Full wwPDB EM Validation Report

Jul 14, 2024 – 02:09 pm BST

PDB ID	:	7ZGX
EMDB ID	:	EMD-14714
Title	:	S-layer Deinoxanthin Binding Complex, C1 symmetry
Authors	:	Farci, D.; Piano, D.
Deposited on	:	2022-04-04
Resolution	:	2.88 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 (i) 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 (i)) were used in the production of this report:

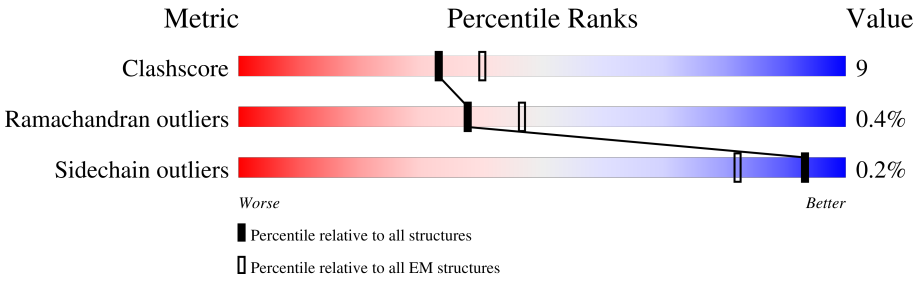
EMDB validation analysis	:	0.0.1.dev92
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 2.88 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 <=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	1167	6% 64% 17% 19%
1	B	1167	7% 64% 17% 19%
1	C	1167	6% 63% 19% 19%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 21351 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 S-layer protein SlpA.

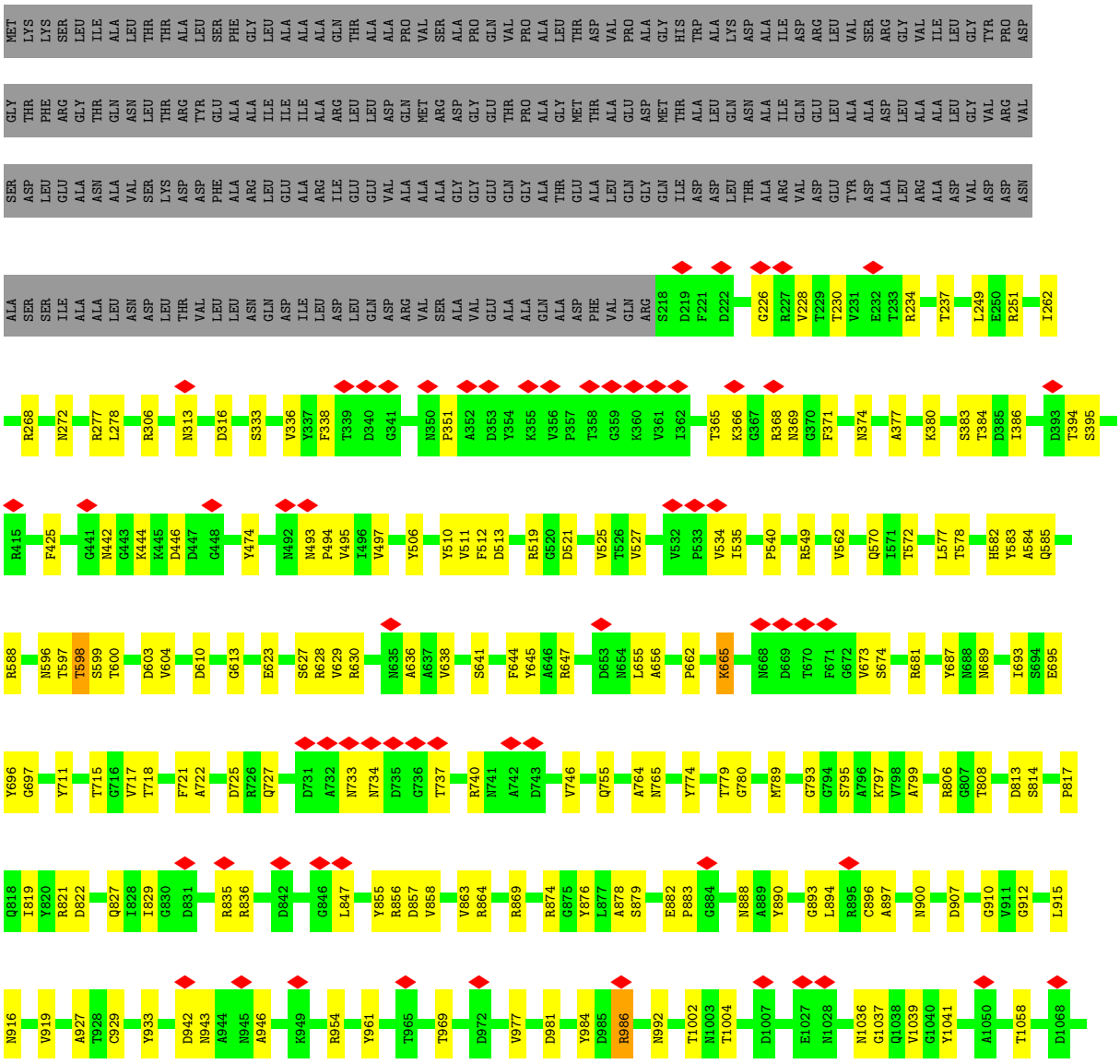
Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	949	Total	C	N	O	S	0	0
			7117	4415	1265	1431	6		
1	B	949	Total	C	N	O	S	0	0
			7117	4415	1265	1431	6		
1	C	949	Total	C	N	O	S	0	0
			7117	4415	1265	1431	6		

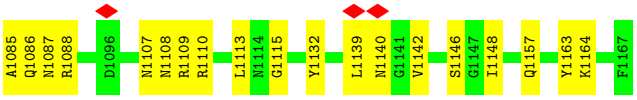
3 Residue-property plots (i)

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

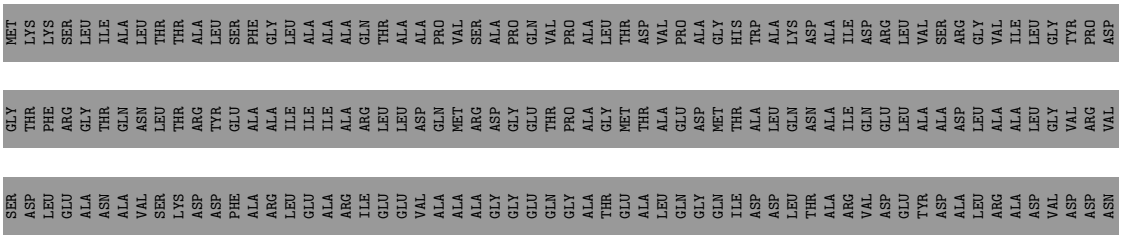
- Molecule 1: S-layer protein SlpA

Chain A:

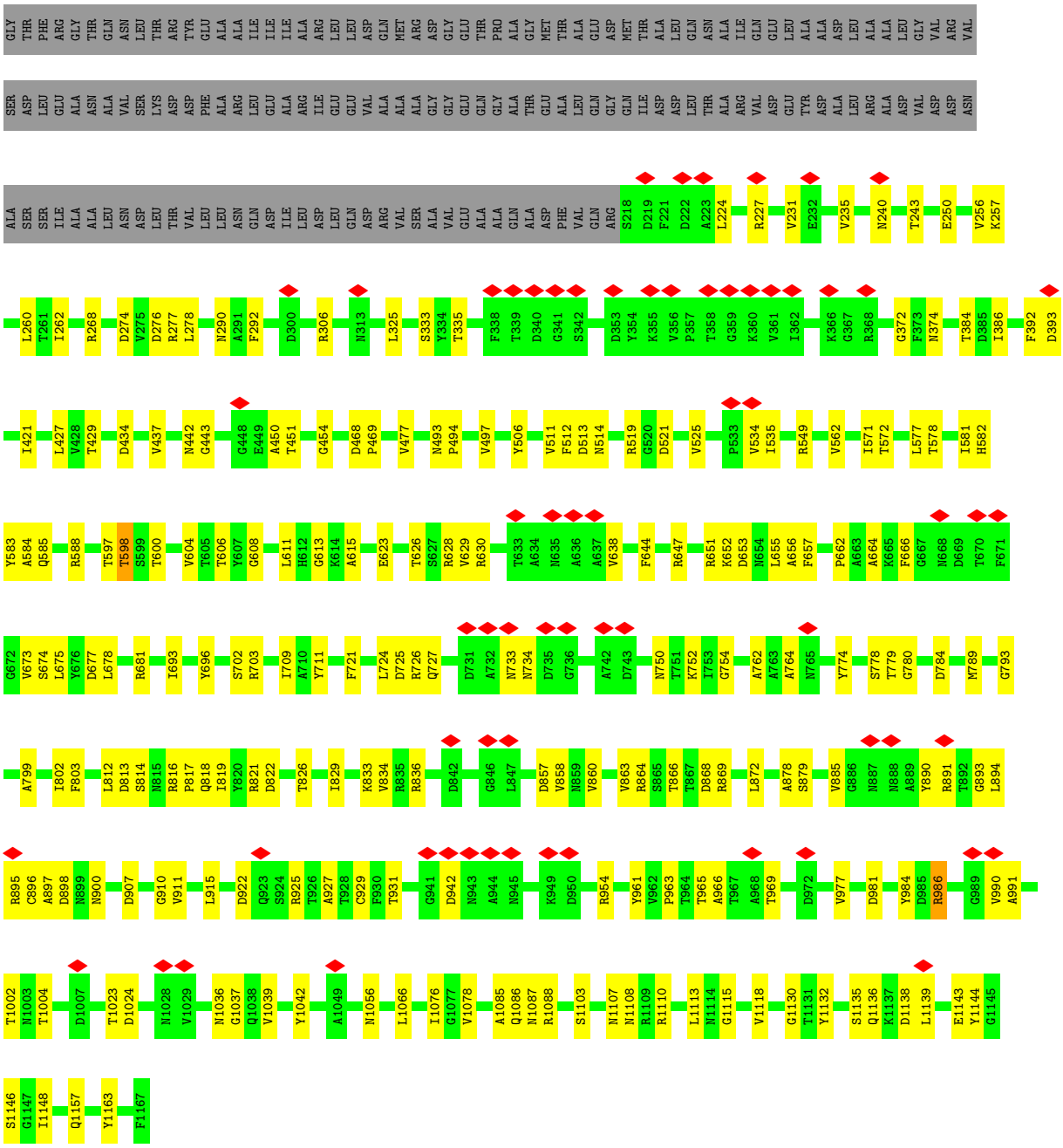




• Molecule 1: S-layer protein SlpA



• Molecule 1: S-layer protein SlpA


GLY THR PHE ARG GLY THR GLN ASN LEU THR ARG TYR GLU ALA ALA ILE ILE ILE ALA ARG LEU LEU LEU ASP GLN MET ARG ASP GLY GLU THR PRO ALA GLY MET THR ALA GLU ASP MET THR ALA LEU GLN GLU LEU ALA ALA ASP LEU ALA ALA LEU GLY VAL ARG VAL
SER ASP LEU GLU ALA ASN ALA VAL SER LYS ASP ASP PHE ALA ARG LEU GLU ALA ARG ILE GLU GLU VAL ALA ALA ALA GLY GLY GLU GLN GLY ALA THR GLU ALA LEU GLN GLY GLN ILE ASP ASP LEU THR ALA ARG VAL ASP GLU TYR ASP ALA LEU ALA ARG ALA ASP VAL ASP ASP ASN
ALA SER SER ILE ALA ALA LEU ASN ASP LEU THR VAL LEU LEU ASN GLN ASP ILE LEU ASP LEU GLN ASP ARG VAL SER ALA VAL GLU ALA ALA GLN ALA ASP PHE VAL GLN ARG S218 D219 F221 D222 A223 L224 R227 V231 E232 V235 N240 T243 E250 V256 K257
L260 T261 I262 R268 D274 V275 D276 R277 L278 N290 A291 F292 D300 R306 N313 L325 S333 Y334 T335 F338 T339 D340 G341 S342 D353 Y354 K355 V356 P357 T358 G359 K360 V361 I362 K366 G367 R368 G372 F373 N374 T384 D385 I386 F392 D393
I421 L427 V428 T429 D434 V437 N442 G443 G448 E449 A450 T451 G454 D468 P469 V477 N493 P494 V497 Y506 V511 F512 D513 N514 R519 G520 D521 V525 P533 V534 I535 R549 V562 I571 T572 L577 T578 I581 H582
Y583 A584 Q585 R588 T597 T598 S599 T600 V604 T605 T606 Y607 G608 L611 H612 G613 K614 A615 E623 T626 S627 R628 V629 R630 T633 A634 N635 A636 A637 V638 F644 R647 R651 K652 D653 N654 L655 A656 F657 P662 A663 A664 K665 F666 G667 N668 D669 T670 F671
G672 V673 S674 L675 V676 D677 L678 R681 I693 Y696 S702 R703 I709 A710 Y711 F721 L724 D725 R726 Q727 D731 A732 N733 N734 D735 G736 A742 D743 N750 T751 K752 I753 G754 A762 A763 A764 N765 Y774 S778 T779 G780 D784 M789 G793
A799 I802 F803 L812 D813 S814 N815 R816 P817 Q818 I819 Y820 R821 D822 T826 I829 K833 V834 R835 R836 D842 G846 L847 D857 V858 N859 V860 V863 R864 S865 T866 T867 D868 R869 L872 A878 S879 V885 G886 N887 N888 A889 Y890 R891 T892 G893 L894
R895 C896 A897 D898 N899 N900 D907 G910 V911 L915 D922 Q923 S924 R925 T926 A927 T928 C929 F930 T931 G941 D942 N943 A944 N945 K949 D950 R954 Y961 V962 P963 T964 T965 A966 T967 A968 T969 D972 V977 D981 Y984 D985 R986 G989 V990 A991
T1002 N1003 T1004 D1007 T1023 D1024 N1028 V1029 N1036 G1037 Q1038 V1039 Y1042 A1049 N1056 L1066 I1076 G1077 V1078 A1085 Q1086 N1087 R1088 S1103 N1107 N1108 R1109 R1110 L1113 N1114 G1115 V1118 G1130 T1131 Y1132 S1135 Q1136 K1137 D1138 L1139 E1143 Y1144 G1145
S1146 G1147 I1148 Q1157 Y1163 F1167

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	252122	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 ($e^-/Å^2$)	1.3	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	1000	Depositor
Magnification	Not provided	
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	1.505	Depositor
Minimum map value	-0.702	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.047	Depositor
Recommended contour level	0.46	Depositor
Map size (Å)	431.90402, 431.90402, 431.90402	wwPDB
Map dimensions	528, 528, 528	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.818, 0.818, 0.818	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	0.35	0/7258	0.55	0/9865
1	B	0.35	0/7258	0.55	0/9865
1	C	0.35	0/7258	0.55	0/9865
All	All	0.35	0/21774	0.55	0/29595

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	696	TYR	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	7117	0	6745	131	0
1	B	7117	0	6745	125	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	7117	0	6745	139	0
All	All	21351	0	20235	382	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 9.

All (382) 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:819:ILE:HG12	1:A:829:ILE:HG12	1.52	0.91
1:A:519:ARG:HH12	1:A:693:ILE:HG22	1.43	0.84
1:B:549:ARG:HB2	1:B:562:VAL:HG23	1.67	0.77
1:A:733:ASN:OD1	1:A:734:ASN:N	2.18	0.76
1:C:878:ALA:HB1	1:C:894:LEU:HD12	1.68	0.76
1:B:384:THR:HG22	1:C:521:ASP:HB3	1.67	0.75
1:C:789:MET:HG3	1:C:814:SER:HB2	1.68	0.74
1:A:384:THR:HG22	1:B:521:ASP:HB3	1.68	0.74
1:A:228:VAL:HG11	1:B:224:LEU:HD11	1.70	0.72
1:B:878:ALA:HB1	1:B:894:LEU:HG	1.71	0.72
1:B:402:THR:HG22	1:B:418:VAL:HG22	1.73	0.71
1:C:630:ARG:HG2	1:C:638:VAL:HG22	1.72	0.71
1:B:630:ARG:HG2	1:B:638:VAL:HG22	1.74	0.69
1:A:910:GLY:O	1:A:1088:ARG:NH1	2.25	0.69
1:B:228:VAL:HG11	1:C:224:LEU:HD11	1.73	0.69
1:C:965:THR:HG23	1:C:966:ALA:H	1.58	0.68
1:C:733:ASN:OD1	1:C:734:ASN:N	2.25	0.68
1:A:878:ALA:HB1	1:A:894:LEU:HG	1.75	0.68
1:B:819:ILE:HG12	1:B:829:ILE:HG12	1.76	0.67
1:A:765:ASN:OD1	1:A:888:ASN:ND2	2.28	0.67
1:C:673:VAL:HA	1:C:764:ALA:HA	1.77	0.67
1:B:806:ARG:NH2	1:B:840:GLN:OE1	2.24	0.67
1:A:1086:GLN:O	1:A:1088:ARG:N	2.29	0.66
1:C:572:THR:HG22	1:C:578:THR:HG22	1.76	0.66
1:B:863:VAL:HG23	1:B:969:THR:HA	1.76	0.66
1:C:268:ARG:NH1	1:C:1157:GLN:OE1	2.28	0.65
1:B:1079:ARG:NH1	1:B:1081:ASP:OD1	2.29	0.65
1:C:549:ARG:HB2	1:C:562:VAL:HG13	1.78	0.65
1:B:722:ALA:O	1:B:755:GLN:NE2	2.30	0.64
1:C:651:ARG:NH1	1:C:655:LEU:O	2.29	0.64
1:B:834:VAL:HG22	1:B:860:VAL:HG22	1.79	0.64
1:B:1133:THR:HG22	1:B:1155:ARG:HG2	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:444:LYS:NZ	1:A:446:ASP:OD1	2.26	0.63
1:A:268:ARG:NH1	1:A:1157:GLN:OE1	2.31	0.63
1:A:1108:ASN:HB3	1:A:1139:LEU:HD13	1.80	0.63
1:B:232:GLU:OE1	1:C:227:ARG:NH1	2.28	0.63
1:A:1115:GLY:HA3	1:A:1132:TYR:CD2	2.34	0.62
1:A:1002:THR:HG22	1:A:1004:THR:H	1.63	0.62
1:C:1002:THR:HG22	1:C:1004:THR:H	1.65	0.62
1:A:836:ARG:NH1	1:A:896:CYS:SG	2.73	0.62
1:A:916:ASN:HB3	1:A:919:VAL:HG12	1.82	0.61
1:A:727:GLN:H	1:A:817:PRO:HG2	1.66	0.61
1:C:878:ALA:HB3	1:C:893:GLY:H	1.64	0.61
1:C:727:GLN:H	1:C:817:PRO:HG2	1.66	0.61
1:A:789:MET:HG2	1:A:814:SER:HB2	1.83	0.60
1:A:836:ARG:HD2	1:A:929:CYS:SG	2.42	0.60
1:B:257:LYS:NZ	1:B:393:ASP:OD2	2.22	0.60
1:A:863:VAL:HG12	1:A:969:THR:HG22	1.84	0.60
1:B:896:CYS:O	1:B:900:ASN:ND2	2.35	0.60
1:B:268:ARG:NH1	1:B:1157:GLN:OE1	2.34	0.59
1:A:779:THR:HG22	1:A:780:GLY:H	1.66	0.59
1:C:910:GLY:O	1:C:1088:ARG:NH1	2.36	0.59
1:A:878:ALA:HB3	1:A:893:GLY:H	1.67	0.59
1:A:549:ARG:HB2	1:A:562:VAL:HG13	1.85	0.58
1:B:1086:GLN:O	1:B:1088:ARG:N	2.35	0.58
1:A:821:ARG:O	1:A:869:ARG:HG2	2.03	0.58
1:B:1117:TYR:OH	1:B:1119:GLU:OE2	2.16	0.58
1:B:572:THR:HG22	1:B:578:THR:HG22	1.85	0.58
1:C:724:LEU:HB2	1:C:754:GLY:O	2.03	0.58
1:A:572:THR:HG22	1:A:578:THR:HG22	1.86	0.58
1:C:858:VAL:HG11	1:C:868:ASP:HB2	1.85	0.58
1:A:673:VAL:HA	1:A:764:ALA:HA	1.86	0.58
1:B:897:ALA:HA	1:B:900:ASN:HD21	1.68	0.58
1:B:1048:VAL:HG23	1:B:1050:ALA:H	1.69	0.58
1:B:988:VAL:HG23	1:B:989:GLY:H	1.69	0.57
1:A:665:LYS:HD2	1:A:665:LYS:O	2.04	0.57
1:C:819:ILE:HG12	1:C:829:ILE:HG12	1.86	0.57
1:B:799:ALA:HB1	1:B:885:VAL:HG12	1.86	0.57
1:C:1115:GLY:HA3	1:C:1132:TYR:CD2	2.40	0.57
1:A:534:VAL:HG13	1:A:535:ILE:HG22	1.86	0.57
1:A:855:TYR:HD1	1:A:933:TYR:HB3	1.68	0.57
1:A:493:ASN:HB3	1:A:494:PRO:HD3	1.87	0.56
1:A:628:ARG:HE	1:A:638:VAL:HG11	1.70	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:836:ARG:NH1	1:B:929:CYS:SG	2.75	0.56
1:A:333:SER:O	1:A:374:ASN:ND2	2.39	0.56
1:B:806:ARG:HH12	1:B:883:PRO:HB3	1.69	0.56
1:A:521:ASP:HB3	1:C:384:THR:HG22	1.88	0.56
1:C:1085:ALA:O	1:C:1110:ARG:HA	2.05	0.56
1:C:834:VAL:HG12	1:C:860:VAL:HG22	1.87	0.56
1:C:588:ARG:NH2	1:C:600:THR:O	2.30	0.56
1:C:812:LEU:HB3	1:C:834:VAL:HG22	1.88	0.56
1:A:588:ARG:NH2	1:A:600:THR:O	2.33	0.56
1:A:278:LEU:HD11	1:A:1113:LEU:HG	1.87	0.55
1:A:896:CYS:SG	1:A:929:CYS:HB2	2.47	0.55
1:C:813:ASP:OD2	1:C:833:LYS:NZ	2.32	0.55
1:C:1108:ASN:HB3	1:C:1139:LEU:HG	1.89	0.55
1:B:333:SER:O	1:B:374:ASN:ND2	2.40	0.55
1:B:779:THR:HG22	1:B:780:GLY:H	1.71	0.55
1:C:262:ILE:HG23	1:C:1163:TYR:HB3	1.88	0.55
1:C:277:ARG:NH2	1:C:306:ARG:O	2.40	0.55
1:C:1086:GLN:O	1:C:1088:ARG:N	2.40	0.55
1:A:722:ALA:O	1:A:755:GLN:NE2	2.38	0.55
1:B:368:ARG:HG3	1:B:369:ASN:H	1.72	0.55
1:A:583:TYR:OH	1:A:585:GLN:OE1	2.25	0.55
1:A:597:THR:OG1	1:A:598:THR:N	2.38	0.54
1:C:437:VAL:H	1:C:450:ALA:HB3	1.72	0.54
1:A:896:CYS:O	1:A:900:ASN:ND2	2.40	0.54
1:C:647:ARG:NH2	1:C:677:ASP:OD2	2.37	0.54
1:C:597:THR:OG1	1:C:598:THR:N	2.40	0.54
1:C:991:ALA:HA	1:C:1023:THR:HA	1.89	0.54
1:C:274:ASP:OD2	1:C:276:ASP:N	2.41	0.54
1:C:1088:ARG:HD3	1:C:1103:SER:O	2.08	0.54
1:C:519:ARG:HD2	1:C:549:ARG:HG2	1.90	0.54
1:A:512:PHE:CZ	1:A:584:ALA:HB1	2.43	0.54
1:A:907:ASP:OD1	1:A:907:ASP:N	2.41	0.54
1:B:583:TYR:OH	1:B:585:GLN:OE1	2.26	0.53
1:C:990:VAL:HG22	1:C:1024:ASP:HB2	1.90	0.53
1:C:497:VAL:HG22	1:C:525:VAL:HG22	1.88	0.53
1:A:689:ASN:ND2	1:A:695:GLU:O	2.41	0.53
1:A:1085:ALA:O	1:A:1110:ARG:HA	2.08	0.53
1:B:368:ARG:HG3	1:B:369:ASN:N	2.23	0.53
1:B:858:VAL:HG11	1:B:868:ASP:HB3	1.91	0.53
1:B:662:PRO:HB3	1:B:674:SER:HB3	1.91	0.53
1:A:540:PRO:HA	1:A:570:GLN:O	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1060:TYR:HE2	1:B:1080:TYR:HE1	1.57	0.53
1:A:338:PHE:O	1:A:366:LYS:NZ	2.42	0.53
1:A:740:ARG:HG2	1:A:746:VAL:HG12	1.91	0.53
1:A:954:ARG:NH2	1:A:981:ASP:OD2	2.41	0.53
1:A:864:ARG:HD2	1:A:961:TYR:CE1	2.44	0.52
1:A:474:TYR:CE1	1:B:480:ARG:HG3	2.45	0.52
1:C:857:ASP:HA	1:C:931:THR:HG23	1.92	0.52
1:C:325:LEU:HB3	1:C:1136:GLN:OE1	2.10	0.52
1:A:942:ASP:OD2	1:A:943:ASN:N	2.43	0.52
1:C:278:LEU:HD11	1:C:1113:LEU:HG	1.90	0.52
1:C:392:PHE:HB2	1:C:427:LEU:HB2	1.92	0.52
1:C:512:PHE:CZ	1:C:584:ALA:HB1	2.45	0.52
1:A:623:GLU:O	1:A:644:PHE:HA	2.10	0.52
1:A:813:ASP:OD1	1:A:835:ARG:NH1	2.28	0.52
1:B:351:PRO:HB2	1:B:371:PHE:CD2	2.45	0.51
1:C:534:VAL:HG13	1:C:535:ILE:HG12	1.92	0.51
1:A:610:ASP:N	1:A:610:ASP:OD2	2.43	0.51
1:C:429:THR:HG22	1:C:477:VAL:HG22	1.91	0.51
1:C:866:THR:HB	1:C:963:PRO:HD3	1.91	0.51
1:A:251:ARG:O	1:A:395:SER:OG	2.24	0.51
1:B:597:THR:OG1	1:B:598:THR:N	2.42	0.51
1:B:336:VAL:HG12	1:B:371:PHE:CD1	2.46	0.51
1:A:351:PRO:HB2	1:A:371:PHE:CD2	2.46	0.51
1:C:333:SER:O	1:C:374:ASN:ND2	2.44	0.51
1:C:907:ASP:N	1:C:907:ASP:OD1	2.44	0.51
1:A:506:TYR:HA	1:A:512:PHE:O	2.11	0.51
1:B:1115:GLY:HA3	1:B:1132:TYR:CD2	2.46	0.51
1:A:836:ARG:HG3	1:A:858:VAL:HG22	1.93	0.51
1:B:623:GLU:O	1:B:644:PHE:HA	2.11	0.50
1:B:673:VAL:HA	1:B:764:ALA:HA	1.92	0.50
1:C:493:ASN:HB3	1:C:494:PRO:HD3	1.93	0.50
1:A:662:PRO:HB3	1:A:674:SER:HB3	1.92	0.50
1:C:451:THR:O	1:C:454:GLY:N	2.30	0.50
1:B:262:ILE:HG23	1:B:1163:TYR:HB3	1.94	0.50
1:C:709:ILE:HG22	1:C:711:TYR:H	1.76	0.50
1:B:450:ALA:O	1:B:451:THR:OG1	2.29	0.50
1:B:836:ARG:HD2	1:B:929:CYS:SG	2.52	0.50
1:C:836:ARG:HG3	1:C:858:VAL:HG22	1.93	0.49
1:B:821:ARG:O	1:B:869:ARG:HG2	2.12	0.49
1:C:656:ALA:HB2	1:C:711:TYR:CZ	2.48	0.49
1:B:512:PHE:HE1	1:B:693:ILE:HB	1.78	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:519:ARG:HH21	1:A:549:ARG:HD2	1.78	0.49
1:B:779:THR:HG22	1:B:780:GLY:N	2.28	0.49
1:B:855:TYR:HD1	1:B:933:TYR:HB3	1.76	0.49
1:C:583:TYR:OH	1:C:585:GLN:OE1	2.30	0.49
1:A:226:GLY:O	1:A:230:THR:HG23	2.13	0.49
1:B:400:GLN:OE1	1:B:420:GLN:NE2	2.46	0.49
1:B:620:LEU:HD13	1:B:648:VAL:HG22	1.95	0.49
1:C:965:THR:HG23	1:C:966:ALA:N	2.27	0.49
1:C:1138:ASP:HB3	1:C:1144:TYR:HE2	1.77	0.49
1:A:521:ASP:HB3	1:C:384:THR:H	1.79	0.48
1:B:1108:ASN:HB3	1:B:1139:LEU:HG	1.95	0.48
1:C:512:PHE:HE1	1:C:693:ILE:HB	1.79	0.48
1:C:611:LEU:O	1:C:611:LEU:HD23	2.13	0.48
1:A:497:VAL:HG22	1:A:525:VAL:HG22	1.96	0.48
1:C:577:LEU:HA	1:C:613:GLY:HA3	1.95	0.48
1:A:262:ILE:HG23	1:A:1163:TYR:HB3	1.95	0.48
1:B:836:ARG:HG3	1:B:858:VAL:HG22	1.95	0.48
1:B:260:LEU:HD22	1:C:421:ILE:HD12	1.95	0.47
1:C:664:ALA:HB1	1:C:666:PHE:CZ	2.48	0.47
1:C:879:SER:HB3	1:C:890:TYR:CE2	2.48	0.47
1:A:272:ASN:ND2	1:A:316:ASP:OD2	2.37	0.47
1:A:656:ALA:HB2	1:A:711:TYR:CZ	2.50	0.47
1:A:882:GLU:OE2	1:A:883:PRO:HD2	2.14	0.47
1:A:977:VAL:HG22	1:A:1002:THR:HG23	1.95	0.47
1:A:1164:LYS:O	1:B:404:GLY:N	2.47	0.47
1:A:681:ARG:NH1	1:A:876:TYR:OH	2.48	0.47
1:A:681:ARG:HD3	1:A:721:PHE:CD1	2.49	0.47
1:C:802:ILE:HG13	1:C:803:PHE:CD1	2.50	0.47
1:A:627:SER:HB3	1:A:641:SER:H	1.79	0.47
1:A:879:SER:HB3	1:A:890:TYR:CE2	2.50	0.47
1:C:606:THR:HA	1:C:626:THR:O	2.14	0.47
1:A:819:ILE:HG21	1:A:827:GLN:HE21	1.79	0.47
1:A:510:TYR:HD2	1:A:623:GLU:HG2	1.79	0.47
1:C:779:THR:HG22	1:C:780:GLY:H	1.78	0.47
1:C:821:ARG:O	1:C:869:ARG:HG2	2.14	0.47
1:C:675:LEU:HD21	1:C:678:LEU:HB2	1.97	0.47
1:A:819:ILE:CG2	1:A:827:GLN:HE21	2.28	0.47
1:C:725:ASP:HB3	1:C:752:LYS:HD3	1.97	0.47
1:A:249:LEU:HD21	1:C:250:GLU:HG3	1.97	0.47
1:B:227:ARG:O	1:B:230:THR:HG22	2.15	0.47
1:B:588:ARG:NH2	1:B:600:THR:O	2.35	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:234:ARG:O	1:B:237:THR:HG22	2.15	0.46
1:B:1056:ASN:OD1	1:B:1086:GLN:HB2	2.15	0.46
1:C:581:ILE:HD12	1:C:608:GLY:O	2.14	0.46
1:C:335:THR:O	1:C:372:GLY:N	2.43	0.46
1:A:512:PHE:HE1	1:A:693:ILE:HB	1.80	0.46
1:A:645:TYR:CD2	1:A:647:ARG:HG3	2.51	0.46
1:C:514:ASN:OD1	1:C:519:ARG:HB2	2.15	0.46
1:C:675:LEU:HD12	1:C:762:ALA:HB2	1.96	0.46
1:A:1036:ASN:OD1	1:A:1037:GLY:N	2.42	0.46
1:B:988:VAL:HG23	1:B:989:GLY:N	2.29	0.46
1:A:313:ASN:OD1	1:A:380:LYS:HG3	2.16	0.46
1:C:726:ARG:NH1	1:C:817:PRO:HD3	2.31	0.46
1:C:879:SER:HA	1:C:891:ARG:O	2.16	0.46
1:B:1066:LEU:HB2	1:B:1076:ILE:HG22	1.98	0.46
1:A:697:GLY:HA3	1:A:717:VAL:HG11	1.97	0.46
1:A:984:TYR:OH	1:A:986:ARG:HD2	2.15	0.46
1:B:506:TYR:HD1	1:B:513:ASP:HA	1.81	0.46
1:B:657:PHE:CE2	1:B:720:PRO:HB3	2.50	0.46
1:A:495:VAL:HG22	1:A:527:VAL:HG13	1.97	0.45
1:A:262:ILE:CD1	1:A:386:ILE:HG13	2.45	0.45
1:A:655:LEU:HB3	1:A:718:THR:HG21	1.98	0.45
1:A:806:ARG:NH1	1:A:883:PRO:HD3	2.31	0.45
1:A:894:LEU:O	1:A:896:CYS:N	2.48	0.45
1:C:778:SER:O	1:C:816:ARG:NH1	2.47	0.45
1:A:856:ARG:HH22	1:A:900:ASN:HB3	1.82	0.45
1:B:1085:ALA:O	1:B:1110:ARG:HA	2.16	0.45
1:B:727:GLN:HG2	1:B:750:ASN:OD1	2.16	0.45
1:B:907:ASP:OD1	1:B:1102:PHE:HB2	2.16	0.45
1:A:681:ARG:HG2	1:A:721:PHE:CD2	2.51	0.45
1:B:1029:VAL:HG13	1:B:1033:PRO:HD2	1.99	0.45
1:C:864:ARG:HB3	1:C:961:TYR:CE2	2.50	0.45
1:A:336:VAL:HG12	1:A:371:PHE:CD1	2.52	0.45
1:B:779:THR:OG1	1:B:788:ARG:NH2	2.48	0.45
1:C:984:TYR:OH	1:C:986:ARG:HD2	2.17	0.45
1:A:864:ARG:HB3	1:A:961:TYR:CE2	2.52	0.45
1:B:666:PHE:HB2	1:B:673:VAL:HG13	1.99	0.45
1:B:519:ARG:HG2	1:B:549:ARG:HG2	1.99	0.45
1:A:857:ASP:OD1	1:A:864:ARG:NH1	2.50	0.45
1:B:580:GLY:O	1:B:609:ALA:HA	2.17	0.45
1:B:652:LYS:HG3	1:B:658:ASP:HB2	1.98	0.44
1:B:869:ARG:N	1:B:869:ARG:HD2	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:577:LEU:HG	1:C:615:ALA:HB2	2.00	0.44
1:C:628:ARG:HE	1:C:638:VAL:HG11	1.82	0.44
1:C:681:ARG:HD3	1:C:721:PHE:CG	2.52	0.44
1:B:757:GLY:HA3	1:B:777:THR:O	2.16	0.44
1:C:260:LEU:HD11	1:C:386:ILE:HG23	1.99	0.44
1:C:647:ARG:HD3	1:C:657:PHE:CE2	2.52	0.44
1:C:662:PRO:HB3	1:C:674:SER:HB3	1.99	0.44
1:A:795:SER:HB3	1:A:808:THR:HG23	1.98	0.44
1:B:632:ASN:HB3	1:B:633:THR:H	1.58	0.44
1:C:262:ILE:CD1	1:C:386:ILE:HG13	2.47	0.44
1:C:1078:VAL:HG13	1:C:1118:VAL:HG22	1.99	0.44
1:B:292:PHE:CE2	1:B:1130:GLY:HA3	2.52	0.44
1:A:588:ARG:NH1	1:A:596:ASN:HD22	2.16	0.44
1:A:869:ARG:HD2	1:A:869:ARG:N	2.33	0.44
1:B:512:PHE:CZ	1:B:584:ALA:HB1	2.52	0.44
1:C:512:PHE:CE1	1:C:693:ILE:HB	2.52	0.44
1:A:442:ASN:HD21	1:A:446:ASP:CG	2.21	0.44
1:A:588:ARG:CZ	1:A:596:ASN:HD22	2.31	0.44
1:B:510:TYR:O	1:B:687:TYR:OH	2.22	0.44
1:B:437:VAL:H	1:B:450:ALA:HB3	1.83	0.44
1:C:240:ASN:HA	1:C:243:THR:HG22	2.00	0.44
1:B:392:PHE:HD2	1:B:427:LEU:HB2	1.83	0.44
1:B:368:ARG:NH1	1:B:369:ASN:HB2	2.32	0.44
1:B:1109:ARG:HB3	1:B:1136:GLN:HG2	1.99	0.44
1:C:571:ILE:O	1:C:578:THR:HA	2.17	0.44
1:A:1108:ASN:HB3	1:A:1139:LEU:CD1	2.46	0.43
1:B:677:ASP:OD2	1:B:678:LEU:N	2.51	0.43
1:B:897:ALA:HB2	1:B:927:ALA:HA	1.99	0.43
1:C:506:TYR:HA	1:C:512:PHE:O	2.18	0.43
1:A:383:SER:OG	1:B:552:LEU:HD23	2.18	0.43
1:A:394:THR:HG21	1:A:425:PHE:CE2	2.53	0.43
1:A:779:THR:HG22	1:A:780:GLY:N	2.32	0.43
1:B:256:VAL:HG22	1:B:392:PHE:HD1	1.83	0.43
1:B:506:TYR:HA	1:B:512:PHE:O	2.18	0.43
1:C:262:ILE:HD13	1:C:386:ILE:HG13	1.99	0.43
1:C:604:VAL:HG23	1:C:629:VAL:HG22	1.99	0.43
1:C:1146:SER:O	1:C:1148:ILE:N	2.51	0.43
1:A:506:TYR:HD1	1:A:513:ASP:HA	1.83	0.43
1:B:577:LEU:HA	1:B:613:GLY:HA3	2.00	0.43
1:C:623:GLU:O	1:C:644:PHE:HA	2.18	0.43
1:C:942:ASP:N	1:C:942:ASP:OD1	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1036:ASN:OD1	1:C:1037:GLY:N	2.51	0.43
1:A:277:ARG:NH2	1:A:306:ARG:O	2.51	0.43
1:A:630:ARG:HG2	1:A:636:ALA:HB1	2.01	0.43
1:A:879:SER:HB3	1:A:890:TYR:CZ	2.53	0.43
1:B:493:ASN:HB3	1:B:494:PRO:HD3	2.00	0.43
1:C:257:LYS:HZ1	1:C:393:ASP:CG	2.21	0.43
1:A:510:TYR:O	1:A:687:TYR:OH	2.23	0.43
1:B:743:ASP:OD1	1:B:744:GLY:N	2.51	0.43
1:C:290:ASN:OD1	1:C:290:ASN:N	2.51	0.43
1:C:784:ASP:OD1	1:C:784:ASP:N	2.52	0.43
1:B:511:VAL:HG21	1:B:582:HIS:NE2	2.34	0.43
1:C:231:VAL:O	1:C:235:VAL:HG23	2.18	0.43
1:B:510:TYR:HD2	1:B:623:GLU:HG2	1.84	0.42
1:B:571:ILE:HG13	1:B:573:PRO:HD3	2.00	0.42
1:B:1057:ALA:HB2	1:B:1088:ARG:HD3	2.00	0.42
1:A:897:ALA:HB2	1:A:927:ALA:HA	2.00	0.42
1:A:797:LYS:HE3	1:A:799:ALA:HB2	2.00	0.42
1:B:364:THR:HG22	1:B:366:LYS:HG3	1.99	0.42
1:C:774:TYR:CZ	1:C:793:GLY:HA3	2.54	0.42
1:C:897:ALA:O	1:C:925:ARG:HG2	2.18	0.42
1:B:351:PRO:CG	1:B:368:ARG:HH21	2.33	0.42
1:B:401:VAL:HG23	1:B:419:ASN:HB2	2.01	0.42
1:B:990:VAL:HG22	1:B:1024:ASP:HB2	2.01	0.42
1:C:868:ASP:HB3	1:C:929:CYS:SG	2.59	0.42
1:A:577:LEU:HA	1:A:613:GLY:HA3	2.01	0.42
1:A:1146:SER:O	1:A:1148:ILE:N	2.52	0.42
1:C:511:VAL:HG21	1:C:582:HIS:CD2	2.54	0.42
1:C:1066:LEU:HB2	1:C:1076:ILE:HG22	2.00	0.42
1:B:847:LEU:O	1:B:946:ALA:HA	2.19	0.42
1:B:864:ARG:HB3	1:B:961:TYR:CE2	2.54	0.42
1:C:895:ARG:HB3	1:C:898:ASP:OD2	2.19	0.42
1:C:1107:ASN:N	1:C:1107:ASN:OD1	2.53	0.42
1:C:834:VAL:HG21	1:C:872:LEU:HD22	2.02	0.42
1:C:863:VAL:HG23	1:C:969:THR:HA	2.00	0.42
1:A:696:TYR:CD2	1:A:715:THR:HB	2.55	0.42
1:B:848:GLY:HA2	1:B:943:ASN:HD22	1.85	0.42
1:B:1142:VAL:HB	1:B:1144:TYR:CE1	2.54	0.42
1:A:603:ASP:OD1	1:A:604:VAL:N	2.53	0.42
1:B:517:ASP:HB2	1:B:695:GLU:OE1	2.20	0.42
1:C:651:ARG:HD3	1:C:655:LEU:HA	2.01	0.42
1:C:664:ALA:HB3	1:C:675:LEU:H	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:365:THR:HG23	1:A:369:ASN:HA	2.02	0.42
1:A:511:VAL:HG21	1:A:582:HIS:NE2	2.35	0.42
1:A:598:THR:HB	1:A:599:SER:H	1.73	0.42
1:B:445:LYS:HE3	1:B:449:GLU:H	1.85	0.42
1:B:702:SER:O	1:B:703:ARG:HB2	2.20	0.42
1:B:791:GLU:OE1	1:B:875:GLY:HA3	2.19	0.42
1:A:819:ILE:O	1:A:874:ARG:NH2	2.53	0.41
1:C:468:ASP:OD1	1:C:469:PRO:HD2	2.19	0.41
1:B:251:ARG:O	1:B:395:SER:OG	2.21	0.41
1:B:725:ASP:HB3	1:B:752:LYS:HD3	2.02	0.41
1:C:869:ARG:HD2	1:C:869:ARG:N	2.36	0.41
1:A:1041:TYR:HD1	1:A:1058:THR:HG1	1.68	0.41
1:A:1107:ASN:O	1:A:1109:ARG:N	2.53	0.41
1:B:515:ASN:O	1:B:516:TYR:HB3	2.19	0.41
1:B:710:ALA:HB2	1:B:722:ALA:HA	2.02	0.41
1:C:434:ASP:OD1	1:C:434:ASP:N	2.43	0.41
1:C:896:CYS:HB2	1:C:929:CYS:HB3	2.02	0.41
1:C:897:ALA:HB2	1:C:927:ALA:HA	2.01	0.41
1:A:512:PHE:CE1	1:A:693:ILE:HB	2.56	0.41
1:A:627:SER:OG	1:A:629:VAL:HG23	2.20	0.41
1:B:442:ASN:HD21	1:B:446:ASP:CG	2.23	0.41
1:A:377:ALA:HB1	1:B:591:PHE:CZ	2.56	0.41
1:A:822:ASP:OD2	1:A:822:ASP:N	2.53	0.41
1:B:512:PHE:CE1	1:B:693:ILE:HB	2.55	0.41
1:C:577:LEU:HD22	1:C:611:LEU:HD23	2.01	0.41
1:A:774:TYR:CZ	1:A:793:GLY:HA3	2.55	0.41
1:C:652:LYS:HG2	1:C:653:ASP:H	1.85	0.41
1:C:822:ASP:OD2	1:C:826:THR:OG1	2.38	0.41
1:C:1135:SER:OG	1:C:1143:GLU:OE1	2.37	0.41
1:C:437:VAL:HB	1:C:450:ALA:HB2	2.02	0.41
1:B:351:PRO:HG2	1:B:368:ARG:HH21	1.85	0.41
1:C:292:PHE:CE2	1:C:1130:GLY:HA3	2.55	0.41
1:C:442:ASN:OD1	1:C:443:GLY:N	2.54	0.41
1:C:506:TYR:HD1	1:C:513:ASP:HA	1.86	0.41
1:C:702:SER:O	1:C:703:ARG:HB2	2.20	0.41
1:C:725:ASP:OD1	1:C:725:ASP:N	2.54	0.41
1:C:1056:ASN:OD1	1:C:1086:GLN:HB2	2.20	0.41
1:A:847:LEU:O	1:A:946:ALA:HA	2.21	0.41
1:A:907:ASP:OD2	1:A:912:GLY:HA2	2.21	0.41
1:B:595:GLN:O	1:B:595:GLN:HG2	2.20	0.41
1:B:774:TYR:CZ	1:B:793:GLY:HA3	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:950:ASP:OD1	1:B:950:ASP:N	2.45	0.41
1:C:896:CYS:O	1:C:900:ASN:ND2	2.54	0.41
1:C:954:ARG:HE	1:C:954:ARG:HB3	1.69	0.41
1:A:734:ASN:ND2	1:A:737:THR:OG1	2.54	0.41
1:A:1140:ASN:HB2	1:A:1142:VAL:HG23	2.03	0.41
1:B:262:ILE:CD1	1:B:386:ILE:HG12	2.51	0.41
1:B:506:TYR:CD1	1:B:513:ASP:HA	2.56	0.41
1:B:907:ASP:OD2	1:B:912:GLY:HA2	2.21	0.41
1:C:256:VAL:HG22	1:C:392:PHE:HD1	1.86	0.41
1:C:922:ASP:HA	1:C:981:ASP:OD2	2.21	0.41
1:A:725:ASP:N	1:A:725:ASP:OD1	2.54	0.40
1:B:512:PHE:O	1:B:514:ASN:N	2.54	0.40
1:B:606:THR:HA	1:B:626:THR:O	2.21	0.40
1:C:799:ALA:HB1	1:C:885:VAL:HG12	2.02	0.40
1:C:911:VAL:HG23	1:C:1042:TYR:HB2	2.03	0.40
1:C:977:VAL:HG22	1:C:1002:THR:HG23	2.04	0.40
1:A:234:ARG:HA	1:A:237:THR:HG22	2.04	0.40
1:A:915:LEU:HD21	1:A:1039:VAL:O	2.21	0.40
1:B:262:ILE:HD13	1:B:386:ILE:HG12	2.03	0.40
1:B:333:SER:HA	1:B:346:PHE:O	2.22	0.40
1:C:727:GLN:HG2	1:C:750:ASN:OD1	2.21	0.40
1:C:915:LEU:HD21	1:C:1039:VAL:O	2.22	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	947/1167 (81%)	826 (87%)	118 (12%)	3 (0%)	41	70
1	B	947/1167 (81%)	838 (88%)	104 (11%)	5 (0%)	29	59
1	C	947/1167 (81%)	844 (89%)	99 (10%)	4 (0%)	34	64

Continued on next page...

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	2841/3501 (81%)	2508 (88%)	321 (11%)	12 (0%)	38 64

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	598	THR
1	B	986	ARG
1	B	818	GLN
1	C	818	GLN
1	C	1087	ASN
1	A	1087	ASN
1	C	986	ARG
1	A	986	ARG
1	B	598	THR
1	B	1087	ASN
1	B	636	ALA
1	C	598	THR

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	726/891 (82%)	723 (100%)	3 (0%)	91 97
1	B	726/891 (82%)	725 (100%)	1 (0%)	93 98
1	C	726/891 (82%)	726 (100%)	0	100 100
All	All	2178/2673 (82%)	2174 (100%)	4 (0%)	93 98

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	368	ARG
1	A	665	LYS
1	A	992	ASN
1	B	681	ARG

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

Mol	Chain	Res	Type
1	A	596	ASN
1	A	708	ASN
1	A	734	ASN
1	A	992	ASN
1	B	570	GLN
1	B	708	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

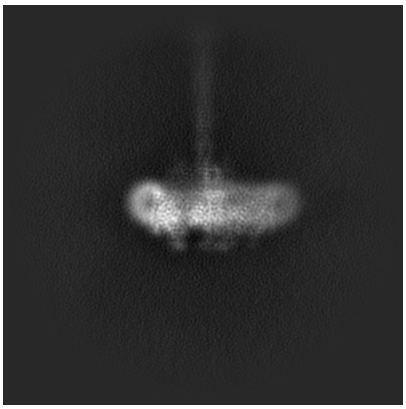
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-14714. These allow visual inspection of the internal detail of the map and identification of artifacts.

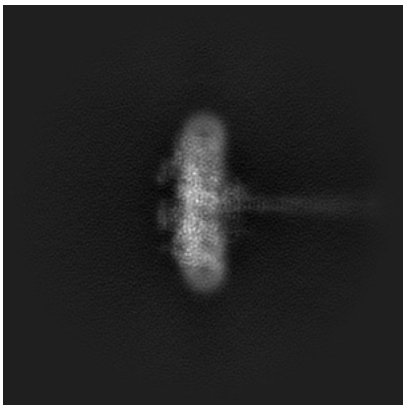
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

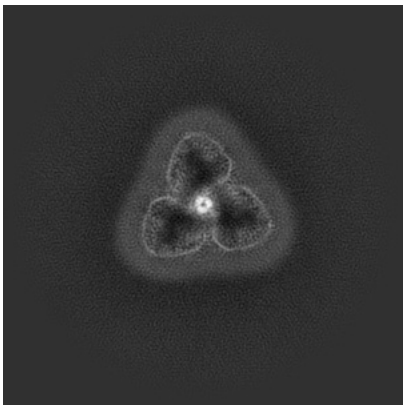
6.1.1 Primary map



X

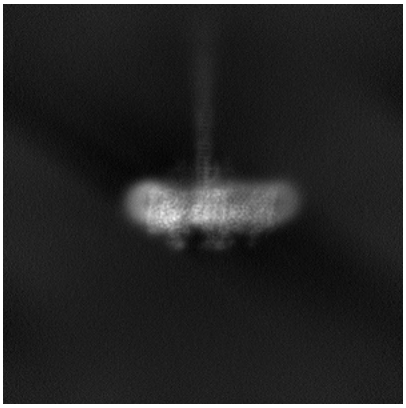


Y

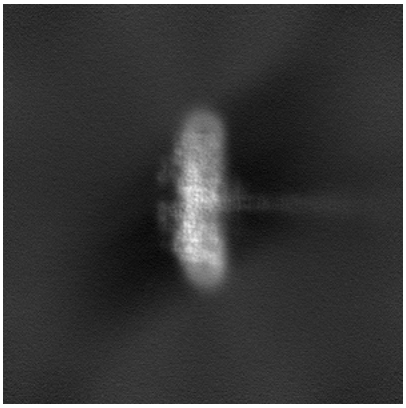


Z

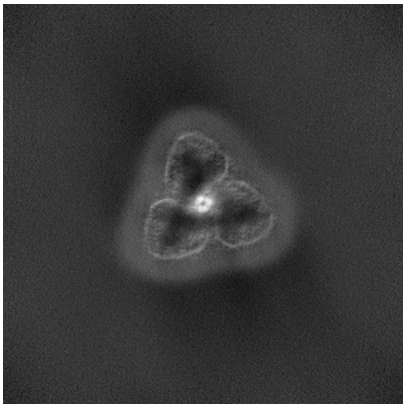
6.1.2 Raw map



X



Y

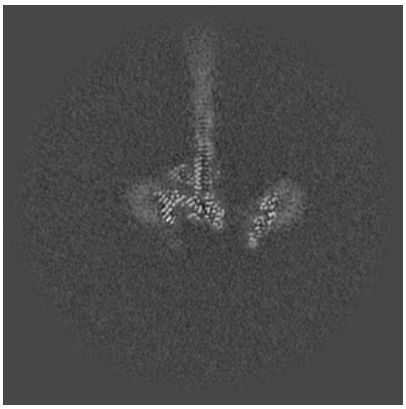


Z

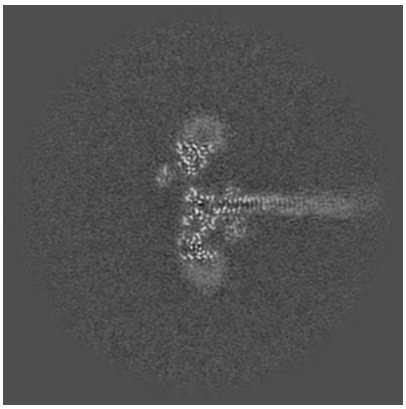
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

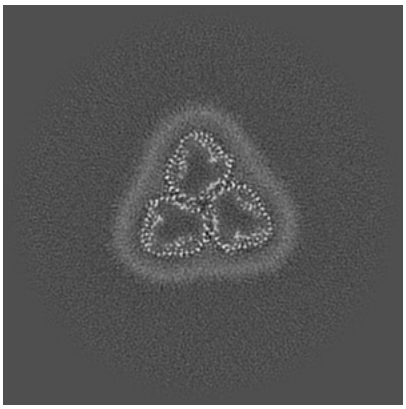
6.2.1 Primary map



X Index: 264

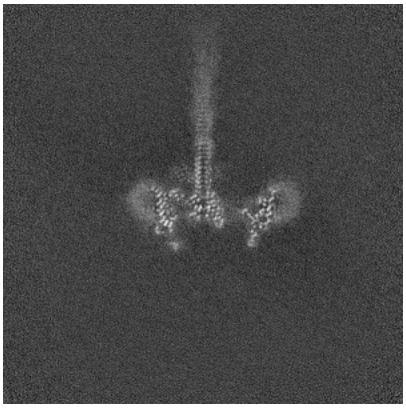


Y Index: 264

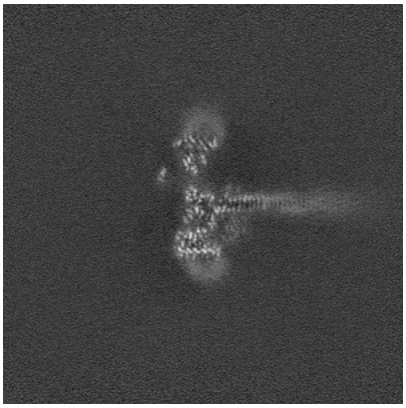


Z Index: 264

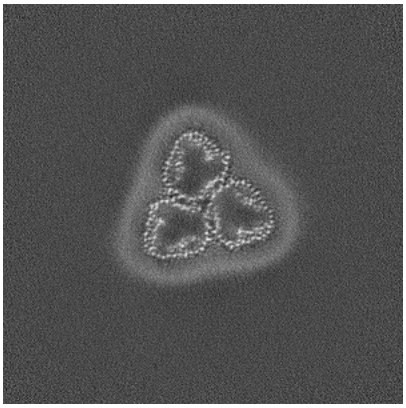
6.2.2 Raw map



X Index: 264



Y Index: 264

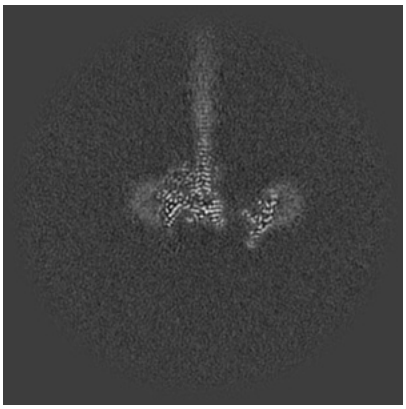


Z Index: 264

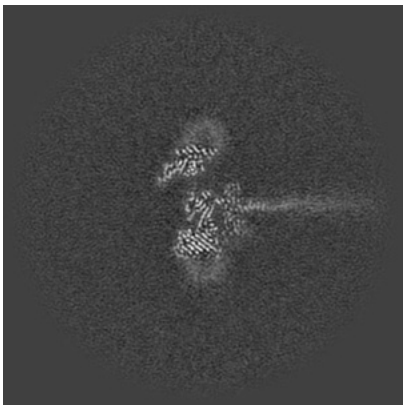
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

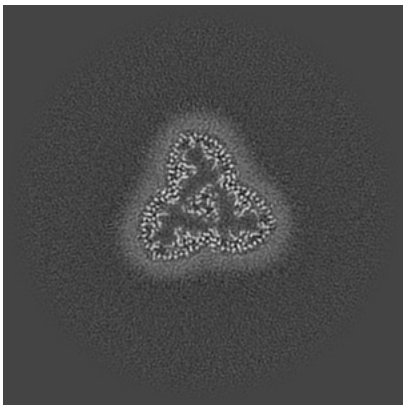
6.3.1 Primary map



X Index: 268

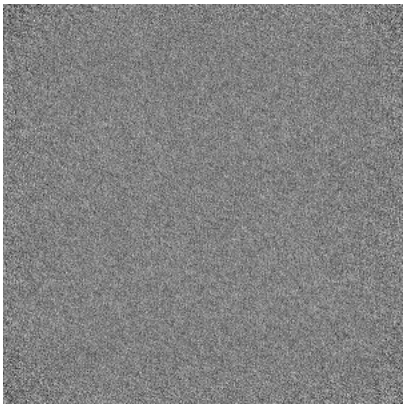


Y Index: 272

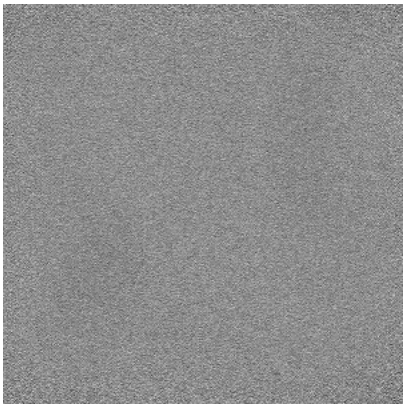


Z Index: 246

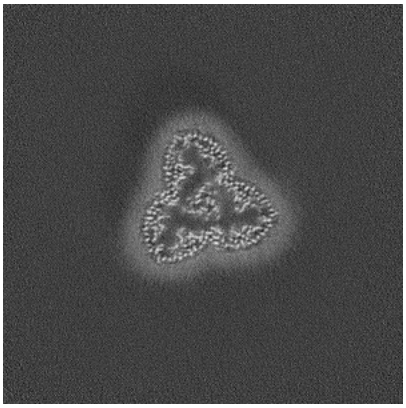
6.3.2 Raw map



X Index: 0



Y Index: 0

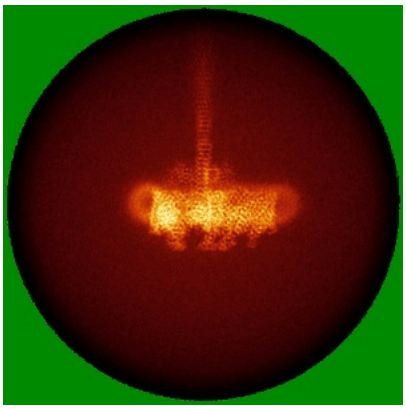


Z Index: 246

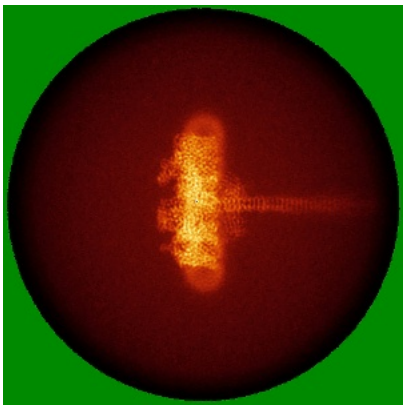
The images above show the largest variance slices of the map in three orthogonal directions.

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

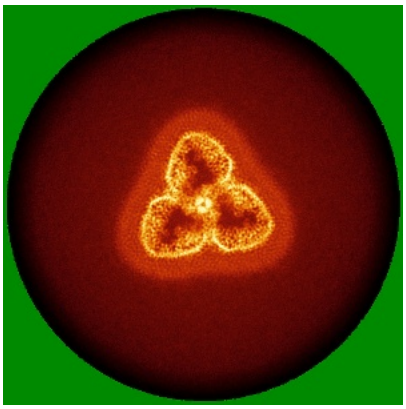
6.4.1 Primary map



X

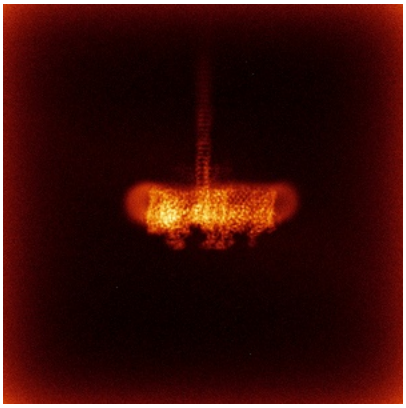


Y

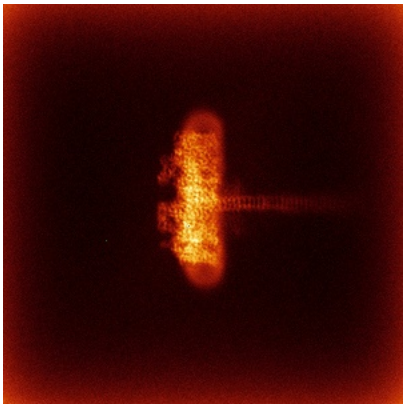


Z

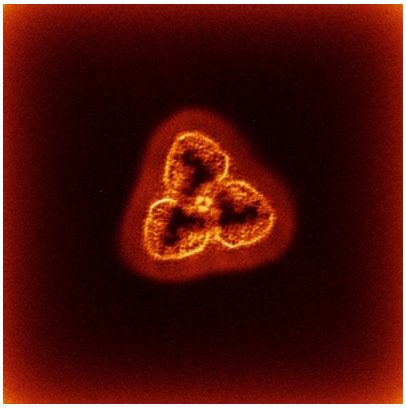
6.4.2 Raw map



X



Y



Z

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

6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.46. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map

X Y Z

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

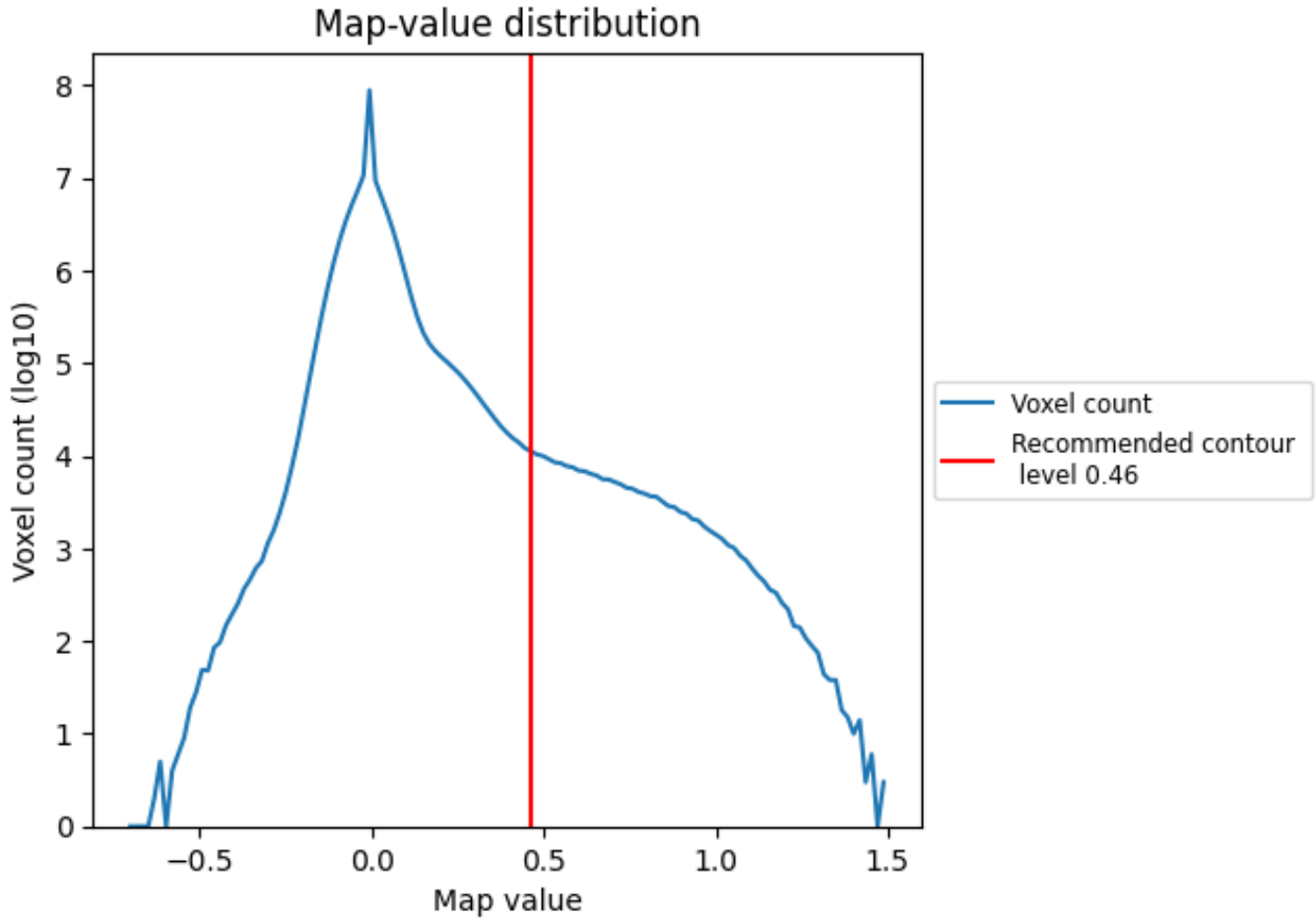
6.6 Mask visualisation (i)

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

7 Map analysis

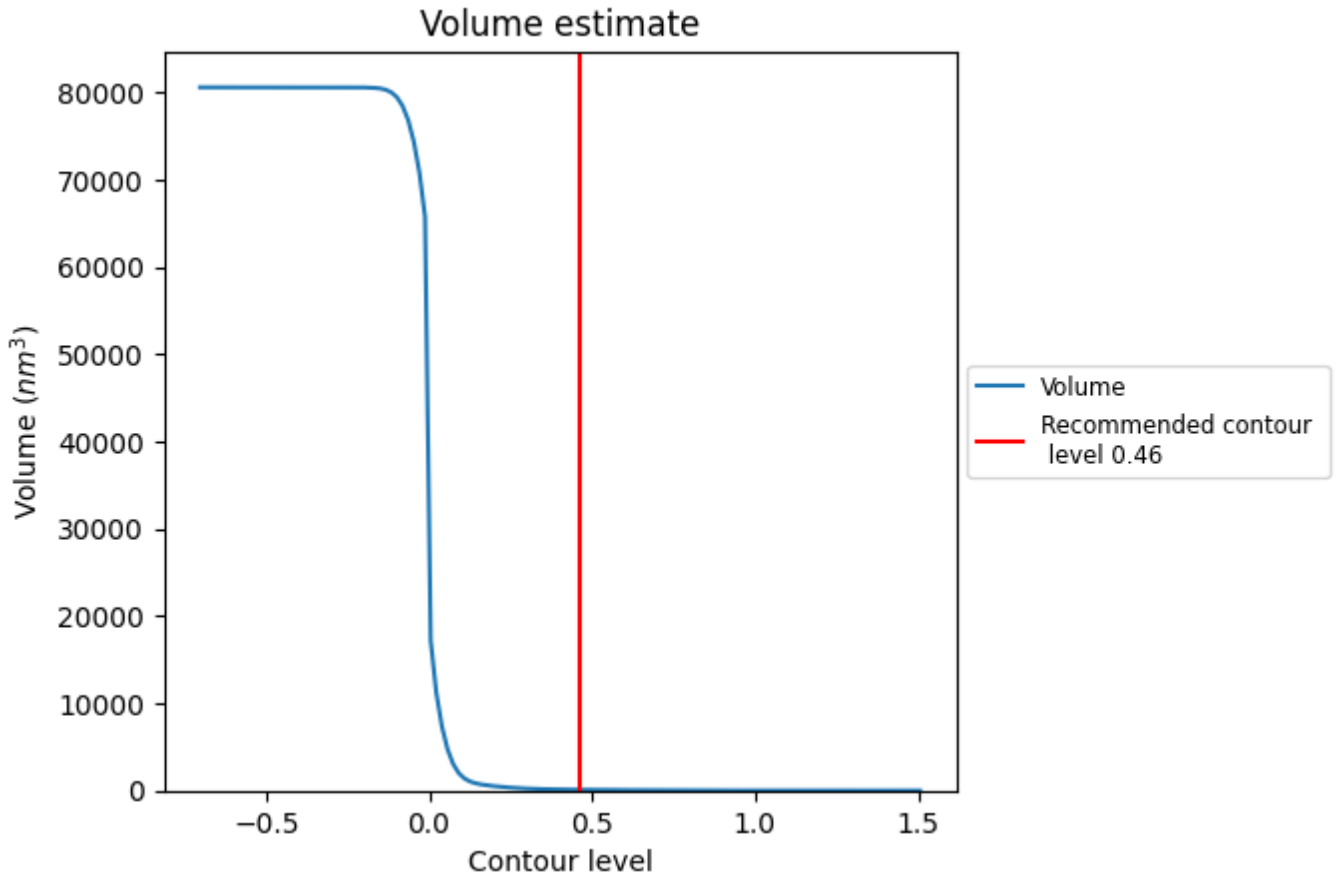
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

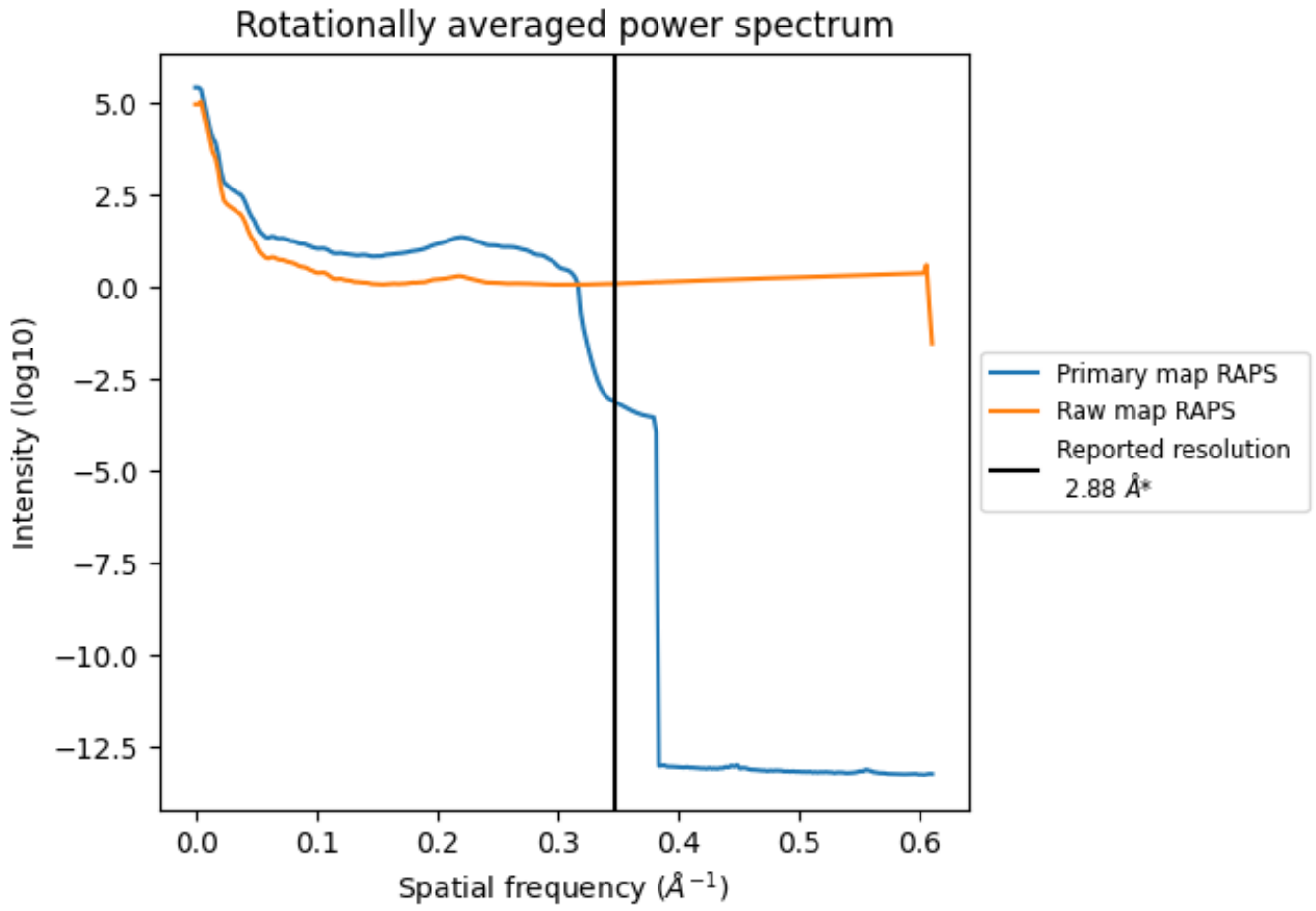
7.2 Volume estimate (i)



The volume at the recommended contour level is 97 nm^3; this corresponds to an approximate mass of 88 kDa.

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

7.3 Rotationally averaged power spectrum (i)

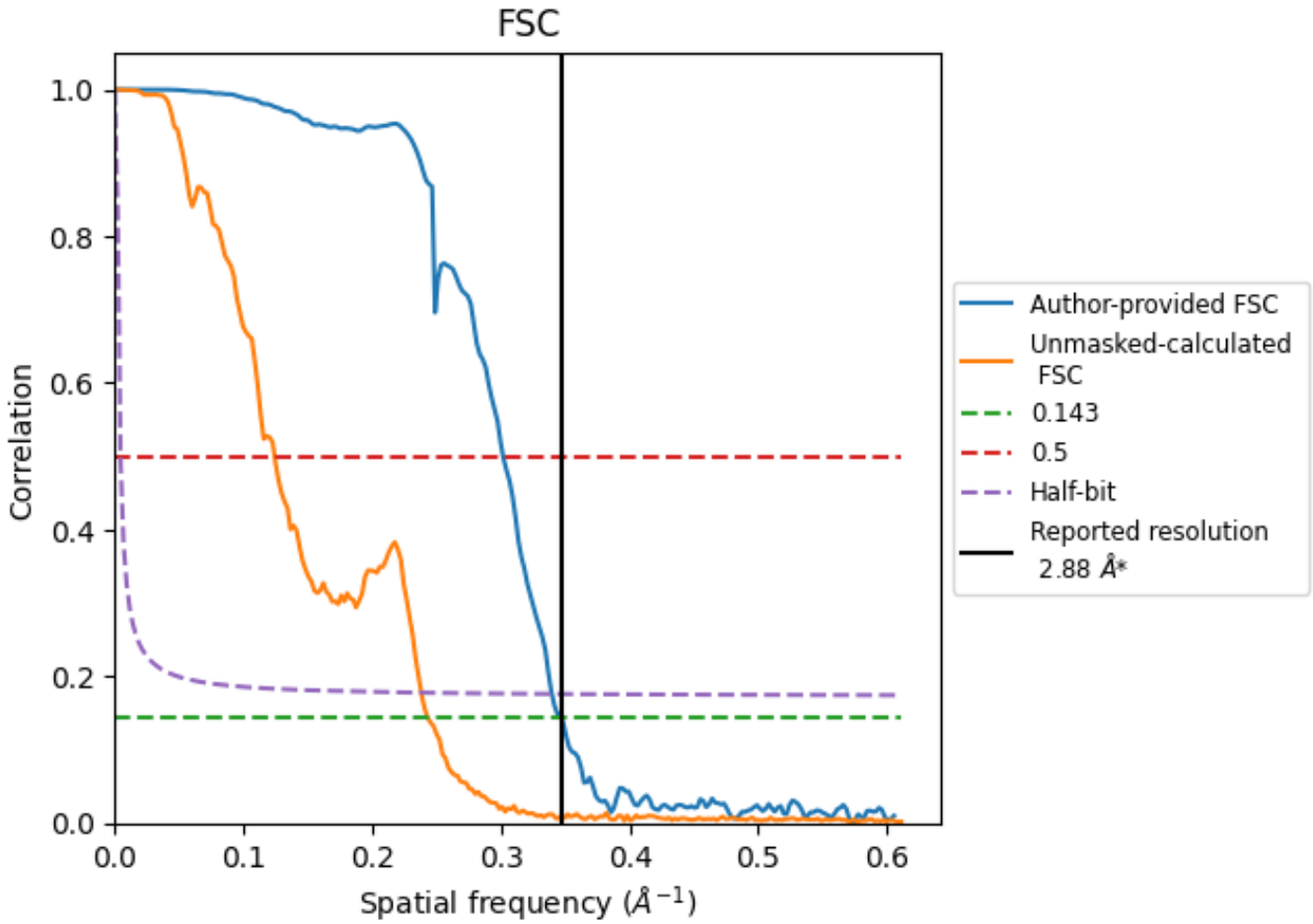


*Reported resolution corresponds to spatial frequency of 0.347 Å^{-1}

8 Fourier-Shell correlation

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

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.347 Å^{-1}

8.2 Resolution estimates (i)

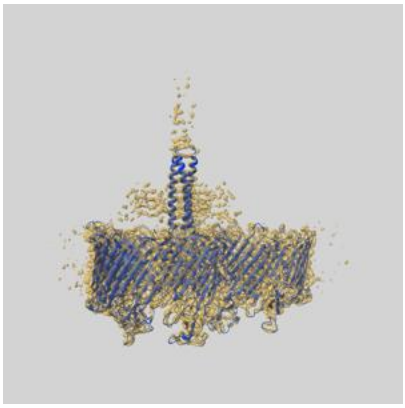
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.88	-	-
Author-provided FSC curve	2.88	3.31	2.94
Unmasked-calculated*	4.11	8.05	4.20

*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 4.11 differs from the reported value 2.88 by more than 10 %

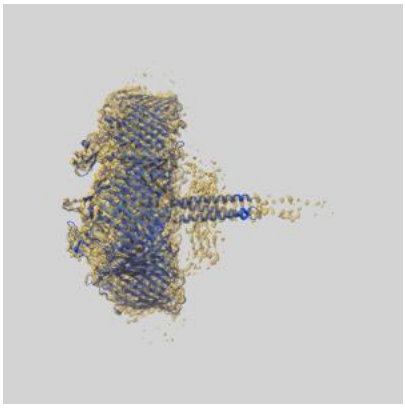
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-14714 and PDB model 7ZGX. Per-residue inclusion information can be found in section 3 on page 4.

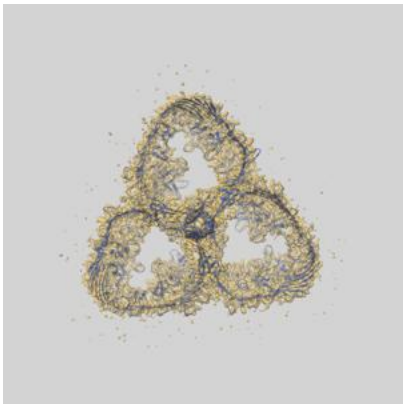
9.1 Map-model overlay



X



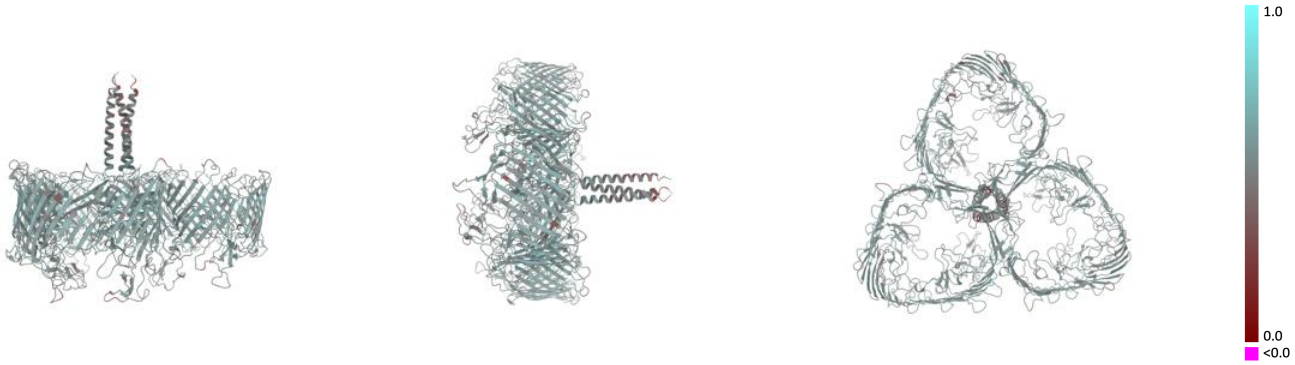
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.46 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.

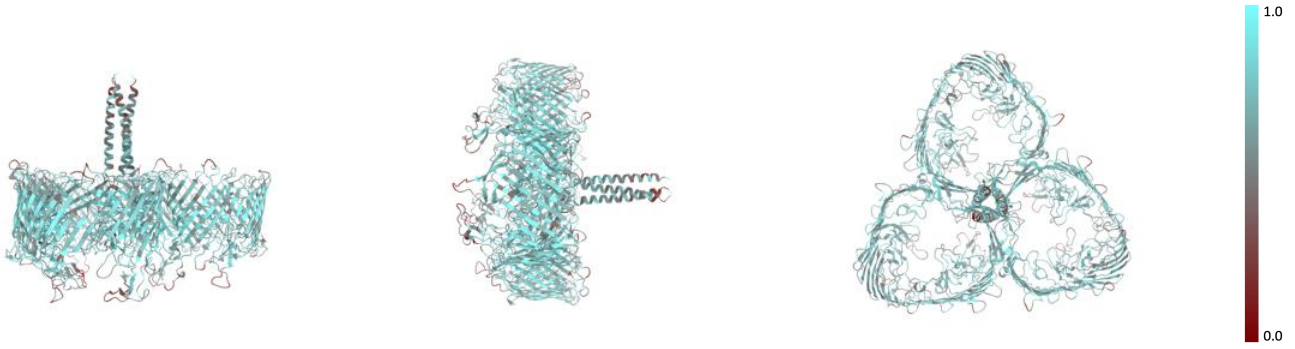
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

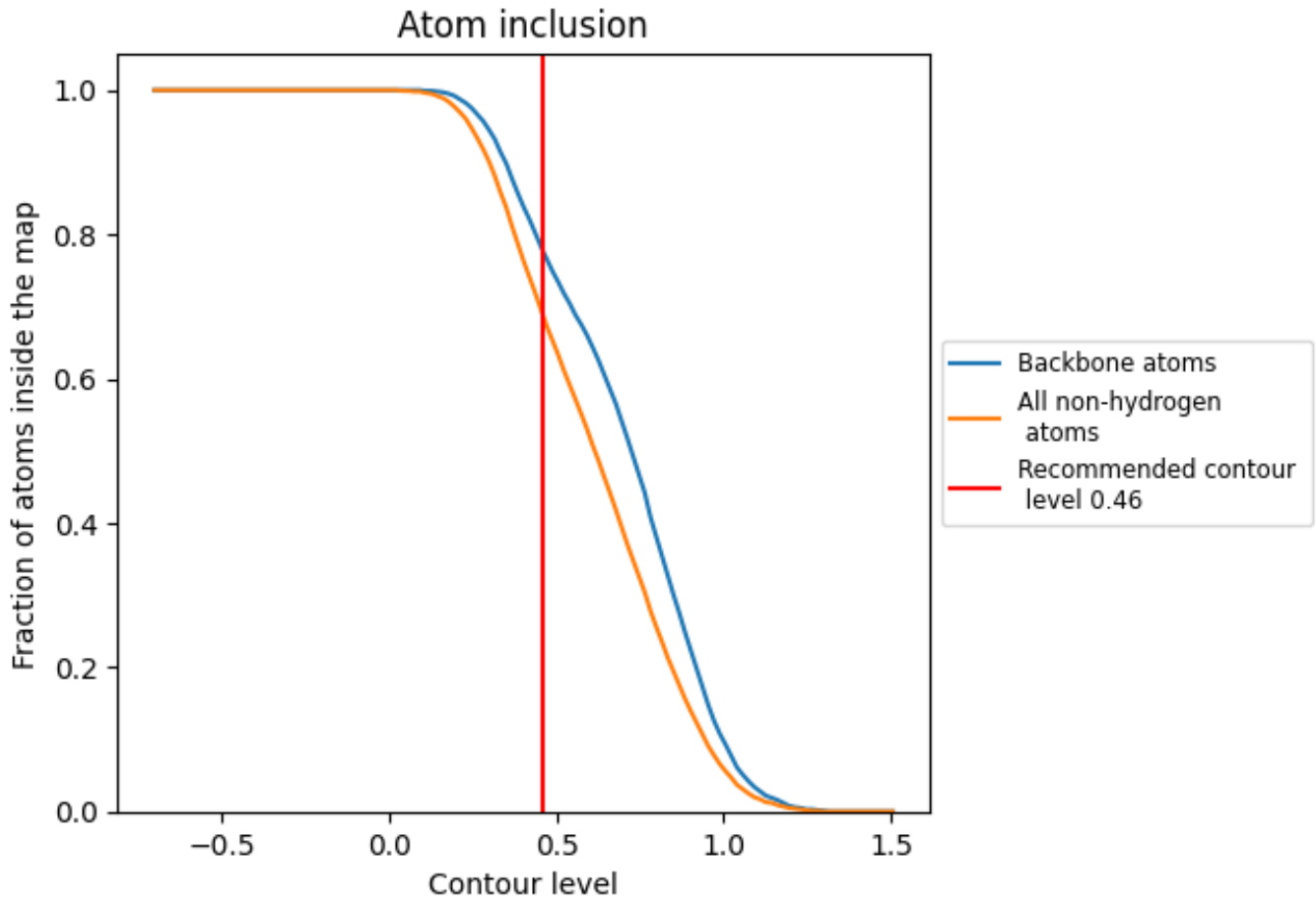
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.46).

9.4 Atom inclusion (i)



At the recommended contour level, 78% of all backbone atoms, 69% 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 (0.46) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6870	0.5310
A	0.6900	0.5300
B	0.6840	0.5310
C	0.6880	0.5320