



Full wwPDB EM Validation Report ⓘ

Nov 5, 2024 – 07:38 pm GMT

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 ⓘ 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.dev113
MolProbity : 4.02b-467
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.39

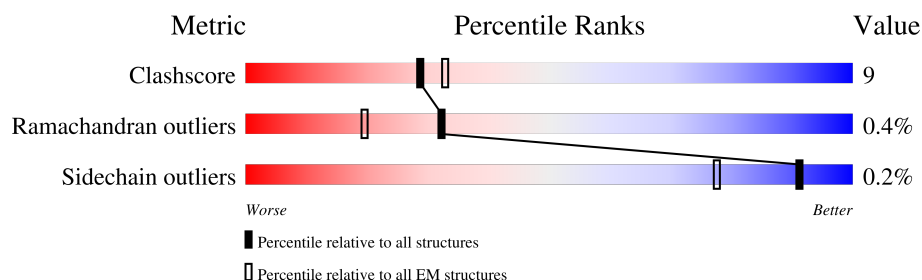
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 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	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	1167	<div> <div>6%</div> <div>64%</div> <div>17%</div> <div>19%</div> </div>
1	B	1167	<div> <div>7%</div> <div>64%</div> <div>17%</div> <div>19%</div> </div>
1	C	1167	<div> <div>6%</div> <div>63%</div> <div>19%</div> <div>19%</div> </div>

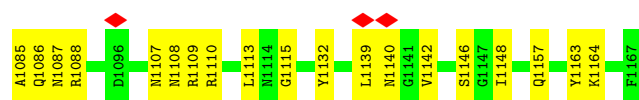
2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 21351 atoms, of which 0 are hydrogens and 0 are deuteriums.

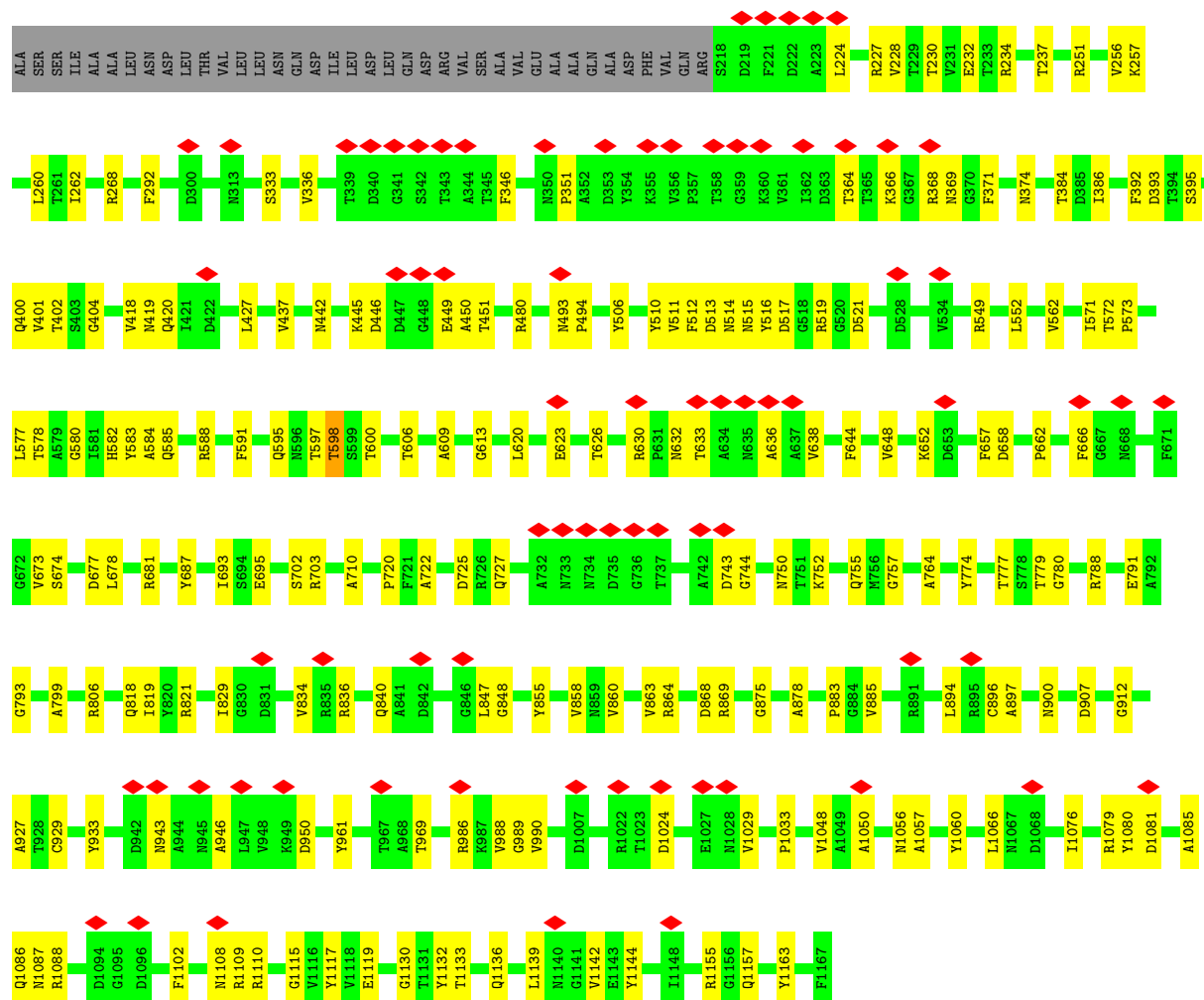
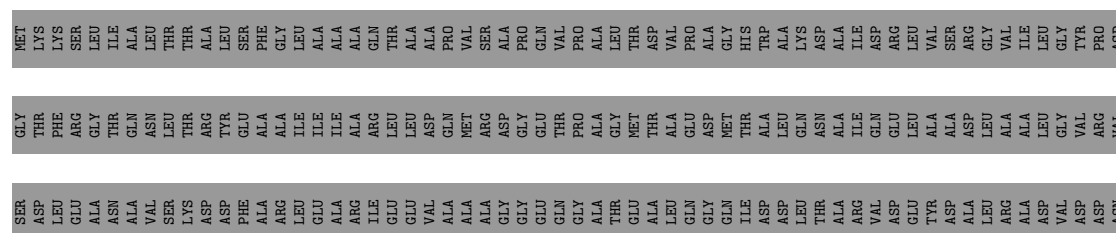
In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called S-layer protein SlpA.

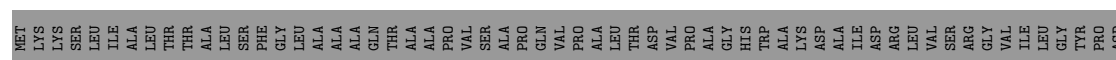
Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	949	Total	C	N	O	S	0	0
			7117	4415	1265	1431	6		
1	B	949	Total	C	N	O	S	0	0
			7117	4415	1265	1431	6		
1	C	949	Total	C	N	O	S	0	0
			7117	4415	1265	1431	6		



• Molecule 1: S-layer protein SlpA



• Molecule 1: S-layer protein SlpA



S1146	T1002	R895	G872	Y883	I421	L260	ALA
G1147	N1003	C896	V673	A884	L260	L260	SER
I1148	T1004	A897	L675	Q885	T261	T261	THR
Q1157	D1007	D898	L676	R888	V428	V428	PHE
Y1163	T1023	N899	D677	T897	R268	R268	GLY
F1167	D1024	N900	L678	T898	D274	D274	THR
	N1028	D907	R681	S899	V275	V275	GLN
	V1029	G910	I693	T800	D276	D276	ASN
	N1036	V911	Y696	V604	R277	R277	ALA
	G1037	I915	S702	T605	L278	L278	VAL
	Q1038	D922	R703	T606	N290	N290	ASP
	V1039	Q923	R709	Y607	A291	A291	THR
	Y1042	S924	A710	A450	LEU	LEU	ASP
	A1049	R925	Y711	T451	D300	D300	TYR
	N1056	A927	F721	G454	R306	R306	GLY
	L1066	T928	L724	D468	N313	N313	ALA
	I1076	C929	L725	P469	LEU	LEU	ARG
	Q1077	F930	R726	V477	ASP	ASP	GLN
	V1078	T931	Q727	N493	GLN	GLN	ASP
	A1085	G941	D731	P494	VAL	VAL	ALA
	Q1086	D942	N733	N497	SER	SER	GLY
	N1087	N943	N734	Y506	ALA	ALA	GLY
	R1088	A944	D735	V511	THR	THR	ALA
	S1103	N945	G736	F512	GLY	GLY	GLY
	N1107	K949	A742	D513	PRO	PRO	ALA
	N1108	D950	A743	N514	ALA	ALA	ALA
	R1109	R954	D743	R519	GLN	GLN	THR
	R1110	Y961	N750	G520	ALA	ALA	GLY
	L1113	P963	T751	D521	ASP	ASP	GLY
	N1114	T964	K752	V825	LEU	LEU	ASP
	G1115	T965	L753	P357	GLN	GLN	ASP
	V1118	A966	G754	T358	ASN	ASN	GLN
	G1130	T967	A762	K360	ALA	ALA	ALA
	T1131	A968	A763	V361	ARG	ARG	ILE
	Y1132	T969	N765	I362	VAL	VAL	GLN
	S1135	D972	Y774	K366	GLY	GLY	GLY
	Q1136	V977	S778	G367	ASP	ASP	ALA
	K1137	D981	T779	R368	LEU	LEU	ALA
	D1138	Y984	G780	G372	ALA	ALA	ALA
	L1139	D985	D784	F373	LEU	LEU	LEU
	E1143	R986	M789	N374	ASP	ASP	GLY
	Y1144	G989	T892	T384	VAL	VAL	VAL
	G1145	V990	L894	I386	ASP	ASP	ASP
		A991		F392	ASN	ASN	VAL
				D393			

4 Experimental information

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 ($e^-/\text{\AA}^2$)	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 [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	0.35	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 [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	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%)	37	63
1	B	947/1167 (81%)	838 (88%)	104 (11%)	5 (0%)	25	53
1	C	947/1167 (81%)	844 (89%)	99 (10%)	4 (0%)	30	58

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%)	32	58

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%)	89	96
1	B	726/891 (82%)	725 (100%)	1 (0%)	92	98
1	C	726/891 (82%)	726 (100%)	0	100	100
All	All	2178/2673 (82%)	2174 (100%)	4 (0%)	91	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 [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 [i](#)

There are no chain breaks in this entry.

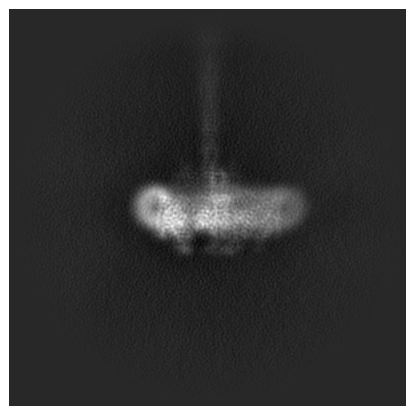
6 Map visualisation [i](#)

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.

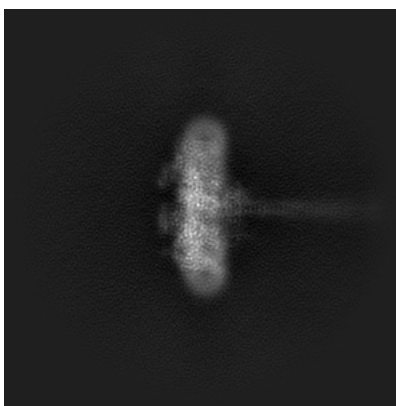
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

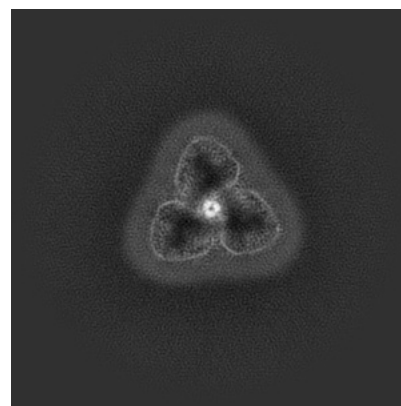
6.1.1 Primary map



X

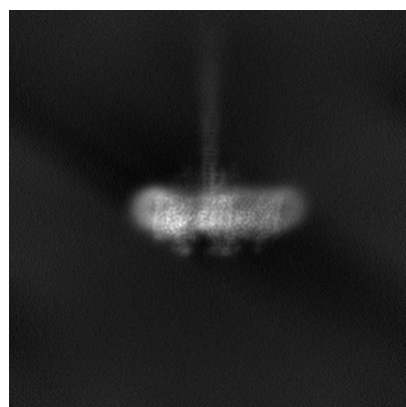


Y

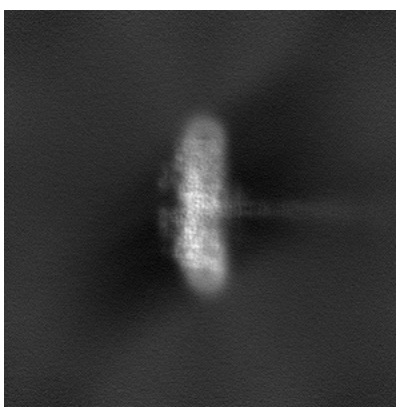


Z

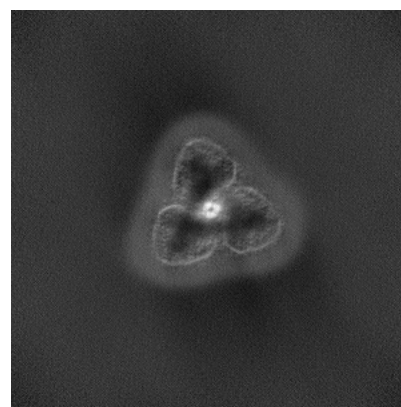
6.1.2 Raw map



X



Y

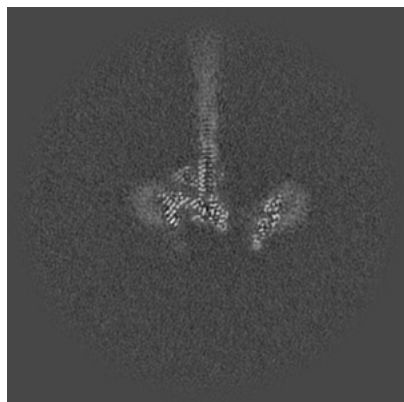


Z

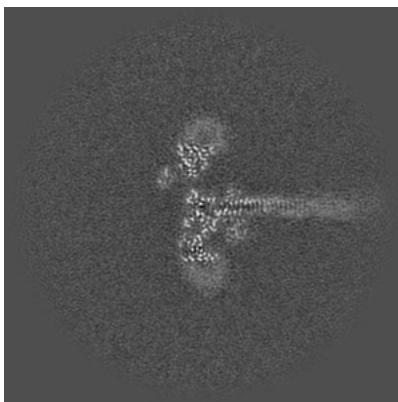
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

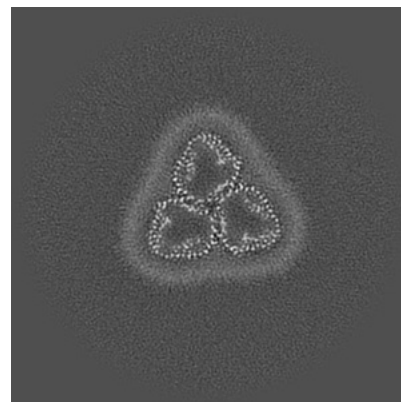
6.2.1 Primary map



X Index: 264

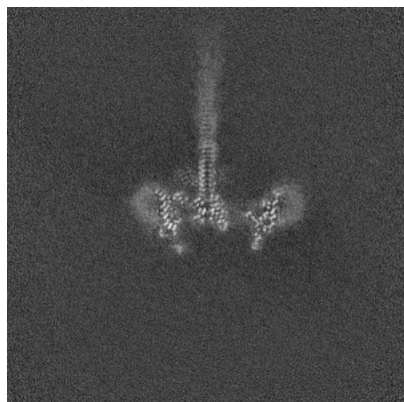


Y Index: 264

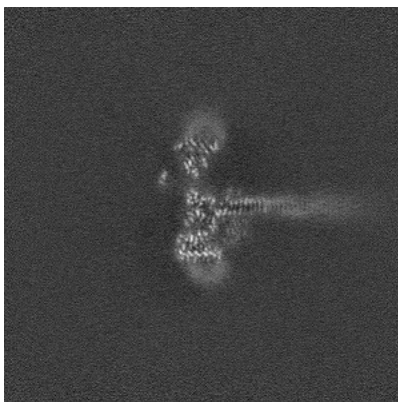


Z Index: 264

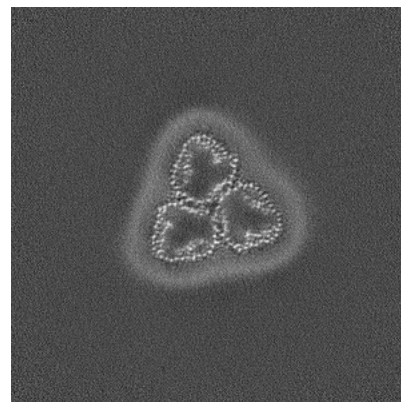
6.2.2 Raw map



X Index: 264



Y Index: 264

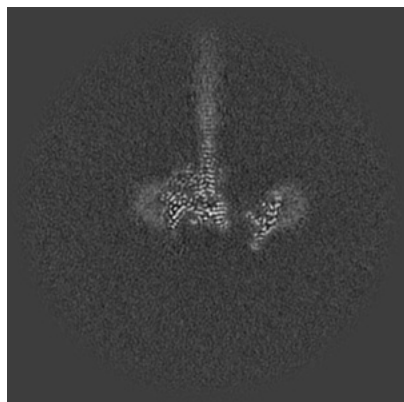


Z Index: 264

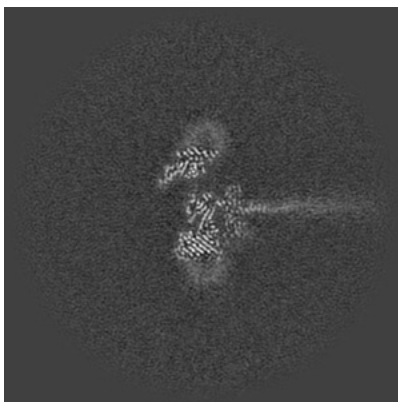
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

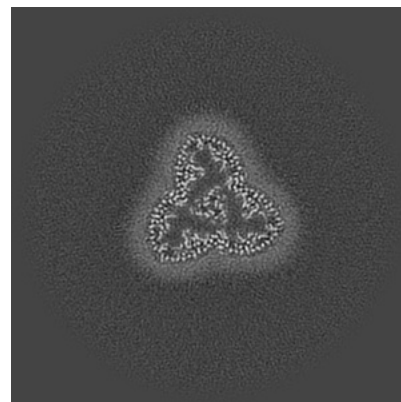
6.3.1 Primary map



X Index: 268

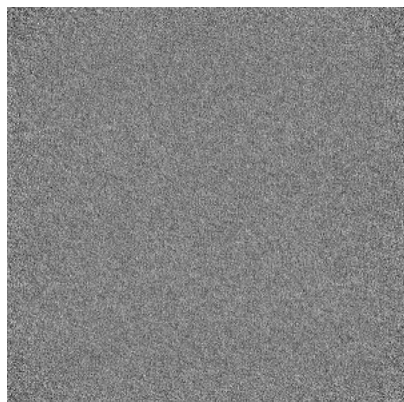


Y Index: 272

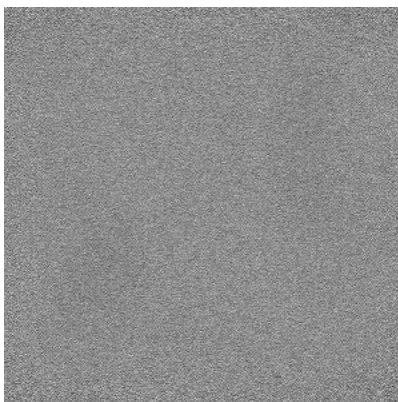


Z Index: 246

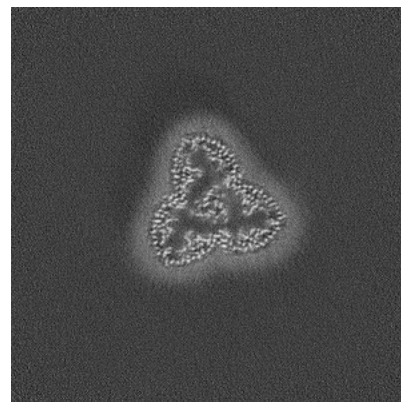
6.3.2 Raw map



X Index: 0



Y Index: 0

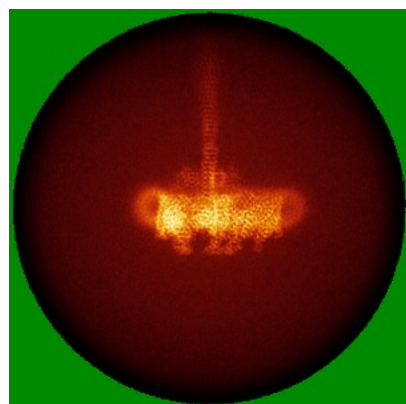


Z Index: 246

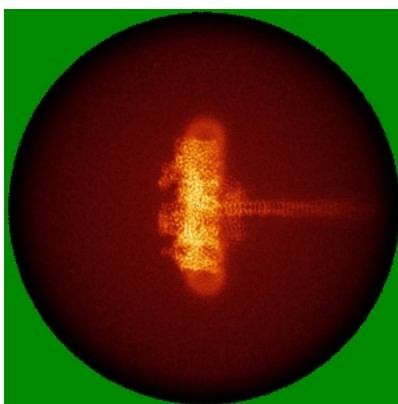
The images above show the largest variance slices of the map in three orthogonal directions.

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

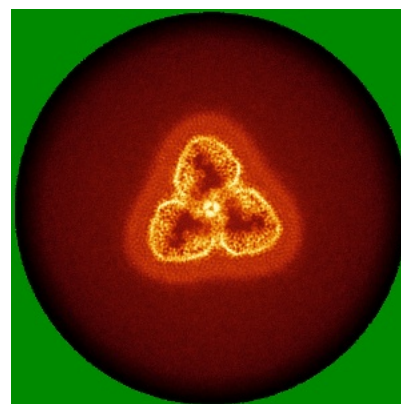
6.4.1 Primary map



X

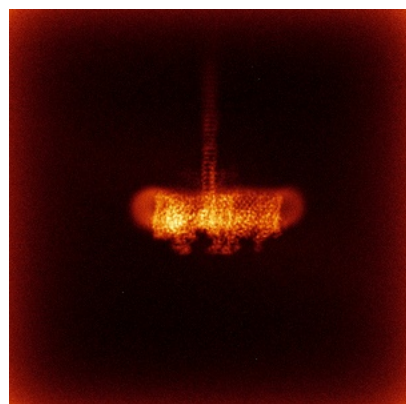


Y

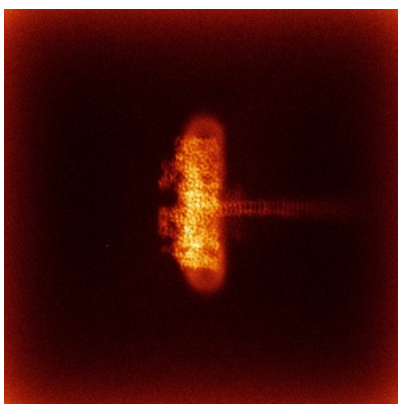


Z

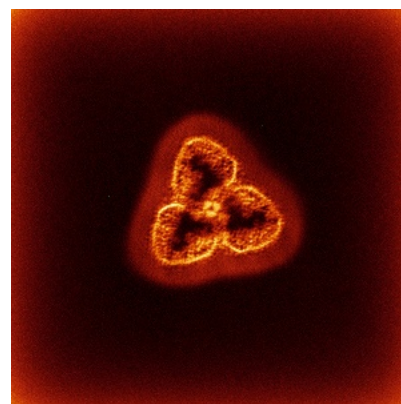
6.4.2 Raw map



X



Y

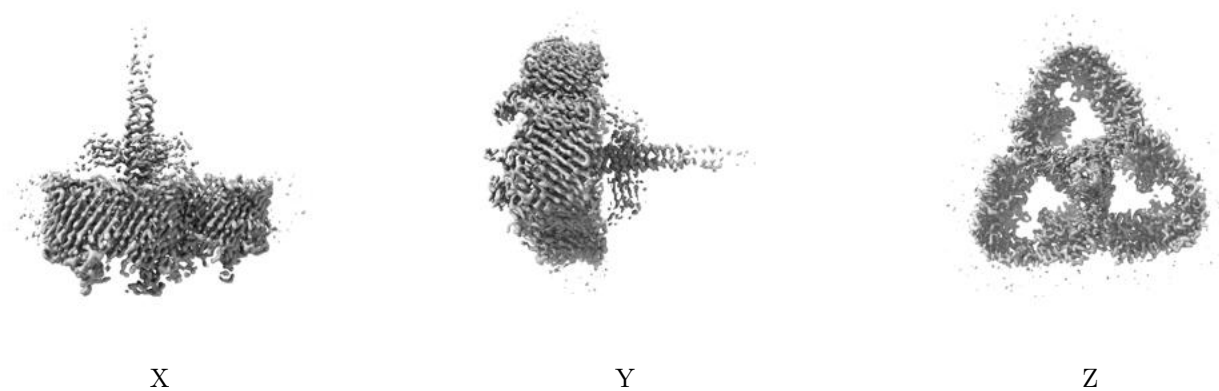


Z

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



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



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.

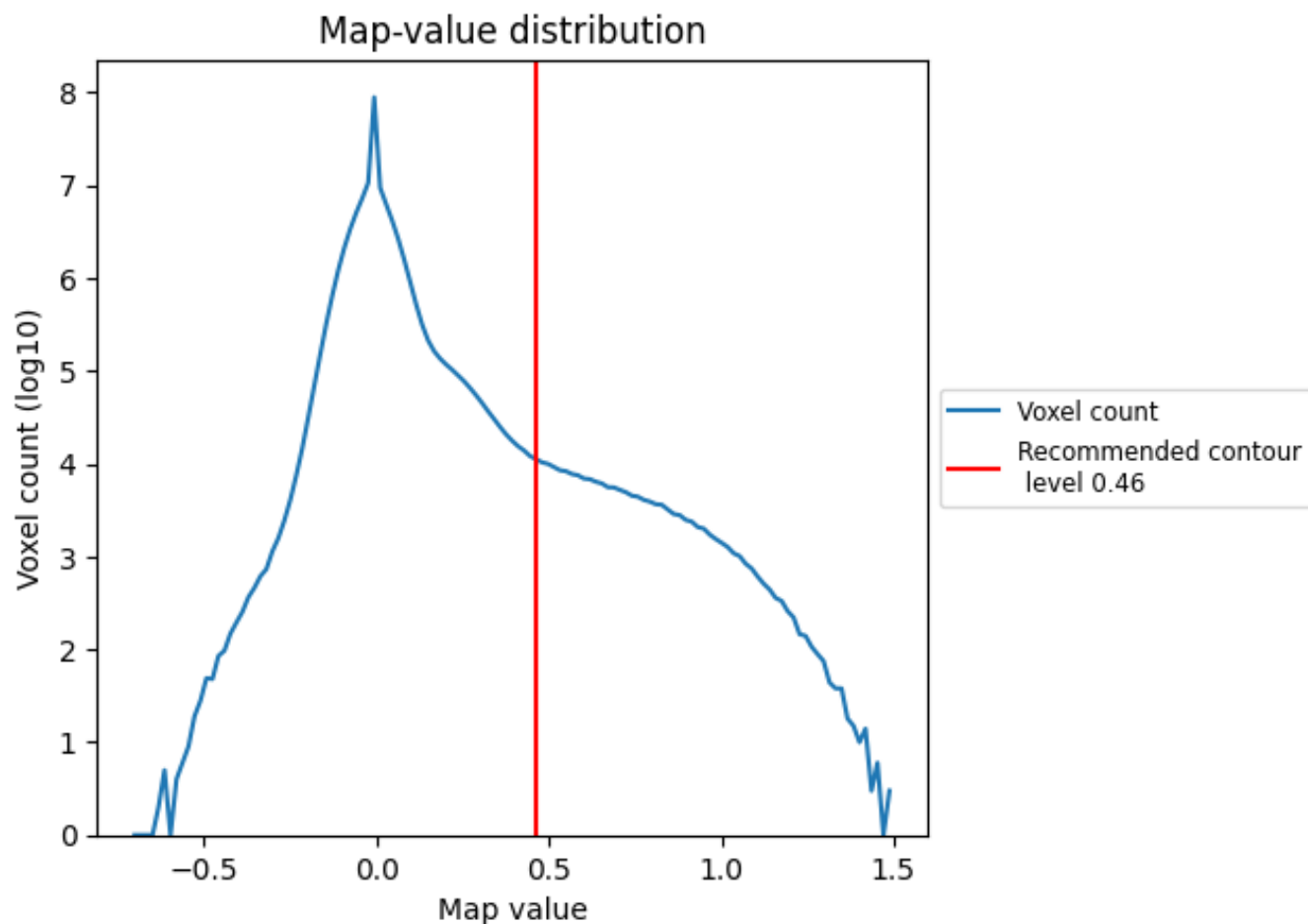
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

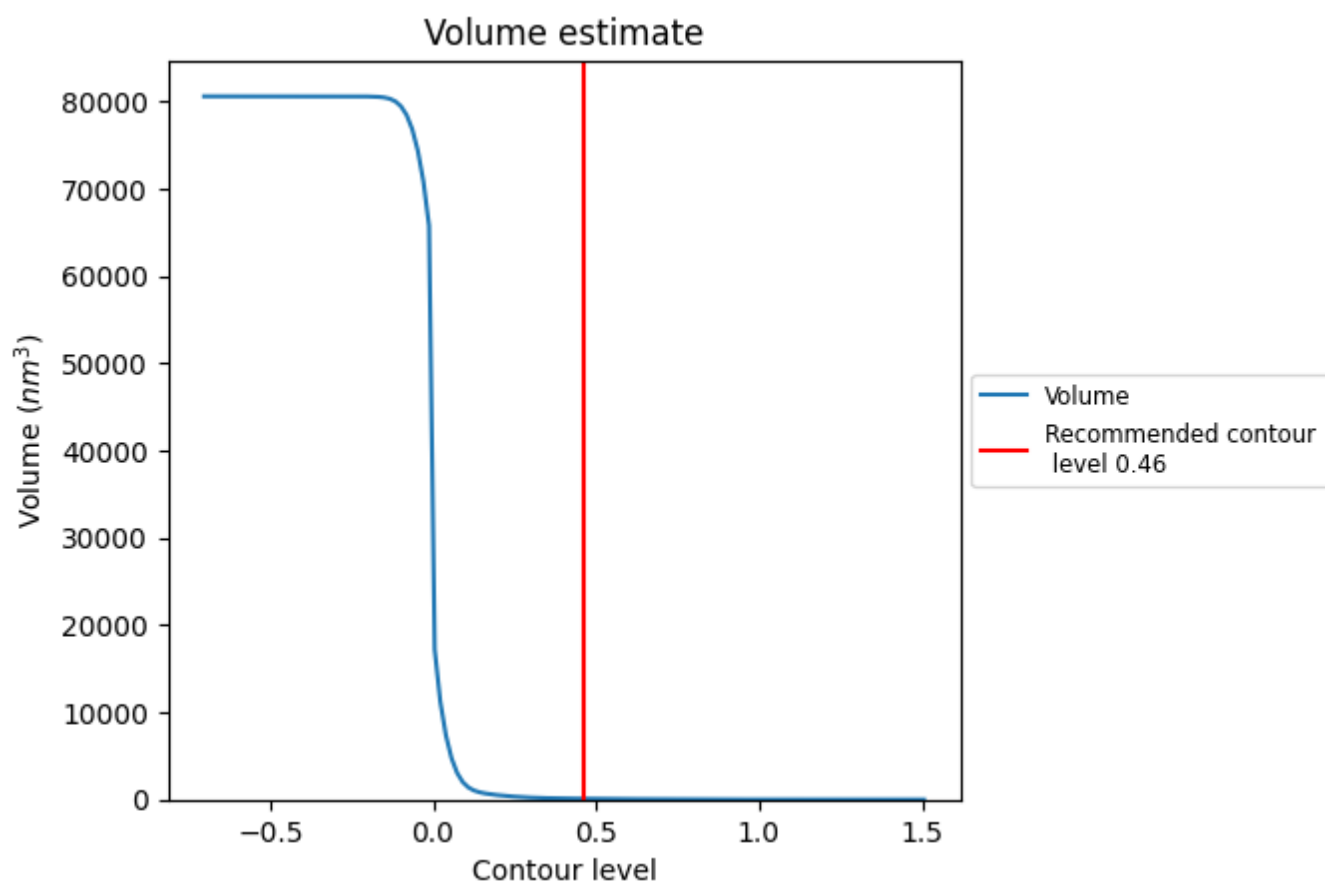
This section contains the results of statistical analysis of the map.

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.

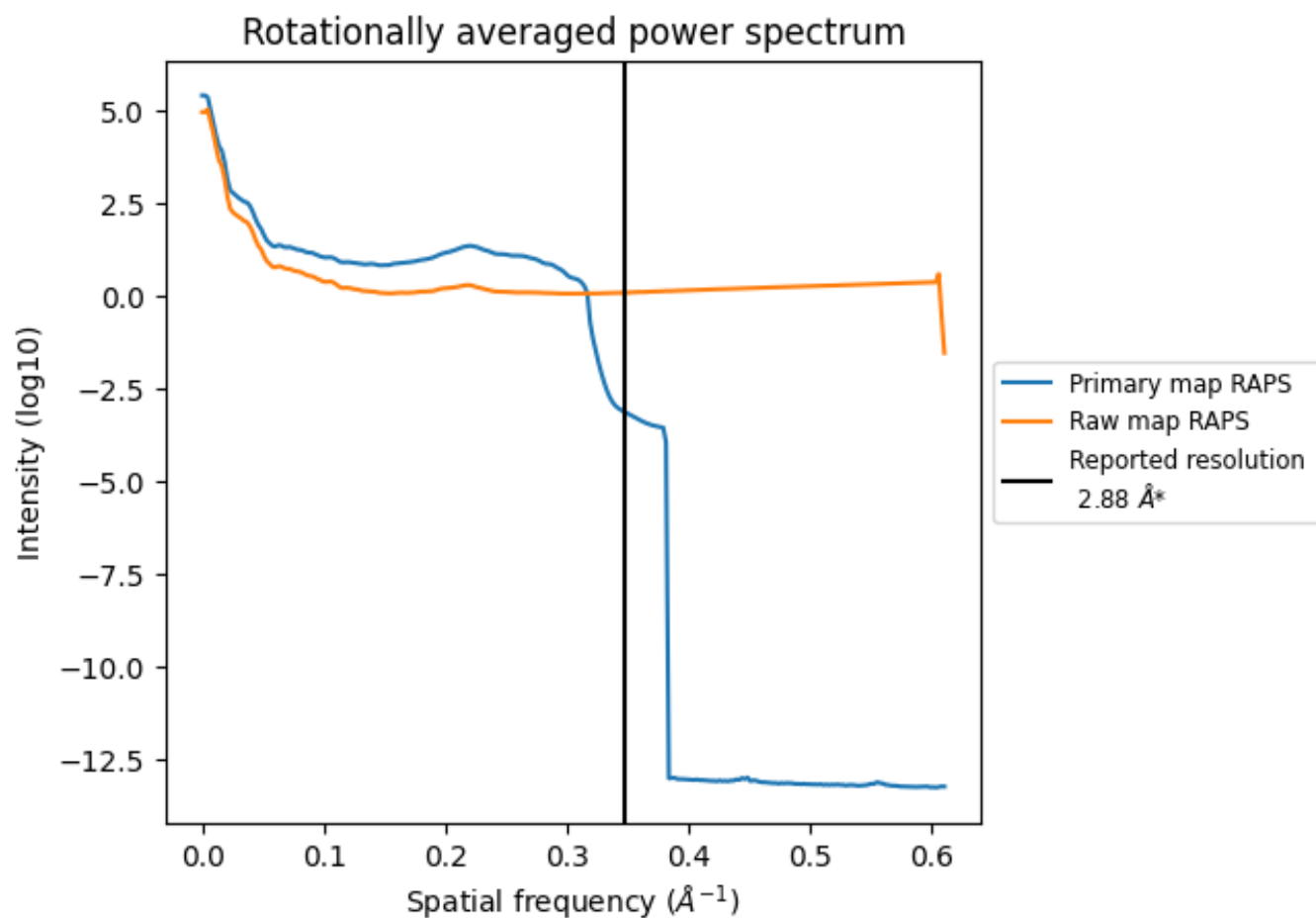
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 97 nm³; 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 ⓘ

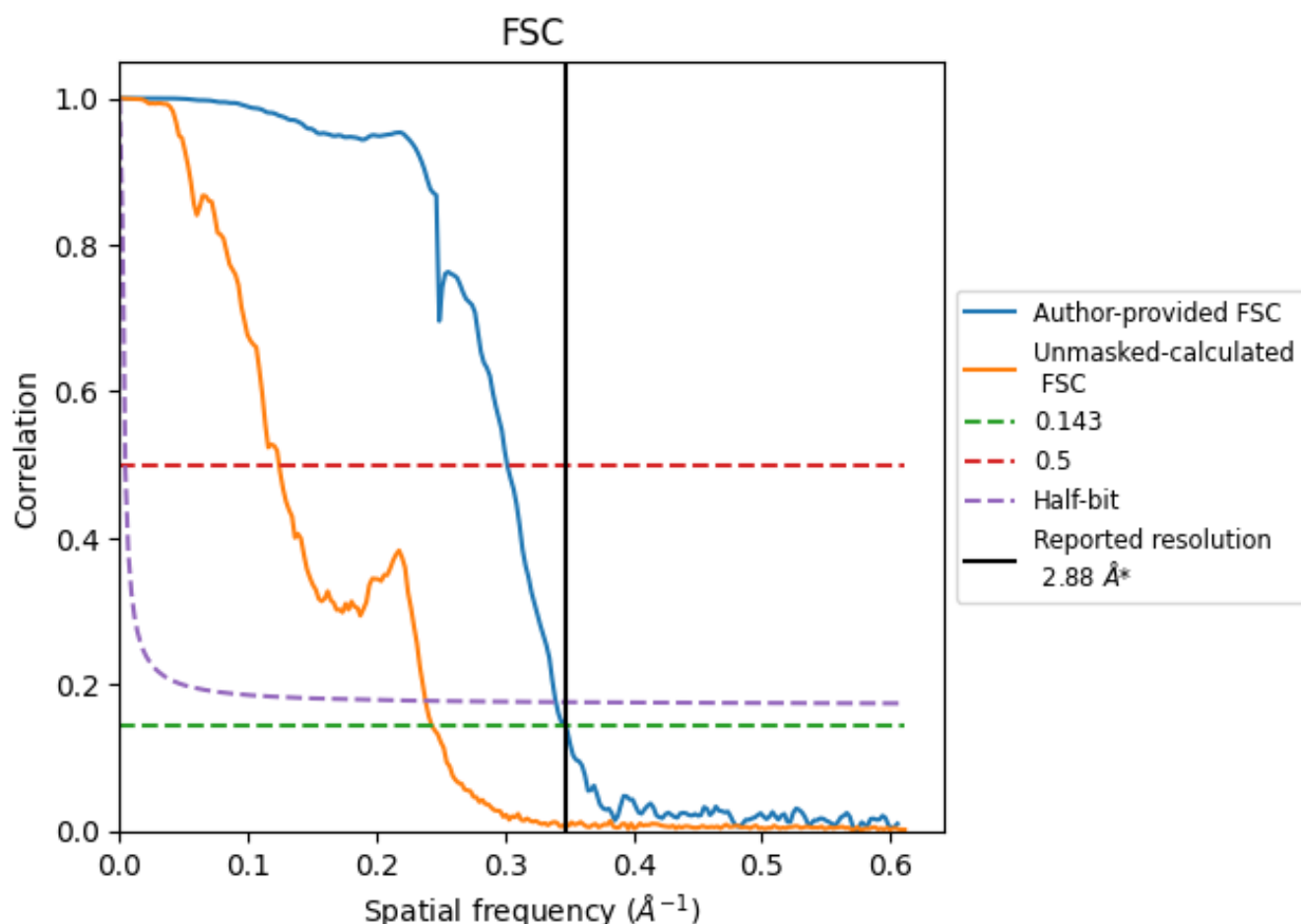


*Reported resolution corresponds to spatial frequency of 0.347 Å⁻¹

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 0.347 \AA^{-1}

8.2 Resolution estimates [i](#)

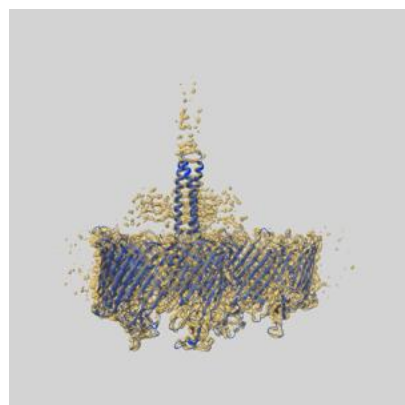
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.88	-	-
Author-provided FSC curve	2.88	3.31	2.94
Unmasked-calculated*	4.11	8.05	4.20

*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 %

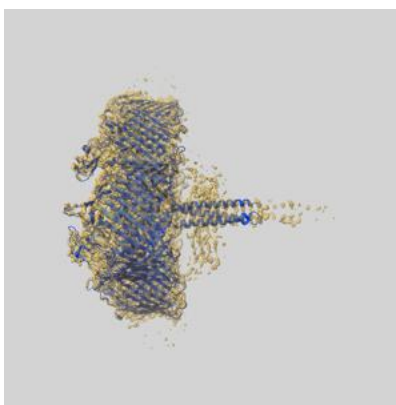
9 Map-model fit [i](#)

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](#).

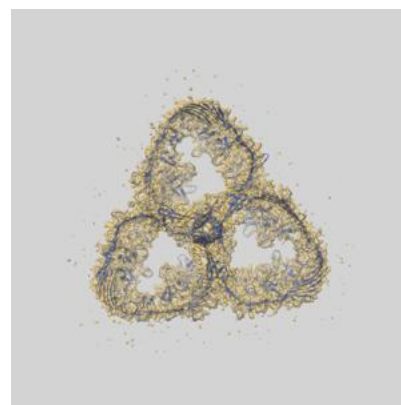
9.1 Map-model overlay [i](#)



X



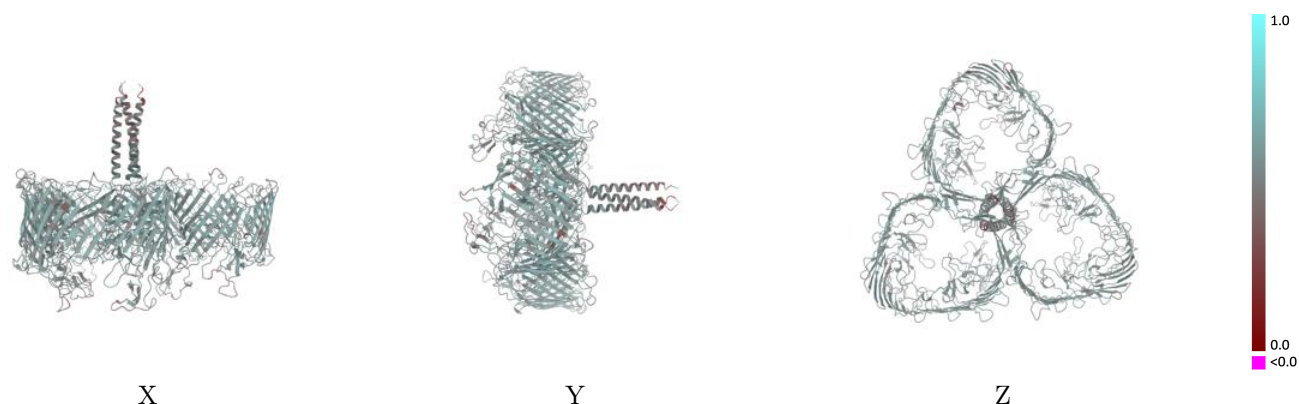
Y



Z

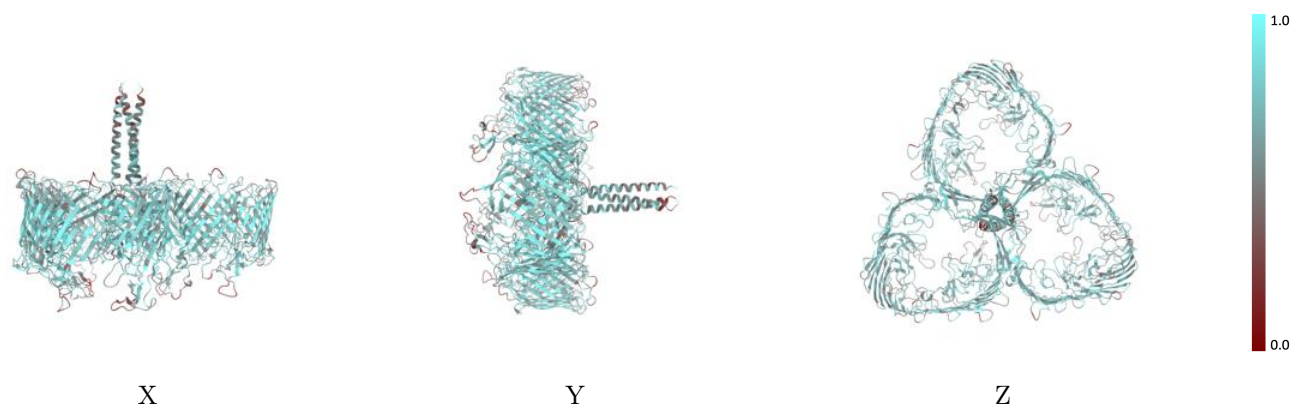
The images above show the 3D surface view of the map at the recommended contour level 0.46 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



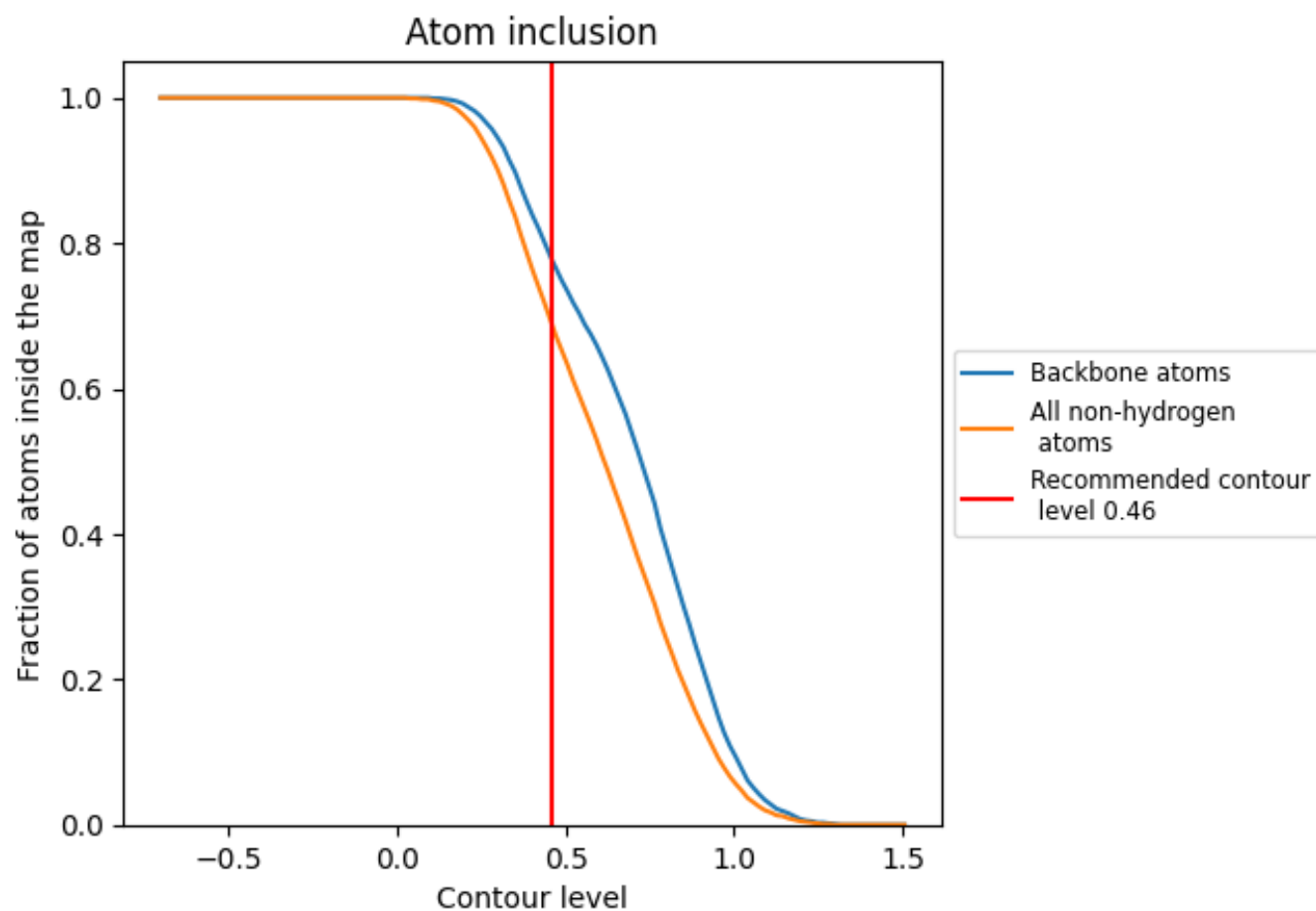
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.46).

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	<div></div> 0.6870	<div></div> 0.5310
A	<div></div> 0.6900	<div></div> 0.5300
B	<div></div> 0.6840	<div></div> 0.5310
C	<div></div> 0.6880	<div></div> 0.5320

