



Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 05:13 AM UTC

PDB ID : 8ALZ / pdb_00008alz
EMDB ID : EMD-15521
Title : Cryo-EM structure of ASCC3 in complex with ASC1
Authors : Jia, J.; Hilal, T.; Loll, B.; Wahl, M.C.
Deposited on : 2022-08-01
Resolution : 3.40 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

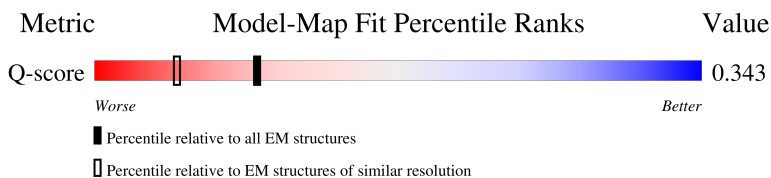
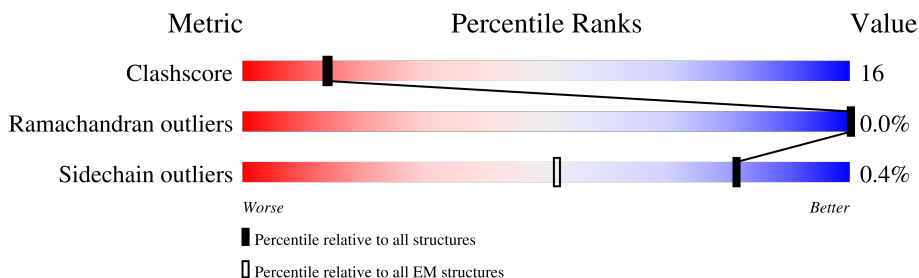
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.40 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	14717 (2.90 - 3.90)

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	585	 30% 14% 56%
2	B	1806	 65% 34%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 16409 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 Activating signal cointegrator 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	258	Total	C	N	O	S	0	0
			2052	1299	367	370	16		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	GLY	-	expression tag	UNP Q15650
A	-2	ALA	-	expression tag	UNP Q15650
A	-1	GLU	-	expression tag	UNP Q15650
A	0	PHE	-	expression tag	UNP Q15650

- Molecule 2 is a protein called Activating signal cointegrator 1 complex subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	1783	Total	C	N	O	S	0	0
			14355	9201	2482	2609	63		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	397	GLY	-	expression tag	UNP Q8N3C0
B	398	ALA	-	expression tag	UNP Q8N3C0
B	399	GLU	-	expression tag	UNP Q8N3C0
B	400	PHE	-	expression tag	UNP Q8N3C0

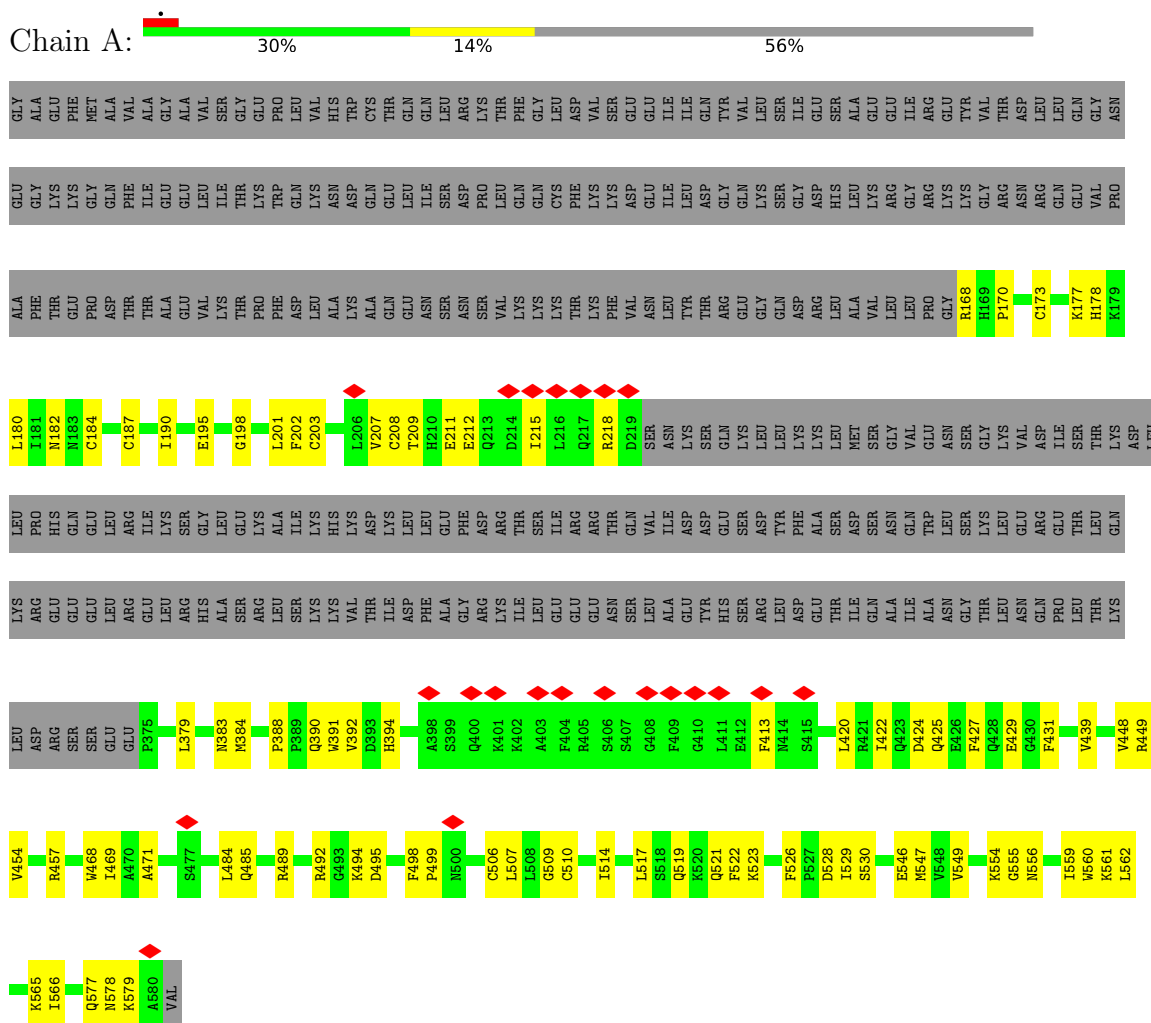
- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
3	A	2	Total	Zn	0
			2	2	

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: Activating signal cointegrator 1



• Molecule 2: Activating signal cointegrator 1 complex subunit 3



V1723	L1608	F1529	D1410	M1286	R1155	Q1023	T908	L806	T728	S648	R577	Q481	GLY
L1727	L1612	H1533	T1412	L1302	D1157	V1026	Y910	V807	V729	A649	T578	V484	ALA
D1733	A1613	C1534	P1413	L1303	E1158	V1026	E912	C808	M733	D656	L581	F485	GLU
N1736	H1619	C1535	D1414	P1307	I1159	I1031	A913	L812	L735	V657	T583	T487	PHE
T1743	H1619	M1538	M1415	L1308	T1162	L1034	V914	A813	T736	A658	T584	T491	H401
D1749	H1624	M1541	K1420	L1321	L1163	N1040	A915	V816	E737	V663	K587	T491	S408
A1750	H1624	M1541	A1421	L1321	Q1178	F1041	V916	V817	R738	V664	K587	T491	A410
L1751	R1626	P1544	L1423	H1326	M1183	K1056	Y923	A822	T745	V665	D588	M495	E411
D1627	R1628	F1546	V1425	M1328	M1184	K1056	Y924	E823	P746	V666	D589	M495	A412
T1757	V1631	Q1547	E1429	M1329	Q1189	I1065	R925	I824	F749	I667	V590	I497	A413
Y1758	E1632	I1548	T1332	T1332	T1192	S1066	Y926	I825	F670	V668	V591	P500	K414
F1759	E1632	I1549	Q1333	Q1333	R1193	R1067	R927	K826	F671	T501	T592	G502	M413
R1762	F1635	S1551	Q1439	I1334	R1193	S1072	A928	G827	F672	F672	K594	T501	K414
L1763	H1635	H1552	Y1443	I1334	L1196	F1073	T935	T828	Q752	R677	G597	K505	A417
I1764	K1639	S1553	V1444	Y1339	R1197	S1074	P944	Y831	G753	P678	D598	T506	F418
M1765	V1640	P1554	Q1445	Y1339	T1202	L1075	R949	A832	H754	R678	V599	N507	I419
N1766	Q1641	A1555	Q1446	D1342	T1202	D1078	R950	K834	D755	L681	A600	L508	K423
P1767	V1642	K1556	T1447	C1343	W1208	D1078	R950	K835	L758	L686	Q603	M510	M424
L1772	A1645	P1557	L1448	N1344	N1209	Y1081	R961	K836	K761	I688	I604	L511	I425
S1776	L1659	L1560	T1455	G1354	Q1211	V1082	D962	A833	V763	R689	L608	V525	L426
V1780	V1660	F1561	I1455	T1356	Q1212	N1085	Q965	K834	Q764	I688	I609	H515	P427
K1781	I1662	S1562	E1460	T1356	H1213	N1085	R966	V846	R765	I688	L610	E530	E428
N1782	I1662	S1563	E1461	E1360	G1217	R1088	R967	M847	R766	R689	E612	K532	G429
F1783	K1663	Q1567	R1462	R1366	D1226	I1089	R968	Q848	N768	Q695	V613	L533	I430
L1784	G1670	T1568	G1463	V1366	E970	W1101	F969	F850	V771	Q696	L616	E535	L437
L1797	R1673	L1573	E1467	K1369	N1229	P1103	E971	R855	R772	N698	H617	Y535	Y438
R1808	A1690	I1576	T1473	K1374	H1231	T1106	Y975	P856	L774	M700	G621	P538	E439
Y1821	G1691	A1577	H1479	A1375	H1234	S1113	F976	G864	G778	D701	L624	R540	Y441
Y1823	R1692	F1578	H1479	Y1377	K1242	K1114	S977	I865	F779	E702	E625	L542	R442
L1824	K1700	E1583	R1485	P1380	K1243	I1115	L981	D871	H782	C704	I627	M546	P450
Q1827	A1701	K1586	I1486	L1381	Q1244	D1117	G982	K872	H783	M707	R630	T547	L451
K1830	V1702	Q1587	S1490	L1381	S1247	K1118	R983	L873	M786	V708	T631	F550	D462
T1842	H1704	W1588	A1494	L1384	E1249	W1121	Y992	I886	L787	L709	L632	S551	L463
E1843	D1707	N1590	N1495	D1390	V1254	I1137	T994	F830	Q789	W712	Q634	R552	D464
E1844	I1708	M1591	D1498	D1391	V1254	I1137	I995	F830	D790	K713	V635	R553	E465
L1845	D1711	R1594	W1502	R1393	I1259	R1140	E996	A895	N792	Q639	Q639	E555	G467
S1847	F1712	E1595	W1502	R1393	I1259	L1141	T997	D896	N796	M719	S640	P556	Q468
I1848	K1714	E1597	V1517	R1395	I1269	L1146	L1001	N897	E795	M641	M641	V561	L469
L1849	L1717	M1598	R1518	L1400	S1273	T1147	A1004	I902	R643	F471	I642	D567	K472
S1850	P1720	V1603	V1524	G1401	L1277	L1147	A1004	A903	L797	H723	I644	M668	G473
E1853		R1604	H1525	K1403	L1277	K1150	D1010	T906	H802	A724	G646	E574	M474
		D1605	I1526	V1404	C1283	M1154	E1019	V907	V805		L647		L477
													R478
													I480



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	244064	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 ($e^-/\text{\AA}^2$)	42	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	1.657	Depositor
Minimum map value	0.000	Depositor
Average map value	0.006	Depositor
Map value standard deviation	0.044	Depositor
Recommended contour level	0.157	Depositor
Map size (Å)	266.24, 266.24, 266.24	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.83199996, 0.83199996, 0.83199996	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN

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	0.11	0/2104	0.33	0/2838
2	B	0.13	0/14692	0.39	2/19926 (0.0%)
All	All	0.13	0/16796	0.38	2/22764 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	665	PRO	CA-N-CD	-5.84	103.82	112.00
2	B	944	PRO	CA-N-CD	-5.24	104.66	112.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2052	0	2016	66	0
2	B	14355	0	14437	457	0
3	A	2	0	0	0	0
All	All	16409	0	16453	512	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 16.

All (512) 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:B:1591:MET:HE3	2:B:1591:MET:H	1.41	0.85
1:A:187:CYS:SG	1:A:203:CYS:HB3	2.17	0.83
1:A:424:ASP:HA	2:B:2131:LYS:HZ2	1.47	0.79
2:B:690:CYS:HB2	2:B:696:GLN:HG3	1.65	0.78
2:B:825:ILE:HG23	2:B:827:GLY:H	1.50	0.77
2:B:500:PRO:HB2	2:B:677:ARG:HD3	1.68	0.76
2:B:966:MET:HE1	2:B:992:TYR:HB2	1.68	0.76
2:B:1328:ASN:ND2	2:B:1331:GLN:OE1	2.24	0.71
2:B:723:HIS:HB3	2:B:828:THR:HB	1.73	0.71
2:B:414:LYS:HD2	2:B:417:ALA:HB2	1.74	0.70
2:B:472:LYS:HB2	2:B:474:MET:HE1	1.74	0.70
2:B:591:VAL:HA	2:B:594:LYS:HG2	1.74	0.69
2:B:1321:LEU:HB3	2:B:1395:ARG:HH21	1.57	0.69
2:B:606:ARG:HH21	2:B:642:ILE:HD11	1.57	0.69
2:B:1969:ASN:HA	2:B:1972:LEU:HG	1.74	0.69
2:B:1366:VAL:HG11	2:B:1375:ALA:HB2	1.75	0.68
2:B:542:LEU:HD11	2:B:814:TRP:HE3	1.56	0.68
2:B:633:ARG:HD3	2:B:906:THR:HB	1.76	0.68
2:B:766:SER:O	2:B:772:ARG:NH1	2.26	0.67
2:B:1234:HIS:O	2:B:1234:HIS:ND1	2.29	0.66
2:B:484:VAL:HG11	2:B:508:ILE:HD12	1.77	0.65
2:B:1765:MET:HE3	2:B:1765:MET:HA	1.78	0.65
2:B:507:ASN:HA	2:B:510:MET:HE3	1.77	0.65
2:B:1026:VAL:HG22	2:B:1056:LYS:HD2	1.78	0.65
2:B:1596:MET:SD	2:B:1596:MET:N	2.70	0.64
2:B:502:GLY:HA2	2:B:505:LYS:HD2	1.80	0.64
2:B:1936:TRP:HA	2:B:2126:GLU:HA	1.78	0.64
2:B:783:HIS:O	2:B:791:ARG:NH1	2.31	0.64
2:B:1954:ARG:NH2	2:B:1967:ILE:O	2.29	0.64
2:B:1997:PRO:HG3	2:B:2169:LEU:HD13	1.80	0.64
2:B:1861:ARG:O	2:B:1862:HIS:ND1	2.30	0.63
1:A:506:CYS:SG	1:A:507:LEU:N	2.71	0.63
2:B:782:HIS:HB2	2:B:806:LEU:HD11	1.80	0.63
2:B:1727:LEU:HD22	2:B:1757:THR:HG21	1.81	0.63
2:B:1945:ASN:HA	2:B:1948:GLN:HE21	1.63	0.63
2:B:1308:LEU:HD23	2:B:1332:THR:HG23	1.80	0.63
1:A:429:GLU:OE2	1:A:429:GLU:N	2.25	0.63
2:B:434:ASN:HB3	2:B:439:GLU:HG3	1.79	0.62
2:B:746:PRO:HA	2:B:749:PHE:HE1	1.64	0.62
2:B:1184:MET:HB2	2:B:1202:ILE:HG22	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:577:GLN:NE2	1:A:578:ASN:OD1	2.33	0.62
2:B:1608:LEU:HB3	2:B:1612:LEU:HD23	1.80	0.62
2:B:1498:ASP:OD2	2:B:1762:ARG:NH1	2.32	0.62
2:B:1623:LEU:HG	2:B:1627:ASP:HB2	1.82	0.61
2:B:1380:PRO:HG2	2:B:1381:LEU:HD22	1.83	0.61
2:B:474:MET:SD	2:B:474:MET:N	2.69	0.61
2:B:695:GLN:HA	2:B:698:ASN:ND2	2.15	0.60
2:B:1661:ILE:HG22	2:B:1702:VAL:HG22	1.83	0.60
2:B:471:PHE:HZ	2:B:477:LEU:HD21	1.67	0.60
2:B:612:GLU:N	2:B:647:LEU:O	2.35	0.60
2:B:1085:ASN:O	2:B:1089:ILE:HG12	2.01	0.60
2:B:1390:ASP:O	2:B:1394:VAL:HG22	2.01	0.59
2:B:1595:GLU:HG2	2:B:1596:MET:SD	2.43	0.59
1:A:528:ASP:OD1	1:A:528:ASP:N	2.36	0.59
1:A:168:ARG:HH22	1:A:198:GLY:HA3	1.68	0.59
2:B:707:ASN:HD22	2:B:865:ILE:HG21	1.68	0.59
2:B:1706:HIS:HD2	2:B:1708:ILE:HG12	1.68	0.59
2:B:426:LEU:HD11	2:B:430:ILE:HG12	1.85	0.58
2:B:1561:PHE:HE1	2:B:1662:ILE:HG22	1.68	0.58
2:B:1365:ARG:HE	2:B:1369:LYS:HG3	1.69	0.58
2:B:1843:GLU:OE2	2:B:1843:GLU:N	2.28	0.58
2:B:1824:LEU:HD21	2:B:1923:VAL:HG12	1.84	0.58
1:A:170:PRO:HG3	1:A:201:LEU:HG	1.85	0.58
1:A:190:ILE:HD11	2:B:1333:GLN:HA	1.84	0.58
2:B:1597:GLU:OE2	2:B:1598:ASN:ND2	2.36	0.58
1:A:579:LYS:HZ3	2:B:1479:HIS:HA	1.68	0.58
2:B:762:GLN:HG2	2:B:765:ARG:HH21	1.69	0.58
2:B:1594:ARG:NH1	2:B:1595:GLU:HB3	2.18	0.58
2:B:1949:MET:O	2:B:1953:GLY:N	2.36	0.58
2:B:719:MET:HE1	2:B:721:PHE:CZ	2.38	0.58
2:B:850:PHE:HE2	2:B:864:GLY:HA3	1.67	0.58
2:B:1114:LYS:O	2:B:1118:LYS:HB2	2.04	0.58
2:B:1502:TRP:CD2	2:B:1758:TYR:HB2	2.39	0.58
2:B:1040:ASN:OD1	2:B:1041:PHE:N	2.37	0.57
2:B:1563:SER:HA	2:B:1567:GLN:HB3	1.84	0.57
2:B:466:ILE:HD13	2:B:469:LEU:HD21	1.86	0.57
2:B:617:HIS:HB2	2:B:886:ILE:HG13	1.85	0.57
2:B:677:ARG:HD2	2:B:678:PRO:HD2	1.86	0.57
2:B:755:ASP:OD1	2:B:755:ASP:N	2.35	0.57
2:B:1157:ASP:OD1	2:B:1158:GLU:N	2.38	0.57
1:A:468:TRP:HB3	1:A:507:LEU:HD11	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:720:VAL:HG22	2:B:824:ILE:HB	1.85	0.57
2:B:1560:ILE:O	2:B:1645:ALA:N	2.29	0.57
2:B:1749:ASP:OD1	2:B:1749:ASP:N	2.38	0.57
2:B:788:ARG:O	2:B:788:ARG:HD3	2.04	0.57
2:B:1533:HIS:ND1	2:B:1533:HIS:O	2.36	0.57
2:B:542:LEU:H	2:B:542:LEU:HD12	1.68	0.56
2:B:710:LYS:HA	2:B:713:LYS:HE2	1.86	0.56
2:B:423:LYS:HE3	2:B:425:ILE:HD13	1.86	0.56
2:B:479:ARG:NH1	2:B:480:ILE:HG13	2.20	0.56
2:B:923:TYR:O	2:B:927:ARG:HG2	2.05	0.56
2:B:1594:ARG:O	2:B:1597:GLU:HG3	2.05	0.56
2:B:626:SER:OG	2:B:630:ARG:NH2	2.38	0.56
2:B:786:MET:HE2	2:B:790:ASP:HB2	1.87	0.56
2:B:711:GLN:HG3	2:B:718:VAL:HG11	1.88	0.56
2:B:1331:GLN:NE2	2:B:1354:GLY:O	2.39	0.56
2:B:1558:VAL:HG12	2:B:1659:LEU:H	1.70	0.56
2:B:535:TYR:HB3	2:B:582:VAL:HG22	1.87	0.55
2:B:855:ARG:HD3	2:B:856:PRO:HD2	1.87	0.55
2:B:1183:MET:HA	2:B:1183:MET:HE2	1.88	0.55
2:B:1662:ILE:HG13	2:B:1703:ILE:HA	1.88	0.55
2:B:1972:LEU:O	2:B:1976:LYS:N	2.40	0.55
2:B:1518:ARG:NH2	2:B:1690:ALA:O	2.40	0.55
2:B:847:MET:HE2	2:B:847:MET:HA	1.89	0.55
2:B:1067:ARG:HA	2:B:1119:ARG:HH21	1.72	0.55
2:B:471:PHE:HA	2:B:553:ARG:HH22	1.72	0.55
2:B:1550:ARG:HE	2:B:1554:PRO:HB3	1.72	0.55
2:B:902:ILE:HG22	2:B:978:SER:HB2	1.89	0.55
2:B:758:LEU:O	2:B:761:LYS:HG3	2.07	0.54
2:B:1974:LEU:HD13	2:B:2017:GLU:HG2	1.90	0.54
1:A:450:GLY:O	1:A:492:ARG:NH2	2.39	0.54
2:B:1661:ILE:HD12	2:B:1663:LYS:HB2	1.89	0.54
2:B:546:MET:HE3	2:B:546:MET:HA	1.89	0.54
2:B:704:CYS:HB2	2:B:826:LYS:NZ	2.23	0.54
2:B:491:THR:O	2:B:515:HIS:NE2	2.36	0.54
1:A:173:CYS:HB2	1:A:177:LYS:HB3	1.88	0.54
1:A:469:ILE:HB	1:A:509:GLY:HA3	1.89	0.54
2:B:1247:SER:OG	2:B:1249:GLU:OE1	2.24	0.54
2:B:707:ASN:ND2	2:B:865:ILE:HG21	2.23	0.54
2:B:789:GLN:NE2	2:B:793:LEU:HD21	2.23	0.54
2:B:1767:PRO:HB3	2:B:1772:LEU:HD22	1.90	0.54
2:B:693:LYS:HB2	2:B:694:MET:HE2	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:825:ILE:HG22	2:B:866:ILE:HA	1.90	0.53
2:B:733:MET:HA	2:B:736:ILE:HD12	1.90	0.53
2:B:1141:LEU:HB3	2:B:1146:LEU:HD11	1.89	0.53
2:B:1550:ARG:HH22	2:B:1588:TRP:HE1	1.53	0.53
2:B:1467:GLU:OE2	2:B:1759:PHE:N	2.40	0.53
2:B:1526:ILE:HG23	2:B:1703:ILE:HD11	1.89	0.53
1:A:526:PHE:O	1:A:530:SER:OG	2.25	0.53
2:B:415:THR:HG21	2:B:426:LEU:HB3	1.89	0.53
2:B:616:LEU:HA	2:B:621:GLY:HA3	1.90	0.53
2:B:746:PRO:HA	2:B:749:PHE:CE1	2.42	0.53
2:B:1226:ASP:OD1	2:B:1226:ASP:N	2.38	0.53
2:B:1342:ASP:HB2	2:B:1365:ARG:NH2	2.22	0.53
2:B:2050:VAL:HG12	2:B:2052:GLY:H	1.73	0.53
2:B:1078:ASP:O	2:B:1082:VAL:HG13	2.08	0.53
2:B:1868:ASN:OD1	2:B:1869:SER:N	2.41	0.53
2:B:589:ASP:OD2	2:B:593:ARG:NH2	2.40	0.53
2:B:1210:ASP:OD1	2:B:1242:LYS:NZ	2.39	0.53
2:B:1404:VAL:HG22	2:B:1423:LEU:HD22	1.91	0.53
2:B:677:ARG:HH21	2:B:681:LEU:HD11	1.73	0.53
2:B:1156:LYS:O	2:B:1159:ILE:HG12	2.09	0.53
2:B:786:MET:SD	2:B:787:LEU:N	2.82	0.53
2:B:1140:ARG:NH1	2:B:1163:LEU:O	2.42	0.53
2:B:1975:PHE:O	2:B:1978:TRP:NE1	2.42	0.52
2:B:2033:LEU:HD12	2:B:2034:PRO:HD2	1.91	0.52
2:B:495:MET:O	2:B:645:LEU:HA	2.09	0.52
2:B:913:ALA:O	2:B:917:ILE:HG12	2.10	0.52
2:B:1415:MET:HE2	2:B:1415:MET:HA	1.90	0.52
2:B:419:ILE:HD13	2:B:424:MET:HB3	1.90	0.52
2:B:1952:GLN:NE2	2:B:1963:THR:OG1	2.42	0.52
2:B:567:ASP:OD2	2:B:568:MET:N	2.40	0.52
2:B:574:GLU:OE2	2:B:577:ARG:NH2	2.43	0.52
2:B:816:VAL:HG12	2:B:818:LEU:HD22	1.91	0.52
1:A:449:ARG:HD2	1:A:546:GLU:OE2	2.10	0.52
2:B:1140:ARG:HD2	2:B:1163:LEU:HG	1.90	0.52
2:B:2013:MET:SD	2:B:2013:MET:N	2.70	0.52
2:B:2040:ILE:HG13	2:B:2058:VAL:HG13	1.92	0.52
2:B:2123:ASP:OD1	2:B:2124:LYS:N	2.43	0.52
2:B:1552:HIS:HB3	2:B:1700:LYS:HD3	1.92	0.52
1:A:579:LYS:NZ	2:B:1479:HIS:HA	2.25	0.52
2:B:480:ILE:HG22	2:B:508:ILE:HD11	1.91	0.52
2:B:692:ASN:HB3	2:B:695:GLN:HG2	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:627:ILE:O	2:B:631:THR:HG22	2.10	0.52
1:A:495:ASP:OD1	1:A:495:ASP:N	2.43	0.51
2:B:711:GLN:HG3	2:B:718:VAL:CG1	2.39	0.51
2:B:2040:ILE:HB	2:B:2082:LEU:HD11	1.91	0.51
2:B:1494:ALA:HB2	2:B:1720:PRO:HB2	1.92	0.51
2:B:909:ASN:HB3	2:B:975:TYR:HD2	1.75	0.51
2:B:1101:ARG:HH22	2:B:1231:HIS:HD2	1.57	0.51
2:B:1209:ASN:HB3	2:B:1212:VAL:HB	1.92	0.51
2:B:610:LEU:O	2:B:647:LEU:HB3	2.09	0.51
2:B:718:VAL:O	2:B:805:VAL:HA	2.10	0.51
2:B:1661:ILE:HG22	2:B:1702:VAL:CG2	2.41	0.51
2:B:589:ASP:O	2:B:593:ARG:HG2	2.11	0.51
2:B:793:LEU:HA	2:B:796:ASN:HD21	1.76	0.51
2:B:981:LEU:HD11	2:B:995:ILE:HD11	1.92	0.51
2:B:1660:VAL:O	2:B:1701:ALA:HA	2.11	0.51
2:B:496:LEU:HD21	2:B:669:LEU:HD13	1.92	0.51
2:B:1374:LYS:HG2	2:B:1422:ASP:HA	1.93	0.51
2:B:1460:GLU:OE1	2:B:1462:ARG:N	2.43	0.51
1:A:392:VAL:HG12	1:A:394:HIS:H	1.75	0.51
2:B:909:ASN:HB3	2:B:975:TYR:CD2	2.47	0.51
2:B:1548:ALA:O	2:B:1552:HIS:ND1	2.33	0.51
2:B:439:GLU:O	2:B:687:GLY:N	2.45	0.50
2:B:965:GLN:HA	2:B:968:ARG:HH22	1.77	0.50
2:B:1541:MET:HB3	2:B:1704:LEU:HB3	1.93	0.50
2:B:2047:ASP:OD1	2:B:2047:ASP:N	2.45	0.50
2:B:484:VAL:HG23	2:B:495:MET:HE1	1.94	0.50
2:B:542:LEU:HD11	2:B:814:TRP:CE3	2.44	0.50
2:B:635:VAL:HG22	2:B:642:ILE:HD13	1.93	0.50
2:B:1229:ASN:HB3	2:B:1231:HIS:CE1	2.46	0.50
2:B:1937:LEU:HA	2:B:2127:LEU:HD23	1.93	0.50
2:B:1529:PHE:HZ	2:B:1544:PRO:HG2	1.75	0.50
2:B:1968:GLU:H	2:B:1971:HIS:HE1	1.60	0.50
1:A:449:ARG:HG3	1:A:499:PRO:HG3	1.93	0.50
2:B:1081:TYR:O	2:B:1085:ASN:ND2	2.44	0.50
2:B:1307:PRO:HB2	2:B:1326:HIS:HB3	1.94	0.50
2:B:1558:VAL:HG23	2:B:1642:VAL:HG23	1.94	0.50
2:B:2025:GLN:HA	2:B:2028:ASN:HD21	1.77	0.50
1:A:168:ARG:HD3	1:A:195:GLU:HB2	1.93	0.50
2:B:598:ASP:N	2:B:598:ASP:OD1	2.44	0.50
2:B:764:GLN:O	2:B:772:ARG:NH2	2.40	0.50
2:B:583:THR:OG1	2:B:584:THR:N	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1711:ASP:OD1	2:B:1711:ASP:N	2.44	0.49
2:B:2161:PHE:HD2	2:B:2171:GLN:HE21	1.59	0.49
2:B:907:VAL:HG12	2:B:976:PHE:HE1	1.76	0.49
1:A:184:CYS:HA	1:A:207:VAL:HG21	1.94	0.49
1:A:379:LEU:HD13	2:B:1749:ASP:HB2	1.94	0.49
2:B:534:VAL:HG12	2:B:581:LEU:HB2	1.95	0.49
2:B:639:GLN:OE1	2:B:639:GLN:HA	2.12	0.49
2:B:547:THR:O	2:B:551:SER:OG	2.30	0.49
2:B:935:ILE:HD11	2:B:949:HIS:CE1	2.47	0.49
1:A:448:VAL:HG21	1:A:509:GLY:HA2	1.93	0.49
2:B:612:GLU:HA	2:B:648:SER:HA	1.94	0.49
2:B:722:VAL:HG21	2:B:728:THR:HB	1.95	0.49
2:B:1495:ASN:ND2	2:B:1723:VAL:O	2.43	0.49
2:B:1879:SER:OG	2:B:1880:ASN:N	2.46	0.49
2:B:1971:HIS:HB2	2:B:1974:LEU:HD12	1.94	0.49
2:B:1910:ASP:O	2:B:1913:THR:HB	2.13	0.49
2:B:469:LEU:HD13	2:B:556:PRO:HB2	1.93	0.48
2:B:605:VAL:HG12	2:B:607:LEU:H	1.77	0.48
2:B:1781:ASN:OD1	2:B:1782:LYS:N	2.46	0.48
2:B:603:GLN:O	2:B:606:ARG:NH2	2.46	0.48
2:B:2067:ASP:H	2:B:2070:LYS:HZ1	1.60	0.48
1:A:420:LEU:C	1:A:422:ILE:H	2.21	0.48
2:B:464:ASP:O	2:B:468:GLN:HG2	2.13	0.48
2:B:1561:PHE:HB3	2:B:1645:ALA:HB3	1.95	0.48
2:B:1524:VAL:HA	2:B:1701:ALA:O	2.13	0.48
2:B:782:HIS:HB3	2:B:808:CYS:HA	1.95	0.48
2:B:2043:LYS:HB2	2:B:2055:GLU:HG2	1.94	0.48
2:B:2131:LYS:HA	2:B:2131:LYS:HE3	1.94	0.48
1:A:182:ASN:H	1:A:209:THR:HG22	1.77	0.48
2:B:1849:LEU:HD13	2:B:1927:MET:HE1	1.95	0.48
2:B:2163:SER:N	2:B:2170:ASP:OD1	2.44	0.48
2:B:825:ILE:HG21	2:B:866:ILE:HG22	1.96	0.48
2:B:721:PHE:HE2	2:B:849:ILE:HG23	1.79	0.48
2:B:1065:ILE:HD12	2:B:1115:VAL:HG12	1.94	0.48
2:B:1163:LEU:O	2:B:1163:LEU:HD23	2.14	0.48
2:B:1229:ASN:HB3	2:B:1231:HIS:HE1	1.79	0.48
2:B:2024:LYS:O	2:B:2028:ASN:ND2	2.46	0.48
2:B:735:LEU:HB3	2:B:779:PHE:HE2	1.78	0.48
2:B:1031:ILE:HD12	2:B:1034:LEU:HD23	1.96	0.48
2:B:1619:HIS:HB2	2:B:1628:ARG:HE	1.78	0.48
2:B:2117:LEU:HG	2:B:2131:LYS:HB2	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1625:GLU:HA	2:B:1628:ARG:HD3	1.96	0.47
1:A:431:PHE:HZ	2:B:1821:TYR:HB2	1.78	0.47
2:B:1114:LYS:HE3	2:B:1277:LEU:HA	1.97	0.47
2:B:890:PHE:HB3	2:B:922:LEU:HD22	1.97	0.47
2:B:462:ASP:OD1	2:B:462:ASP:N	2.43	0.47
2:B:774:LEU:HB3	2:B:779:PHE:O	2.14	0.47
2:B:962:ASP:OD1	2:B:968:ARG:NH2	2.44	0.47
2:B:1529:PHE:CZ	2:B:1544:PRO:HG2	2.49	0.47
2:B:1595:GLU:OE2	2:B:1595:GLU:N	2.24	0.47
2:B:486:GLU:OE1	2:B:486:GLU:N	2.28	0.47
2:B:530:GLU:HG3	2:B:531:PHE:CD1	2.50	0.47
2:B:734:SER:O	2:B:737:GLU:HG3	2.14	0.47
2:B:1377:TYR:HD2	2:B:1425:VAL:HG12	1.79	0.47
2:B:1196:LEU:HD22	2:B:1259:ILE:HG21	1.95	0.47
2:B:1331:GLN:HA	2:B:1334:ILE:HG12	1.95	0.47
2:B:721:PHE:HD2	2:B:825:ILE:HA	1.79	0.47
2:B:408:SER:O	2:B:409:GLN:HG3	2.15	0.46
2:B:1137:ILE:O	2:B:1141:LEU:HG	2.15	0.46
2:B:1192:THR:HG22	2:B:1193:ARG:H	1.79	0.46
2:B:1460:GLU:OE1	2:B:1461:GLU:N	2.48	0.46
2:B:440:GLU:HB3	2:B:686:LEU:HD13	1.96	0.46
2:B:495:MET:HG3	2:B:668:GLY:HA3	1.97	0.46
2:B:663:VAL:HG23	2:B:667:ILE:HD11	1.97	0.46
2:B:702:GLU:HG3	2:B:738:ARG:HH22	1.79	0.46
2:B:1243:LYS:HD2	2:B:1244:GLN:N	2.31	0.46
2:B:1535:CYS:O	2:B:1538:MET:HE3	2.15	0.46
2:B:1586:LYS:HB3	2:B:1589:LEU:HB2	1.96	0.46
2:B:1901:ARG:HH12	2:B:2106:ARG:HG3	1.80	0.46
2:B:656:ASP:N	2:B:656:ASP:OD1	2.48	0.46
2:B:697:LEU:HA	2:B:700:MET:SD	2.56	0.46
2:B:1439:GLN:HG3	2:B:1743:THR:HG22	1.98	0.46
2:B:1605:ASP:HB3	2:B:1608:LEU:HG	1.97	0.46
2:B:745:ILE:N	2:B:746:PRO:HD2	2.30	0.46
2:B:1072:SER:HB3	2:B:1075:LEU:HB3	1.98	0.46
2:B:1286:ASN:OD1	2:B:1286:ASN:N	2.48	0.46
2:B:778:GLY:O	2:B:805:VAL:HG22	2.15	0.46
2:B:895:ALA:HB1	2:B:961:LEU:HD21	1.97	0.46
2:B:1619:HIS:O	2:B:1619:HIS:ND1	2.49	0.46
2:B:1969:ASN:OD1	2:B:1970:HIS:N	2.49	0.46
2:B:597:GLY:HA2	2:B:1535:CYS:SG	2.55	0.46
2:B:648:SER:OG	2:B:649:ALA:N	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:688:ILE:HD11	2:B:699:ASN:HB3	1.98	0.46
2:B:793:LEU:HA	2:B:796:ASN:ND2	2.31	0.46
2:B:1557:PRO:HD2	2:B:1692:ARG:HH22	1.81	0.46
2:B:1968:GLU:H	2:B:1971:HIS:CE1	2.33	0.46
2:B:718:VAL:CG1	2:B:822:ALA:HB3	2.46	0.46
2:B:1842:THR:HA	2:B:1845:LEU:HD23	1.98	0.46
2:B:698:ASN:HA	2:B:701:ASP:OD2	2.16	0.45
2:B:1450:LEU:HD22	2:B:1473:THR:HG21	1.98	0.45
2:B:1847:SER:O	2:B:1850:SER:OG	2.28	0.45
2:B:2006:LYS:HB3	2:B:2009:VAL:HG22	1.99	0.45
2:B:725:ARG:O	2:B:728:THR:HG22	2.17	0.45
2:B:925:ARG:HH12	2:B:928:ALA:HB3	1.80	0.45
2:B:1415:MET:HE1	2:B:1443:TYR:CE1	2.50	0.45
2:B:2007:ASP:HB3	2:B:2027:TRP:NE1	2.32	0.45
2:B:480:ILE:HD12	2:B:480:ILE:H	1.82	0.45
2:B:738:ARG:HA	2:B:738:ARG:HD2	1.72	0.45
2:B:2042:VAL:HG12	2:B:2080:TYR:HD2	1.81	0.45
2:B:2042:VAL:HG22	2:B:2082:LEU:HD13	1.97	0.45
2:B:2056:LEU:HD12	2:B:2072:ILE:HG23	1.99	0.45
1:A:424:ASP:OD1	2:B:2132:ARG:HG2	2.15	0.45
2:B:417:ALA:HA	2:B:423:LYS:HD3	1.99	0.45
2:B:1670:GLY:O	2:B:1673:ARG:NH1	2.50	0.45
1:A:514:ILE:HD12	1:A:514:ILE:HA	1.87	0.45
1:A:177:LYS:HG2	1:A:178:HIS:HD1	1.81	0.45
1:A:546:GLU:OE1	1:A:546:GLU:HA	2.16	0.45
2:B:466:ILE:HG13	2:B:525:VAL:HG11	1.99	0.45
2:B:672:PHE:CD1	2:B:672:PHE:N	2.85	0.45
2:B:1412:THR:OG1	2:B:1413:PRO:HD3	2.17	0.45
2:B:2041:SER:HA	2:B:2057:SER:HA	1.99	0.45
2:B:832:ALA:O	2:B:836:GLY:N	2.41	0.45
2:B:1269:ILE:HB	2:B:1283:CYS:SG	2.57	0.45
2:B:1449:ILE:HD12	2:B:1485:ARG:HB3	1.98	0.45
2:B:1576:ILE:HD12	2:B:1576:ILE:HA	1.88	0.45
1:A:180:LEU:HD22	2:B:1303:LEU:HD13	1.98	0.45
2:B:550:PHE:HB3	2:B:561:VAL:HG11	1.98	0.45
2:B:791:ARG:HA	2:B:794:VAL:HG12	1.99	0.45
2:B:1088:ARG:HG3	2:B:1089:ILE:HD13	1.99	0.45
2:B:1559:LEU:O	2:B:1560:ILE:HD13	2.17	0.45
2:B:1662:ILE:CG1	2:B:1703:ILE:HA	2.46	0.45
2:B:1845:LEU:HA	2:B:1848:ILE:HG22	1.99	0.45
1:A:413:PHE:HA	1:A:561:LYS:HB3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:440:GLU:HB2	2:B:686:LEU:HD22	1.99	0.45
2:B:539:MET:SD	2:B:539:MET:N	2.90	0.45
1:A:383:ASN:C	1:A:384:MET:HE2	2.42	0.44
1:A:439:VAL:HA	1:A:457:ARG:HH22	1.82	0.44
2:B:430:ILE:HB	2:B:442:ARG:HB2	1.99	0.44
2:B:1573:LEU:HA	2:B:1576:ILE:HG22	1.99	0.44
1:A:547:MET:HE3	1:A:547:MET:N	2.31	0.44
2:B:1356:THR:O	2:B:1360:GLU:HG3	2.18	0.44
2:B:1624:HIS:HD2	2:B:1626:ARG:HG2	1.82	0.44
1:A:211:GLU:OE2	1:A:211:GLU:N	2.30	0.44
1:A:388:PRO:HG2	1:A:390:GLN:NE2	2.32	0.44
1:A:391:TRP:CE3	2:B:1751:LEU:HD12	2.52	0.44
2:B:541:ALA:HB1	2:B:815:GLY:HA2	2.00	0.44
2:B:1189:GLN:HB2	2:B:1197:ARG:O	2.17	0.44
2:B:870:HIS:O	2:B:873:LEU:HG	2.18	0.44
2:B:903:ALA:O	2:B:983:ARG:NH2	2.39	0.44
2:B:1004:ALA:HB2	2:B:1102:TRP:CE2	2.53	0.44
2:B:1827:GLN:HG3	2:B:1853:GLU:HG2	2.00	0.44
2:B:1867:MET:HA	2:B:1870:GLU:HG3	1.99	0.44
2:B:1990:ARG:NH2	2:B:1992:SER:O	2.49	0.44
1:A:468:TRP:CE3	1:A:510:CYS:HB3	2.53	0.44
2:B:472:LYS:NZ	2:B:555:GLU:OE2	2.41	0.44
2:B:608:LEU:HB3	2:B:644:ILE:HD13	1.98	0.44
2:B:1113:SER:HA	2:B:1116:ILE:HG22	1.98	0.44
2:B:1556:LYS:HB2	2:B:1556:LYS:HE2	1.69	0.44
2:B:695:GLN:HA	2:B:698:ASN:HD21	1.79	0.44
2:B:1591:MET:HB3	2:B:1639:LYS:HD3	2.00	0.44
2:B:789:GLN:O	2:B:793:LEU:HG	2.18	0.44
2:B:1154:MET:HE1	2:B:1162:ILE:HD12	2.00	0.44
2:B:1154:MET:SD	2:B:1159:ILE:HG22	2.57	0.44
2:B:1533:HIS:ND1	2:B:1535:CYS:SG	2.90	0.44
2:B:1635:PHE:HD1	2:B:1640:VAL:HB	1.82	0.44
2:B:505:LYS:HG2	2:B:647:LEU:HD11	2.00	0.44
2:B:1178:GLN:O	2:B:1213:HIS:NE2	2.51	0.44
2:B:1429:GLU:HB2	2:B:1823:TYR:HE2	1.82	0.44
2:B:1541:MET:HB2	2:B:1663:LYS:HG3	2.00	0.44
2:B:1603:VAL:HG13	2:B:1623:LEU:HD11	1.98	0.44
2:B:505:LYS:HG2	2:B:505:LYS:HZ2	1.50	0.43
2:B:611:ASP:HA	2:B:647:LEU:HB3	1.99	0.43
2:B:761:LYS:O	2:B:765:ARG:HG3	2.18	0.43
2:B:1302:LEU:HD22	2:B:1517:VAL:HG13	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:897:ASN:HB3	2:B:916:TRP:HH2	1.83	0.43
2:B:1628:ARG:O	2:B:1631:VAL:HG22	2.19	0.43
2:B:1628:ARG:NH2	2:B:1632:GLU:OE2	2.51	0.43
2:B:1945:ASN:C	2:B:1949:MET:HE3	2.43	0.43
1:A:425:GLN:OE1	2:B:2131:LYS:NZ	2.29	0.43
2:B:534:VAL:HG23	2:B:608:LEU:HD13	1.99	0.43
2:B:2038:VAL:HG23	2:B:2060:THR:HG21	2.00	0.43
1:A:484:LEU:HA	1:A:484:LEU:HD23	1.84	0.43
1:A:526:PHE:HE2	1:A:529:ILE:HB	1.83	0.43
2:B:616:LEU:HD21	2:B:624:LEU:HB3	2.01	0.43
2:B:667:ILE:HG13	2:B:668:GLY:N	2.33	0.43
2:B:1733:ASP:O	2:B:1736:ASN:HB3	2.18	0.43
2:B:2067:ASP:H	2:B:2070:LYS:NZ	2.17	0.43
2:B:2074:LEU:HD13	2:B:2148:THR:HG21	2.01	0.43
1:A:208:CYS:HB3	1:A:212:GLU:HG3	1.99	0.43
1:A:562:LEU:HD21	1:A:566:ILE:HG22	2.00	0.43
2:B:497:ILE:O	2:B:647:LEU:HA	2.18	0.43
2:B:600:ALA:H	2:B:603:GLN:HE22	1.67	0.43
2:B:864:GLY:C	2:B:865:ILE:HD13	2.43	0.43
2:B:1339:TYR:O	2:B:1365:ARG:HD3	2.18	0.43
2:B:2137:ARG:HG2	2:B:2138:ASN:N	2.34	0.43
2:B:471:PHE:CZ	2:B:477:LEU:HD21	2.51	0.43
2:B:768:ASN:HB3	2:B:771:VAL:HG12	2.00	0.43
2:B:997:THR:O	2:B:1001:LEU:HB2	2.19	0.43
1:A:424:ASP:HB3	1:A:427:PHE:CD1	2.54	0.43
2:B:437:LEU:HD23	2:B:437:LEU:H	1.84	0.43
2:B:613:VAL:HG22	2:B:648:SER:HB2	2.00	0.43
2:B:694:MET:HE2	2:B:694:MET:N	2.34	0.43
2:B:729:VAL:O	2:B:733:MET:SD	2.77	0.43
2:B:1381:LEU:HB2	2:B:1384:LEU:HB2	2.00	0.43
2:B:1546:PHE:CG	2:B:1578:PHE:HE2	2.36	0.43
1:A:494:LYS:HA	1:A:494:LYS:HD3	1.78	0.43
1:A:182:ASN:HB2	1:A:209:THR:HA	2.00	0.42
1:A:454:VAL:HG11	1:A:522:PHE:HZ	1.84	0.42
2:B:2011:SER:HA	2:B:2014:VAL:HG22	1.99	0.42
2:B:1114:LYS:NZ	2:B:1273:SER:O	2.43	0.42
2:B:1560:ILE:HD12	2:B:1661:ILE:HG13	2.01	0.42
2:B:1619:HIS:HB2	2:B:1628:ARG:HH21	1.85	0.42
2:B:871:ASP:OD1	2:B:871:ASP:N	2.52	0.42
2:B:1328:ASN:HB2	2:B:1329:PRO:HD2	2.00	0.42
2:B:1360:GLU:HG2	2:B:1392:TRP:CH2	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1450:LEU:HD12	2:B:1450:LEU:HA	1.87	0.42
2:B:437:LEU:HG	2:B:438:TYR:CD2	2.54	0.42
1:A:177:LYS:HG2	1:A:178:HIS:ND1	2.35	0.42
2:B:497:ILE:HD11	2:B:672:PHE:CZ	2.54	0.42
2:B:1763:LEU:HD21	2:B:1772:LEU:HD13	2.00	0.42
1:A:517:LEU:HD12	1:A:521:GLN:HB3	2.01	0.42
1:A:547:MET:HG2	1:A:549:VAL:H	1.85	0.42
2:B:603:GLN:HG2	2:B:604:ILE:HG23	2.00	0.42
2:B:616:LEU:HD22	2:B:621:GLY:HA2	2.01	0.42
2:B:1526:ILE:HG21	2:B:1714:LYS:HD2	2.01	0.42
2:B:1546:PHE:HA	2:B:1549:ILE:HD12	2.00	0.42
2:B:2113:GLU:HG3	2:B:2166:TYR:HE2	1.84	0.42
2:B:812:LEU:HD22	2:B:818:LEU:HD21	2.02	0.42
2:B:914:VAL:HG22	2:B:950:ARG:HB3	2.02	0.42
2:B:969:PHE:CE2	2:B:971:GLU:HG2	2.54	0.42
2:B:1460:GLU:OE1	2:B:1462:ARG:HG3	2.20	0.42
2:B:1589:LEU:HA	2:B:1591:MET:HE1	2.01	0.42
2:B:1865:ASP:O	2:B:1869:SER:OG	2.20	0.42
2:B:2054:ASN:OD1	2:B:2054:ASN:N	2.50	0.42
2:B:2063:ALA:O	2:B:2070:LYS:HD3	2.19	0.42
1:A:454:VAL:HG11	1:A:522:PHE:CZ	2.55	0.42
1:A:529:ILE:HG22	1:A:529:ILE:O	2.19	0.42
2:B:477:LEU:HD22	2:B:481:GLN:HG3	2.01	0.42
2:B:909:ASN:OD1	2:B:911:GLU:HG2	2.20	0.42
2:B:1560:ILE:HD12	2:B:1661:ILE:CG1	2.49	0.42
1:A:391:TRP:CD1	2:B:1808:ARG:HH22	2.38	0.42
1:A:554:LYS:NZ	1:A:555:GLY:O	2.50	0.42
2:B:1569:ARG:O	2:B:1573:LEU:HD13	2.19	0.42
1:A:485:GLN:HB3	1:A:489:ARG:HH12	1.84	0.42
2:B:479:ARG:HD2	2:B:480:ILE:N	2.35	0.42
2:B:786:MET:HE3	2:B:787:LEU:O	2.20	0.42
2:B:2095:LYS:HA	2:B:2095:LYS:HD3	1.81	0.42
2:B:677:ARG:HH11	2:B:678:PRO:HD2	1.83	0.41
2:B:737:GLU:HA	2:B:740:LYS:HE2	2.01	0.41
2:B:788:ARG:HH11	2:B:792:ASN:ND2	2.18	0.41
2:B:1420:LYS:HA	2:B:1420:LYS:HD2	1.83	0.41
2:B:1446:GLN:H	2:B:1446:GLN:HG3	1.73	0.41
2:B:1937:LEU:HB3	2:B:2127:LEU:HB3	2.02	0.41
2:B:1776:SER:O	2:B:1780:VAL:HG12	2.20	0.41
2:B:1859:PRO:HG2	2:B:1861:ARG:HH12	1.85	0.41
2:B:1898:HIS:NE2	2:B:1917:LEU:HD11	2.34	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:215:ILE:HG13	1:A:218:ARG:HH12	1.85	0.41
1:A:485:GLN:O	1:A:489:ARG:HG2	2.21	0.41
1:A:565:LYS:HB2	1:A:565:LYS:HE2	1.81	0.41
2:B:812:LEU:HB2	2:B:818:LEU:HD21	2.02	0.41
2:B:1713:TYR:O	2:B:1717:LEU:N	2.46	0.41
2:B:1927:MET:HE3	2:B:1927:MET:HB2	1.87	0.41
2:B:831:TYR:CD2	2:B:1074:SER:HB2	2.55	0.41
2:B:1984:GLY:N	2:B:1985:PRO:HD2	2.35	0.41
2:B:2120:GLY:HA2	2:B:2128:ILE:HG13	2.02	0.41
2:B:719:MET:SD	2:B:719:MET:C	3.03	0.41
2:B:1066:SER:HB3	2:B:1121:TRP:HE1	1.86	0.41
2:B:1147:THR:HG23	2:B:1150:LYS:H	1.86	0.41
2:B:1404:VAL:HG13	2:B:1423:LEU:HD22	2.03	0.41
2:B:1444:VAL:O	2:B:1447:VAL:HG12	2.21	0.41
2:B:1529:PHE:HE2	2:B:1704:LEU:HD22	1.86	0.41
2:B:1797:LEU:O	2:B:1830:LYS:NZ	2.45	0.41
2:B:1880:ASN:HD22	2:B:1883:SER:HB3	1.85	0.41
2:B:2024:LYS:HB2	2:B:2024:LYS:HE2	1.85	0.41
1:A:471:ALA:HB3	1:A:506:CYS:H	1.85	0.41
1:A:519:GLN:O	1:A:523:LYS:HG2	2.21	0.41
2:B:495:MET:HG2	2:B:496:LEU:N	2.35	0.41
2:B:1010:ASP:OD1	2:B:1010:ASP:N	2.52	0.41
2:B:1784:LEU:HD23	2:B:1784:LEU:HA	1.89	0.41
2:B:658:ALA:HB2	2:B:669:LEU:HD11	2.03	0.41
2:B:914:VAL:HG13	2:B:950:ARG:HD2	2.03	0.41
2:B:1400:LEU:HD23	2:B:1401:GLY:N	2.35	0.41
2:B:1550:ARG:HH22	2:B:1588:TRP:NE1	2.16	0.41
1:A:187:CYS:SG	1:A:202:PHE:HB3	2.61	0.41
2:B:1439:GLN:HE21	2:B:1743:THR:HG22	1.85	0.41
2:B:487:THR:O	2:B:491:THR:OG1	2.32	0.41
2:B:640:SER:OG	2:B:641:MET:N	2.54	0.41
2:B:708:VAL:O	2:B:712:VAL:HG13	2.19	0.41
2:B:812:LEU:HD12	2:B:813:ALA:N	2.35	0.41
2:B:1344:ASN:HB3	2:B:1486:ILE:H	1.85	0.41
2:B:1410:ASP:HB3	2:B:1413:PRO:HD2	2.03	0.41
2:B:1463:GLY:N	2:B:1464:PRO:HD3	2.36	0.41
1:A:485:GLN:HB3	1:A:489:ARG:NH1	2.35	0.41
1:A:485:GLN:HG2	1:A:498:PHE:CE2	2.55	0.41
2:B:532:LYS:O	2:B:605:VAL:HA	2.20	0.41
2:B:718:VAL:HG12	2:B:822:ALA:HB3	2.03	0.41
2:B:552:ARG:O	2:B:552:ARG:HG2	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:704:CYS:HB2	2:B:826:LYS:HZ3	1.86	0.40
2:B:794:VAL:HA	2:B:797:LEU:HG	2.04	0.40
2:B:845:ASP:O	2:B:849:ILE:HG12	2.21	0.40
2:B:1529:PHE:CD2	2:B:1541:MET:HG2	2.56	0.40
2:B:2006:LYS:HG3	2:B:2093:PHE:CE2	2.56	0.40
2:B:532:LYS:HE2	2:B:578:THR:O	2.22	0.40
2:B:1208:TRP:HH2	2:B:1217:GLY:HA2	1.86	0.40
2:B:486:GLU:H	2:B:486:GLU:CD	2.21	0.40
2:B:609:ILE:HD13	2:B:609:ILE:HA	1.90	0.40
2:B:994:THR:N	2:B:1019:GLU:OE2	2.54	0.40
2:B:1455:ILE:H	2:B:1490:SER:HB3	1.85	0.40
1:A:556:ASN:HB2	1:A:560:TRP:CD2	2.56	0.40
2:B:1321:LEU:HD23	2:B:1395:ARG:HB3	2.04	0.40
2:B:481:GLN:HE22	2:B:511:LEU:HD23	1.85	0.40
2:B:538:PRO:HD2	2:B:542:LEU:HD22	2.04	0.40
2:B:587:LYS:HA	2:B:590:VAL:HG22	2.04	0.40
2:B:670:PHE:HB3	2:B:672:PHE:HE1	1.86	0.40
2:B:834:LYS:O	2:B:1023:GLN:NE2	2.37	0.40
2:B:1103:PRO:HA	2:B:1106:THR:HG22	2.04	0.40
2:B:1400:LEU:HD22	2:B:1402:LYS:HG2	2.04	0.40
2:B:2067:ASP:O	2:B:2070:LYS:HG2	2.21	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	254/585 (43%)	243 (96%)	10 (4%)	1 (0%)	30	59
2	B	1781/1806 (99%)	1699 (95%)	82 (5%)	0	100	100
All	All	2035/2391 (85%)	1942 (95%)	92 (4%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	559	ILE

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	227/519 (44%)	227 (100%)	0	100	100
2	B	1579/1598 (99%)	1572 (100%)	7 (0%)	84	83
All	All	1806/2117 (85%)	1799 (100%)	7 (0%)	81	83

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	672	PHE
2	B	802	HIS
2	B	844	LEU
2	B	849	ILE
2	B	886	ILE
2	B	1254	VAL
2	B	1996	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	381	ASN
1	A	417	GLN
1	A	423	GLN
1	A	577	GLN
2	B	435	ASN
2	B	490	ASN
2	B	492	ASN
2	B	717	GLN
2	B	829	GLN

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Mol	Chain	Res	Type
2	B	941	GLN
2	B	993	ASN
2	B	1085	ASN
2	B	1136	HIS
2	B	1231	HIS
2	B	1306	GLN
2	B	1598	ASN
2	B	1607	ASN
2	B	1620	HIS
2	B	1948	GLN
2	B	1971	HIS
2	B	2028	ASN
2	B	2078	GLN

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](#)

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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.

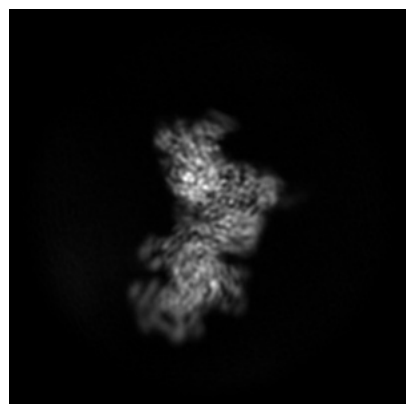
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-15521. These allow visual inspection of the internal detail of the map and identification of artifacts.

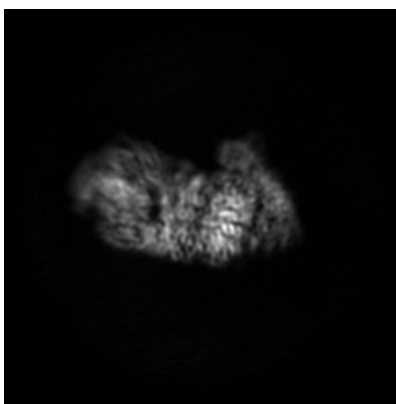
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

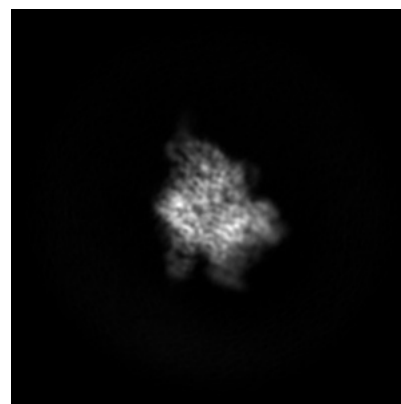
6.1.1 Primary map



X

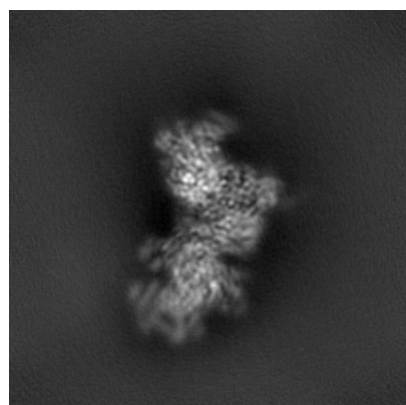


Y

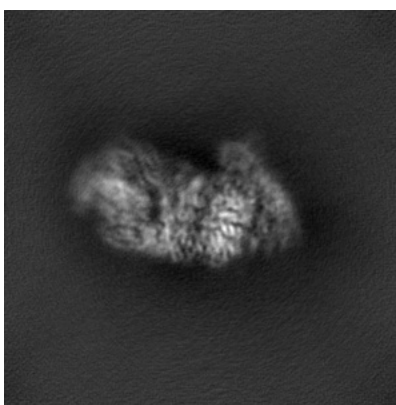


Z

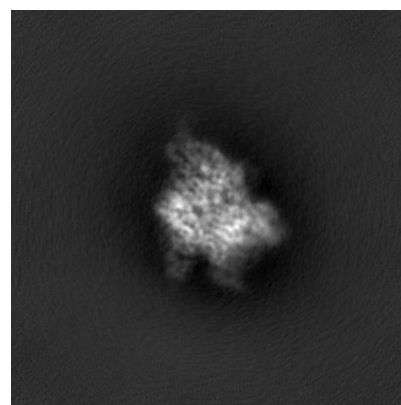
6.1.2 Raw map



X



Y

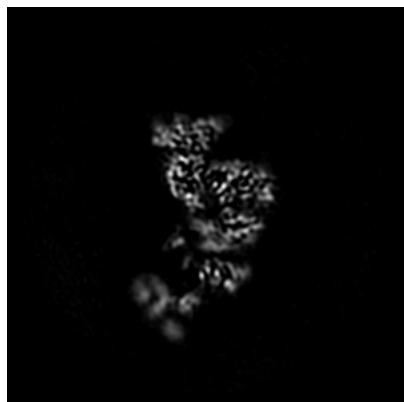


Z

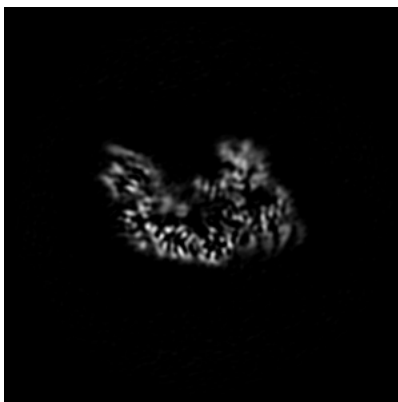
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

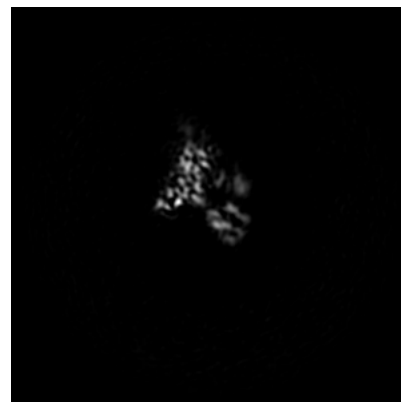
6.2.1 Primary map



X Index: 160

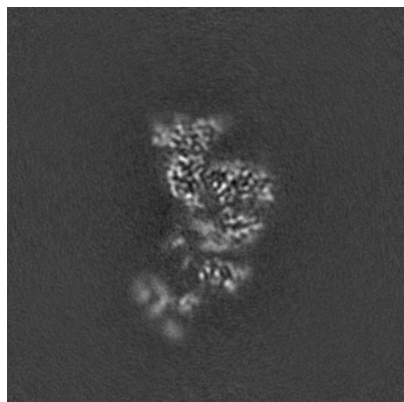


Y Index: 160

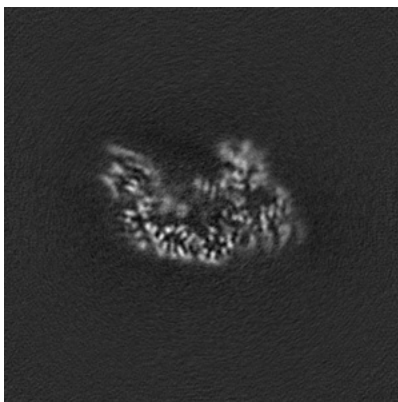


Z Index: 160

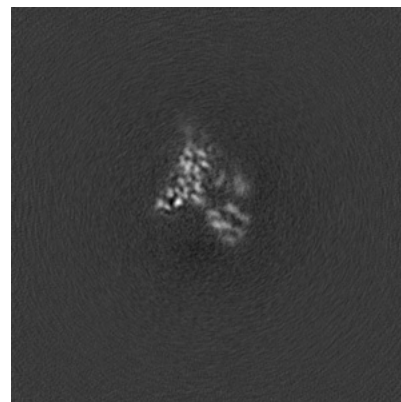
6.2.2 Raw map



X Index: 160



Y Index: 160

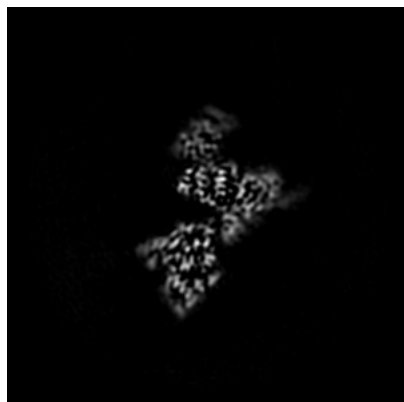


Z Index: 160

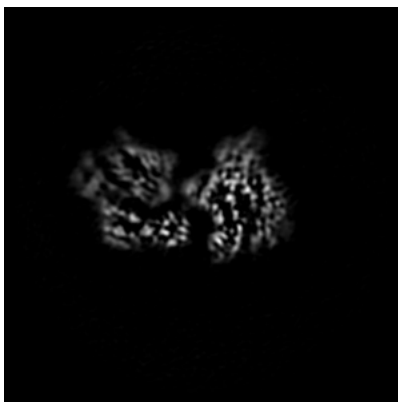
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

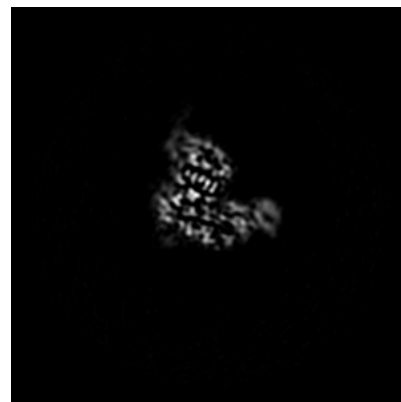
6.3.1 Primary map



X Index: 142

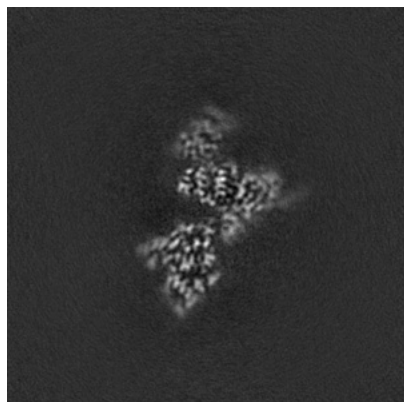


Y Index: 146

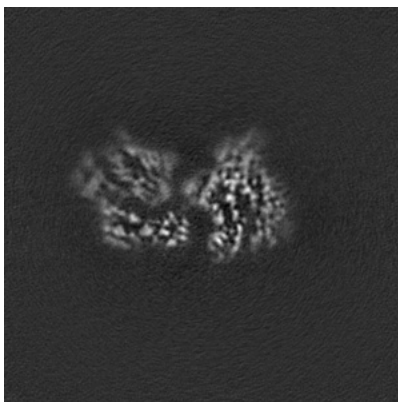


Z Index: 176

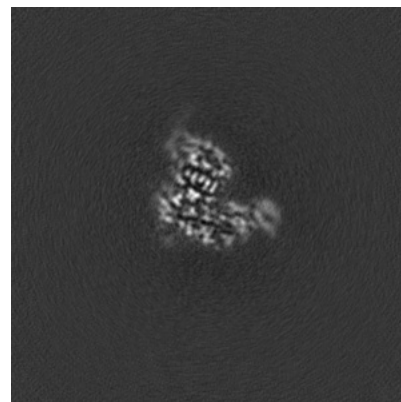
6.3.2 Raw map



X Index: 142



Y Index: 146

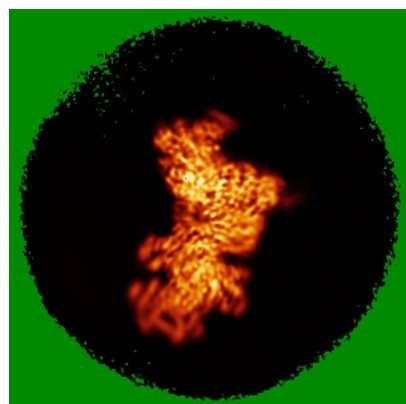


Z Index: 176

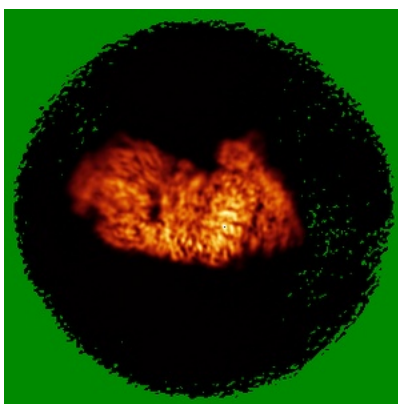
The images above show the largest variance slices of the map in three orthogonal directions.

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

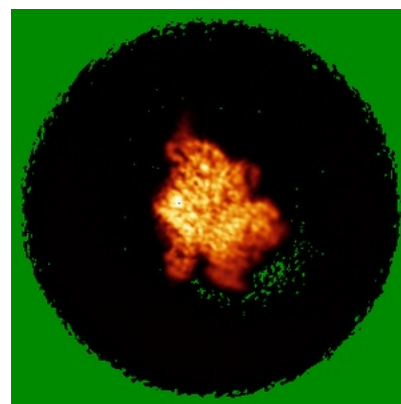
6.4.1 Primary map



X

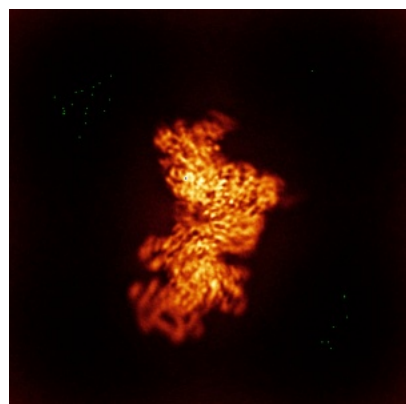


Y

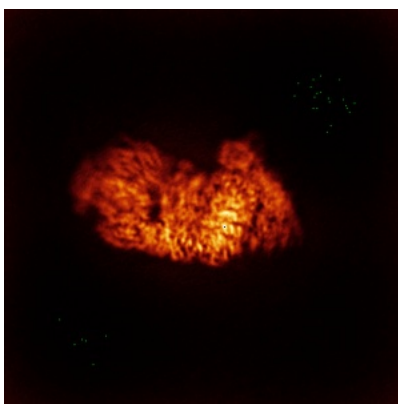


Z

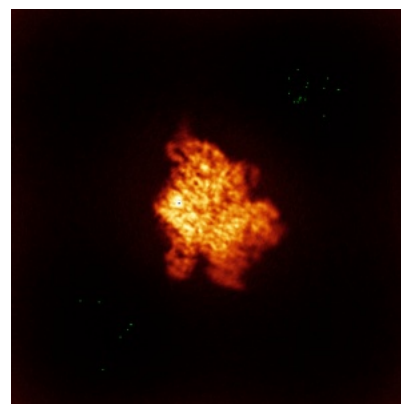
6.4.2 Raw map



X



Y

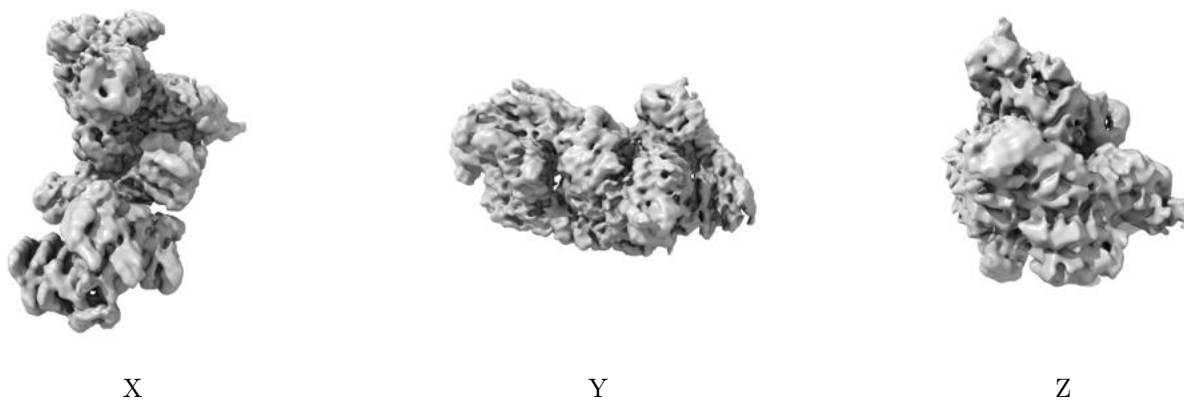


Z

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.

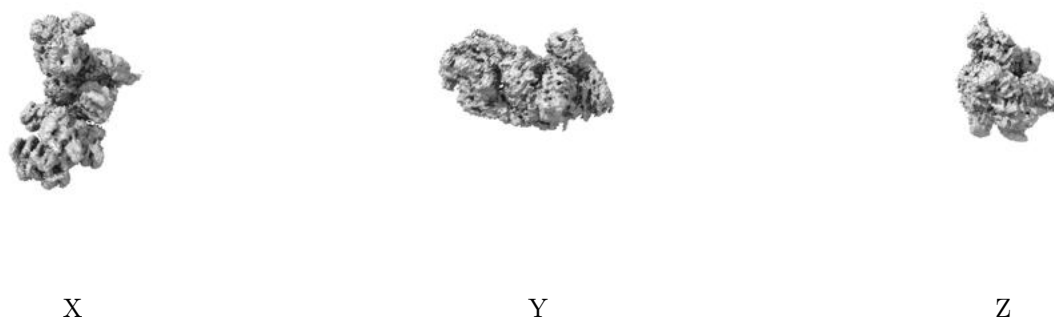
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.157. 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.

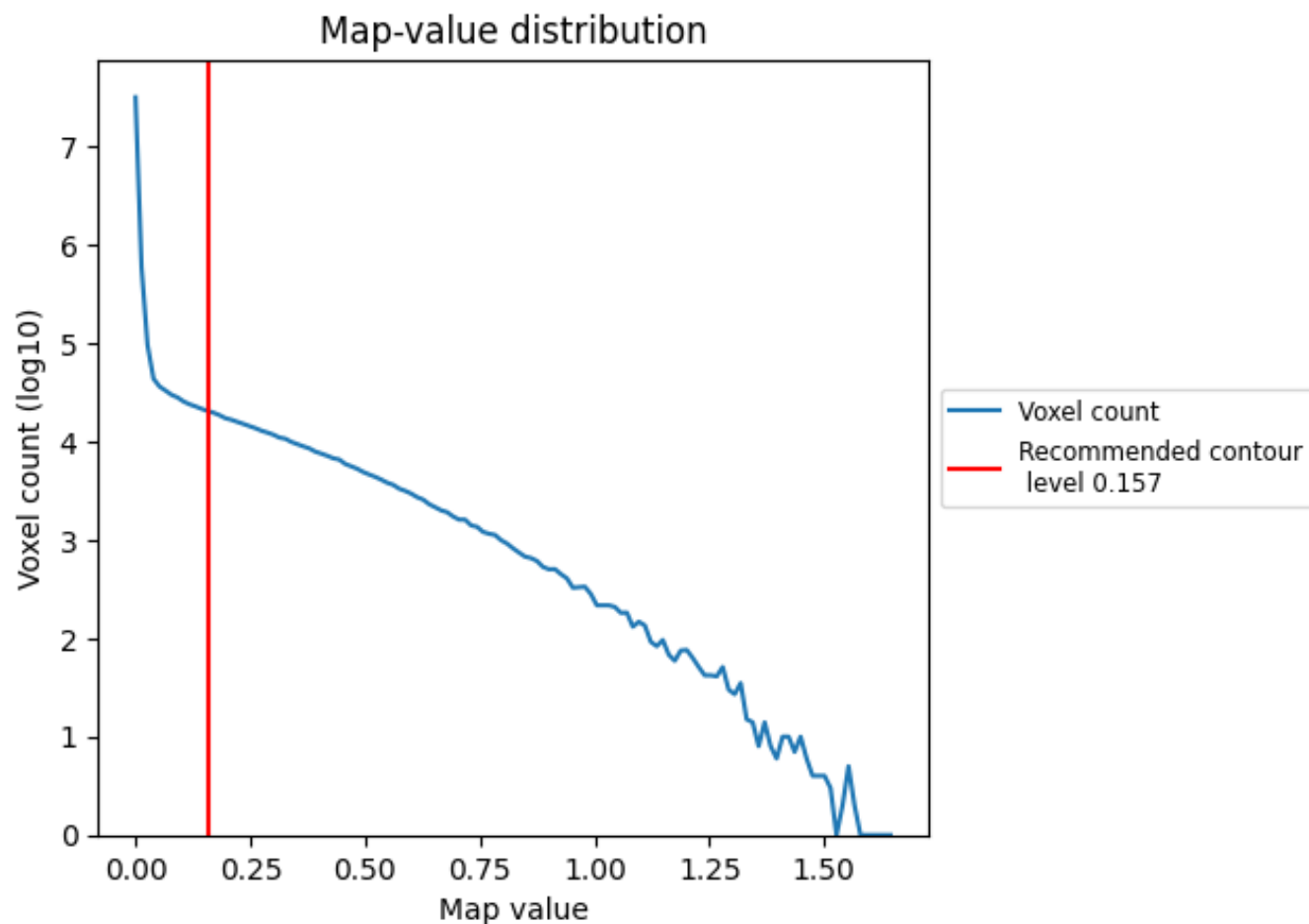
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

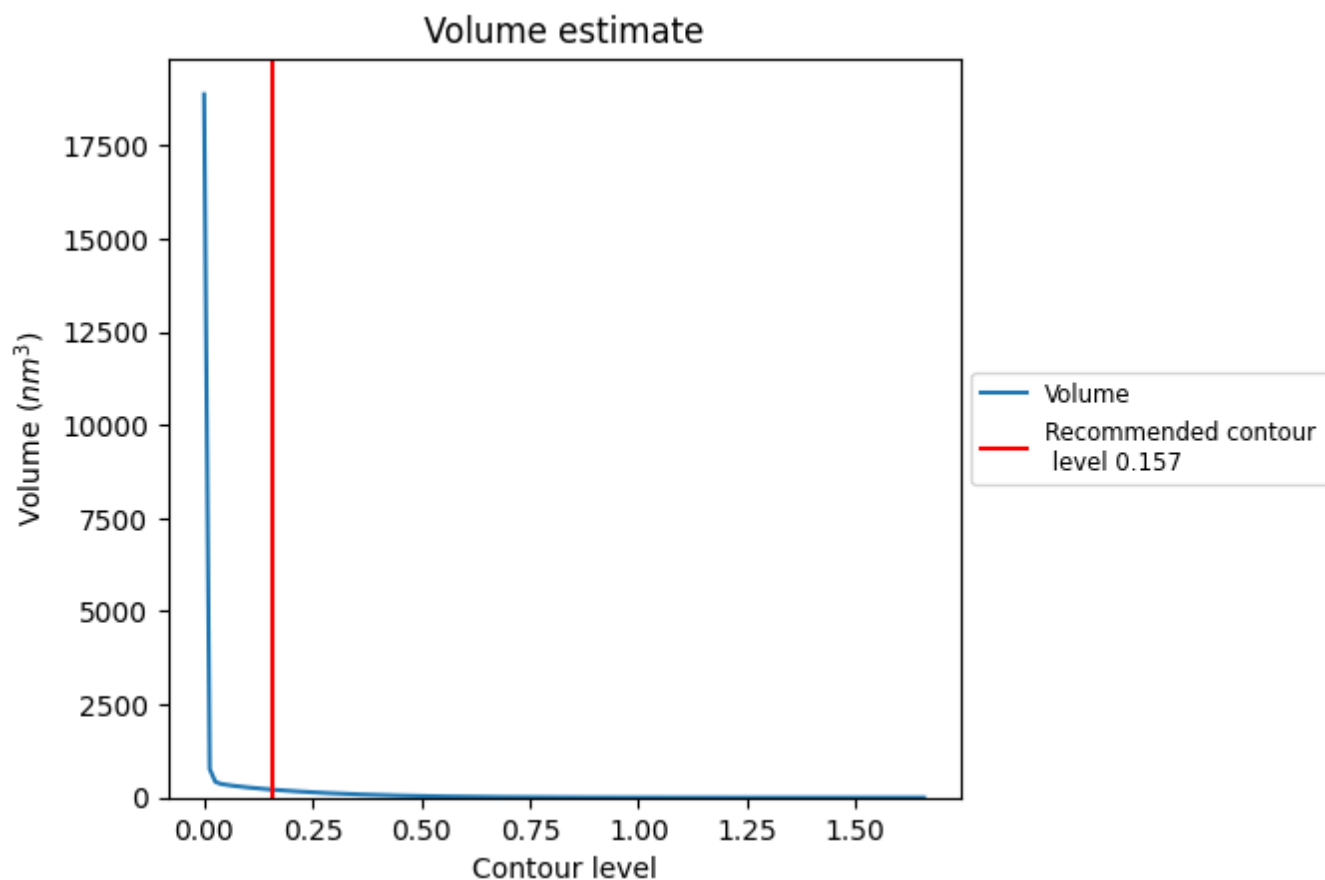
This section contains the results of statistical analysis of the map.

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.

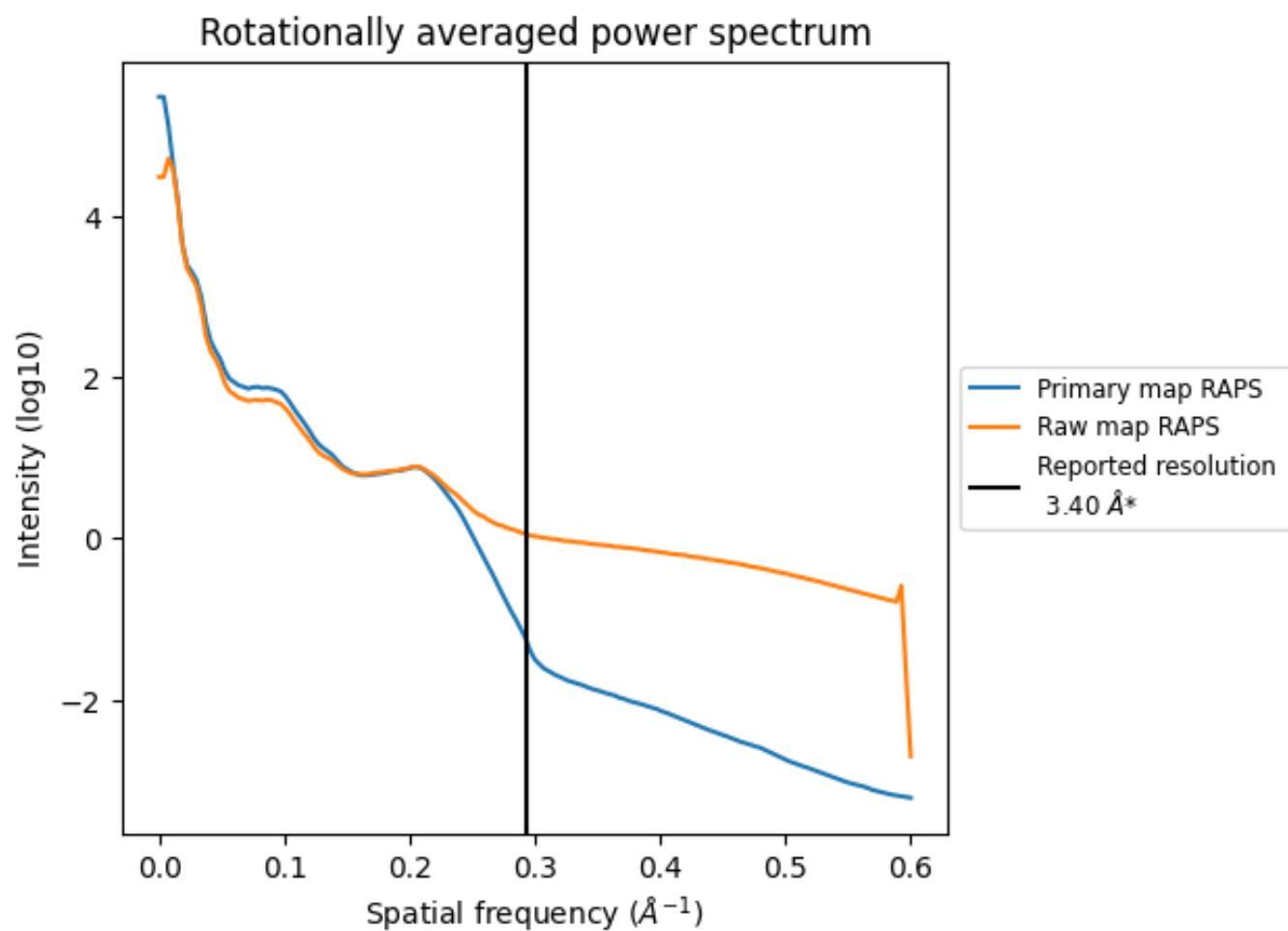
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 213 nm^3 ; this corresponds to an approximate mass of 192 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 ⓘ

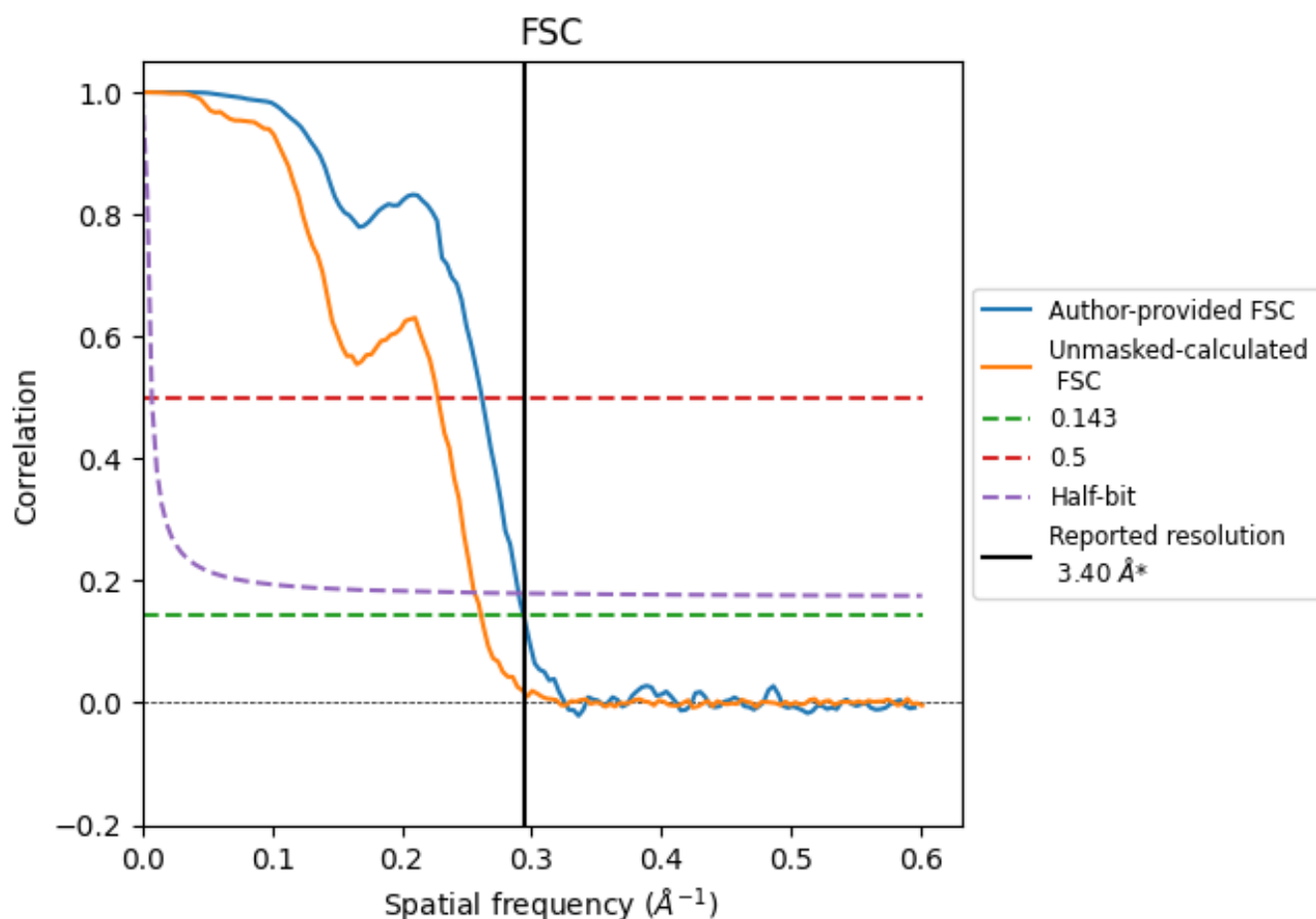


*Reported resolution corresponds to spatial frequency of 0.294 $\text{\AA}^{-1}$

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 $0.294 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

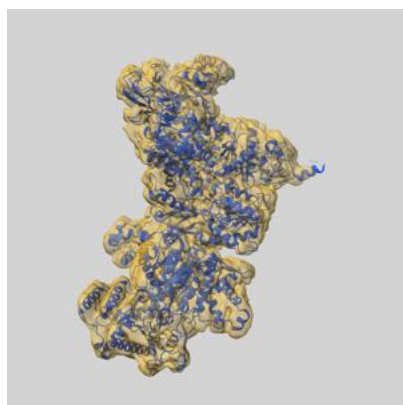
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.40	-	-
Author-provided FSC curve	3.40	3.82	3.45
Unmasked-calculated*	3.83	4.39	3.90

*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 3.83 differs from the reported value 3.4 by more than 10 %

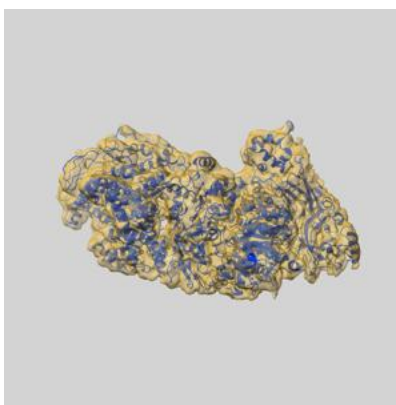
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-15521 and PDB model 8ALZ. Per-residue inclusion information can be found in [section 3](#) on [page 4](#).

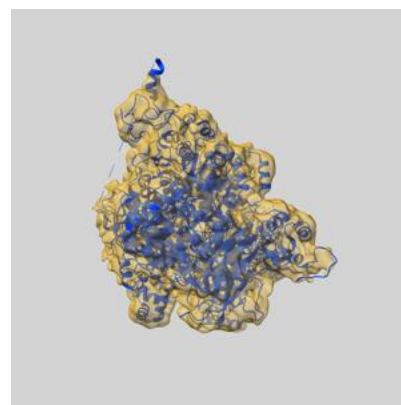
9.1 Map-model overlay [i](#)



X



Y



Z

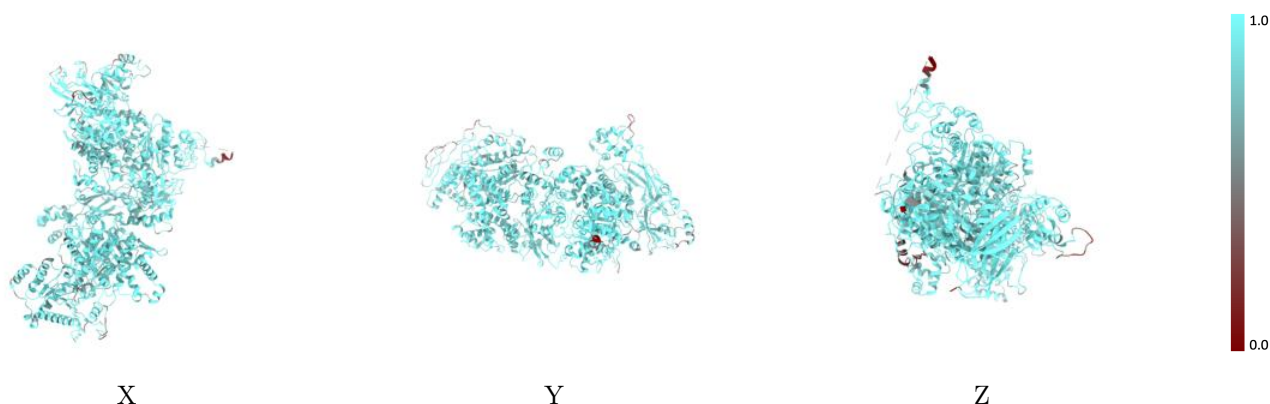
The images above show the 3D surface view of the map at the recommended contour level 0.157 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



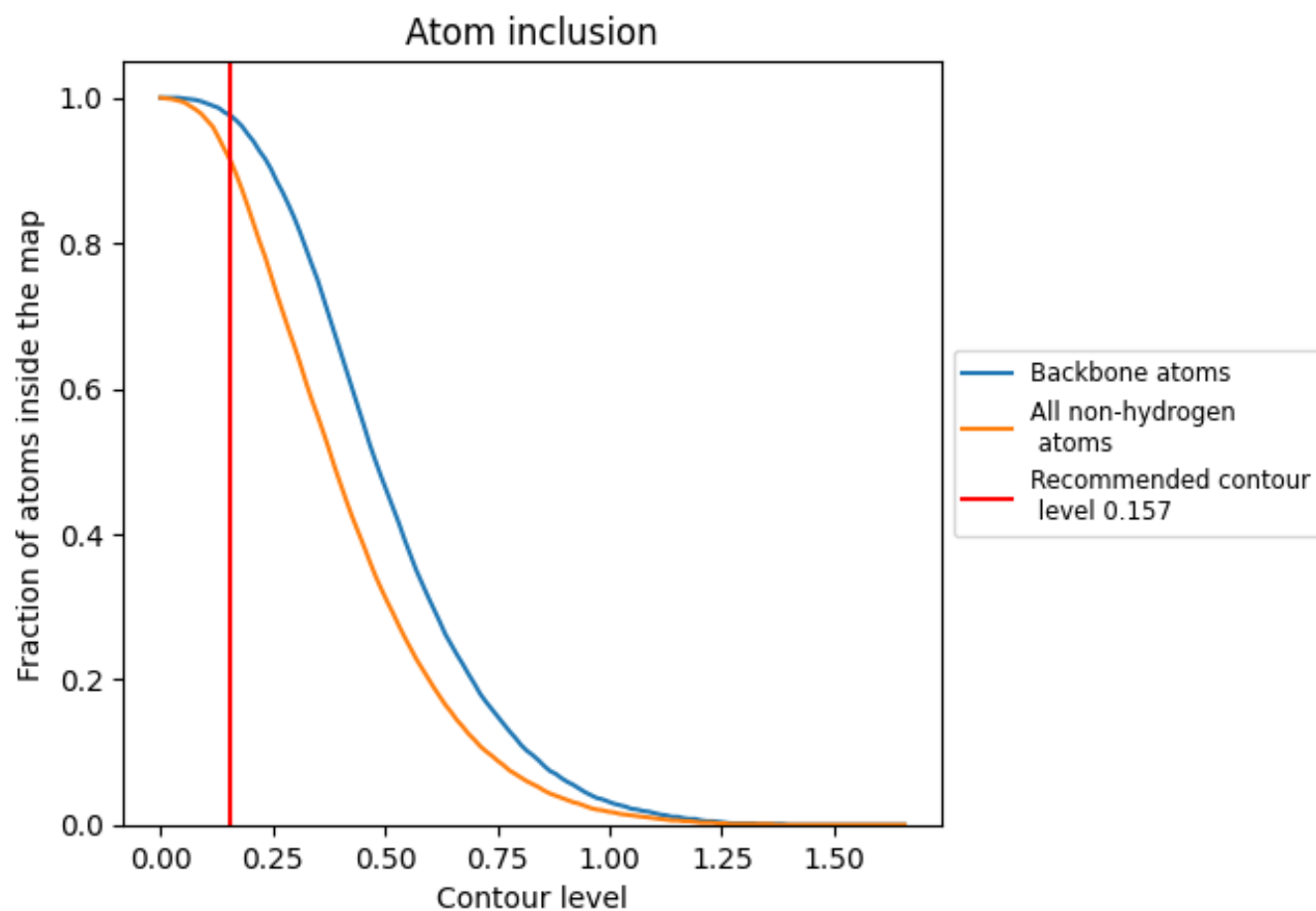
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.157).

9.4 Atom inclusion [i](#)



At the recommended contour level, 98% of all backbone atoms, 91% 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 (0.157) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9120	0.3430
A	0.8290	0.3300
B	0.9240	0.3450

