



Full wwPDB EM Validation Report ⓘ

Mar 10, 2026 – 03:12 AM UTC

PDB ID : 8IOB / pdb_00008iob
EMDB ID : EMD-35614
Title : Herg1a-herg1b closed state 1
Authors : Zhang, M.F.
Deposited on : 2023-03-10
Resolution : 3.90 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.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

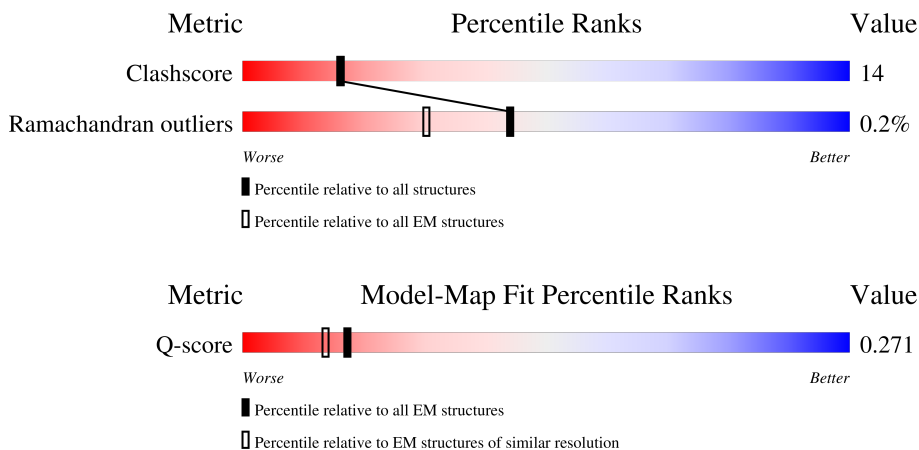
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.90 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Q-score	-	25397	8855 (3.40 - 4.40)

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	1159	35% 25% 12% 63%
1	B	1159	35% 25% 13% 63%
1	C	1159	35% 25% 12% 63%
1	D	1159	35% 25% 12% 63%

2 Entry composition

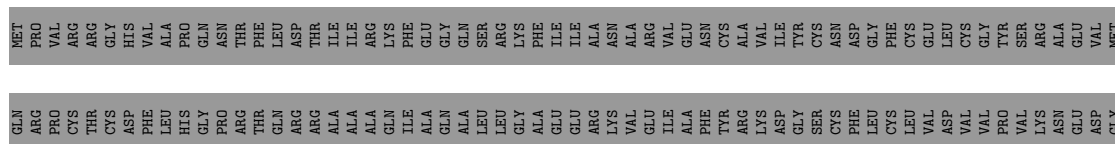
There is only 1 type of molecule in this entry. The entry contains 13736 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Potassium voltage-gated channel subfamily H member 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	431	Total	C	N	O	S	0	0
			3434	2252	581	584	17		
1	B	431	Total	C	N	O	S	0	0
			3434	2252	581	584	17		
1	C	431	Total	C	N	O	S	0	0
			3434	2252	581	584	17		
1	D	431	Total	C	N	O	S	0	0
			3434	2252	581	584	17		







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- Molecule 1: Potassium voltage-gated channel subfamily H member 2

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

ARG	HIS	ALA	SER	THR	GLY	ALA	MET	HIS	PRO	LEU	ARG	SER	GLY	LEU	LEU	ASN	SER	THR	SER	ASP	ASP	ASP	LEU	VAL	ARG	TYR	ARG	THR	ILE	SER	SER	LYS	ILE	PRO	PRO	GLN	ILE	THR	LEU	ASN	PHE	VAL	ASP	LEU	LYS	GLY	ASP	PRO	PHE	LEU	LEU	SER	PRO	ALA	THR	THR	SER	ASP	ARG	GLU	ILE	ILE	ALA
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PRO	LYS	GLU	ARG	THR	HIS	ASN	VAL	GLU	LYS	VAL	GLN	VAL	LEU	SER	LEU	GLY	ALA	ASP	VAL	LEU	PRO	GLU	TYR	LYS	LEU	GLN	ALA	PRO	ARG	ILE	HIS	ARG	W398
LYS	GLU	ARG	THR	HIS	ASN	VAL	GLU	LYS	VAL	GLN	VAL	LEU	SER	LEU	GLY	ALA	ASP	VAL	LEU	PRO	GLU	TYR	LYS	LEU	GLN	ALA	PRO	ARG	ILE	HIS	ARG	T399	
GLU	ARG	THR	HIS	ASN	VAL	GLU	LYS	VAL	GLN	VAL	LEU	SER	LEU	GLY	ALA	ASP	VAL	LEU	PRO	GLU	TYR	LYS	LEU	GLN	ALA	PRO	ARG	ILE	HIS	ARG	T400		
ARG	THR	HIS	ASN	VAL	GLU	LYS	VAL	GLN	VAL	LEU	SER	LEU	GLY	ALA	ASP	VAL	LEU	PRO	GLU	TYR	LYS	LEU	GLN	ALA	PRO	ARG	ILE	HIS	ARG	T401			
THR	HIS	ASN	VAL	GLU	LYS	VAL	GLN	VAL	LEU	SER	LEU	GLY	ALA	ASP	VAL	LEU	PRO	GLU	TYR	LYS	LEU	GLN	ALA	PRO	ARG	ILE	HIS	ARG	T402				
HIS	ASN	VAL	GLU	LYS	VAL	GLN	VAL	LEU	SER	LEU	GLY	ALA	ASP	VAL	LEU	PRO	GLU	TYR	LYS	LEU	GLN	ALA	PRO	ARG	ILE	HIS	ARG	T403					
ASN	VAL	GLU	LYS	VAL	GLN	VAL	LEU	SER	LEU	GLY	ALA	ASP	VAL	LEU	PRO	GLU	TYR	LYS	LEU	GLN	ALA	PRO	ARG	ILE	HIS	ARG	T404						
VAL	GLU	LYS	VAL	GLN	VAL	LEU	SER	LEU	GLY	ALA	ASP	VAL	LEU	PRO	GLU	TYR	LYS	LEU	GLN	ALA	PRO	ARG	ILE	HIS	ARG	T405							
GLU	LYS	VAL	GLN	VAL	LEU	SER	LEU	GLY	ALA	ASP	VAL	LEU	PRO	GLU	TYR	LYS	LEU	GLN	ALA	PRO	ARG	ILE	HIS	ARG	T406								
LYS	VAL	GLN	VAL	LEU	SER	LEU	GLY	ALA	ASP	VAL	LEU	PRO	GLU	TYR	LYS	LEU	GLN	ALA	PRO	ARG	ILE	HIS	ARG	T407									
VAL	GLN	VAL	LEU	SER	LEU	GLY	ALA	ASP	VAL	LEU	PRO	GLU	TYR	LYS	LEU	GLN	ALA	PRO	ARG	ILE	HIS	ARG	T408										
GLN	VAL	LEU	SER	LEU	GLY	ALA	ASP	VAL	LEU	PRO	GLU	TYR	LYS	LEU	GLN	ALA	PRO	ARG	ILE	HIS	ARG	T409											
VAL	LEU	SER	LEU	GLY	ALA	ASP	VAL	LEU	PRO	GLU	TYR	LYS	LEU	GLN	ALA	PRO	ARG	ILE	HIS	ARG	T410												
LEU	SER	LEU	GLY	ALA	ASP	VAL	LEU	PRO	GLU	TYR	LYS	LEU	GLN	ALA	PRO	ARG	ILE	HIS	ARG	T411													
SER	LEU	GLY	ALA	ASP	VAL	LEU	PRO	GLU	TYR	LYS	LEU	GLN	ALA	PRO	ARG	ILE	HIS	ARG	T412														
LEU	GLY	ALA	ASP	VAL	LEU	PRO	GLU	TYR	LYS	LEU	GLN	ALA	PRO	ARG	ILE	HIS	ARG	T413															
ALA	ASP	VAL	LEU	PRO	GLU	TYR	LYS	LEU	GLN	ALA	PRO	ARG	ILE	HIS	ARG	T414																	
ASP	VAL	LEU	PRO	GLU	TYR	LYS	LEU	GLN	ALA	PRO	ARG	ILE	HIS	ARG	T415																		
VAL	LEU	PRO	GLU	TYR	LYS	LEU	GLN	ALA	PRO	ARG	ILE	HIS	ARG	T416																			
LEU	PRO	GLU	TYR	LYS	LEU	GLN	ALA	PRO	ARG	ILE	HIS	ARG	T417																				
PRO	GLU	TYR	LYS	LEU	GLN	ALA	PRO	ARG	ILE	HIS	ARG	T418																					
GLU	TYR	LYS	LEU	GLN	ALA	PRO	ARG	ILE	HIS	ARG	T419																						
TYR	LYS	LEU	GLN	ALA	PRO	ARG	ILE	HIS	ARG	T420																							

T421	T422	T423	T424	T425	P426	T427	S428	A429	A430	F431	L432	LEU	LYS	GLU	THR	GLU	GLY	PRO	PRO	ALA	THR	GLU	CYS	GLY	TYR	ALA	C449	Q450	P451	L452	A453	V454	V455	D456	L457	I458	V459	D460	I461	M462	F463	I464	V465	D466	L467	L468	L469	M470	F471	R472	T473	T474	V475	V476	M477	A478	N479	F480
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E481	V482	S483	S484	H485	P486	G487	R488	I489	A490	V491	H492	Y493	F494	K495	G496	W497	F498	L499	I500	D501	M502	V503	A504	A505	I506	P507	F508	D509	L510	LEU	ILE	PHE	GLY	SER	GLY	SER	GLU	GLU	L520	I521	G522	L523	L524	K525	T526	A527	R528	L529	L530	R531	L532	V533	R534	V535	A536	R537	K538	L539	D540
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L666	Y667	S668	G669	T670	A671	R672	Y673	H674	T675	Q676	M677	L678	R679	V680	R681	E682	F683	L684	R685	F686	H687	Q688	T689	P690	N691	P692	L693	R694	Q695	R696	L697	E698	E699	Y700	F701	Q702	Q703	H704	A705	W706	S707	T708	N709	G710	I711	D712	M713	N714	A715	Y716	L717	K718	G719	F720	P721	E722	C723	L724	U725
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A726	D727	I728	L729	L730	H731	L732	N733	R734	S735	L736	L737	Q738	H739	C740	C741	P742	F743	R744	G745	A746	T747	K748	G749	C750	L751	R752	A753	L754	A755	H756	K757	F758	K759	T760	T761	H762	A763	P764	P765	G766	D767	T768	L769	V770	H771	A772	G773	D774	L775	L776	T777	A778	L779	V780	F781	L782	S783	R784	G785
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[illegible]

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	35000	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	1500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.494	Depositor
Minimum map value	-0.291	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.011	Depositor
Recommended contour level	0.22	Depositor
Map size ($\text{\AA}$)	339.59998, 339.59998, 339.59998	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.8489999, 0.8489999, 0.8489999	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	0.15	0/3524	0.43	0/4788
1	B	0.16	0/3524	0.45	0/4788
1	C	0.16	0/3524	0.46	0/4788
1	D	0.15	0/3524	0.42	0/4788
All	All	0.16	0/14096	0.44	0/19152

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 [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	3434	0	3453	106	0
1	B	3434	0	3453	105	0
1	C	3434	0	3453	105	0
1	D	3434	0	3453	98	0
All	All	13736	0	13812	395	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 14.

All (395) 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:757:LYS:HE3	1:A:841:VAL:HG11	1.60	0.84
1:C:819:ASN:HB2	1:C:862:LEU:HB3	1.65	0.79
1:C:489:ILE:HA	1:C:492:HIS:CE1	2.18	0.78
1:B:489:ILE:HA	1:B:492:HIS:CE1	2.18	0.78
1:B:632:PRO:O	1:C:629:ASN:ND2	2.17	0.78
1:C:632:PRO:O	1:D:629:ASN:ND2	2.19	0.75
1:A:819:ASN:HB2	1:A:862:LEU:HB3	1.68	0.75
1:D:819:ASN:HB2	1:D:862:LEU:HB3	1.67	0.74
1:A:632:PRO:O	1:B:629:ASN:ND2	2.21	0.74
1:A:629:ASN:ND2	1:D:632:PRO:O	2.21	0.73
1:D:762:HIS:HE2	1:D:827:TYR:HH	1.35	0.73
1:C:676:GLN:HG3	1:C:679:ARG:HH22	1.54	0.72
1:B:504:ALA:HA	1:B:527:ALA:HB1	1.73	0.71
1:C:504:ALA:HA	1:C:527:ALA:HB1	1.72	0.71
1:D:670:THR:O	1:D:674:HIS:ND1	2.23	0.71
1:D:504:ALA:HA	1:D:527:ALA:HB1	1.72	0.71
1:A:679:ARG:HG3	1:D:711:ILE:HD13	1.73	0.70
1:B:676:GLN:HG3	1:B:679:ARG:HH22	1.54	0.70
1:B:684:ILE:HA	1:B:689:ILE:HG13	1.74	0.69
1:C:711:ILE:HD13	1:D:679:ARG:HG3	1.73	0.69
1:B:788:GLU:HG3	1:B:825:LEU:HD22	1.75	0.69
1:C:670:THR:O	1:C:674:HIS:ND1	2.23	0.69
1:C:788:GLU:HG3	1:C:825:LEU:HD22	1.75	0.69
1:B:670:THR:O	1:B:674:HIS:ND1	2.23	0.68
1:C:684:ILE:HA	1:C:689:ILE:HG13	1.75	0.68
1:A:788:GLU:HG3	1:A:825:LEU:HD22	1.74	0.68
1:A:670:THR:O	1:A:674:HIS:ND1	2.23	0.67
1:B:735:SER:OG	1:B:802:ASN:OD1	2.13	0.67
1:D:788:GLU:HG3	1:D:825:LEU:HD22	1.76	0.67
1:A:735:SER:OG	1:A:802:ASN:OD1	2.13	0.67
1:C:735:SER:OG	1:C:802:ASN:OD1	2.13	0.67
1:D:684:ILE:HA	1:D:689:ILE:HG13	1.76	0.67
1:C:486:PRO:HA	1:C:489:ILE:HD12	1.76	0.66
1:D:411:ASP:HA	1:D:414:ILE:HD12	1.77	0.66
1:B:486:PRO:HA	1:B:489:ILE:HD12	1.76	0.66
1:A:834:HIS:ND1	1:A:836:ASP:OD1	2.28	0.66
1:A:684:ILE:HA	1:A:689:ILE:HG13	1.77	0.66
1:C:754:LEU:HB3	1:C:758:PHE:CZ	2.30	0.66
1:A:772:ALA:HB2	1:A:820:GLY:HA2	1.78	0.65
1:D:497:TRP:HB3	1:D:534:ARG:HH12	1.61	0.65
1:B:672:ARG:O	1:B:675:THR:OG1	2.12	0.65
1:B:411:ASP:HA	1:B:414:ILE:HD12	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:504:ALA:HA	1:A:527:ALA:HB1	1.78	0.64
1:A:423:VAL:HG23	1:A:424:PHE:HD1	1.63	0.64
1:B:819:ASN:HB2	1:B:862:LEU:HB3	1.79	0.64
1:D:735:SER:OG	1:D:802:ASN:OD1	2.14	0.64
1:C:592:GLN:NE2	1:C:629:ASN:O	2.30	0.63
1:B:718:LYS:HE3	1:B:718:LYS:HA	1.81	0.63
1:D:747:THR:OG1	1:D:750:CYS:SG	2.57	0.63
1:A:833:ILE:HB	1:A:838:LEU:HD21	1.79	0.63
1:D:486:PRO:HA	1:D:489:ILE:HD12	1.81	0.63
1:D:718:LYS:HE3	1:D:718:LYS:HA	1.81	0.63
1:D:762:HIS:NE2	1:D:827:TYR:OH	2.24	0.63
1:B:754:LEU:HB3	1:B:758:PHE:CZ	2.34	0.63
1:A:676:GLN:HG2	1:A:679:ARG:HH21	1.63	0.63
1:B:572:GLY:HA3	1:B:585:TRP:HE1	1.62	0.62
1:A:728:ILE:HA	1:A:731:HIS:HD2	1.64	0.62
1:A:676:GLN:HA	1:A:679:ARG:HE	1.65	0.62
1:C:772:ALA:HB2	1:C:820:GLY:HA2	1.80	0.62
1:B:423:VAL:HG23	1:B:424:PHE:HD1	1.64	0.62
1:C:672:ARG:O	1:C:675:THR:OG1	2.12	0.62
1:C:754:LEU:HA	1:C:757:LYS:HG2	1.80	0.62
1:D:728:ILE:HA	1:D:731:HIS:HD2	1.65	0.61
1:D:772:ALA:HB2	1:D:820:GLY:HA2	1.82	0.61
1:A:708:THR:HG22	1:A:713:MET:HE1	1.83	0.60
1:A:718:LYS:HE3	1:A:718:LYS:HA	1.82	0.60
1:C:728:ILE:HA	1:C:731:HIS:HD2	1.65	0.60
1:B:772:ALA:HB2	1:B:820:GLY:HA2	1.83	0.60
1:B:410:TRP:NE1	1:B:466:ASP:OD1	2.35	0.60
1:B:592:GLN:NE2	1:B:629:ASN:O	2.30	0.60
1:C:718:LYS:HE3	1:C:718:LYS:HA	1.82	0.60
1:D:410:TRP:NE1	1:D:466:ASP:OD1	2.33	0.60
1:A:486:PRO:HA	1:A:489:ILE:HD12	1.84	0.59
1:A:833:ILE:HD12	1:A:838:LEU:HG	1.84	0.58
1:B:728:ILE:HA	1:B:731:HIS:HD2	1.66	0.58
1:A:592:GLN:NE2	1:A:629:ASN:O	2.31	0.58
1:C:642:ILE:HA	1:C:645:MET:HE3	1.84	0.58
1:A:475:TYR:HD1	1:A:489:ILE:HG12	1.69	0.58
1:C:489:ILE:HA	1:C:492:HIS:HE1	1.68	0.58
1:B:781:PHE:HB2	1:B:831:HIS:HB3	1.87	0.57
1:D:708:THR:HG22	1:D:713:MET:HE1	1.85	0.57
1:C:757:LYS:HD3	1:C:837:ASP:OD2	2.05	0.57
1:B:782:ILE:HG21	1:B:800:GLY:HA2	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:687:HIS:O	1:B:689:ILE:N	2.38	0.57
1:C:411:ASP:HA	1:C:414:ILE:HD12	1.87	0.57
1:C:633:ASN:O	1:C:638:LYS:NZ	2.33	0.57
1:A:687:HIS:O	1:A:689:ILE:N	2.38	0.57
1:B:711:ILE:HD13	1:C:679:ARG:HG2	1.87	0.56
1:C:789:ILE:HB	1:C:796:VAL:HG23	1.87	0.56
1:C:672:ARG:HG2	1:C:676:GLN:HE22	1.71	0.56
1:B:489:ILE:HA	1:B:492:HIS:HE1	1.67	0.56
1:B:708:THR:HG22	1:B:713:MET:HE1	1.87	0.56
1:D:687:HIS:O	1:D:689:ILE:N	2.38	0.56
1:B:497:TRP:HB3	1:B:534:ARG:HH12	1.70	0.56
1:A:557:PHE:CD2	1:A:651:MET:HE2	2.41	0.55
1:B:672:ARG:HG2	1:B:676:GLN:HE22	1.71	0.55
1:C:687:HIS:O	1:C:689:ILE:N	2.38	0.55
1:B:488:ARG:HA	1:B:491:VAL:HG22	1.88	0.55
1:C:497:TRP:HB3	1:C:534:ARG:HH12	1.72	0.55
1:A:711:ILE:HD13	1:B:679:ARG:HG2	1.88	0.55
1:B:703:HIS:O	1:B:706:SER:OG	2.22	0.55
1:A:789:ILE:HB	1:A:796:VAL:HG23	1.87	0.55
1:B:789:ILE:HB	1:B:796:VAL:HG23	1.88	0.55
1:A:411:ASP:HA	1:A:414:ILE:HD12	1.87	0.54
1:C:557:PHE:CD2	1:C:651:MET:HE2	2.41	0.54
1:D:633:ASN:O	1:D:638:LYS:NZ	2.34	0.54
1:D:557:PHE:CD2	1:D:651:MET:HE2	2.42	0.54
1:D:789:ILE:HB	1:D:796:VAL:HG23	1.90	0.54
1:A:418:VAL:HG22	1:A:531:ARG:HD2	1.88	0.54
1:B:833:ILE:HD12	1:B:838:LEU:HD22	1.89	0.54
1:C:488:ARG:HA	1:C:491:VAL:HG22	1.89	0.54
1:D:592:GLN:NE2	1:D:629:ASN:O	2.32	0.54
1:A:455:VAL:O	1:A:459:VAL:HG23	2.08	0.54
1:D:475:TYR:HD1	1:D:489:ILE:HG12	1.71	0.54
1:C:812:TYR:O	1:C:814:ARG:HG2	2.06	0.54
1:D:493:TYR:OH	1:D:534:ARG:NH2	2.41	0.53
1:D:639:ILE:HA	1:D:642:ILE:HD12	1.89	0.53
1:A:754:LEU:HB3	1:A:758:PHE:CE1	2.44	0.53
1:D:617:PHE:HB2	1:D:630:VAL:HG11	1.91	0.53
1:C:734:ARG:O	1:C:738:GLN:NE2	2.41	0.53
1:A:812:TYR:O	1:A:814:ARG:HG2	2.09	0.53
1:B:845:TYR:CE2	1:B:848:PHE:HB3	2.43	0.53
1:A:703:HIS:ND1	1:A:764:PRO:HB3	2.24	0.52
1:C:776:LEU:HB2	1:C:815:PRO:HA	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:693:LEU:HG	1:D:731:HIS:NE2	2.24	0.52
1:D:812:TYR:O	1:D:814:ARG:HG2	2.09	0.52
1:A:782:ILE:HD13	1:A:800:GLY:HA2	1.91	0.52
1:D:676:GLN:HG2	1:D:679:ARG:HH21	1.72	0.52
1:D:776:LEU:HB2	1:D:815:PRO:HA	1.91	0.52
1:A:497:TRP:CD1	1:A:537:ARG:HH11	2.28	0.52
1:C:617:PHE:HB2	1:C:630:VAL:HG11	1.91	0.51
1:A:766:GLY:HA2	1:A:824:ALA:HB1	1.93	0.51
1:B:782:ILE:HD13	1:B:800:GLY:HA2	1.92	0.51
1:C:410:TRP:NE1	1:C:466:ASP:OD1	2.44	0.51
1:C:845:TYR:CE2	1:C:848:PHE:HB3	2.46	0.51
1:D:763:ALA:HB3	1:D:828:CYS:HB2	1.93	0.51
1:B:776:LEU:HB2	1:B:815:PRO:HA	1.91	0.51
1:C:418:VAL:HG22	1:C:531:ARG:HD2	1.93	0.51
1:C:703:HIS:O	1:C:706:SER:OG	2.21	0.51
1:B:674:HIS:O	1:B:678:LEU:HG	2.11	0.51
1:B:812:TYR:O	1:B:814:ARG:HG2	2.09	0.51
1:D:766:GLY:HA2	1:D:824:ALA:HB1	1.92	0.51
1:C:766:GLY:HA2	1:C:824:ALA:HB1	1.92	0.51
1:A:776:LEU:HB2	1:A:815:PRO:HA	1.93	0.50
1:A:731:HIS:NE2	1:B:693:LEU:HG	2.27	0.50
1:C:720:PHE:O	1:C:725:GLN:NE2	2.44	0.50
1:B:418:VAL:HG22	1:B:531:ARG:HD2	1.93	0.50
1:B:790:LEU:HD12	1:B:823:ARG:HG3	1.94	0.50
1:C:674:HIS:O	1:C:678:LEU:HG	2.11	0.50
1:C:758:PHE:C	1:C:759:LYS:HD2	2.37	0.50
1:A:797:ALA:HB2	1:A:860:PHE:HD2	1.77	0.50
1:C:746:ALA:HB2	1:C:848:PHE:CZ	2.46	0.50
1:A:781:PHE:O	1:A:831:HIS:N	2.43	0.50
1:A:790:LEU:HD12	1:A:823:ARG:HG3	1.94	0.50
1:C:464:ILE:HG13	1:C:505:ALA:HB1	1.93	0.50
1:C:708:THR:HG22	1:C:713:MET:HE1	1.94	0.50
1:A:720:PHE:O	1:A:725:GLN:NE2	2.45	0.50
1:B:731:HIS:NE2	1:C:693:LEU:HG	2.27	0.50
1:C:536:ALA:HA	1:C:539:LEU:HD23	1.94	0.50
1:D:418:VAL:HG22	1:D:531:ARG:HD2	1.93	0.50
1:A:528:ARG:O	1:A:532:LEU:HD12	2.11	0.50
1:D:703:HIS:O	1:D:706:SER:OG	2.24	0.50
1:B:746:ALA:HB2	1:B:848:PHE:CZ	2.47	0.49
1:B:755:ALA:HA	1:B:758:PHE:CD1	2.47	0.49
1:C:731:HIS:NE2	1:D:693:LEU:HG	2.27	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:642:ILE:HA	1:B:645:MET:HE3	1.93	0.49
1:B:766:GLY:HA2	1:B:824:ALA:HB1	1.93	0.49
1:B:692:PRO:O	1:B:696:ARG:HG3	2.13	0.49
1:B:757:LYS:HE3	1:B:841:VAL:HG21	1.94	0.49
1:B:536:ALA:HA	1:B:539:LEU:HD23	1.95	0.49
1:C:541:ARG:HD2	1:C:541:ARG:O	2.13	0.49
1:D:414:ILE:HD11	1:D:466:ASP:OD1	2.13	0.49
1:A:534:ARG:NH1	1:A:537:ARG:HH12	2.11	0.49
1:C:479:ASN:OD1	1:C:480:GLU:N	2.46	0.49
1:C:790:LEU:HD12	1:C:823:ARG:HG3	1.95	0.49
1:D:692:PRO:O	1:D:696:ARG:HG3	2.12	0.49
1:D:541:ARG:HD2	1:D:541:ARG:O	2.13	0.49
1:A:479:ASN:OD1	1:A:480:GLU:N	2.46	0.49
1:A:754:LEU:HB3	1:A:758:PHE:CZ	2.47	0.49
1:B:720:PHE:O	1:B:725:GLN:NE2	2.46	0.49
1:B:734:ARG:O	1:B:738:GLN:NE2	2.40	0.49
1:B:617:PHE:HB2	1:B:630:VAL:HG11	1.94	0.48
1:C:781:PHE:O	1:C:831:HIS:N	2.42	0.48
1:B:464:ILE:HG13	1:B:505:ALA:HB1	1.94	0.48
1:B:753:ALA:HB1	1:B:757:LYS:HZ1	1.77	0.48
1:B:765:PRO:HG3	1:B:827:TYR:HA	1.95	0.48
1:C:475:TYR:HD1	1:C:489:ILE:HG12	1.78	0.48
1:C:692:PRO:O	1:C:696:ARG:HG3	2.13	0.48
1:D:676:GLN:HA	1:D:679:ARG:HE	1.77	0.48
1:C:765:PRO:HG3	1:C:827:TYR:HA	1.95	0.48
1:D:691:ASN:HA	1:D:694:ARG:HE	1.79	0.48
1:B:541:ARG:HD2	1:B:541:ARG:O	2.13	0.48
1:C:648:GLY:O	1:C:652:TYR:HB2	2.13	0.48
1:C:691:ASN:HA	1:C:694:ARG:HE	1.78	0.48
1:A:765:PRO:HG3	1:A:827:TYR:HA	1.94	0.48
1:D:464:ILE:HG13	1:D:505:ALA:HB1	1.95	0.48
1:A:617:PHE:HB2	1:A:630:VAL:HG11	1.95	0.48
1:A:648:GLY:O	1:A:652:TYR:HB2	2.13	0.48
1:A:691:ASN:HA	1:A:694:ARG:HE	1.78	0.48
1:B:414:ILE:HD11	1:B:466:ASP:OD1	2.13	0.48
1:A:825:LEU:HG	1:A:826:THR:H	1.79	0.48
1:A:834:HIS:O	1:A:838:LEU:HD23	2.14	0.48
1:B:479:ASN:OD1	1:B:480:GLU:N	2.46	0.48
1:C:837:ASP:O	1:C:840:GLU:HG3	2.14	0.48
1:D:790:LEU:HD12	1:D:823:ARG:HG3	1.95	0.48
1:A:464:ILE:HG13	1:A:505:ALA:HB1	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:692:PRO:O	1:A:696:ARG:HG3	2.13	0.48
1:D:489:ILE:O	1:D:492:HIS:ND1	2.47	0.48
1:D:738:GLN:HG2	1:D:739:HIS:CD2	2.49	0.47
1:A:734:ARG:O	1:A:738:GLN:NE2	2.44	0.47
1:A:738:GLN:HG2	1:A:739:HIS:CD2	2.49	0.47
1:B:781:PHE:HE2	1:B:833:ILE:HD11	1.79	0.47
1:B:799:LEU:HB3	1:B:803:ASP:CG	2.39	0.47
1:D:488:ARG:HA	1:D:491:VAL:HG22	1.96	0.47
1:D:703:HIS:ND1	1:D:764:PRO:HB3	2.29	0.47
1:D:720:PHE:O	1:D:725:GLN:NE2	2.48	0.47
1:A:703:HIS:O	1:A:706:SER:OG	2.26	0.47
1:B:557:PHE:CE2	1:B:651:MET:HE3	2.49	0.47
1:A:758:PHE:C	1:A:759:LYS:HD3	2.39	0.47
1:B:455:VAL:O	1:B:459:VAL:HG23	2.15	0.47
1:B:651:MET:O	1:B:655:ILE:HG12	2.15	0.47
1:B:825:LEU:HG	1:B:826:THR:H	1.79	0.47
1:C:825:LEU:HG	1:C:826:THR:H	1.78	0.47
1:B:475:TYR:HD1	1:B:489:ILE:HG12	1.80	0.47
1:D:479:ASN:OD1	1:D:480:GLU:N	2.46	0.47
1:C:738:GLN:HG2	1:C:739:HIS:CD2	2.50	0.47
1:D:825:LEU:HG	1:D:826:THR:H	1.80	0.47
1:B:738:GLN:HG2	1:B:739:HIS:CD2	2.51	0.46
1:D:458:ILE:HA	1:D:461:ILE:HD12	1.96	0.46
1:D:734:ARG:O	1:D:738:GLN:NE2	2.46	0.46
1:B:665:ARG:HG2	1:B:665:ARG:HH11	1.80	0.46
1:B:845:TYR:HE2	1:B:848:PHE:HB3	1.80	0.46
1:D:461:ILE:O	1:D:465:VAL:HG23	2.15	0.46
1:B:703:HIS:ND1	1:B:764:PRO:HB3	2.30	0.46
1:C:455:VAL:O	1:C:459:VAL:HG23	2.15	0.46
1:C:461:ILE:O	1:C:465:VAL:HG23	2.16	0.46
1:B:461:ILE:O	1:B:465:VAL:HG23	2.16	0.46
1:B:640:PHE:O	1:B:644:VAL:HG23	2.16	0.46
1:C:782:ILE:HD13	1:C:800:GLY:HA2	1.98	0.46
1:A:476:VAL:HG13	1:A:481:GLU:HA	1.97	0.46
1:A:488:ARG:HA	1:A:491:VAL:HG22	1.97	0.46
1:B:691:ASN:HA	1:B:694:ARG:HE	1.80	0.46
1:A:461:ILE:O	1:A:465:VAL:HG23	2.15	0.46
1:A:619:PHE:CE2	1:D:642:ILE:HG23	2.50	0.46
1:B:402:HIS:HB3	1:B:474:THR:O	2.16	0.46
1:C:402:HIS:HB3	1:C:474:THR:O	2.16	0.46
1:C:640:PHE:O	1:C:644:VAL:HG23	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:476:VAL:HG13	1:D:481:GLU:HA	1.98	0.46
1:B:804:ILE:O	1:B:859:THR:OG1	2.24	0.46
1:D:758:PHE:HD2	1:D:833:ILE:HG22	1.81	0.46
1:B:818:SER:OG	1:B:862:LEU:O	2.31	0.46
1:D:455:VAL:O	1:D:459:VAL:HG23	2.16	0.46
1:D:568:TRP:HB2	1:D:640:PHE:HE2	1.81	0.46
1:C:557:PHE:HD2	1:C:651:MET:HE2	1.80	0.45
1:C:761:THR:OG1	1:C:830:LEU:HB2	2.16	0.45
1:D:417:LEU:O	1:D:421:THR:HG23	2.16	0.45
1:A:753:ALA:C	1:A:757:LYS:HZ3	2.24	0.45
1:B:417:LEU:O	1:B:421:THR:HG23	2.16	0.45
1:B:759:LYS:N	1:B:759:LYS:HD2	2.32	0.45
1:C:766:GLY:N	1:C:825:LEU:O	2.50	0.45
1:D:414:ILE:O	1:D:418:VAL:HG23	2.17	0.45
1:D:648:GLY:O	1:D:652:TYR:HB2	2.16	0.45
1:B:414:ILE:O	1:B:418:VAL:HG23	2.16	0.45
1:A:568:TRP:HB2	1:A:640:PHE:HE2	1.81	0.45
1:C:845:TYR:HE2	1:C:848:PHE:HB3	1.81	0.45
1:D:536:ALA:HA	1:D:539:LEU:HD23	1.98	0.45
1:D:769:LEU:HB2	1:D:822:VAL:HG11	1.99	0.45
1:C:776:LEU:HG	1:C:816:GLY:H	1.81	0.45
1:D:781:PHE:HB2	1:D:831:HIS:HB3	1.99	0.45
1:A:414:ILE:O	1:A:418:VAL:HG23	2.17	0.45
1:B:425:THR:OG1	1:B:426:PRO:HD3	2.17	0.45
1:C:458:ILE:HA	1:C:461:ILE:HD12	1.97	0.45
1:D:766:GLY:N	1:D:825:LEU:O	2.50	0.45
1:D:838:LEU:HA	1:D:841:VAL:HG12	1.99	0.45
1:B:776:LEU:HG	1:B:816:GLY:H	1.82	0.45
1:C:414:ILE:O	1:C:418:VAL:HG23	2.17	0.45
1:D:837:ASP:O	1:D:840:GLU:HG3	2.17	0.45
1:A:691:ASN:O	1:A:694:ARG:HG2	2.17	0.44
1:C:417:LEU:O	1:C:421:THR:HG23	2.17	0.44
1:D:765:PRO:HG3	1:D:827:TYR:HA	2.00	0.44
1:C:487:GLY:O	1:C:491:VAL:HG13	2.17	0.44
1:A:674:HIS:O	1:A:678:LEU:HG	2.17	0.44
1:A:414:ILE:HD11	1:A:466:ASP:OD1	2.18	0.44
1:A:762:HIS:HE1	1:A:827:TYR:OH	2.01	0.44
1:C:425:THR:OG1	1:C:426:PRO:HD3	2.17	0.44
1:D:489:ILE:HA	1:D:492:HIS:HD1	1.83	0.44
1:A:425:THR:OG1	1:A:426:PRO:HD3	2.17	0.44
1:A:489:ILE:HA	1:A:492:HIS:HD1	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:846:PRO:O	1:C:849:SER:OG	2.26	0.44
1:A:458:ILE:HA	1:A:461:ILE:HD12	1.99	0.44
1:B:762:HIS:HE1	1:B:827:TYR:OH	2.01	0.44
1:B:455:VAL:HA	1:B:458:ILE:HG12	2.00	0.44
1:A:755:ALA:HA	1:A:758:PHE:HD1	1.83	0.44
1:A:421:THR:OG1	1:A:531:ARG:NH1	2.51	0.43
1:B:645:MET:HG2	1:C:625:VAL:HG21	2.00	0.43
1:C:703:HIS:ND1	1:C:764:PRO:HB3	2.32	0.43
1:C:769:LEU:HB2	1:C:822:VAL:HG11	1.99	0.43
1:A:455:VAL:HA	1:A:458:ILE:HG12	2.00	0.43
1:C:455:VAL:HA	1:C:458:ILE:HG12	2.00	0.43
1:D:425:THR:OG1	1:D:426:PRO:HD3	2.17	0.43
1:B:642:ILE:HG23	1:C:619:PHE:CD2	2.54	0.43
1:B:487:GLY:O	1:B:491:VAL:HG13	2.17	0.43
1:B:691:ASN:O	1:B:694:ARG:HG2	2.18	0.43
1:A:799:LEU:HB3	1:A:803:ASP:CG	2.43	0.43
1:B:743:PHE:HA	1:B:848:PHE:HZ	1.83	0.43
1:A:833:ILE:HB	1:A:838:LEU:CD2	2.48	0.43
1:A:812:TYR:CE1	1:A:814:ARG:HB2	2.53	0.43
1:B:458:ILE:HA	1:B:461:ILE:HD12	1.99	0.43
1:B:766:GLY:N	1:B:825:LEU:O	2.51	0.43
1:D:725:GLN:HA	1:D:728:ILE:HG22	2.01	0.43
1:D:685:ARG:HA	1:D:685:ARG:HD3	1.81	0.43
1:D:753:ALA:HB1	1:D:757:LYS:NZ	2.34	0.43
1:D:776:LEU:HG	1:D:816:GLY:H	1.83	0.43
1:A:842:LEU:HG	1:A:849:SER:HB3	2.00	0.43
1:D:833:ILE:HB	1:D:838:LEU:CD2	2.49	0.43
1:B:812:TYR:CE1	1:B:814:ARG:HB2	2.54	0.43
1:C:691:ASN:O	1:C:694:ARG:HG2	2.18	0.43
1:D:691:ASN:O	1:D:694:ARG:HG2	2.18	0.43
1:D:761:THR:OG1	1:D:830:LEU:HB2	2.19	0.43
1:D:812:TYR:CE1	1:D:814:ARG:HB2	2.53	0.43
1:A:782:ILE:HG21	1:A:800:GLY:HA2	2.00	0.42
1:B:725:GLN:HA	1:B:728:ILE:HG22	2.01	0.42
1:B:763:ALA:HB3	1:B:828:CYS:HB2	2.00	0.42
1:B:846:PRO:O	1:B:849:SER:OG	2.28	0.42
1:D:773:GLY:H	1:D:817:LYS:HB3	1.84	0.42
1:D:842:LEU:HG	1:D:849:SER:HB3	2.01	0.42
1:C:651:MET:O	1:C:655:ILE:HG12	2.19	0.42
1:D:455:VAL:HA	1:D:458:ILE:HG12	2.00	0.42
1:A:651:MET:O	1:A:655:ILE:HG12	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:720:PHE:HA	1:A:721:PRO:HD3	1.91	0.42
1:B:791:ARG:HB3	1:B:820:GLY:HA3	2.02	0.42
1:D:674:HIS:O	1:D:678:LEU:HG	2.19	0.42
1:C:476:VAL:HG13	1:C:481:GLU:HA	2.02	0.42
1:C:749:GLY:O	1:C:752:ARG:HG2	2.20	0.42
1:C:762:HIS:HE1	1:C:827:TYR:OH	2.03	0.42
1:C:747:THR:OG1	1:C:750:CYS:SG	2.67	0.42
1:C:754:LEU:HA	1:C:757:LYS:CG	2.49	0.42
1:D:640:PHE:O	1:D:644:VAL:HG23	2.19	0.42
1:A:665:ARG:HG2	1:A:665:ARG:HH11	1.84	0.42
1:A:725:GLN:HA	1:A:728:ILE:HG22	2.02	0.42
1:A:766:GLY:N	1:A:825:LEU:O	2.52	0.42
1:A:769:LEU:HB2	1:A:822:VAL:HG11	2.01	0.42
1:A:797:ALA:HB2	1:A:860:PHE:CD2	2.55	0.42
1:B:769:LEU:HB2	1:B:822:VAL:HG11	2.02	0.42
1:B:476:VAL:HG13	1:B:481:GLU:HA	2.01	0.42
1:C:725:GLN:HA	1:C:728:ILE:HG22	2.02	0.42
1:A:463:PHE:O	1:A:467:ILE:HG13	2.19	0.41
1:B:781:PHE:O	1:B:831:HIS:N	2.42	0.41
1:C:782:ILE:HA	1:C:830:LEU:HA	2.02	0.41
1:A:419:ILE:O	1:A:423:VAL:HG22	2.20	0.41
1:A:781:PHE:HB2	1:A:831:HIS:HB3	2.01	0.41
1:A:498:PHE:HA	1:A:501:ASP:OD2	2.20	0.41
1:C:665:ARG:HH21	1:D:674:HIS:CG	2.38	0.41
1:C:759:LYS:HD2	1:C:759:LYS:N	2.35	0.41
1:D:641:SER:O	1:D:645:MET:HE2	2.21	0.41
1:D:757:LYS:HD2	1:D:837:ASP:OD2	2.21	0.41
1:C:417:LEU:HD23	1:C:417:LEU:HA	1.89	0.41
1:D:749:GLY:HA2	1:D:752:ARG:HG2	2.03	0.41
1:D:781:PHE:O	1:D:831:HIS:N	2.40	0.41
1:A:782:ILE:HA	1:A:830:LEU:HA	2.02	0.41
1:A:856:LEU:HG	1:A:858:ILE:HD11	2.03	0.41
1:B:676:GLN:O	1:B:680:VAL:HG23	2.21	0.41
1:A:674:HIS:CG	1:D:665:ARG:HH21	2.38	0.41
1:A:844:MET:HE1	1:B:775:LEU:HD21	2.02	0.41
1:C:676:GLN:HG3	1:C:679:ARG:NH2	2.30	0.41
1:C:773:GLY:H	1:C:817:LYS:HB3	1.85	0.41
1:A:489:ILE:O	1:A:492:HIS:ND1	2.54	0.41
1:C:676:GLN:O	1:C:680:VAL:HG23	2.21	0.41
1:A:541:ARG:C	1:A:541:ARG:HH11	2.28	0.41
1:A:707:TYR:HB2	1:B:686:PHE:CE1	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:761:THR:OG1	1:A:830:LEU:HB2	2.20	0.41
1:A:776:LEU:HG	1:A:816:GLY:H	1.86	0.41
1:C:781:PHE:HB2	1:C:831:HIS:HB3	2.02	0.41
1:D:720:PHE:HA	1:D:721:PRO:HD3	1.91	0.41
1:A:729:CYS:HB3	1:A:755:ALA:O	2.21	0.41
1:C:414:ILE:HD11	1:C:466:ASP:OD1	2.21	0.41
1:C:763:ALA:HB3	1:C:828:CYS:HB2	2.02	0.41
1:C:782:ILE:HG23	1:C:830:LEU:HD23	2.03	0.41
1:D:808:PRO:HG2	1:D:812:TYR:HB3	2.02	0.41
1:D:818:SER:OG	1:D:862:LEU:O	2.36	0.41
1:A:416:LEU:HD11	1:A:420:TYR:CZ	2.56	0.41
1:C:755:ALA:HA	1:C:758:PHE:CD1	2.56	0.41
1:D:651:MET:O	1:D:655:ILE:HG12	2.20	0.41
1:A:763:ALA:HB3	1:A:828:CYS:HB2	2.02	0.40
1:A:779:LEU:HD21	1:A:809:LEU:HD21	2.03	0.40
1:B:609:ASP:O	1:B:613:THR:OG1	2.30	0.40
1:D:405:PRO:O	1:D:409:VAL:HG23	2.21	0.40
1:B:419:ILE:O	1:B:423:VAL:HG22	2.20	0.40
1:B:473:THR:O	1:B:489:ILE:HD13	2.21	0.40
1:B:761:THR:OG1	1:B:830:LEU:HB2	2.22	0.40
1:D:402:HIS:HB3	1:D:474:THR:O	2.20	0.40
1:A:676:GLN:HG2	1:A:679:ARG:NH2	2.33	0.40
1:C:685:ARG:HA	1:C:685:ARG:HD3	1.79	0.40
1:C:757:LYS:NZ	1:C:841:VAL:HG21	2.37	0.40
1:C:825:LEU:HD12	1:C:825:LEU:HA	1.93	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	421/1159 (36%)	392 (93%)	28 (7%)	1 (0%)	43 74

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	421/1159 (36%)	391 (93%)	29 (7%)	1 (0%)	43	74
1	C	421/1159 (36%)	391 (93%)	29 (7%)	1 (0%)	43	74
1	D	421/1159 (36%)	392 (93%)	28 (7%)	1 (0%)	43	74
All	All	1684/4636 (36%)	1566 (93%)	114 (7%)	4 (0%)	44	74

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	521	ILE
1	B	521	ILE
1	C	521	ILE
1	D	521	ILE

5.3.2 Protein sidechains [i](#)

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

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

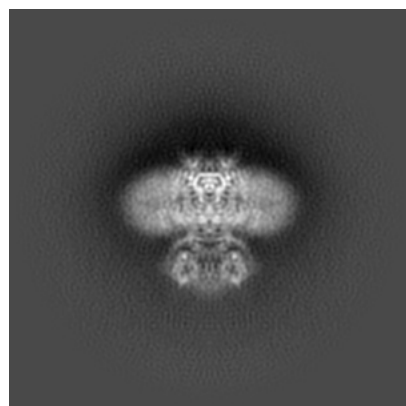
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-35614. These allow visual inspection of the internal detail of the map and identification of artifacts.

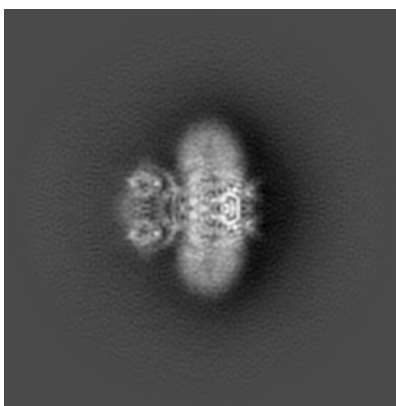
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

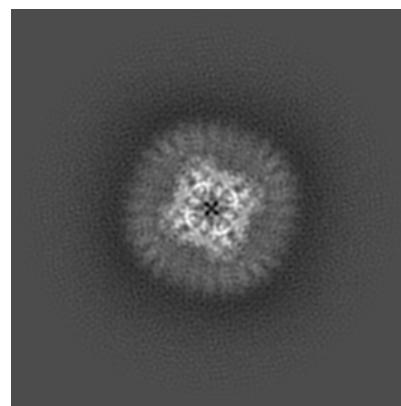
6.1.1 Primary map



X

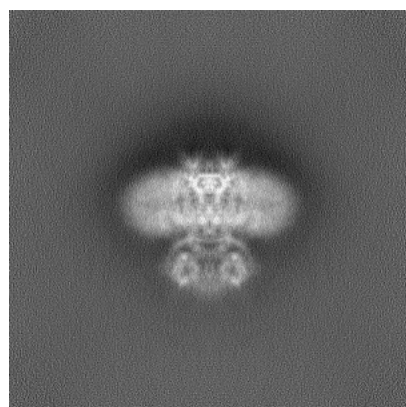


Y

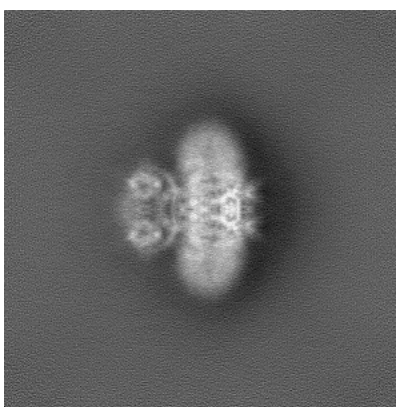


Z

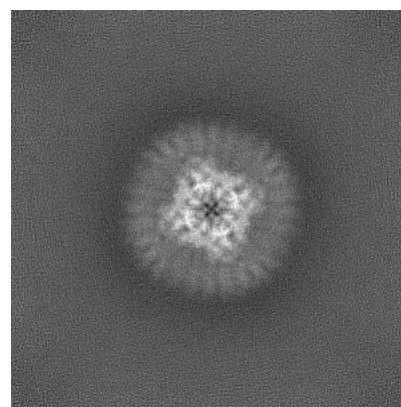
6.1.2 Raw map



X



Y

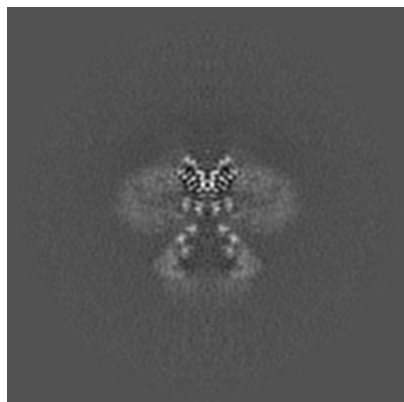


Z

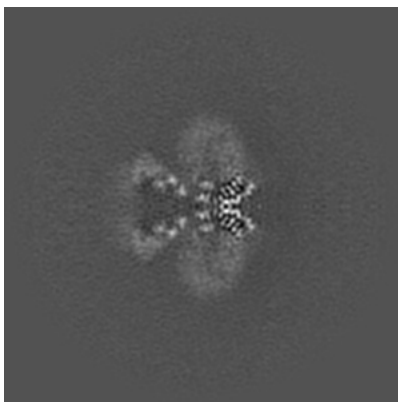
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

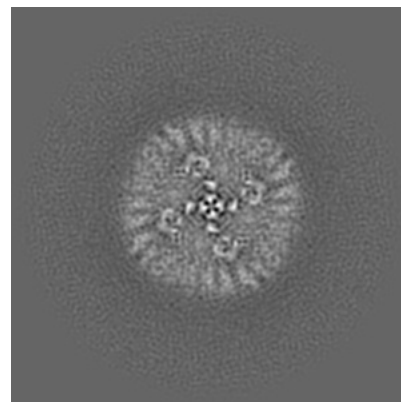
6.2.1 Primary map



X Index: 200

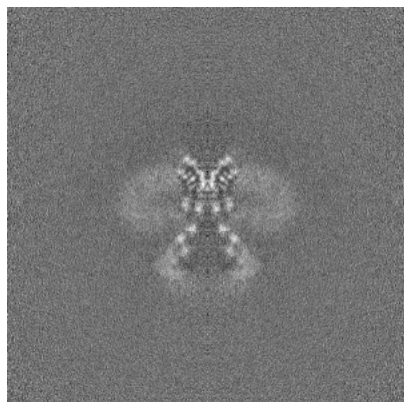


Y Index: 200

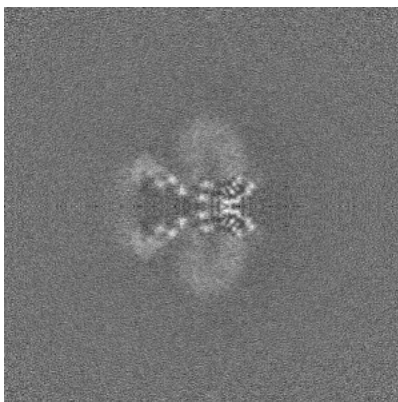


Z Index: 200

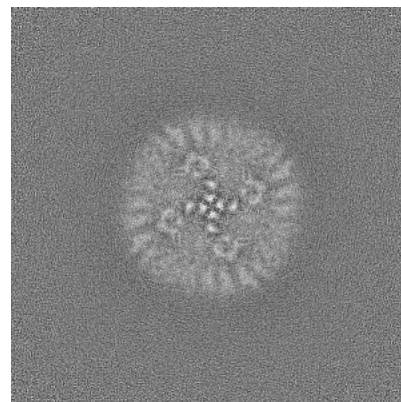
6.2.2 Raw map



X Index: 200



Y Index: 200

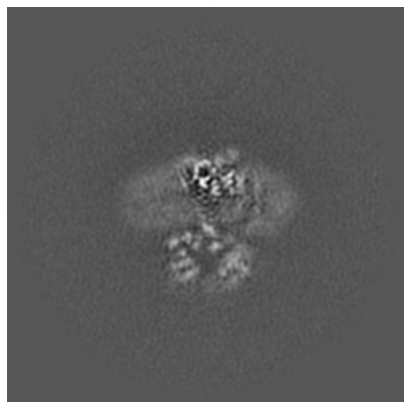


Z Index: 200

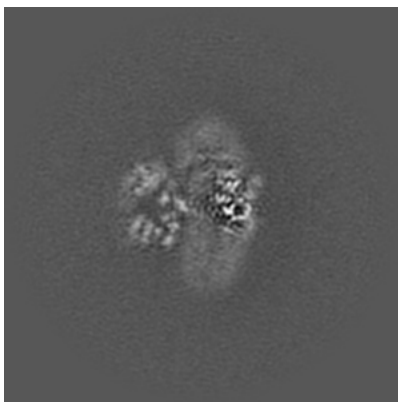
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

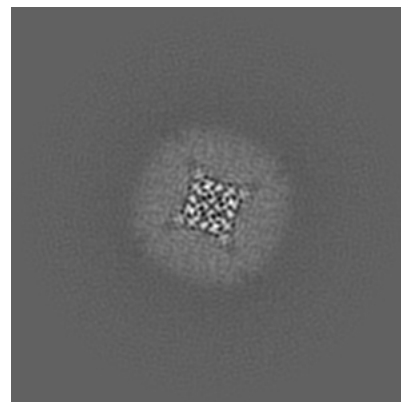
6.3.1 Primary map



X Index: 186

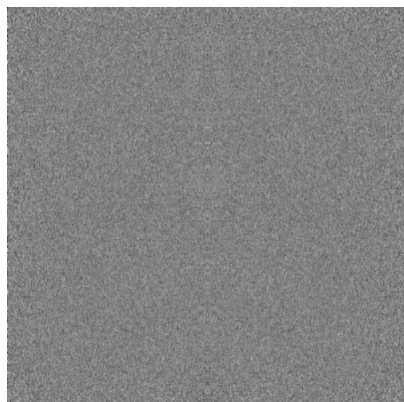


Y Index: 214

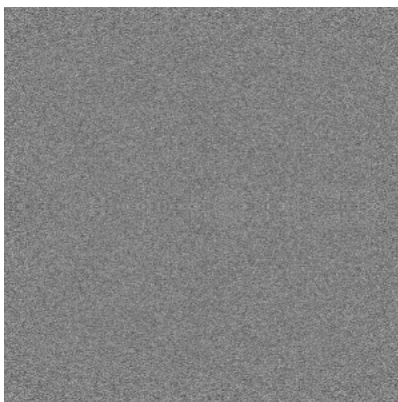


Z Index: 229

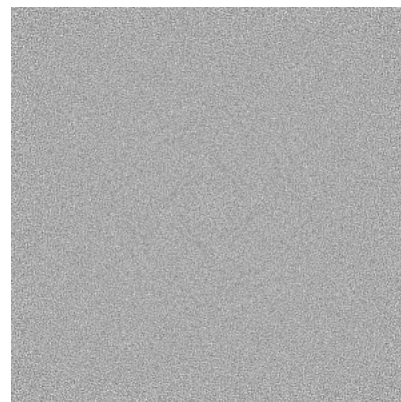
6.3.2 Raw map



X Index: 0



Y Index: 0

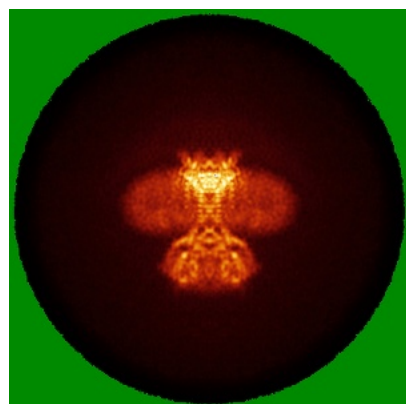


Z Index: 399

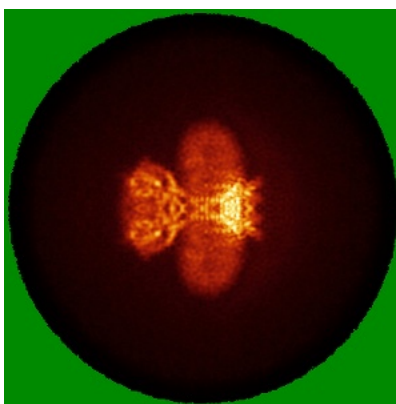
The images above show the largest variance slices of the map in three orthogonal directions.

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

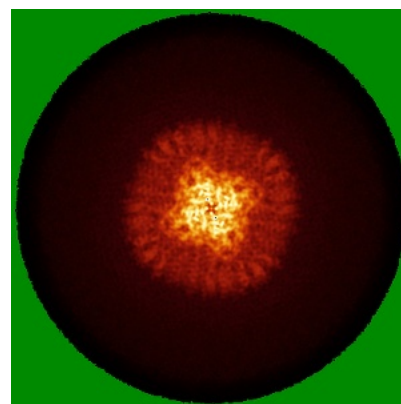
6.4.1 Primary map



X

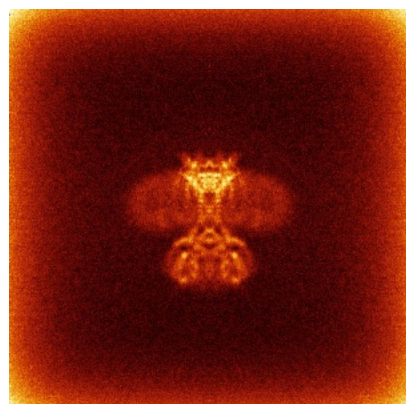


Y

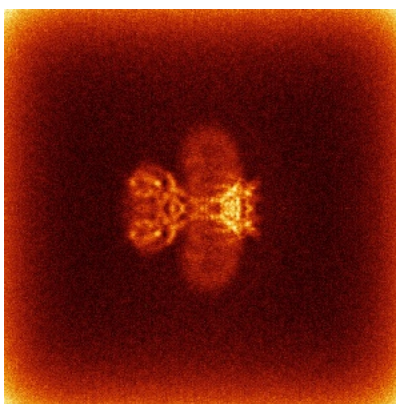


Z

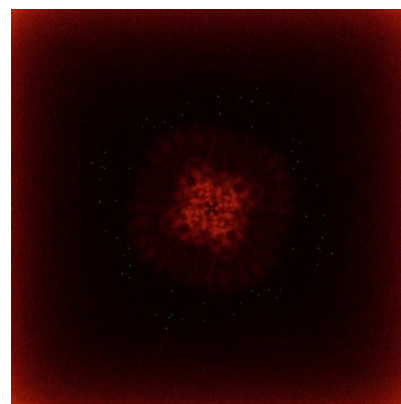
6.4.2 Raw map



X



Y

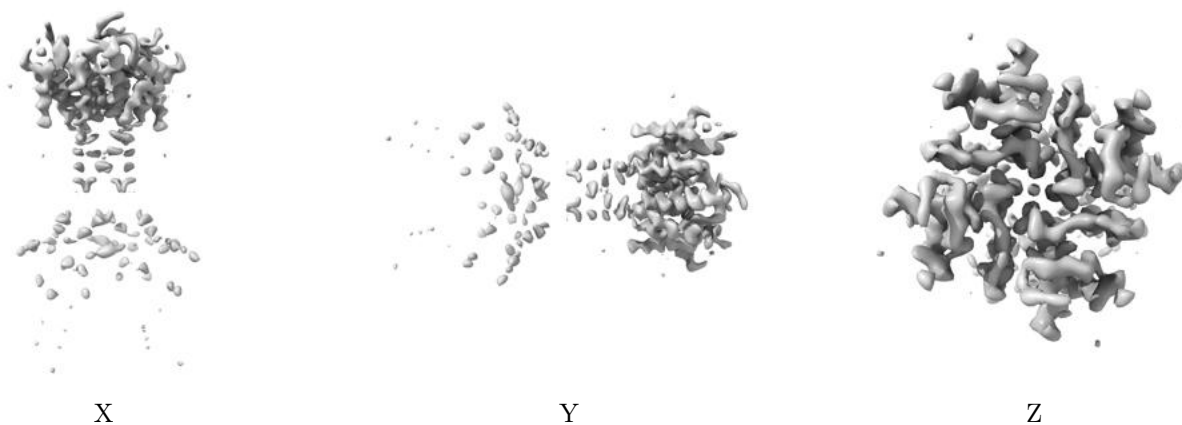


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.22. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

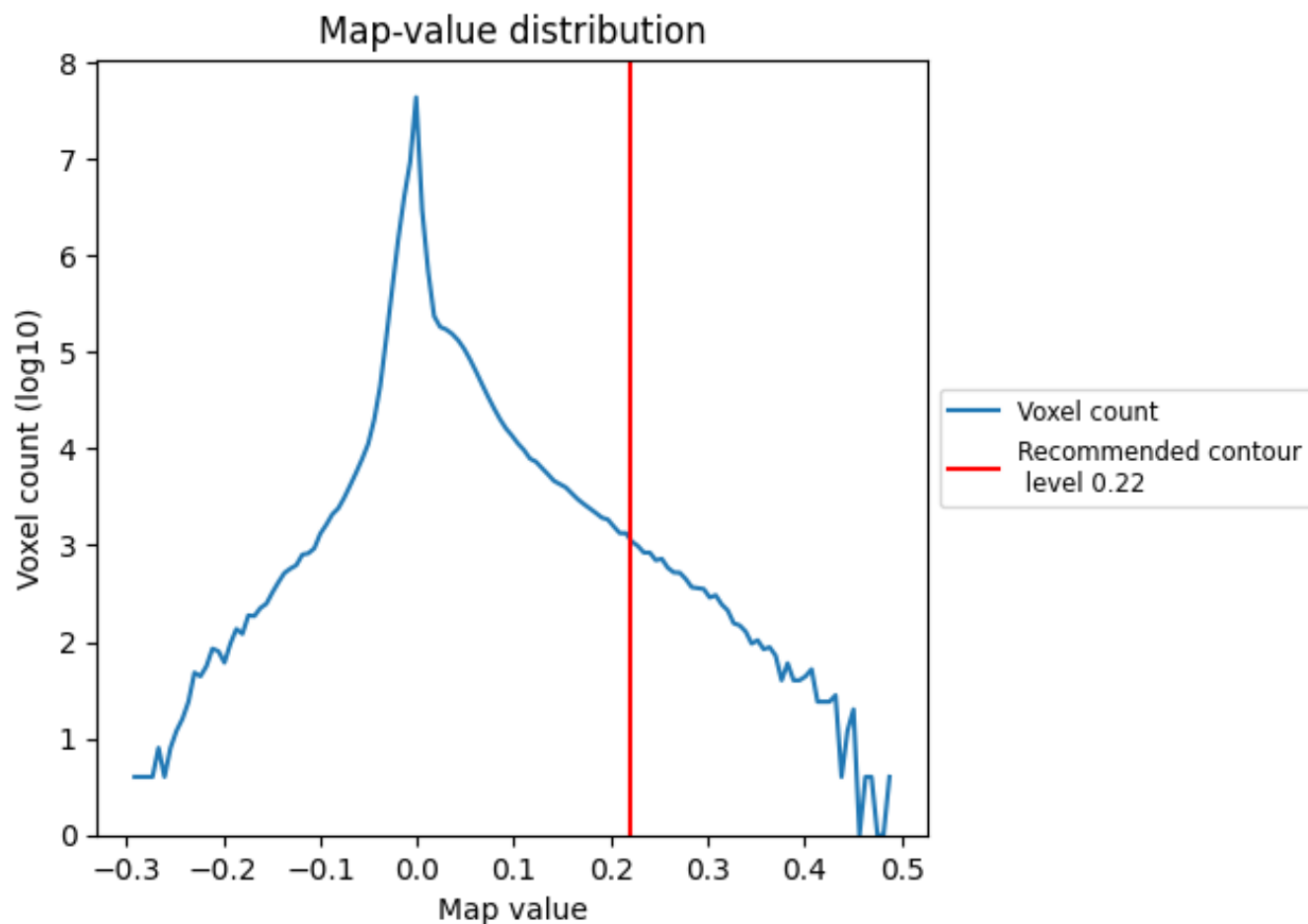
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

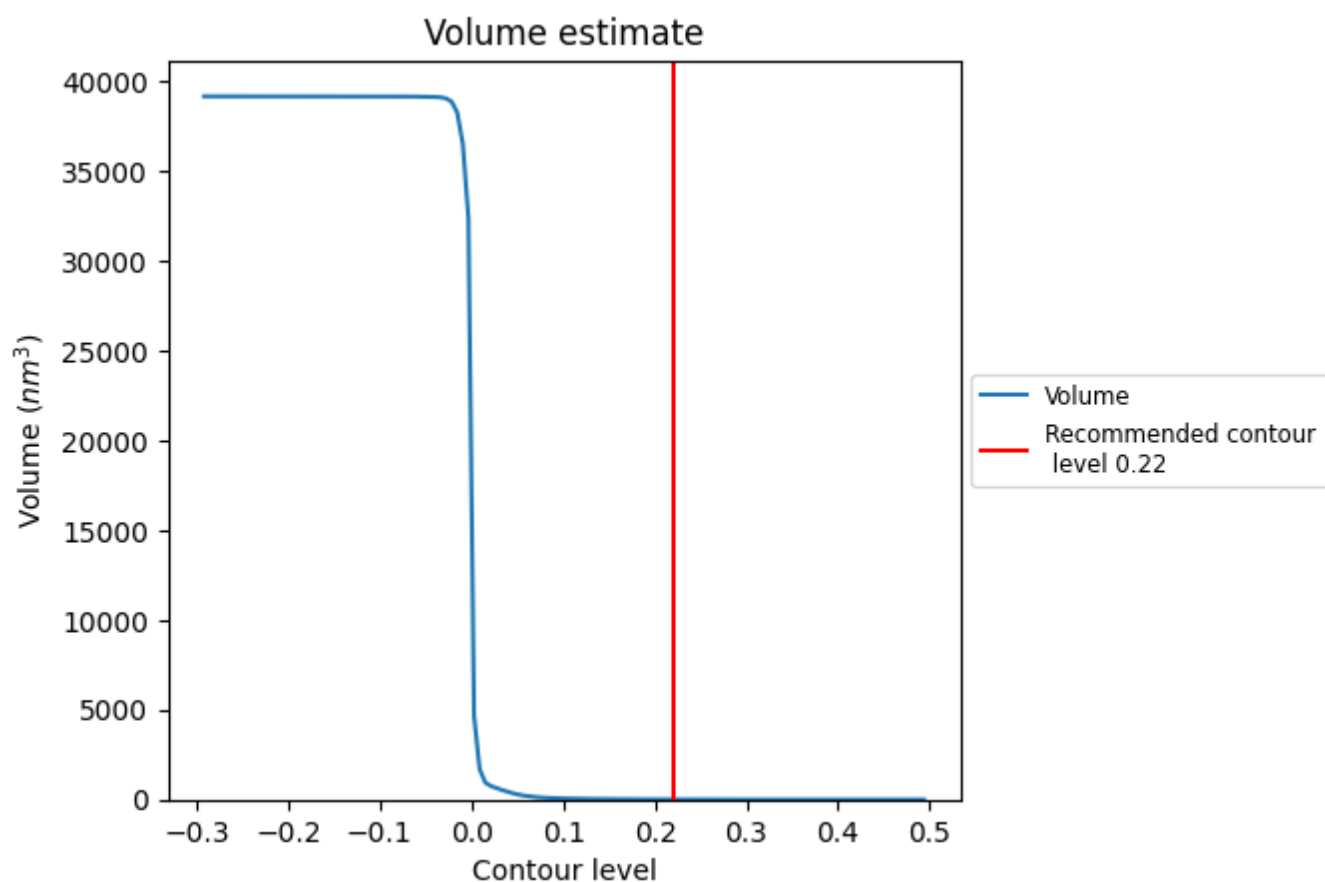
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

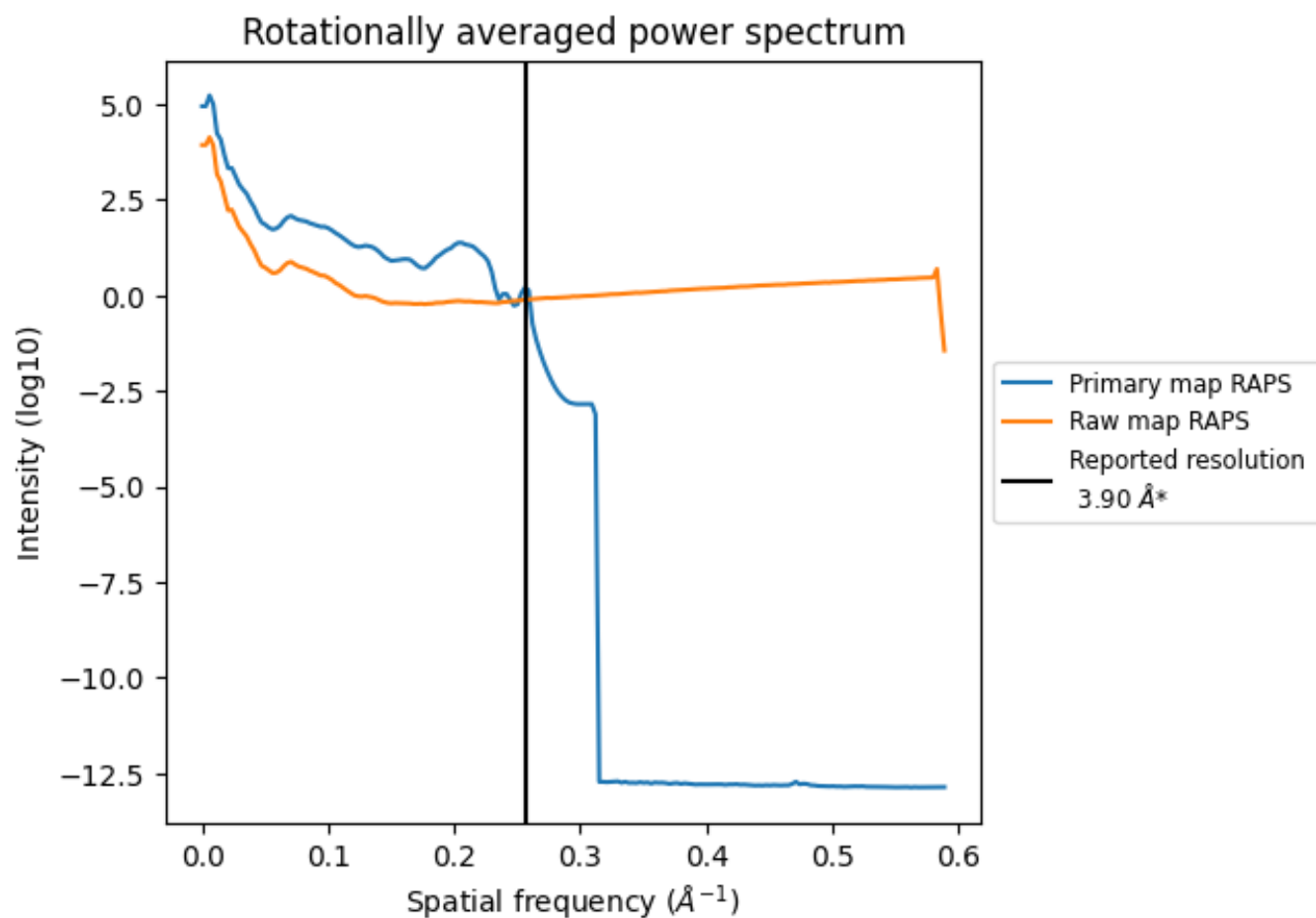
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 7 nm³; this corresponds to an approximate mass of 6 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 ⓘ

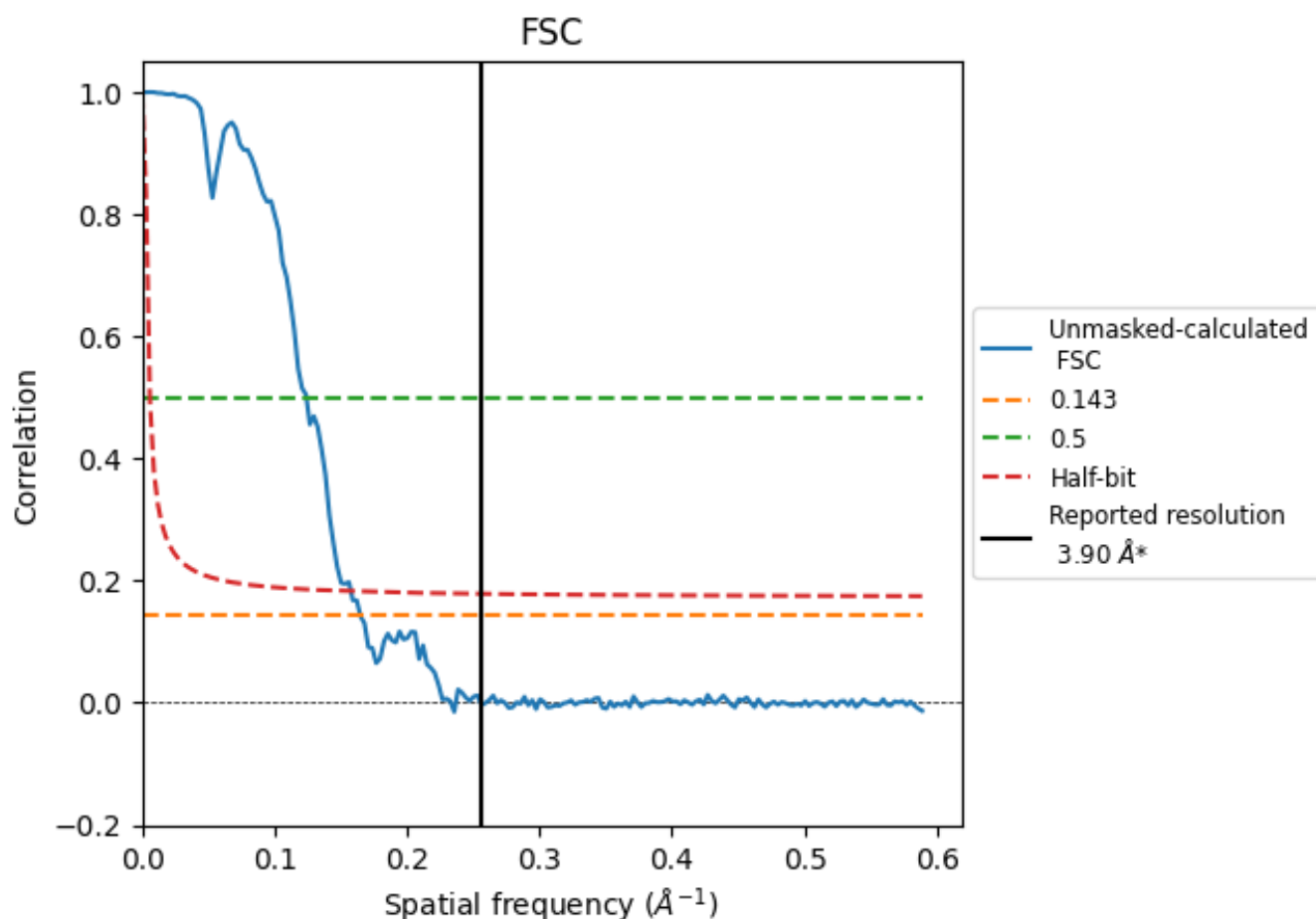


*Reported resolution corresponds to spatial frequency of 0.256 Å⁻¹

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 0.256 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

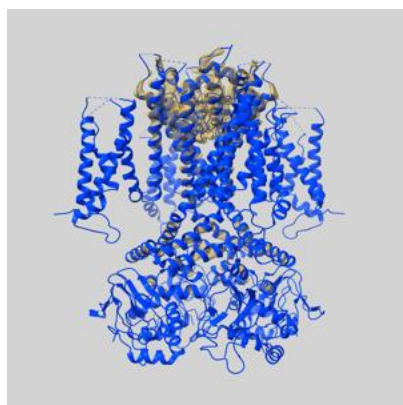
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.90	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	6.07	8.07	6.35

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 6.07 differs from the reported value 3.9 by more than 10 %

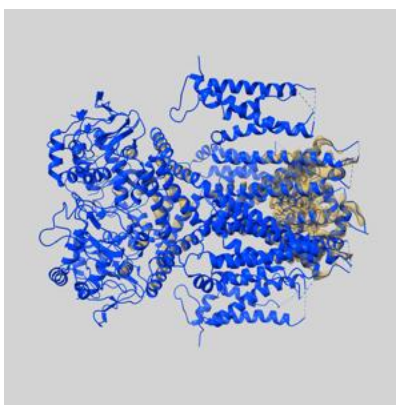
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-35614 and PDB model 8IOB. Per-residue inclusion information can be found in [section 3](#) on [page 4](#).

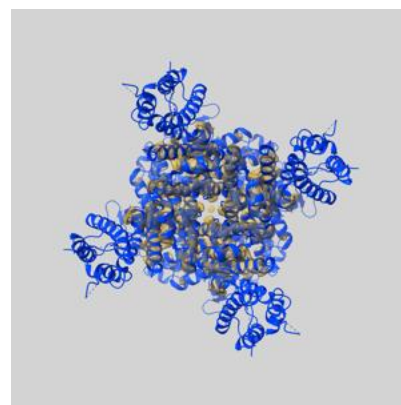
9.1 Map-model overlay [i](#)



X



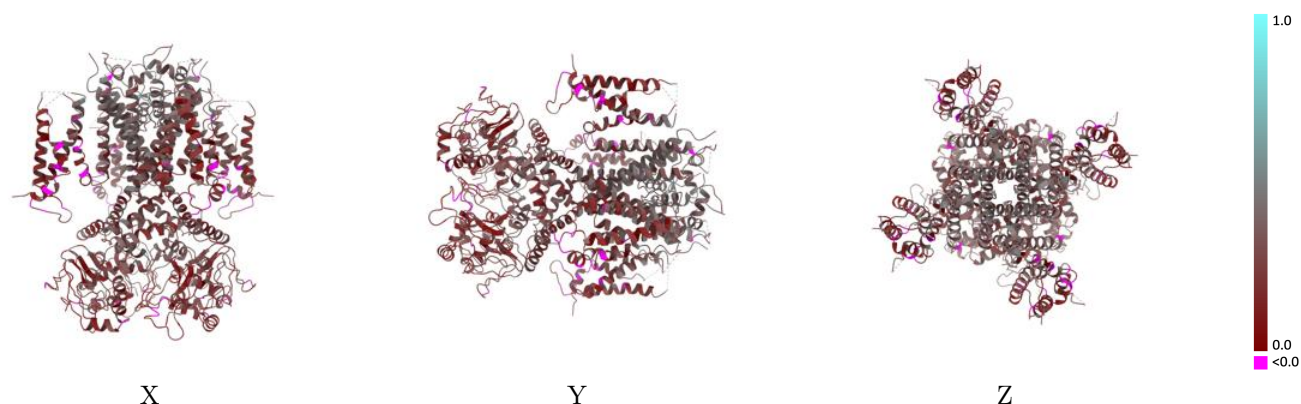
Y



Z

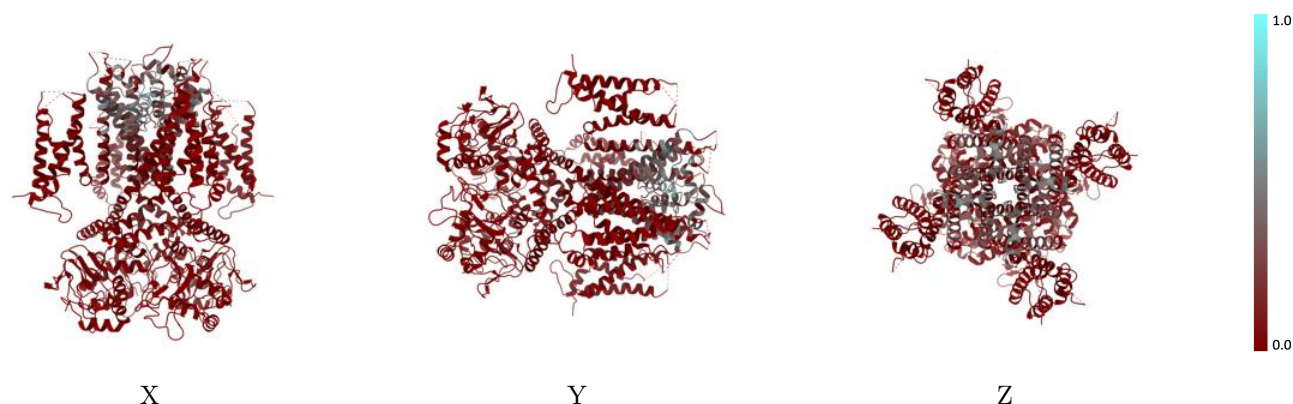
The images above show the 3D surface view of the map at the recommended contour level 0.22 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



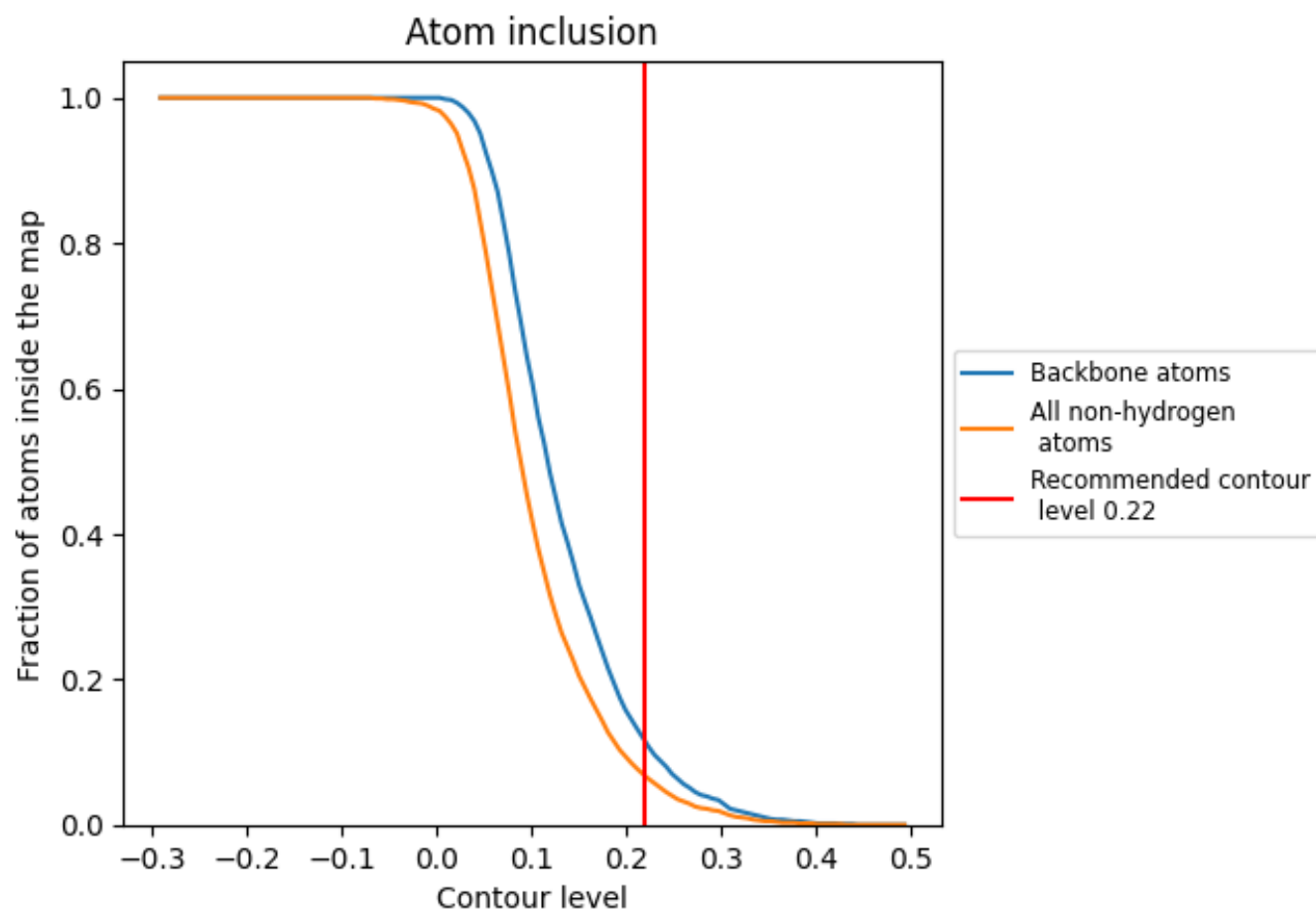
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.22).

9.4 Atom inclusion [i](#)



At the recommended contour level, 12% of all backbone atoms, 7% 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 (0.22) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.0670	0.2710
A	0.0680	0.2700
B	0.0690	0.2720
C	0.0670	0.2730
D	0.0660	0.2710

