



Full wwPDB EM Validation Report ⓘ

Nov 14, 2022 – 09:26 PM EST

PDB ID : 7KFT
EMDB ID : EMD-22855
Title : Partial Cas6-RT-Cas1–Cas2 complex
Authors : Hoel, C.M.; Wang, J.Y.; Doudna, J.A.; Brohawn, S.G.
Deposited on : 2020-10-14
Resolution : 3.40 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

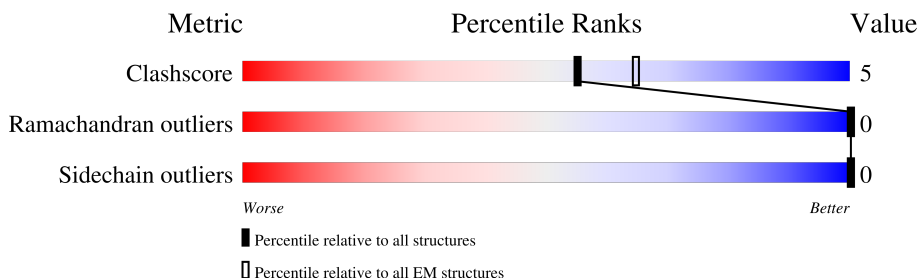
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.40 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	99	
1	B	99	
2	C	984	
2	D	984	
2	E	984	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 11680 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.

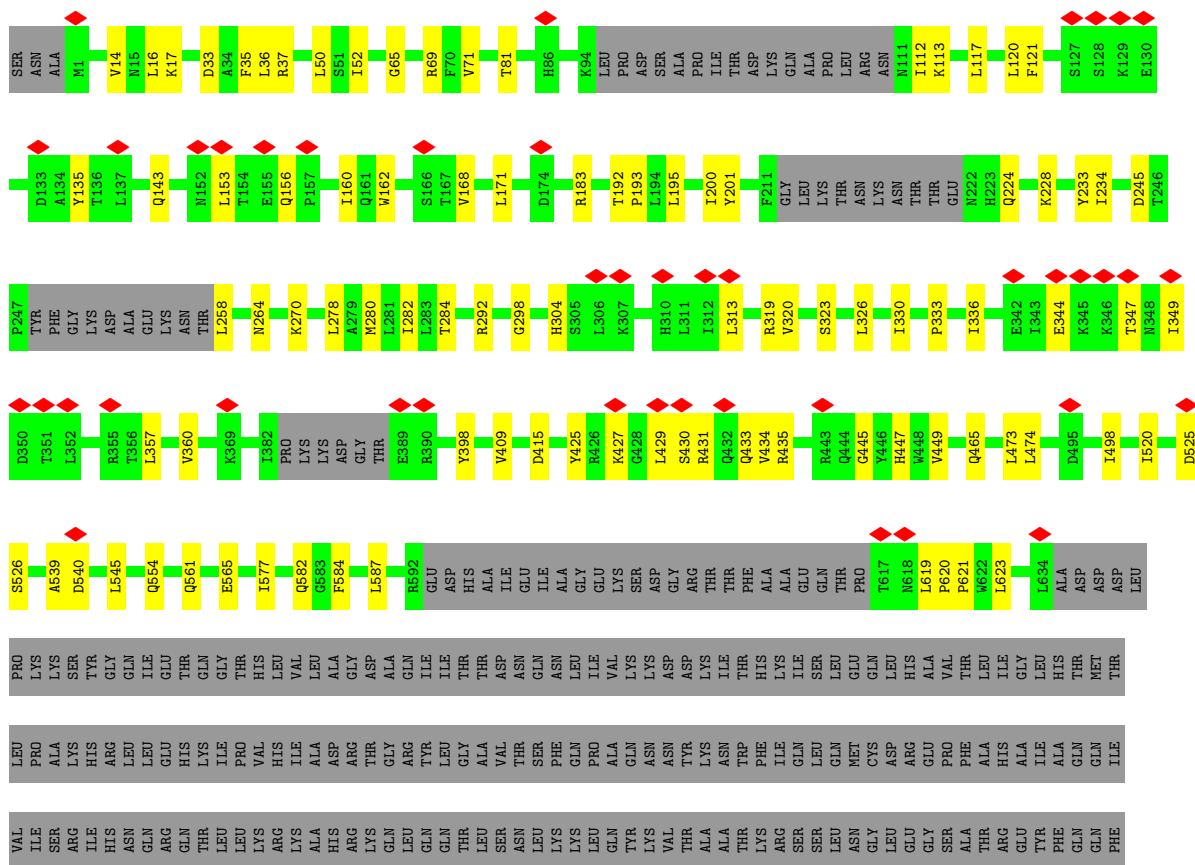
- Molecule 1 is a protein called Cas2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	B	96	Total	C	N	O	S	0	0
			796	505	147	142	2		
1	A	90	Total	C	N	O	S	0	0
			756	477	141	136	2		

- Molecule 2 is a protein called Cas6-RT-Cas1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	D	332	Total	C	N	O	S	0	0
			2727	1728	513	481	5		
2	C	568	Total	C	N	O	S	0	0
			4601	2949	809	832	11		
2	E	341	Total	C	N	O	S	0	0
			2800	1774	525	496	5		

- Molecule 2: Cas6-RT-Cas1



ASN	ARG	PHE	GLN	LYS	PHE	SER	LYS	ASP	LYS	THR	LEU	HIS	GLN	HIS	LEU	TYR	GLN	GLN	ALA	GLN	LEU	LYS	ASN	ALA	MET	HIS	ASN	GLN	GLN	SER	SER	GLN	PHE	GLN	VAL	TRP	LYS	GLU	LEU	LYS
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- Molecule 2: Cas6-RT-Cas1

Chain E:  31% 65%

ASN	ASP	LEU	PHE	ASP	GLY	ILE	PRO	VAL	SER	SER	LYS	GLU	LEU	SER	ASP	ALA	ALA	TYR	THR	LEU	GLN	ARG	ALA	MET	GLU	GLN	GLY	LEU	ALA	TRP	HIS	LYS	ALA	ALA	ASN	LEU	THR	GLN	GLU	PRO	LEU	ASP	ILE	GLN	LEU	TRP	TYR	TRP	TRP	GLN	SER	THR	VAL	ARG	ILE	LEU	HIS	ASP	LYS	THR	TRP	ASN
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HIS	PRO	ASP	LEU	TRP	ILE	ASP	THR	PRO	TYR	PHE	GLY	LYS	ASP	ALA	GLU	LYS	ASN	THR	LEU	GLY	GLY	ALA	ASN	PHE	THR	LEU	SER	LYS	PRO	GLY	ILE	GLU	PRO	GLY	LEU	LEU	ALA	MET	LEU	ILE	LEU	THR	GLN	MET	VAL	GLY	VAL	GLN	ARG	ARG	THR	SER	GLY	LEU
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SER	GLN	VAL	GLN	SER	ALA	ILE	GLY	GLN	LEU	ARG	LYS	HIS	GLN	TYR	ALA	GLN	PRO	LYS	LEU	GLN	GLY	PHE	THR	ILE	PRO	LYS	LYS	LYS	ASP	GLY	THR	GLU	ARG	LEU	LEU	ALA	VAL	SER	PRO	PRO	LEU	LEU	LYS	ALA	ALA	ALA	ILE	VAL	THR	PRO	GLY	LEU	ASP	ILE	THR
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[illegible][illegible]

GLU	641	Green
ILE	650	Yellow
ALA	653	Yellow
GLY	666	Orange
LYS	669	Yellow
SER	685	Yellow
ASP	689	Yellow
GLY	690	Yellow
ARG	699	Yellow
THR	700	Yellow
THR	703	Yellow
PHE	705	Yellow
ALA	706	Yellow
ALA	707	Yellow
GLU	708	Yellow
GLN	709	Yellow
THR	710	Yellow
PRO	711	Yellow
THR	712	Yellow
ASN	713	Yellow
LEU	714	Yellow
PRO	715	Yellow
PRO	716	Yellow
TRP	717	Yellow
LEU	718	Yellow
ALA	719	Yellow
ASN	720	Yellow
LEU	721	Yellow
GLY	722	Yellow
THR	723	Yellow
LYS	724	Yellow
SER	725	Yellow
PRO	726	Yellow
GLN	727	Yellow
PRO	728	Yellow
LEU	729	Yellow
ALA	730	Yellow
ASP	731	Yellow
ASP	732	Yellow
ASP	733	Yellow
LEU	734	Yellow
PRO	735	Yellow
PRO	736	Yellow
GLU	737	Yellow
ILE	738	Yellow
ALA	739	Yellow
GLY	740	Yellow
LYS	741	Yellow
SER	742	Yellow
PRO	743	Yellow
GLN	744	Yellow
PRO	745	Yellow
LEU	746	Yellow
ALA	747	Yellow
ASP	748	Yellow
ASP	749	Yellow
LEU	750	Yellow
PRO	751	Yellow
PRO	752	Yellow
GLU	753	Yellow
ILE	754	Yellow
ALA	755	Yellow
GLY	756	Yellow
LYS	757	Yellow
SER	758	Yellow
PRO	759	Yellow
GLN	760	Yellow
PRO	761	Yellow
LEU	762	Yellow
ALA	763	Yellow
ASP	764	Yellow
ASP	765	Yellow
LEU	766	Yellow
PRO	767	Yellow
PRO	768	Yellow
GLU	769	Yellow
ILE	770	Yellow
ALA	771	Yellow
GLY	772	Yellow
LYS	773	Yellow
SER	774	Yellow
PRO	775	Yellow
GLN	776	Yellow
PRO	777	Yellow
LEU	778	Yellow
ALA	779	Yellow
ASP	780	Yellow
ASP	781	Yellow
LEU	782	Yellow
PRO	783	Yellow
PRO	784	Yellow
GLU	785	Yellow
ILE	786	Yellow
ALA	787	Yellow
GLY	788	Yellow
LYS	789	Yellow
SER	790	Yellow
PRO	791	Yellow
GLN	792	Yellow
PRO	793	Yellow
LEU	794	Yellow
ALA	795	Yellow
ASP	796	Yellow
ASP	797	Yellow
LEU	798	Yellow
PRO	799	Yellow
PRO	800	Yellow
GLU	801	Yellow
ILE	802	Yellow
ALA	803	Yellow
GLY	804	Yellow
LYS	805	Yellow
SER	806	Yellow
PRO	807	Yellow
GLN	808	Yellow
PRO	809	Yellow
LEU	810	Yellow
ALA	811	Yellow
ASP	812	Yellow
ASP	813	Yellow
LEU	814	Yellow
PRO	815	Yellow
PRO	816	Yellow
GLU	817	Yellow
ILE	818	Yellow
ALA	819	Yellow
GLY	820	Yellow
LYS	821	Yellow
SER	822	Yellow
PRO	823	Yellow
GLN	824	Yellow
PRO	825	Yellow
LEU	826	Yellow
ALA	827	Yellow
ASP	828	Yellow
ASP	829	Yellow
LEU	830	Yellow
PRO	831	Yellow
PRO	832	Yellow
GLU	833	Yellow
ILE	834	Yellow
ALA	835	Yellow
GLY	836	Yellow
LYS	837	Yellow
SER	838	Yellow
PRO	839	Yellow
GLN	840	Yellow
PRO	841	Yellow
LEU	842	Yellow
ALA	843	Yellow
ASP	844	Yellow
ASP	845	Yellow
LEU	846	Yellow
PRO	847	Yellow
PRO	848	Yellow
GLU	849	Yellow
ILE	850	Yellow
ALA	851	Yellow
GLY	852	Yellow
LYS	853	Yellow
SER	854	Yellow
PRO	855	Yellow
GLN	856	Yellow
PRO	857	Yellow
LEU	858	Yellow
ALA	859	Yellow
ASP	860	Yellow
ASP	861	Yellow
LEU	862	Yellow
PRO	863	Yellow
PRO	864	Yellow
GLU	865	Yellow
ILE	866	Yellow
ALA	867	Yellow
GLY	868	Yellow
LYS	869	Yellow
SER	870	Yellow
PRO	871	Yellow
GLN	872	Yellow
PRO	873	Yellow
LEU	874	Yellow
ALA	875	Yellow
ASP	876	Yellow
ASP	877	Yellow
LEU	878	Yellow
PRO	879	Yellow
PRO	880	Yellow
GLU	881	Yellow
ILE	882	Yellow
ALA	883	Yellow
GLY	884	Yellow
LYS	885	Yellow
SER	886	Yellow
PRO	887	Yellow
GLN	888	Yellow
PRO	889	Yellow
LEU	890	Yellow
ALA	891	Yellow
ASP	892	Yellow
ASP	893	Yellow
LEU	894	Yellow
PRO	895	Yellow
PRO	896	Yellow
GLU	897	Yellow
ILE	898	Yellow
ALA	899	Yellow
GLY	900	Yellow
LYS	901	Yellow
SER	902	Yellow
PRO	903	Yellow
GLN	904	Yellow
PRO	905	Yellow
LEU	906	Yellow
ALA	907	Yellow
ASP	908	Yellow
ASP	909	Yellow
LEU	910	Yellow
PRO	911	Yellow
PRO	912	Yellow
GLU	913	Yellow
ILE	914	Yellow
ALA	915	Yellow
GLY	916	Yellow
LYS	917	Yellow
SER	918	Yellow
PRO	919	Yellow
GLN	920	Yellow
PRO	921	Yellow
LEU	922	Yellow
ALA	923	Yellow
ASP	924	Yellow
ASP	925	Yellow
LEU	926	Yellow
PRO	927	Yellow
PRO	928	Yellow
GLU	929	Yellow
ILE	930	Yellow
ALA	931	Yellow
GLY	932	Yellow
LYS	933	Yellow
SER	934	Yellow
PRO	935	Yellow
GLN	936	Yellow
PRO	937	Yellow
LEU	938	Yellow
ALA	939	Yellow
ASP	940	Yellow
ASP	941	Yellow
LEU	942	Yellow
PRO	943	Yellow
PRO	944	Yellow
GLU	945	Yellow
ILE	946	Yellow
ALA	947	Yellow
GLY	948	Yellow
LYS	949	Yellow
SER	950	Yellow
PRO	951	Yellow
GLN	952	Yellow
PRO	953	Yellow
LEU	954	Yellow
ALA	955	Yellow
ASP	956	Yellow
ASP	957	Yellow
LEU	958	Yellow
PRO	959	Yellow
PRO	960	Yellow
GLU	961	Yellow
ILE	962	Yellow
ALA	963	Yellow
GLY	964	Yellow
LYS	965	Yellow
SER	966	Yellow
PRO	967	Yellow
GLN	968	Yellow
PRO	969	Yellow
LEU	970	Yellow
ALA	971	Yellow
ASP	972	Yellow
ASP	973	Yellow
LEU	974	Yellow
PRO	975	Yellow
PRO	976	Yellow
GLU	977	Yellow
ILE	978	Yellow
ALA	979	Yellow
GLY	980	Yellow
LYS	981	Yellow
SER	982	Yellow
PRO	983	Yellow
GLN	984	Yellow
PRO	985	Yellow
LEU	986	Yellow
ALA	987	Yellow
ASP	988	Yellow
ASP	989	Yellow
LEU	990	Yellow
PRO	991	Yellow
PRO	992	Yellow
GLU	993	Yellow
ILE	994	Yellow
ALA	995	Yellow
GLY	996	Yellow
LYS	997	Yellow
SER	998	Yellow
PRO	999	Yellow
GLN	1000	Yellow

Year	Publications
2007	1
2008	1
2009	1
2010	1
2011	2
2012	2
2013	9
2014	2
2015	3
2016	3
2017	3
2018	3
2019	3
2020	10

L961	H952	L956	Q961	F974	K981
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4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	129175	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 ($e^-/\text{\AA}^2$)	49.9	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	62.598	Depositor
Minimum map value	-41.692	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	1.000	Depositor
Recommended contour level	9.0	Depositor
Map size (Å)	474.80002, 474.80002, 474.80002	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.187, 1.187, 1.187	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	0.28	0/771	0.55	0/1034
1	B	0.32	0/812	0.56	0/1092
2	C	0.29	0/4706	0.51	1/6379 (0.0%)
2	D	0.32	0/2787	0.48	0/3759
2	E	0.34	0/2861	0.53	1/3857 (0.0%)
All	All	0.31	0/11937	0.52	2/16121 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	540	ASP	CB-CG-OD1	6.07	123.76	118.30
2	E	666	ASP	CB-CG-OD2	5.59	123.33	118.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	756	0	765	21	0
1	B	796	0	813	13	0
2	C	4601	0	4613	55	0
2	D	2727	0	2751	21	0
2	E	2800	0	2826	24	0
All	All	11680	0	11768	124	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 (124) 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:D:699:THR:HG22	2:D:701:PRO:HD2	1.67	0.75
2:E:860:LEU:HD11	2:E:886:ILE:HD12	1.74	0.69
2:E:714:HIS:NE2	2:E:857:ASP:OD2	2.25	0.68
2:C:200:ILE:HG12	2:C:284:THR:HG21	1.76	0.67
2:E:906:GLN:O	2:E:933:ARG:NH2	2.28	0.67
2:E:699:THR:HG22	2:E:701:PRO:HD2	1.78	0.65
1:B:31:GLN:HB3	1:B:34:VAL:HB	1.78	0.65
2:C:14:VAL:HG12	2:C:117:LEU:HG	1.77	0.65
2:C:427:LYS:HA	2:C:539:ALA:HA	1.78	0.64
2:E:766:ASN:HB3	2:E:892:HIS:HD2	1.63	0.63
1:B:44:ARG:NE	2:E:685:GLU:OE1	2.29	0.63
1:B:5:LEU:HD23	1:B:71:LEU:HD11	1.81	0.62
1:A:10:VAL:HB	1:A:16:ARG:HB3	1.81	0.62
2:C:120:LEU:O	2:C:319:ARG:NH1	2.34	0.60
2:E:916:LYS:HB3	2:E:920:GLY:HA2	1.82	0.60
2:C:33:ASP:OD2	2:C:37:ARG:NH1	2.35	0.60
1:B:75:THR:HG23	1:A:70:ASN:HB3	1.82	0.60
2:C:153:LEU:HD23	2:C:156:GLN:HE21	1.66	0.60
2:C:620:PRO:HD2	2:C:623:LEU:HD12	1.83	0.60
2:D:863:ALA:O	2:D:963:LYS:NZ	2.33	0.59
2:C:17:LYS:HB3	2:C:113:LYS:HB2	1.85	0.59
2:C:233:TYR:HB3	2:C:270:LYS:HB2	1.83	0.59
2:C:445:GLY:O	2:C:447:HIS:ND1	2.37	0.58
2:C:449:VAL:HG12	2:C:545:LEU:HD23	1.86	0.57
2:C:16:LEU:HD13	2:C:112:ILE:HG23	1.85	0.57
2:D:667:ASN:HB3	2:E:918:HIS:HE1	1.70	0.57
2:D:801:ARG:NH2	2:D:874:GLN:OE1	2.38	0.57
1:A:31:GLN:HG2	1:A:32:GLY:H	1.70	0.57
1:B:64:ASN:ND2	1:A:83:ASN:OD1	2.38	0.56
2:C:333:PRO:HA	2:C:336:ILE:HD12	1.88	0.56
2:E:801:ARG:NH2	2:E:871:ILE:O	2.38	0.56
1:B:46:ARG:NH2	2:C:554:GLN:OE1	2.31	0.56
2:C:465:GLN:HG3	2:C:520:ILE:HD11	1.87	0.56
2:D:707:LEU:HD21	2:D:726:VAL:HG12	1.87	0.56
1:A:10:VAL:HG13	1:A:63:GLU:HG3	1.88	0.56
2:C:35:PHE:HD1	2:C:36:LEU:HD12	1.71	0.55
1:A:70:ASN:OD1	1:A:71:LEU:N	2.39	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:258:LEU:HD22	2:C:292:ARG:HH12	1.72	0.55
2:D:831:LYS:HE2	2:C:577:ILE:HD11	1.88	0.55
1:B:10:VAL:HG13	1:B:63:GLU:HG3	1.89	0.55
2:C:582:GLN:HG2	2:C:621:PRO:HB3	1.88	0.55
2:E:832:ARG:NH2	2:E:846:SER:OG	2.32	0.54
1:B:8:PHE:HB2	1:B:66:ILE:HG12	1.90	0.54
2:C:193:PRO:HB3	2:C:234:ILE:HG13	1.90	0.54
2:E:666:ASP:HB3	2:E:669:ASN:H	1.73	0.53
2:D:834:ARG:HG2	2:C:577:ILE:HB	1.91	0.53
2:E:835:ARG:HB2	2:E:836:PRO:HD3	1.91	0.52
2:C:525:ASP:OD1	2:C:526:SER:N	2.43	0.52
2:E:690:VAL:HG13	2:E:713:VAL:HG23	1.91	0.52
1:A:81:ASP:OD1	1:A:82:ILE:N	2.41	0.51
2:C:168:VAL:HG23	2:C:298:GLY:HA2	1.92	0.51
2:E:836:PRO:O	2:E:838:LYS:HG3	2.09	0.51
1:B:31:GLN:NE2	1:A:65:ASN:OD1	2.44	0.50
2:C:561:GLN:O	2:C:565:GLU:HG3	2.12	0.50
2:C:344:GLU:HA	2:C:347:THR:HB	1.94	0.50
2:C:430:SER:HB2	2:C:433:GLN:HB3	1.94	0.49
2:C:121:PHE:CE2	2:C:135:TYR:HB2	2.47	0.49
2:C:498:ILE:HD13	2:C:587:LEU:HD11	1.94	0.49
1:A:26:TYR:OH	1:A:47:GLN:NE2	2.38	0.49
2:D:726:VAL:HG22	2:E:726:VAL:HG22	1.95	0.49
2:C:233:TYR:HB3	2:C:270:LYS:HE2	1.94	0.48
1:B:20:SER:O	1:B:24:GLU:HG3	2.13	0.48
1:A:53:HIS:HA	1:A:56:ILE:HG12	1.95	0.48
1:A:13:ASP:OD1	1:A:14:LYS:N	2.47	0.48
2:C:429:LEU:HD12	2:C:434:VAL:HG21	1.94	0.48
2:E:961:GLN:HG2	2:E:974:PHE:HA	1.94	0.48
2:C:415:ASP:OD1	2:C:425:TYR:OH	2.24	0.48
2:C:619:LEU:HD23	2:C:623:LEU:HD13	1.95	0.48
2:C:71:VAL:HG21	2:C:320:VAL:HG12	1.97	0.47
1:A:16:ARG:HA	1:A:19:LEU:HD23	1.95	0.47
1:A:20:SER:O	1:A:24:GLU:HG2	2.15	0.47
1:A:48:LEU:O	1:A:52:ILE:HG12	2.14	0.47
2:D:771:LEU:HD12	2:D:781:LEU:HD13	1.96	0.47
2:C:201:TYR:OH	2:C:224:GLN:OE1	2.32	0.47
2:C:50:LEU:HD11	2:C:81:THR:HG21	1.98	0.46
2:E:650:GLN:OE1	2:E:952:HIS:NE2	2.46	0.46
2:C:431:ARG:HB3	2:C:435:ARG:HH21	1.81	0.46
2:E:881:ALA:O	2:E:885:ASP:HB2	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:48:LEU:HA	1:A:51:LYS:HE2	1.98	0.46
2:D:653:HIS:CD2	2:D:689:ALA:HB3	2.50	0.46
2:D:775:LYS:HG2	2:D:778:ARG:HH21	1.81	0.46
2:C:326:LEU:O	2:C:330:ILE:HG12	2.16	0.46
2:C:473:LEU:HG	2:C:474:LEU:HD12	1.98	0.45
2:C:36:LEU:HD22	2:C:52:ILE:HD11	1.99	0.45
2:D:820:ASN:O	2:D:828:HIS:NE2	2.49	0.45
1:B:31:GLN:HG3	1:B:32:GLY:H	1.82	0.45
1:A:47:GLN:O	1:A:51:LYS:HG3	2.17	0.45
1:A:8:PHE:HB3	1:A:66:ILE:HD12	1.98	0.44
2:C:143:GLN:HB3	2:C:313:LEU:HB2	1.99	0.44
2:E:849:TYR:OH	2:E:895:GLU:OE2	2.35	0.44
2:D:881:ALA:O	2:D:885:ASP:HB2	2.18	0.43
1:A:77:LYS:HB3	1:A:77:LYS:HE2	1.75	0.43
2:C:245:ASP:OD1	2:C:245:ASP:N	2.44	0.43
2:D:773:LYS:NZ	2:D:979:GLU:OE2	2.48	0.43
2:C:584:PHE:O	2:C:587:LEU:HB2	2.18	0.43
2:E:705:ARG:HA	2:E:705:ARG:HD3	1.85	0.43
2:D:840:PRO:HB3	2:D:912:PHE:CZ	2.54	0.43
2:C:278:LEU:O	2:C:282:ILE:HG12	2.19	0.43
2:D:778:ARG:O	2:D:782:GLN:HG2	2.19	0.43
2:C:360:VAL:HG12	2:C:398:TYR:HB2	2.00	0.43
2:C:228:LYS:HA	2:C:228:LYS:HD3	1.86	0.42
2:E:951:LEU:HG	2:E:955:LEU:HD23	2.01	0.42
2:D:884:SER:HA	2:D:887:MET:HG2	2.01	0.42
2:E:790:LYS:HE3	2:E:790:LYS:HB2	1.86	0.42
2:C:160:ILE:HG22	2:C:304:HIS:HA	2.02	0.42
2:C:347:THR:HG23	2:C:349:ILE:H	1.84	0.42
2:D:764:ILE:HA	2:D:767:GLN:HG2	2.02	0.41
2:C:200:ILE:HG22	2:C:280:MET:HE2	2.02	0.41
2:E:653:HIS:ND1	2:E:689:ALA:HB3	2.34	0.41
2:C:17:LYS:HE2	2:C:65:GLY:HA2	2.02	0.41
1:A:6:ILE:HB	1:A:35:PHE:HB2	2.03	0.41
2:C:162:TRP:O	2:C:264:ASN:HA	2.20	0.41
1:B:74:ASP:N	1:B:74:ASP:OD1	2.54	0.41
2:D:765:HIS:O	2:D:769:GLN:HG2	2.21	0.41
2:D:869:LYS:HA	2:D:869:LYS:HD2	1.92	0.41
2:C:69:ARG:HB2	2:C:323:SER:HB2	2.03	0.41
2:C:330:ILE:HD13	2:C:409:VAL:HG21	2.03	0.41
2:C:171:LEU:HD22	2:C:183:ARG:HG2	2.02	0.41
1:B:87:ILE:HA	1:B:87:ILE:HD12	1.81	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:8:PHE:HB3	1:A:66:ILE:CD1	2.52	0.40
1:A:51:LYS:O	1:A:55:ILE:HD12	2.21	0.40
2:C:192:THR:HB	2:C:195:LEU:HB3	2.03	0.40
2:D:667:ASN:HB3	2:E:918:HIS:CE1	2.53	0.40
2:C:357:LEU:HA	2:C:360:VAL:HG22	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	88/99 (89%)	86 (98%)	2 (2%)	0	100	100
1	B	94/99 (95%)	89 (95%)	5 (5%)	0	100	100
2	C	556/984 (56%)	531 (96%)	25 (4%)	0	100	100
2	D	330/984 (34%)	318 (96%)	12 (4%)	0	100	100
2	E	339/984 (34%)	316 (93%)	23 (7%)	0	100	100
All	All	1407/3150 (45%)	1340 (95%)	67 (5%)	0	100	100

There are no Ramachandran outliers to report.

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	85/91 (93%)	85 (100%)	0	100	100
1	B	89/91 (98%)	89 (100%)	0	100	100
2	C	499/859 (58%)	499 (100%)	0	100	100
2	D	291/859 (34%)	291 (100%)	0	100	100
2	E	299/859 (35%)	299 (100%)	0	100	100
All	All	1263/2759 (46%)	1263 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	64	ASN
1	A	83	ASN
2	D	738	ASN
2	C	156	GLN
2	E	892	HIS
2	E	973	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 ⓘ

There are no chain breaks in this entry.

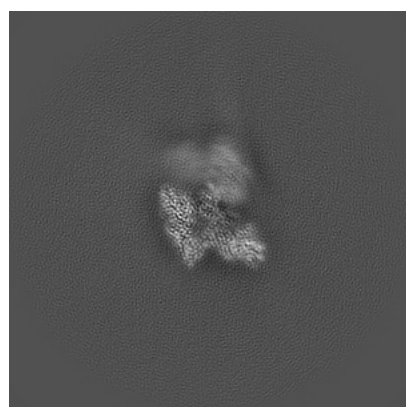
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-22855. These allow visual inspection of the internal detail of the map and identification of artifacts.

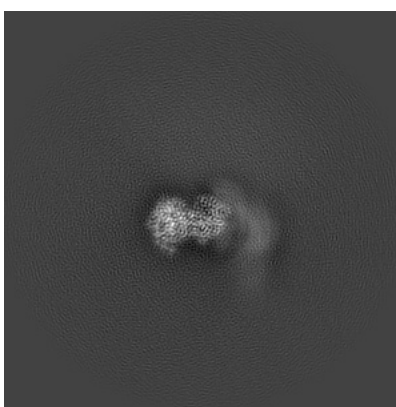
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

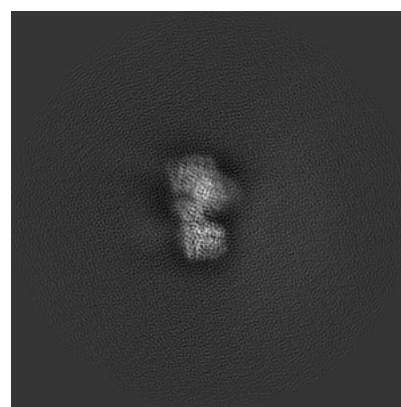
6.1.1 Primary map



X



Y

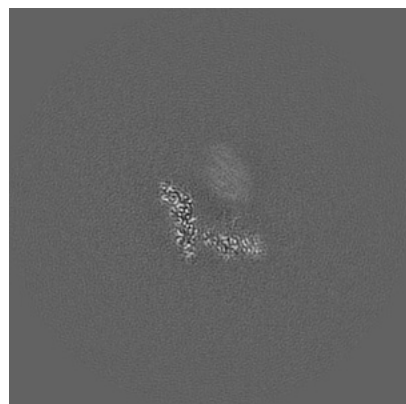


Z

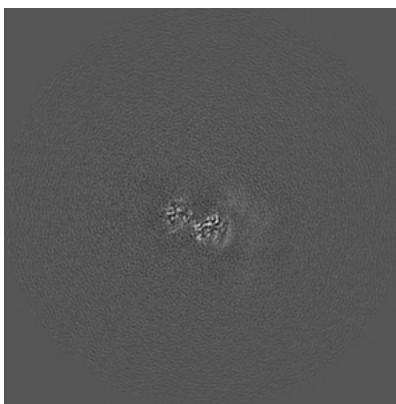
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

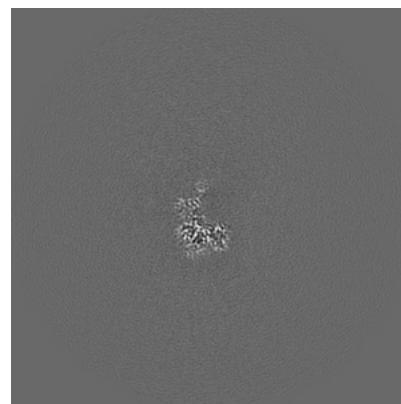
6.2.1 Primary map



X Index: 200



Y Index: 200

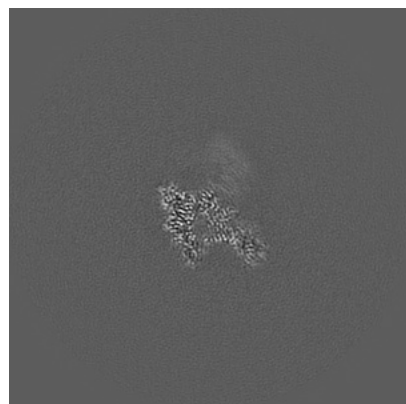


Z Index: 200

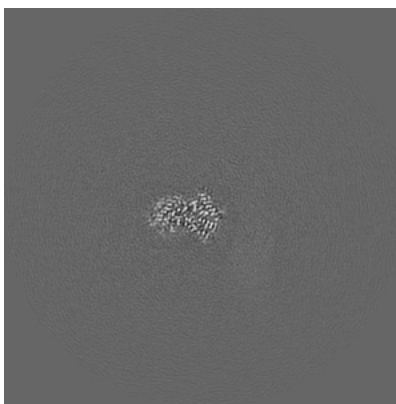
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

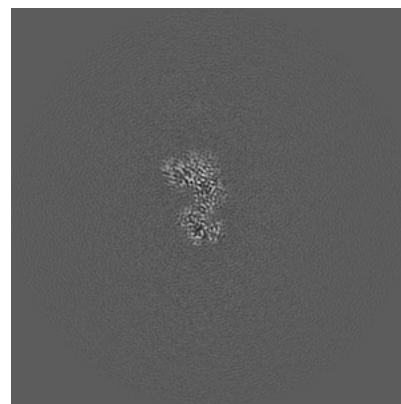
6.3.1 Primary map



X Index: 186



Y Index: 178



Z Index: 166

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 9.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

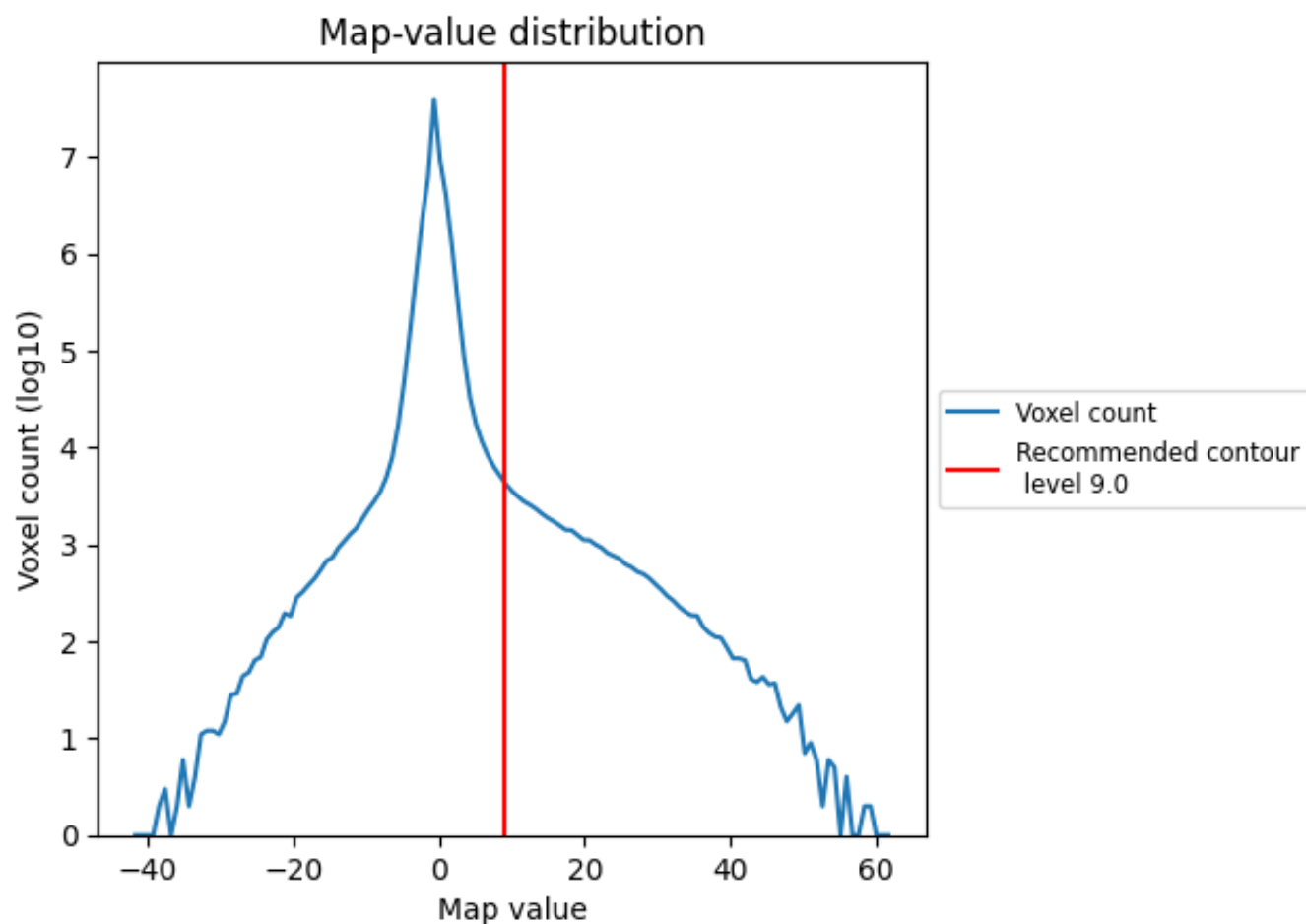
6.5 Mask visualisation

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

7 Map analysis [i](#)

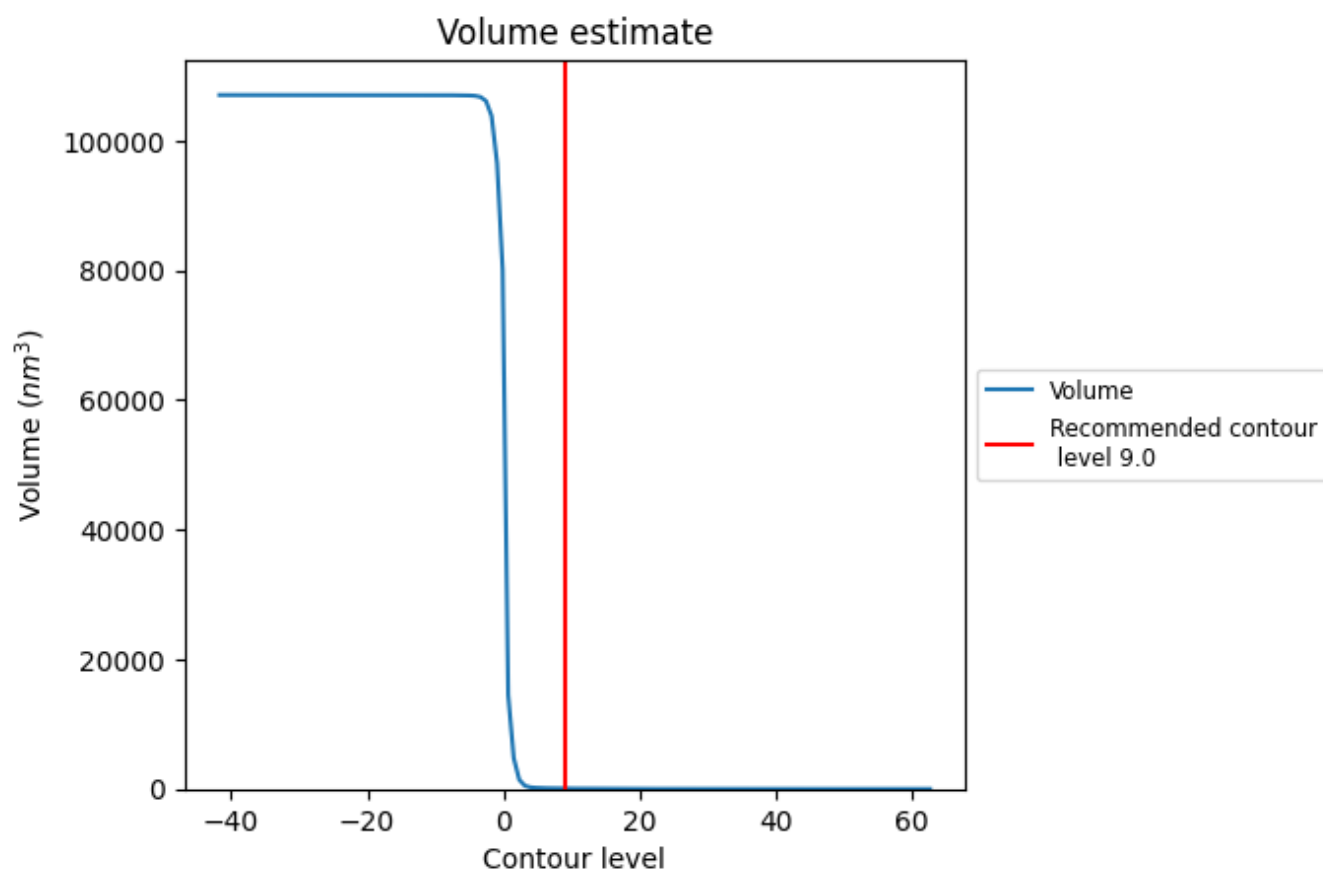
This section contains the results of statistical analysis of the map.

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.

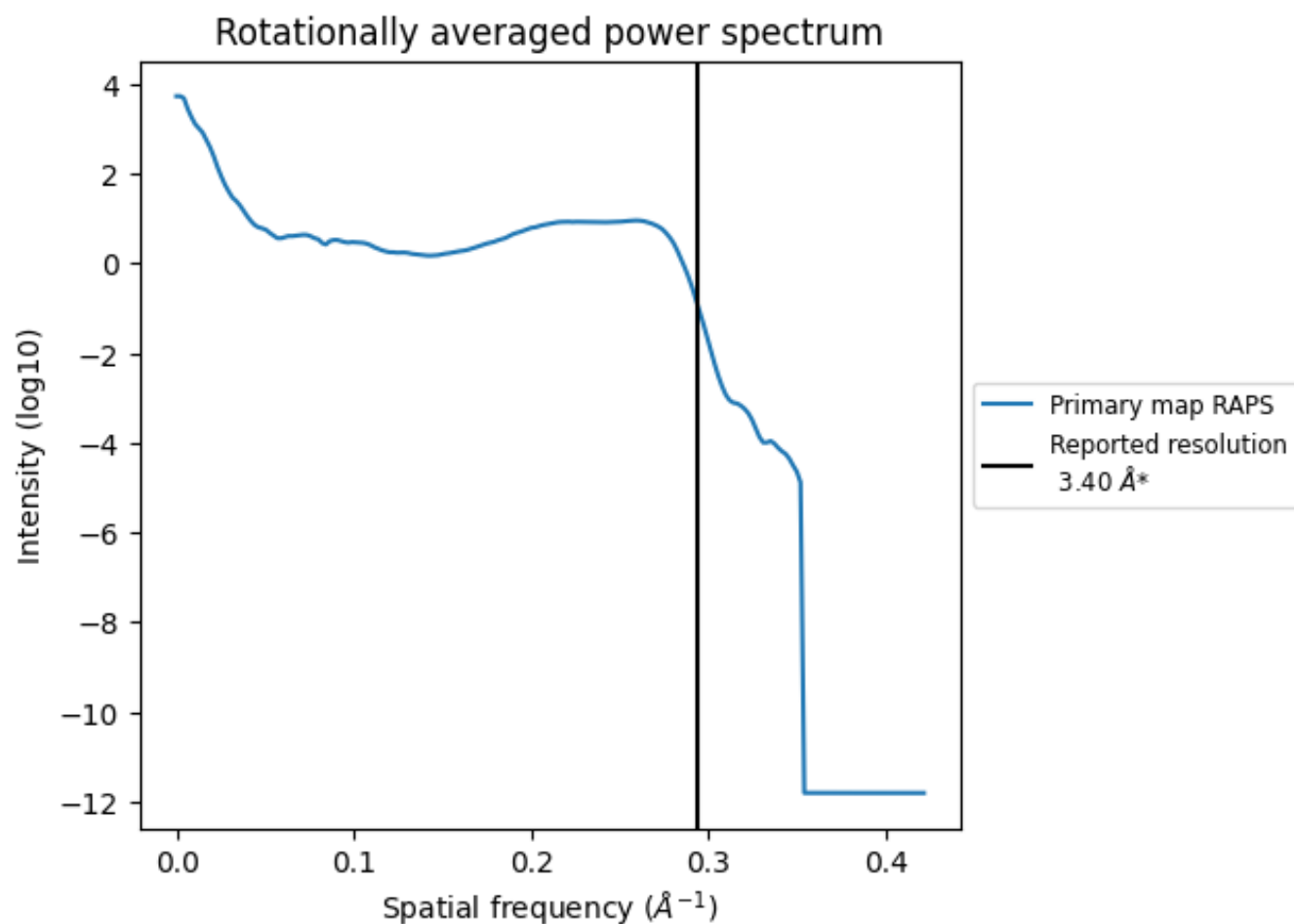
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 73 nm^3 ; this corresponds to an approximate mass of 66 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 0.294 Å⁻¹

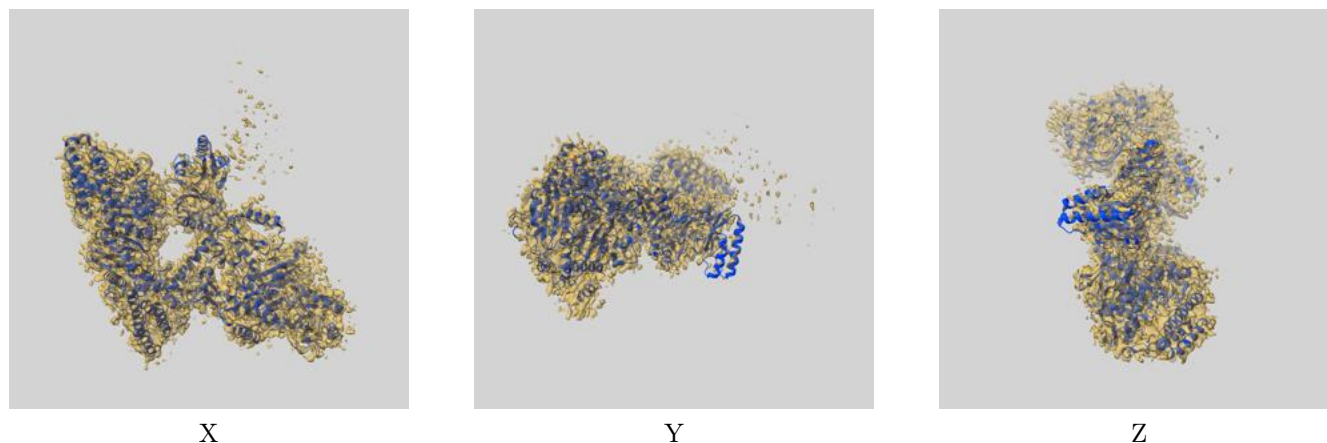
8 Fourier-Shell correlation ⓘ

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-22855 and PDB model 7KFT. Per-residue inclusion information can be found in [section 3](#) on [page 4](#).

9.1 Map-model overlay [i](#)



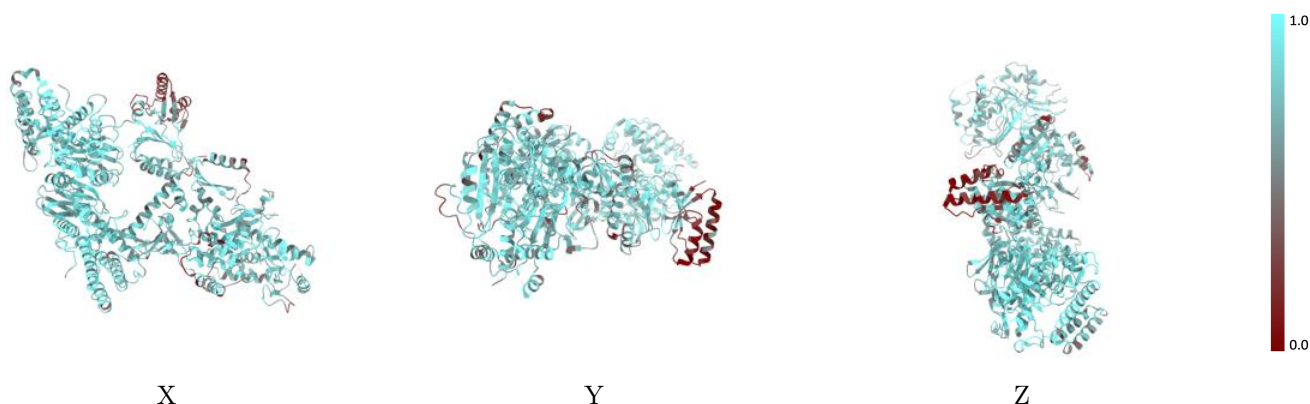
The images above show the 3D surface view of the map at the recommended contour level 9.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



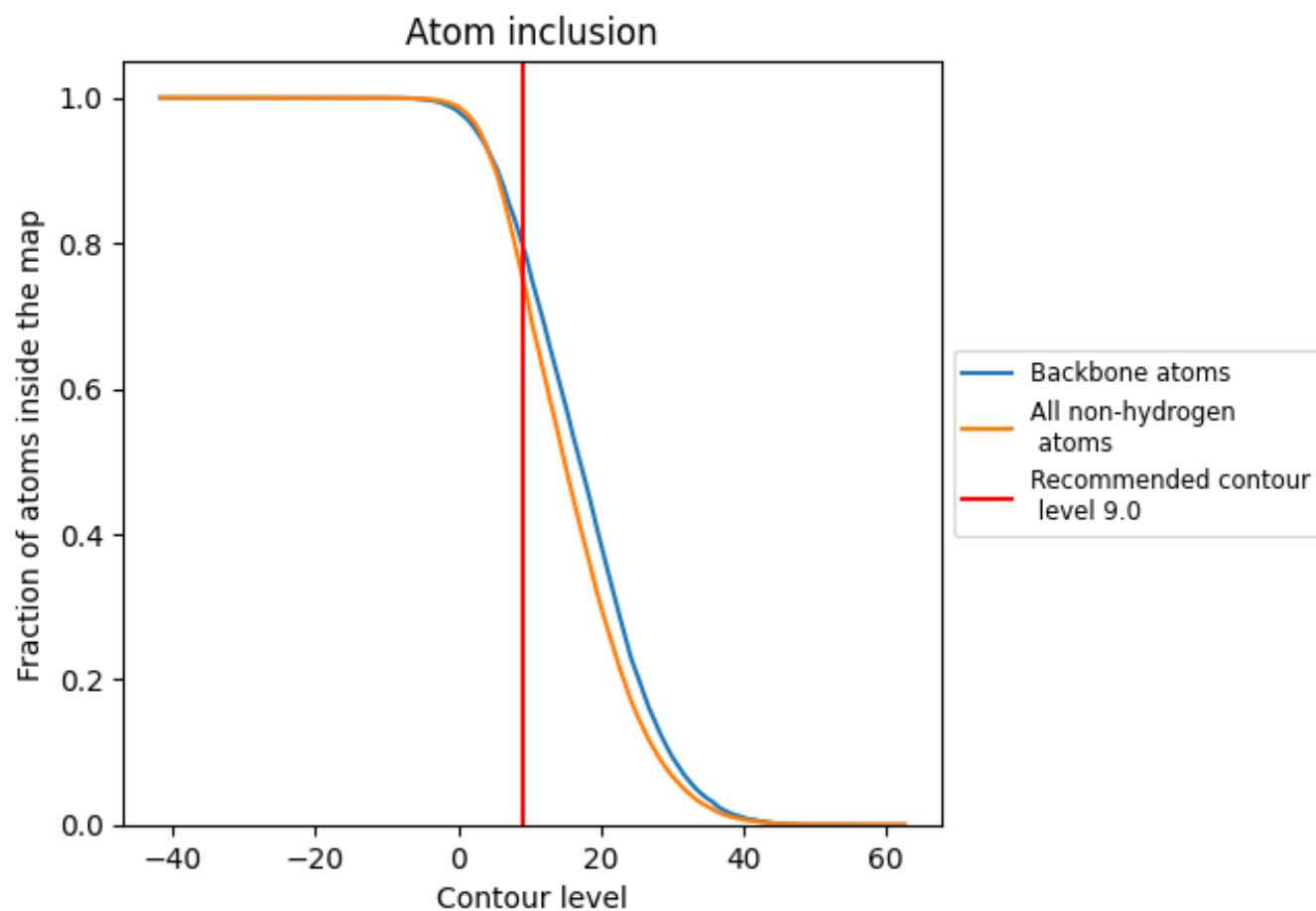
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (9.0).

9.4 Atom inclusion [i](#)



At the recommended contour level, 80% of all backbone atoms, 75% 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 (9.0) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.7545	<div></div> 0.5020
A	<div></div> 0.4000	<div></div> 0.4250
B	<div></div> 0.7026	<div></div> 0.5060
C	<div></div> 0.7366	<div></div> 0.4820
D	<div></div> 0.8224	<div></div> 0.5280
E	<div></div> 0.8282	<div></div> 0.5300

