB ID : EMD-6991
Title : Structure of the human PKD1/PKD2 complex
Authors : Su, Q.; Hu, F.; Ge, X.; Lei, J.; Yu, S.; Wang, T.; Zhou, Q.; Mei, C.; Shi, Y.
Deposited on : 2018-06-29
Resolution : 3.60 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.dev43
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.2

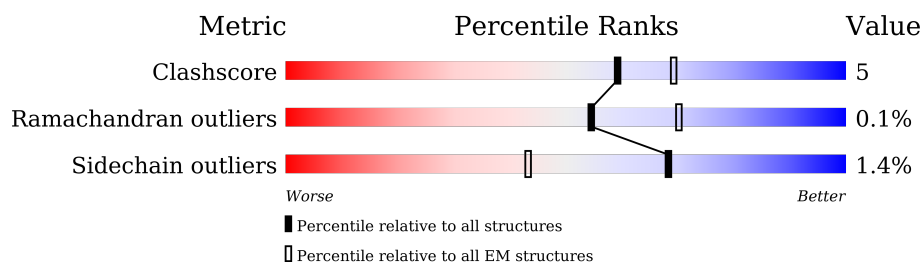
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.60 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	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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

Mol	Chain	Length	Quality of chain
1	A	577	
1	F	577	
1	G	577	
2	B	1153	

2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 15142 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 Polycystin-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	448	Total	C	N	O	S	0	0
			2579	1608	472	492	7		
1	F	463	Total	C	N	O	S	0	0
			3762	2476	593	674	19		
1	G	471	Total	C	N	O	S	0	0
			3841	2534	604	684	19		

There are 114 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	147	MET	-	expression tag	UNP Q13563
A	148	GLY	-	expression tag	UNP Q13563
A	149	SER	-	expression tag	UNP Q13563
A	150	ALA	-	expression tag	UNP Q13563
A	151	GLY	-	expression tag	UNP Q13563
A	152	TRP	-	expression tag	UNP Q13563
A	153	SER	-	expression tag	UNP Q13563
A	154	HIS	-	expression tag	UNP Q13563
A	155	PRO	-	expression tag	UNP Q13563
A	156	GLN	-	expression tag	UNP Q13563
A	157	PHE	-	expression tag	UNP Q13563
A	158	GLU	-	expression tag	UNP Q13563
A	159	LYS	-	expression tag	UNP Q13563
A	160	GLY	-	expression tag	UNP Q13563
A	161	GLY	-	expression tag	UNP Q13563
A	162	GLY	-	expression tag	UNP Q13563
A	163	SER	-	expression tag	UNP Q13563
A	164	GLY	-	expression tag	UNP Q13563
A	165	GLY	-	expression tag	UNP Q13563
A	166	GLY	-	expression tag	UNP Q13563
A	167	SER	-	expression tag	UNP Q13563
A	168	GLY	-	expression tag	UNP Q13563
A	169	GLY	-	expression tag	UNP Q13563
A	170	SER	-	expression tag	UNP Q13563

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Chain	Residue	Modelled	Actual	Comment	Reference
A	171	ALA	-	expression tag	UNP Q13563
A	172	TRP	-	expression tag	UNP Q13563
A	173	SER	-	expression tag	UNP Q13563
A	174	HIS	-	expression tag	UNP Q13563
A	175	PRO	-	expression tag	UNP Q13563
A	176	GLN	-	expression tag	UNP Q13563
A	177	PHE	-	expression tag	UNP Q13563
A	178	GLU	-	expression tag	UNP Q13563
A	179	LYS	-	expression tag	UNP Q13563
A	180	GLY	-	expression tag	UNP Q13563
A	181	SER	-	expression tag	UNP Q13563
A	182	ALA	-	expression tag	UNP Q13563
A	183	ALA	-	expression tag	UNP Q13563
A	184	ALA	-	expression tag	UNP Q13563
F	147	MET	-	expression tag	UNP Q13563
F	148	GLY	-	expression tag	UNP Q13563
F	149	SER	-	expression tag	UNP Q13563
F	150	ALA	-	expression tag	UNP Q13563
F	151	GLY	-	expression tag	UNP Q13563
F	152	TRP	-	expression tag	UNP Q13563
F	153	SER	-	expression tag	UNP Q13563
F	154	HIS	-	expression tag	UNP Q13563
F	155	PRO	-	expression tag	UNP Q13563
F	156	GLN	-	expression tag	UNP Q13563
F	157	PHE	-	expression tag	UNP Q13563
F	158	GLU	-	expression tag	UNP Q13563
F	159	LYS	-	expression tag	UNP Q13563
F	160	GLY	-	expression tag	UNP Q13563
F	161	GLY	-	expression tag	UNP Q13563
F	162	GLY	-	expression tag	UNP Q13563
F	163	SER	-	expression tag	UNP Q13563
F	164	GLY	-	expression tag	UNP Q13563
F	165	GLY	-	expression tag	UNP Q13563
F	166	GLY	-	expression tag	UNP Q13563
F	167	SER	-	expression tag	UNP Q13563
F	168	GLY	-	expression tag	UNP Q13563
F	169	GLY	-	expression tag	UNP Q13563
F	170	SER	-	expression tag	UNP Q13563
F	171	ALA	-	expression tag	UNP Q13563
F	172	TRP	-	expression tag	UNP Q13563
F	173	SER	-	expression tag	UNP Q13563
F	174	HIS	-	expression tag	UNP Q13563

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Chain	Residue	Modelled	Actual	Comment	Reference
F	175	PRO	-	expression tag	UNP Q13563
F	176	GLN	-	expression tag	UNP Q13563
F	177	PHE	-	expression tag	UNP Q13563
F	178	GLU	-	expression tag	UNP Q13563
F	179	LYS	-	expression tag	UNP Q13563
F	180	GLY	-	expression tag	UNP Q13563
F	181	SER	-	expression tag	UNP Q13563
F	182	ALA	-	expression tag	UNP Q13563
F	183	ALA	-	expression tag	UNP Q13563
F	184	ALA	-	expression tag	UNP Q13563
G	147	MET	-	expression tag	UNP Q13563
G	148	GLY	-	expression tag	UNP Q13563
G	149	SER	-	expression tag	UNP Q13563
G	150	ALA	-	expression tag	UNP Q13563
G	151	GLY	-	expression tag	UNP Q13563
G	152	TRP	-	expression tag	UNP Q13563
G	153	SER	-	expression tag	UNP Q13563
G	154	HIS	-	expression tag	UNP Q13563
G	155	PRO	-	expression tag	UNP Q13563
G	156	GLN	-	expression tag	UNP Q13563
G	157	PHE	-	expression tag	UNP Q13563
G	158	GLU	-	expression tag	UNP Q13563
G	159	LYS	-	expression tag	UNP Q13563
G	160	GLY	-	expression tag	UNP Q13563
G	161	GLY	-	expression tag	UNP Q13563
G	162	GLY	-	expression tag	UNP Q13563
G	163	SER	-	expression tag	UNP Q13563
G	164	GLY	-	expression tag	UNP Q13563
G	165	GLY	-	expression tag	UNP Q13563
G	166	GLY	-	expression tag	UNP Q13563
G	167	SER	-	expression tag	UNP Q13563
G	168	GLY	-	expression tag	UNP Q13563
G	169	GLY	-	expression tag	UNP Q13563
G	170	SER	-	expression tag	UNP Q13563
G	171	ALA	-	expression tag	UNP Q13563
G	172	TRP	-	expression tag	UNP Q13563
G	173	SER	-	expression tag	UNP Q13563
G	174	HIS	-	expression tag	UNP Q13563
G	175	PRO	-	expression tag	UNP Q13563
G	176	GLN	-	expression tag	UNP Q13563
G	177	PHE	-	expression tag	UNP Q13563
G	178	GLU	-	expression tag	UNP Q13563

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Chain	Residue	Modelled	Actual	Comment	Reference
G	179	LYS	-	expression tag	UNP Q13563
G	180	GLY	-	expression tag	UNP Q13563
G	181	SER	-	expression tag	UNP Q13563
G	182	ALA	-	expression tag	UNP Q13563
G	183	ALA	-	expression tag	UNP Q13563
G	184	ALA	-	expression tag	UNP Q13563

- Molecule 2 is a protein called Polycystin-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	704	Total	C	N	O	S	0	0
			4960	3194	905	845	16		

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	3017	MET	-	expression tag	UNP P98161
B	3018	GLY	-	expression tag	UNP P98161
B	3019	SER	-	expression tag	UNP P98161
B	3020	ALA	-	expression tag	UNP P98161
B	3021	GLY	-	expression tag	UNP P98161
B	3022	ASP	-	expression tag	UNP P98161
B	3023	TYR	-	expression tag	UNP P98161
B	3024	LYS	-	expression tag	UNP P98161
B	3025	ASP	-	expression tag	UNP P98161
B	3026	HIS	-	expression tag	UNP P98161
B	3027	ASP	-	expression tag	UNP P98161
B	3028	GLY	-	expression tag	UNP P98161
B	3029	ASP	-	expression tag	UNP P98161
B	3030	TYR	-	expression tag	UNP P98161
B	3031	LYS	-	expression tag	UNP P98161
B	3032	ASP	-	expression tag	UNP P98161
B	3033	HIS	-	expression tag	UNP P98161
B	3034	ASP	-	expression tag	UNP P98161
B	3035	ILE	-	expression tag	UNP P98161
B	3036	ASP	-	expression tag	UNP P98161
B	3037	TYR	-	expression tag	UNP P98161
B	3038	LYS	-	expression tag	UNP P98161
B	3039	ASP	-	expression tag	UNP P98161
B	3040	ASP	-	expression tag	UNP P98161
B	3041	ASP	-	expression tag	UNP P98161
B	3042	ASP	-	expression tag	UNP P98161

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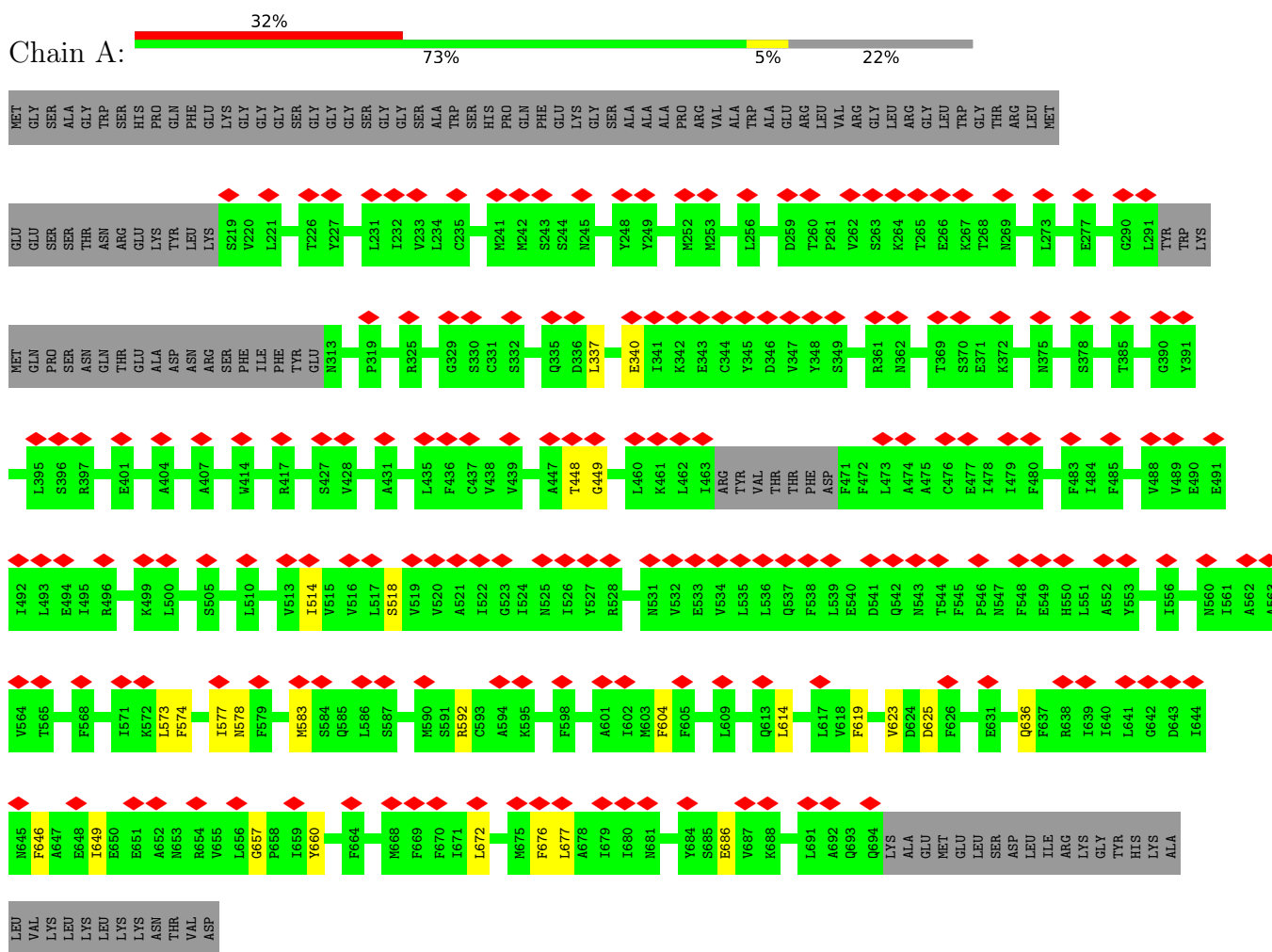
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Chain	Residue	Modelled	Actual	Comment	Reference
B	3043	LYS	-	expression tag	UNP P98161
B	3044	GLY	-	expression tag	UNP P98161
B	3045	SER	-	expression tag	UNP P98161
B	3046	ALA	-	expression tag	UNP P98161
B	3047	ALA	-	expression tag	UNP P98161
B	3048	ALA	-	expression tag	UNP P98161

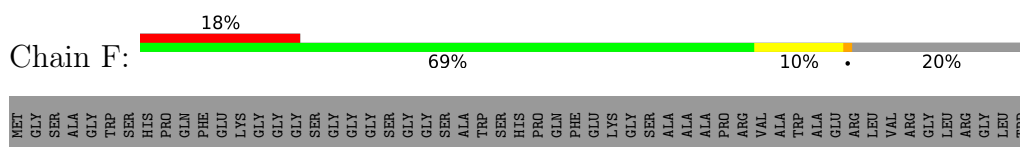
3 Residue-property plots

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

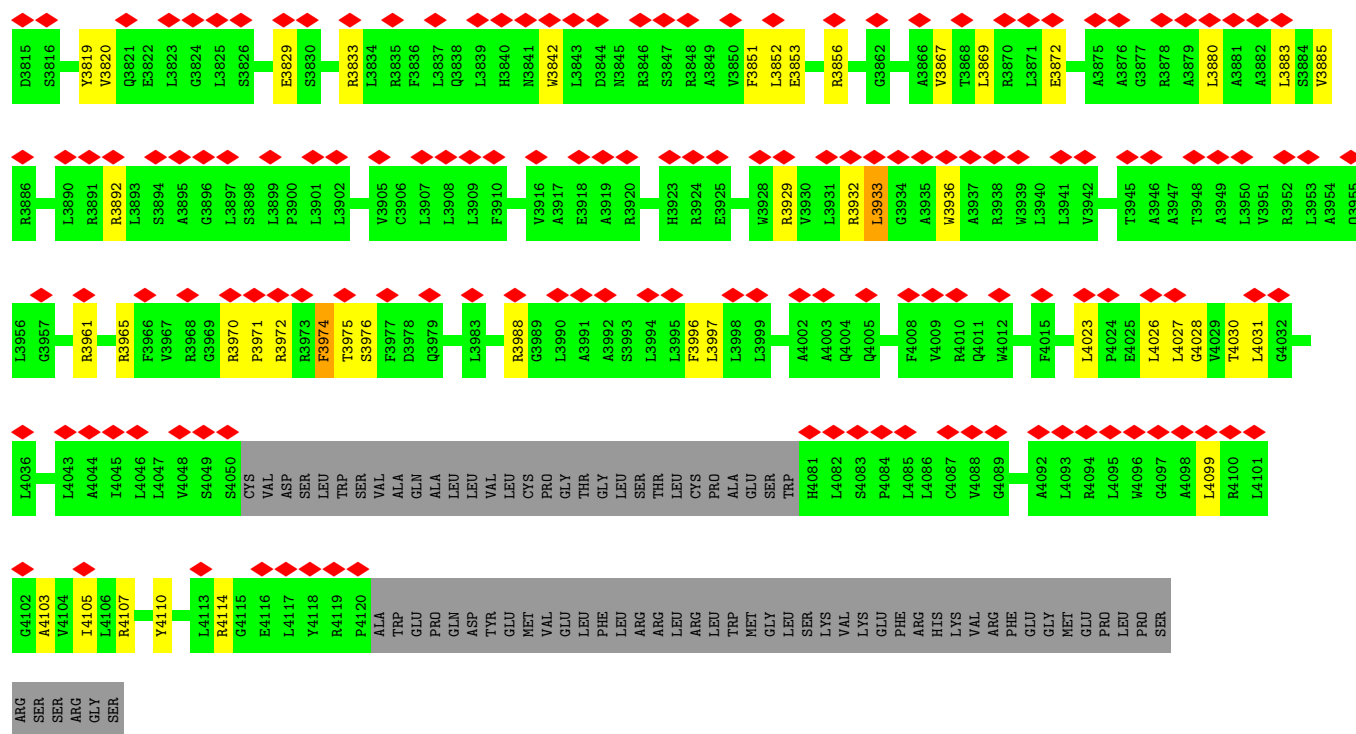
• Molecule 1: Polycystin-2



• Molecule 1: Polycystin-2







4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	27296	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.085	Depositor
Minimum map value	-0.033	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.03	Depositor
Map size (Å)	279.296, 279.296, 279.296	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.091, 1.091, 1.091	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	0.34	0/2600	0.52	0/3584
1	F	0.48	0/3860	0.67	6/5247 (0.1%)
1	G	0.51	0/3943	0.67	9/5358 (0.2%)
2	B	0.36	0/5065	0.70	2/6920 (0.0%)
All	All	0.43	0/15468	0.66	17/21109 (0.1%)

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	F	0	1
1	G	0	2
2	B	0	7
All	All	0	10

There are no bond length outliers.

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	460	LEU	CA-CB-CG	8.23	134.23	115.30
1	F	500	LEU	CA-CB-CG	7.90	133.47	115.30
1	F	460	LEU	CA-CB-CG	7.74	133.11	115.30
1	F	395	LEU	CA-CB-CG	7.68	132.97	115.30
1	F	337	LEU	CA-CB-CG	7.37	132.24	115.30
2	B	3686	LEU	CA-CB-CG	6.54	130.34	115.30
1	G	435	LEU	CA-CB-CG	6.44	130.12	115.30
1	G	287	LEU	CA-CB-CG	5.72	128.45	115.30
1	G	435	LEU	CB-CG-CD2	-5.70	101.31	111.00
1	G	315	LEU	CA-CB-CG	5.70	128.40	115.30
1	F	551	LEU	CA-CB-CG	5.49	127.92	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	573	LEU	CA-CB-CG	5.45	127.83	115.30
1	G	510	LEU	CA-CB-CG	5.42	127.76	115.30
1	G	395	LEU	CA-CB-CG	5.33	127.56	115.30
1	G	551	LEU	CA-CB-CG	5.22	127.30	115.30
1	G	536	LEU	CA-CB-CG	5.18	127.23	115.30
2	B	3933	LEU	CA-CB-CG	5.14	127.13	115.30

There are no chirality outliers.

All (10) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	3304	ASP	Peptide
2	B	3306	ALA	Peptide
2	B	3699	TYR	Peptide
2	B	3820	VAL	Peptide
2	B	3974	PHE	Peptide
2	B	3975	THR	Peptide
2	B	3976	SER	Peptide
1	F	577	ILE	Peptide
1	G	463	ILE	Peptide
1	G	577	ILE	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2579	0	1634	23	0
1	F	3762	0	3656	41	0
1	G	3841	0	3741	43	0
2	B	4960	0	4566	52	0
All	All	15142	0	13597	137	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 5.

All (137) 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:448:THR:HA	1:F:312:GLU:HB3	1.16	1.10
1:A:448:THR:HA	1:F:312:GLU:CB	2.05	0.84
1:A:448:THR:CA	1:F:312:GLU:HB3	2.05	0.82
1:A:573:LEU:O	1:A:577:ILE:N	2.29	0.66
2:B:3702:GLN:OE1	2:B:3706:LYS:NZ	2.28	0.65
2:B:3269:ARG:NH1	2:B:3273:SER:O	2.30	0.65
1:F:319:PRO:HB3	1:F:426:PHE:HB3	1.78	0.64
1:G:319:PRO:HB3	1:G:426:PHE:HB3	1.78	0.64
1:G:380:TRP:HD1	1:G:385:THR:HG22	1.63	0.63
1:A:578:ASN:HA	1:A:583:MET:HB3	1.80	0.63
1:A:677:LEU:HD12	1:F:677:LEU:HD21	1.82	0.62
1:G:229:LEU:HD12	1:G:232:ILE:HD11	1.81	0.62
1:G:492:ILE:HA	1:G:495:ILE:HG22	1.81	0.61
2:B:4028:GLY:HA2	2:B:4031:LEU:HD13	1.83	0.60
2:B:3933:LEU:HA	2:B:3936:TRP:HB3	1.84	0.59
1:A:574:PHE:HA	1:A:577:ILE:CB	2.33	0.59
2:B:3748:ARG:NH1	2:B:3853:GLU:OE1	2.36	0.58
1:F:319:PRO:HG2	1:F:395:LEU:HD11	1.84	0.58
2:B:3970:ARG:HH12	1:G:340:GLU:HG3	1.68	0.58
2:B:3829:GLU:O	2:B:3833:ARG:N	2.39	0.56
1:F:322:ARG:NH1	1:F:387:SER:O	2.40	0.55
2:B:3317:PRO:HB3	2:B:3587:ALA:HB2	1.87	0.55
1:G:313:ASN:OD1	1:G:430:ASN:ND2	2.39	0.55
1:G:227:TYR:OH	1:G:569:VAL:O	2.25	0.54
2:B:3139:GLY:N	2:B:3185:TRP:O	2.40	0.54
2:B:3867:VAL:HG22	2:B:3885:VAL:HG22	1.91	0.53
1:A:573:LEU:O	1:A:577:ILE:CB	2.58	0.52
1:F:674:ASN:HB3	1:G:677:LEU:HD23	1.92	0.51
1:F:278:ASP:HA	1:F:281:LYS:HG2	1.92	0.51
1:F:320:ARG:HH12	1:F:374:LEU:HD21	1.75	0.51
1:A:578:ASN:CA	1:A:583:MET:HB3	2.41	0.51
1:A:449:GLY:N	1:F:312:GLU:OE1	2.44	0.51
1:A:604:PHE:HD1	1:A:672:LEU:HD12	1.76	0.51
2:B:3749:LEU:HA	2:B:3852:LEU:HA	1.93	0.50
1:F:321:ILE:HG12	1:F:424:ILE:HG12	1.92	0.50
2:B:3706:LYS:HE3	2:B:3856:ARG:HD2	1.93	0.50
2:B:3872:GLU:HB2	2:B:3880:LEU:HB2	1.92	0.50
1:A:337:LEU:CB	1:F:539:LEU:HD11	2.41	0.50
2:B:3929:ARG:HE	2:B:3932:ARG:HB2	1.77	0.50
2:B:3263:TRP:HE1	2:B:3284:CYS:HB3	1.77	0.50
1:F:604:PHE:HD1	1:F:672:LEU:HD12	1.76	0.50
2:B:3808:TRP:HB3	2:B:3813:VAL:HG22	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:3869:LEU:HD23	2:B:3883:LEU:HB2	1.95	0.49
1:G:604:PHE:HD1	1:G:672:LEU:HD12	1.76	0.49
2:B:3705:ILE:HG21	1:G:448:THR:HB	1.94	0.49
1:G:280:TRP:HB3	1:G:410:LYS:HE2	1.95	0.49
2:B:4026:LEU:HD13	2:B:4105:ILE:HD12	1.94	0.49
2:B:3712:ARG:HB3	2:B:3715:LEU:HD23	1.93	0.49
1:A:614:LEU:HD12	1:F:567:PHE:HB2	1.93	0.49
1:G:619:PHE:HZ	1:G:657:GLY:HA2	1.77	0.49
1:A:619:PHE:HZ	1:A:657:GLY:HA2	1.77	0.49
2:B:3599:SER:HA	2:B:3603:TRP:HB2	1.94	0.48
2:B:3751:GLN:O	2:B:3819:TYR:N	2.39	0.48
1:F:624:ASP:OD1	1:G:247:TYR:OH	2.20	0.48
2:B:3138:VAL:HA	2:B:3186:HIS:HA	1.96	0.48
1:F:434:ASN:HD21	1:F:463:ILE:HB	1.78	0.48
1:F:619:PHE:HZ	1:F:657:GLY:HA2	1.77	0.48
1:G:434:ASN:ND2	1:G:463:ILE:O	2.47	0.48
1:F:320:ARG:HH22	1:F:374:LEU:HD11	1.80	0.47
1:G:593:CYS:HB2	1:G:683:THR:HG21	1.96	0.47
1:F:334:PRO:HG3	1:G:463:ILE:HG21	1.96	0.47
2:B:4023:LEU:HG	2:B:4027:LEU:HD23	1.96	0.47
2:B:4110:TYR:OH	2:B:4114:ARG:NH2	2.36	0.47
2:B:3748:ARG:HG2	2:B:3974:PHE:CG	2.49	0.47
1:F:335:GLN:HG3	1:F:338:ARG:NH2	2.29	0.47
1:F:224:LEU:HG	1:F:576:PHE:CZ	2.50	0.46
1:G:328:ASN:ND2	1:G:343:GLU:OE1	2.38	0.46
1:A:340:GLU:CB	1:F:314:LEU:HD13	2.45	0.46
2:B:3284:CYS:SG	2:B:3285:VAL:N	2.89	0.45
1:G:293:TRP:CD1	1:G:309:ILE:HA	2.51	0.45
2:B:3291:PHE:O	2:B:3295:ASN:ND2	2.50	0.45
2:B:3971:PRO:HG2	2:B:3972:ARG:CZ	2.47	0.45
2:B:3996:PHE:HD2	2:B:3997:LEU:HD22	1.82	0.45
1:F:379:HIS:CE1	1:F:386:TYR:HB2	2.51	0.45
1:F:470:ASP:N	1:F:470:ASP:OD1	2.46	0.44
2:B:3140:ILE:HA	2:B:3184:VAL:HA	1.99	0.44
1:A:578:ASN:CB	1:A:583:MET:HB3	2.48	0.44
1:F:440:ARG:NH2	1:F:549:GLU:OE1	2.50	0.44
1:F:592:ARG:NH1	1:F:686:GLU:OE1	2.50	0.44
1:F:623:VAL:HG12	1:F:625:ASP:H	1.83	0.44
1:G:499:LYS:HB2	1:G:502:TYR:HB3	2.00	0.44
2:B:3139:GLY:O	2:B:3185:TRP:N	2.51	0.44
2:B:3705:ILE:O	2:B:3709:LEU:N	2.35	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:499:LYS:HB2	1:F:502:TYR:HB3	2.00	0.44
1:G:592:ARG:NH1	1:G:686:GLU:OE1	2.50	0.44
2:B:4027:LEU:O	2:B:4030:THR:OG1	2.34	0.43
1:G:423:PHE:HB3	1:G:442:LEU:HA	2.00	0.43
1:A:592:ARG:NH1	1:A:686:GLU:OE1	2.50	0.43
1:A:623:VAL:HG12	1:A:625:ASP:H	1.83	0.43
1:G:291:LEU:O	1:G:307:SER:OG	2.28	0.43
1:G:326:VAL:HG11	1:G:346:ASP:H	1.84	0.43
1:G:577:ILE:HG23	1:G:578:ASN:H	1.83	0.43
2:B:3269:ARG:NH1	2:B:3274:ARG:O	2.45	0.43
1:G:623:VAL:HG12	1:G:625:ASP:H	1.83	0.43
1:A:514:ILE:O	1:A:518:SER:N	2.51	0.43
1:A:636:GLN:NE2	1:A:660:TYR:OH	2.44	0.43
2:B:3268:ASP:OD1	2:B:3268:ASP:N	2.51	0.43
1:G:423:PHE:HB3	1:G:442:LEU:HD23	2.01	0.43
1:F:326:VAL:HG11	1:F:346:ASP:H	1.84	0.43
1:F:577:ILE:HG23	1:F:578:ASN:H	1.83	0.43
2:B:4099:LEU:HA	1:G:670:PHE:HE1	1.83	0.43
1:F:280:TRP:HB3	1:F:410:LYS:HE2	2.00	0.43
1:A:337:LEU:CB	1:F:539:LEU:CD1	2.96	0.42
1:F:423:PHE:HB3	1:F:442:LEU:HA	2.00	0.42
1:F:503:PHE:CE2	1:F:508:ASN:HB3	2.55	0.42
2:B:3741:SER:O	2:B:3856:ARG:NH2	2.52	0.42
2:B:3799:ALA:HA	2:B:3800:PRO:HD3	1.80	0.42
1:G:501:HIS:O	1:G:501:HIS:ND1	2.52	0.42
2:B:4103:ALA:HA	1:G:674:ASN:HB3	2.00	0.42
2:B:3751:GLN:NE2	2:B:3842:TRP:O	2.52	0.42
1:F:337:LEU:HD11	1:G:429:TYR:CE2	2.55	0.42
1:G:262:VAL:HG12	1:G:282:PHE:HD1	1.85	0.42
2:B:3079:LEU:HD13	2:B:3685:LEU:HG	2.01	0.42
1:G:416:ASP:OD1	1:G:416:ASP:N	2.53	0.42
1:A:578:ASN:HA	1:A:583:MET:CB	2.49	0.42
2:B:4099:LEU:HD13	1:G:669:PHE:CD1	2.55	0.42
1:F:646:PHE:HE1	1:G:638:ARG:HD2	1.85	0.42
2:B:3748:ARG:HH22	2:B:3750:ARG:HD2	1.84	0.41
1:F:595:LYS:HG3	1:G:582:THR:HG21	2.01	0.41
1:A:646:PHE:HB2	1:A:649:ILE:HB	2.02	0.41
2:B:3988:ARG:HG2	1:G:617:LEU:HD12	2.01	0.41
1:G:462:LEU:HD12	1:G:462:LEU:HA	1.86	0.41
1:G:309:ILE:HB	1:G:313:ASN:HB2	2.01	0.41
2:B:4099:LEU:HA	1:G:670:PHE:CE1	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:646:PHE:HB2	1:G:649:ILE:HB	2.02	0.41
2:B:3929:ARG:HD2	2:B:3929:ARG:HA	1.94	0.41
2:B:3750:ARG:HD3	2:B:3851:PHE:O	2.21	0.41
2:B:3802:LEU:HD22	2:B:3803:LEU:H	1.86	0.41
1:F:646:PHE:HB2	1:F:649:ILE:HB	2.02	0.41
2:B:3705:ILE:HG13	2:B:3709:LEU:HD23	2.02	0.41
2:B:3335:PRO:O	2:B:3339:ALA:N	2.41	0.40
1:G:383:ILE:HD11	1:G:446:PRO:HG3	2.04	0.40
1:G:510:LEU:HD12	1:G:572:LYS:HE2	2.03	0.40
1:G:580:ASN:HB2	1:G:583:MET:HG2	2.02	0.40
2:B:3286:LEU:HD11	2:B:3565:LEU:HD23	2.02	0.40
1:F:356:ALA:HA	1:F:357:PRO:HD3	1.95	0.40
1:F:605:PHE:HA	1:F:608:PHE:HB3	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	442/577 (77%)	398 (90%)	44 (10%)	0	100	100
1	F	459/577 (80%)	438 (95%)	20 (4%)	1 (0%)	47	79
1	G	467/577 (81%)	446 (96%)	20 (4%)	1 (0%)	47	79
2	B	690/1153 (60%)	584 (85%)	105 (15%)	1 (0%)	51	83
All	All	2058/2884 (71%)	1866 (91%)	189 (9%)	3 (0%)	54	83

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	578	ASN
1	G	578	ASN

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Mol	Chain	Res	Type
2	B	3788	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	98/508 (19%)	97 (99%)	1 (1%)	76	88
1	F	404/508 (80%)	398 (98%)	6 (2%)	65	84
1	G	413/508 (81%)	407 (98%)	6 (2%)	65	84
2	B	410/946 (43%)	404 (98%)	6 (2%)	65	84
All	All	1325/2470 (54%)	1306 (99%)	19 (1%)	68	85

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	676	PHE
2	B	3345	ARG
2	B	3750	ARG
2	B	3892	ARG
2	B	3961	ARG
2	B	3965	ARG
2	B	4107	ARG
1	F	320	ARG
1	F	395	LEU
1	F	434	ASN
1	F	495	ILE
1	F	500	LEU
1	F	676	PHE
1	G	256	LEU
1	G	287	LEU
1	G	510	LEU
1	G	525	ASN
1	G	573	LEU
1	G	676	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	613	GLN
2	B	3840	HIS
1	F	434	ASN
1	F	458	GLN
1	F	613	GLN
1	F	681	ASN
1	G	458	GLN
1	G	613	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 monosaccharides 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.

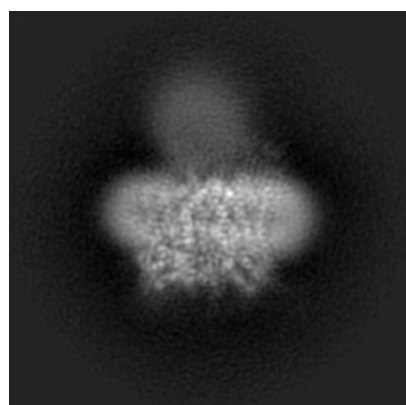
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-6991. These allow visual inspection of the internal detail of the map and identification of artifacts.

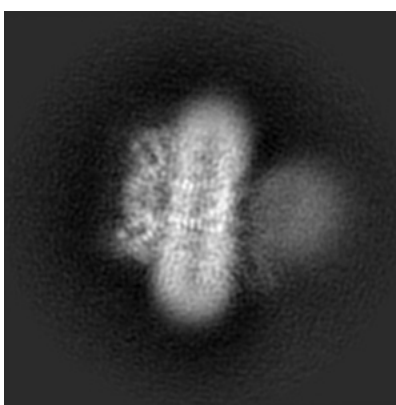
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

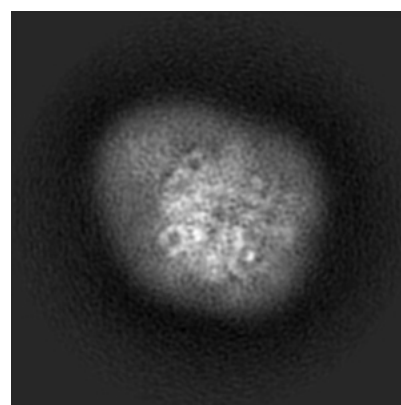
6.1.1 Primary map



X



Y

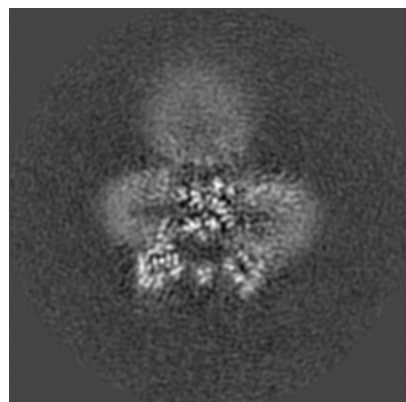


Z

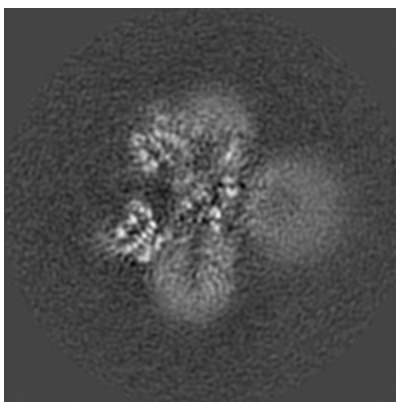
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

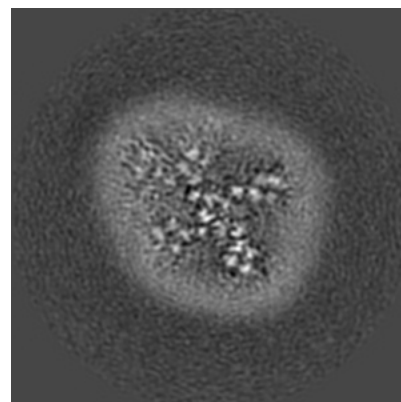
6.2.1 Primary map



X Index: 128



Y Index: 128

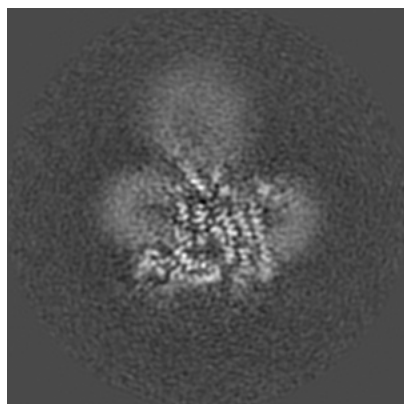


Z Index: 128

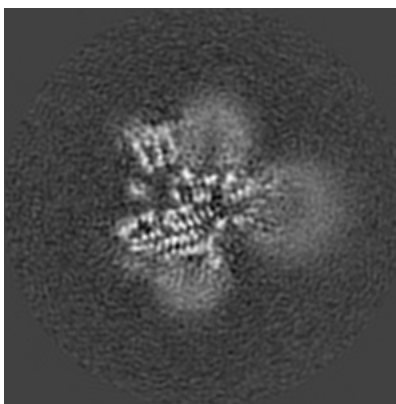
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

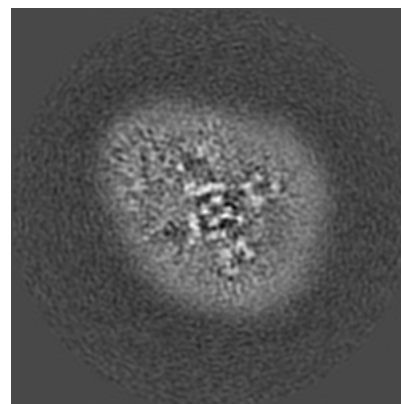
6.3.1 Primary map



X Index: 121



Y Index: 115

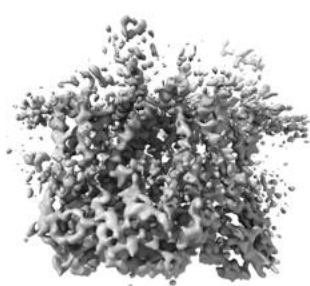


Z Index: 138

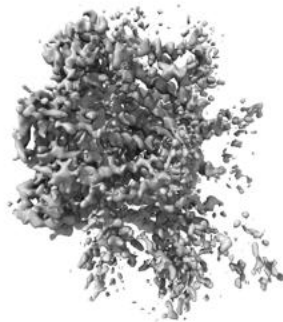
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views [i](#)

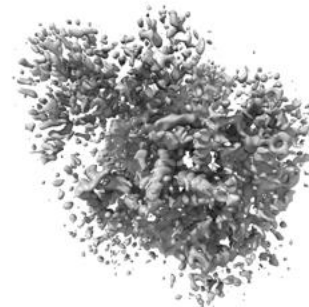
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.03. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

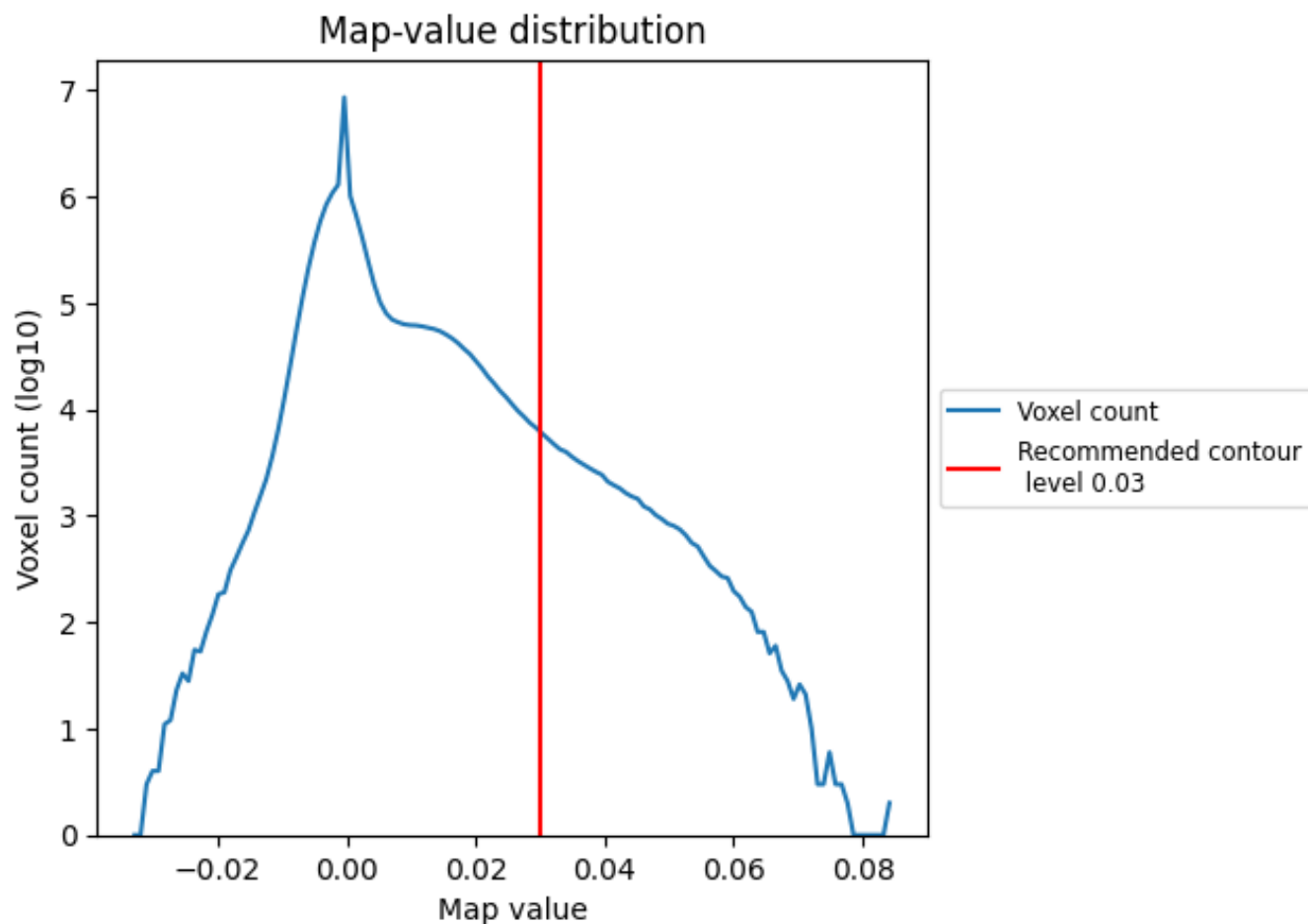
6.5 Mask visualisation

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

7 Map analysis [i](#)

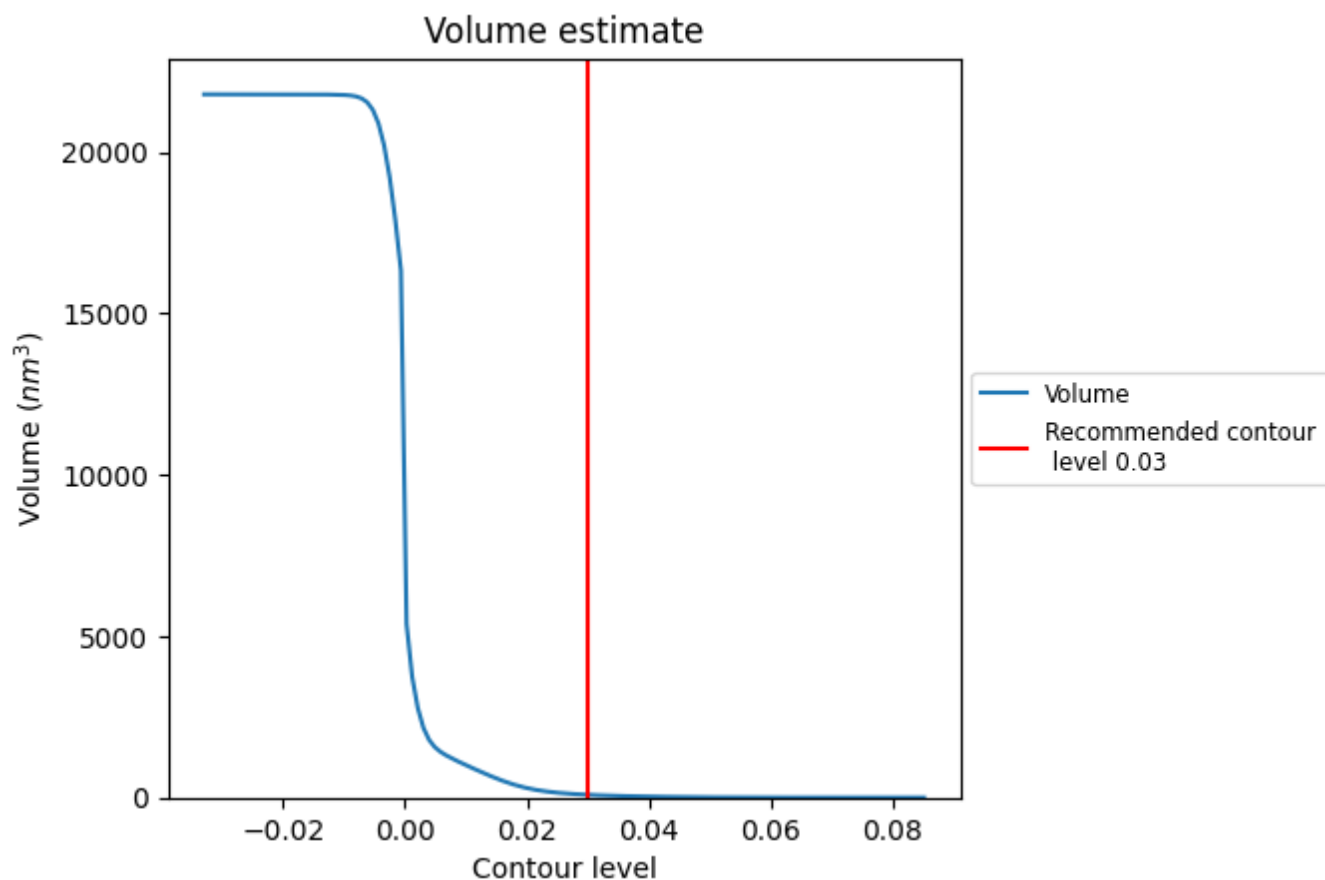
This section contains the results of statistical analysis of the map.

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.

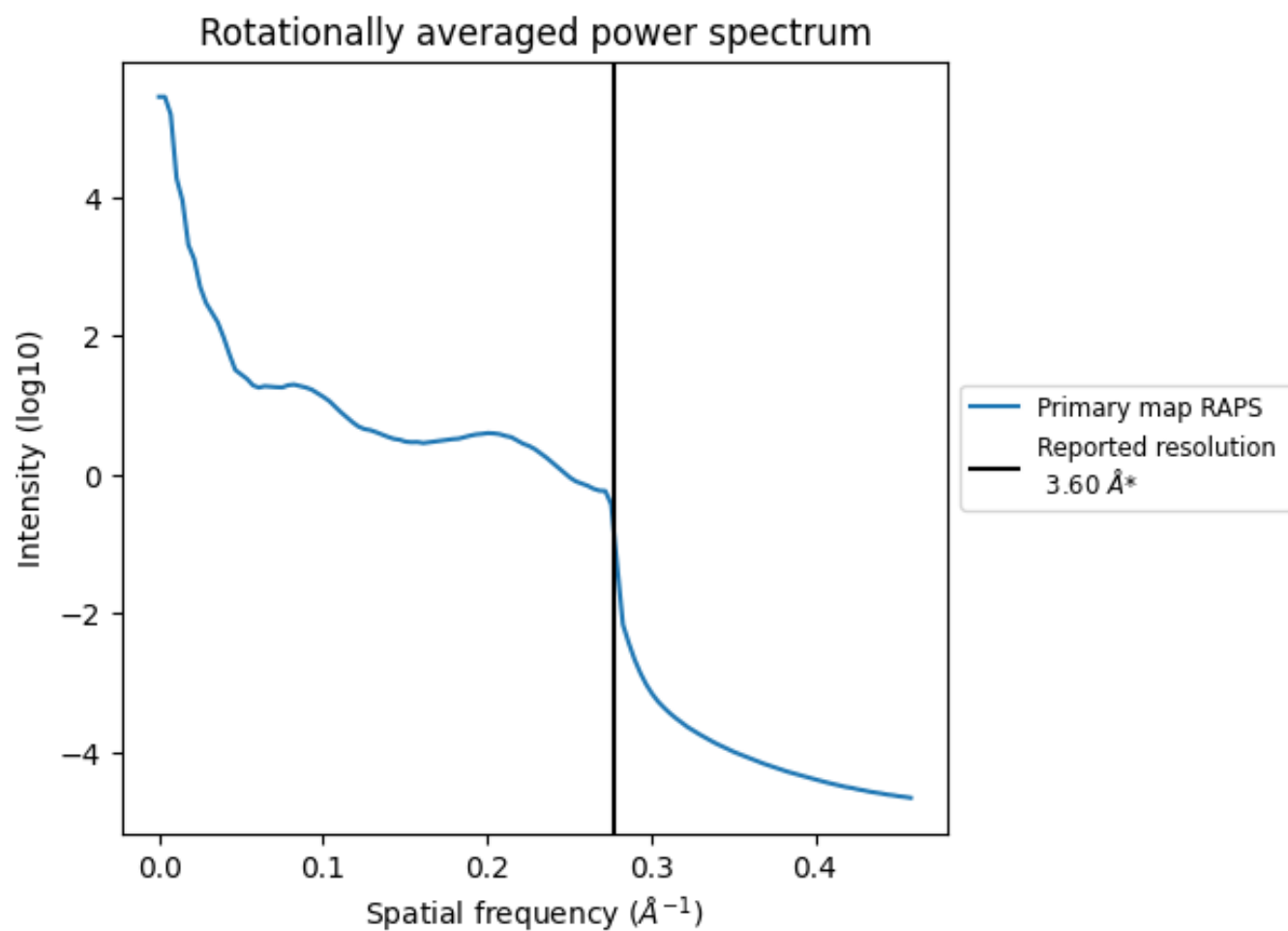
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 85 nm³; this corresponds to an approximate mass of 77 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ



*Reported resolution corresponds to spatial frequency of 0.278 Å⁻¹

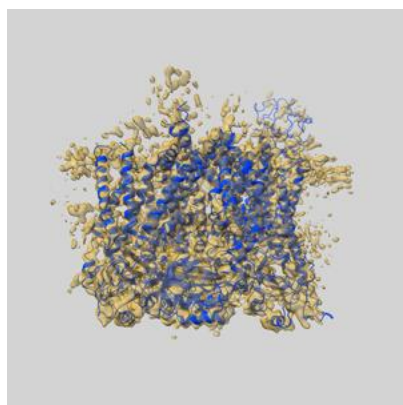
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

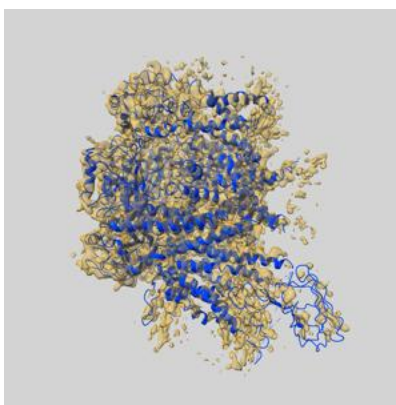
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-6991 and PDB model 6A70. Per-residue inclusion information can be found in section [3](#) on page [8](#).

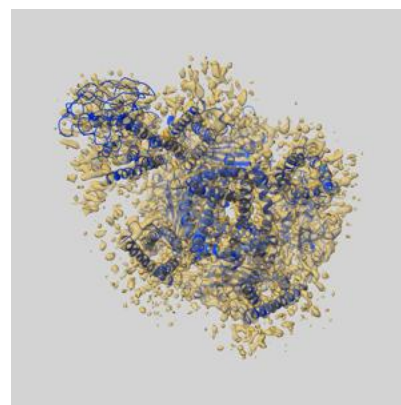
9.1 Map-model overlay [i](#)



X



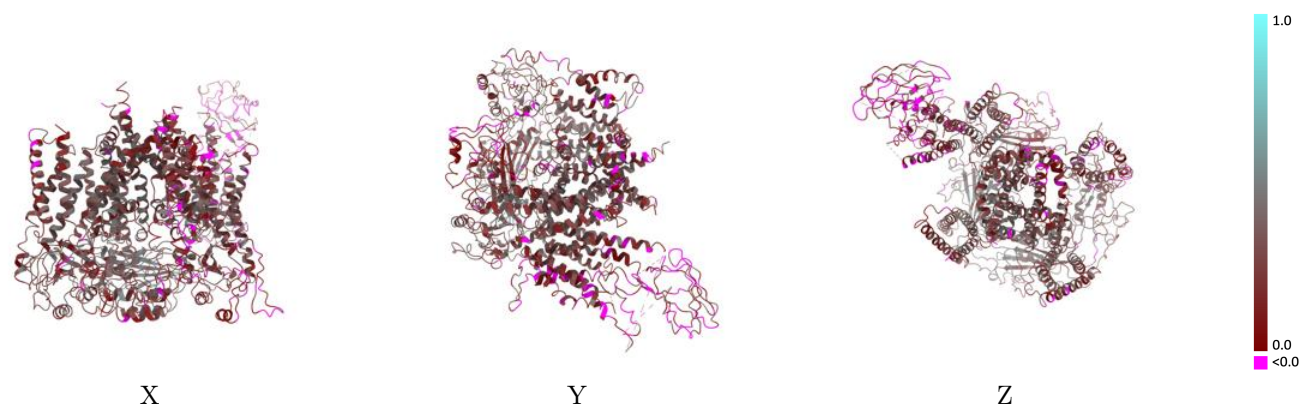
Y



Z

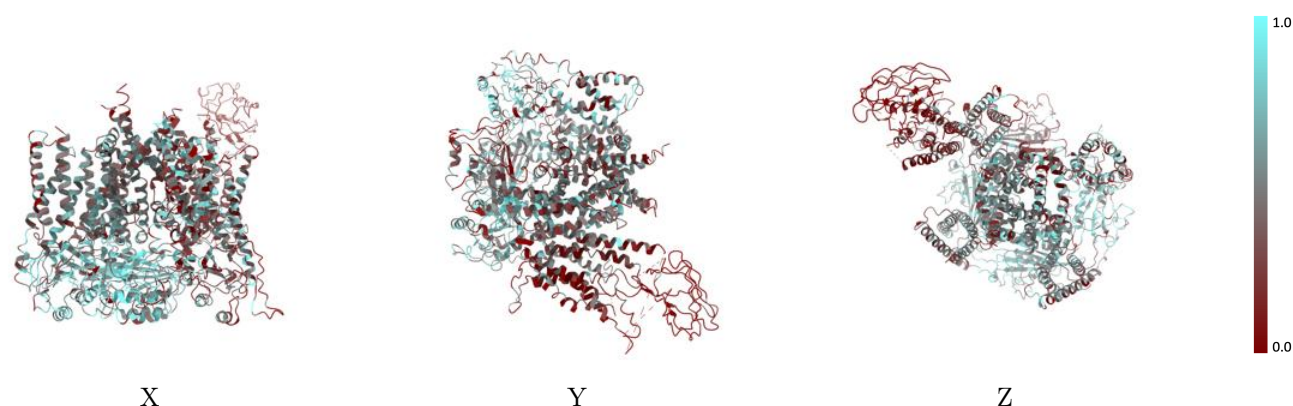
The images above show the 3D surface view of the map at the recommended contour level 0.03 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



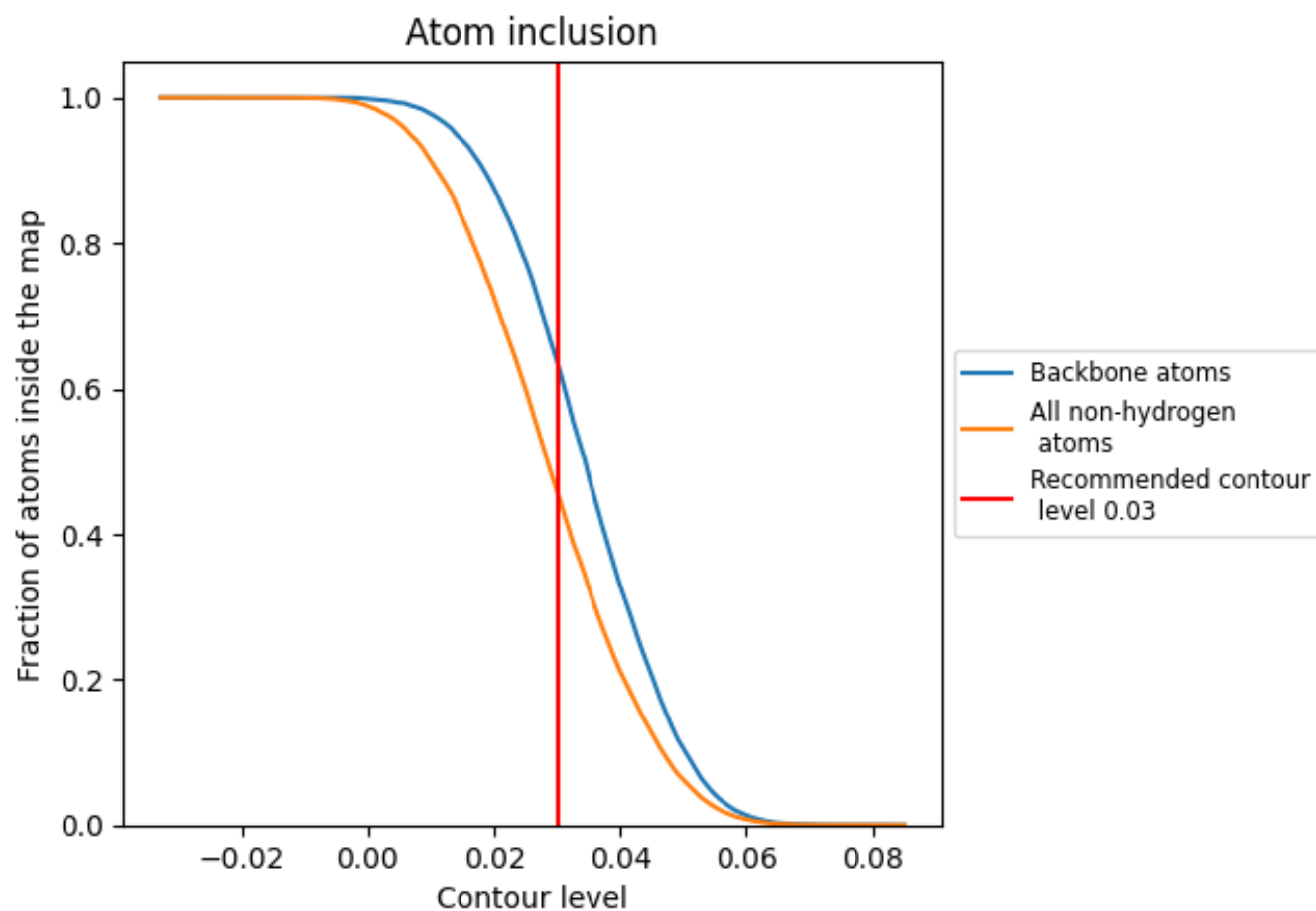
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.03).

9.4 Atom inclusion [i](#)



At the recommended contour level, 64% of all backbone atoms, 46% 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 (0.03) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.4583	<div></div> 0.2630
A	<div></div> 0.5205	<div></div> 0.2610
B	<div></div> 0.2898	<div></div> 0.1770
F	<div></div> 0.5564	<div></div> 0.3210
G	<div></div> 0.5366	<div></div> 0.3200

