



Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 01:02 PM UTC

PDB ID : 9CYX / pdb_00009cyx
EMDB ID : EMD-46053
Title : Cryo-EM structure of MRV full core
Authors : Liu, X.Y.; Xia, X.; Martynowycz, M.W.; Gonen, T.; Zhou, Z.H.
Deposited on : 2024-08-02
Resolution : 3.30 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:

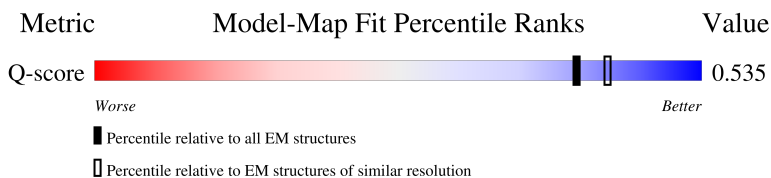
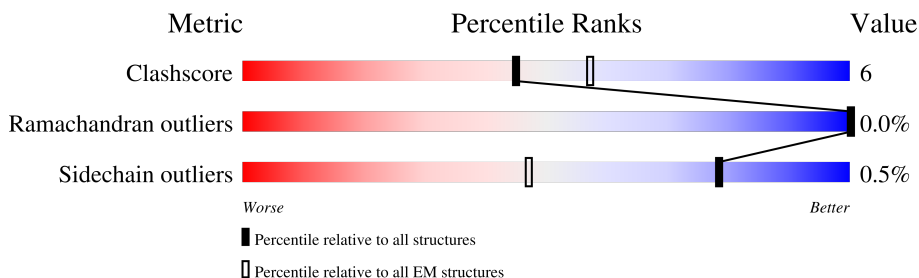
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDb archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & 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 3.30 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	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	15087 (2.80 - 3.80)

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	B	1275	 10% 89%
1	H	1275	 70% 11% 19%
1	I	1275	 76% 9% 15%
2	A	1288	 66% 77% 22%

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Mol	Chain	Length	Quality of chain
3	Q	417	 88%11%
3	R	417	 7%88%12%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 34537 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 Lambda 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	H	1034	Total	C	N	O	S	0	0
			8164	5220	1378	1517	49		
1	I	1085	Total	C	N	O	S	0	0
			8562	5471	1450	1590	51		
1	B	140	Total	C	N	O	S	0	0
			1050	622	198	226	4		

- Molecule 2 is a protein called Outer capsid protein lambda-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A	1284	Total	C	N	O	S	0	0
			10127	6468	1700	1917	42		

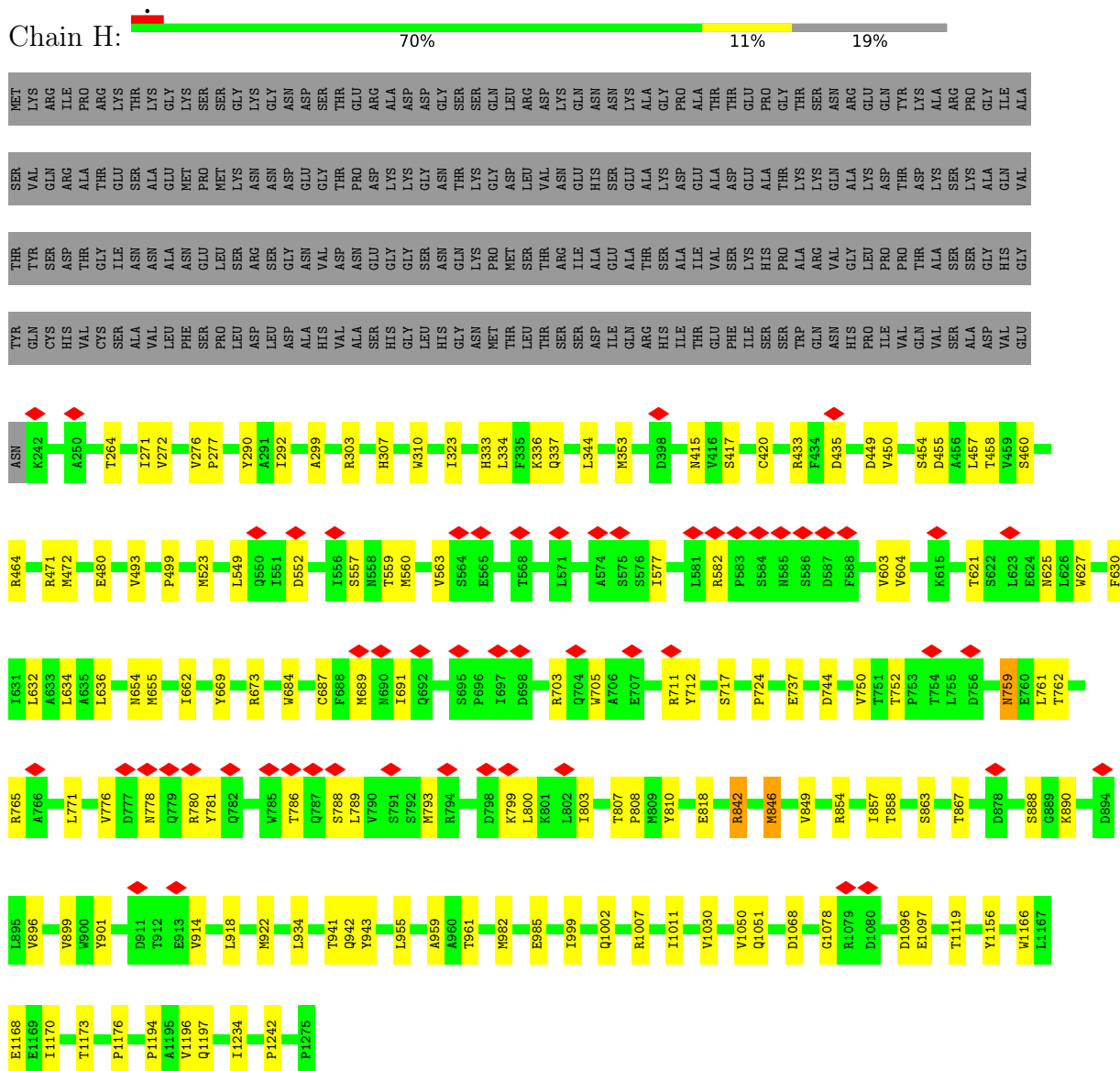
- Molecule 3 is a protein called Inner capsid protein sigma-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	Q	417	Total	C	N	O	S	0	0
			3317	2096	599	605	17		
3	R	417	Total	C	N	O	S	0	0
			3317	2096	599	605	17		

3 Residue-property plots

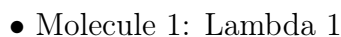
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: Lambda 1



• Molecule 1: Lambda 1

Frequency	Percentage
Daily	76%
Weekly	9%
Monthly	15%



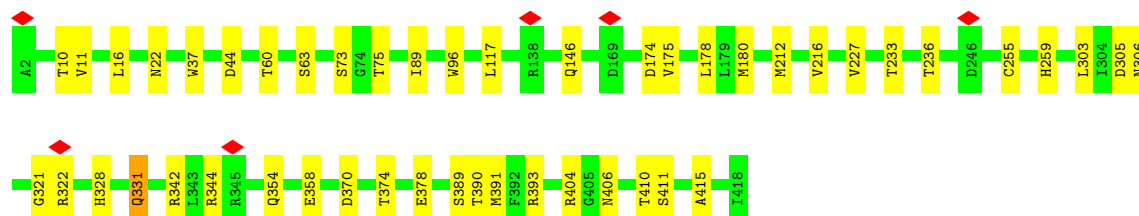
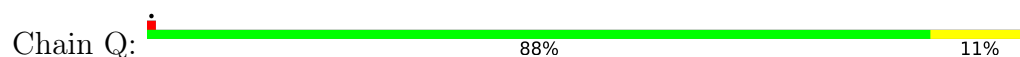
10% 89%



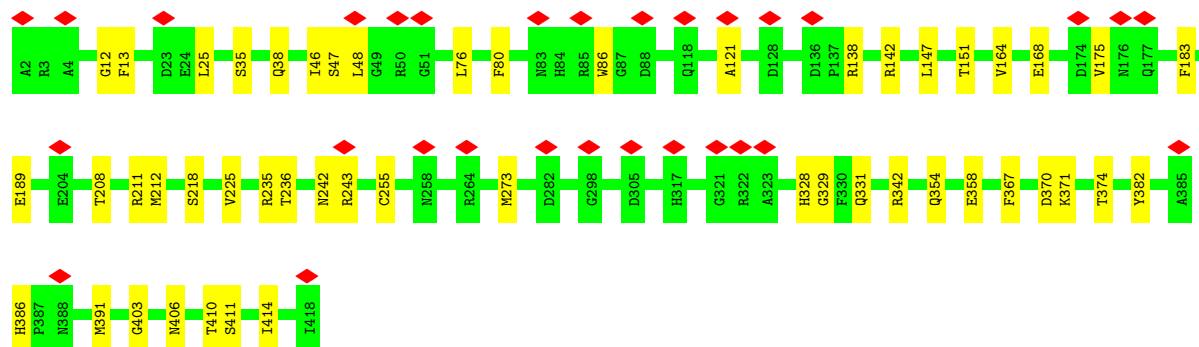
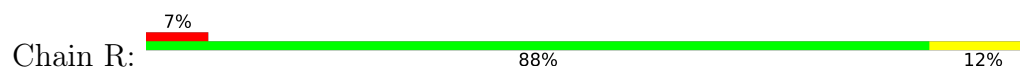
A1096	V1036	P975	T854	V793	G729	Q660	L594	Q526	P457	D389	T298
G1097	G1037	N976	A855	L794	L730	H661	V595	P527	D458	D389	S305
I1098	Q1038	C977	Q856	F795	C731	S662	E596	L528	T459	S392	N310
Y1099	M1039	S978	P857	E796	A732	S663	S997	V529	Y460	Q395	G311
T1100	C1040	S979	S858	W797	W733	L664	L599	E531	G463	Q395	Y312
Q1102	S1041	T980	C859	W798	W734	T665	S900	P532	G464	Y400	A315
A1103	L1042	W981	C960	S799	G735	W666	S601	W333	D465	T401	
L1104	V1043	W982	C860	G800	W736	W667	C602	Q535	G468	I402	R320
L1105	I1044	W861	A801	S802	W737	S668	M603	G536	R469	D403	Q321
V1106	P1045	W863	S802	R803	R738	G669	H604	K537	S470	Q404	
G1106	G1046	W864	H804	W805	S740	F672	T606	I538	A605	A405	R325
S1107	F1047	F867	W805	C806	I743	F673	A607	S539	R476	A406	W326
M1108	M1048	L868	C806	L807	Y744	L674	P608	G540	K477	M407	L327
A1109	A1049	E869	L807	T808	E745	V675	G609	V541	I478	D408	L328
M1110	Q1050	L870	T808	W746	W745	D676	G609	P542	G479	E409	S329
P1111	D1051	D871	W809	W747	S746	H677	G610	F943	D480	G410	
V1112	V1052	W872	W810	H810	H747	F678	S611	P544	S482	D411	S332
S1113	F1053	L873	F813	F813	G748	Y679	F612	V547	R483	L412	D337
L1114	M1054	S874	E814	E814	A749	R680	V613	R548	L483	M413	
G1115	C1055	D875	W815	W815	R750	Y681	V614	V484	K485	V414	E341
S1116	Y1056	C876	S816	S816	W751	G682	K615	D486	V484	S415	W345
F1117	F1057	W877	S817	S817	L752	T683	I616	G551	D486	R416	
M1118	M1058	L878	A818	A818	T753	1687	N617	Y552	V489	L417	
V1119	S1059	T879	W819	W819	I754	S688	F618	D553	L490	T418	E348
D1120	A1060	C880	W820	W820	T755	R689	F619	V554	K91	Q419	R349
S1121	L1061	W881	Y820	Y820	S756	R689	T620	A555	H492	L420	Y350
P1122	A1062	D821	D821	D821	R757	S693	R621	R556	A493	P421	Q352
D1123	F1063	C822	C822	C822	A761	D698	P622	G557	L422	L422	
V1124	S1064	D823	D823	D823	S762	D699	V623	D561	R423	R423	Y355
I1126	T1065	W824	W824	W824	W762	G700	W624	L562	P424	P424	D356
D1127	E1066	W825	W825	W825	A763	S701	H625	A563	A496	D425	S357
M1128	M1067	L826	L826	L826	R764	S702	Y626	R564	I497	I429	V361
A1129	C1068	D827	D827	D827	R765	S702	K630	P567	D498	W430	D362
M1130	A1070	C829	C829	C829	W766	V703	I631	S568	P499	G363	G363
P1131	L1071	T830	T830	T830	R770	I706	L632	G569	T501	A434	A364
A1132	M1072	S831	S831	S831	Y771	E707	P633	D570	G502	L435	T365
Q1133	K1073	P832	P832	P832	L772	T708	N634	Y571	K503	S436	Q366
L1134	I1074	E833	E833	E833	P773	I709	I635	Q572	E504	Y437	N373
D1135	P1074	K835	K835	K835	L774	S710	T636	Y575	Y506	Y438	Q374
F1136	Q1075	1836	1836	1836	I775	S711	S637	Y575	R507	Y439	L375
T1137	I1076	A896	A896	A896	E712	I711	Y638	D579	S508	D440	R376
I1138	S1077	L837	L837	L837	W713	E712	M639	Q580	Y441	L377	L377
A1139	A1078	E838	E838	E838	P777	N713	L640	V581	M442	R443	G378
G1140	Q1079	P839	P839	P839	R778	G715	F644	V582	S511	R443	M379
T1141	F1080	L839	L839	L839	S779	F716	V645	D583	V512	S444	R380
D1142	D1081	1840	1840	1840	W781	W717	T646	H647	A513	H445	I381
V1143	H1024	P841	P841	P841	E782	N718	N647	G584	G516	R446	A383
K1084	G1025	A842	A842	A842	Q783	W719	E650	H585	V447	V447	S386
T1145	L1026	S844	S844	S844	A784	T720	L651	D586	V448	V448	L384
F1027	P1027	P845	P845	P845	W785	Q721	F652	L588	L449	L449	Q385
M1028	M1028	T847	T847	T847	I787	A722	V654	L588	G520	S450	S386
E1029	E1029	F907	F907	F907	1787	A723	A655	S589	H521	S451	L387
M1148	M1088	Q908	Q908	Q908	L788	R724	A655	I590	S522	E452	S388
P1149	K1030	Q909	Q909	Q909	P789	I725	F656	S591	G523	L453	
Y1150	L1089	L910	L910	L910	W789	G726	F656	S592	A524	P454	
G1032	D1090	C970	C970	C970	A790	I727	H659	G593	D525	L456	
M1091	M1091	T851	T851	T851	D791	S728					
V1092	F1092	R852	R852	R852	P792						
F1093	T972	P853	P853	P853							
M1151	F1034										
R1152	F1034										
L1153	F1093										
M1154	S1094										
T1155	D1095										



• Molecule 3: Inner capsid protein sigma-2



• Molecule 3: Inner capsid protein sigma-2



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C5	Depositor
Number of particles used	10857	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1800	Depositor
Maximum defocus (nm)	2600	Depositor
Magnification	81000	Depositor
Image detector	GATAN K3 BIOCONTINUUM (6k x 4k)	Depositor
Maximum map value	0.086	Depositor
Minimum map value	-0.057	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.02	Depositor
Map size ($\text{\AA}$)	422.40002, 422.40002, 422.40002	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.1, 1.1, 1.1	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	B	0.23	0/1060	0.41	0/1420
1	H	0.32	1/8385 (0.0%)	0.53	1/11486 (0.0%)
1	I	0.28	0/8795	0.47	0/12048
2	A	0.29	0/10385	0.49	0/14172
3	Q	0.25	0/3403	0.41	0/4634
3	R	0.24	0/3403	0.44	0/4634
All	All	0.29	1/35431 (0.0%)	0.48	1/48394 (0.0%)

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
2	A	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	854	ARG	N-CA	5.08	1.49	1.46

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	854	ARG	CB-CA-C	-5.11	109.72	117.07

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	A	992	ARG	Sidechain

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	B	1050	0	1035	10	0
1	H	8164	0	8082	93	0
1	I	8562	0	8451	71	0
2	A	10127	0	9910	211	0
3	Q	3317	0	3216	30	0
3	R	3317	0	3216	30	0
All	All	34537	0	33910	434	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 6.

All (434) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:1237:GLU:HB2	2:A:1289:LEU:HB2	1.48	0.93
2:A:8:ARG:HB2	2:A:716:PHE:CD2	2.05	0.90
2:A:413:MET:SD	2:A:722:ALA:HB1	2.14	0.88
1:I:186:CYS:SG	1:I:199:HIS:NE2	2.48	0.86
1:H:1234:ILE:HD11	1:H:1242:PRO:HA	1.58	0.85
3:Q:391:MET:HE1	3:Q:393:ARG:HG3	1.60	0.83
2:A:413:MET:SD	2:A:722:ALA:CB	2.66	0.83
2:A:810:MET:HB3	2:A:984:LEU:HD21	1.63	0.80
2:A:976:ASN:HB3	2:A:1025:GLY:O	1.83	0.78
2:A:710:SER:OG	2:A:751:VAL:CG2	2.34	0.76
2:A:531:GLU:HG3	2:A:532:PRO:HD3	1.69	0.75
3:Q:178:LEU:HD23	3:Q:212:MET:HG3	1.66	0.75
2:A:387:LEU:HB2	2:A:785:ARG:HD3	1.68	0.74
2:A:349:ARG:HG2	2:A:350:TYR:HD1	1.51	0.74
1:H:271:ILE:CD1	1:H:303:ARG:HD2	2.18	0.73
2:A:974:TRP:HB2	2:A:977:CYS:HB3	1.69	0.72
2:A:178:TYR:HE1	2:A:180:ASN:OD1	1.71	0.72
2:A:1238:TRP:HB2	2:A:1250:LEU:HB2	1.71	0.72
2:A:1238:TRP:HD1	2:A:1251:ASN:HD22	1.37	0.72
2:A:984:LEU:HD23	2:A:1013:TYR:CE1	2.26	0.71
1:H:691:ILE:O	1:H:703:ARG:NH1	2.25	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:1028:MET:HE1	2:A:1044:ILE:HG12	1.74	0.69
2:A:1236:ARG:O	2:A:1251:ASN:HB2	1.92	0.68
3:R:328:HIS:HB3	3:R:410:THR:HG22	1.76	0.68
1:H:272:VAL:O	1:H:299:ALA:HB1	1.95	0.67
1:I:1065:LEU:O	1:I:1136:ARG:NH2	2.25	0.67
2:A:711:ILE:HD12	2:A:752:LEU:HD22	1.75	0.67
2:A:8:ARG:HB2	2:A:716:PHE:HD2	1.59	0.67
2:A:1101:MET:HB2	2:A:1114:LEU:HB2	1.77	0.67
3:R:25:LEU:HD11	3:R:391:MET:HE2	1.79	0.65
2:A:23:ARG:NH1	2:A:24:GLN:O	2.30	0.65
2:A:1153:LEU:O	2:A:1154:MET:HE2	1.96	0.65
2:A:481:ARG:NH1	2:A:646:THR:OG1	2.30	0.65
1:H:669:TYR:HA	1:H:673:ARG:HG3	1.80	0.64
3:R:12:GLY:HA2	3:R:121:ALA:HB1	1.79	0.64
2:A:807:LEU:HA	2:A:810:MET:HE2	1.80	0.64
2:A:940:LEU:HG	2:A:942:ILE:HD11	1.80	0.64
1:H:786:THR:HB	1:H:789:LEU:HD23	1.80	0.63
1:H:1119:THR:HG21	1:H:1170:ILE:O	1.97	0.63
1:I:250:ALA:HB2	1:I:913:GLU:OE1	1.98	0.63
1:H:271:ILE:HD11	1:H:303:ARG:HD2	1.81	0.63
2:A:460:TYR:O	2:A:469:ARG:NH2	2.31	0.63
2:A:387:LEU:CB	2:A:785:ARG:HD3	2.28	0.63
1:H:499:PRO:HD3	3:Q:180:MET:HE3	1.80	0.62
1:H:765:ARG:HH12	1:H:803:ILE:HG22	1.63	0.62
2:A:433:ASP:OD1	2:A:434:ALA:N	2.32	0.62
3:Q:354:GLN:O	3:Q:358:GLU:HG2	1.99	0.62
2:A:724:ARG:NE	2:A:774:LEU:HD23	2.13	0.62
1:H:455:ASP:OD1	1:H:458:THR:HG22	2.00	0.62
1:I:765:ARG:NH1	1:I:801:LYS:O	2.31	0.62
2:A:1083:THR:HG23	2:A:1084:LYS:HG3	1.82	0.62
2:A:851:ILE:HG22	2:A:851:ILE:O	1.99	0.62
2:A:8:ARG:CB	2:A:716:PHE:CD2	2.81	0.61
1:H:765:ARG:NH1	1:H:800:LEU:O	2.33	0.61
1:H:717:SER:HB3	1:H:744:ASP:HA	1.82	0.61
2:A:980:THR:HG23	2:A:980:THR:O	2.00	0.61
3:Q:370:ASP:O	3:Q:374:THR:HG23	2.00	0.61
3:Q:89:ILE:HD12	3:Q:117:LEU:HB2	1.82	0.61
1:H:711:ARG:HG3	1:H:712:TYR:CD2	2.35	0.61
2:A:621:ARG:HA	2:A:624:TRP:CD1	2.35	0.61
2:A:112:ASN:OD1	2:A:142:MET:HG3	2.01	0.61
1:H:334:LEU:O	1:H:337:GLN:NE2	2.34	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:750:VAL:HG12	1:H:752:THR:H	1.66	0.60
1:I:630:PHE:HB2	1:I:772:MET:HE1	1.83	0.60
2:A:809:MET:SD	2:A:994:ALA:HB2	2.42	0.59
2:A:809:MET:HG2	2:A:993:LEU:HD23	1.83	0.59
1:H:552:ASP:HB2	1:H:890:LYS:HE2	1.85	0.59
1:H:857:ILE:HG21	1:H:863:SER:HB3	1.84	0.59
2:A:445:HIS:NE2	2:A:1095:ASP:OD1	2.28	0.59
1:H:1051:GLN:HG3	1:H:1196:VAL:HG22	1.84	0.59
1:I:850:THR:HG1	1:I:1000:GLN:HE22	1.49	0.59
2:A:8:ARG:CB	2:A:716:PHE:CE2	2.86	0.59
2:A:456:LEU:HD22	2:A:618:PHE:HB3	1.85	0.59
2:A:635:ILE:HG21	2:A:655:ALA:HB1	1.85	0.59
2:A:727:ILE:HD11	2:A:780:LEU:CD1	2.33	0.59
1:I:1165:ALA:O	1:I:1169:GLU:HG3	2.02	0.58
2:A:178:TYR:CE1	2:A:180:ASN:OD1	2.55	0.58
2:A:498:ASP:HA	2:A:505:TYR:HE1	1.68	0.58
1:B:152:THR:O	1:B:156:GLU:HG3	2.04	0.58
2:A:506:LEU:HD23	2:A:510:GLN:HE22	1.67	0.58
2:A:710:SER:OG	2:A:751:VAL:HG21	2.03	0.58
3:R:147:LEU:O	3:R:151:THR:HG23	2.04	0.58
1:H:603:VAL:HG13	1:H:604:VAL:HG23	1.84	0.58
2:A:966:LEU:HD23	2:A:969:ILE:HD12	1.85	0.58
3:R:46:ILE:HG22	3:R:48:LEU:H	1.69	0.58
1:H:759:ASN:HD21	1:H:762:THR:HG23	1.68	0.58
1:H:858:THR:HB	1:H:942:GLN:HB2	1.85	0.58
1:I:1121:TYR:O	1:I:1125:GLN:HG2	2.03	0.58
3:Q:406:ASN:O	3:Q:410:THR:HG23	2.03	0.58
2:A:530:ILE:O	2:A:534:ILE:HG13	2.04	0.57
1:I:1163:THR:HG21	1:I:1198:TYR:HB2	1.87	0.57
1:H:435:ASP:HB2	1:H:449:ASP:HB2	1.86	0.57
2:A:580:GLN:HG3	2:A:594:LEU:HD23	1.86	0.57
2:A:710:SER:OG	2:A:751:VAL:HG23	2.04	0.57
2:A:816:SER:HB2	2:A:839:LEU:HD12	1.86	0.57
2:A:878:ILE:HD12	2:A:881:VAL:HB	1.85	0.57
2:A:1170:LYS:NZ	2:A:1186:LYS:O	2.22	0.56
3:R:370:ASP:O	3:R:374:THR:HG23	2.06	0.56
1:I:435:ASP:HB3	1:I:449:ASP:HB2	1.87	0.56
1:I:1081:CYS:HB2	1:I:1094:ILE:HD11	1.88	0.56
2:A:529:VAL:O	2:A:532:PRO:HD2	2.05	0.56
2:A:903:PHE:HB3	2:A:961:SER:HB3	1.88	0.56
2:A:723:ALA:O	2:A:727:ILE:HG22	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:778:ASN:OD1	1:H:780:ARG:NE	2.39	0.56
1:I:472:MET:HE3	1:I:506:PRO:HB2	1.88	0.55
2:A:345:TRP:O	2:A:352:GLN:NE2	2.39	0.55
1:H:1007:ARG:NH2	2:A:290:GLN:O	2.39	0.55
1:I:1096:ASP:OD1	1:I:1097:GLU:N	2.40	0.55
3:R:235:ARG:O	3:R:236:THR:OG1	2.21	0.55
2:A:1238:TRP:HD1	2:A:1251:ASN:ND2	2.04	0.55
1:I:987:LEU:HD22	1:I:994:MET:HE1	1.87	0.55
2:A:1164:GLN:HG2	2:A:1270:TRP:CZ3	2.42	0.55
2:A:1238:TRP:CD1	2:A:1251:ASN:HD22	2.22	0.55
3:R:35:SER:OG	3:R:38:GLN:OE1	2.24	0.55
2:A:988:LEU:O	2:A:991:THR:OG1	2.25	0.54
1:I:943:TYR:HD1	1:I:995:THR:HG23	1.71	0.54
2:A:1188:ASP:OD1	2:A:1189:ILE:N	2.40	0.54
2:A:203:THR:HG22	2:A:205:GLU:H	1.72	0.54
2:A:687:ILE:HD12	2:A:992:ARG:HG3	1.89	0.54
1:I:333:HIS:HA	1:I:336:LYS:HG2	1.90	0.54
2:A:196:ALA:HB2	2:A:255:MET:HE1	1.88	0.54
1:I:242:LYS:HD2	1:I:247:LEU:HG	1.89	0.54
2:A:980:THR:HG21	2:A:1020:ARG:HD3	1.90	0.54
2:A:41:GLU:OE2	2:A:43:TRP:NE1	2.42	0.53
2:A:1067:ASP:O	2:A:1069:ASN:N	2.37	0.53
1:H:577:ILE:HD11	1:H:627:TRP:CE3	2.43	0.53
1:H:307:HIS:CE1	1:H:323:ILE:HD12	2.44	0.53
2:A:418:THR:HG22	2:A:420:LEU:H	1.74	0.53
2:A:734:VAL:HG11	2:A:756:SER:HB3	1.91	0.53
2:A:1089:LEU:HB2	2:A:1091:MET:HE1	1.91	0.53
1:H:761:LEU:HD12	1:H:808:PRO:HA	1.91	0.53
2:A:40:ARG:HA	2:A:40:ARG:CZ	2.39	0.53
2:A:449:LEU:HD23	2:A:449:LEU:H	1.74	0.53
2:A:486:ASP:HB3	2:A:529:VAL:HG21	1.91	0.53
3:R:406:ASN:O	3:R:410:THR:HG23	2.09	0.53
3:R:354:GLN:O	3:R:358:GLU:HG2	2.09	0.52
2:A:419:GLN:HB2	2:A:708:THR:HG23	1.90	0.52
2:A:836:ILE:O	2:A:839:LEU:N	2.42	0.52
3:Q:344:ARG:NH1	3:Q:354:GLN:OE1	2.41	0.52
2:A:711:ILE:HG22	2:A:712:GLU:N	2.24	0.52
2:A:716:PHE:CD1	2:A:716:PHE:C	2.85	0.52
2:A:807:LEU:HD22	2:A:1012:MET:SD	2.50	0.52
1:H:457:LEU:HD13	1:H:1030:VAL:HG21	1.92	0.52
1:I:641:ASP:OD2	1:I:647:LYS:NZ	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:941:GLU:HG3	2:A:950:ARG:HB2	1.91	0.52
1:H:762:THR:HG22	1:H:765:ARG:HH21	1.75	0.52
1:I:239:VAL:HG22	1:I:241:ASN:H	1.73	0.52
2:A:1045:PRO:HA	2:A:1086:GLU:HA	1.92	0.52
1:H:778:ASN:ND2	1:H:780:ARG:HB2	2.24	0.52
2:A:387:LEU:HB2	2:A:785:ARG:HB3	1.91	0.52
1:I:518:GLN:OE1	1:I:829:PRO:HG2	2.09	0.52
2:A:86:MET:HA	2:A:86:MET:HE2	1.91	0.52
1:I:237:ALA:HA	1:I:247:LEU:HD22	1.92	0.52
2:A:713:ASN:N	2:A:714:PRO:HD3	2.25	0.51
2:A:967:GLU:O	2:A:971:ARG:HG2	2.09	0.51
3:Q:37:TRP:HB3	3:Q:146:GLN:OE1	2.09	0.51
1:I:1166:TRP:CD1	1:I:1176:PRO:HG2	2.45	0.51
1:H:807:THR:N	1:H:808:PRO:HD2	2.25	0.51
1:I:552:ASP:HB2	1:I:890:LYS:HZ2	1.75	0.51
3:Q:331:GLN:HG2	3:Q:404:ARG:HA	1.91	0.51
3:Q:374:THR:O	3:Q:378:GLU:HG2	2.11	0.51
2:A:711:ILE:O	2:A:751:VAL:HG23	2.11	0.51
2:A:727:ILE:HD11	2:A:780:LEU:HD11	1.93	0.51
2:A:61:ARG:HB3	2:A:62:PRO:HD3	1.91	0.51
3:R:242:ASN:ND2	3:R:243:ARG:HG2	2.26	0.51
1:H:759:ASN:ND2	1:H:762:THR:H	2.08	0.51
2:A:683:THR:O	2:A:687:ILE:HG12	2.11	0.51
2:A:947:LYS:O	2:A:948:ARG:HD2	2.09	0.51
2:A:1191:ASP:HB3	2:A:1217:LEU:HG	1.93	0.51
1:H:1096:ASP:OD1	1:H:1097:GLU:N	2.43	0.50
2:A:242:VAL:HG12	2:A:248:ILE:HD12	1.93	0.50
2:A:825:VAL:HB	2:A:846:VAL:HG12	1.92	0.50
2:A:85:PHE:CE1	2:A:89:LYS:HD3	2.45	0.50
2:A:1143:VAL:HB	2:A:1183:MET:HB3	1.94	0.50
3:Q:75:THR:HG22	3:Q:96:TRP:CZ2	2.46	0.50
1:I:625:ASN:HB3	1:I:655:MET:HE3	1.93	0.50
2:A:727:ILE:CD1	2:A:780:LEU:CD1	2.90	0.50
1:H:415:ASN:OD1	1:H:417:SER:N	2.44	0.50
2:A:711:ILE:O	2:A:751:VAL:HA	2.12	0.50
2:A:949:TYR:N	2:A:958:GLU:O	2.38	0.50
2:A:1237:GLU:CB	2:A:1289:LEU:HB2	2.32	0.50
1:H:276:VAL:HB	1:H:277:PRO:HD3	1.93	0.49
1:I:253:PRO:HG3	1:I:923:ILE:HG13	1.92	0.49
2:A:925:GLN:NE2	2:A:1016:MET:HB3	2.26	0.49
3:R:225:VAL:HG21	3:R:414:ILE:HG21	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:654:ASN:ND2	1:H:673:ARG:O	2.42	0.49
2:A:8:ARG:HB2	2:A:716:PHE:CE2	2.48	0.49
2:A:93:LEU:HD13	2:A:123:PHE:CD2	2.47	0.49
2:A:887:THR:HG22	2:A:889:MET:HG2	1.93	0.49
1:H:705:TRP:HE3	1:H:771:LEU:HD13	1.76	0.49
1:I:182:GLN:NE2	1:B:44:GLU:OE1	2.46	0.49
1:B:158:THR:O	1:B:161:ILE:HG22	2.13	0.49
1:I:335:PHE:CE1	1:I:1040:ILE:HD11	2.48	0.49
3:Q:328:HIS:HB3	3:Q:410:THR:HG22	1.94	0.49
1:H:1166:TRP:CD1	1:H:1176:PRO:HG2	2.47	0.49
1:H:982:MET:HG2	1:H:985:GLU:OE1	2.12	0.49
1:H:1156:TYR:HD1	1:H:1194:PRO:HG2	1.77	0.49
2:A:8:ARG:HB3	2:A:716:PHE:CE2	2.47	0.49
2:A:1128:ASP:HB3	2:A:1145:ILE:HG12	1.93	0.49
1:I:242:LYS:HD3	1:I:247:LEU:HD11	1.95	0.49
1:I:264:THR:HB	1:I:454:SER:HA	1.95	0.49
3:Q:303:LEU:HD23	3:Q:321:GLY:HA3	1.95	0.49
2:A:826:LEU:N	2:A:885:ILE:O	2.39	0.48
3:Q:16:LEU:HD22	3:Q:390:THR:HB	1.94	0.48
1:H:705:TRP:CE3	1:H:771:LEU:HD13	2.48	0.48
1:H:778:ASN:HD21	1:H:780:ARG:HB2	1.78	0.48
1:H:961:THR:HG22	1:I:893:PRO:O	2.12	0.48
3:R:367:PHE:O	3:R:371:LYS:HG2	2.13	0.48
3:R:382:TYR:CE1	3:R:386:HIS:CD2	3.02	0.48
2:A:455:GLN:HB2	2:A:620:THR:HA	1.94	0.48
2:A:478:ILE:HD11	2:A:484:VAL:HG11	1.94	0.48
1:H:344:LEU:HD22	1:B:52:GLN:HB3	1.94	0.48
1:I:446:GLU:CD	1:I:502:ASN:HD22	2.20	0.48
2:A:813:PHE:CZ	2:A:989:ARG:HB3	2.48	0.48
2:A:825:VAL:HB	2:A:846:VAL:CG1	2.43	0.48
1:H:914:VAL:O	1:H:918:LEU:HG	2.14	0.48
2:A:310:ASN:O	2:A:357:SER:OG	2.32	0.48
1:I:1015:MET:HG3	1:I:1016:PRO:O	2.14	0.48
2:A:1056:TYR:CE1	2:A:1061:LEU:HD12	2.49	0.47
1:I:352:LEU:HB3	1:I:955:LEU:HD22	1.96	0.47
1:I:507:TYR:CE1	1:I:915:PHE:HB3	2.50	0.47
2:A:8:ARG:HG3	2:A:315:ALA:HB3	1.96	0.47
2:A:1056:TYR:HE1	2:A:1061:LEU:HD12	1.78	0.47
3:Q:322:ARG:HG3	3:Q:322:ARG:HH11	1.78	0.47
3:R:208:THR:O	3:R:212:MET:HG3	2.12	0.47
1:I:870:THR:OG1	1:I:872:GLY:O	2.32	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:1002:GLN:HG2	1:I:1003:GLN:O	2.14	0.47
1:H:959:ALA:HB3	1:I:806:MET:HE2	1.97	0.47
2:A:851:ILE:O	2:A:851:ILE:CG2	2.62	0.47
2:A:964:ASP:OD1	2:A:965:ALA:N	2.48	0.47
3:R:331:GLN:HG3	3:R:403:GLY:O	2.15	0.47
1:H:625:ASN:HB3	1:H:655:MET:CE	2.44	0.47
2:A:491:LYS:O	2:A:495:GLN:HG2	2.14	0.47
1:H:896:VAL:HG23	1:H:899:VAL:HB	1.96	0.47
3:R:183:PHE:CZ	3:R:255:CYS:HB2	2.50	0.47
2:A:1031:ARG:CZ	2:A:1043:VAL:HG21	2.44	0.47
3:Q:10:THR:HB	3:Q:73:SER:HB3	1.96	0.47
3:Q:212:MET:O	3:Q:216:VAL:HG23	2.15	0.47
1:H:480:GLU:HG3	1:H:493:VAL:HG23	1.96	0.47
1:I:943:TYR:HD2	1:I:945:VAL:HG23	1.79	0.47
2:A:1170:LYS:HG3	2:A:1186:LYS:HB2	1.96	0.47
3:Q:322:ARG:HG3	3:Q:322:ARG:NH1	2.30	0.46
1:H:523:MET:HB3	1:H:849:VAL:HG21	1.96	0.46
1:H:621:THR:HA	1:H:781:TYR:HE1	1.80	0.46
1:I:190:LEU:HD12	1:I:196:LEU:HD12	1.97	0.46
1:I:503:ARG:NH2	3:R:189:GLU:OE2	2.46	0.46
2:A:498:ASP:HB3	2:A:501:THR:HB	1.98	0.46
2:A:712:GLU:OE2	2:A:749:ALA:HB1	2.16	0.46
3:Q:342:ARG:NH2	3:Q:411:SER:OG	2.49	0.46
1:I:763:ASN:O	1:I:767:ARG:HG2	2.16	0.46
2:A:413:MET:HE3	2:A:722:ALA:HA	1.97	0.46
1:H:552:ASP:O	1:H:888:SER:HB2	2.16	0.46
1:H:786:THR:HG22	1:H:788:SER:H	1.81	0.46
2:A:494:TYR:CE2	2:A:541:VAL:HG13	2.50	0.46
3:R:86:TRP:H	3:R:86:TRP:CD1	2.33	0.46
1:H:333:HIS:HA	1:H:336:LYS:HG2	1.98	0.46
1:H:625:ASN:HB3	1:H:655:MET:HE1	1.98	0.46
1:H:799:LYS:HE2	1:H:799:LYS:HA	1.98	0.46
1:H:818:GLU:OE2	1:H:901:TYR:OH	2.31	0.46
2:A:421:PRO:HA	2:A:698:ASP:O	2.15	0.46
2:A:50:ARG:HB2	2:A:183:ASP:OD2	2.16	0.46
2:A:120:VAL:O	2:A:124:LEU:HG	2.16	0.46
2:A:1136:PHE:HE2	2:A:1220:ILE:HD12	1.81	0.46
3:R:175:VAL:HG21	3:R:211:ARG:HH12	1.81	0.46
1:H:1168:GLU:OE1	1:B:50:ARG:NE	2.38	0.46
2:A:512:VAL:HG11	2:A:533:TRP:CH2	2.51	0.45
1:H:662:ILE:HD12	1:H:687:CYS:SG	2.55	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:392:ARG:HD3	1:I:452:GLU:OE2	2.17	0.45
2:A:826:LEU:HD21	2:A:878:ILE:CD1	2.47	0.45
1:I:242:LYS:CD	1:I:247:LEU:HG	2.45	0.45
1:I:845:THR:O	1:I:846:MET:HB2	2.16	0.45
2:A:413:MET:SD	2:A:722:ALA:HB2	2.53	0.45
2:A:711:ILE:CG2	2:A:712:GLU:N	2.78	0.45
1:H:934:LEU:HD23	1:H:934:LEU:HA	1.77	0.45
1:I:248:LEU:HG	1:I:913:GLU:OE2	2.16	0.45
2:A:770:ARG:HB2	2:A:862:ASN:HA	1.98	0.45
3:R:168:GLU:OE2	3:R:235:ARG:NE	2.50	0.45
2:A:828:LEU:HD13	2:A:828:LEU:HA	1.79	0.45
2:A:933:VAL:O	2:A:934:ARG:NH1	2.49	0.45
2:A:455:GLN:HG2	2:A:621:ARG:HG3	1.98	0.45
1:H:999:ILE:HG22	1:H:1011:ILE:HB	1.98	0.45
1:I:341:THR:HG21	1:B:84:LYS:HB2	1.98	0.45
2:A:1135:ASP:HB3	2:A:1141:THR:HB	1.99	0.45
3:Q:22:ASN:HD22	3:Q:389:SER:HB3	1.82	0.45
1:H:264:THR:HB	1:H:454:SER:HA	1.99	0.45
1:I:1061:PRO:HG3	1:I:1201:SER:O	2.16	0.45
2:A:50:ARG:NH1	2:A:181:ASP:OD2	2.44	0.45
2:A:1232:ALA:HB1	2:A:1251:ASN:HD21	1.81	0.45
1:I:1044:ASP:OD2	1:I:1138:ARG:NH2	2.46	0.45
2:A:903:PHE:CE2	2:A:927:ASN:HB2	2.52	0.45
2:A:146:LEU:HD22	2:A:157:PHE:CZ	2.51	0.45
2:A:1122:PRO:HG2	2:A:1151:TYR:CZ	2.53	0.44
2:A:253:ASP:OD1	2:A:298:THR:OG1	2.29	0.44
2:A:716:PHE:O	2:A:716:PHE:CG	2.70	0.44
3:Q:227:VAL:HG21	3:Q:415:ALA:HA	1.98	0.44
1:H:1050:VAL:HG13	1:H:1197:GLN:HB2	2.00	0.44
2:A:433:ASP:O	2:A:1003:SER:OG	2.22	0.44
2:A:455:GLN:HG3	2:A:621:ARG:NH1	2.31	0.44
2:A:1234:ASP:OD1	2:A:1236:ARG:HB2	2.16	0.44
2:A:772:LEU:HD12	2:A:773:PRO:HD2	1.99	0.44
2:A:1264:LEU:HD13	2:A:1278:ILE:HD11	1.99	0.44
1:I:249:HIS:O	1:I:250:ALA:C	2.60	0.44
1:I:940:GLU:OE2	1:I:956:ARG:HD3	2.17	0.44
1:I:955:LEU:HD23	1:I:955:LEU:H	1.82	0.44
1:H:759:ASN:ND2	1:H:808:PRO:HB2	2.33	0.44
2:A:829:GLY:HA3	2:A:891:SER:HB2	2.00	0.44
2:A:925:GLN:HE21	2:A:1016:MET:HB3	1.83	0.44
2:A:1065:THR:HA	2:A:1068:VAL:HG22	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:290:TYR:HB2	1:H:292:ILE:CD1	2.47	0.44
1:H:460:SER:O	1:H:464:ARG:HG2	2.18	0.44
1:H:724:PRO:HG3	1:H:737:GLU:OE2	2.18	0.44
3:R:175:VAL:HG21	3:R:211:ARG:NH1	2.32	0.44
1:H:290:TYR:HB2	1:H:292:ILE:HD12	2.00	0.44
1:H:632:LEU:O	1:H:636:LEU:HD23	2.17	0.44
2:A:1189:ILE:HD11	2:A:1228:LEU:HD13	1.99	0.44
2:A:1267:THR:OG1	2:A:1274:ILE:O	2.30	0.44
1:I:773:LYS:O	1:I:777:ASP:HB2	2.18	0.44
2:A:1052:VAL:HG13	2:A:1065:THR:OG1	2.17	0.44
3:R:76:LEU:O	3:R:80:PHE:HD2	1.99	0.44
2:A:743:ILE:O	2:A:787:ILE:N	2.49	0.43
2:A:1073:ILE:HD13	2:A:1093:PHE:CE1	2.53	0.43
1:H:415:ASN:HB3	1:H:420:CYS:SG	2.58	0.43
1:H:630:PHE:CZ	1:H:634:LEU:HD11	2.54	0.43
2:A:561:ASP:OD1	2:A:561:ASP:N	2.46	0.43
1:H:1068:ASP:OD1	1:H:1068:ASP:N	2.50	0.43
1:I:249:HIS:HD2	1:B:70:GLU:HB3	1.83	0.43
2:A:206:VAL:HA	2:A:209:ARG:HG2	2.01	0.43
2:A:940:LEU:HD13	2:A:951:PHE:CE1	2.53	0.43
1:H:472:MET:SD	1:H:922:MET:HE2	2.58	0.43
1:I:691:ILE:HD12	1:I:706:ALA:HB1	2.00	0.43
2:A:38:PRO:C	2:A:40:ARG:H	2.27	0.43
2:A:976:ASN:O	2:A:1025:GLY:O	2.35	0.43
1:I:1159:ALA:O	1:I:1163:THR:HG23	2.18	0.43
2:A:289:ALA:HB2	2:A:348:GLU:OE1	2.19	0.43
2:A:509:ARG:HA	2:A:544:PRO:HA	1.99	0.43
2:A:1034:PHE:HA	2:A:1040:CYS:SG	2.59	0.43
2:A:1172:GLN:HB3	2:A:1184:ASN:HB3	2.01	0.43
3:R:342:ARG:NH2	3:R:411:SER:OG	2.48	0.43
2:A:413:MET:HE2	2:A:413:MET:HB2	1.85	0.43
2:A:902:THR:HG23	2:A:905:ALA:H	1.83	0.43
3:R:13:PHE:CE1	3:R:121:ALA:HB2	2.54	0.43
3:R:138:ARG:O	3:R:142:ARG:HG2	2.18	0.43
3:Q:174:ASP:OD1	3:Q:175:VAL:N	2.52	0.43
1:H:336:LYS:HB2	1:H:336:LYS:HE3	1.84	0.42
1:H:684:TRP:HE3	1:H:689:MET:HE1	1.83	0.42
1:H:1173:THR:O	1:H:1173:THR:OG1	2.36	0.42
2:A:260:CYS:HA	2:A:282:CYS:SG	2.58	0.42
2:A:827:ASP:OD2	2:A:836:ILE:HG12	2.19	0.42
1:H:549:LEU:HD22	1:H:810:TYR:CD2	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:846:MET:HB3	1:H:846:MET:HE3	1.71	0.42
1:I:332:ILE:HG21	1:I:347:ARG:HD3	2.00	0.42
1:I:552:ASP:HB2	1:I:890:LYS:NZ	2.34	0.42
1:I:630:PHE:CB	1:I:772:MET:HE1	2.49	0.42
2:A:439:VAL:HG11	2:A:673:PHE:HB2	2.01	0.42
2:A:948:ARG:NH2	2:A:959:PRO:HD3	2.34	0.42
1:B:82:ASP:N	1:B:86:ASN:O	2.49	0.42
1:H:471:ARG:NH1	3:Q:44:ASP:OD1	2.51	0.42
1:I:309:ARG:NH2	1:I:317:ASP:OD1	2.52	0.42
2:A:38:PRO:HG2	2:A:40:ARG:HB2	2.02	0.42
2:A:889:MET:HE3	2:A:889:MET:HA	2.00	0.42
3:Q:11:VAL:HG12	3:Q:73:SER:CB	2.49	0.42
2:A:407:MET:HG3	2:A:771:TYR:HA	2.02	0.42
2:A:1157:VAL:HG12	2:A:1159:ILE:HG12	2.01	0.42
1:H:759:ASN:HD22	1:H:762:THR:H	1.67	0.42
1:H:1050:VAL:CG1	1:H:1197:GLN:HB2	2.50	0.42
1:I:573:PRO:HB3	1:I:793:MET:SD	2.60	0.42
2:A:404:GLN:HB3	2:A:771:TYR:CE1	2.55	0.42
2:A:527:PRO:HB2	2:A:530:ILE:HG12	2.01	0.42
2:A:405:ALA:O	2:A:771:TYR:HB2	2.19	0.42
3:Q:11:VAL:HG12	3:Q:73:SER:HB2	2.01	0.42
1:B:64:ARG:HA	1:B:64:ARG:HD3	1.86	0.42
1:H:941:THR:HG23	1:H:943:TYR:H	1.85	0.42
2:A:770:ARG:NH1	2:A:862:ASN:OD1	2.53	0.42
1:H:582:ARG:O	1:H:582:ARG:HD3	2.20	0.42
2:A:9:LEU:HD13	2:A:312:TYR:CD2	2.55	0.42
1:I:440:MET:HE2	1:I:440:MET:HB3	1.78	0.42
2:A:662:SER:OG	2:A:664:LEU:HD23	2.19	0.42
2:A:1240:VAL:HA	2:A:1285:THR:O	2.19	0.42
2:A:992:ARG:O	2:A:996:LEU:HB2	2.20	0.42
1:I:1111:PRO:HG2	1:I:1114:LEU:HG	2.02	0.41
2:A:570:ASP:HB3	2:A:607:ALA:HB2	2.02	0.41
2:A:613:VAL:HG23	2:A:654:VAL:HG22	2.01	0.41
2:A:1155:THR:HG21	2:A:1171:PHE:CG	2.54	0.41
2:A:439:VAL:O	2:A:639:MET:HG3	2.21	0.41
3:Q:236:THR:O	3:Q:255:CYS:HA	2.19	0.41
1:H:353:MET:HE1	1:H:955:LEU:HD13	2.01	0.41
1:I:502:ASN:C	1:I:502:ASN:OD1	2.63	0.41
1:I:982:MET:HG2	1:I:985:GLU:CG	2.50	0.41
2:A:486:ASP:OD1	2:A:575:TYR:CZ	2.73	0.41
2:A:1232:ALA:HA	2:A:1233:PRO:HD3	1.95	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:60:ALA:O	1:B:64:ARG:HG2	2.21	0.41
1:H:761:LEU:HB2	1:H:808:PRO:HB3	2.03	0.41
2:A:42:PRO:HD2	2:A:43:TRP:CZ3	2.55	0.41
1:H:842:ARG:HE	1:H:842:ARG:HB3	1.62	0.41
1:H:846:MET:CE	1:H:1002:GLN:HB2	2.51	0.41
2:A:1034:PHE:HD2	2:A:1119:VAL:HG22	1.85	0.41
2:A:498:ASP:HA	2:A:505:TYR:CE1	2.53	0.41
2:A:1026:LEU:HD23	2:A:1026:LEU:HA	1.89	0.41
2:A:1128:ASP:OD1	2:A:1128:ASP:N	2.53	0.41
2:A:1145:ILE:HG22	2:A:1147:VAL:HG23	2.02	0.41
1:I:248:LEU:HD21	1:I:250:ALA:HB3	2.02	0.41
2:A:130:TYR:HA	2:A:133:LEU:HD12	2.03	0.41
2:A:1073:ILE:HD13	2:A:1093:PHE:HE1	1.85	0.41
1:H:867:THR:O	1:H:867:THR:HG22	2.20	0.41
1:H:1078:GLY:N	1:H:1097:GLU:OE2	2.54	0.41
1:I:254:ARG:HE	1:I:254:ARG:HB2	1.71	0.41
1:I:603:VAL:HG23	1:I:604:VAL:HG23	2.03	0.41
2:A:9:LEU:HD13	2:A:312:TYR:HD2	1.85	0.41
2:A:355:TYR:CD1	2:A:373:ASN:HA	2.56	0.41
2:A:529:VAL:C	2:A:532:PRO:HD2	2.46	0.41
2:A:1238:TRP:HA	2:A:1287:THR:O	2.21	0.41
2:A:1280:PRO:O	2:A:1284:TYR:OH	2.30	0.41
3:Q:233:THR:OG1	3:Q:259:HIS:O	2.32	0.41
3:Q:305:ASP:OD1	3:Q:306:ASN:N	2.53	0.41
3:Q:60:THR:OG1	3:Q:63:SER:OG	2.30	0.41
3:R:164:VAL:HG13	3:R:218:SER:HA	2.03	0.41
2:A:282:CYS:HB3	2:A:305:SER:OG	2.21	0.40
2:A:981:TRP:CZ3	2:A:1017:PRO:HG2	2.57	0.40
2:A:996:LEU:HA	2:A:996:LEU:HD13	1.85	0.40
3:R:273:MET:O	3:R:329:GLY:HA2	2.21	0.40
2:A:971:ARG:HD3	2:A:977:CYS:SG	2.61	0.40
3:R:47:SER:O	3:R:48:LEU:HD23	2.21	0.40
1:H:307:HIS:ND1	1:H:310:TRP:HB3	2.36	0.40
3:R:382:TYR:CE1	3:R:386:HIS:HD2	2.39	0.40
1:H:433:ARG:HA	1:H:450:VAL:HG12	2.04	0.40
1:I:253:PRO:CG	1:I:923:ILE:HG13	2.51	0.40
2:A:494:TYR:CE2	2:A:542:PRO:HD2	2.57	0.40
2:A:947:LYS:O	2:A:959:PRO:HA	2.21	0.40
2:A:963:MET:HE3	2:A:981:TRP:CD1	2.56	0.40
1:H:776:VAL:HG11	1:H:793:MET:HG2	2.02	0.40
1:I:422:PHE:O	1:I:425:SER:OG	2.38	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:610:ASP:N	1:I:610:ASP:OD1	2.54	0.40
1:I:1150:TYR:HB3	1:I:1184:ILE:HD11	2.03	0.40
2:A:980:THR:CG2	2:A:1020:ARG:HB3	2.51	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	B	136/1275 (11%)	131 (96%)	5 (4%)	0	100	100
1	H	1032/1275 (81%)	999 (97%)	33 (3%)	0	100	100
1	I	1081/1275 (85%)	1031 (95%)	50 (5%)	0	100	100
2	A	1280/1288 (99%)	1203 (94%)	76 (6%)	1 (0%)	48	75
3	Q	415/417 (100%)	403 (97%)	12 (3%)	0	100	100
3	R	415/417 (100%)	405 (98%)	10 (2%)	0	100	100
All	All	4359/5947 (73%)	4172 (96%)	186 (4%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	850	ASP

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	B	115/1114 (10%)	115 (100%)	0	100	100
1	H	914/1114 (82%)	907 (99%)	7 (1%)	73	79
1	I	959/1114 (86%)	959 (100%)	0	100	100
2	A	1118/1120 (100%)	1108 (99%)	10 (1%)	70	78
3	Q	353/353 (100%)	352 (100%)	1 (0%)	86	86
3	R	353/353 (100%)	353 (100%)	0	100	100
All	All	3812/5168 (74%)	3794 (100%)	18 (0%)	78	83

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	557	SER
1	H	559	THR
1	H	560	MET
1	H	563	VAL
1	H	759	ASN
1	H	842	ARG
1	H	846	MET
2	A	384	LEU
2	A	387	LEU
2	A	716	PHE
2	A	719	MET
2	A	828	LEU
2	A	836	ILE
2	A	847	THR
2	A	984	LEU
2	A	996	LEU
2	A	1248	CYS
3	Q	331	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (40) such sidechains are listed below:

Mol	Chain	Res	Type
1	H	307	HIS
1	H	527	ASN
1	H	759	ASN
1	H	812	GLN
1	H	1003	GLN
1	H	1010	ASN
1	H	1088	ASN

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Mol	Chain	Res	Type
1	H	1118	ASN
1	H	1155	GLN
1	H	1218	GLN
1	H	1226	HIS
1	I	690	ASN
1	I	937	GLN
1	I	1033	HIS
1	I	1107	ASN
1	I	1118	ASN
2	A	214	HIS
2	A	284	HIS
2	A	324	ASN
2	A	395	GLN
2	A	549	GLN
2	A	580	GLN
2	A	661	HIS
2	A	783	GLN
2	A	1133	GLN
2	A	1251	ASN
3	Q	18	ASN
3	Q	28	HIS
3	Q	214	GLN
3	Q	300	GLN
3	Q	315	ASN
3	R	110	GLN
3	R	114	GLN
3	R	146	GLN
3	R	280	ASN
3	R	300	GLN
3	R	315	ASN
3	R	328	HIS
3	R	386	HIS
1	B	146	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 [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.

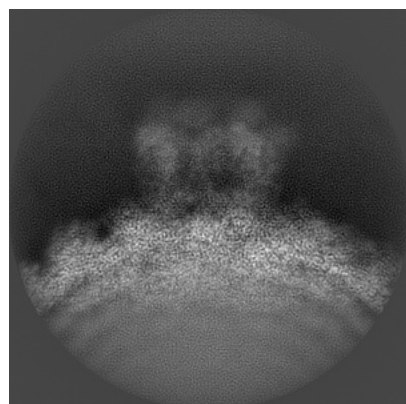
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-46053. These allow visual inspection of the internal detail of the map and identification of artifacts.

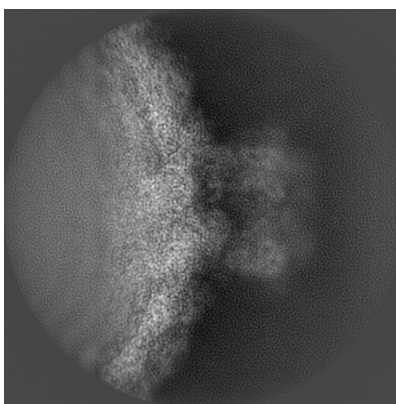
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

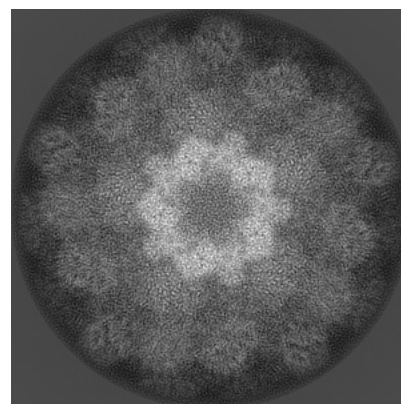
6.1.1 Primary map



X

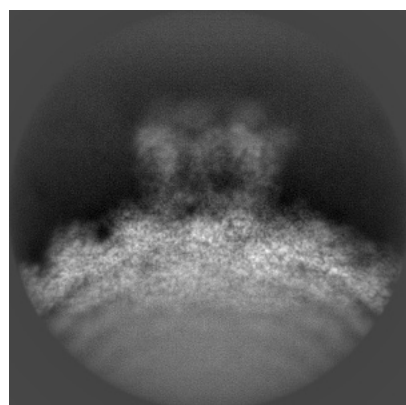


Y

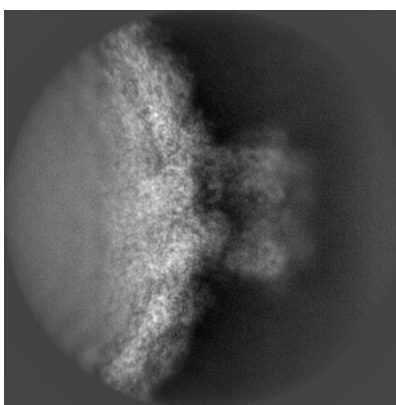


Z

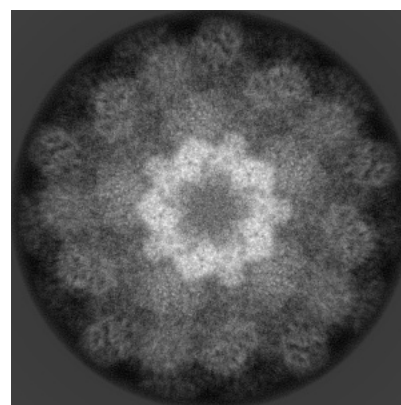
6.1.2 Raw map



X



Y

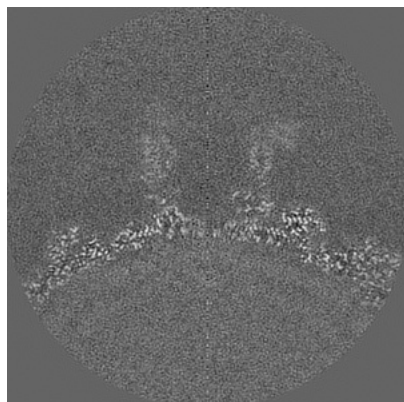


Z

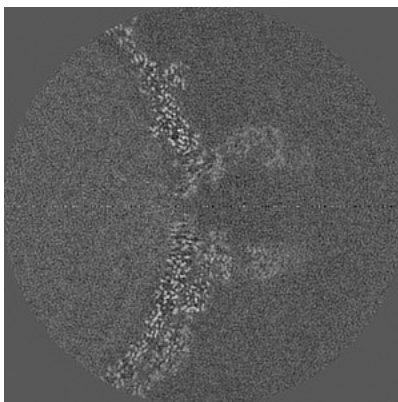
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

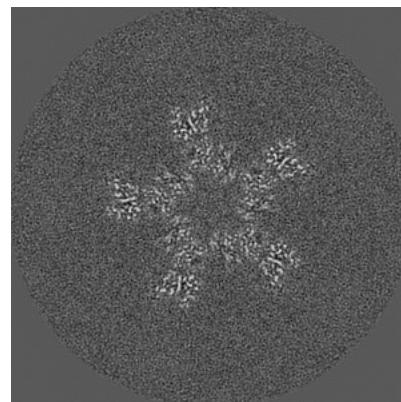
6.2.1 Primary map



X Index: 192

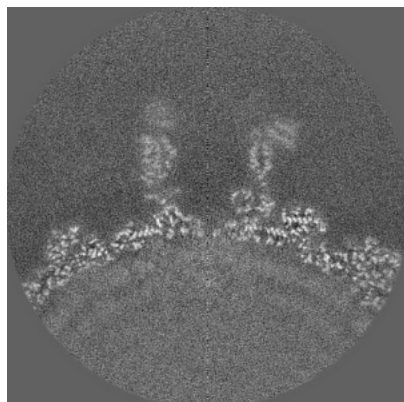


Y Index: 192

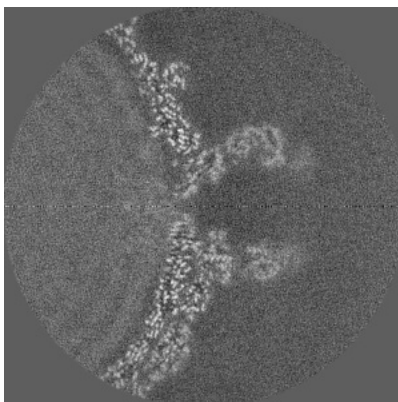


Z Index: 192

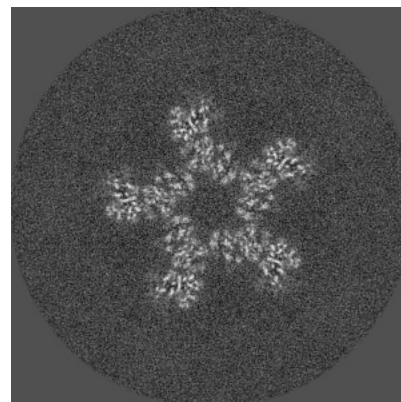
6.2.2 Raw map



X Index: 192



Y Index: 192

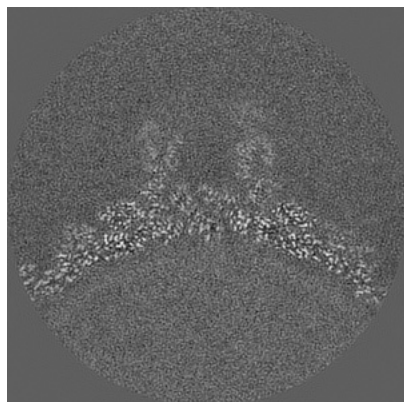


Z Index: 192

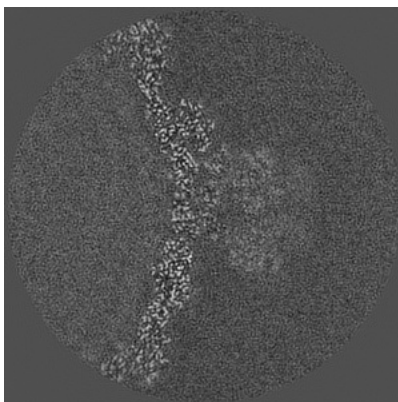
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

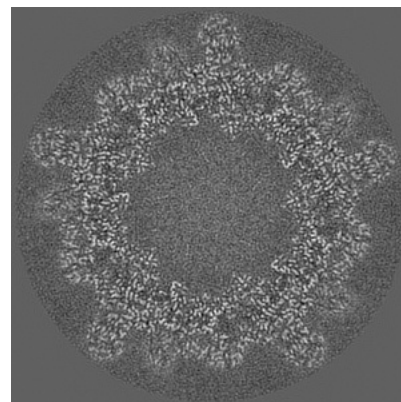
6.3.1 Primary map



X Index: 165

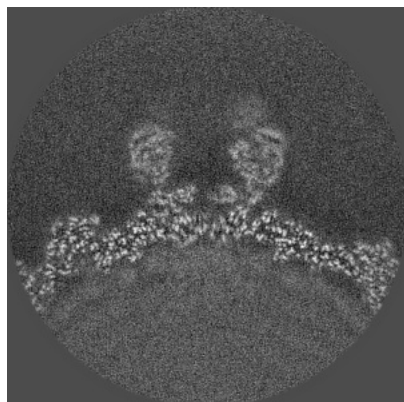


Y Index: 235

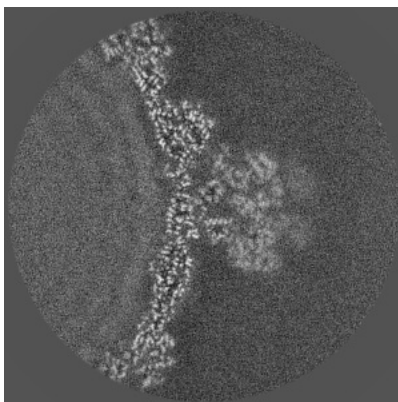


Z Index: 146

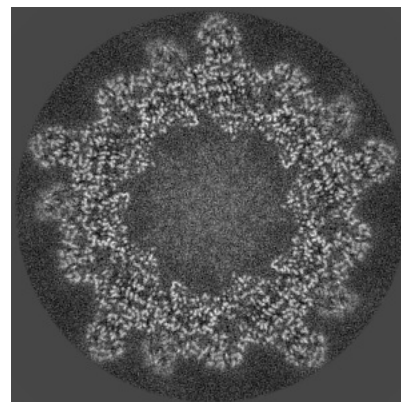
6.3.2 Raw map



X Index: 214



Y Index: 238

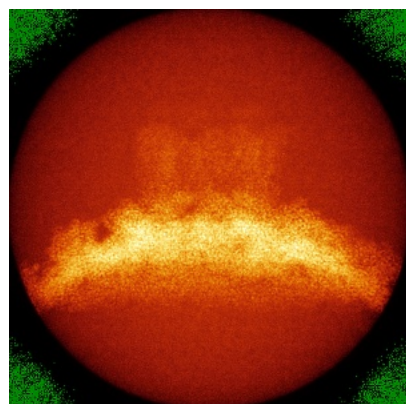


Z Index: 146

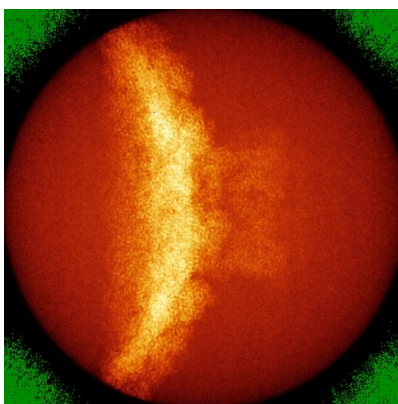
The images above show the largest variance slices of the map in three orthogonal directions.

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

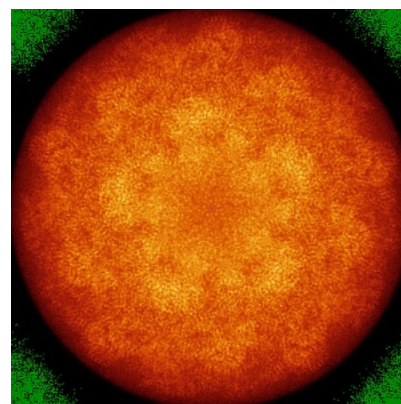
6.4.1 Primary map



X

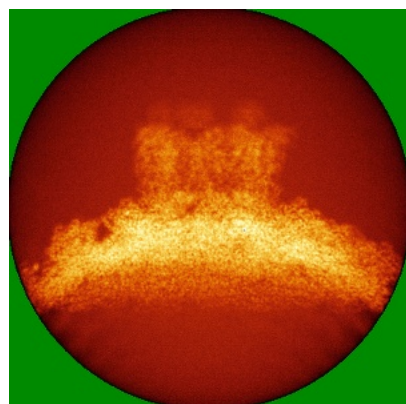


Y

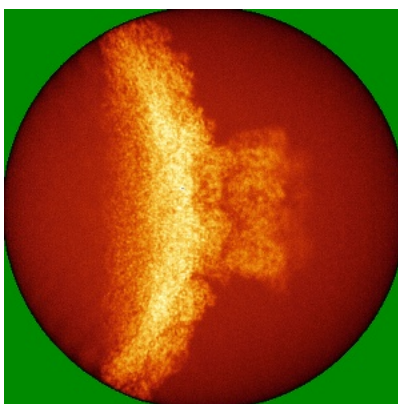


Z

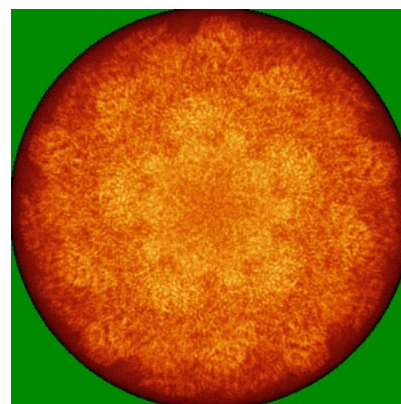
6.4.2 Raw map



X



Y

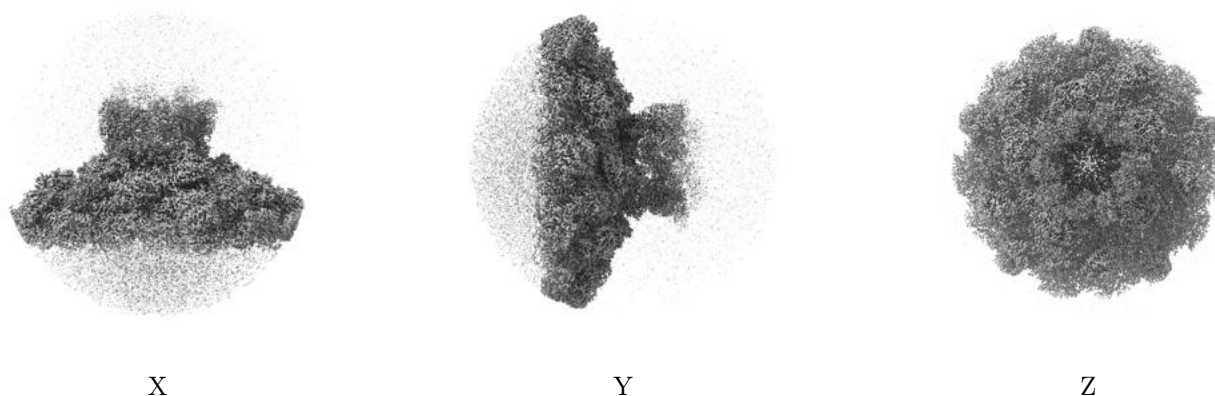


Z

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

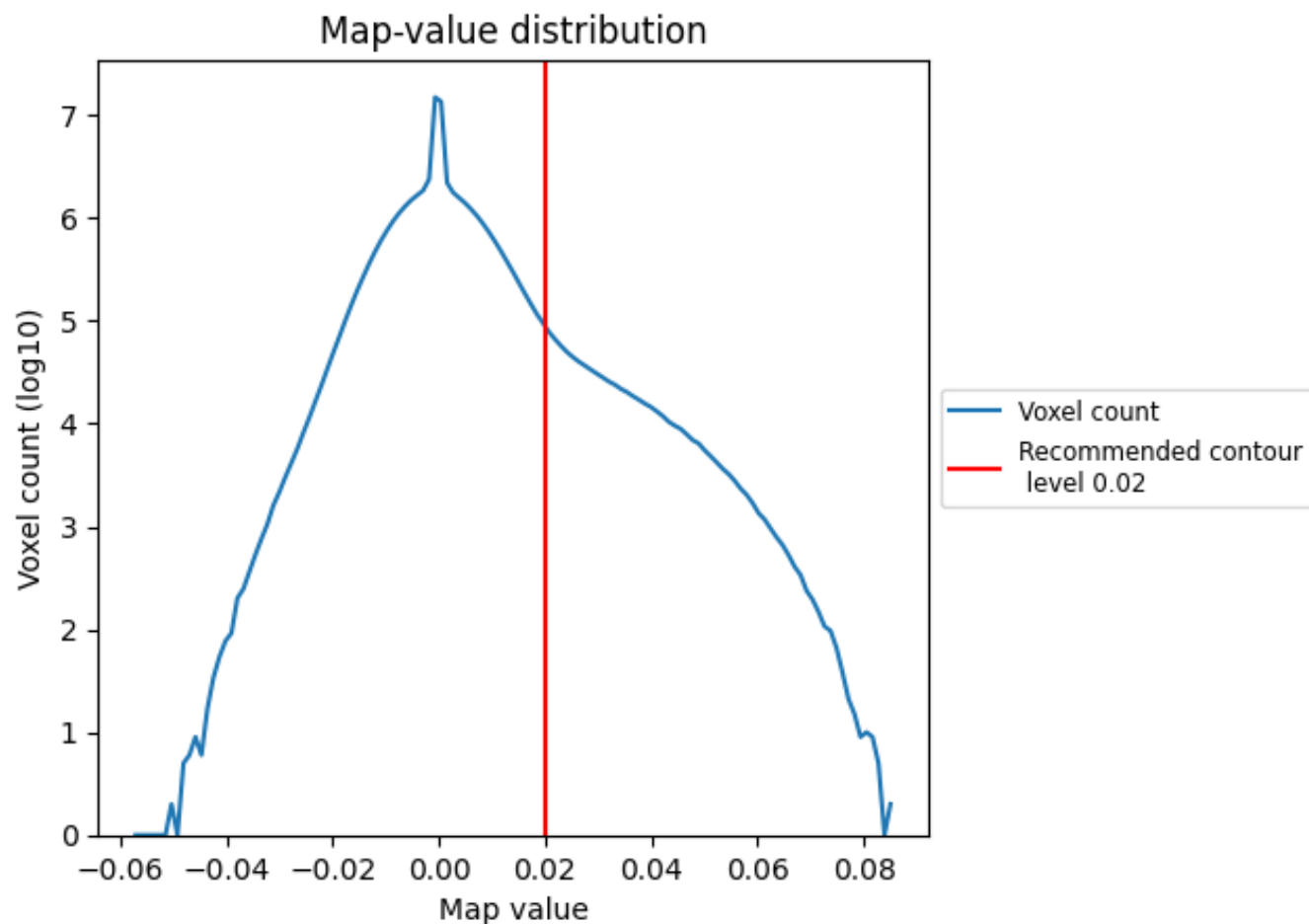
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

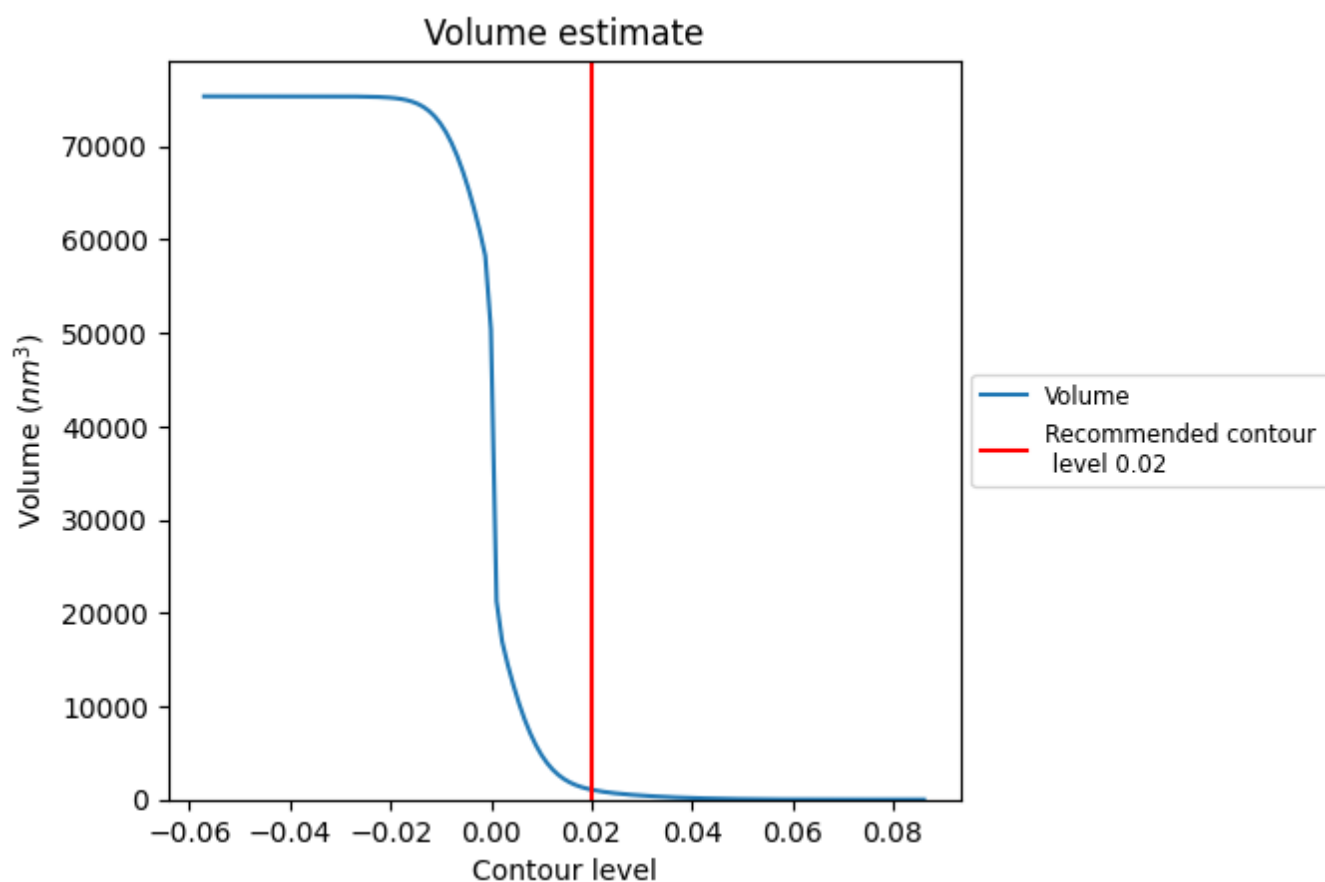
This section contains the results of statistical analysis of the map.

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.

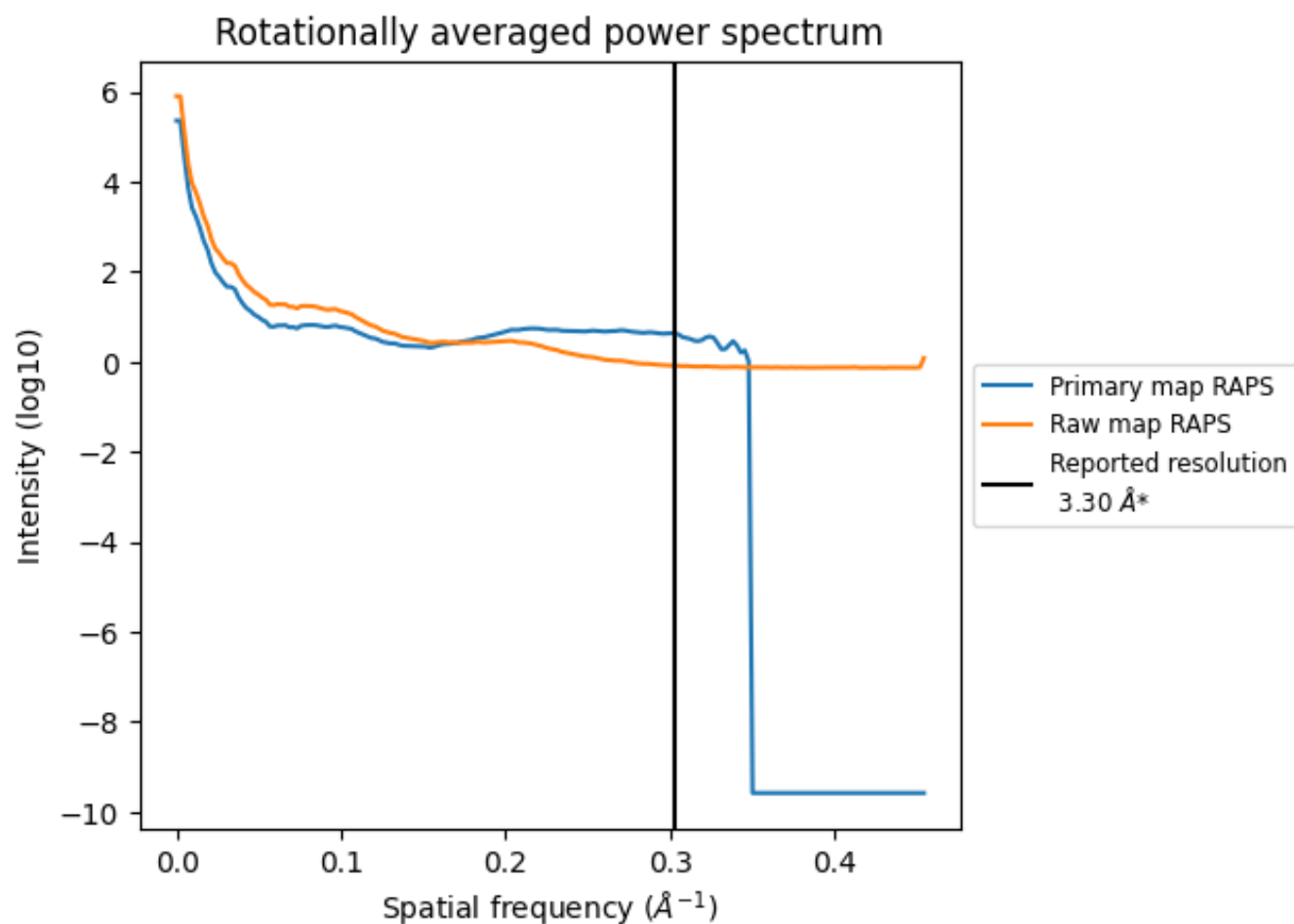
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1064 nm³; this corresponds to an approximate mass of 961 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 ⓘ

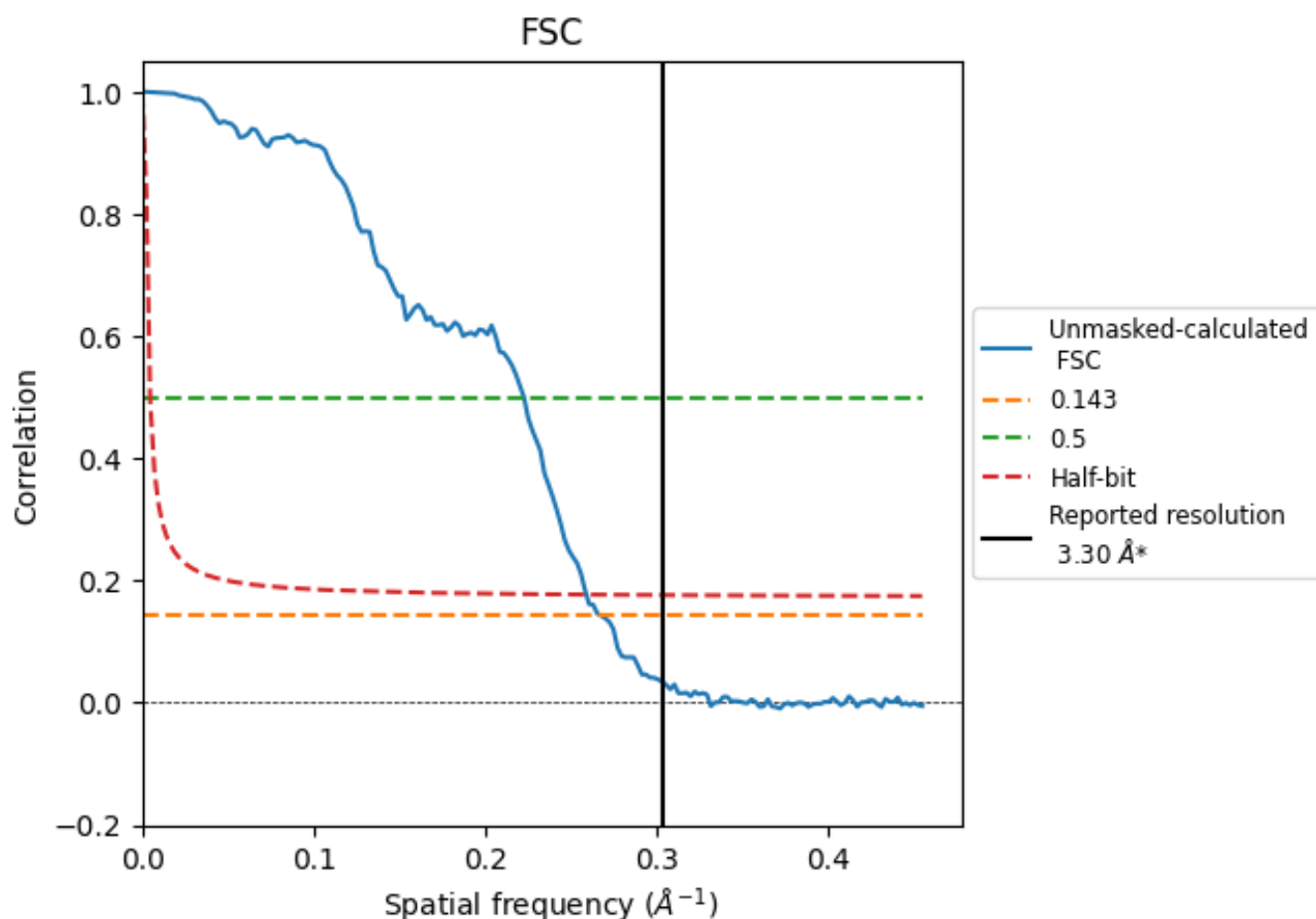


*Reported resolution corresponds to spatial frequency of 0.303 $\text{\AA}^{-1}$

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.303 Å⁻¹

8.2 Resolution estimates [i](#)

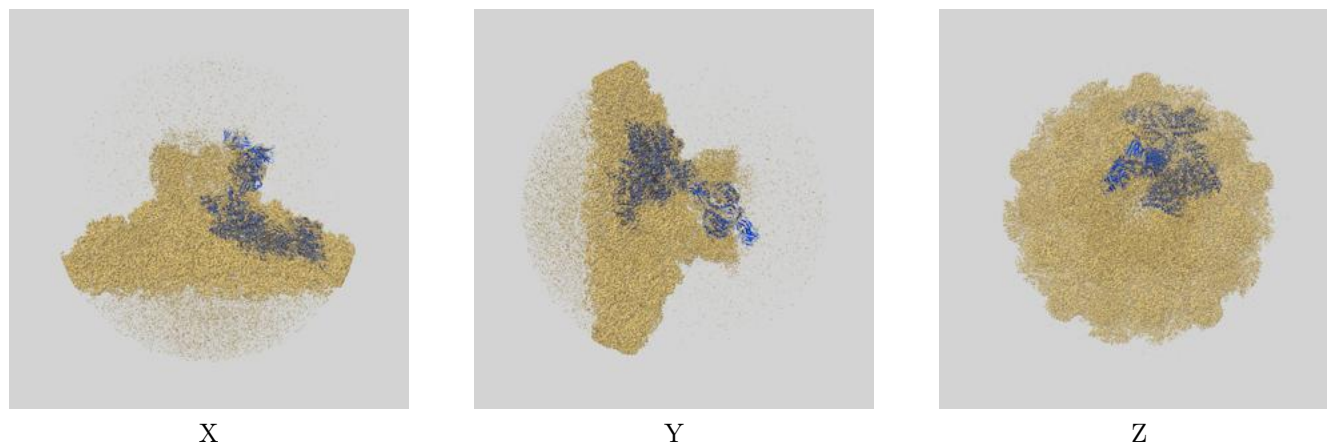
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.30	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.74	4.49	3.86

*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 3.74 differs from the reported value 3.3 by more than 10 %

9 Map-model fit [i](#)

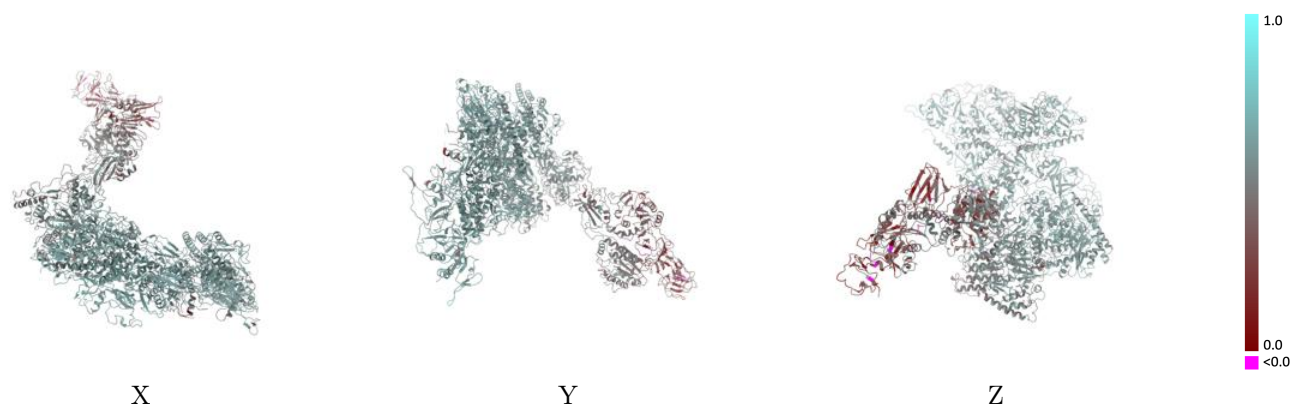
This section contains information regarding the fit between EMDB map EMD-46053 and PDB model 9CYX. Per-residue inclusion information can be found in [section 3](#) on [page 5](#).

9.1 Map-model overlay [i](#)



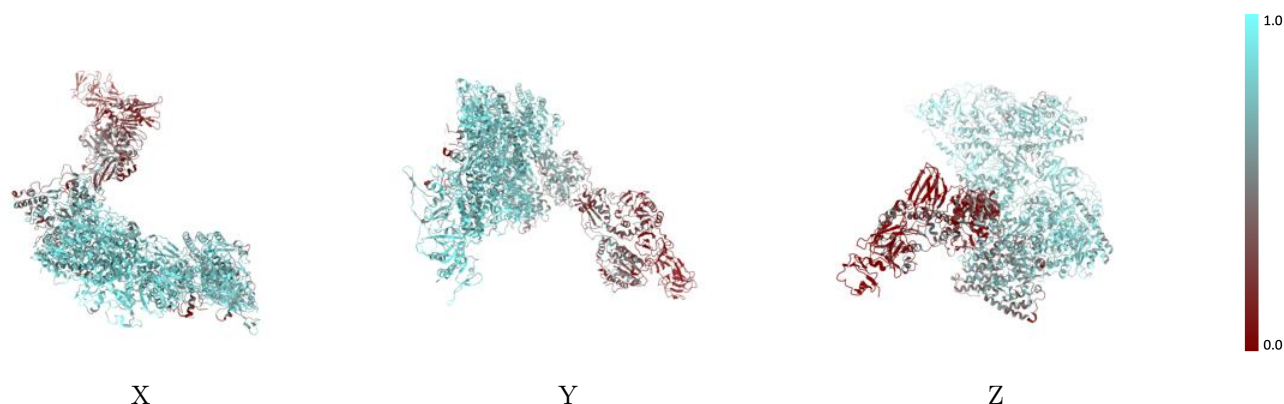
The images above show the 3D surface view of the map at the recommended contour level 0.02 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



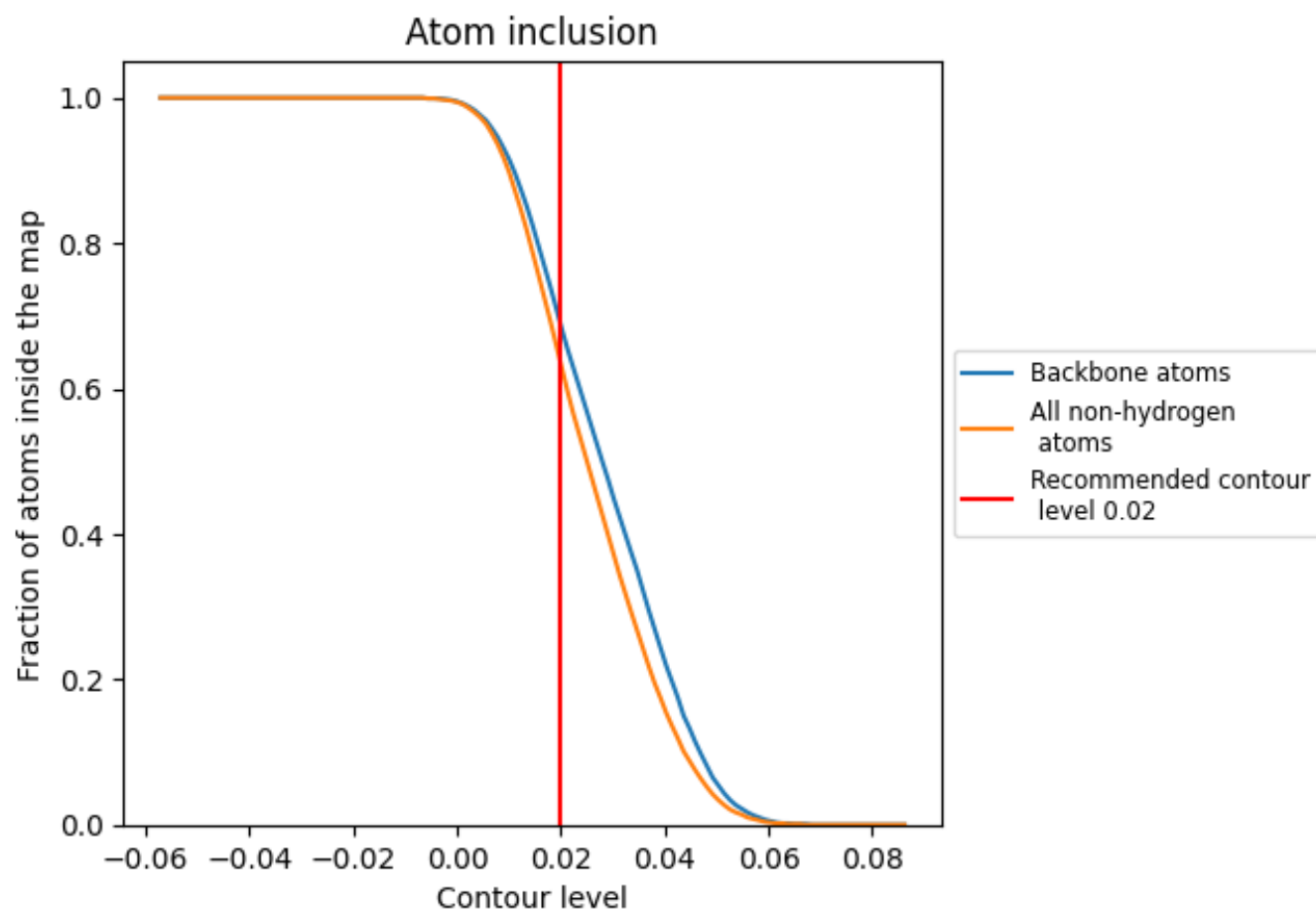
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.02).

9.4 Atom inclusion [i](#)



At the recommended contour level, 69% of all backbone atoms, 63% 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 (0.02) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6340	0.5350
A	0.3150	0.4260
B	0.6570	0.5750
H	0.7700	0.5740
I	0.7710	0.5810
Q	0.8140	0.5950
R	0.7310	0.5740

1.0

0.0

<0.0