



Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 11:59 PM UTC

PDB ID : 9CQ9 / pdb_00009cq9
EMDB ID : EMD-45812
Title : Modifying region of EcPKS1
Authors : Schubert, H.L.; Hill, C.P.
Deposited on : 2024-07-19
Resolution : 3.50 Å(reported)
Based on initial model : .

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

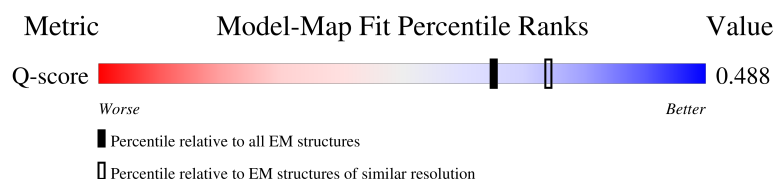
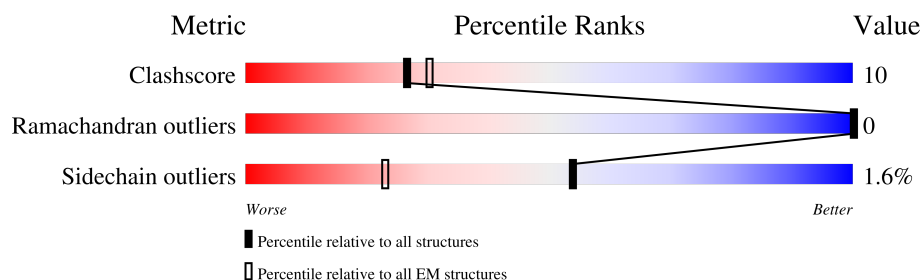
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.50 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	13950 (3.00 - 4.00)

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	2272	 43% 12% 45%
1	B	2272	 43% 12% 45%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 38874 atoms, of which 19370 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 Polyketide synthase 1.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	1256	Total	C	H	N	O	S	0	0
			19437	6164	9685	1709	1825	54		
1	B	1256	Total	C	H	N	O	S	0	0
			19437	6164	9685	1709	1825	54		

Y1638	VAL	T1563	D1217	V1100	L923	GLU	GLU	LEU	SER	VAL	GLY	SER	ASP	ASN	ALA	CYS	THR
V1643	THR	L1354	F1218	L1101	M947	PHE	PHE	ALA	LEU	VAL	PRO	GLU	ALA	GLY	ILE	LYS	ALA
S1644	P1480	A1224	A1224	D1110	I1111	VAL	VAL	PRO	ILE	CYS	THR	LYS	THR	ALA	THR	ASN	THR
D1646	D1488	T1568	E1226	V1112	V957	PRO	PRO	HIS	SER	HIS	GLY	ALA	GLY	SER	VAL	LYS	SER
L1647	L1489	ASP	R1227	S1113	M962	LEU	GLY	ASN	PRO	ALA	VAL	ALA	MET	LEU	ILE	GLU	LEU
D1657	A1362	PRO	I1228	A1114	Q969	LEU	THR	GLU	PRO	GLU	CYS	VAL	PRO	ILE	VAL	ILE	GLU
E1658	A1369	Q1231	Q1232	G1115	L976	GLN	ARG	ASP	ARG	ASP	THR	VAL	TYR	TYR	ALA	VAL	ALA
M1663	V1497	H1372	GLY	V1117	L977	VAL	LEU	ILE	THR	THR	CYS	GLY	ALA	SER	GLY	GLU	ALA
T1669	D1510	D1373	HIS	E1118	A978	LYS	ASP	TRP	TRP	ILE	CYS	VAL	ALA	SER	GLY	CYS	ALA
L1670	L1515	L1374	GLN	I1119	V982	ARG	MET	LEU	PRO	GLY	CYS	ASP	THR	LEU	ILE	LYS	GLN
I1672	H1238	Q1383	H1238	T1124	D986	ALA	ALA	ASN	SER	GLY	THR	LEU	GLY	ASN	THR	LYS	THR
E1673	H1238	R1130	E1242	R1130	K987	GLY	GLY	GLY	VAL	ASP	ALA	GLU	GLY	GLN	PRO	GLY	ARG
F1674	M1391	E1139	F1243	E1139	V988	TRP	ASP	VAL	PRO	VAL	VAL	VAL	ASP	THR	LEU	PRO	THR
D1678	G1523	V1144	F1243	V1144	V989	ASP	HIS	GLU	GLU	MET	GLU	LEU	ASP	ALA	HIS	ALA	GLY
T1679	M1524	G1396	L1248	V1144	L990	VAL	VAL	GLU	GLU	THR	VAL	GLU	PHE	LYS	PHE	LYS	VAL
K1680	F1528	F1397	L1248	H1147	E991	VAL	ALA	TRP	TRP	PHE	THR	GLY	VAL	PRO	SER	ARG	ILE
N1529	V1410	V1410	L1254	VAL	T992	GLN	GLY	GLY	ASP	GLY	THR	THR	VAL	GLN	SER	ARG	SER
C1530	L1413	L1413	R1270	THR	S1000	LEU	TRP	LEU	SER	GLU	ALA	GLU	LYS	LEU	ASN	CYS	ALA
Q1533	P1514	P1514	R1270	GLY	S1001	GLN	LEU	GLN	ALA	GLU	ALA	ASP	LYS	THR	THR	THR	ILE
E1534	T1415	C1688	M1273	ARG	L1002	LYS	VAL	LYS	PRO	LEU	ARG	THR	CYS	THR	VAL	VAL	VAL
A1689	L1416	L1416	V1274	ASP	Q1003	ASN	PRO	ARG	ALA	LYS	GLY	LEU	LYS	THR	ILE	ASN	VAL
P1690	L1417	L1417	D1276	PRO	L1022	THR	ASN	GLN	GLN	ALA	LYS	THR	LYS	THR	GLY	VAL	VAL
P1691	D1276	GLY	D1276	ALA	L1022	ALA	SER	ASP	SER	ASP	ASP	ILE	ALA	ARG	GLY	ASN	LYS
A1692	L1427	ALA	C1277	ALA	E1026	ASP	ASP	ASP	SER	VAL	VAL	LEU	ALA	THR	LEU	THR	THR
R1697	P1428	LYS	L1278	LYS	L1278	ASN	PHE	ASN	ALA	PHE	GLU	ASN	ARG	GLU	ASP	ASN	CYS
C1699	R1429	ARG	M1279	ARG	R1036	GLU	GLU	LEU	GLU	VAL	VAL	PRO	THR	VAL	GLY	ASN	THR
L1700	LYS	S1280	S1280	PRO	GLY	THR	GLY	PHE	PHE	ARG	GLY	ILE	THR	GLY	THR	GLN	LYS
Y1562	SER	GLY	GLY	GLY	I1046	ARG	VAL	VAL	VAL	VAL	VAL	VAL	THR	GLY	ALA	THR	THR
M1566	D1433	GLY	L1290	ALA	T1162	GLN	GLN	PHE	ASN	ASN	ASN	ALA	ILE	ARG	ALA	PHE	LYS
D1567	L1436	Q1178	H1302	Q1178	D1057	ALA	ALA	ALA	ASN	ASN	SER	SER	ALA	THR	VAL	VAL	ASN
L1568	Y1440	V1191	V1306	V1191	V1059	GLY	GLY	LEU	VAL	VAL	ASN	ILE	GLY	GLY	GLU	GLU	VAL
H1583	S1441	L1192	L1307	L1192	L1061	SER	SER	GLY	PRO	ALA	THR	VAL	GLY	GLY	ALA	LEU	THR
T1586	A1442	E1308	E1308	K1195	M1062	CYS	PHE	CYS	VAL	TYR	HIS	ALA	ALA	TRP	THR	PRO	ASN
T1587	Q1444	A1311	A1311	L1198	R1067	THR	ALA	ALA	VAL	VAL	VAL	VAL	VAL	ALA	TRP	ILE	ILE
Q1590	H1452	Y1317	Y1317	L1198	M1073	GLY	GLY	ASN	THR	THR	GLY	GLY	GLY	GLY	GLY	GLY	GLY
E1598	E1456	R1318	R1318	L1204	T1081	SER	SER	LEU	ALA	GLY	THR	TRP	ALA	SER	TYR	ILE	ASN
T1604	V1457	D1332	D1332	Q1207	N1082	LEU	LEU	LEU	GLN	ASN	ASN	SER	CYS	GLY	GLY	GLU	GLU
L1613	I1458	Y1335	Y1335	ASP	I1083	PRO	ASN	ASN	LYS	LYS	ILE	MET	THR	PHE	ILE	GLN	GLN
S1625	F1469	T1336	T1336	LEU	P1092	GLY	LEU	LEU	PRO	ALA	THR	GLY	GLY	ALA	ASN	LEU	LYS
D1740	L1470	G1338	G1338	SER	P1092	LYS	ALA	ALA	PRO	ALA	GLN	ARG	LEU	PHE	ALA	ARG	ALA
T1741	L1471	G1338	G1338	LYS	D1095	THR	CYS	CYS	THR	LEU	CYS	PRO	ASP	GLY	THR	GLY	ALA
E1633	E1374	M1343	M1343	SER	E1096	ALA	TYR	TYR	ALA	LYS	PRO	ASP	VAL	MET	GLY	VAL	ASP
L1634	VAL	D1344	D1344	SER	D1097	PRO	PRO	PRO	ILE	ASP	GLY	GLY	PHE	ALA	GLY	ALA	SER
V1637	GLU	D1345	D1345	SER	V1099	VAL	VAL	VAL	ILE	LEU	ALA	ILE	ARG	ALA	SER	ALA	ASP



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	143694	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.226	Depositor
Minimum map value	-0.124	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.008	Depositor
Recommended contour level	0.0229	Depositor
Map size (Å)	271.36, 271.36, 271.36	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.53, 0.53, 0.53	Depositor

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.20	0/9950	0.36	0/13478
1	B	0.20	0/9950	0.36	0/13478
All	All	0.20	0/19900	0.36	0/26956

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	9752	9685	9684	198	0
1	B	9752	9685	9684	198	0
All	All	19504	19370	19368	389	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 10.

All (389) 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:1311:ALA:HB2	1:A:1337:VAL:HG13	1.23	1.11
1:B:1311:ALA:HB2	1:B:1337:VAL:HG13	1.23	1.10

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1311:ALA:CB	1:A:1337:VAL:HG13	1.84	1.08
1:B:1311:ALA:CB	1:B:1337:VAL:HG13	1.84	1.05
1:A:1308:GLU:OE1	1:A:1335:TYR:OH	1.83	0.96
1:B:1308:GLU:OE1	1:B:1335:TYR:OH	1.83	0.96
1:B:1311:ALA:CB	1:B:1337:VAL:CG1	2.44	0.95
1:A:1311:ALA:CB	1:A:1337:VAL:CG1	2.44	0.94
1:B:1489:LEU:HD23	1:B:1489:LEU:O	1.71	0.91
1:A:1489:LEU:O	1:A:1489:LEU:HD23	1.71	0.89
1:B:1092:PRO:HG3	1:B:1099:VAL:HG23	1.61	0.82
1:B:2010:VAL:HG21	1:B:2032:LEU:HD21	1.62	0.82
1:A:1092:PRO:HG3	1:A:1099:VAL:HG23	1.61	0.82
1:A:2010:VAL:HG21	1:A:2032:LEU:HD21	1.62	0.81
1:B:2114:ASP:OD2	1:B:2131:GLN:NE2	2.17	0.78
1:B:1756:ILE:HD13	1:B:1766:ILE:HG21	1.67	0.77
1:A:2114:ASP:OD2	1:A:2131:GLN:NE2	2.17	0.77
1:A:1756:ILE:HD13	1:A:1766:ILE:HG21	1.67	0.76
1:B:2058:TYR:HH	1:B:2104:THR:HG1	1.32	0.76
1:A:1192:LEU:HD11	1:A:1198:LEU:HD12	1.70	0.74
1:A:1022:LEU:HD21	1:A:2158:MET:HG2	1.70	0.73
1:A:1861:SER:OG	1:B:1733:ARG:NH2	2.23	0.72
1:B:1192:LEU:HD11	1:B:1198:LEU:HD12	1.70	0.72
1:B:1022:LEU:HD21	1:B:2158:MET:HG2	1.70	0.72
1:A:905:ASP:OD2	1:A:1130:ARG:N	2.23	0.71
1:B:905:ASP:OD2	1:B:1130:ARG:N	2.23	0.71
1:A:1733:ARG:NH2	1:B:1861:SER:OG	2.24	0.71
1:B:1709:GLN:O	1:B:1710:HIS:ND1	2.25	0.69
1:A:1709:GLN:O	1:A:1710:HIS:ND1	2.25	0.69
1:B:1598:GLU:OE2	1:B:1940:LYS:NZ	2.18	0.68
1:B:1302:HIS:NE2	1:B:1332:ASP:OD1	2.27	0.68
1:B:1960:VAL:HG21	1:B:2072:LEU:HD11	1.76	0.68
1:A:1960:VAL:HG21	1:A:2072:LEU:HD11	1.76	0.67
1:A:1302:HIS:NE2	1:A:1332:ASP:OD1	2.27	0.66
1:A:1897:LEU:O	1:A:1899:ARG:NH1	2.29	0.66
1:A:2058:TYR:HH	1:A:2104:THR:HG1	1.36	0.66
1:B:1897:LEU:O	1:B:1899:ARG:NH1	2.29	0.66
1:B:2061:THR:HG21	1:B:2105:ASN:HB2	1.78	0.66
1:A:2061:THR:HG21	1:A:2105:ASN:HB2	1.78	0.65
1:B:1633:GLU:OE2	1:B:1701:ARG:NH2	2.29	0.65
1:A:1633:GLU:OE2	1:A:1701:ARG:NH2	2.29	0.64
1:B:1800:GLU:OE2	1:B:1829:ARG:NH1	2.30	0.64
1:A:1800:GLU:OE2	1:A:1829:ARG:NH1	2.30	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1969:GLU:OE2	1:A:1998:LYS:NZ	2.20	0.64
1:A:1598:GLU:OE2	1:A:1940:LYS:NZ	2.18	0.64
1:B:1969:GLU:OE2	1:B:1998:LYS:NZ	2.20	0.62
1:A:1337:VAL:CG1	1:A:1343:MET:SD	2.88	0.62
1:A:1456:GLU:N	1:A:1456:GLU:OE1	2.30	0.62
1:B:1337:VAL:CG1	1:B:1343:MET:SD	2.88	0.62
1:B:1587:THR:OG1	1:B:1590:GLN:OE1	2.18	0.62
1:A:1587:THR:OG1	1:A:1590:GLN:OE1	2.17	0.62
1:A:1638:TYR:HD2	1:A:1713:LEU:HD13	1.64	0.61
1:B:1638:TYR:HD2	1:B:1713:LEU:HD13	1.64	0.61
1:A:1337:VAL:HG11	1:A:1343:MET:SD	2.40	0.61
1:B:1003:GLN:OE1	1:B:1036:ARG:NE	2.34	0.61
1:B:1337:VAL:HG11	1:B:1343:MET:SD	2.40	0.61
1:B:1494:LEU:HD13	1:B:2058:TYR:CE2	2.36	0.61
1:A:1003:GLN:OE1	1:A:1036:ARG:NE	2.34	0.61
1:A:1494:LEU:HD13	1:A:2058:TYR:CE2	2.36	0.60
1:B:1456:GLU:N	1:B:1456:GLU:OE1	2.31	0.60
1:B:1678:ASP:OD1	1:B:1679:THR:N	2.33	0.60
1:B:1311:ALA:HB3	1:B:1337:VAL:CG1	2.31	0.60
1:A:969:GLN:HB2	1:B:962:MET:HE1	1.84	0.60
1:A:1311:ALA:HB2	1:A:1337:VAL:CG1	2.08	0.60
1:A:1756:ILE:HD11	1:A:1768:ILE:HG12	1.84	0.60
1:B:1690:PRO:O	1:B:1692:ALA:N	2.34	0.60
1:A:962:MET:HE1	1:B:969:GLN:HB2	1.84	0.60
1:B:2044:ASN:O	1:B:2061:THR:HG23	2.03	0.59
1:A:2044:ASN:O	1:A:2061:THR:HG23	2.03	0.59
1:B:1417:LEU:CD1	1:B:1436:LEU:HD13	2.33	0.59
1:A:1417:LEU:CD1	1:A:1436:LEU:HD13	2.33	0.59
1:A:2167:TYR:OH	1:A:2173:ARG:NH2	2.36	0.58
1:A:947:MET:HE1	1:A:957:VAL:HG11	1.86	0.58
1:B:1756:ILE:HD11	1:B:1768:ILE:HG12	1.84	0.58
1:B:1523:GLY:O	1:B:2111:SER:OG	2.17	0.58
1:B:2167:TYR:OH	1:B:2173:ARG:NH2	2.36	0.58
1:A:1417:LEU:HD23	1:A:1417:LEU:O	2.04	0.58
1:B:947:MET:HE1	1:B:957:VAL:HG11	1.85	0.58
1:B:1457:VAL:HG21	1:B:1568:LEU:HD11	1.86	0.58
1:B:1417:LEU:O	1:B:1417:LEU:HD23	2.04	0.57
1:B:1457:VAL:HG13	1:B:1458:ILE:HG13	1.87	0.57
1:B:1276:ASP:OD1	1:B:1278:LEU:N	2.37	0.57
1:B:1927:ILE:O	1:B:1941:LYS:NZ	2.38	0.57
1:A:1678:ASP:OD1	1:A:1679:THR:N	2.33	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1927:ILE:O	1:A:1941:LYS:NZ	2.38	0.57
1:B:1139:GLU:OE2	1:B:1583:HIS:ND1	2.38	0.57
1:A:1311:ALA:HB3	1:A:1337:VAL:CG1	2.31	0.56
1:A:1457:VAL:HG13	1:A:1458:ILE:HG13	1.86	0.56
1:A:1139:GLU:OE2	1:A:1583:HIS:ND1	2.38	0.56
1:B:1518:LYS:O	1:B:1518:LYS:HG3	2.05	0.56
1:A:1276:ASP:OD1	1:A:1278:LEU:N	2.37	0.56
1:A:1457:VAL:HG21	1:A:1568:LEU:HD11	1.86	0.56
1:A:1523:GLY:O	1:A:2111:SER:OG	2.17	0.56
1:A:906:GLY:N	1:A:1026:GLU:OE2	2.39	0.56
1:A:1518:LYS:O	1:A:1518:LYS:HG3	2.05	0.56
1:B:1658:GLU:OE1	1:B:1658:GLU:O	2.23	0.56
1:B:1510:ASP:OD1	1:B:1510:ASP:C	2.49	0.55
1:A:1992:THR:OG1	1:A:1993:GLY:N	2.38	0.55
1:B:899:LEU:HD21	1:B:910:PHE:HE1	1.71	0.55
1:A:1658:GLU:O	1:A:1658:GLU:OE1	2.23	0.55
1:B:1992:THR:OG1	1:B:1993:GLY:N	2.38	0.55
1:B:1756:ILE:HD11	1:B:1768:ILE:CG1	2.37	0.55
1:A:1690:PRO:O	1:A:1692:ALA:N	2.34	0.55
1:B:906:GLY:N	1:B:1026:GLU:OE2	2.39	0.55
1:B:1291:CYS:CB	1:B:1470:LEU:HD12	2.37	0.55
1:A:1510:ASP:C	1:A:1510:ASP:OD1	2.49	0.55
1:A:1056:MET:HE1	1:A:1083:ILE:HD11	1.90	0.54
1:A:1291:CYS:CB	1:A:1470:LEU:HD12	2.37	0.54
1:B:1688:CYS:SG	1:B:1697:VAL:HG11	2.47	0.54
1:A:1096:GLU:N	1:A:1096:GLU:OE1	2.41	0.54
1:A:1756:ILE:HD11	1:A:1768:ILE:CG1	2.37	0.54
1:A:1688:CYS:SG	1:A:1697:VAL:HG11	2.47	0.54
1:B:2010:VAL:CG2	1:B:2032:LEU:HD21	2.36	0.54
1:B:2124:GLY:O	1:B:2125:LEU:HD12	2.08	0.54
1:A:1604:THR:HG22	1:A:1613:LEU:HG	1.89	0.54
1:B:1687:LEU:HD13	1:B:1878:TRP:HH2	1.73	0.54
1:B:1291:CYS:HB3	1:B:1470:LEU:HD12	1.90	0.54
1:B:1515:LEU:HB3	1:B:1524:MET:SD	2.47	0.54
1:A:899:LEU:HD21	1:A:910:PHE:HE1	1.71	0.54
1:A:1291:CYS:HB3	1:A:1470:LEU:HD12	1.90	0.54
1:A:2124:GLY:O	1:A:2125:LEU:HD12	2.08	0.54
1:B:1699:CYS:HG	1:B:1703:SER:HG	1.55	0.54
1:A:1634:LEU:HD23	1:A:1634:LEU:O	2.08	0.54
1:B:1056:MET:HE1	1:B:1083:ILE:HD11	1.90	0.54
1:A:1515:LEU:HB3	1:A:1524:MET:SD	2.47	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1096:GLU:OE1	1:B:1096:GLU:N	2.41	0.54
1:B:1881:LEU:C	1:B:1881:LEU:HD23	2.34	0.53
1:A:899:LEU:HD21	1:A:910:PHE:CE1	2.43	0.53
1:B:899:LEU:HD21	1:B:910:PHE:CE1	2.43	0.53
1:A:1687:LEU:HD13	1:A:1878:TRP:HH2	1.73	0.53
1:B:1604:THR:HG22	1:B:1613:LEU:HG	1.89	0.53
1:B:1634:LEU:HD23	1:B:1634:LEU:O	2.08	0.53
1:B:1337:VAL:HG12	1:B:1343:MET:SD	2.50	0.52
1:A:1803:VAL:O	1:A:1807:THR:HG22	2.10	0.52
1:B:1353:THR:O	1:B:1354:LEU:HD23	2.09	0.52
1:A:1881:LEU:HD23	1:A:1881:LEU:C	2.34	0.52
1:A:1990:ILE:CD1	1:A:2011:VAL:HG21	2.40	0.52
1:B:1990:ILE:CD1	1:B:2011:VAL:HG21	2.40	0.52
1:A:1494:LEU:HD22	1:A:2058:TYR:CD2	2.45	0.52
1:B:2171:GLN:O	1:B:2171:GLN:NE2	2.43	0.52
1:A:1344:ASP:OD1	1:A:1344:ASP:N	2.43	0.51
1:B:1494:LEU:HD22	1:B:2058:TYR:CD2	2.45	0.51
1:B:1344:ASP:N	1:B:1344:ASP:OD1	2.43	0.51
1:B:1803:VAL:O	1:B:1807:THR:HG22	2.10	0.51
1:A:1967:GLY:HA2	1:A:2041:LEU:HD22	1.93	0.51
1:A:2076:SER:OG	1:A:2085:LEU:HD22	2.11	0.51
1:A:1353:THR:O	1:A:1354:LEU:HD23	2.09	0.51
1:A:1699:CYS:HG	1:A:1703:SER:HG	1.57	0.51
1:A:1337:VAL:HG12	1:A:1343:MET:SD	2.50	0.51
1:B:1248:LEU:HD23	1:B:1248:LEU:C	2.36	0.51
1:B:1417:LEU:HD12	1:B:1436:LEU:HD13	1.93	0.51
1:A:1469:PHE:HB3	1:A:1471:LEU:HD21	1.92	0.51
1:A:947:MET:HE1	1:A:957:VAL:CG1	2.41	0.51
1:A:1248:LEU:C	1:A:1248:LEU:HD23	2.36	0.51
1:B:1469:PHE:HB3	1:B:1471:LEU:HD21	1.92	0.51
1:B:1967:GLY:HA2	1:B:2041:LEU:HD22	1.93	0.51
1:B:947:MET:HE1	1:B:957:VAL:CG1	2.41	0.51
1:A:2168:PHE:CD1	1:A:2176:VAL:HG21	2.46	0.50
1:B:1311:ALA:CB	1:B:1337:VAL:HG11	2.38	0.50
1:B:1720:PRO:O	1:B:1722:ALA:N	2.44	0.50
1:A:1990:ILE:HD11	1:A:2011:VAL:HG21	1.92	0.50
1:B:2168:PHE:CD1	1:B:2176:VAL:HG21	2.46	0.50
1:B:1990:ILE:HD11	1:B:2011:VAL:HG21	1.92	0.50
1:A:2171:GLN:O	1:A:2171:GLN:NE2	2.43	0.50
1:A:1337:VAL:HG12	1:A:1338:GLY:N	2.27	0.49
1:A:2035:LEU:HD23	1:A:2081:ILE:HG21	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1643:VAL:HG12	1:B:1644:SER:N	2.27	0.49
1:A:1417:LEU:HD12	1:A:1436:LEU:HD13	1.93	0.49
1:A:1733:ARG:NH1	1:B:1859:ASP:OD1	2.36	0.49
1:A:1311:ALA:CB	1:A:1337:VAL:HG11	2.38	0.49
1:A:1391:MET:HB3	1:A:1452:HIS:CD2	2.47	0.49
1:B:1688:CYS:SG	1:B:1692:ALA:HB2	2.53	0.49
1:B:2076:SER:OG	1:B:2085:LEU:HD22	2.10	0.49
1:A:1101:LEU:HD23	1:A:1115:GLY:HA3	1.95	0.49
1:B:1101:LEU:HD23	1:B:1115:GLY:HA3	1.95	0.49
1:B:1337:VAL:HG12	1:B:1338:GLY:N	2.27	0.49
1:B:1279:MET:SD	1:B:1416:LEU:HD11	2.53	0.49
1:B:1391:MET:HB3	1:B:1452:HIS:CD2	2.47	0.49
1:A:1643:VAL:HG12	1:A:1644:SER:N	2.27	0.49
1:A:1901:VAL:HG11	1:A:1926:LYS:HE3	1.94	0.49
1:A:2092:SER:OG	1:A:2093:SER:N	2.46	0.49
1:A:1881:LEU:HD23	1:A:1881:LEU:O	2.13	0.48
1:B:1881:LEU:HD23	1:B:1881:LEU:O	2.13	0.48
1:B:2124:GLY:C	1:B:2125:LEU:HD12	2.38	0.48
1:A:1533:GLN:NE2	1:A:2151:GLU:OE2	2.45	0.48
1:A:1688:CYS:SG	1:A:1692:ALA:HB2	2.53	0.48
1:B:1533:GLN:NE2	1:B:2151:GLU:OE2	2.45	0.48
1:A:2124:GLY:C	1:A:2125:LEU:HD12	2.38	0.48
1:A:1415:THR:O	1:A:1416:LEU:HB2	2.13	0.48
1:B:1488:ASP:OD2	1:B:1489:LEU:N	2.47	0.48
1:B:2035:LEU:HD23	1:B:2081:ILE:HG21	1.94	0.48
1:A:1097:ASP:OD1	1:A:1098:VAL:N	2.47	0.48
1:A:1720:PRO:O	1:A:1722:ALA:N	2.44	0.48
1:A:1957:TYR:HD2	1:A:1979:VAL:HG13	1.79	0.48
1:B:1901:VAL:HG11	1:B:1926:LYS:HE3	1.94	0.48
1:B:1957:TYR:HD2	1:B:1979:VAL:HG13	1.79	0.48
1:A:1488:ASP:OD2	1:A:1489:LEU:N	2.47	0.48
1:B:1415:THR:O	1:B:1416:LEU:HB2	2.13	0.48
1:A:2010:VAL:CG2	1:A:2032:LEU:HD21	2.36	0.48
1:A:992:THR:HG21	1:A:1113:SER:HB3	1.95	0.48
1:A:1279:MET:SD	1:A:1416:LEU:HD11	2.53	0.47
1:A:1859:ASP:OD1	1:B:1733:ARG:NH1	2.34	0.47
1:B:992:THR:HG21	1:B:1113:SER:HB3	1.95	0.47
1:B:1679:THR:O	1:B:1680:LYS:HB2	2.15	0.47
1:B:1242:LEU:N	1:B:1276:ASP:OD2	2.39	0.47
1:B:1056:MET:CE	1:B:1083:ILE:HD11	2.45	0.47
1:B:1111:ILE:HD11	1:B:1118:GLU:CG	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1056:MET:CE	1:A:1083:ILE:HD11	2.45	0.46
1:B:1097:ASP:OD1	1:B:1098:VAL:N	2.47	0.46
1:B:2092:SER:OG	1:B:2093:SER:N	2.46	0.46
1:A:1111:ILE:HD11	1:A:1118:GLU:CG	2.45	0.46
1:A:1679:THR:O	1:A:1680:LYS:HB2	2.15	0.46
1:B:1057:ASP:OD2	1:B:1061:GLN:NE2	2.49	0.46
1:B:1311:ALA:HB2	1:B:1337:VAL:CG1	2.09	0.46
1:A:2047:ASP:OD1	1:A:2047:ASP:N	2.48	0.46
1:A:1280:SER:O	1:A:1280:SER:OG	2.25	0.46
1:B:1534:GLU:O	1:B:1537:SER:OG	2.26	0.46
1:A:1168:TYR:HE1	1:A:1172:CYS:HG	1.60	0.46
1:A:1306:VAL:HG22	1:A:1374:LEU:HB3	1.98	0.46
1:A:1410:VAL:HG11	1:A:1442:ALA:HB2	1.98	0.46
1:B:1683:ARG:NH1	1:B:1930:GLU:OE2	2.49	0.46
1:A:1489:LEU:HD21	1:A:2066:ILE:HG21	1.98	0.46
1:B:1306:VAL:HG22	1:B:1374:LEU:HB3	1.98	0.46
1:B:1657:ASP:OD2	1:B:1658:GLU:N	2.50	0.46
1:A:1057:ASP:OD2	1:A:1061:GLN:NE2	2.49	0.45
1:B:1489:LEU:HD21	1:B:2066:ILE:HG21	1.98	0.45
1:A:1683:ARG:NH1	1:A:1930:GLU:OE2	2.49	0.45
1:B:1410:VAL:HG11	1:B:1442:ALA:HB2	1.98	0.45
1:A:1657:ASP:OD2	1:A:1658:GLU:N	2.50	0.45
1:B:1963:LEU:HD12	1:B:1968:LEU:HD21	1.97	0.45
1:B:1493:TRP:O	1:B:1497:VAL:HG13	2.17	0.45
1:B:2047:ASP:OD1	1:B:2047:ASP:N	2.48	0.45
1:B:1227:ARG:O	1:B:1231:GLN:HG3	2.17	0.45
1:A:957:VAL:HG23	1:A:957:VAL:O	2.16	0.45
1:B:986:ASP:O	1:B:987:LYS:C	2.60	0.45
1:B:1280:SER:O	1:B:1280:SER:OG	2.25	0.45
1:A:1493:TRP:O	1:A:1497:VAL:HG13	2.17	0.45
1:A:2086:ASP:N	1:A:2086:ASP:OD1	2.50	0.45
1:B:1721:VAL:CG2	1:B:1722:ALA:N	2.80	0.45
1:B:2086:ASP:OD1	1:B:2086:ASP:N	2.50	0.45
1:A:1963:LEU:HD12	1:A:1968:LEU:HD21	1.97	0.45
1:A:1721:VAL:CG2	1:A:1722:ALA:N	2.80	0.44
1:B:1062:MET:HE3	1:B:1062:MET:HB2	1.93	0.44
1:B:1081:ILE:HG23	1:B:1119:ILE:HG12	1.99	0.44
1:A:1081:ILE:HG23	1:A:1119:ILE:HG12	1.99	0.44
1:B:1700:LEU:O	1:B:1701:ARG:HB3	2.17	0.44
1:A:1410:VAL:O	1:A:1413:LEU:HD21	2.18	0.44
1:A:969:GLN:HG3	1:A:976:LEU:HD13	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:957:VAL:O	1:B:957:VAL:HG23	2.16	0.44
1:A:1227:ARG:O	1:A:1231:GLN:HG3	2.17	0.44
1:A:1663:MET:SD	1:A:1690:PRO:HG3	2.58	0.44
1:B:1067:ARG:NH2	1:B:1110:ASP:OD2	2.50	0.44
1:B:918:LEU:CD2	1:B:957:VAL:HG21	2.48	0.44
1:B:1663:MET:SD	1:B:1690:PRO:HG3	2.58	0.44
1:B:1671:GLY:O	1:B:1692:ALA:HB3	2.18	0.44
1:A:918:LEU:CD2	1:A:957:VAL:HG21	2.48	0.43
1:A:1700:LEU:O	1:A:1701:ARG:HB3	2.17	0.43
1:A:1701:ARG:O	1:A:1701:ARG:HG3	2.18	0.43
1:A:1225:LEU:HD13	1:A:1243:PHE:CD1	2.54	0.43
1:A:1369:ALA:O	1:A:1396:GLY:O	2.37	0.43
1:A:923:LEU:HD22	1:A:982:VAL:HG22	2.00	0.43
1:A:986:ASP:O	1:A:987:LYS:C	2.60	0.43
1:A:1046:ILE:HD11	1:A:1062:MET:HE1	2.01	0.43
1:A:1709:GLN:O	1:A:1710:HIS:CG	2.70	0.43
1:A:1307:LEU:HB2	1:A:1372:HIS:NE2	2.34	0.43
1:A:1225:LEU:HD13	1:A:1243:PHE:HD1	1.83	0.43
1:A:2069:THR:HG23	1:A:2090:MET:HE2	2.00	0.43
1:B:969:GLN:HG3	1:B:976:LEU:HD13	1.99	0.43
1:B:1144:VAL:HG11	1:B:1290:LEU:HD22	2.00	0.43
1:B:1701:ARG:HG3	1:B:1701:ARG:O	2.18	0.43
1:B:891:SER:OG	1:B:892:ALA:N	2.52	0.43
1:B:1410:VAL:O	1:B:1413:LEU:HD21	2.18	0.43
1:A:976:LEU:HD11	1:A:978:ALA:O	2.19	0.43
1:A:1067:ARG:NH2	1:A:1110:ASP:OD2	2.50	0.43
1:A:1417:LEU:HD13	1:A:1436:LEU:HD13	2.01	0.43
1:A:1144:VAL:HG11	1:A:1290:LEU:HD22	2.00	0.43
1:A:1671:GLY:O	1:A:1692:ALA:HB3	2.18	0.43
1:B:923:LEU:HD22	1:B:982:VAL:HG22	2.00	0.43
1:B:1046:ILE:HD13	1:B:1114:ALA:HB1	2.01	0.43
1:B:1225:LEU:HD13	1:B:1243:PHE:HD1	1.83	0.43
1:A:1311:ALA:HB3	1:A:1343:MET:SD	2.59	0.43
1:B:1225:LEU:HD13	1:B:1243:PHE:CD1	2.54	0.43
1:B:1311:ALA:HB3	1:B:1343:MET:SD	2.59	0.43
1:B:1489:LEU:O	1:B:1489:LEU:CD2	2.55	0.43
1:B:1494:LEU:HD22	1:B:2058:TYR:HD2	1.84	0.43
1:A:1046:ILE:HD13	1:A:1114:ALA:HB1	2.01	0.43
1:B:1046:ILE:HD11	1:B:1062:MET:HE1	2.01	0.43
1:B:1372:HIS:HB2	1:B:1397:PHE:O	2.19	0.43
1:B:2149:VAL:HG12	1:B:2154:TRP:CE3	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1372:HIS:HB2	1:A:1397:PHE:O	2.19	0.42
1:A:2040:ASN:OD1	1:A:2040:ASN:C	2.62	0.42
1:B:1059:VAL:HG21	1:B:1117:VAL:CG2	2.50	0.42
1:B:1073:MET:SD	1:B:1124:THR:HG21	2.59	0.42
1:B:1383:GLN:O	1:B:1427:LEU:HD11	2.19	0.42
1:B:2069:THR:HG23	1:B:2090:MET:HE2	2.00	0.42
1:A:1383:GLN:O	1:A:1427:LEU:HD11	2.19	0.42
1:A:2149:VAL:HG12	1:A:2154:TRP:CE3	2.54	0.42
1:B:1192:LEU:HD23	1:B:1195:LYS:CB	2.49	0.42
1:B:1224:ALA:HA	1:B:1227:ARG:HE	1.84	0.42
1:B:1369:ALA:O	1:B:1396:GLY:O	2.37	0.42
1:B:1671:GLY:O	1:B:1690:PRO:O	2.37	0.42
1:A:1059:VAL:HG21	1:A:1117:VAL:CG2	2.49	0.42
1:B:2040:ASN:OD1	1:B:2040:ASN:C	2.62	0.42
1:A:1637:VAL:HG22	1:A:1674:PHE:CD2	2.54	0.42
1:A:2168:PHE:CE1	1:A:2176:VAL:HG21	2.54	0.42
1:B:1307:LEU:HB2	1:B:1372:HIS:NE2	2.34	0.42
1:B:1637:VAL:HG22	1:B:1674:PHE:CD2	2.54	0.42
1:B:1709:GLN:O	1:B:1710:HIS:CG	2.70	0.42
1:A:891:SER:OG	1:A:892:ALA:N	2.52	0.42
1:A:1317:TYR:O	1:A:1318:ARG:C	2.63	0.42
1:A:1534:GLU:O	1:A:1537:SER:OG	2.26	0.42
1:A:2171:GLN:OE1	1:A:2173:ARG:NE	2.42	0.42
1:B:2168:PHE:CE1	1:B:2176:VAL:HG21	2.54	0.42
1:A:1192:LEU:HD23	1:A:1195:LYS:CB	2.50	0.42
1:B:976:LEU:HD11	1:B:978:ALA:O	2.19	0.42
1:B:2150:ILE:N	1:B:2150:ILE:HD12	2.35	0.42
1:A:1073:MET:SD	1:A:1124:THR:HG21	2.59	0.42
1:A:1671:GLY:O	1:A:1690:PRO:O	2.37	0.42
1:A:1562:TYR:CZ	1:A:1566:MET:CE	3.03	0.42
1:A:1720:PRO:O	1:A:1721:VAL:HG22	2.20	0.42
1:B:1528:PHE:HE2	1:B:1540:VAL:HG12	1.85	0.42
1:B:1741:THR:HG22	1:B:1765:GLU:HB3	2.01	0.42
1:A:1673:GLU:HB3	1:A:1721:VAL:HG13	2.01	0.42
1:A:1528:PHE:HE2	1:A:1540:VAL:HG12	1.85	0.42
1:A:1657:ASP:OD2	1:A:1657:ASP:C	2.63	0.42
1:B:1713:LEU:HD12	1:B:1930:GLU:CD	2.45	0.42
1:A:889:ASP:O	1:A:896:ASP:HB2	2.21	0.41
1:B:1225:LEU:O	1:B:1228:ILE:HG22	2.20	0.41
1:B:1440:TYR:CD2	1:B:1444:GLN:HB3	2.55	0.41
1:A:1637:VAL:HG22	1:A:1674:PHE:HD2	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1637:VAL:HG22	1:B:1674:PHE:HD2	1.85	0.41
1:A:1494:LEU:HD22	1:A:2058:TYR:HD2	1.84	0.41
1:A:2045:LEU:HD23	1:A:2045:LEU:HA	1.94	0.41
1:B:1657:ASP:OD2	1:B:1657:ASP:C	2.63	0.41
1:B:1720:PRO:O	1:B:1721:VAL:HG22	2.20	0.41
1:A:1133:HIS:NE2	1:A:2157:ARG:HG2	2.35	0.41
1:A:1440:TYR:CD2	1:A:1444:GLN:HB3	2.55	0.41
1:A:989:VAL:HG13	1:A:990:LEU:N	2.36	0.41
1:A:1224:ALA:HA	1:A:1227:ARG:HE	1.84	0.41
1:B:1562:TYR:CZ	1:B:1566:MET:CE	3.03	0.41
1:B:1647:LEU:HD21	1:B:1915:GLU:HB2	2.02	0.41
1:A:1345:ASP:OD1	1:A:1345:ASP:N	2.53	0.41
1:B:1337:VAL:CG1	1:B:1338:GLY:N	2.84	0.41
1:B:1528:PHE:CD1	1:B:1528:PHE:C	2.99	0.41
1:A:1646:ASP:OD1	1:A:1671:GLY:N	2.46	0.41
1:A:2150:ILE:HD12	1:A:2150:ILE:N	2.35	0.41
1:B:1270:ARG:HA	1:B:1273:MET:HB3	2.03	0.41
1:A:1000:SER:O	1:A:1001:SER:HB3	2.21	0.41
1:A:1735:HIS:NE2	1:B:1735:HIS:NE2	2.69	0.41
1:A:1741:THR:HG22	1:A:1765:GLU:HB3	2.01	0.41
1:B:1191:VAL:HG21	1:B:1254:LEU:O	2.21	0.41
1:B:1317:TYR:O	1:B:1318:ARG:C	2.63	0.41
1:B:1345:ASP:OD1	1:B:1345:ASP:N	2.53	0.41
1:B:1673:GLU:HB3	1:B:1721:VAL:HG13	2.01	0.41
1:A:1191:VAL:HG21	1:A:1254:LEU:O	2.21	0.41
1:A:1232:GLN:OE1	1:A:1232:GLN:C	2.64	0.41
1:A:1690:PRO:N	1:A:1691:PRO:HD2	2.35	0.41
1:A:1713:LEU:HD12	1:A:1930:GLU:CD	2.45	0.41
1:A:2135:ILE:H	1:A:2135:ILE:HD12	1.85	0.41
1:B:1000:SER:O	1:B:1001:SER:HB3	2.21	0.41
1:B:1232:GLN:C	1:B:1232:GLN:OE1	2.64	0.41
1:B:1308:GLU:O	1:B:1308:GLU:HG2	2.21	0.41
1:B:1646:ASP:OD1	1:B:1671:GLY:N	2.46	0.41
1:B:2171:GLN:OE1	1:B:2173:ARG:NE	2.42	0.41
1:A:1178:GLN:OE1	1:A:1218:PHE:HA	2.21	0.41
1:B:1178:GLN:OE1	1:B:1218:PHE:HA	2.21	0.41
1:B:1689:ALA:HB1	1:B:1690:PRO:HD2	2.03	0.41
1:A:1189:ASP:OD1	1:A:1189:ASP:N	2.52	0.40
1:A:1719:VAL:N	1:A:1720:PRO:HD2	2.36	0.40
1:B:889:ASP:O	1:B:896:ASP:HB2	2.20	0.40
1:B:1908:VAL:HG23	1:B:1909:ASP:N	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1225:LEU:O	1:A:1228:ILE:HG22	2.20	0.40
1:A:1908:VAL:HG23	1:A:1909:ASP:N	2.36	0.40
1:B:2065:LYS:HE2	1:B:2110:ASN:ND2	2.36	0.40
1:B:2172:ASN:OD1	1:B:2172:ASN:C	2.64	0.40
1:A:1337:VAL:CG1	1:A:1338:GLY:N	2.84	0.40
1:A:1424:ASP:OD1	1:A:1425:HIS:N	2.54	0.40
1:A:1689:ALA:HB1	1:A:1690:PRO:HD2	2.03	0.40
1:A:976:LEU:HD12	1:A:977:LEU:N	2.36	0.40
1:A:1046:ILE:HG21	1:A:1055:PHE:CE1	2.57	0.40
1:A:1082:ASN:OD1	1:A:1082:ASN:N	2.55	0.40
1:A:1933:GLU:HG3	1:A:1935:ILE:H	1.87	0.40
1:B:1690:PRO:N	1:B:1691:PRO:HD2	2.35	0.40
1:B:2073:ASP:OD2	1:B:2116:LEU:HD11	2.22	0.40
1:B:2135:ILE:HD12	1:B:2135:ILE:H	1.85	0.40
1:A:1647:LEU:HD21	1:A:1915:GLU:HB2	2.02	0.40
1:B:989:VAL:HG13	1:B:990:LEU:N	2.36	0.40
1:B:1095:ASP:OD1	1:B:1095:ASP:N	2.54	0.40
1:B:2045:LEU:HD23	1:B:2045:LEU:HA	1.94	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	1240/2272 (55%)	1137 (92%)	103 (8%)	0	100	100
1	B	1240/2272 (55%)	1137 (92%)	103 (8%)	0	100	100
All	All	2480/4544 (55%)	2274 (92%)	206 (8%)	0	100	100

There are no Ramachandran outliers to report.

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	1050/1892 (56%)	1033 (98%)	17 (2%)	55	70
1	B	1050/1892 (56%)	1034 (98%)	16 (2%)	57	71
All	All	2100/3784 (56%)	2067 (98%)	33 (2%)	54	70

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1095	ASP
1	A	1275	ASP
1	A	1440	TYR
1	A	1530	CYS
1	A	1534	GLU
1	A	1542	CYS
1	A	1560	PHE
1	A	1586	ILE
1	A	1587	THR
1	A	1625	SER
1	A	1669	THR
1	A	1721	VAL
1	A	1740	ASP
1	A	1766	ILE
1	A	2026	VAL
1	A	2149	VAL
1	A	2175	VAL
1	B	1095	ASP
1	B	1275	ASP
1	B	1440	TYR
1	B	1530	CYS
1	B	1534	GLU
1	B	1542	CYS
1	B	1586	ILE
1	B	1587	THR
1	B	1625	SER
1	B	1669	THR

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Mol	Chain	Res	Type
1	B	1721	VAL
1	B	1740	ASP
1	B	1766	ILE
1	B	2026	VAL
1	B	2149	VAL
1	B	2175	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	969	GLN
1	A	1452	HIS
1	A	1571	ASN
1	A	1972	HIS
1	A	2103	GLN
1	B	969	GLN
1	B	1452	HIS
1	B	1571	ASN
1	B	1874	GLN
1	B	1972	HIS
1	B	2103	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](#)

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.

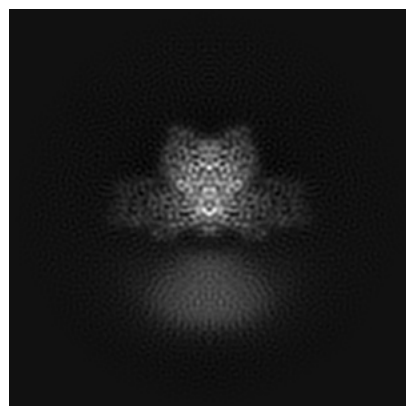
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-45812. These allow visual inspection of the internal detail of the map and identification of artifacts.

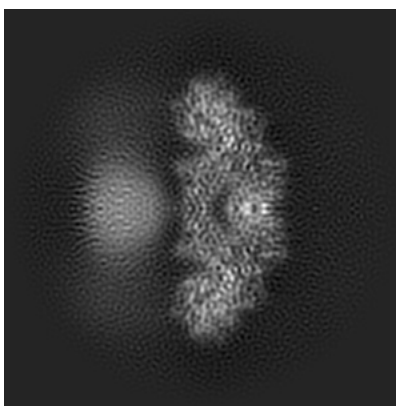
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

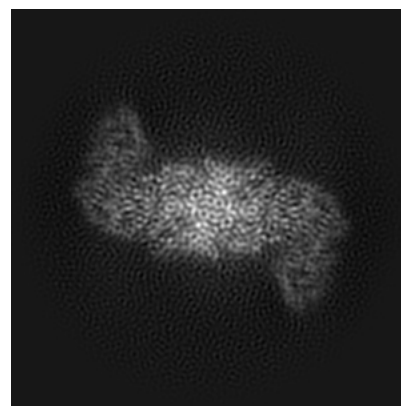
6.1.1 Primary map



X

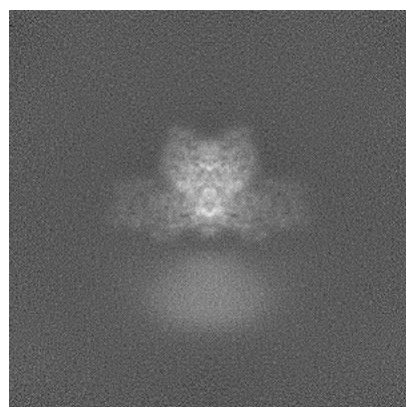


Y

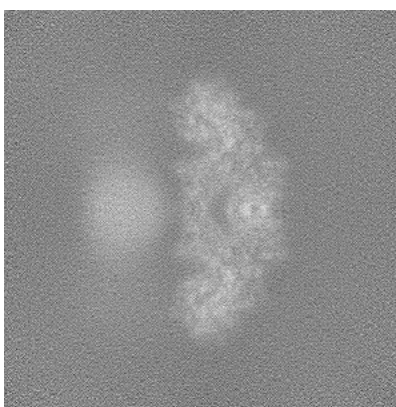


Z

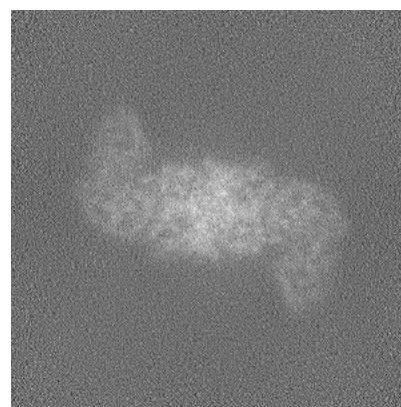
6.1.2 Raw map



X



Y

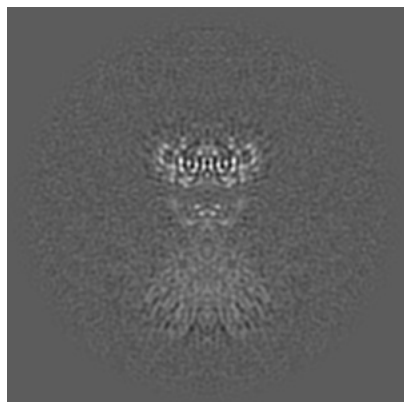


Z

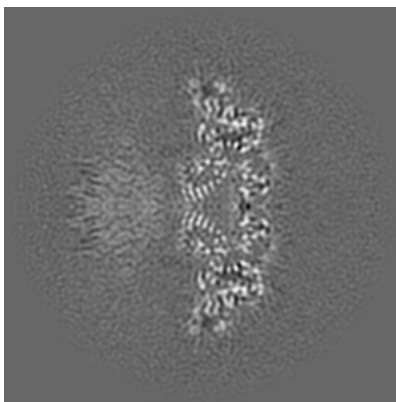
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

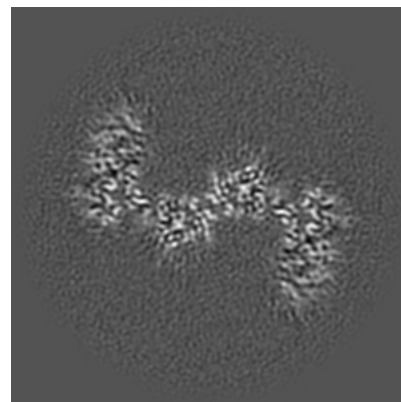
6.2.1 Primary map



X Index: 256

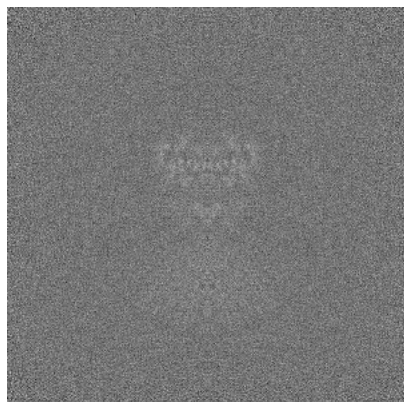


Y Index: 256

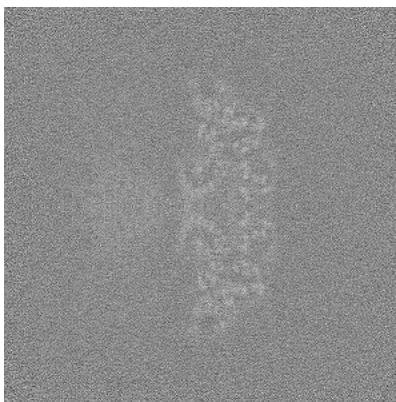


Z Index: 256

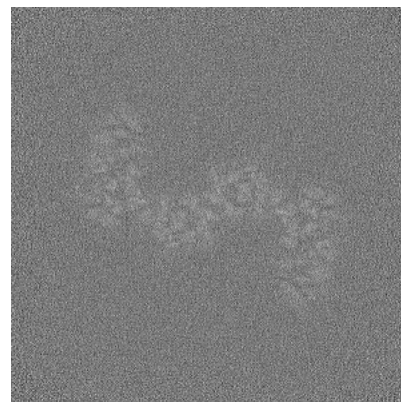
6.2.2 Raw map



X Index: 256



Y Index: 256

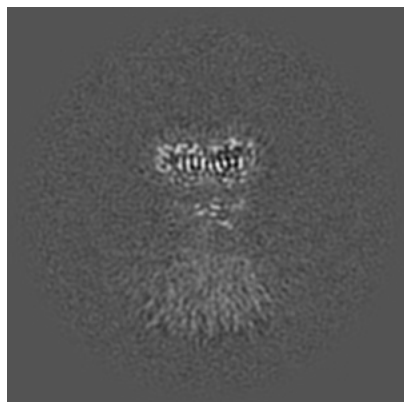


Z Index: 256

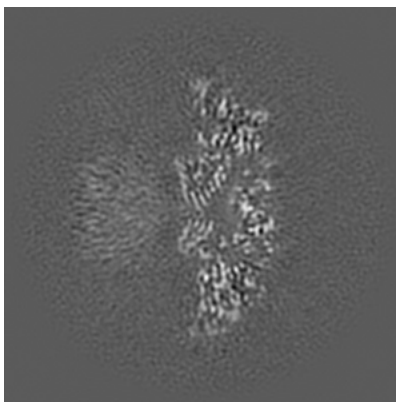
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

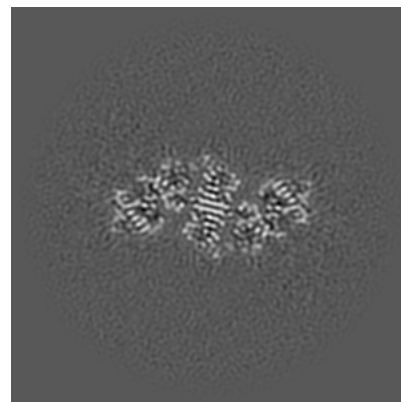
6.3.1 Primary map



X Index: 259

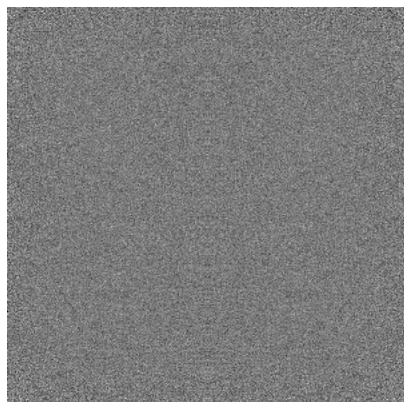


Y Index: 261

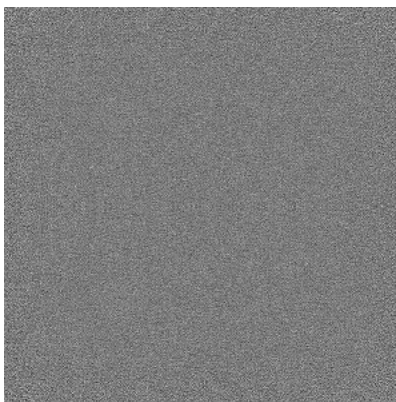


Z Index: 309

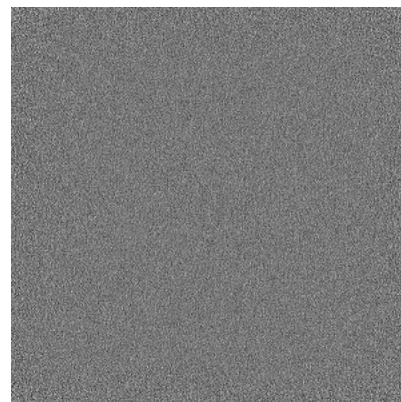
6.3.2 Raw map



X Index: 0



Y Index: 0

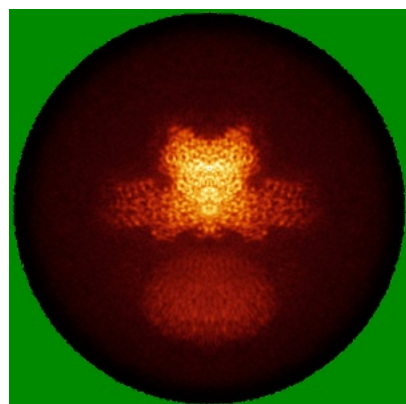


Z Index: 0

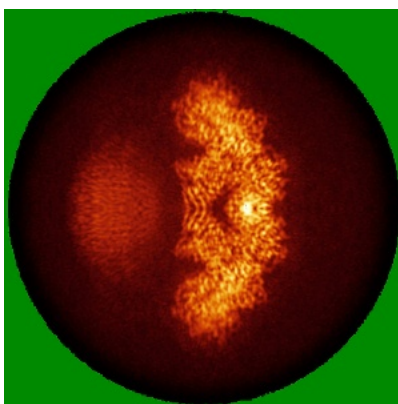
The images above show the largest variance slices of the map in three orthogonal directions.

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

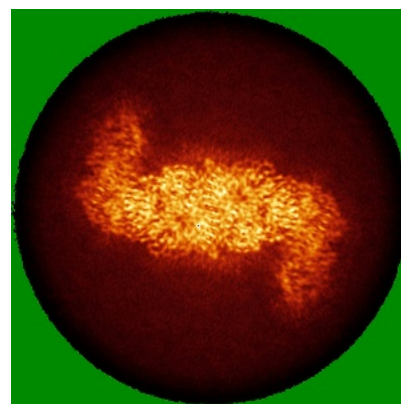
6.4.1 Primary map



X

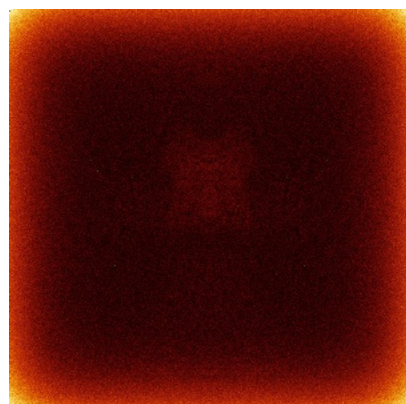


Y

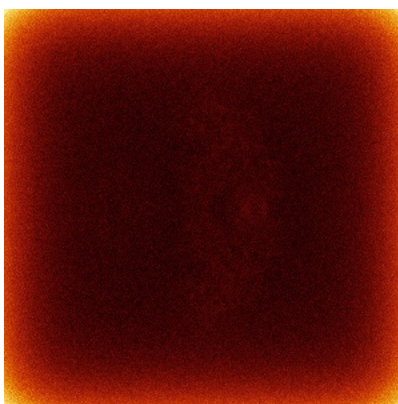


Z

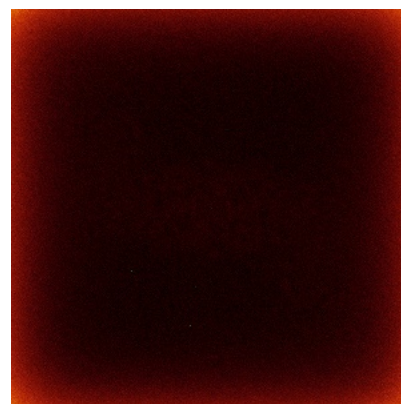
6.4.2 Raw map



X



Y

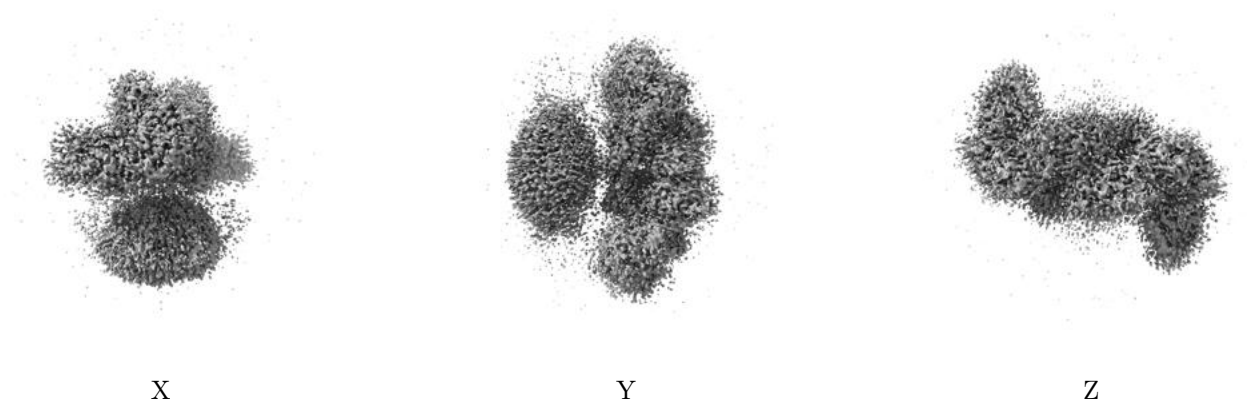


Z

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.

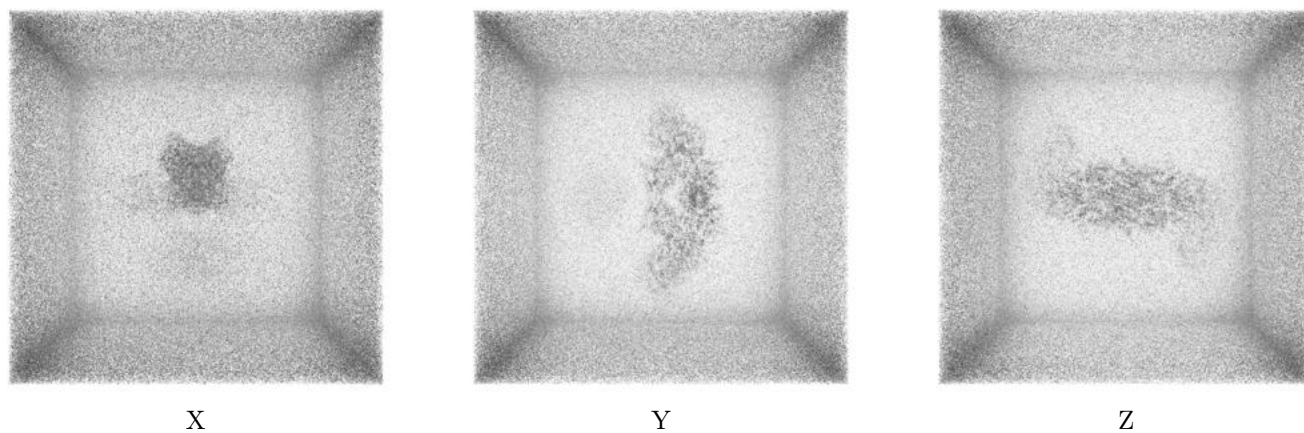
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0229. 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.

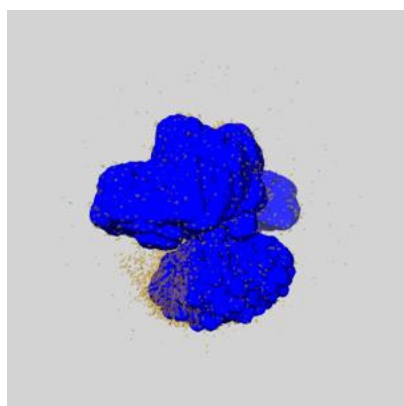
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

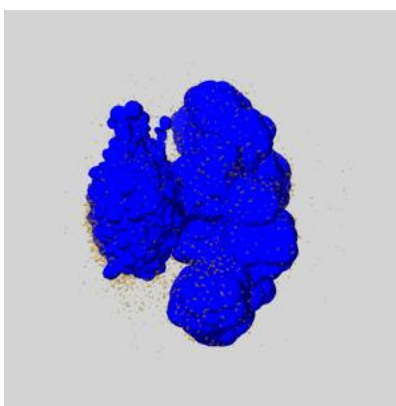
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

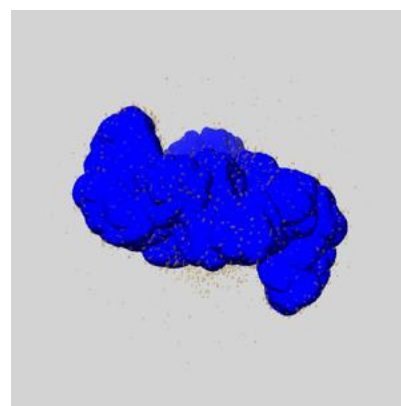
6.6.1 emd_45812_msk_1.map [i](#)



X



Y

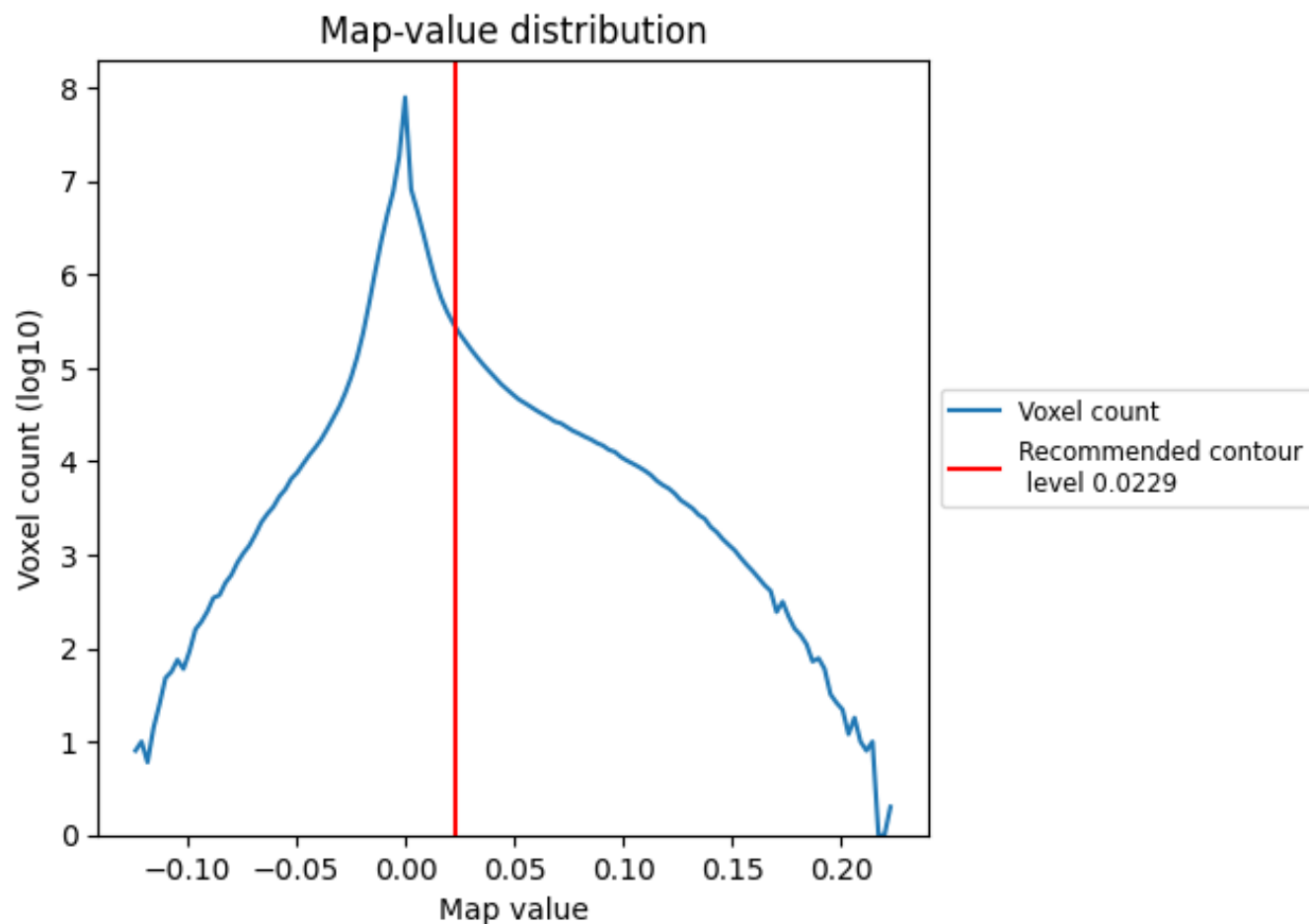


Z

7 Map analysis [i](#)

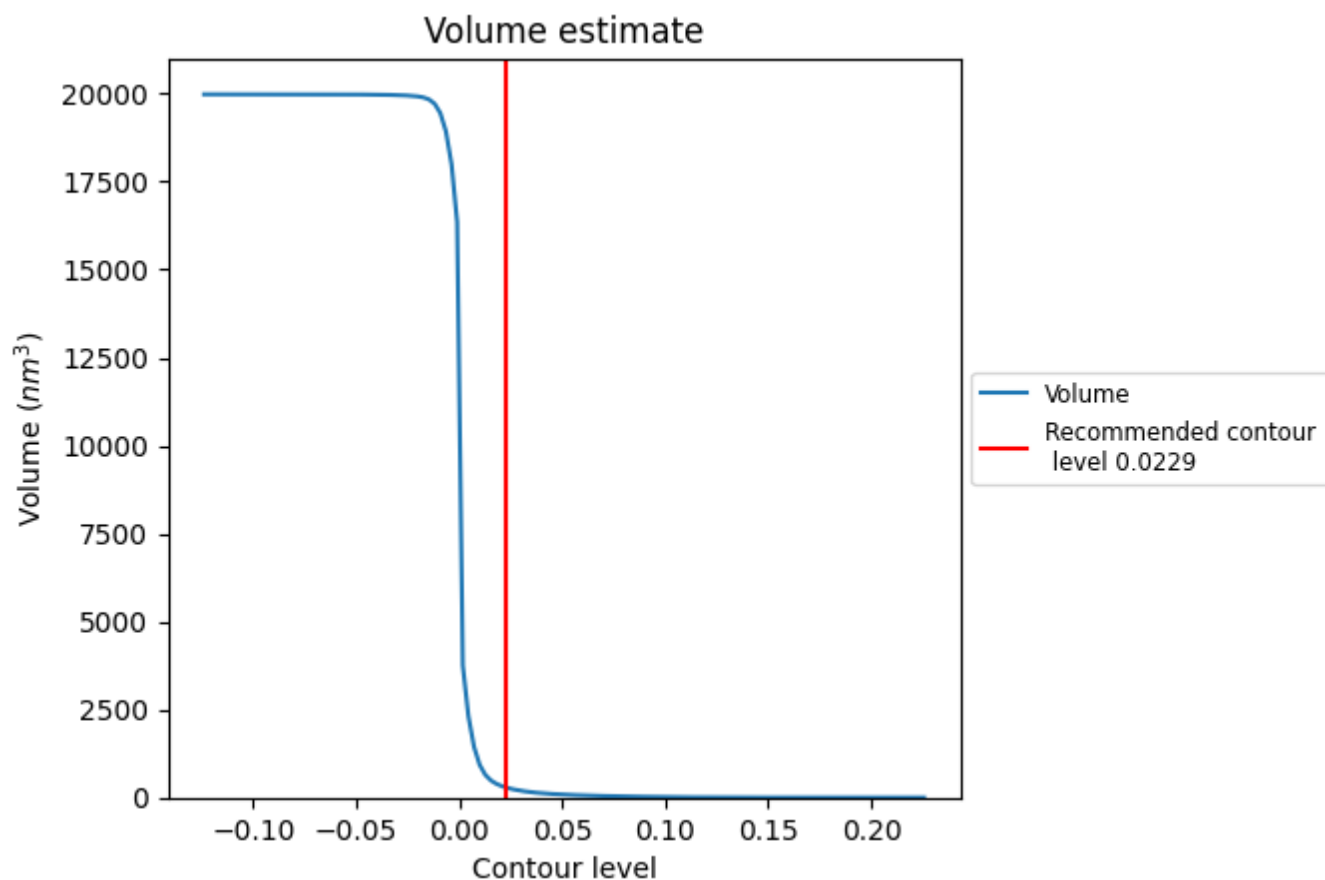
This section contains the results of statistical analysis of the map.

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.

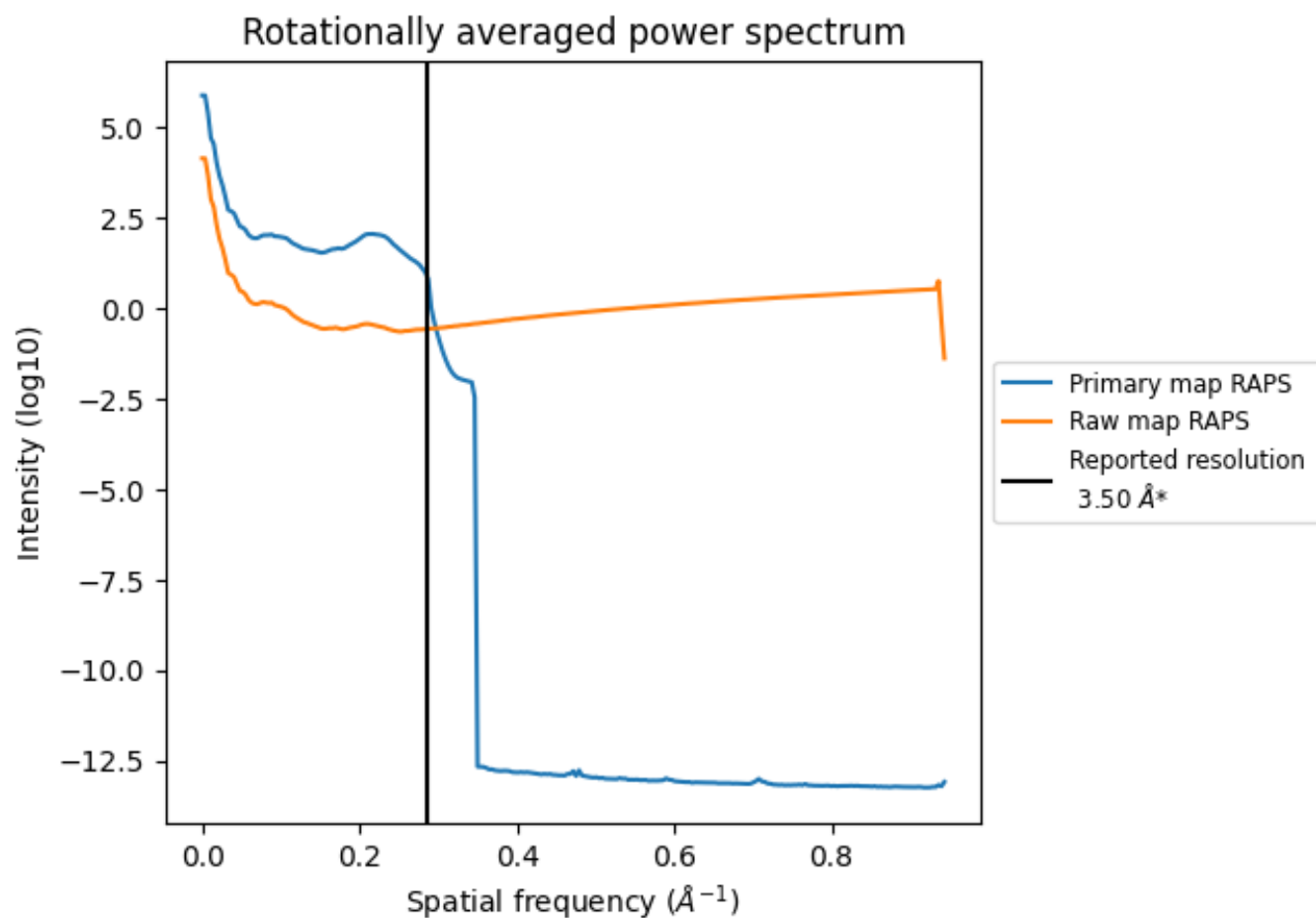
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 284 nm³; this corresponds to an approximate mass of 256 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 ⓘ

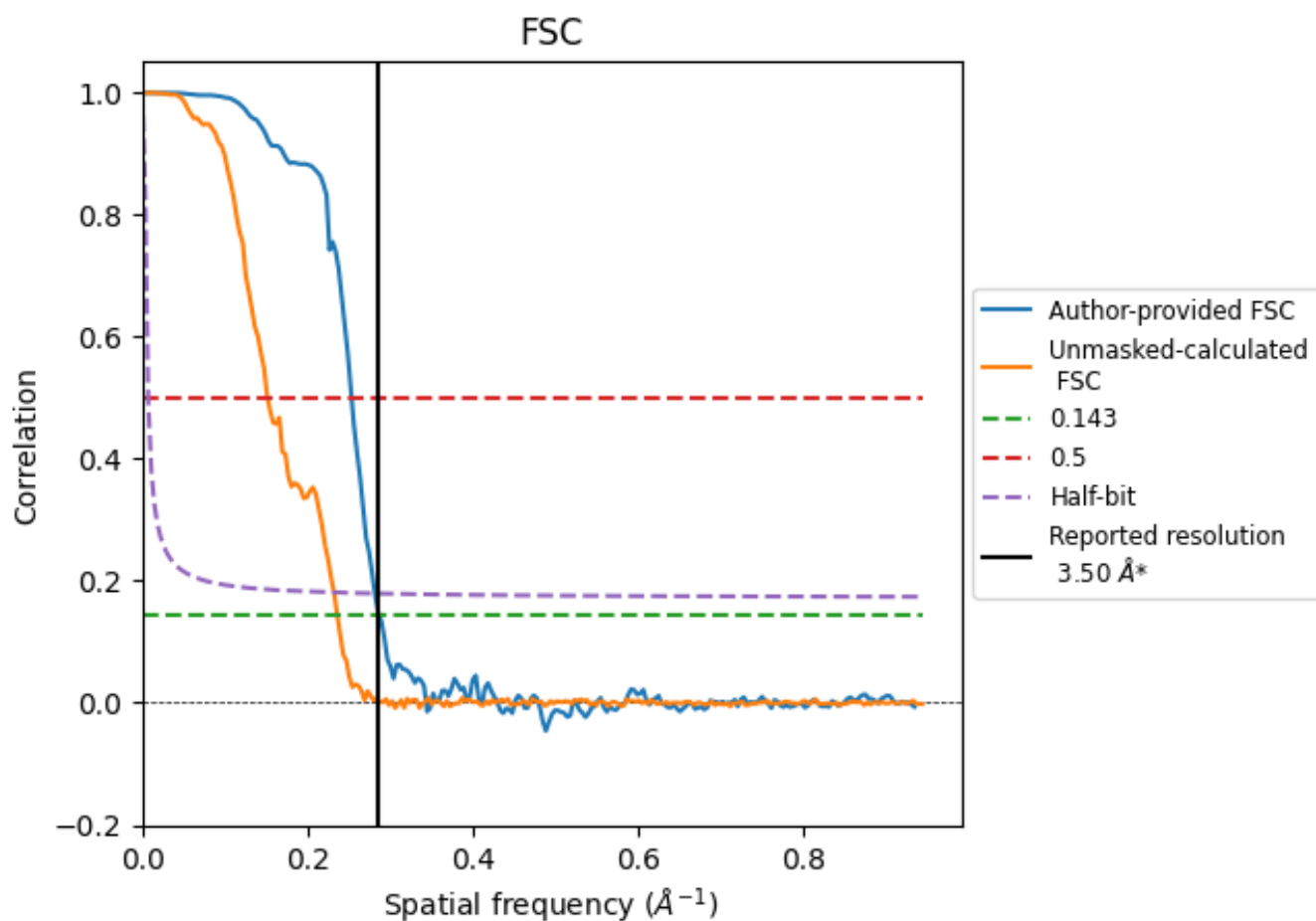


*Reported resolution corresponds to spatial frequency of 0.286 Å⁻¹

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 $0.286 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

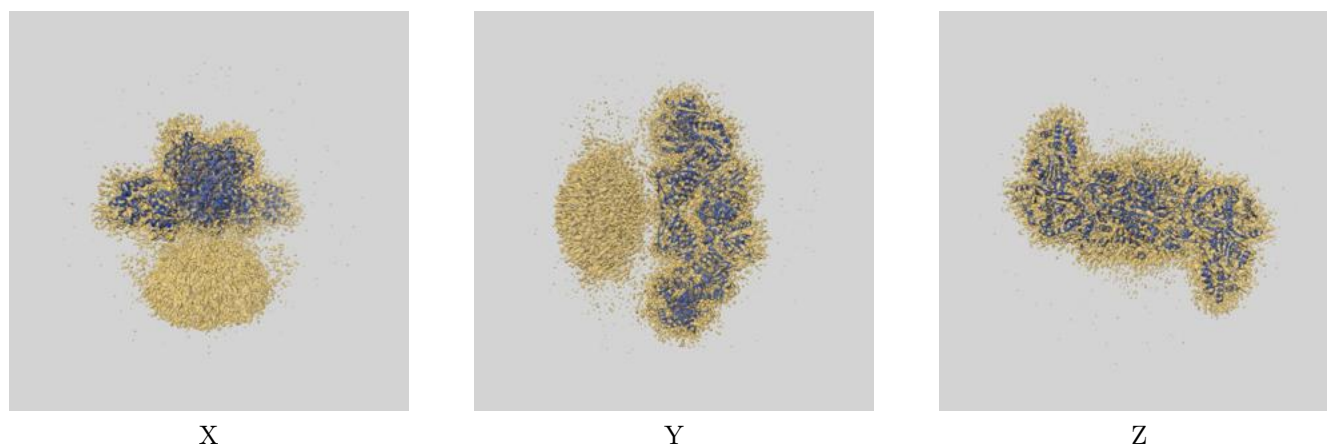
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.50	-	-
Author-provided FSC curve	3.49	3.95	3.55
Unmasked-calculated*	4.24	6.60	4.31

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.24 differs from the reported value 3.5 by more than 10 %

9 Map-model fit [i](#)

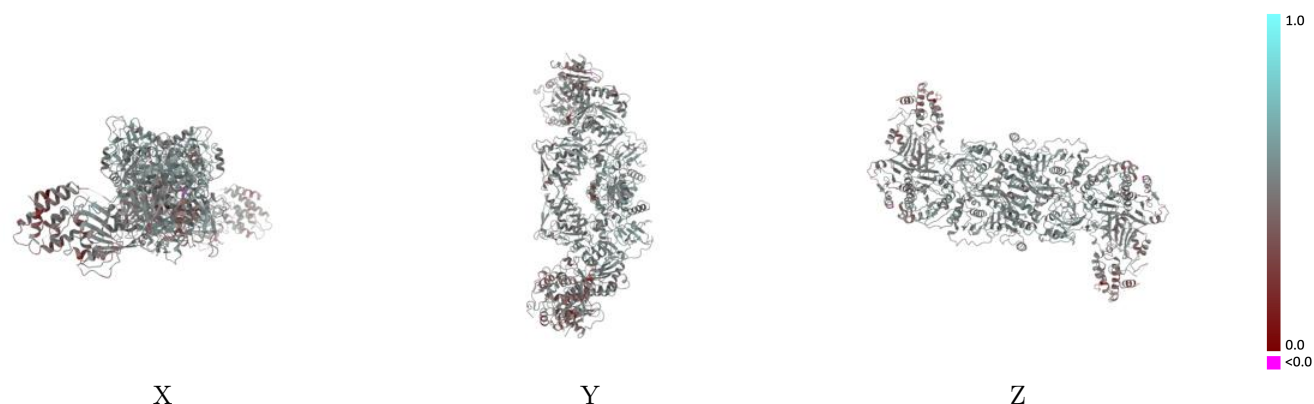
This section contains information regarding the fit between EMDB map EMD-45812 and PDB model 9CQ9. Per-residue inclusion information can be found in [section 3](#) on [page 4](#).

9.1 Map-model overlay [i](#)



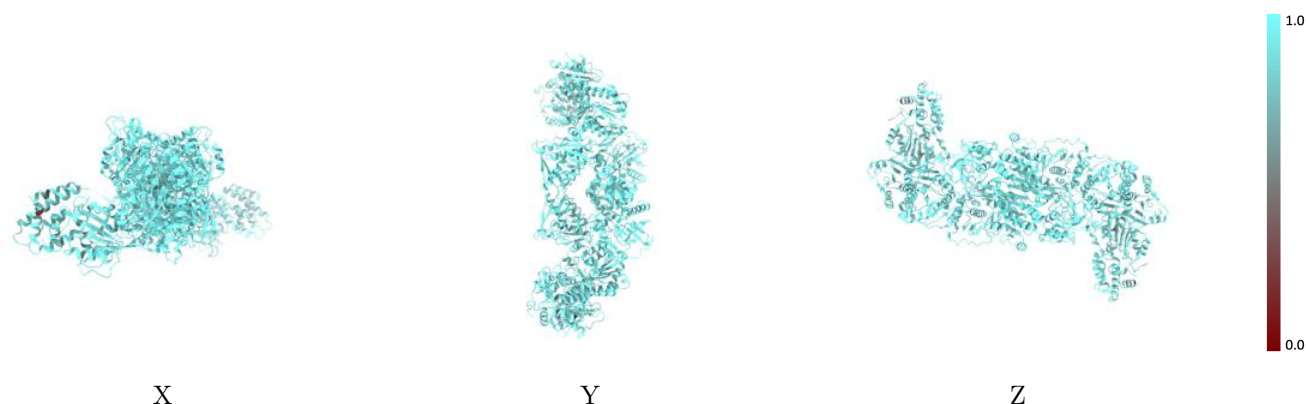
The images above show the 3D surface view of the map at the recommended contour level 0.0229 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



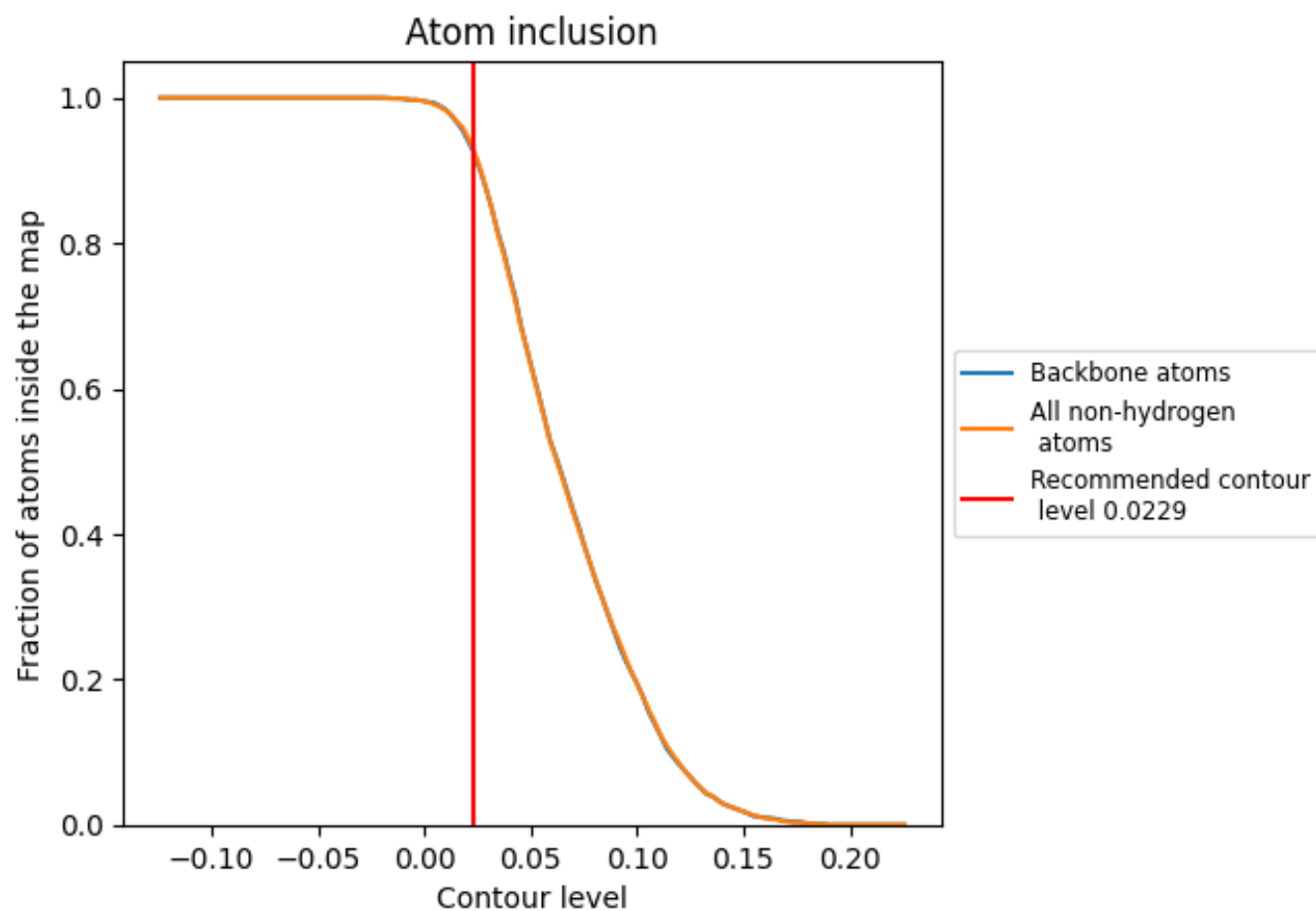
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0229).

9.4 Atom inclusion [i](#)



At the recommended contour level, 93% of all backbone atoms, 93% 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 (0.0229) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9310	0.4880
A	0.9290	0.4880
B	0.9290	0.4890

