



Full wwPDB EM Validation Report ⓘ

Nov 14, 2022 – 12:22 PM EST

PDB ID : 7UVK
EMDB ID : EMD-26812
Title : G. haemolysans IgA1 protease
Authors : Eisenmesser, E.Z.; Zheng, H.
Deposited on : 2022-05-02
Resolution : 3.28 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.dev43
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.2

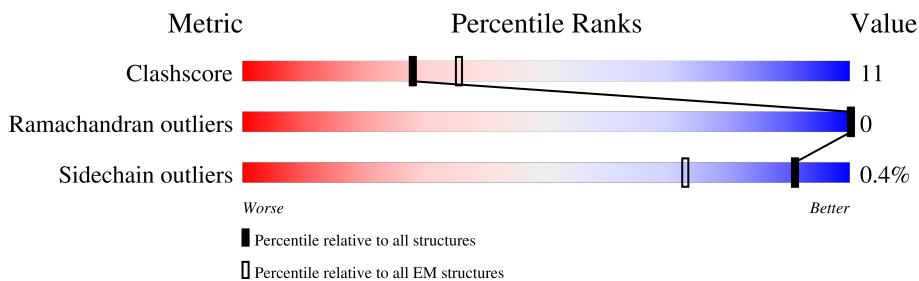
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.28 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	2201	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 10350 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.

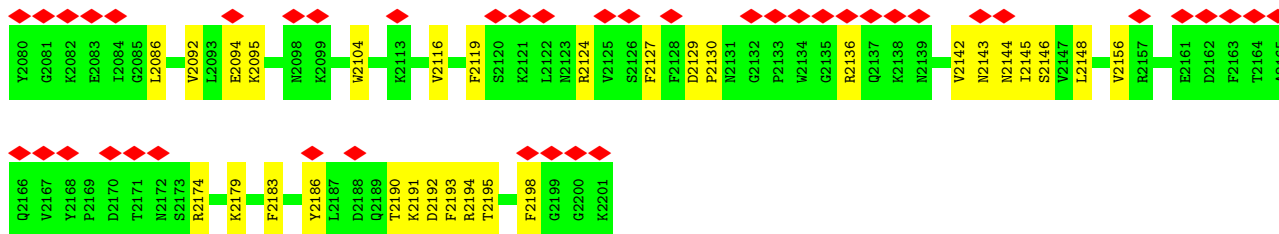
- Molecule 1 is a protein called IgA1 Protease.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	1295	10350	6536	1750	2045	19	0	0

There are 23 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	initiating methionine	UNP C5NYF3
A	2	ARG	-	expression tag	UNP C5NYF3
A	3	LYS	-	expression tag	UNP C5NYF3
A	4	TYR	-	expression tag	UNP C5NYF3
A	5	LEU	-	expression tag	UNP C5NYF3
A	6	GLU	-	expression tag	UNP C5NYF3
A	7	GLU	-	expression tag	UNP C5NYF3
A	8	LYS	-	expression tag	UNP C5NYF3
A	9	TYR	-	expression tag	UNP C5NYF3
A	10	ASN	-	expression tag	UNP C5NYF3
A	11	LYS	-	expression tag	UNP C5NYF3
A	12	PHE	-	expression tag	UNP C5NYF3
A	13	SER	-	expression tag	UNP C5NYF3
A	14	LEU	-	expression tag	UNP C5NYF3
A	15	ARG	-	expression tag	UNP C5NYF3
A	16	LYS	-	expression tag	UNP C5NYF3
A	17	LEU	-	expression tag	UNP C5NYF3
A	18	THR	-	expression tag	UNP C5NYF3
A	19	VAL	-	expression tag	UNP C5NYF3
A	20	GLY	-	expression tag	UNP C5NYF3
A	21	VAL	-	expression tag	UNP C5NYF3
A	22	CYS	-	expression tag	UNP C5NYF3
A	23	SER	-	expression tag	UNP C5NYF3

ALA	ARG	ASN	ASP	GLN	GLY	ILE	LEU	LYS	PRO	THR	TRP	TYR	ASP
S978	S982	S983	S984	S985	S986	S987	S988	S989	S990	S991	S992	S993	S994
Q1057	Q1058	Q1059	Q1060	K1063	K1064	E1065	F1066	S1067	K1068	K1069	L1070	L1071	L1072
T1169	I1162	D1167	T1168	T1169	A1170	T1171	Q1172	Q1173	K1174	L1175	L1176	L1177	L1181
V1239	V1242	V1243	D1248	R1249	E1250	L1251	S1252	E1253	L1260	M1261	M1262	L1264	S1265
N1321	N1322	V1323	V1324	L1325	K1326	K1327	K1328	L1329	L1330	L1331	V1332	P1333	K1334
S1401	V1402	V1403	K1406	D1407	I1411	N1417	K1418	T1419	S1420	I1421	N1422	L1426	D1430
D1487	R1490	K1491	D1494	N1498	I1499	D1507	E1508	Q1509	T1513	L1525	D1528	M1534	S1535
N1646	K1655	S1663	T1664	I1665	P1666	E1667	S1668	Q1672	G1676	T1677	E1678	S1691	W1692
V1778	Y1779	D1780	A1781	R1782	R1783	T1788	N1789	T1792	Q1793	E1794	A1795	T1799	N1800
N1646	K1655	S1663	T1664	I1665	P1666	E1667	S1668	Q1672	G1676	T1677	E1678	S1691	W1692
V1778	Y1779	D1780	A1781	R1782	R1783	T1788	N1789	T1792	Q1793	E1794	A1795	T1799	N1800
V1894	L1895	D1898	D1899	S1900	E1901	R1905	L1906	Q1907	I1908	A1909	D1910	T1916	E1919
K1993	L1994	I1995	E1996	N1997	D1998	V1999	T2000	R2002	R2003	L2006	D2007	Q2008	G2009
S2023	P2024	I2025	L2029	S2030	S2031	K2032	I2033	G2034	M2040	R2042	R2043	E2047	L2048
G2041	K1984	L1985	P1966	D1967	G1968	M1969	S1970	V1971	R1978	E1979	L1980	T1981	S1982
R2073	I2077	R2078	S2079	L1988	F1991	D1992	K1986	L1988	F1991	D1992	K1986	L1988	F1991
L1056	L1054	E1053	E1051	R1050	N965	N966	N965	N966	N965	N966	N965	N966	N965
L1048	A1049	R1050	E1051	V1052	E1053	L1054	L1056	D1056	L1056	D1056	L1056	L1056	D1056
V1023	Y1023	T1024	L1029	V1030	D1031	V1035	Y1038	L1043	C1044	D1048	A1049	R1050	E1051
I1108	E1111	A1114	A1117	K1118	I1135	A1136	R1139	S1140	I1141	I1145	V1148	I1153	I1153
V1211	V1214	V1215	D1216	A1219	E1205	V1207	V1208	V1211	V1214	V1215	D1216	A1219	E1205
V1300	Q1301	V1302	V1302	E1305	V1306	L1307	S1308	K1309	D1310	S1311	N1312	V1313	Q1314
N1351	N1352	N1353	N1354	L1355	K1356	D1357	A1358	D1359	V1360	R1364	N1368	I1369	E1370
K1396	K1397	N1391	N1392	N1391	N1392	S1486	D1486	S1486	S1486	S1486	S1486	S1486	S1486



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	443908	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	30	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	5000	Depositor
Magnification	Not provided	
Image detector	GATAN K2 BASE (4k x 4k)	Depositor
Maximum map value	1.738	Depositor
Minimum map value	-1.169	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.045	Depositor
Recommended contour level	0.43	Depositor
Map size (\AA)	298.8, 298.8, 298.8	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	0.83, 0.83, 0.83	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.29	2/10533 (0.0%)	0.50	4/14226 (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
1	A	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	954	PRO	CG-CD	-8.92	1.21	1.50
1	A	954	PRO	N-CD	5.05	1.54	1.47

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	954	PRO	CA-N-CD	-11.03	96.05	111.50
1	A	954	PRO	N-CD-CG	-10.91	86.83	103.20
1	A	954	PRO	CA-CB-CG	-6.55	91.55	104.00
1	A	953	ASN	C-N-CD	6.05	141.11	128.40

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1055	SER	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	10350	0	10260	218	0
All	All	10350	0	10260	218	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 11.

All (218) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1969:ASN:HD21	1:A:2077:ILE:HB	1.48	0.78
1:A:1204:GLY:O	1:A:1238:LYS:NZ	2.17	0.76
1:A:1655:LYS:HB3	1:A:1707:GLU:HA	1.68	0.75
1:A:1370:GLU:OE1	1:A:1378:ARG:NH1	2.20	0.74
1:A:2191:LYS:HG3	1:A:2192:ASP:H	1.54	0.72
1:A:1159:THR:HG22	1:A:1194:SER:HB3	1.70	0.72
1:A:1162:ILE:HB	1:A:1197:MET:HG2	1.72	0.71
1:A:993:ALA:HB3	1:A:996:LEU:HB2	1.73	0.70
1:A:1756:HIS:HB2	1:A:1894:VAL:HG12	1.74	0.69
1:A:2073:ARG:NH2	1:A:2094:GLU:OE2	2.24	0.69
1:A:1616:TYR:HA	1:A:1620:LEU:HB2	1.74	0.68
1:A:1242:VAL:HG12	1:A:1243:VAL:HG23	1.76	0.68
1:A:2124:ARG:HD2	1:A:2198:PHE:HD2	1.59	0.67
1:A:1170:ALA:O	1:A:1206:GLN:NE2	2.27	0.67
1:A:1745:ASN:HB3	1:A:1837:LEU:HB3	1.76	0.66
1:A:1490:ARG:NH2	1:A:1499:ILE:O	2.28	0.66
1:A:1264:LEU:HD11	1:A:1319:LEU:HD22	1.78	0.65
1:A:1148:VAL:HG11	1:A:1153:ILE:HD11	1.77	0.65
1:A:1971:VAL:HG23	1:A:2033:ILE:HG22	1.79	0.65
1:A:1509:GLN:HG2	1:A:1563:ARG:HB2	1.79	0.65
1:A:1242:VAL:HG11	1:A:1263:VAL:HG11	1.77	0.65
1:A:2029:LEU:HB3	1:A:2040:MET:HG2	1.79	0.64
1:A:1570:ASP:HB2	1:A:1641:LEU:HD12	1.78	0.64
1:A:1208:VAL:HB	1:A:1239:VAL:HG22	1.77	0.64
1:A:1665:ILE:HB	1:A:1668:VAL:HG12	1.80	0.64
1:A:944:VAL:HG23	1:A:947:LEU:HB3	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1905:ARG:NH2	1:A:2192:ASP:OD1	2.32	0.63
1:A:1905:ARG:HH21	1:A:1909:ALA:H	1.47	0.62
1:A:1471:ILE:HG23	1:A:1544:ILE:HG22	1.82	0.62
1:A:1618:VAL:HG23	1:A:1619:LEU:HD13	1.81	0.62
1:A:1368:ASN:ND2	1:A:1396:THR:O	2.33	0.61
1:A:1207:VAL:HG21	1:A:1214:VAL:HG23	1.82	0.61
1:A:1077:LYS:HE3	1:A:1334:LYS:HD2	1.83	0.61
1:A:2031:SER:OG	1:A:2034:GLY:O	2.19	0.60
1:A:1019:GLU:HG3	1:A:1020:ASN:H	1.66	0.60
1:A:2116:VAL:HA	1:A:2119:PHE:CE1	2.37	0.59
1:A:997:ILE:HD11	1:A:1004:THR:HB	1.85	0.59
1:A:1757:TYR:HE2	1:A:1845:TYR:HH	1.51	0.59
1:A:1931:LEU:HD22	1:A:2186:TYR:CD2	2.37	0.58
1:A:1417:ASN:OD1	1:A:1418:LYS:N	2.37	0.58
1:A:2191:LYS:HG3	1:A:2192:ASP:N	2.18	0.58
1:A:1048:ASP:OD2	1:A:1049:ALA:N	2.37	0.57
1:A:1663:SER:O	1:A:1669:SER:OG	2.22	0.57
1:A:1139:ARG:HG3	1:A:1139:ARG:HH11	1.70	0.57
1:A:1291:ASN:HB2	1:A:1319:LEU:HD11	1.87	0.57
1:A:1312:GLU:OE2	1:A:1313:GLU:N	2.38	0.57
1:A:1070:LEU:HD13	1:A:1096:THR:HB	1.87	0.56
1:A:990:VAL:HG23	1:A:1009:THR:HG22	1.86	0.56
1:A:927:ASN:HD22	1:A:965:ASN:HB2	1.71	0.55
1:A:1067:SER:HB3	1:A:1089:PHE:CD1	2.41	0.55
1:A:1831:TYR:OH	1:A:1845:TYR:HB2	2.06	0.55
1:A:1230:LEU:HD22	1:A:1269:VAL:HG23	1.88	0.55
1:A:1297:VAL:HG21	1:A:1309:LYS:HD3	1.88	0.55
1:A:1273:ASN:HA	1:A:1309:LYS:HG2	1.88	0.55
1:A:1875:LYS:HG2	1:A:2016:TYR:HB3	1.88	0.55
1:A:1988:LEU:HD21	1:A:1999:VAL:HG21	1.88	0.54
1:A:1043:LEU:HG	1:A:1073:GLU:HG3	1.90	0.54
1:A:1248:ASP:HB2	1:A:1252:SER:HB2	1.88	0.54
1:A:2022:PHE:HB3	1:A:2179:LYS:HD2	1.90	0.54
1:A:1344:PHE:HB3	1:A:1378:ARG:HG2	1.90	0.53
1:A:1022:VAL:HG23	1:A:1029:LEU:HD12	1.91	0.53
1:A:1181:LEU:HD21	1:A:1188:ILE:HG13	1.89	0.53
1:A:1621:SER:O	1:A:1622:LYS:HG3	2.09	0.53
1:A:1714:ALA:O	1:A:1715:ASN:ND2	2.41	0.53
1:A:1634:GLU:OE1	1:A:1646:ASN:ND2	2.38	0.53
1:A:1876:GLY:HA3	1:A:2042:ARG:HE	1.73	0.53
1:A:1441:LEU:HG	1:A:1442:GLN:HB2	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1174:ILE:HD11	1:A:1208:VAL:HG22	1.91	0.52
1:A:1892:ASN:ND2	1:A:1908:ILE:O	2.39	0.52
1:A:1339:ILE:HG13	1:A:1340:GLU:N	2.24	0.52
1:A:1971:VAL:HG21	1:A:2086:LEU:HD21	1.91	0.52
1:A:1980:LEU:HD21	1:A:1985:ILE:HD11	1.92	0.51
1:A:1232:ASN:OD1	1:A:1233:VAL:N	2.41	0.51
1:A:2048:LEU:HD11	1:A:2104:TRP:HH2	1.75	0.51
1:A:2129:ASP:OD1	1:A:2129:ASP:N	2.43	0.51
1:A:1189:GLU:OE2	1:A:1190:LYS:NZ	2.37	0.51
1:A:1243:VAL:HG21	1:A:1260:LEU:HD11	1.92	0.50
1:A:1779:TYR:HB2	1:A:1830:TYR:HD1	1.77	0.50
1:A:919:VAL:HG21	1:A:1379:GLU:HB3	1.94	0.50
1:A:1946:LEU:HB3	1:A:1951:LYS:HG3	1.94	0.50
1:A:2000:ILE:HG13	1:A:2025:ILE:HG23	1.94	0.50
1:A:1285:ALA:O	1:A:1286:THR:HG22	2.11	0.50
1:A:1859:LEU:HD13	1:A:2063:SER:HB2	1.94	0.50
1:A:1936:GLU:HG2	1:A:2024:PRO:HB3	1.92	0.50
1:A:1079:TYR:HE1	1:A:1334:LYS:HD3	1.76	0.50
1:A:1471:ILE:O	1:A:1475:VAL:HG12	2.12	0.50
1:A:1403:VAL:HB	1:A:1421:ILE:HG21	1.93	0.50
1:A:1525:LEU:HD21	1:A:1547:ILE:HD11	1.94	0.50
1:A:1023:TYR:HB3	1:A:1044:GLY:HA3	1.94	0.49
1:A:2127:PHE:HB2	1:A:2142:VAL:HB	1.94	0.49
1:A:1417:ASN:OD1	1:A:1418:LYS:HG2	2.12	0.49
1:A:1692:TRP:NE1	1:A:1694:TYR:O	2.44	0.49
1:A:1406:LYS:HE3	1:A:1422:ASN:ND2	2.28	0.48
1:A:2060:PRO:HB3	1:A:2066:TYR:CE2	2.48	0.48
1:A:1195:ILE:O	1:A:1228:GLY:HA3	2.12	0.48
1:A:1729:SER:OG	1:A:1730:SER:N	2.47	0.48
1:A:1850:THR:HG22	1:A:1858:TYR:HE2	1.78	0.48
1:A:936:LEU:HD23	1:A:936:LEU:O	2.13	0.48
1:A:1442:GLN:OE1	1:A:1444:PHE:HB2	2.14	0.48
1:A:1203:THR:HB	1:A:1206:GLN:OE1	2.13	0.48
1:A:1715:ASN:HB2	1:A:1718:THR:HG22	1.96	0.48
1:A:954:PRO:HD2	1:A:954:PRO:O	2.13	0.48
1:A:1264:LEU:HD23	1:A:1265:SER:N	2.29	0.48
1:A:2077:ILE:HD13	1:A:2086:LEU:HD13	1.95	0.47
1:A:1668:VAL:O	1:A:1672:GLN:HG3	2.14	0.47
1:A:1048:ASP:OD2	1:A:1050:ARG:HG2	2.14	0.47
1:A:1655:LYS:HD3	1:A:1707:GLU:HB2	1.96	0.47
1:A:1048:ASP:OD1	1:A:1083:ASN:ND2	2.40	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1215:VAL:HG13	1:A:1219:ALA:HB3	1.96	0.47
1:A:1795:ALA:HB1	1:A:1799:THR:HG21	1.95	0.47
1:A:1965:ASP:OD2	1:A:1966:PRO:HD2	2.15	0.47
1:A:1326:GLU:O	1:A:1326:GLU:HG2	2.14	0.47
1:A:1655:LYS:HD2	1:A:1704:LEU:O	2.15	0.47
1:A:1355:LEU:HD22	1:A:1382:VAL:HG11	1.95	0.46
1:A:1621:SER:C	1:A:1623:ASN:H	2.19	0.46
1:A:1783:ARG:HB3	1:A:1792:THR:HB	1.98	0.46
1:A:1172:TYR:CE2	1:A:1206:GLN:HG2	2.50	0.46
1:A:1566:ASN:HB2	1:A:1703:THR:HG23	1.97	0.46
1:A:1211:VAL:HG23	1:A:1226:VAL:HB	1.96	0.46
1:A:1100:LEU:HD12	1:A:1101:SER:H	1.81	0.46
1:A:1991:PHE:HA	1:A:1994:LEU:HD12	1.98	0.46
1:A:1019:GLU:HG3	1:A:1020:ASN:N	2.31	0.46
1:A:1069:LYS:HE3	1:A:1093:SER:O	2.15	0.46
1:A:1238:LYS:HD2	1:A:1278:TYR:HB2	1.98	0.46
1:A:1905:ARG:NH2	1:A:1909:ALA:H	2.12	0.46
1:A:1181:LEU:HD11	1:A:1188:ILE:HD11	1.98	0.45
1:A:1355:LEU:HB2	1:A:1358:ALA:HB2	1.98	0.45
1:A:2144:ASN:OD1	1:A:2146:SER:HB3	2.17	0.45
1:A:1139:ARG:HG3	1:A:1139:ARG:NH1	2.31	0.45
1:A:936:LEU:HD12	1:A:941:TYR:CZ	2.51	0.45
1:A:1757:TYR:HE2	1:A:1845:TYR:OH	1.98	0.45
1:A:1931:LEU:HD22	1:A:2186:TYR:HD2	1.82	0.45
1:A:1940:GLY:HA2	1:A:1943:VAL:HG22	1.98	0.45
1:A:2001:THR:HG22	1:A:2003:ARG:H	1.81	0.45
1:A:1444:PHE:CZ	1:A:1446:LYS:HD2	2.51	0.45
1:A:1756:HIS:CE1	1:A:1846:THR:HG23	2.52	0.45
1:A:1052:VAL:HG12	1:A:1054:LEU:H	1.81	0.45
1:A:1441:LEU:HB2	1:A:1451:GLU:HG2	1.98	0.45
1:A:2119:PHE:CD2	1:A:2145:ILE:HG12	2.51	0.45
1:A:1087:PRO:HG2	1:A:1118:LYS:NZ	2.32	0.45
1:A:1117:ALA:HB3	1:A:1145:ILE:HG12	1.97	0.45
1:A:1176:GLY:HA3	1:A:1195:ILE:HG21	1.98	0.45
1:A:1447:VAL:HG12	1:A:1460:THR:HB	1.99	0.45
1:A:1957:LYS:NZ	1:A:1978:ARG:HH21	2.14	0.45
1:A:1536:ASN:OD1	1:A:1537:SER:N	2.48	0.44
1:A:1141:ILE:HG21	1:A:1162:ILE:HG23	1.99	0.44
1:A:1969:ASN:HD22	1:A:2077:ILE:HD12	1.81	0.44
1:A:1509:GLN:O	1:A:1513:THR:HG23	2.18	0.44
1:A:1980:LEU:HD23	1:A:1980:LEU:H	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1401:SER:HB3	1:A:1426:LEU:HD23	2.00	0.43
1:A:2191:LYS:HG2	1:A:2194:ARG:HG2	2.00	0.43
1:A:1054:LEU:HD21	1:A:1085:LYS:HG2	2.00	0.43
1:A:2010:GLU:HG2	1:A:2011:TYR:O	2.19	0.43
1:A:1829:PHE:HE1	1:A:1848:GLU:HG3	1.83	0.43
1:A:1177:LEU:HD21	1:A:1191:SER:HB3	2.00	0.43
1:A:1071:ILE:HG12	1:A:1073:GLU:OE2	2.18	0.43
1:A:1114:ALA:HB3	1:A:1117:ALA:O	2.19	0.43
1:A:1324:VAL:HG12	1:A:1324:VAL:O	2.19	0.43
1:A:1873:TYR:O	1:A:1877:LEU:HB2	2.19	0.43
1:A:2142:VAL:HG21	1:A:2148:LEU:HD13	2.01	0.43
1:A:1906:LEU:O	1:A:1907:GLN:NE2	2.52	0.43
1:A:923:LEU:O	1:A:997:ILE:HG22	2.18	0.43
1:A:1296:VAL:HA	1:A:1307:LEU:O	2.19	0.43
1:A:1339:ILE:HG13	1:A:1340:GLU:HG2	2.01	0.43
1:A:1448:ALA:HB2	1:A:1465:LEU:HD11	2.01	0.43
1:A:1762:LYS:HD3	1:A:1916:THR:HA	2.00	0.43
1:A:1894:VAL:HG23	1:A:1895:LEU:HG	2.00	0.43
1:A:1846:THR:O	1:A:1850:THR:HG23	2.19	0.42
1:A:965:ASN:O	1:A:1588:SER:HB3	2.19	0.42
1:A:1547:ILE:HG23	1:A:1554:LEU:HD22	2.00	0.42
1:A:1290:SER:HB2	1:A:1312:GLU:CD	2.39	0.42
1:A:1389:ASP:HB3	1:A:1392:ASN:HB2	2.00	0.42
1:A:1761:TYR:CE1	1:A:1769:LYS:HB2	2.55	0.42
1:A:1894:VAL:HG23	1:A:1895:LEU:N	2.33	0.42
1:A:2055:LYS:HA	1:A:2055:LYS:HD3	1.67	0.42
1:A:2061:TYR:HD1	1:A:2092:VAL:HG11	1.83	0.42
1:A:1859:LEU:HD22	1:A:2063:SER:HB3	2.01	0.42
1:A:2143:ASN:OD1	1:A:2144:ASN:ND2	2.53	0.42
1:A:1291:ASN:OD1	1:A:1292:LYS:N	2.48	0.42
1:A:1107:VAL:HG23	1:A:1135:ILE:HG23	2.01	0.42
1:A:1487:ASP:O	1:A:1491:LYS:HG2	2.20	0.42
1:A:2006:ILE:O	1:A:2008:GLN:NE2	2.53	0.42
1:A:1840:SER:O	1:A:1844:THR:HG22	2.19	0.42
1:A:1469:ASN:O	1:A:1473:LYS:HG2	2.19	0.42
1:A:1707:GLU:O	1:A:1707:GLU:HG2	2.20	0.42
1:A:2190:THR:HG21	1:A:2195:THR:H	1.84	0.42
1:A:1162:ILE:HD12	1:A:1176:GLY:HA2	2.02	0.42
1:A:1192:ILE:HG23	1:A:1225:TYR:CD2	2.55	0.42
1:A:1087:PRO:HG2	1:A:1118:LYS:HZ1	1.84	0.41
1:A:1541:ASN:HA	1:A:1544:ILE:HG12	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1778:VAL:HG22	1:A:1829:PHE:HD2	1.85	0.41
1:A:2130:PRO:HB3	1:A:2136:ARG:HH11	1.85	0.41
1:A:1228:GLY:O	1:A:1267:VAL:HA	2.20	0.41
1:A:1262:ASN:H	1:A:1287:ASN:HB3	1.86	0.41
1:A:1388:VAL:HG22	1:A:1457:LEU:HD11	2.01	0.41
1:A:1108:SER:HA	1:A:1136:ALA:O	2.20	0.41
1:A:1172:TYR:OH	1:A:1200:ASN:O	2.35	0.41
1:A:1060:SER:CB	1:A:1090:LYS:HB2	2.50	0.41
1:A:1444:PHE:HD2	1:A:1447:VAL:O	2.03	0.41
1:A:1781:ALA:O	1:A:1782:PHE:HB2	2.20	0.41
1:A:2186:TYR:HE2	1:A:2193:PHE:CE2	2.39	0.41
1:A:930:ASN:HA	1:A:1339:ILE:HG12	2.01	0.41
1:A:1717:SER:HB2	1:A:1772:LEU:O	2.20	0.41
1:A:1421:ILE:O	1:A:1438:ILE:HG13	2.21	0.41
1:A:2030:SER:HB3	1:A:2104:TRP:CD1	2.55	0.41
1:A:2119:PHE:CE2	1:A:2145:ILE:HG12	2.55	0.41
1:A:1327:LYS:O	1:A:1329:ILE:HG12	2.20	0.41
1:A:1939:GLU:HG3	1:A:2156:VAL:HG21	2.02	0.41
1:A:933:LEU:HD11	1:A:957:TYR:HB3	2.03	0.41
1:A:1931:LEU:HD23	1:A:2183:PHE:CD2	2.55	0.41
1:A:2095:LYS:HA	1:A:2095:LYS:HD3	1.74	0.41
1:A:1225:TYR:OH	1:A:1323:ILE:HD13	2.20	0.40
1:A:2043:ARG:NE	1:A:2047:GLU:OE2	2.50	0.40
1:A:1870:PRO:HD2	1:A:2014:ASN:HD21	1.86	0.40
1:A:923:LEU:HA	1:A:1375:PHE:O	2.21	0.40
1:A:959:MET:HE2	1:A:971:LEU:HD21	2.03	0.40
1:A:1807:PHE:C	1:A:1809:GLY:H	2.25	0.40
1:A:1853:SER:HB2	1:A:1857:ILE:HB	2.04	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	1293/2201 (59%)	1176 (91%)	117 (9%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	1148/1915 (60%)	1143 (100%)	5 (0%)	91	95

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	926	ARG
1	A	1605	ASN
1	A	1622	LYS
1	A	2002	ARG
1	A	2174	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1322	ASN
1	A	1715	ASN
1	A	1969	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides 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.

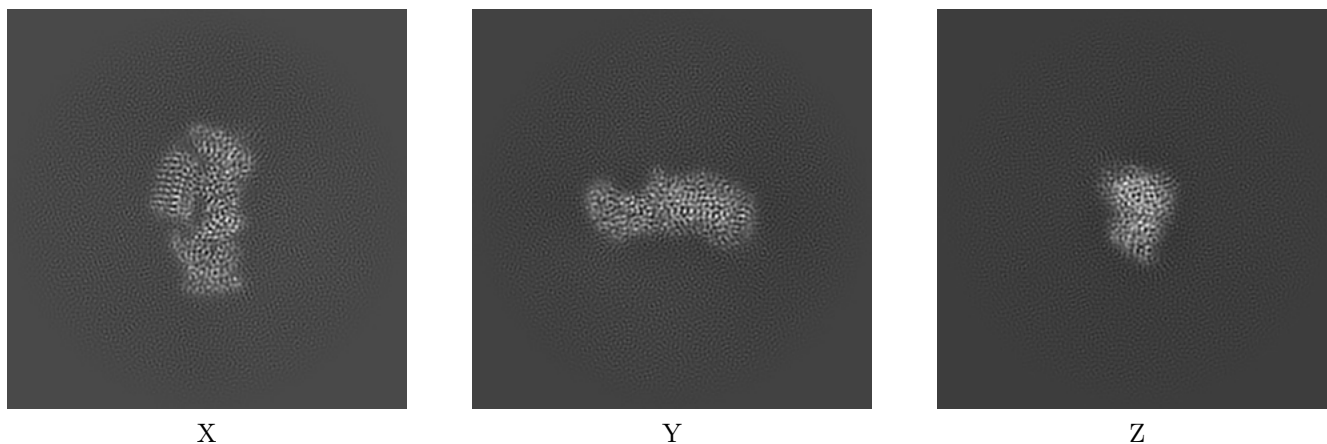
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-26812. These allow visual inspection of the internal detail of the map and identification of artifacts.

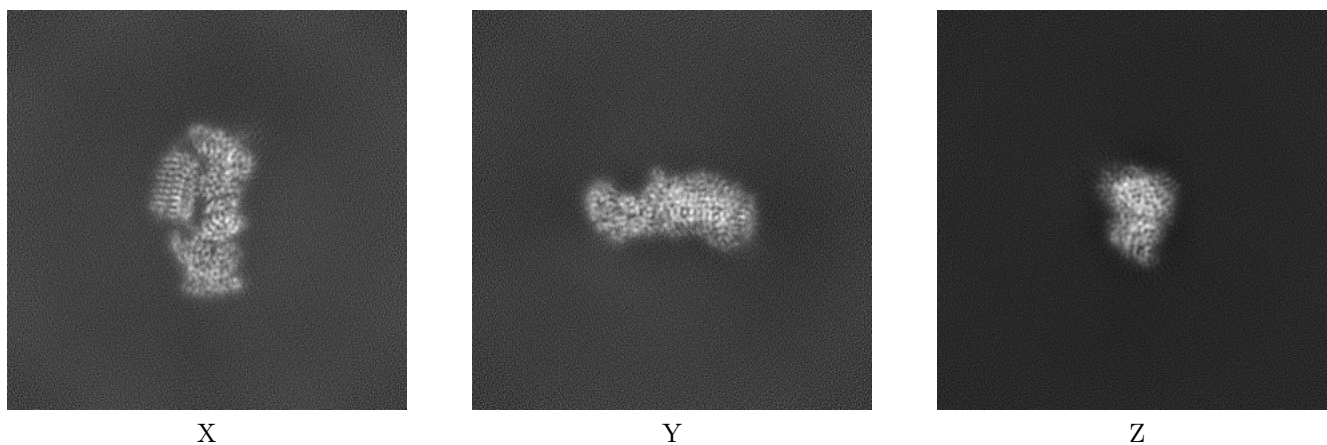
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

6.1.1 Primary map



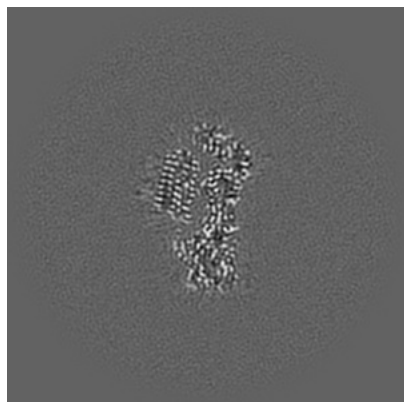
6.1.2 Raw map



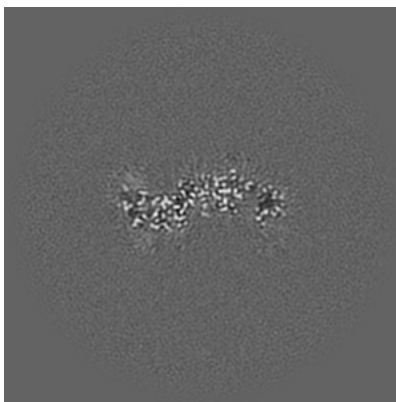
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

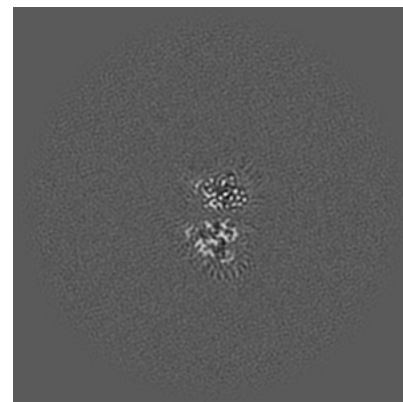
6.2.1 Primary map



X Index: 180

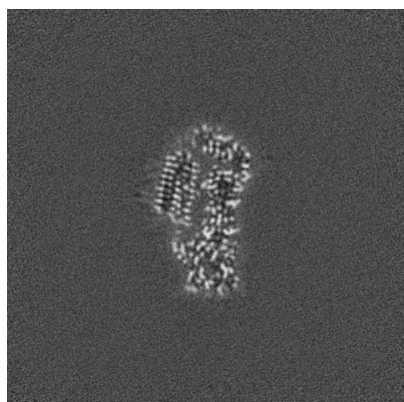


Y Index: 180

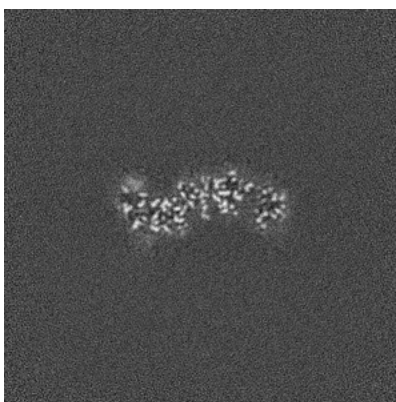


Z Index: 180

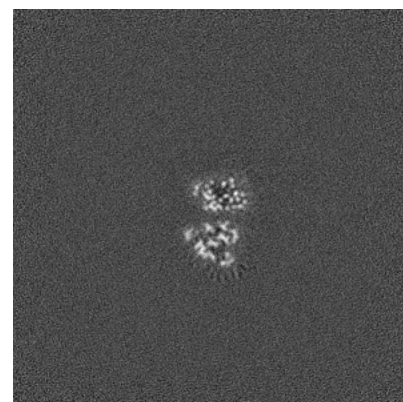
6.2.2 Raw map



X Index: 180



Y Index: 180

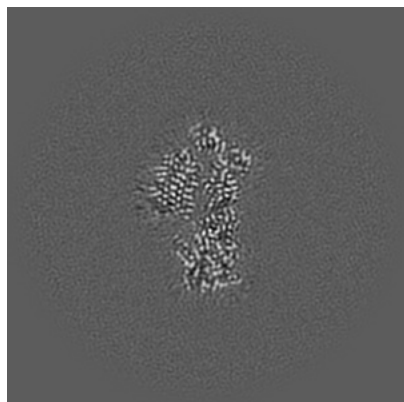


Z Index: 180

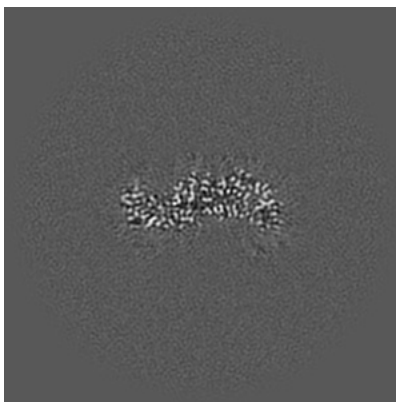
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

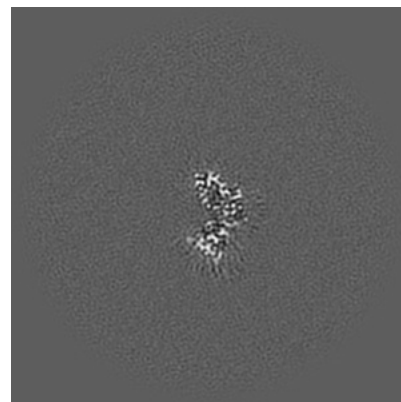
6.3.1 Primary map



X Index: 184

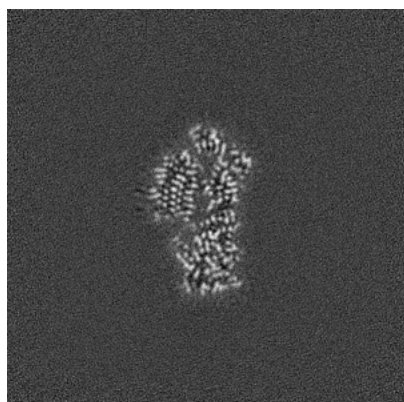


Y Index: 188

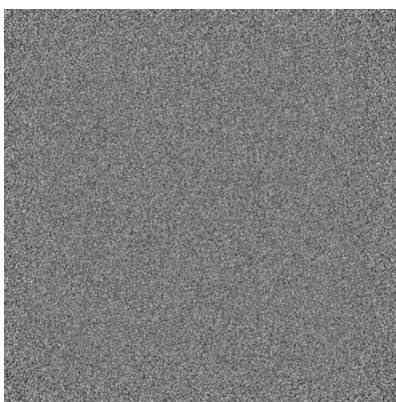


Z Index: 197

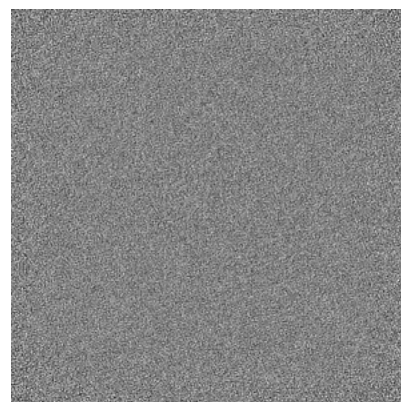
6.3.2 Raw map



X Index: 184



Y Index: 0

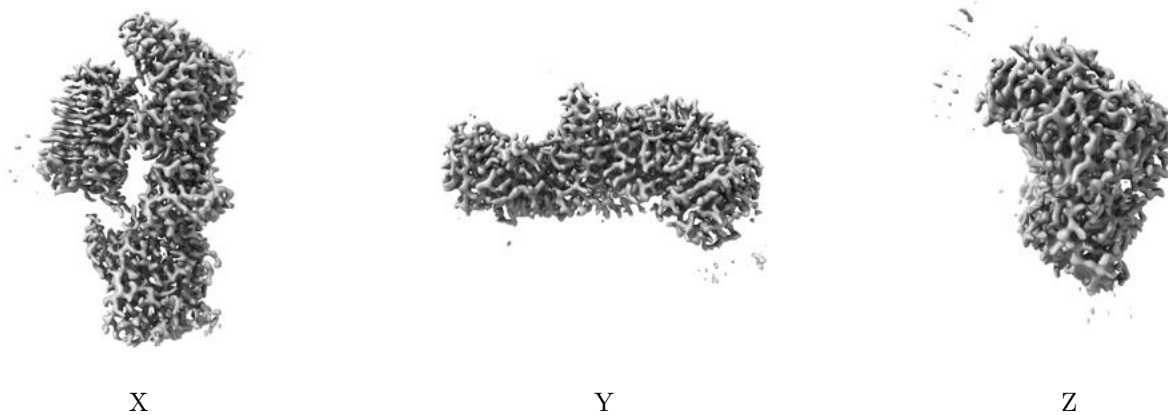


Z Index: 0

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

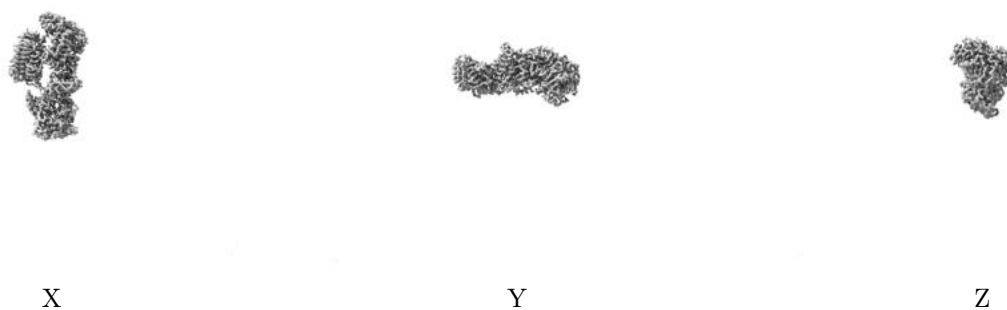
6.4 Orthogonal surface views [i](#)

6.4.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.43. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 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.

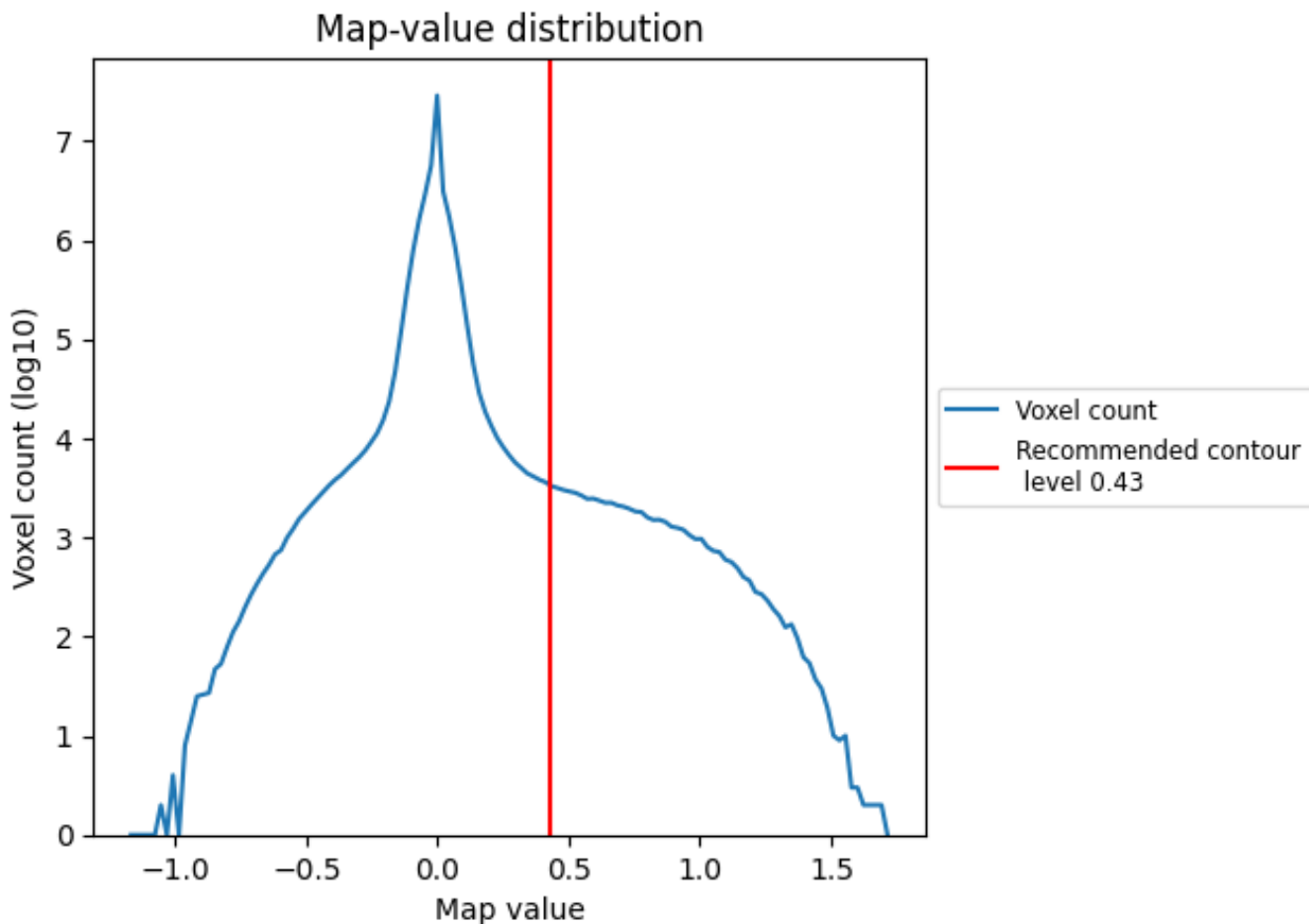
6.5 Mask visualisation [i](#)

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

7 Map analysis [i](#)

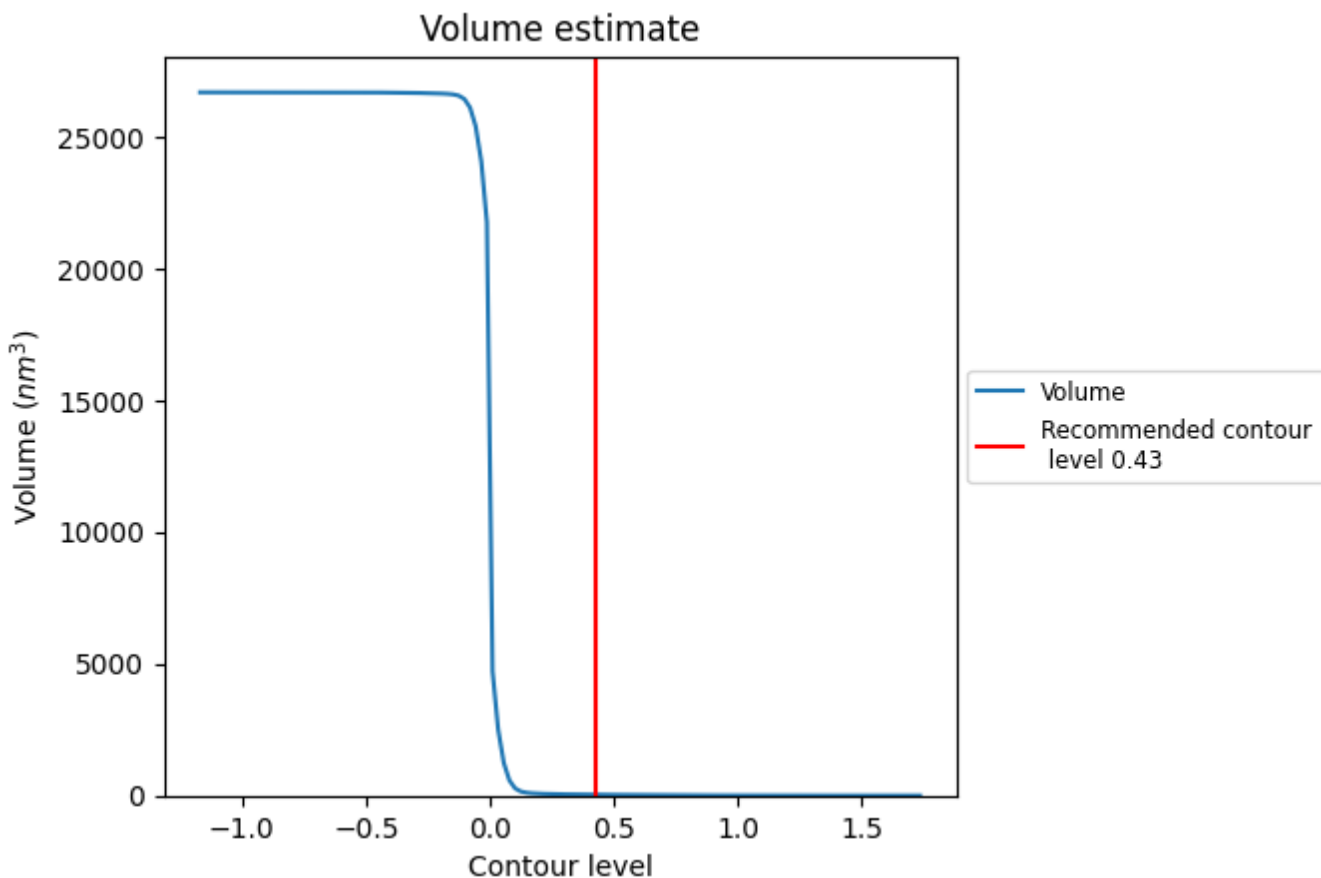
This section contains the results of statistical analysis of the map.

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.

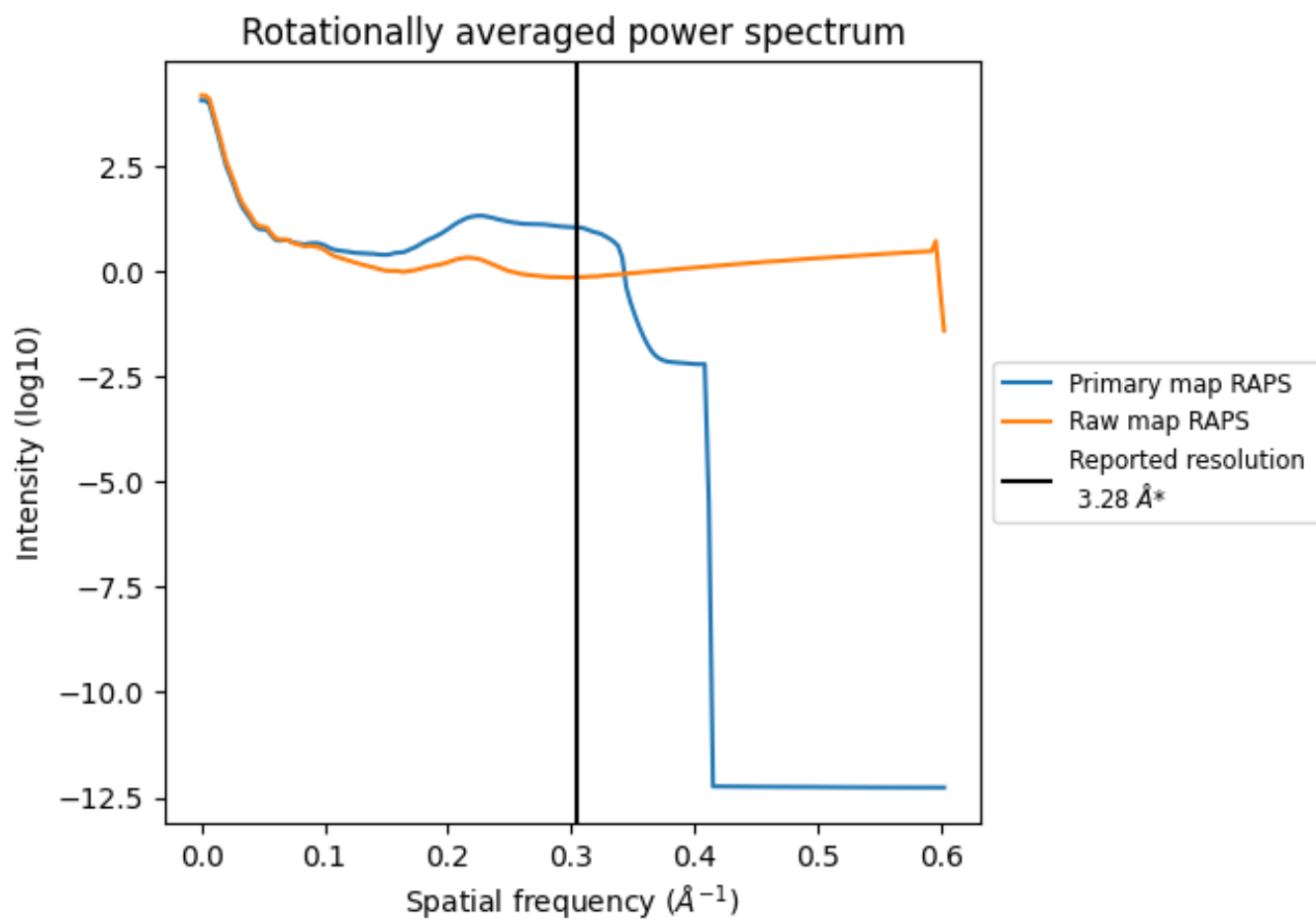
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 34 nm³; this corresponds to an approximate mass of 31 kDa.

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

7.3 Rotationally averaged power spectrum [i](#)

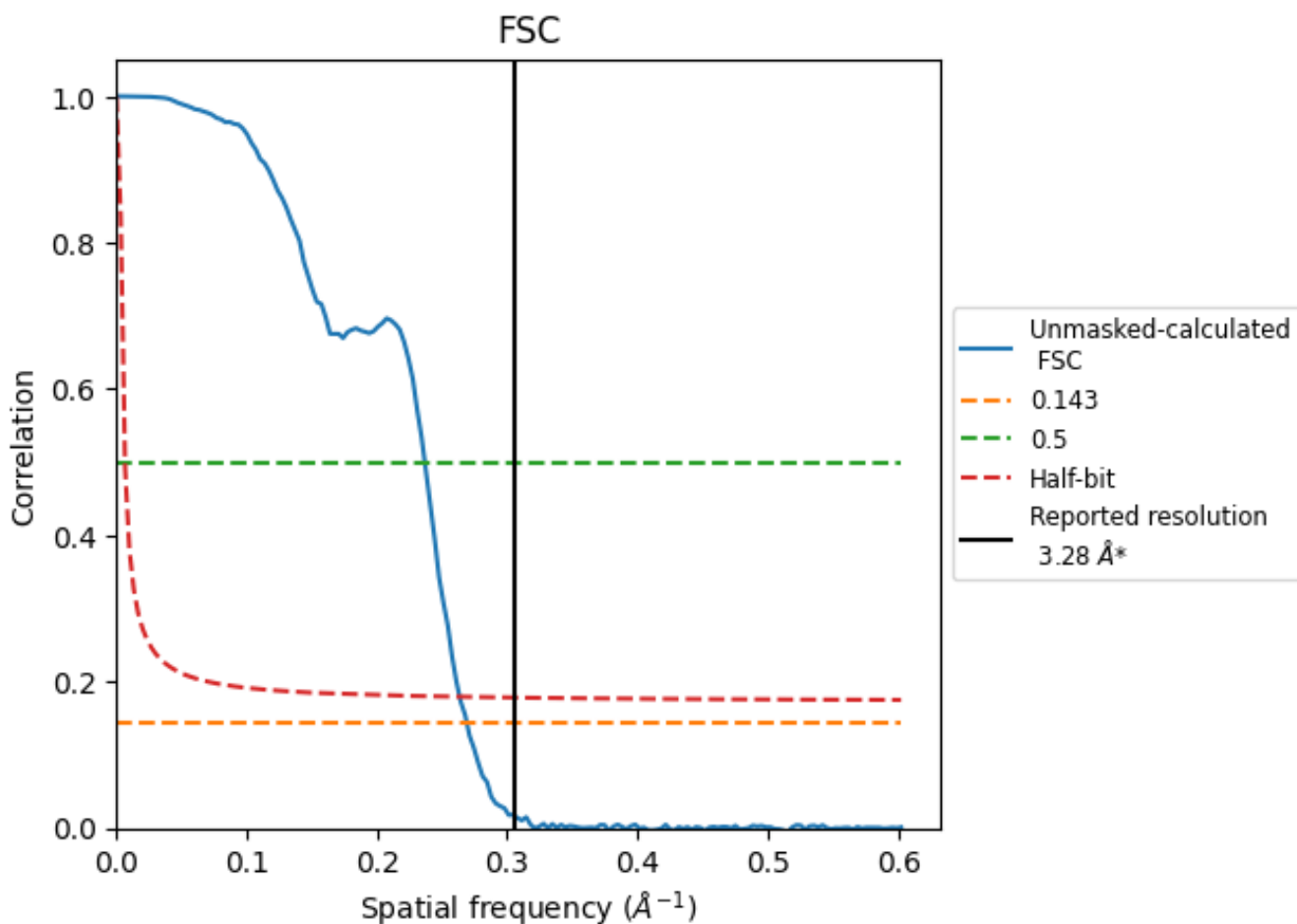


*Reported resolution corresponds to spatial frequency of 0.305 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.305 Å⁻¹

8.2 Resolution estimates [i](#)

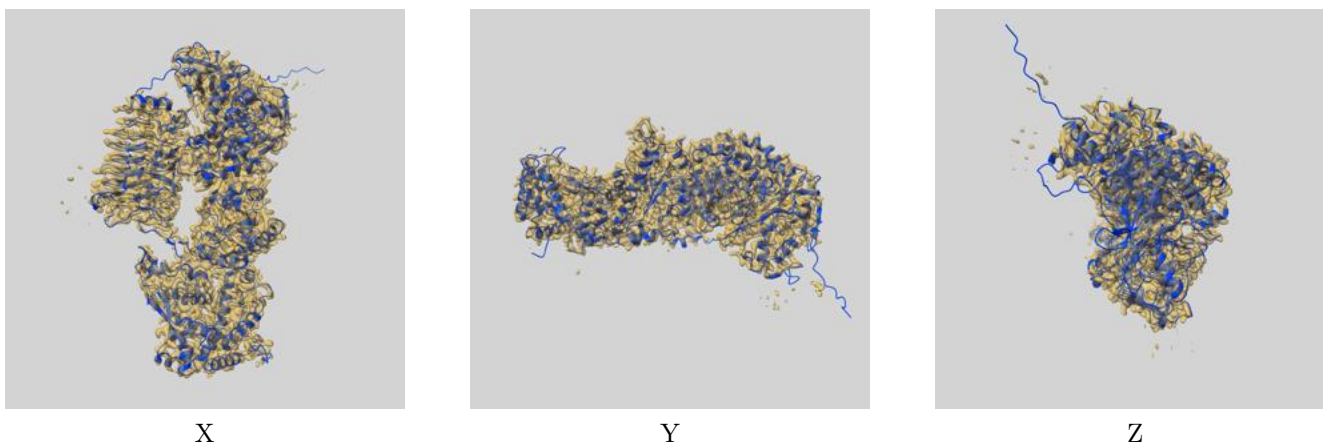
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.28	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.72	4.22	3.80

*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 3.72 differs from the reported value 3.28 by more than 10 %

9 Map-model fit [i](#)

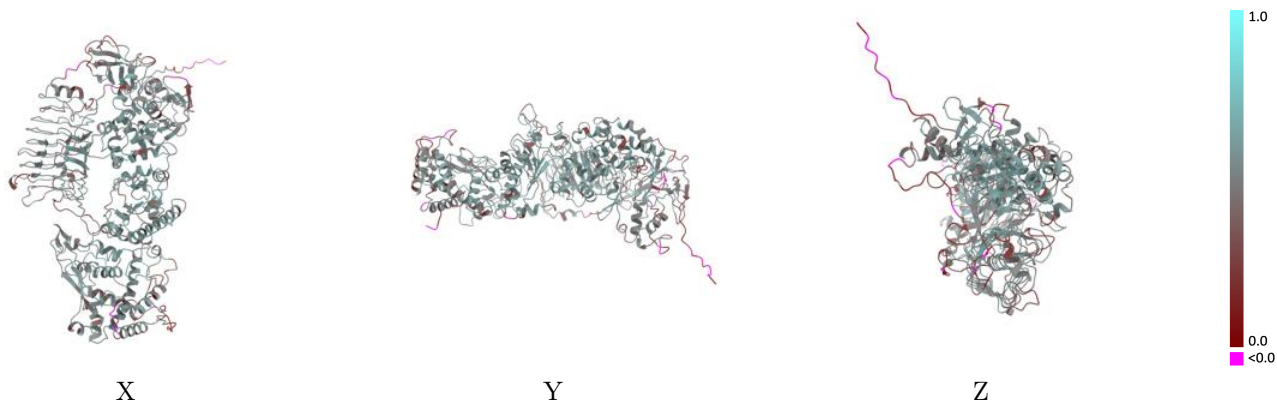
This section contains information regarding the fit between EMDB map EMD-26812 and PDB model 7UVK. Per-residue inclusion information can be found in section [3](#) on page [4](#).

9.1 Map-model overlay [i](#)



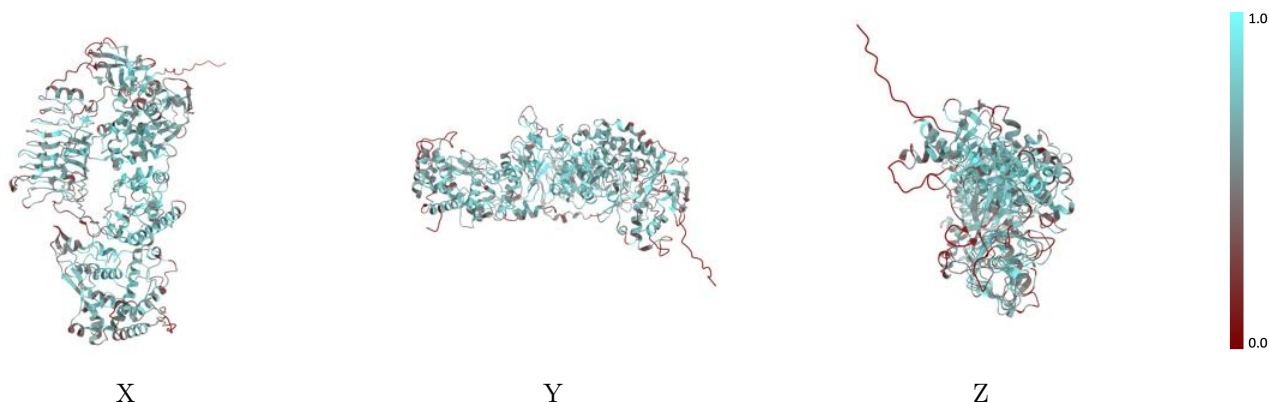
The images above show the 3D surface view of the map at the recommended contour level 0.43 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



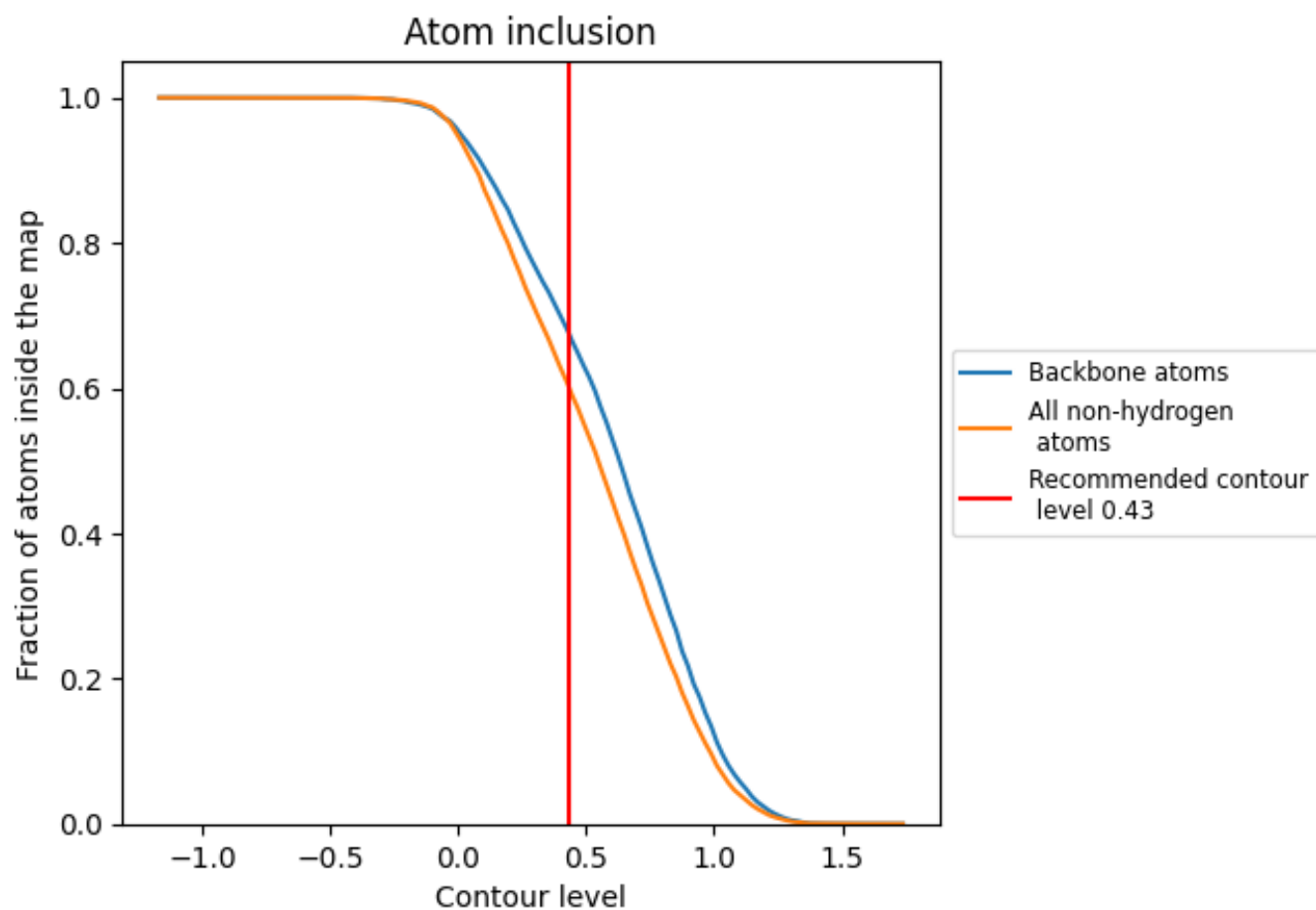
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.43).




9.4 Atom inclusion [i](#)



At the recommended contour level, 68% of all backbone atoms, 60% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary [i](#)

The table lists the average atom inclusion at the recommended contour level (0.43) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6037	 0.4820
A	 0.6037	 0.4820

