



## Full wwPDB EM Validation Report ⓘ

Nov 6, 2022 – 06:31 AM EST

PDB ID : 6B7Y  
EMDB ID : EMD-7065  
Title : Cryo-EM structure of human insulin degrading enzyme  
Authors : Liang, W.G.; Zhang, Z.; Bailey, L.J.; Kossiakoff, A.A.; Tan, Y.Z.; Wei, H.; Carragher, B.; Potter, S.C.; Tang, W.J.  
Deposited on : 2017-10-05  
Resolution : 6.50 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.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

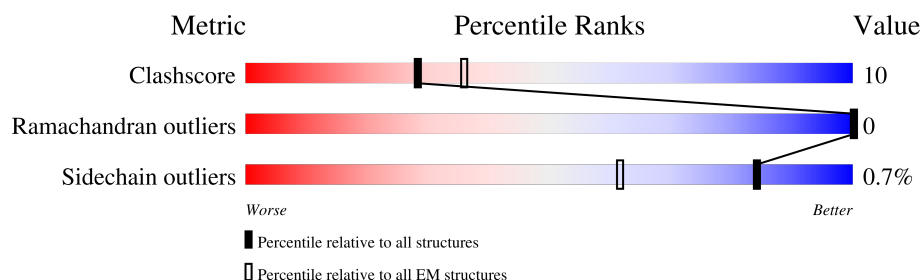
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 6.50 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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion  $< 40\%$ ). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	966	
1	B	966	

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 15410 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 Insulin-degrading enzyme.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	949	Total	C	N	O	S	0	0
			7748	4995	1302	1429	22		
1	B	939	Total	C	N	O	S	0	0
			7662	4942	1284	1415	21		

There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	110	LEU	CYS	conflict	UNP P14735
A	171	SER	CYS	conflict	UNP P14735
A	178	ALA	CYS	conflict	UNP P14735
A	257	VAL	CYS	conflict	UNP P14735
A	414	LEU	CYS	conflict	UNP P14735
A	573	ASN	CYS	conflict	UNP P14735
A	590	SER	CYS	conflict	UNP P14735
A	789	SER	CYS	conflict	UNP P14735
A	812	ALA	CYS	conflict	UNP P14735
A	819	ALA	CYS	conflict	UNP P14735
A	904	SER	CYS	conflict	UNP P14735
B	110	LEU	CYS	conflict	UNP P14735
B	171	SER	CYS	conflict	UNP P14735
B	178	ALA	CYS	conflict	UNP P14735
B	257	VAL	CYS	conflict	UNP P14735
B	414	LEU	CYS	conflict	UNP P14735
B	573	ASN	CYS	conflict	UNP P14735
B	590	SER	CYS	conflict	UNP P14735
B	789	SER	CYS	conflict	UNP P14735
B	812	ALA	CYS	conflict	UNP P14735
B	819	ALA	CYS	conflict	UNP P14735
B	904	SER	CYS	conflict	UNP P14735



R950	K953	H957	V958	L959	E962	MET	ASP	SER	CYS	PRO	VAL	GLY	GLU	PHE	PRO	CYS	GLN	ASN	ASP	ILE	ASN	LEU	SER	GLN	ALA	PRO	ALA	LEU	PRO	GLN	P989	K999	R1000	G1001	L1002	P1003	L1004	L1007	H1011								
K826	E827	I832	V833	F834	L846	I849	I850	Q851	P855	P856	H857	Y858	F866	M870	S873	Q883	I886	Q887	A888	R892	H893	L894	D895	K896	L900	E903	S904	A905	K906	F918	V925	A926	Y927	L931	E934	I937	Y940	M943	L944								
P878	E692	D706	V707	R711	L712	H724	I725	E726	A727	L728	G731	N732	Q743	E746	D747	T748	L749	L758	L759	V764	R765	Y766	W776	Q780	Q781	R782	N783	E784	N788	S789	G790	Y795	D798	S803	E804	L810	I815	T822	L823	R824	T825						
W560	F561	K562	Q563	D564	F568	K571	A572	N573	L574	N575	F576	E577	F578	F579	D586	F587	L588	H589	M592	Y596	L600	K601	L604	N605	A608	A611	L616	D619	L620	T623	T624	Y625	G626	M627	Y628	L629	S630	Q633	Y634	Q638	L642	M649					
E428	S435	I436	I437	V449	L450	E457	E458	P461	I464	L468	D469	R472	P473	E474	N475	V476	R477	V478	A479	I480	T489	I505	E508	V509	I510	Q514	F522	P525	F530	I537	L538	Y547	P548	A549	L550	I551	K552	D553	T554	S557	K558	L559					
P284	L285	H291	P292	F293	K299	Q300	L301	Y302	K303	Y314	V315	T316	F317	P318	L322	K327	P330	H340	L346	L350	Q363	K364	M371	F372	L253	M254	A255	L259	G260	L264	D265	D266	L267	T268	N269	L270	V271	V272	K273	L274	F275	S276	E277	V278	K281	N282	V283

## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	24425	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 ( $e^-/\text{\AA}^2$ )	7.9, 6.8	Depositor
Minimum defocus (nm)	940	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	46598	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k), GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.082	Depositor
Minimum map value	-0.132	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.014	Depositor
Map size ( $\text{\AA}$ )	343.36, 343.36, 343.36	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	1.073, 1.073, 1.073	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	A	0.39	0/7942	0.65	0/10744
1	B	0.39	0/7853	0.64	0/10620
All	All	0.39	0/15795	0.65	0/21364

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	A	7748	0	7686	165	0
1	B	7662	0	7581	163	0
All	All	15410	0	15267	321	0

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

All (321) 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:B:244:PHE:O	1:B:248:TYR:HB2	1.84	0.78
1:B:419:ALA:O	1:B:423:ARG:HB2	1.86	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:839:ARG:HG2	1:A:844:GLN:HA	1.71	0.71
1:B:245:HIS:HA	1:B:249:TYR:HB2	1.72	0.70
1:A:317:PHE:HB2	1:A:373:PHE:HB3	1.73	0.69
1:B:150:TYR:HB3	1:B:435:SER:HB3	1.73	0.69
1:A:437:ILE:O	1:A:441:LEU:HB2	1.91	0.69
1:B:314:TYR:HB2	1:B:479:ALA:HB3	1.74	0.69
1:A:897:PRO:HG2	1:A:903:GLU:HB3	1.75	0.69
1:B:782:ARG:HA	1:B:959:LEU:HB2	1.75	0.68
1:B:822:THR:O	1:B:826:LYS:HB3	1.93	0.68
1:A:1000:ARG:HH12	1:B:764:VAL:HA	1.59	0.68
1:B:317:PHE:HB2	1:B:373:PHE:HB3	1.76	0.67
1:B:623:THR:HB	1:B:626:GLY:H	1.60	0.67
1:B:834:PHE:HB3	1:B:849:ILE:HB	1.76	0.67
1:B:855:PRO:HB2	1:B:858:TYR:HB3	1.76	0.66
1:B:269:ASN:O	1:B:273:LYS:HB3	1.95	0.66
1:A:838:ARG:HH12	1:A:840:ALA:HB2	1.61	0.65
1:B:823:LEU:HD21	1:B:866:PHE:HB2	1.79	0.65
1:B:346:LEU:HD11	1:B:393:HIS:HB3	1.77	0.65
1:B:795:TYR:HB2	1:B:846:LEU:HB3	1.78	0.65
1:A:78:ILE:HB	1:A:259:LEU:HA	1.79	0.65
1:B:576:PHE:HB2	1:B:629:LEU:HB3	1.80	0.64
1:B:92:VAL:HG22	1:B:254:MET:HG3	1.80	0.63
1:A:782:ARG:HA	1:A:959:LEU:HB2	1.80	0.63
1:B:586:ASP:HB2	1:B:589:HIS:H	1.62	0.63
1:B:578:PHE:HB2	1:B:627:MET:HB2	1.79	0.63
1:A:382:GLU:O	1:A:386:HIS:ND1	2.30	0.63
1:A:103:ILE:HG23	1:A:226:LEU:HA	1.81	0.63
1:A:395:PHE:HE2	1:A:513:TRP:HB3	1.64	0.62
1:B:266:ASP:O	1:B:270:LEU:HB2	2.00	0.62
1:A:74:LYS:HB2	1:A:255:ALA:HA	1.81	0.62
1:B:788:ASN:HB2	1:B:851:GLN:HE21	1.65	0.62
1:B:125:ASN:O	1:B:129:GLN:N	2.32	0.61
1:A:1001:GLY:HA2	1:B:1007:LEU:H	1.65	0.61
1:B:409:TRP:O	1:B:413:GLU:HB2	2.01	0.61
1:A:415:LYS:HG3	1:A:456:LEU:HB2	1.82	0.61
1:B:363:GLN:NE2	1:B:371:MET:SD	2.74	0.60
1:A:109:PHE:HB2	1:A:226:LEU:HD11	1.81	0.60
1:B:293:PHE:HB2	1:B:318:PRO:HG3	1.84	0.60
1:A:93:HIS:HB3	1:A:253:LEU:HB3	1.84	0.60
1:A:621:GLN:O	1:A:628:TYR:N	2.32	0.60
1:B:260:GLY:HA3	1:B:267:LEU:HD21	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:300:GLN:HB3	1:A:502:GLN:HE22	1.67	0.60
1:A:678:PRO:HG3	1:A:783:ASN:HD22	1.67	0.60
1:B:248:TYR:HA	1:B:283:VAL:HG21	1.82	0.59
1:A:1006:PRO:HG3	1:B:1003:PRO:HG3	1.84	0.59
1:B:322:LEU:HD13	1:B:330:PRO:HD2	1.84	0.59
1:B:316:THR:HB	1:B:477:ARG:HB2	1.83	0.59
1:A:646:ILE:O	1:A:650:ALA:HB2	2.03	0.59
1:A:312:ASN:ND2	1:A:377:VAL:O	2.34	0.58
1:B:253:LEU:HD21	1:B:285:LEU:HG	1.84	0.58
1:B:571:LYS:HA	1:B:634:TYR:HA	1.85	0.58
1:B:579:PHE:HB3	1:B:724:HIS:HB3	1.84	0.58
1:A:759:LEU:H	1:A:762:GLN:HE21	1.51	0.58
1:A:538:LEU:O	1:A:563:GLN:NE2	2.36	0.58
1:A:942:GLU:HG3	1:A:950:ARG:HD3	1.86	0.58
1:B:538:LEU:H	1:B:732:ASN:HB3	1.68	0.58
1:A:190:HIS:HE1	1:A:495:TRP:HB3	1.68	0.57
1:A:200:ARG:HD3	1:A:498:THR:HB	1.86	0.57
1:A:790:GLY:N	1:A:958:VAL:O	2.35	0.57
1:B:894:LEU:HD11	1:B:925:VAL:HG11	1.85	0.57
1:A:92:VAL:HG22	1:A:254:MET:HG3	1.87	0.57
1:B:127:TYR:HA	1:B:164:ARG:HD3	1.86	0.57
1:A:575:ASN:HB2	1:A:728:LEU:HB3	1.86	0.57
1:A:489:THR:HA	1:A:501:LYS:HG2	1.86	0.57
1:A:108:HIS:HD2	1:A:186:VAL:HG13	1.69	0.57
1:B:69:LEU:HD21	1:B:272:VAL:HG22	1.87	0.57
1:A:87:SER:HA	1:A:152:ASP:HA	1.87	0.56
1:A:102:ASN:HD22	1:A:235:ILE:HD13	1.70	0.56
1:A:587:PRO:HG3	1:A:695:TRP:HB3	1.86	0.56
1:A:692:GLU:HB2	1:A:766:TYR:HB3	1.88	0.56
1:B:126:GLU:HG3	1:B:164:ARG:HE	1.69	0.56
1:B:327:LYS:HB3	1:B:458:GLU:H	1.70	0.56
1:A:364:LYS:HB2	1:A:374:ILE:HG12	1.88	0.56
1:B:389:ASP:O	1:B:393:HIS:ND1	2.35	0.56
1:B:575:ASN:HB2	1:B:728:LEU:HB3	1.88	0.55
1:A:873:SER:HA	1:A:876:ASP:HB2	1.88	0.55
1:B:63:GLU:HB2	1:B:79:SER:HB3	1.87	0.55
1:B:87:SER:HB2	1:B:259:LEU:HB3	1.88	0.55
1:B:823:LEU:O	1:B:827:GLU:HB2	2.05	0.55
1:B:402:ARG:HG3	1:B:468:LEU:HD21	1.89	0.55
1:B:692:GLU:HB3	1:B:766:TYR:HD1	1.72	0.55
1:A:402:ARG:HA	1:A:468:LEU:HD21	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:943:MET:HA	1:B:950:ARG:HB2	1.88	0.55
1:A:389:ASP:O	1:A:393:HIS:ND1	2.38	0.55
1:B:303:LYS:HE3	1:B:489:THR:HG22	1.87	0.55
1:B:62:ARG:NH1	1:B:428:GLU:OE2	2.40	0.55
1:A:764:VAL:HA	1:B:1000:ARG:HH12	1.72	0.55
1:A:948:ALA:HB3	1:A:951:ARG:HB2	1.89	0.55
1:B:552:LYS:HB3	1:B:559:LEU:HB3	1.89	0.55
1:A:781:GLN:O	1:A:959:LEU:N	2.29	0.54
1:B:91:ASP:HB3	1:B:255:ALA:HB3	1.89	0.54
1:B:575:ASN:HD22	1:B:728:LEU:HD23	1.73	0.54
1:B:69:LEU:HB2	1:B:73:ILE:HB	1.89	0.54
1:B:562:LYS:NZ	1:B:563:GLN:O	2.35	0.54
1:B:575:ASN:ND2	1:B:904:SER:OG	2.40	0.54
1:A:245:HIS:O	1:A:249:TYR:HB2	2.08	0.54
1:A:765:ARG:HB2	1:A:1007:LEU:HD21	1.88	0.54
1:B:776:TRP:CD1	1:B:953:LYS:HG2	2.43	0.54
1:B:299:LYS:NZ	1:B:474:GLU:O	2.39	0.53
1:B:187:ASP:HB2	1:B:223:LYS:HB2	1.89	0.53
1:A:91:ASP:O	1:A:255:ALA:N	2.38	0.53
1:A:572:ALA:HB3	1:A:638:GLN:HE22	1.73	0.53
1:A:595:LEU:HD22	1:A:662:ILE:HG22	1.91	0.53
1:B:382:GLU:O	1:B:386:HIS:ND1	2.31	0.53
1:A:638:GLN:O	1:A:642:LEU:HB3	2.08	0.53
1:A:677:GLN:OE1	1:A:786:HIS:NE2	2.42	0.53
1:A:999:LYS:HA	1:A:1002:LEU:HD12	1.91	0.52
1:B:322:LEU:HD22	1:B:330:PRO:HG2	1.91	0.52
1:A:538:LEU:HD22	1:A:539:PRO:HD2	1.91	0.52
1:B:134:HIS:HB3	1:B:154:SER:H	1.74	0.52
1:A:104:ALA:HB1	1:A:218:PHE:HB3	1.90	0.52
1:A:578:PHE:HD2	1:A:627:MET:HB2	1.75	0.52
1:A:808:LEU:HD12	1:A:839:ARG:HH21	1.75	0.52
1:A:344:GLY:HA3	1:A:523:LYS:H	1.75	0.52
1:B:264:LEU:O	1:B:268:THR:OG1	2.25	0.52
1:A:299:LYS:N	1:A:476:VAL:O	2.40	0.52
1:B:91:ASP:HA	1:B:148:ASN:HA	1.92	0.52
1:B:999:LYS:HA	1:B:1002:LEU:HD12	1.91	0.52
1:A:357:ASN:HB2	1:A:378:ASP:HB3	1.91	0.52
1:B:508:GLU:HG3	1:B:509:VAL:HG23	1.92	0.52
1:A:769:VAL:O	1:A:796:GLN:NE2	2.40	0.51
1:B:71:ASN:ND2	1:B:276:SER:O	2.43	0.51
1:B:780:GLN:HA	1:B:957:HIS:HB2	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:49:ARG:HB2	1:A:67:LEU:HD22	1.91	0.51
1:A:319:ILE:HG22	1:A:470:LYS:HG2	1.93	0.51
1:B:547:TYR:CG	1:B:918:PHE:HB3	2.46	0.51
1:A:297:HIS:HB3	1:A:477:ARG:HH11	1.76	0.51
1:A:638:GLN:O	1:A:642:LEU:CB	2.59	0.51
1:B:268:THR:O	1:B:272:VAL:HB	2.11	0.51
1:A:119:LYS:HE2	1:A:167:GLN:HE22	1.77	0.50
1:A:789:SER:N	1:A:852:SER:O	2.37	0.50
1:B:832:ILE:HB	1:B:851:GLN:HB3	1.92	0.50
1:B:269:ASN:O	1:B:273:LYS:CB	2.60	0.50
1:B:301:LEU:HA	1:B:478:VAL:HB	1.94	0.50
1:A:96:SER:HB2	1:A:219:GLY:HA2	1.94	0.50
1:A:673:PHE:HA	1:A:676:GLU:HG2	1.93	0.50
1:A:760:PRO:HA	1:A:763:LEU:HB3	1.93	0.50
1:A:190:HIS:CE1	1:A:495:TRP:HB3	2.47	0.49
1:A:686:LEU:HD11	1:A:838:ARG:HG2	1.93	0.49
1:B:400:LYS:HG3	1:B:522:PHE:HB2	1.93	0.49
1:A:824:ARG:HB2	1:A:833:VAL:HG21	1.92	0.49
1:B:73:ILE:HD11	1:B:278:VAL:HB	1.93	0.49
1:B:473:PRO:HG2	1:B:514:GLN:HA	1.94	0.49
1:B:299:LYS:N	1:B:476:VAL:O	2.43	0.49
1:A:131:LEU:O	1:A:136:GLY:N	2.41	0.49
1:A:722:ARG:HG3	1:A:756:LYS:HB2	1.95	0.49
1:B:131:LEU:O	1:B:136:GLY:N	2.45	0.49
1:A:823:LEU:O	1:A:828:GLN:N	2.46	0.49
1:B:592:MET:HB3	1:B:712:LEU:HD13	1.95	0.49
1:B:601:LYS:HD2	1:B:620:LEU:HB2	1.95	0.49
1:B:619:ASP:HB3	1:B:630:SER:HB3	1.93	0.49
1:A:388:GLU:HG2	1:A:509:VAL:HG11	1.94	0.49
1:B:449:VAL:HG23	1:B:450:LEU:HG	1.95	0.49
1:B:810:LEU:HD23	1:B:931:LEU:HD22	1.95	0.49
1:B:943:MET:HG2	1:B:950:ARG:HD2	1.95	0.49
1:A:571:LYS:HA	1:A:634:TYR:HA	1.94	0.48
1:B:469:ASP:HA	1:B:472:ARG:HE	1.77	0.48
1:A:646:ILE:O	1:A:650:ALA:CB	2.61	0.48
1:A:832:ILE:HB	1:A:851:GLN:H	1.78	0.48
1:B:400:LYS:HE3	1:B:522:PHE:HB2	1.95	0.48
1:A:244:PHE:O	1:A:248:TYR:HB2	2.13	0.48
1:B:623:THR:HG22	1:B:625:TYR:H	1.79	0.48
1:A:404:GLU:OE1	1:A:407:GLN:NE2	2.46	0.48
1:A:940:TYR:HA	1:A:944:LEU:HD12	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:834:PHE:N	1:B:849:ILE:O	2.41	0.48
1:A:73:ILE:HA	1:A:254:MET:HB2	1.96	0.48
1:B:63:GLU:N	1:B:79:SER:O	2.36	0.48
1:B:461:PRO:HA	1:B:464:ILE:HD12	1.95	0.48
1:B:934:GLU:HA	1:B:937:ILE:HD12	1.95	0.48
1:A:1007:LEU:H	1:B:1001:GLY:HA2	1.78	0.48
1:B:315:VAL:HB	1:B:375:ILE:HB	1.94	0.47
1:B:505:ILE:HB	1:B:510:ILE:HD11	1.96	0.47
1:A:342:GLY:H	1:A:345:SER:HB2	1.77	0.47
1:A:829:LEU:O	1:A:852:SER:OG	2.27	0.47
1:A:210:ASN:HB3	1:A:213:HIS:HB2	1.95	0.47
1:A:639:PRO:HG3	1:A:741:ILE:HD11	1.95	0.47
1:B:573:ASN:HB2	1:B:900:LEU:HD22	1.96	0.47
1:A:317:PHE:HD1	1:A:475:ASN:HB3	1.80	0.47
1:B:798:ASP:HB3	1:B:804:GLU:HG3	1.97	0.47
1:B:596:TYR:O	1:B:600:LEU:HB2	2.14	0.47
1:A:103:ILE:HG21	1:A:106:LEU:HD13	1.96	0.47
1:A:395:PHE:HD1	1:A:398:ILE:HD12	1.80	0.47
1:B:91:ASP:O	1:B:255:ALA:N	2.42	0.47
1:B:706:ASP:O	1:B:711:ARG:NE	2.47	0.47
1:A:552:LYS:HB3	1:A:559:LEU:HB3	1.96	0.47
1:B:746:GLU:HA	1:B:749:LEU:HD12	1.97	0.47
1:B:76:LEU:HD23	1:B:437:ILE:HD13	1.96	0.47
1:A:224:TYR:HA	1:A:228:THR:HB	1.97	0.46
1:B:103:ILE:HG12	1:B:230:PRO:HG3	1.97	0.46
1:B:271:VAL:O	1:B:275:PHE:HB2	2.15	0.46
1:B:795:TYR:O	1:B:846:LEU:N	2.48	0.46
1:A:119:LYS:N	1:A:171:SER:OG	2.42	0.46
1:A:210:ASN:N	1:A:292:PRO:O	2.49	0.46
1:A:572:ALA:HA	1:A:731:GLY:HA3	1.97	0.46
1:B:419:ALA:O	1:B:423:ARG:CB	2.60	0.46
1:A:65:ARG:HB3	1:A:77:LEU:HB2	1.96	0.46
1:A:855:PRO:HB2	1:A:858:TYR:HB3	1.97	0.46
1:B:552:LYS:O	1:B:559:LEU:N	2.46	0.46
1:A:87:SER:O	1:A:259:LEU:N	2.49	0.46
1:A:139:ASN:HB3	1:A:150:TYR:CZ	2.50	0.46
1:A:291:HIS:HD2	1:A:293:PHE:HB2	1.81	0.46
1:A:251:SER:HB2	1:A:282:ASN:H	1.81	0.46
1:A:575:ASN:HD22	1:A:728:LEU:HD23	1.80	0.46
1:B:87:SER:HA	1:B:152:ASP:HA	1.97	0.46
1:B:743:GLN:O	1:B:747:ASP:HB2	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:803:SER:HA	1:B:927:TYR:CE2	2.51	0.46
1:A:69:LEU:HB2	1:A:73:ILE:HB	1.96	0.46
1:A:81:PRO:HA	1:A:261:ARG:HB2	1.97	0.45
1:B:115:PHE:HE1	1:B:149:TYR:HE1	1.65	0.45
1:B:131:LEU:HD22	1:B:136:GLY:HA3	1.97	0.45
1:A:673:PHE:HZ	1:A:681:HIS:HA	1.81	0.45
1:A:788:ASN:HB2	1:A:851:GLN:HE21	1.80	0.45
1:B:855:PRO:HA	1:B:856:PRO:HD3	1.84	0.45
1:A:322:LEU:HB2	1:A:325:TYR:HB2	1.97	0.45
1:B:205:GLU:OE1	1:B:364:LYS:NZ	2.49	0.45
1:A:1004:LEU:HD12	1:B:1004:LEU:HB2	1.99	0.45
1:B:623:THR:N	1:B:626:GLY:O	2.43	0.45
1:B:251:SER:HB3	1:B:281:LYS:HB2	1.99	0.45
1:B:558:LYS:HD3	1:B:560:TRP:HE1	1.82	0.45
1:B:225:THR:HA	1:B:229:ARG:HD3	1.98	0.45
1:A:350:LEU:HD13	1:A:356:VAL:HG21	1.98	0.45
1:A:359:LEU:HA	1:A:377:VAL:HA	1.98	0.45
1:A:915:GLN:HE22	1:A:1008:VAL:HG11	1.82	0.45
1:B:588:LEU:HD21	1:B:707:VAL:HG22	1.98	0.45
1:B:409:TRP:O	1:B:413:GLU:CB	2.65	0.45
1:B:616:LEU:HG	1:B:633:GLY:HA3	1.99	0.45
1:A:554:THR:HB	1:A:557:SER:H	1.82	0.45
1:B:154:SER:HB3	1:B:157:HIS:CE1	2.51	0.45
1:A:422:PHE:HE2	1:A:451:THR:HG22	1.82	0.44
1:A:601:LYS:HD2	1:A:620:LEU:HB2	1.98	0.44
1:B:815:ILE:HA	1:B:870:MET:HE2	1.99	0.44
1:A:112:HIS:ND1	1:A:182:GLU:OE2	2.50	0.44
1:B:558:LYS:O	1:B:727:ALA:N	2.50	0.44
1:B:870:MET:HA	1:B:873:SER:HB3	1.98	0.44
1:B:604:LEU:O	1:B:608:ALA:N	2.50	0.44
1:A:621:GLN:HB3	1:A:628:TYR:HB3	2.00	0.44
1:A:780:GLN:HA	1:A:957:HIS:HB2	1.99	0.44
1:B:548:PRO:HA	1:B:562:LYS:HB2	1.99	0.44
1:B:564:ASP:HB2	1:B:731:GLY:HA2	1.98	0.44
1:A:87:SER:HB3	1:A:259:LEU:HB3	1.99	0.44
1:A:726:GLU:OE2	1:A:916:TYR:OH	2.35	0.44
1:A:183:VAL:HG22	1:A:223:LYS:HA	1.99	0.43
1:B:178:ALA:O	1:B:182:GLU:HB2	2.18	0.43
1:B:790:GLY:N	1:B:958:VAL:O	2.35	0.43
1:A:301:LEU:HA	1:A:478:VAL:HB	2.00	0.43
1:A:131:LEU:HB3	1:A:136:GLY:HA3	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:194:VAL:HA	1:A:496:TYR:HD1	1.83	0.43
1:A:556:MET:HB2	1:A:757:PRO:HG3	1.99	0.43
1:A:777:PHE:HB3	1:A:992:ILE:HD11	2.00	0.43
1:A:864:GLU:OE2	1:A:953:LYS:NZ	2.51	0.43
1:A:90:LEU:O	1:A:149:TYR:N	2.42	0.43
1:A:110:LEU:HD21	1:A:241:LEU:HD22	1.99	0.43
1:A:575:ASN:OD1	1:A:628:TYR:OH	2.36	0.43
1:A:63:GLU:HB2	1:A:79:SER:HB3	2.00	0.43
1:A:604:LEU:HD22	1:A:648:LYS:HG2	2.00	0.43
1:A:810:LEU:HD23	1:A:931:LEU:HD22	2.01	0.43
1:A:818:PRO:O	1:A:822:THR:OG1	2.24	0.43
1:A:769:VAL:HA	1:A:1004:LEU:HD23	2.00	0.43
1:B:109:PHE:HZ	1:B:179:LYS:HG3	1.84	0.43
1:B:888:ALA:O	1:B:892:ARG:HB2	2.19	0.43
1:A:671:ASN:HB3	1:A:701:LYS:HD2	2.01	0.42
1:B:301:LEU:HD21	1:B:480:ILE:HD12	2.00	0.42
1:B:327:LYS:HG2	1:B:457:GLU:HB2	2.00	0.42
1:A:227:GLU:HG2	1:A:237:VAL:HG21	2.00	0.42
1:A:803:SER:HA	1:A:927:TYR:CE2	2.54	0.42
1:A:942:GLU:HA	1:A:949:PRO:HD2	2.01	0.42
1:B:364:LYS:HB3	1:B:372:PHE:HB2	2.01	0.42
1:A:110:LEU:HA	1:A:110:LEU:HD23	1.86	0.42
1:A:699:GLU:HG3	1:B:759:LEU:HD21	2.00	0.42
1:A:214:PRO:HB2	1:A:288:PHE:CE1	2.53	0.42
1:A:91:ASP:HA	1:A:148:ASN:HA	2.02	0.42
1:A:152:ASP:N	1:A:152:ASP:OD1	2.53	0.42
1:A:402:ARG:NH2	1:A:472:ARG:HH12	2.18	0.42
1:B:554:THR:OG1	1:B:557:SER:N	2.44	0.42
1:A:350:LEU:HD23	1:A:350:LEU:HA	1.91	0.42
1:B:202:PHE:O	1:B:206:LYS:HG2	2.20	0.42
1:B:110:LEU:HD13	1:B:244:PHE:HD2	1.85	0.42
1:B:883:GLN:HA	1:B:886:ILE:HG12	2.02	0.42
1:A:74:LYS:O	1:A:256:VAL:N	2.43	0.41
1:B:110:LEU:O	1:B:114:LEU:N	2.51	0.41
1:B:210:ASN:N	1:B:292:PRO:O	2.47	0.41
1:A:135:ALA:HB3	1:A:154:SER:HA	2.02	0.41
1:A:776:TRP:CD1	1:A:953:LYS:HG2	2.55	0.41
1:B:100:PRO:HA	1:B:101:PRO:HD3	1.93	0.41
1:A:125:ASN:O	1:A:129:GLN:N	2.36	0.41
1:B:291:HIS:HA	1:B:292:PRO:HD3	1.83	0.41
1:B:724:HIS:HB2	1:B:758:LEU:HD12	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:783:ASN:OD1	1:B:784:GLU:N	2.53	0.41
1:A:564:ASP:OD1	1:A:564:ASP:N	2.53	0.41
1:B:93:HIS:HB3	1:B:253:LEU:HB3	2.01	0.41
1:B:578:PHE:HE1	1:B:725:ILE:HG23	1.86	0.41
1:B:537:ILE:HD12	1:B:568:PHE:HB3	2.02	0.41
1:B:574:LEU:HB3	1:B:576:PHE:CE2	2.56	0.41
1:B:605:ASN:HA	1:B:608:ALA:HB3	2.03	0.41
1:A:93:HIS:CE1	1:A:145:GLU:HB3	2.55	0.41
1:A:210:ASN:ND2	1:A:294:GLN:OE1	2.53	0.41
1:A:666:TYR:HA	1:A:669:SER:HB3	2.01	0.41
1:B:903:GLU:HA	1:B:906:LYS:HE3	2.02	0.41
1:A:577:GLU:HB2	1:A:908:TRP:HH2	1.85	0.41
1:B:586:ASP:H	1:B:589:HIS:HB2	1.85	0.41
1:A:57:SER:O	1:A:59:GLU:N	2.54	0.41
1:A:767:ARG:HD3	1:A:1004:LEU:HB3	2.02	0.41
1:A:870:MET:HA	1:A:873:SER:HB3	2.03	0.41
1:A:936:ILE:HD12	1:A:936:ILE:HA	1.93	0.41
1:B:1004:LEU:HD23	1:B:1004:LEU:HA	1.96	0.41
1:A:355:TRP:HD1	1:A:382:GLU:HG3	1.86	0.41
1:A:670:LEU:HD23	1:A:670:LEU:HA	1.85	0.41
1:A:313:LEU:HD13	1:A:480:ILE:HG12	2.02	0.40
1:A:689:LEU:HD11	1:A:779:TYR:HE1	1.86	0.40
1:B:340:HIS:CD2	1:B:525:PRO:HG3	2.57	0.40
1:B:940:TYR:HA	1:B:944:LEU:HD12	2.02	0.40
1:A:300:GLN:OE1	1:A:502:GLN:NE2	2.55	0.40
1:A:584:TYR:HH	1:A:693:VAL:H	1.66	0.40
1:B:350:LEU:HD23	1:B:350:LEU:HA	1.94	0.40
1:B:638:GLN:O	1:B:642:LEU:CB	2.69	0.40
1:B:550:LEU:HD11	1:B:553:ASP:HB2	2.03	0.40
1:B:678:PRO:HG3	1:B:783:ASN:ND2	2.37	0.40
1:B:530:PHE:HE2	1:B:611:ALA:HA	1.86	0.40
1:A:440:ILE:H	1:A:440:ILE:HG13	1.80	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	945/966 (98%)	906 (96%)	39 (4%)	0	100	100
1	B	933/966 (97%)	902 (97%)	31 (3%)	0	100	100
All	All	1878/1932 (97%)	1808 (96%)	70 (4%)	0	100	100

There are no Ramachandran outliers to report.

### 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	840/861 (98%)	833 (99%)	7 (1%)	81	89
1	B	828/861 (96%)	824 (100%)	4 (0%)	88	93
All	All	1668/1722 (97%)	1657 (99%)	11 (1%)	84	90

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	49	ARG
1	A	229	ARG
1	A	527	LYS
1	A	649	MET
1	A	732	ASN
1	A	824	ARG
1	A	896	LYS
1	B	56	LYS
1	B	649	MET
1	B	824	ARG
1	B	896	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:



Mol	Chain	Res	Type
1	A	167	GLN
1	A	190	HIS
1	A	232	GLN
1	A	291	HIS
1	A	300	GLN
1	A	502	GLN
1	A	575	ASN
1	A	638	GLN
1	A	681	HIS
1	A	762	GLN
1	A	844	GLN
1	B	844	GLN
1	B	957	HIS

### 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.

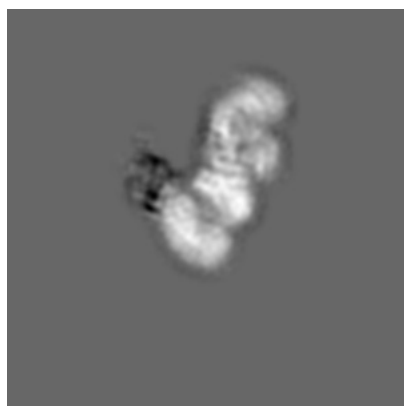
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-7065. These allow visual inspection of the internal detail of the map and identification of artifacts.

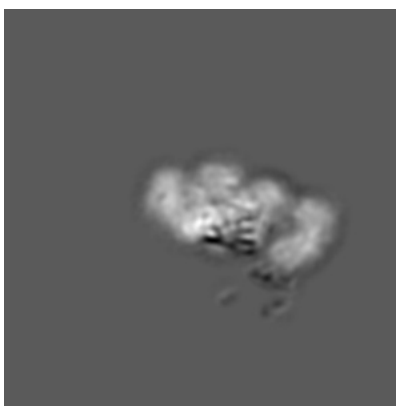
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

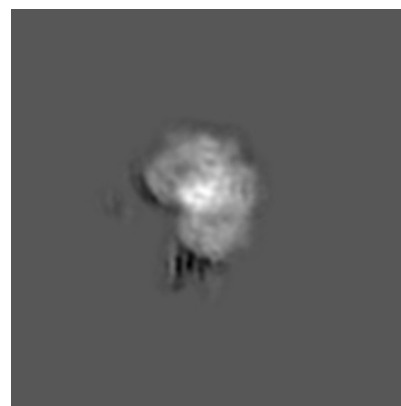
#### 6.1.1 Primary map



X

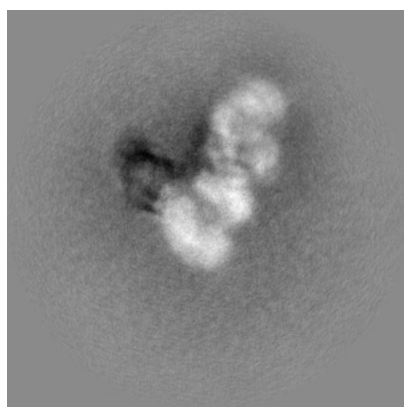


Y

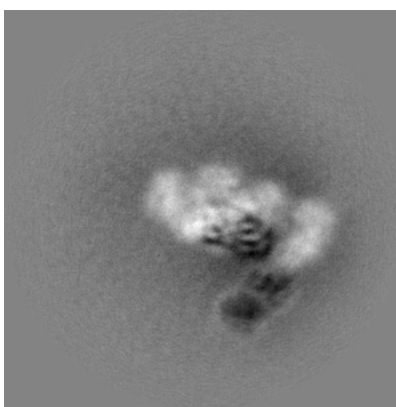


Z

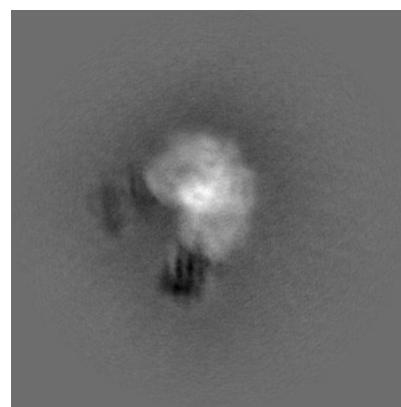
#### 6.1.2 Raw map



X



Y



Z

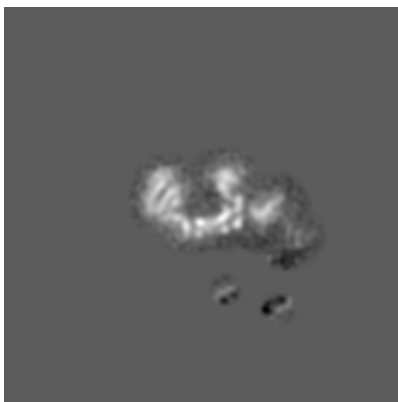
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

### 6.2.1 Primary map



X Index: 160

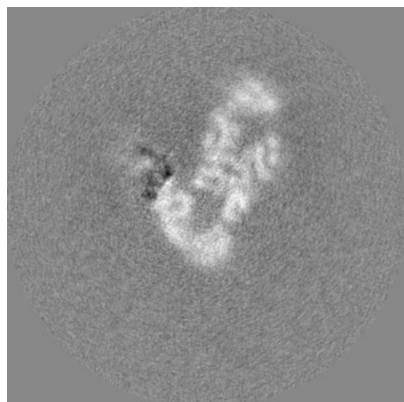


Y Index: 160

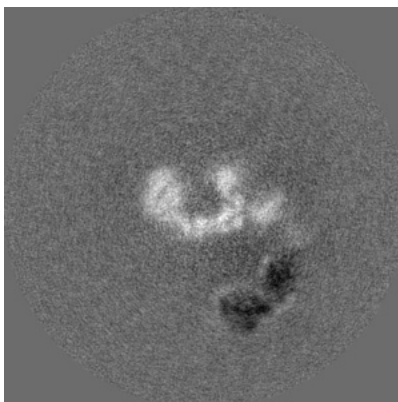


Z Index: 160

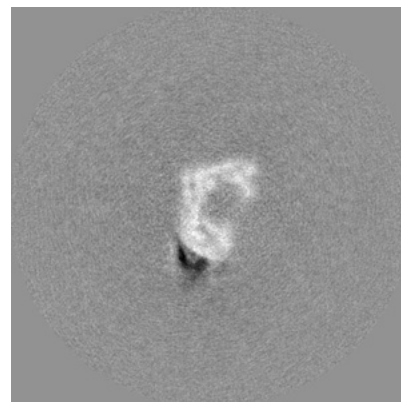
### 6.2.2 Raw map



X Index: 160



Y Index: 160



Z Index: 160

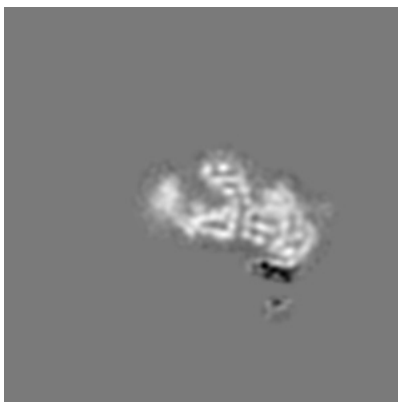
The images above show central slices of the map in three orthogonal directions.

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

### 6.3.1 Primary map



X Index: 151

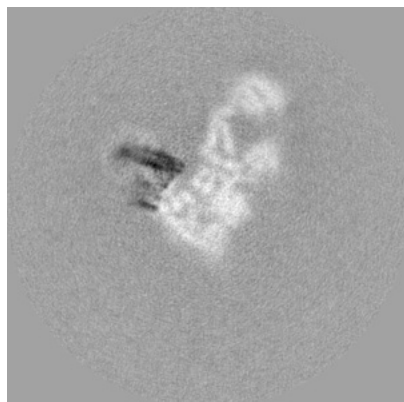


Y Index: 173

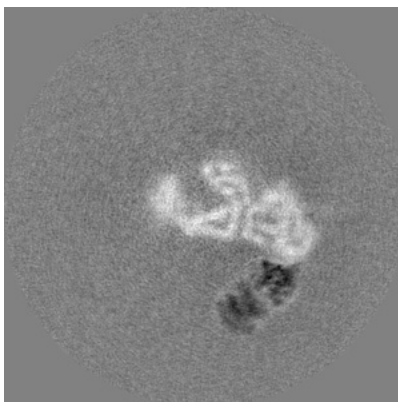


Z Index: 160

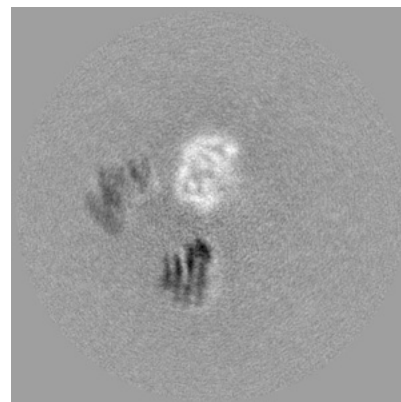
### 6.3.2 Raw map



X Index: 151



Y Index: 171

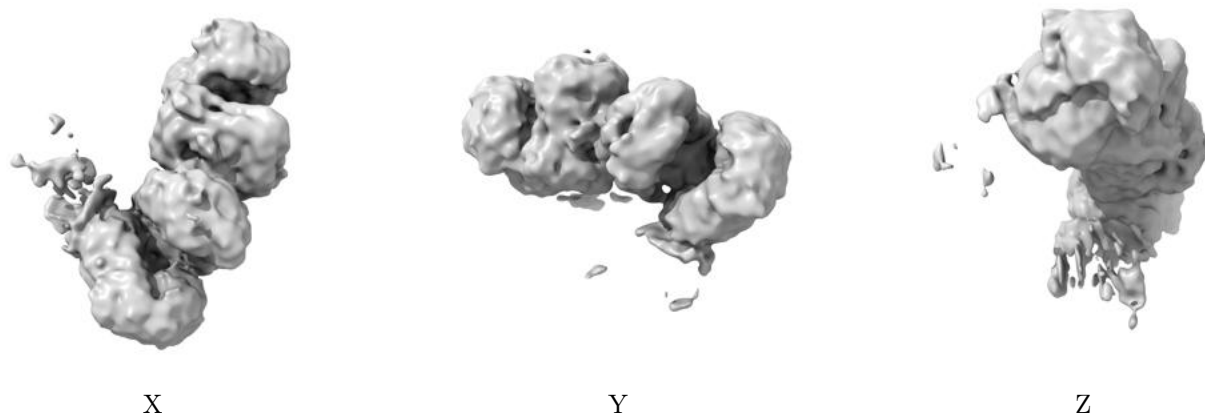


Z Index: 199

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

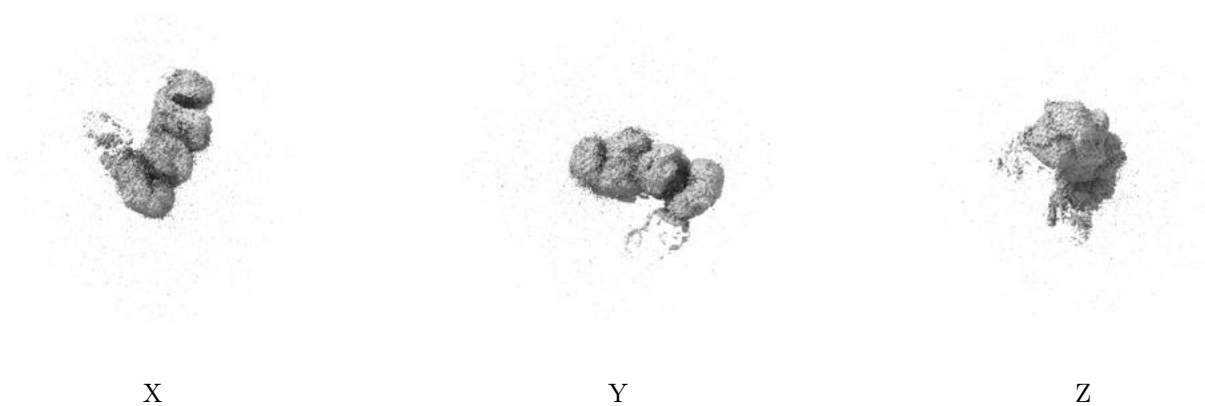
## 6.4 Orthogonal surface views [i](#)

### 6.4.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.014. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.4.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

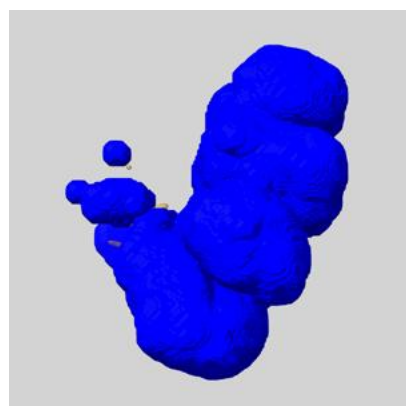
## 6.5 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

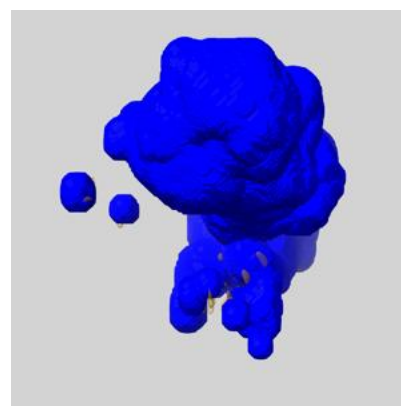
### 6.5.1 emd\_7065\_msk\_1.map [i](#)



X



Y

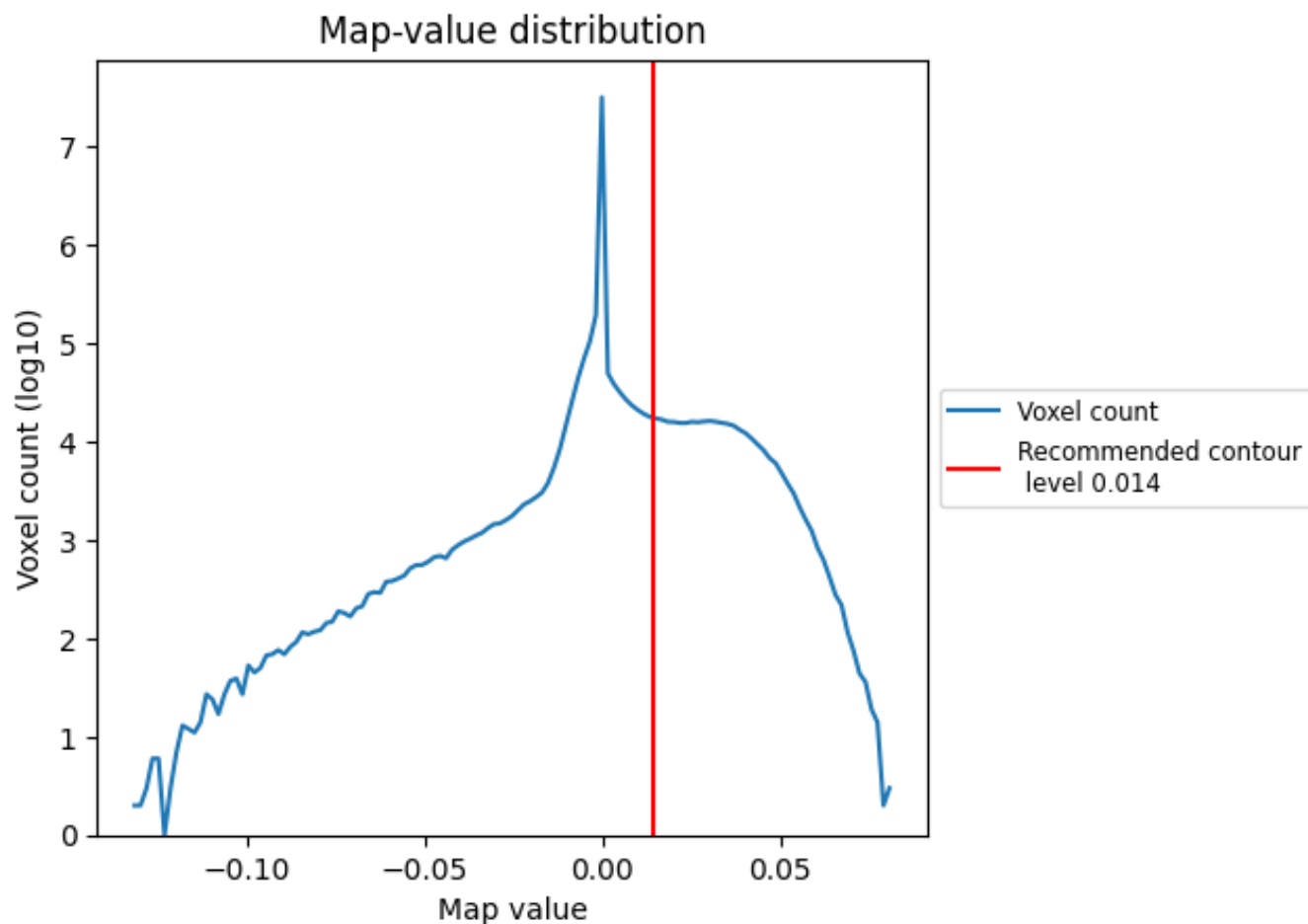


Z

## 7 Map analysis [i](#)

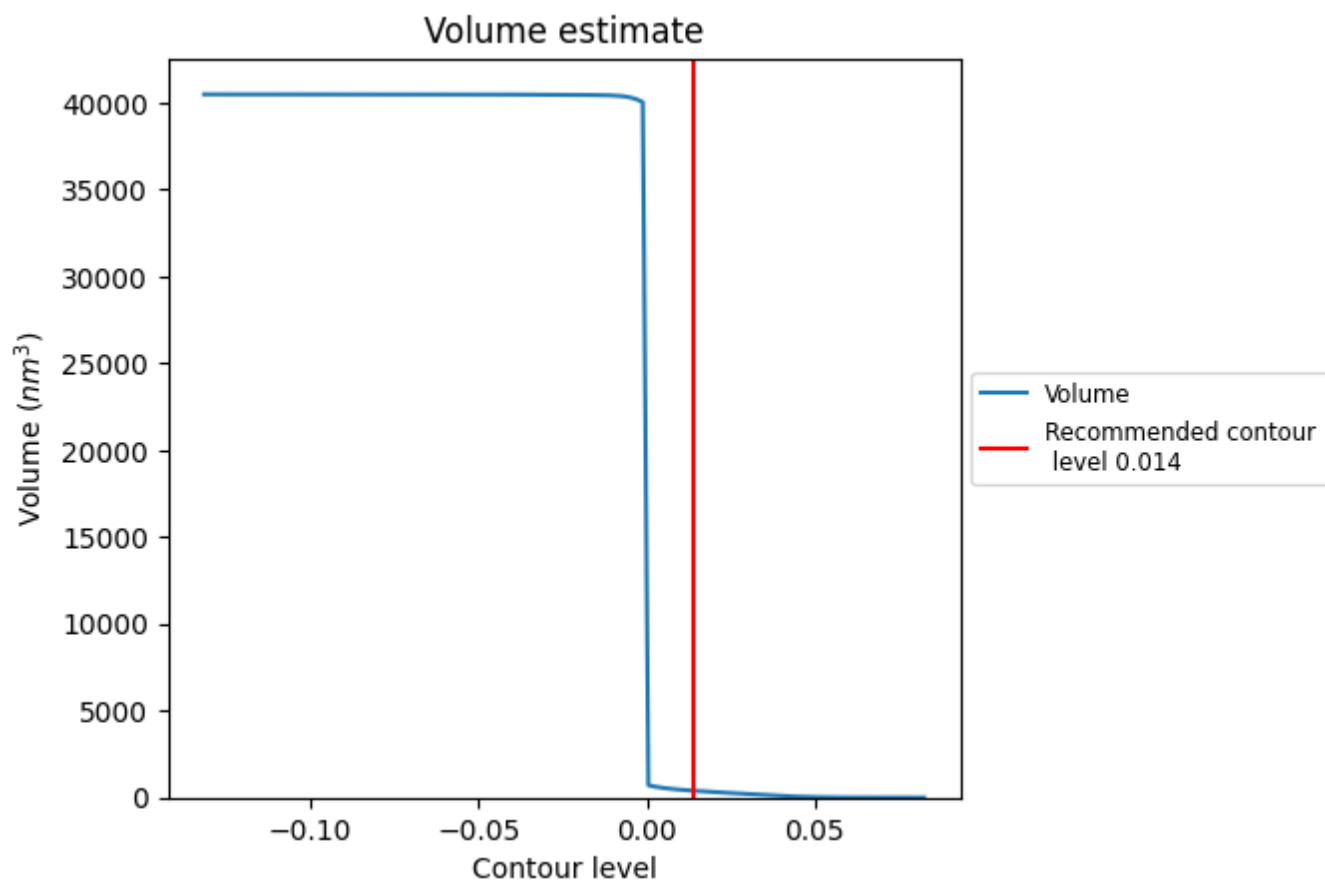
This section contains the results of statistical analysis of the map.

### 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](#)

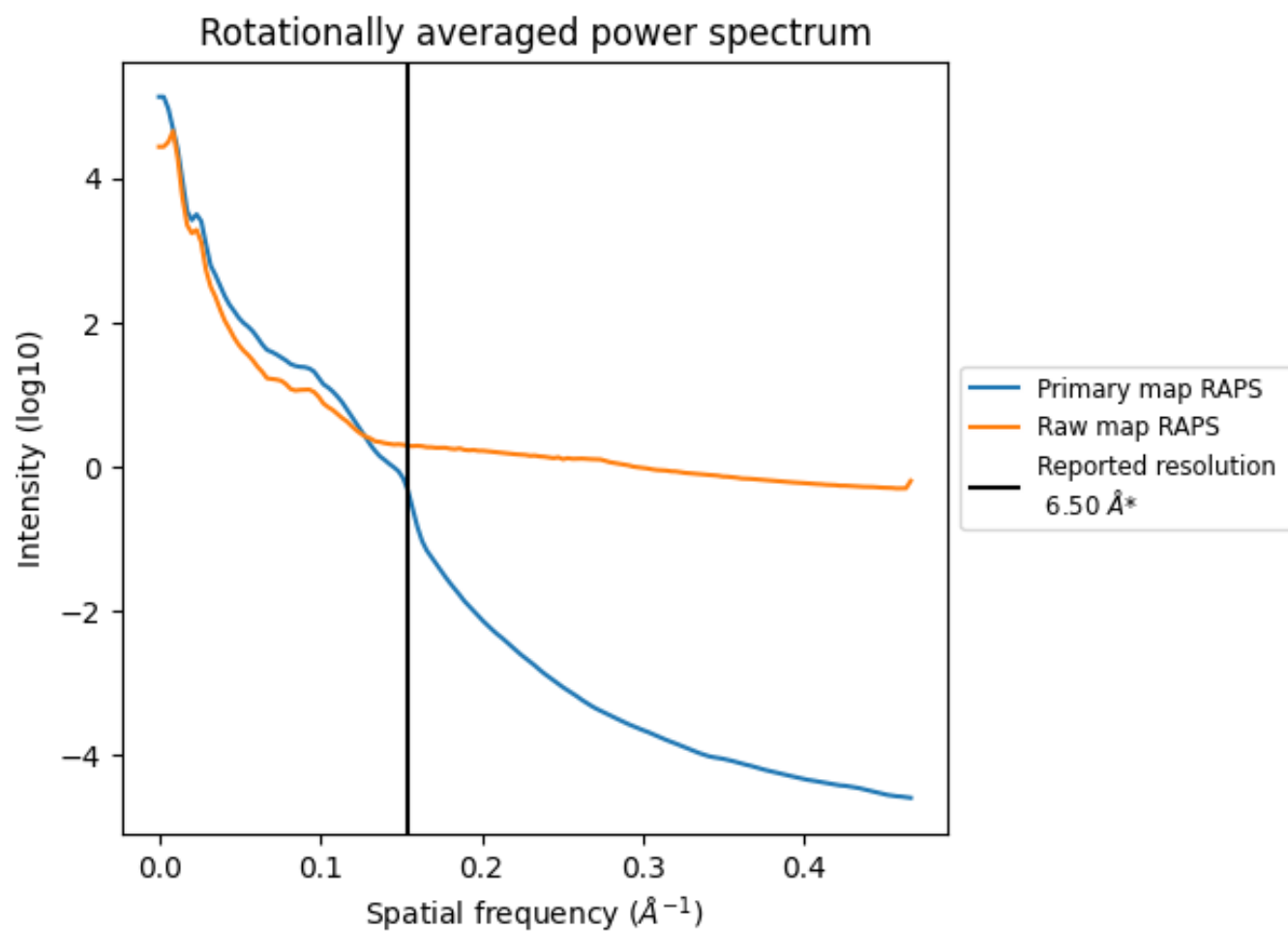


The volume at the recommended contour level is 393 nm<sup>3</sup>; this corresponds to an approximate mass of 355 kDa.

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 ⓘ

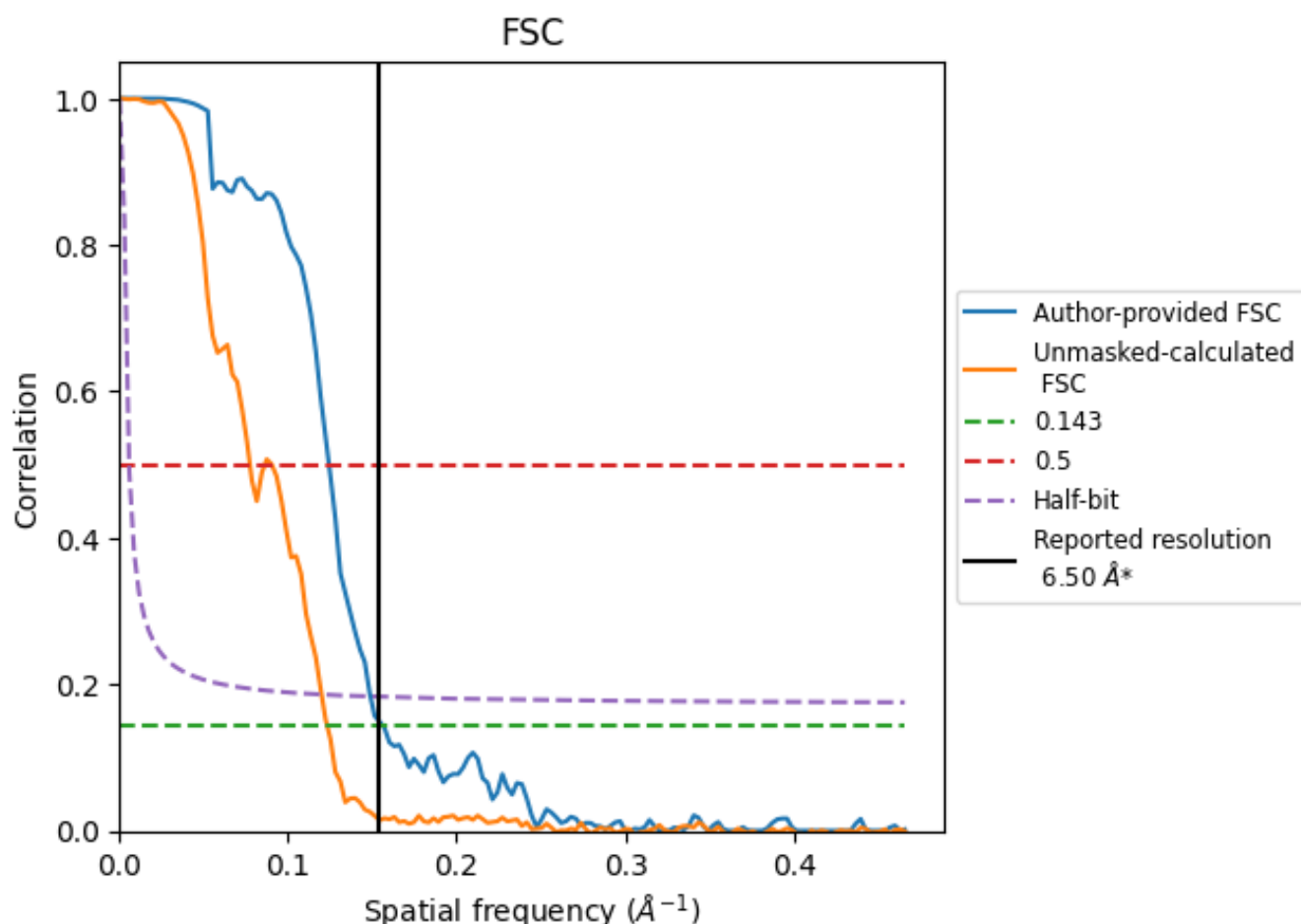


\*Reported resolution corresponds to spatial frequency of 0.154  $\text{\AA}^{-1}$

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

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

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of 0.154 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

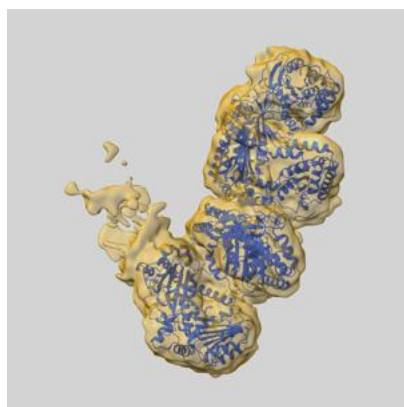
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	6.50	-	-
Author-provided FSC curve	6.40	8.04	6.71
Unmasked-calculated*	8.11	12.92	8.34

\*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 8.11 differs from the reported value 6.5 by more than 10 %

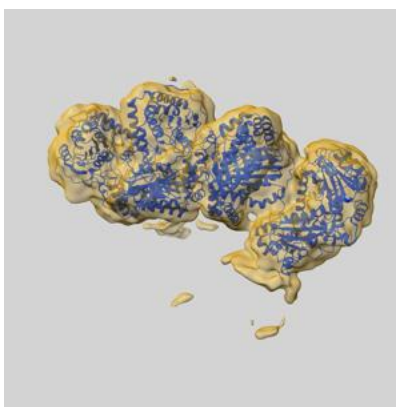
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-7065 and PDB model 6B7Y. Per-residue inclusion information can be found in [section 3](#) on [page 4](#).

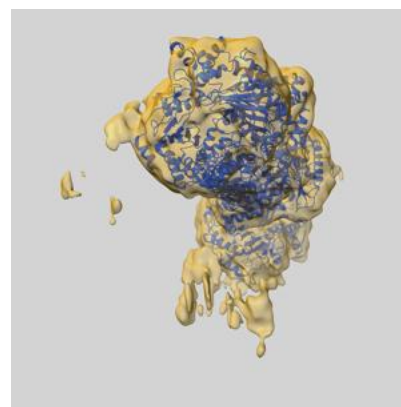
### 9.1 Map-model overlay [i](#)



X



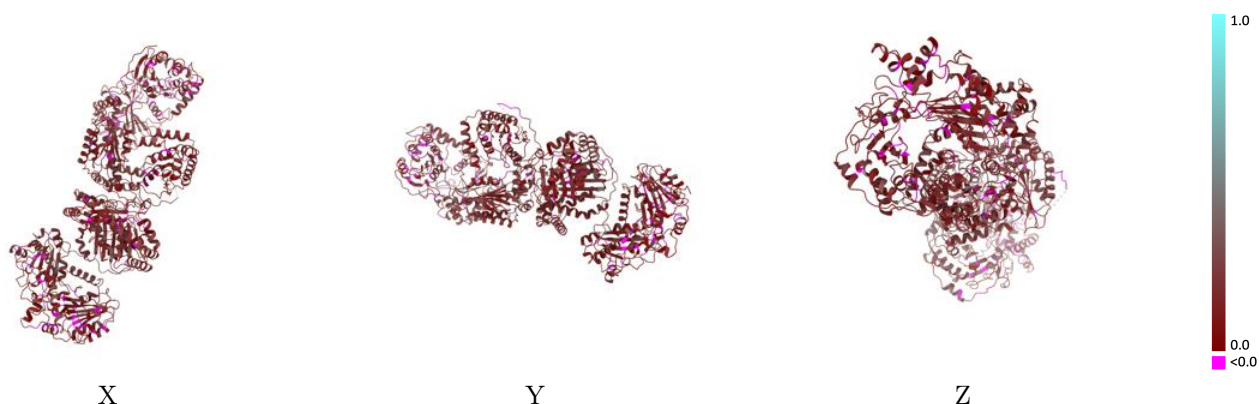
Y



Z

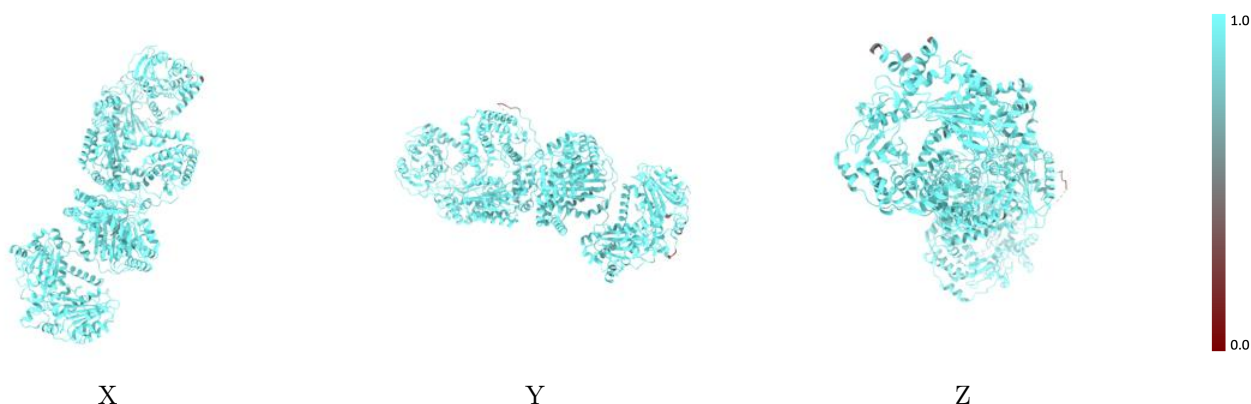
The images above show the 3D surface view of the map at the recommended contour level 0.014 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



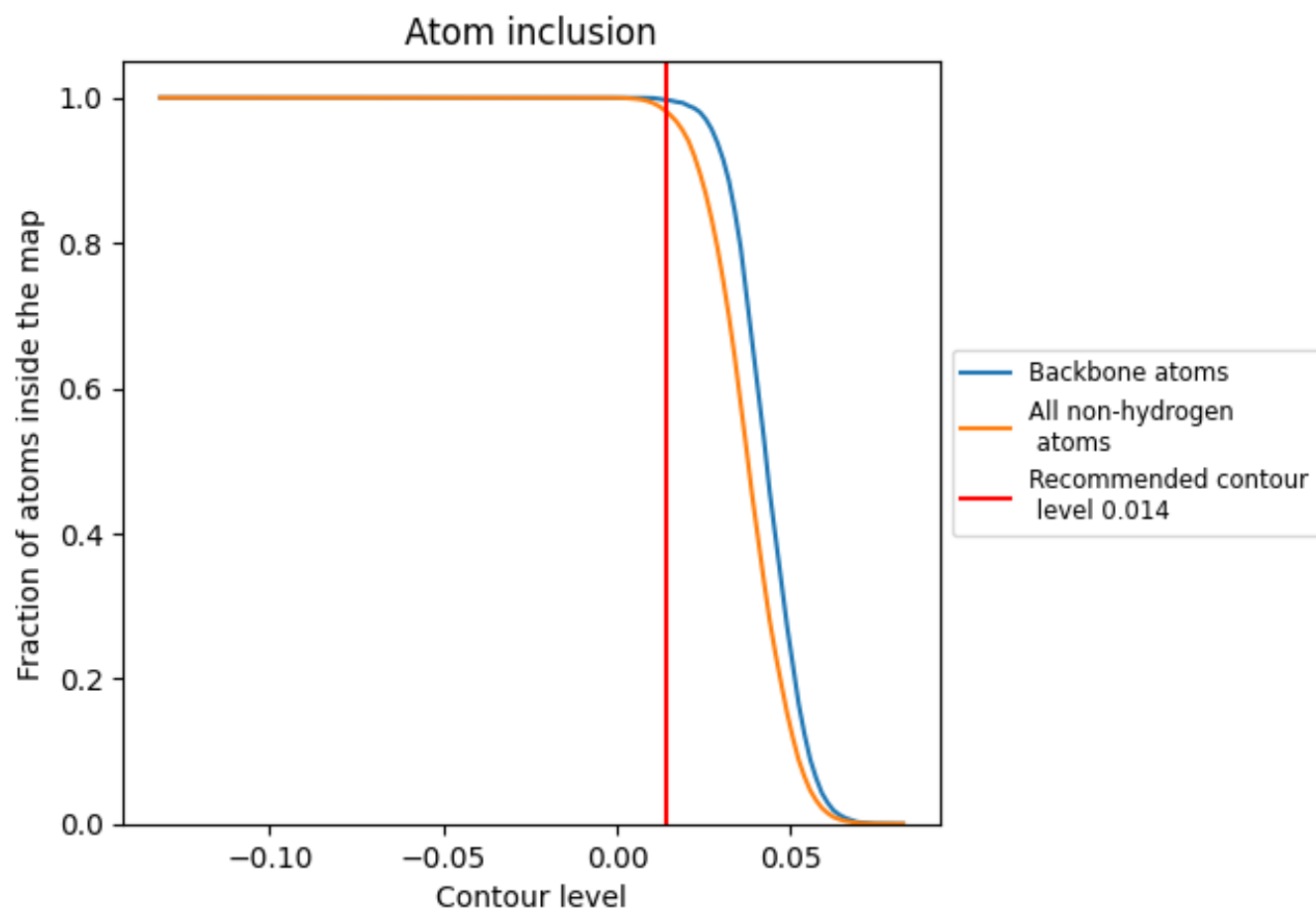
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.014).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 100% of all backbone atoms, 98% 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 (0.014) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.9816	<div></div> 0.1570
A	<div></div> 0.9911	<div></div> 0.1590
B	<div></div> 0.9721	<div></div> 0.1560

