



Full wwPDB EM Validation Report ⓘ

Apr 25, 2026 – 10:23 PM EDT

PDB ID : 9PWQ / pdb_00009pwq
EMDB ID : EMD-71938
Title : Cryo-EM structure of receptor tyrosine kinase ROS1 extracellular domain in complex with NELL2
Authors : Li, H.; Klein, D.
Deposited on : 2025-08-05
Resolution : 4.45 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
Mogul : 2022.3.0, CSD as543be (2022)
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

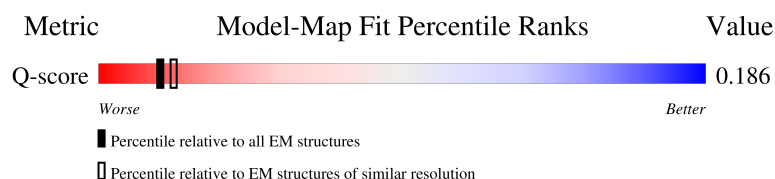
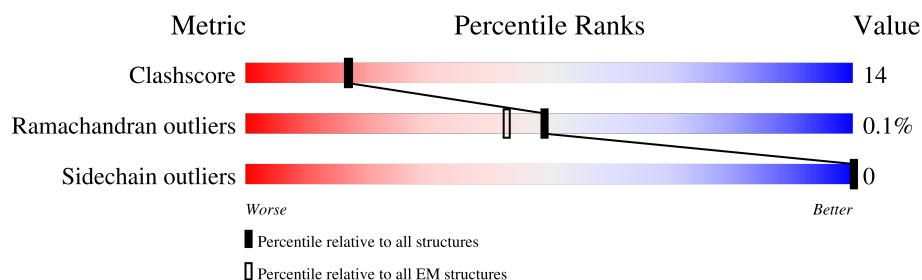
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.45 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	3027 (3.95 - 4.95)

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	1853	 56% 27% 17%
2	B	830	 18% 8% 74%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 14039 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 Proto-oncogene tyrosine-protein kinase ROS.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1542	Total	C	N	O	S	0	0
			12242	7896	2006	2291	49		

There are 34 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1848	GLY	-	expression tag	UNP Q78DX7
A	1849	GLY	-	expression tag	UNP Q78DX7
A	1850	GLY	-	expression tag	UNP Q78DX7
A	1851	SER	-	expression tag	UNP Q78DX7
A	1852	SER	-	expression tag	UNP Q78DX7
A	1853	ALA	-	expression tag	UNP Q78DX7
A	1854	TRP	-	expression tag	UNP Q78DX7
A	1855	SER	-	expression tag	UNP Q78DX7
A	1856	HIS	-	expression tag	UNP Q78DX7
A	1857	PRO	-	expression tag	UNP Q78DX7
A	1858	GLN	-	expression tag	UNP Q78DX7
A	1859	PHE	-	expression tag	UNP Q78DX7
A	1860	GLU	-	expression tag	UNP Q78DX7
A	1861	LYS	-	expression tag	UNP Q78DX7
A	1862	GLY	-	expression tag	UNP Q78DX7
A	1863	GLY	-	expression tag	UNP Q78DX7
A	1864	GLY	-	expression tag	UNP Q78DX7
A	1865	SER	-	expression tag	UNP Q78DX7
A	1866	GLY	-	expression tag	UNP Q78DX7
A	1867	GLY	-	expression tag	UNP Q78DX7
A	1868	GLY	-	expression tag	UNP Q78DX7
A	1869	SER	-	expression tag	UNP Q78DX7
A	1870	GLY	-	expression tag	UNP Q78DX7
A	1871	GLY	-	expression tag	UNP Q78DX7
A	1872	SER	-	expression tag	UNP Q78DX7
A	1873	ALA	-	expression tag	UNP Q78DX7
A	1874	TRP	-	expression tag	UNP Q78DX7
A	1875	SER	-	expression tag	UNP Q78DX7

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1876	HIS	-	expression tag	UNP Q78DX7
A	1877	PRO	-	expression tag	UNP Q78DX7
A	1878	GLN	-	expression tag	UNP Q78DX7
A	1879	PHE	-	expression tag	UNP Q78DX7
A	1880	GLU	-	expression tag	UNP Q78DX7
A	1881	LYS	-	expression tag	UNP Q78DX7

- Molecule 2 is a protein called Protein kinase C-binding protein NELL2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	213	Total	C	N	O	S	0	0
			1657	1000	290	332	35		

There are 35 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	817	GLY	-	expression tag	UNP Q99435
B	818	GLY	-	expression tag	UNP Q99435
B	819	GLY	-	expression tag	UNP Q99435
B	820	GLY	-	expression tag	UNP Q99435
B	821	SER	-	expression tag	UNP Q99435
B	822	SER	-	expression tag	UNP Q99435
B	823	ALA	-	expression tag	UNP Q99435
B	824	TRP	-	expression tag	UNP Q99435
B	825	SER	-	expression tag	UNP Q99435
B	826	HIS	-	expression tag	UNP Q99435
B	827	PRO	-	expression tag	UNP Q99435
B	828	GLN	-	expression tag	UNP Q99435
B	829	PHE	-	expression tag	UNP Q99435
B	830	GLU	-	expression tag	UNP Q99435
B	831	LYS	-	expression tag	UNP Q99435
B	832	GLY	-	expression tag	UNP Q99435
B	833	GLY	-	expression tag	UNP Q99435
B	834	GLY	-	expression tag	UNP Q99435
B	835	SER	-	expression tag	UNP Q99435
B	836	GLY	-	expression tag	UNP Q99435
B	837	GLY	-	expression tag	UNP Q99435
B	838	GLY	-	expression tag	UNP Q99435
B	839	SER	-	expression tag	UNP Q99435
B	840	GLY	-	expression tag	UNP Q99435
B	841	GLY	-	expression tag	UNP Q99435
B	842	SER	-	expression tag	UNP Q99435

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Chain	Residue	Modelled	Actual	Comment	Reference
B	843	ALA	-	expression tag	UNP Q99435
B	844	TRP	-	expression tag	UNP Q99435
B	845	SER	-	expression tag	UNP Q99435
B	846	HIS	-	expression tag	UNP Q99435
B	847	PRO	-	expression tag	UNP Q99435
B	848	GLN	-	expression tag	UNP Q99435
B	849	PHE	-	expression tag	UNP Q99435
B	850	GLU	-	expression tag	UNP Q99435
B	851	LYS	-	expression tag	UNP Q99435

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				AltConf
3	A	1	Total	C	N	O	0
			14	8	1	5	
3	A	1	Total	C	N	O	0
			14	8	1	5	
3	A	1	Total	C	N	O	0
			14	8	1	5	
3	A	1	Total	C	N	O	0
			14	8	1	5	
3	A	1	Total	C	N	O	0
			14	8	1	5	

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Mol	Chain	Residues	Atoms				AltConf
3	A	1	Total	C	N	O	0
			14	8	1	5	
3	A	1	Total	C	N	O	0
			14	8	1	5	
3	A	1	Total	C	N	O	0
			14	8	1	5	
3	A	1	Total	C	N	O	0
			14	8	1	5	

Q962	S1049	S1154	H1268	D1385	V1525	L1611	LYS
1963	S1050	L1155	T1269	D1385	V1525	S1612	TRP
1964	G1051	N1158	T1270	I1389	K1526	L1613	LYS
W965	E1068	K1159	I1271	Y1390	N1527	L1614	TRP
	V1059	I1160	I1272	W1391	Y1528	L1615	GLY
P968	W1060	V1161	P1276	I1392	S1530	T1616	PHE
Y978	V1061	F1162		I1401	E1531	T1617	TRP
S979	E1062	L1163	V1288	Y1402	E1534	L1617	HIS
Y980	E1062	D1164	S1289	Q1403		G1620	VAL
E981	P1068	Q1167	D1290	V1415	Q1545		ALA
	E1071	N1168	L1291	I1423	T1546	L1623	SER
T984	N1072	Q1169	H1292	L1424	K1547		CYS
	L1075	L1171	Q1294	A1425	S1548	M1626	SER
E992	F1078	D1179	M1295	Y1426	P1551	K1627	GLN
Q994	I1084	V1183	Y1297	S1427	G1552	P1633	GLY
P997	S1085	T1187	T1304	S1428	A1553	E1634	VAL
F998	P1104	D1188	Q1305	A1429	T1557	S1641	ALA
T1000	L1111	D1189	Q1306	L1430	N1558	H1642	ASN
		F1194	V1307	K1436	A1559	P1643	ILE
G1003	S1115	A1195	V1308	L1439	T1560	H1647	THR
L1004	P1116	L1200	S1314	D1444	V1561	D1650	THR
E1005	E1117	R1206	N1315	M1445	L1562	THR	GLN
Y1007	Y1118	V1219	Q1316	V1446	T1565	GLU	PRO
T1008	T1119	F1122	R1319	A1447	S1566	GLY	THR
L1009	V1120	R1222	C1322	A1448	L1567	LYS	SER
F1010	A1121	I1230	L1331	T1449	H1568	PRO	PRO
S1013	F1122	I1231	L1332	A1450	V1569	VAL	ALA
V1014	R1125	A1231	S1332	L1451	T1572	PRO	VAL
T1015	V1126	R1232	G1333	Y1452		ASN	VAL
P1016	F1127	H1233	D1337	A1453	P1580	THR	VAL
Y1017	T1128	L1234	V1338	T1454	K1581	GLU	VAL
	P1132	K1239	R1344	T1459	E1582	THR	THR
W1020	G1133	K1247	P1345	L1460	S1583	LEU	THR
S1027	P1134	F1135	I1347	V1465	V1584	GLN	GLY
A1032	F1138	I1249	Y1348	S1479	V1589	LEU	GLY
P1033	V1139	N1249	F1349	M1486	M1590	ASP	ASN
E1034	M1140	V1250	T1350	E1487	L1593	TRP	ASN
S1035	S1141	D1251	K1351	A1488	A1594	ALA	SER
V1036	K1142	L1252	R1352	N1489	P1595	ARG	ILE
P1037	T1143	E1253	Q1353	R1496	E1598	SER	PRO
S1038	S1144	H1254	A1357	R1497	T1599	VAL	GLY
A1039	E1145	K1257	I1369	H1498	P1600	GLU	SER
P1040	I1146	R1260	M1370	Q1504	L1601	THR	VAL
E1041	K1147	E1261	V1371	F1516	G1604	PHE	PHE
R1044	P1148	V1262	P1375	I1521	E1605	GLU	GLY
I1045	Y1151	L1152	I1379		F1606	LEU	VAL
F1046	L1152	I1153			P1607	GLN	GLY
I1048	I1153				S1608	THR	CYS
					A1609	LEU	SER
					K1610	GLN	

● Molecule 2: Protein kinase C-binding protein NELL2

Chain B:  18% 8% 74%

LEU	ARG	PRO	LYS
GLY	ASN	TYR	GLY
VAL	LYS	ILE	ILE
ASP	HIS	LEU	MET
PRO	GLU	ALA	GLN
SER	PHE	ASP	ASP
LEU	THR	ASP	VAL
GLN	ILE	LYS	GLN
ILE	LEU	TRP	LEU
ASP	VAL	HIS	LEU
VAL	THR	LYS	VAL
LEU	LEU	LEU	MET
THR	LYS	SER	PRO
GLU	GLN	LEU	GLN
LEU	THR	ALA	GLY
GLU	HIS	ILE	PHE
LEU	LEU	SER	ILE
GLY	ASN	ALA	ALA
GLU	SER	SER	GLN
SER	GLY	HIS	CYS
THR	VAL	LEU	PRO
THR	ILE	ILE	ASP
GLY	LEU	LEU	LEU
VAL	SER	HIS	ASN
ARG	ILE	ILE	ARG
GLN	HIS	ASP	THR
VAL	HIS	CYS	CYS
PRO	LEU	ASN	PRO
GLY	ASP	LYS	THR
LEU	HIS	ILE	CYS
ASN	ARG	TYR	ASN
HIS	THR	GLU	ASP
GLY	LEU	ARG	PHE
THR	GLU	VAL	HIS
LYS	LEU	VAL	GLY
ALA	GLU	GLU	LEU
PHE	SER	LYS	VAL
LEU	GLY	PRO	GLN
GLN	THR	THR	ILE
ASP	ARG	ASP	MET
THR	ASN	LEU	LEU
THR	GLU	PRO	LEU
PRO	VAL	LEU	GLN
ARG	SER	GLY	ASP
ILE	LEU	THR	ILE
LYS	HIS	THR	LEU
ALA	THR	PHE	ALA
SER	TTR	THR	LYS
ALA	ARG	GLY	THR
THR	THR	LEU	SER
ALA	GLY	GLY	THR
THR	SER	GLN	ALA
ALA	HIS	ARG	LYS
GLU	ARG	ASN	LEU
GLN	PRO	ASN	SER
PHE	HIS	ALA	ARG
THR	THR	HIS	PHE
GLN	GLU	GLY	GLN
LYS	VAL	TYR	LYS



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	59436	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 ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.478	Depositor
Minimum map value	-0.316	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.0248	Depositor
Map size (Å)	532.48, 532.48, 532.48	wwPDB
Map dimensions	640, 640, 640	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: NAG

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	0/12595	0.31	0/17178
2	B	0.11	0/1685	0.34	0/2268
All	All	0.11	0/14280	0.32	0/19446

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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	406	ASN	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	12242	0	12006	342	0
2	B	1657	0	1524	50	0
3	A	140	0	130	2	0
All	All	14039	0	13660	385	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 14.

All (385) 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:320:ALA:HB3	2:B:331:LYS:HD3	1.62	0.80
1:A:682:LEU:HB2	1:A:696:LEU:HB2	1.66	0.78
2:B:400:PHE:HB2	2:B:420:ALA:HB2	1.67	0.76
2:B:428:PHE:HB3	2:B:438:CYS:HB3	1.67	0.76
1:A:488:MET:SD	1:A:499:ARG:NH1	2.58	0.75
1:A:471:LYS:NZ	1:A:514:CYS:O	2.20	0.74
1:A:115:PRO:HD2	1:A:193:SER:HB3	1.70	0.73
2:B:294:CYS:HA	2:B:303:CYS:HA	1.70	0.73
1:A:711:ASN:HA	1:A:727:LEU:HB2	1.71	0.73
1:A:177:ARG:HH22	1:A:189:TYR:HA	1.53	0.72
1:A:382:ILE:HG22	1:A:393:PHE:HB2	1.71	0.72
1:A:1046:PHE:HB2	1:A:1062:GLU:HB3	1.71	0.72
1:A:613:GLN:NE2	1:A:642:THR:OG1	2.24	0.70
1:A:1304:THR:HB	1:A:1306:GLN:HE22	1.56	0.70
1:A:305:LEU:HD21	1:A:540:VAL:HG21	1.74	0.70
1:A:1319:ARG:NH1	1:A:1322:CYS:SG	2.65	0.69
2:B:329:GLU:HB2	2:B:331:LYS:HZ1	1.57	0.69
2:B:300:THR:HG22	2:B:301:ILE:H	1.57	0.69
1:A:303:LEU:HD13	1:A:520:LEU:HD22	1.75	0.69
2:B:452:ARG:HB3	2:B:479:SER:HB2	1.74	0.69
1:A:907:GLN:NE2	1:A:909:THR:OG1	2.26	0.68
1:A:242:LEU:HB3	1:A:249:LEU:HB2	1.75	0.68
1:A:1004:LEU:HD22	1:A:1008:THR:HG21	1.75	0.68
1:A:331:ILE:HG23	1:A:351:GLU:HG3	1.75	0.68
1:A:1152:LEU:HD21	1:A:1390:TYR:CD2	2.29	0.68
1:A:829:VAL:HG22	1:A:845:VAL:HG22	1.76	0.67
1:A:325:CYS:H	1:A:363:MET:HE2	1.60	0.67
2:B:452:ARG:HG3	2:B:453:GLU:H	1.58	0.67
1:A:357:MET:SD	1:A:370:ARG:NH1	2.68	0.66
1:A:835:ASP:HB3	1:A:840:LEU:H	1.60	0.66
1:A:1289:SER:HB3	1:A:1294:GLN:HE22	1.60	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1531:GLU:HB2	1:A:1534:GLU:HB2	1.76	0.66
1:A:572:GLN:HE22	1:A:591:ALA:H	1.43	0.66
1:A:458:ARG:HD3	1:A:461:GLU:HB3	1.77	0.66
1:A:673:PHE:HD2	1:A:675:MET:HE3	1.61	0.66
1:A:1006:PRO:HG3	1:A:1072:ASN:H	1.61	0.66
1:A:746:ALA:HB1	1:A:788:MET:HB2	1.79	0.65
1:A:252:GLY:H	2:B:419:ARG:NH2	1.96	0.64
1:A:981:GLU:HB2	1:A:1013:SER:HB2	1.79	0.64
1:A:408:SER:OG	1:A:409:ASN:N	2.31	0.63
1:A:1232:ARG:HB3	1:A:1252:LEU:HB2	1.80	0.63
1:A:605:THR:HG23	1:A:648:SER:HB2	1.80	0.63
1:A:465:LEU:HA	1:A:480:PHE:HE1	1.63	0.63
1:A:805:VAL:HG23	1:A:818:LEU:HB2	1.80	0.63
2:B:410:ASN:HB3	2:B:438:CYS:HB2	1.79	0.63
1:A:313:LYS:NZ	1:A:360:ALA:O	2.31	0.63
1:A:814:SER:O	1:A:859:ARG:NH2	2.32	0.63
1:A:1516:PHE:N	1:A:1546:THR:OG1	2.32	0.62
2:B:296:CYS:HB2	2:B:302:GLN:HB2	1.81	0.62
1:A:342:ALA:HB2	1:A:563:GLN:HE21	1.64	0.62
1:A:1234:LEU:HB3	1:A:1250:VAL:HB	1.80	0.62
1:A:381:SER:HB3	1:A:394:ILE:HD12	1.82	0.62
1:A:122:SER:HA	1:A:199:HIS:HB2	1.80	0.61
1:A:1127:PHE:HA	1:A:1132:PRO:HA	1.82	0.61
1:A:438:ARG:NH2	1:A:463:GLY:O	2.33	0.61
1:A:767:ARG:HH11	1:A:778:VAL:HG22	1.66	0.61
1:A:314:ARG:HG2	1:A:538:PHE:HE2	1.66	0.61
1:A:756:LEU:HD23	1:A:770:VAL:HG12	1.83	0.60
1:A:585:ILE:HD11	1:A:630:LEU:HD23	1.84	0.60
1:A:673:PHE:CD2	1:A:675:MET:HE3	2.37	0.60
1:A:222:GLU:HG2	1:A:259:GLN:HG3	1.84	0.60
1:A:723:TYR:HB3	1:A:735:ASN:HB2	1.83	0.60
1:A:828:LYS:NZ	1:A:829:VAL:O	2.35	0.59
1:A:1253:GLU:HG3	1:A:1528:TYR:HB2	1.83	0.59
2:B:295:THR:N	2:B:302:GLN:O	2.34	0.59
2:B:329:GLU:HB2	2:B:331:LYS:NZ	2.18	0.59
1:A:1293:HIS:ND1	1:A:1331:LEU:O	2.36	0.58
1:A:1006:PRO:HG3	1:A:1072:ASN:N	2.18	0.58
1:A:1272:ILE:HD11	1:A:1333:GLY:HA3	1.84	0.58
1:A:1195:ALA:HA	1:A:1200:LEU:HA	1.85	0.58
1:A:243:ILE:HG13	1:A:270:ARG:HH21	1.68	0.58
1:A:1047:ILE:H	1:A:1148:PRO:HG3	1.68	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:283:GLU:HA	2:B:299:GLY:HA3	1.85	0.58
1:A:239:ASN:HB2	1:A:274:ALA:HB3	1.85	0.57
1:A:1167:GLN:NE2	1:A:1169:GLN:OE1	2.36	0.57
1:A:459:ILE:HD11	1:A:493:ASP:C	2.29	0.57
1:A:312:ARG:NH2	1:A:548:GLU:OE2	2.37	0.57
1:A:177:ARG:NH2	1:A:179:VAL:HG22	2.19	0.57
1:A:340:VAL:HG23	1:A:347:VAL:HG12	1.87	0.57
1:A:259:GLN:NE2	1:A:260:PHE:O	2.38	0.57
1:A:1117:GLU:HA	1:A:1144:SER:HB3	1.86	0.57
1:A:1344:ARG:HD2	1:A:1344:ARG:O	2.05	0.57
1:A:1385:ASP:HA	1:A:1430:LEU:HD11	1.86	0.57
1:A:608:VAL:HG22	1:A:645:VAL:HG22	1.87	0.57
1:A:142:GLN:HB3	1:A:177:ARG:HG3	1.86	0.57
1:A:252:GLY:O	2:B:419:ARG:NH2	2.38	0.57
1:A:716:SER:HB3	1:A:722:VAL:HG22	1.85	0.56
1:A:871:PHE:HD2	1:A:908:ARG:HH22	1.52	0.56
1:A:669:THR:OG1	1:A:670:GLU:N	2.37	0.56
1:A:980:VAL:HG22	1:A:1014:VAL:HG22	1.88	0.56
1:A:177:ARG:HH12	1:A:189:TYR:HB3	1.71	0.56
1:A:391:MET:N	1:A:402:CYS:O	2.36	0.56
1:A:1551:PRO:HG3	1:A:1584:VAL:HG13	1.87	0.55
1:A:706:MET:HE1	1:A:921:GLN:HB3	1.87	0.55
1:A:951:SER:O	1:A:953:ARG:NH1	2.39	0.55
1:A:265:PRO:HG2	1:A:294:PRO:HG3	1.87	0.55
1:A:547:ILE:HG12	2:B:368:LEU:HD22	1.89	0.55
1:A:691:GLY:HA2	1:A:916:PRO:HD2	1.88	0.55
1:A:242:LEU:HD11	1:A:269:TYR:HB3	1.88	0.55
1:A:301:GLN:NE2	1:A:518:ASP:OD2	2.39	0.55
1:A:738:ILE:HG22	1:A:740:SER:H	1.71	0.55
1:A:1239:LYS:HD2	1:A:1270:THR:HG23	1.89	0.55
1:A:1353:GLN:HG3	1:A:1371:VAL:HB	1.89	0.55
1:A:979:SER:HB2	1:A:1017:TYR:HE2	1.71	0.55
2:B:425:ARG:HE	2:B:428:PHE:HE2	1.54	0.55
1:A:1068:PRO:HG2	1:A:1071:GLU:HG2	1.89	0.54
1:A:566:PRO:HB2	1:A:604:TRP:HH2	1.72	0.54
1:A:684:SER:HB3	1:A:694:GLU:HB3	1.88	0.54
1:A:750:GLU:OE1	1:A:757:TYR:OH	2.23	0.54
1:A:247:GLN:OE1	1:A:269:TYR:OH	2.20	0.54
1:A:512:PHE:HB2	1:A:521:ILE:HG22	1.89	0.54
1:A:978:TYR:HB2	1:A:994:GLN:HG3	1.89	0.54
1:A:142:GLN:N	1:A:177:ARG:O	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:415:PRO:HG2	1:A:418:LEU:HB2	1.88	0.54
1:A:803:TYR:HH	1:A:823:TRP:CD1	2.25	0.54
1:A:841:LEU:N	1:A:856:ALA:O	2.39	0.54
1:A:697:SER:OG	1:A:699:ASP:OD2	2.25	0.54
1:A:959:SER:O	1:A:1003:GLY:N	2.37	0.54
2:B:395:CYS:SG	2:B:396:LYS:N	2.82	0.53
1:A:1557:ILE:HG21	1:A:1626:MET:HE1	1.91	0.53
1:A:115:PRO:HB2	1:A:127:LEU:HD12	1.91	0.53
1:A:789:ALA:HB3	1:A:798:TYR:HB2	1.91	0.53
1:A:1126:VAL:O	1:A:1133:GLY:N	2.41	0.53
1:A:177:ARG:NH2	1:A:189:TYR:HA	2.23	0.52
1:A:1295:MET:HB3	1:A:1308:VAL:HB	1.91	0.52
1:A:1045:ILE:HD13	1:A:1120:VAL:HG23	1.91	0.52
1:A:1392:ILE:HD11	1:A:1423:ILE:HG23	1.91	0.52
1:A:532:SER:OG	1:A:533:LEU:N	2.40	0.52
1:A:798:TYR:HE2	1:A:858:LEU:HD12	1.73	0.52
1:A:303:LEU:HD12	1:A:557:ILE:HG12	1.91	0.52
1:A:1288:VAL:HG22	1:A:1293:HIS:HD2	1.75	0.52
1:A:342:ALA:O	1:A:345:GLN:NE2	2.43	0.52
1:A:1158:ASN:HA	1:A:1179:ASP:HA	1.90	0.52
1:A:431:GLY:HA2	1:A:446:LEU:HD23	1.90	0.52
1:A:782:LYS:HG3	1:A:783:LEU:HD12	1.92	0.52
1:A:413:ILE:HG12	1:A:447:PRO:HG3	1.92	0.52
2:B:276:MET:SD	2:B:276:MET:N	2.83	0.52
1:A:261:TYR:HB3	2:B:339:ARG:HH21	1.75	0.51
1:A:357:MET:HG3	1:A:372:PHE:HB2	1.91	0.51
1:A:979:SER:HB3	1:A:1015:THR:HB	1.91	0.51
1:A:212:ASN:OD1	1:A:224:SER:OG	2.18	0.51
1:A:340:VAL:HG21	1:A:558:PHE:CG	2.46	0.51
1:A:1125:ARG:HB3	1:A:1135:PHE:HA	1.93	0.51
1:A:211:LEU:H	1:A:225:TRP:HA	1.75	0.51
1:A:708:TRP:CG	1:A:925:ILE:HG12	2.46	0.51
1:A:233:GLY:HA3	1:A:277:ASN:HD22	1.74	0.51
1:A:1590:MET:SD	1:A:1593:LEU:HB2	2.51	0.50
2:B:318:ALA:HB3	2:B:333:ILE:HG21	1.92	0.50
1:A:1164:ASP:HB2	1:A:1171:LEU:HD21	1.93	0.50
2:B:296:CYS:HB3	2:B:300:THR:C	2.36	0.50
1:A:391:MET:SD	1:A:393:PHE:HB3	2.51	0.50
1:A:703:VAL:HA	1:A:717:ASP:HA	1.93	0.50
2:B:346:ARG:HH21	2:B:358:LEU:HD22	1.77	0.50
1:A:874:TRP:CD1	1:A:903:GLN:HE21	2.29	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:341:TYR:OH	2:B:347:ASN:ND2	2.45	0.50
1:A:306:SER:HB2	1:A:338:ILE:HD11	1.93	0.50
1:A:242:LEU:HD23	1:A:249:LEU:HD12	1.94	0.50
1:A:706:MET:HG3	1:A:715:TYR:HB3	1.94	0.50
1:A:989:LEU:HD11	1:A:999:PHE:HZ	1.76	0.50
1:A:1058:GLU:HB3	1:A:1206:ARG:HH22	1.75	0.50
1:A:267:THR:H	1:A:291:THR:HG1	1.56	0.49
1:A:406:ASN:OD1	1:A:407:CYS:N	2.44	0.49
2:B:455:THR:HA	2:B:468:CYS:HA	1.93	0.49
1:A:169:HIS:O	1:A:172:THR:OG1	2.25	0.49
1:A:1487:GLU:OE2	1:A:1489:ASN:ND2	2.45	0.49
1:A:721:ASN:ND2	1:A:723:TYR:OH	2.44	0.49
1:A:875:SER:N	1:A:903:GLN:HE22	2.09	0.49
1:A:1084:ILE:HD11	1:A:1111:LEU:HD13	1.94	0.49
2:B:410:ASN:ND2	2:B:438:CYS:O	2.37	0.49
1:A:1351:LYS:O	1:A:1353:GLN:N	2.46	0.49
2:B:387:LEU:HD11	2:B:394:VAL:HB	1.95	0.49
1:A:386:TRP:O	1:A:387:LEU:HB2	2.12	0.49
2:B:315:LEU:O	2:B:316:LYS:HG2	2.13	0.49
2:B:361:CYS:HB2	2:B:366:MET:HE1	1.95	0.49
1:A:217:SER:HB2	1:A:220:THR:OG1	2.12	0.49
1:A:1401:ILE:HB	1:A:1415:VAL:HG23	1.95	0.49
2:B:319:LEU:HB3	2:B:328:LYS:HE3	1.95	0.49
1:A:844:LEU:HD11	1:A:879:ILE:HD13	1.95	0.49
1:A:963:ILE:O	1:A:999:PHE:N	2.45	0.49
1:A:979:SER:OG	1:A:992:GLU:OE2	2.30	0.49
1:A:214:GLU:OE1	1:A:216:TRP:CD1	2.66	0.48
1:A:325:CYS:N	1:A:363:MET:HE2	2.27	0.48
1:A:1254:HIS:ND1	1:A:1504:GLN:OE1	2.46	0.48
1:A:1553:ALA:HB1	1:A:1641:SER:HA	1.95	0.48
2:B:311:PRO:HG2	2:B:319:LEU:HD11	1.94	0.48
1:A:158:VAL:HG21	1:A:163:TYR:HB2	1.95	0.48
1:A:247:GLN:NE2	1:A:262:SER:O	2.37	0.48
1:A:750:GLU:HG2	1:A:753:GLY:H	1.78	0.48
1:A:962:GLN:HG2	1:A:1000:THR:HG23	1.96	0.48
1:A:1037:PRO:HD3	1:A:1128:THR:OG1	2.13	0.48
1:A:713:LEU:N	1:A:725:ARG:O	2.42	0.48
1:A:205:GLU:HB2	1:A:230:PHE:HB3	1.96	0.47
1:A:469:ALA:HB3	1:A:478:ILE:HB	1.96	0.47
1:A:436:LEU:HA	1:A:441:ILE:HD13	1.96	0.47
1:A:573:GLU:OE1	1:A:588:THR:OG1	2.28	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1267:ALA:HB1	1:A:1271:ILE:HD11	1.95	0.47
1:A:520:LEU:HD23	1:A:527:ILE:HG21	1.96	0.47
1:A:984:THR:HG22	1:A:1010:PHE:HB3	1.96	0.47
1:A:302:TRP:CD1	1:A:313:LYS:HE2	2.49	0.47
1:A:336:THR:OG1	1:A:350:SER:OG	2.25	0.47
1:A:487:PHE:HE2	1:A:521:ILE:HG21	1.79	0.47
1:A:206:THR:HG21	1:A:229:HIS:HB2	1.97	0.47
1:A:1162:PHE:HD1	1:A:1171:LEU:HD12	1.80	0.47
1:A:1247:ILE:HG23	1:A:1262:VAL:HB	1.96	0.47
1:A:1288:VAL:HG22	1:A:1293:HIS:CD2	2.50	0.47
1:A:131:PRO:HD3	1:A:161:LEU:HD21	1.97	0.47
1:A:171:PHE:CZ	1:A:234:PRO:HD3	2.51	0.46
1:A:480:PHE:HA	1:A:487:PHE:HA	1.97	0.46
1:A:774:HIS:NE2	1:A:776:ASP:OD2	2.48	0.46
1:A:1044:ARG:NH2	1:A:1167:GLN:OE1	2.48	0.46
1:A:352:GLY:O	1:A:379:VAL:HG22	2.15	0.46
1:A:893:TRP:CZ3	1:A:895:ASN:HA	2.51	0.46
1:A:314:ARG:HD3	1:A:323:ALA:HB2	1.96	0.46
1:A:889:GLY:O	1:A:890:ARG:NH1	2.49	0.46
1:A:958:THR:HG22	1:A:1035:SER:HB2	1.97	0.46
1:A:961:PHE:CG	1:A:1033:PRO:HG2	2.50	0.46
1:A:243:ILE:HB	1:A:270:ARG:HB3	1.96	0.46
1:A:1219:VAL:HG13	1:A:1222:ILE:HD12	1.97	0.46
1:A:1251:ASP:O	1:A:1257:LYS:NZ	2.39	0.46
1:A:1385:ASP:HB3	1:A:1425:ALA:HB1	1.97	0.46
2:B:410:ASN:O	2:B:424:CYS:HB3	2.15	0.46
1:A:1436:LYS:HA	1:A:1529:TYR:CD1	2.51	0.46
2:B:291:CYS:HB2	2:B:437:TYR:CD2	2.50	0.46
1:A:1035:SER:N	1:A:1072:ASN:O	2.37	0.46
1:A:1153:ILE:HG22	1:A:1160:ILE:HD11	1.98	0.46
1:A:1337:VAL:HG22	1:A:1347:ILE:HG12	1.97	0.46
1:A:1460:LEU:HD11	1:A:1521:ILE:HD13	1.96	0.46
2:B:330:CYS:C	2:B:331:LYS:HD2	2.40	0.46
1:A:835:ASP:HB2	1:A:842:TYR:CE2	2.51	0.46
1:A:1268:HIS:CD2	1:A:1269:THR:HG23	2.50	0.46
1:A:799:TRP:HH2	1:A:808:THR:HG23	1.81	0.46
1:A:1155:LEU:HD11	1:A:1183:VAL:HG12	1.98	0.46
1:A:572:GLN:N	1:A:572:GLN:OE1	2.49	0.46
1:A:697:SER:OG	1:A:725:ARG:NH2	2.49	0.46
1:A:1251:ASP:N	1:A:1260:ARG:HH22	2.14	0.45
1:A:243:ILE:N	1:A:270:ARG:O	2.39	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1140:MET:HG3	1:A:1142:LYS:NZ	2.30	0.45
1:A:397:LYS:HB2	1:A:420:ALA:HA	1.97	0.45
2:B:288:ILE:HD12	2:B:306:LEU:HD12	1.98	0.45
1:A:144:LYS:NZ	1:A:145:TYR:O	2.40	0.45
1:A:252:GLY:H	2:B:419:ARG:HH22	1.65	0.45
1:A:926:GLN:HB3	1:A:929:LEU:HG	1.99	0.45
1:A:152:TRP:CZ3	1:A:177:ARG:HG2	2.51	0.45
1:A:506:LEU:HD13	1:A:523:ASP:HB3	1.99	0.45
1:A:844:LEU:HD22	1:A:851:ILE:HD11	1.97	0.45
1:A:751:TRP:CE2	1:A:792:SER:HB3	2.52	0.45
1:A:1051:GLY:HA3	1:A:1206:ARG:HB3	1.99	0.45
1:A:1294:GLN:HG3	1:A:1296:PHE:HE2	1.82	0.45
1:A:1487:GLU:HG2	1:A:1489:ASN:H	1.82	0.45
2:B:313:CYS:SG	2:B:319:LEU:HD22	2.56	0.45
1:A:1039:ALA:HB2	1:A:1134:PRO:HB2	1.99	0.45
1:A:1627:LYS:HE2	1:A:1643:PRO:HD3	1.99	0.45
1:A:1439:LEU:O	1:A:1527:ASN:ND2	2.45	0.45
2:B:287:TRP:HZ2	2:B:301:ILE:HG23	1.82	0.45
1:A:390:ARG:NE	1:A:403:GLU:OE2	2.50	0.44
1:A:525:LYS:HA	1:A:550:PHE:H	1.82	0.44
1:A:853:LEU:HB3	1:A:871:PHE:HB2	1.98	0.44
1:A:1010:PHE:HE1	1:A:1032:ALA:HA	1.82	0.44
1:A:171:PHE:CE2	1:A:233:GLY:HA2	2.52	0.44
1:A:278:GLU:HG2	1:A:279:VAL:HG23	1.99	0.44
1:A:1496:ARG:HD2	1:A:1496:ARG:HA	1.84	0.44
1:A:325:CYS:HB2	1:A:542:CYS:HB2	1.51	0.44
1:A:528:PHE:HD1	1:A:537:GLU:HA	1.82	0.44
2:B:287:TRP:CZ2	2:B:301:ILE:HG23	2.51	0.44
1:A:387:LEU:HD11	1:A:566:PRO:HD3	1.99	0.44
1:A:1008:THR:HB	1:A:1032:ALA:HB2	1.99	0.44
1:A:1122:PHE:O	1:A:1138:ILE:HA	2.18	0.44
1:A:140:ILE:CG2	1:A:179:VAL:HB	2.48	0.44
1:A:685:LYS:NZ	1:A:689:SER:O	2.47	0.44
1:A:962:GLN:OE1	1:A:1000:THR:OG1	2.33	0.44
1:A:1183:VAL:HG23	1:A:1194:PHE:HB3	1.99	0.44
1:A:166:GLU:O	1:A:168:LEU:N	2.46	0.44
1:A:418:LEU:HD23	1:A:437:LEU:HD21	1.98	0.44
1:A:715:TYR:OH	1:A:735:ASN:ND2	2.49	0.44
1:A:878:GLU:O	1:A:896:GLY:N	2.51	0.44
1:A:947:VAL:HG23	1:A:1016:PRO:HG3	1.99	0.44
1:A:324:HIS:HB3	1:A:363:MET:HG3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:349:PHE:CE2	1:A:356:TRP:HB2	2.53	0.44
1:A:835:ASP:HB2	1:A:842:TYR:HE2	1.83	0.44
1:A:1230:ILE:HD12	1:A:1278:PRO:HB2	1.99	0.44
1:A:883:ALA:HB2	1:A:921:GLN:NE2	2.33	0.44
1:A:1350:THR:HG21	1:A:1379:ILE:HG21	1.98	0.44
1:A:751:TRP:CD1	1:A:752:LEU:HG	2.53	0.43
1:A:942:VAL:HG21	1:A:1020:TRP:CD2	2.52	0.43
1:A:1297:TYR:HD1	1:A:1308:VAL:HG22	1.84	0.43
1:A:430:ASN:HD21	1:A:475:LYS:HG2	1.84	0.43
1:A:491:PHE:HD1	1:A:493:ASP:H	1.66	0.43
1:A:239:ASN:N	1:A:274:ALA:O	2.37	0.43
1:A:685:LYS:HE3	1:A:914:SER:HB2	2.00	0.43
1:A:1148:PRO:HG2	1:A:1151:TYR:CE2	2.53	0.43
1:A:1348:TYR:CE2	1:A:1357:ALA:HB2	2.54	0.43
1:A:1454:THR:HA	1:A:1547:LYS:HE2	2.00	0.43
2:B:358:LEU:HB2	2:B:369:VAL:HB	2.00	0.43
1:A:423:LYS:HE3	1:A:467:ASP:HB2	2.00	0.43
2:B:289:ASP:OD1	2:B:289:ASP:N	2.49	0.43
1:A:834:LEU:HD23	1:A:834:LEU:H	1.83	0.43
1:A:1338:ASP:N	1:A:1346:TRP:O	2.43	0.43
1:A:206:THR:HB	1:A:230:PHE:H	1.84	0.43
1:A:208:PRO:HG3	1:A:275:ALA:HB2	2.00	0.43
1:A:769:SER:HB3	1:A:774:HIS:H	1.82	0.43
1:A:1369:ILE:HD11	1:A:1389:ILE:HD12	2.01	0.43
2:B:450:TYR:HB2	2:B:478:TYR:CE2	2.53	0.43
1:A:979:SER:HB2	1:A:1017:TYR:CE2	2.54	0.43
1:A:1059:VAL:HG21	1:A:1143:THR:HB	2.01	0.43
1:A:1075:LEU:HD22	1:A:1126:VAL:HG21	2.00	0.43
1:A:1085:SER:O	1:A:1119:THR:N	2.41	0.43
1:A:764:VAL:HA	1:A:780:HIS:HA	2.00	0.42
1:A:856:ALA:HB2	1:A:868:ILE:HD13	2.00	0.42
1:A:1013:SER:HA	1:A:1027:SER:HA	2.00	0.42
1:A:140:ILE:HG22	1:A:179:VAL:HB	2.01	0.42
1:A:1041:GLU:N	1:A:1041:GLU:OE1	2.52	0.42
1:A:728:ASN:OD1	1:A:728:ASN:N	2.52	0.42
1:A:1044:ARG:HE	1:A:1046:PHE:HZ	1.66	0.42
2:B:359:TYR:HB3	2:B:366:MET:SD	2.60	0.42
1:A:169:HIS:HB2	1:A:172:THR:HG21	2.01	0.42
1:A:336:THR:O	1:A:554:ASN:ND2	2.50	0.42
1:A:648:SER:HA	1:A:653:PRO:HA	2.01	0.42
1:A:833:THR:O	1:A:841:LEU:HD12	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:250:ASP:N	2:B:386:THR:OG1	2.52	0.42
2:B:319:LEU:HD12	2:B:328:LYS:HB3	2.02	0.42
1:A:466:LYS:HD3	1:A:510:LYS:HA	2.02	0.42
1:A:1146:ILE:HB	1:A:1428:SER:HB3	2.01	0.42
1:A:171:PHE:CE2	1:A:200:PRO:HA	2.55	0.42
1:A:732:ILE:HG23	1:A:732:ILE:O	2.20	0.42
1:A:1465:VAL:HG21	1:A:1479:SER:HB2	2.01	0.42
1:A:1249:ASN:ND2	1:A:1260:ARG:HH21	2.18	0.42
1:A:1486:MET:SD	1:A:1498:HIS:HA	2.60	0.42
1:A:808:THR:HG22	1:A:815:SER:HA	2.01	0.42
1:A:947:VAL:HG11	1:A:965:TRP:CD1	2.55	0.42
1:A:1127:PHE:CE2	1:A:1132:PRO:HB3	2.54	0.42
1:A:1163:LEU:HD23	1:A:1170:VAL:HA	2.02	0.42
1:A:120:ILE:HG22	1:A:125:VAL:HG13	2.02	0.41
1:A:235:ILE:HG21	1:A:238:TYR:CZ	2.55	0.41
1:A:278:GLU:O	2:B:414:ARG:NE	2.52	0.41
1:A:674:ILE:HD12	1:A:924:ILE:HG12	2.02	0.41
1:A:738:ILE:O	1:A:741:ILE:HG22	2.20	0.41
1:A:1189:ASP:OD1	1:A:1189:ASP:N	2.52	0.41
1:A:1390:TYR:HE1	1:A:1403:GLN:HG3	1.85	0.41
1:A:302:TRP:CG	1:A:313:LYS:HE2	2.55	0.41
1:A:303:LEU:HB2	1:A:316:LEU:HD11	2.02	0.41
1:A:795:GLY:O	1:A:809:ARG:HG3	2.20	0.41
1:A:683:TRP:CE3	1:A:692:PRO:HB2	2.55	0.41
1:A:895:ASN:HB3	1:A:901:THR:HG21	2.02	0.41
1:A:1580:PRO:HB2	1:A:1583:SER:HB2	2.02	0.41
1:A:355:ILE:HG23	1:A:372:PHE:HB3	2.02	0.41
1:A:510:LYS:H	1:A:523:ASP:HA	1.85	0.41
1:A:964:LEU:HB3	1:A:998:ILE:HG13	2.01	0.41
2:B:452:ARG:O	2:B:455:THR:HG22	2.20	0.41
1:A:675:MET:HE1	1:A:684:SER:HB2	2.02	0.41
1:A:978:TYR:CZ	1:A:997:PRO:HB3	2.56	0.41
1:A:636:GLN:HG3	1:A:639:THR:OG1	2.20	0.41
1:A:827:LYS:HB3	1:A:845:VAL:HG11	2.01	0.41
1:A:1115:SER:HB2	1:A:1118:TYR:CE1	2.55	0.41
1:A:1239:LYS:HE3	1:A:1271:ILE:H	1.86	0.41
1:A:146:ALA:HB3	1:A:173:GLU:HG3	2.03	0.41
1:A:893:TRP:HZ3	1:A:895:ASN:HA	1.86	0.41
1:A:350:SER:HB3	1:A:382:ILE:HD13	2.02	0.41
1:A:765:ILE:HB	1:A:778:VAL:HB	2.02	0.41
1:A:1187:THR:HG22	1:A:1426:TYR:CE1	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:576:VAL:HG12	1:A:585:ILE:HG22	2.03	0.41
1:A:800:THR:OG1	1:A:805:VAL:HG12	2.21	0.41
2:B:347:ASN:OD1	2:B:348:THR:N	2.52	0.41
1:A:328:SER:HB3	1:A:331:ILE:HD12	2.02	0.41
1:A:388:TYR:HB3	1:A:390:ARG:HD3	2.01	0.41
1:A:459:ILE:HD11	1:A:494:GLY:N	2.35	0.41
1:A:898:ARG:O	1:A:919:PHE:N	2.54	0.41
1:A:1078:PHE:CZ	1:A:1104:PRO:HG3	2.56	0.41
1:A:1436:LYS:HD3	1:A:1529:TYR:HD1	1.85	0.41
2:B:447:GLY:HA2	2:B:449:HIS:CE1	2.55	0.41
1:A:462:SER:HB2	1:A:465:LEU:HD13	2.03	0.40
1:A:487:PHE:HD2	1:A:519:PHE:HZ	1.70	0.40
1:A:385:ASP:HB3	1:A:390:ARG:HB2	2.03	0.40
1:A:722:VAL:HG23	1:A:744:ALA:HB3	2.03	0.40
1:A:947:VAL:HG22	1:A:968:PRO:HD3	2.04	0.40
1:A:1061:VAL:HG11	1:A:1120:VAL:HG21	2.03	0.40
1:A:1147:LYS:N	1:A:1148:PRO:HD3	2.36	0.40
1:A:1239:LYS:HA	1:A:1239:LYS:HD3	1.89	0.40
2:B:465:MET:SD	2:B:465:MET:N	2.94	0.40
1:A:406:ASN:HB3	3:A:1901:NAG:H82	2.02	0.40
1:A:483:THR:HG21	3:A:1907:NAG:H62	2.03	0.40
1:A:1445:MET:HE1	1:A:1525:VAL:HB	2.02	0.40
1:A:1548:SER:HB2	1:A:1633:PRO:HG2	2.03	0.40
1:A:728:ASN:HB2	1:A:730:MET:HE1	2.03	0.40
1:A:1049:SER:HA	1:A:1059:VAL:HG12	2.03	0.40
1:A:1589:VAL:HG22	1:A:1595:PRO:HB3	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	1540/1853 (83%)	1458 (95%)	80 (5%)	2 (0%)	48	83
2	B	211/830 (25%)	195 (92%)	16 (8%)	0	100	100
All	All	1751/2683 (65%)	1653 (94%)	96 (6%)	2 (0%)	49	83

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1352	ARG
1	A	1148	PRO

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	1373/1641 (84%)	1373 (100%)	0	100	100
2	B	193/731 (26%)	193 (100%)	0	100	100
All	All	1566/2372 (66%)	1566 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	142	GLN
1	A	343	GLN
1	A	344	GLN
1	A	481	ASN
1	A	554	ASN
1	A	563	GLN
1	A	613	GLN
1	A	811	ASN
1	A	849	GLN
1	A	907	GLN
1	A	1011	ASN
1	A	1249	ASN

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Mol	Chain	Res	Type
1	A	1294	GLN
1	A	1306	GLN
1	A	1414	GLN
2	B	337	GLN
2	B	415	ASN
2	B	417	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

10 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	NAG	A	1906	-	14,14,15	0.71	0	17,19,21	0.76	0
3	NAG	A	1908	1	14,14,15	0.71	0	17,19,21	0.79	0
3	NAG	A	1905	1	14,14,15	0.68	0	17,19,21	0.89	1 (5%)
3	NAG	A	1904	1	14,14,15	0.73	0	17,19,21	1.06	2 (11%)
3	NAG	A	1902	1	14,14,15	0.74	0	17,19,21	0.76	0
3	NAG	A	1901	-	14,14,15	0.73	0	17,19,21	0.77	0
3	NAG	A	1907	-	14,14,15	0.71	0	17,19,21	0.78	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAG	A	1909	-	14,14,15	0.72	0	17,19,21	0.76	0
3	NAG	A	1910	-	14,14,15	0.71	0	17,19,21	0.75	0
3	NAG	A	1903	1	14,14,15	0.72	0	17,19,21	0.84	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	A	1906	-	-	2/6/23/26	0/1/1/1
3	NAG	A	1908	1	-	3/6/23/26	0/1/1/1
3	NAG	A	1905	1	-	2/6/23/26	0/1/1/1
3	NAG	A	1904	1	-	1/6/23/26	0/1/1/1
3	NAG	A	1902	1	-	2/6/23/26	0/1/1/1
3	NAG	A	1901	-	-	2/6/23/26	0/1/1/1
3	NAG	A	1907	-	-	2/6/23/26	0/1/1/1
3	NAG	A	1909	-	-	0/6/23/26	0/1/1/1
3	NAG	A	1910	-	-	0/6/23/26	0/1/1/1
3	NAG	A	1903	1	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1904	NAG	C1-O5-C5	-2.39	108.98	112.19
3	A	1905	NAG	O5-C1-C2	-2.30	107.73	111.29
3	A	1904	NAG	O5-C1-C2	-2.20	107.89	111.29

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1905	NAG	C4-C5-C6-O6
3	A	1908	NAG	O5-C5-C6-O6
3	A	1902	NAG	O5-C5-C6-O6
3	A	1901	NAG	O5-C5-C6-O6
3	A	1903	NAG	O5-C5-C6-O6
3	A	1908	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
3	A	1905	NAG	O5-C5-C6-O6
3	A	1907	NAG	C4-C5-C6-O6
3	A	1902	NAG	C4-C5-C6-O6
3	A	1901	NAG	C4-C5-C6-O6
3	A	1903	NAG	C4-C5-C6-O6
3	A	1907	NAG	O5-C5-C6-O6
3	A	1904	NAG	O5-C5-C6-O6
3	A	1906	NAG	C4-C5-C6-O6
3	A	1906	NAG	O5-C5-C6-O6
3	A	1908	NAG	C1-C2-N2-C7

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1901	NAG	1	0
3	A	1907	NAG	1	0

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.

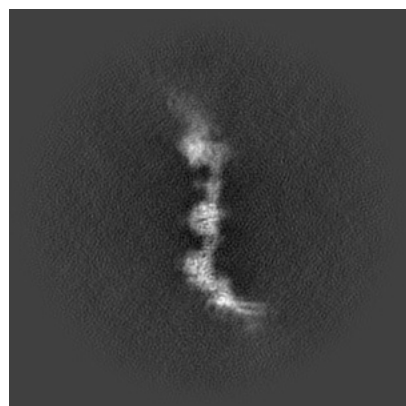
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-71938. These allow visual inspection of the internal detail of the map and identification of artifacts.

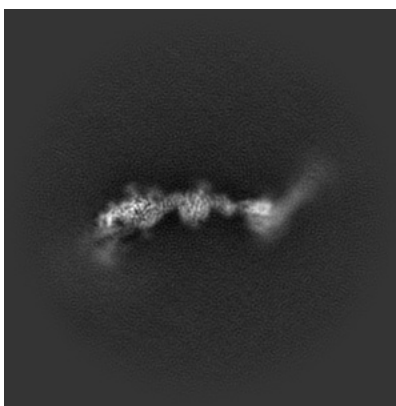
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

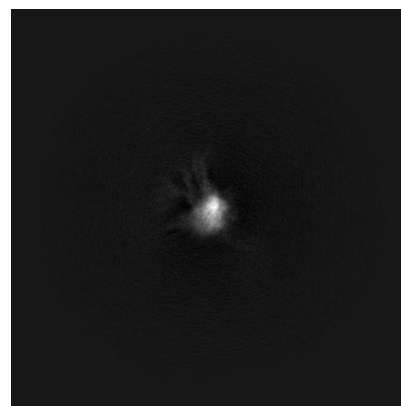
6.1.1 Primary map



X

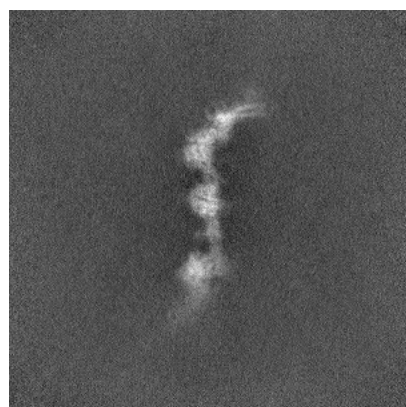


Y

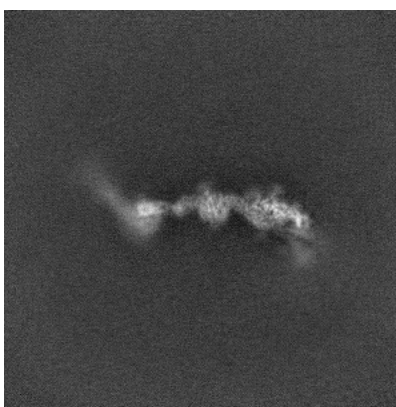


Z

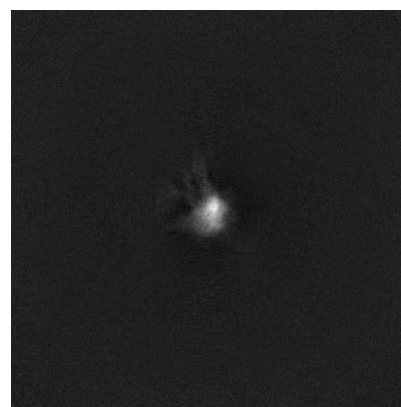
6.1.2 Raw map



X



Y



Z

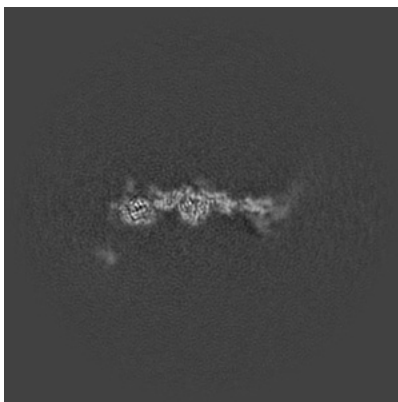
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

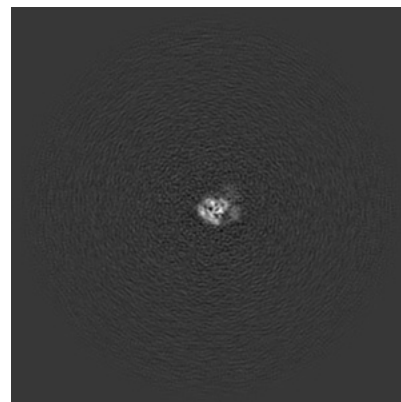
6.2.1 Primary map



X Index: 320



Y Index: 320

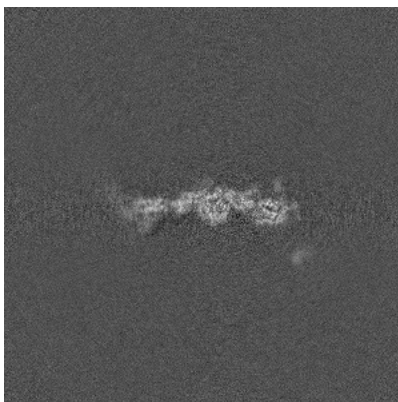


Z Index: 320

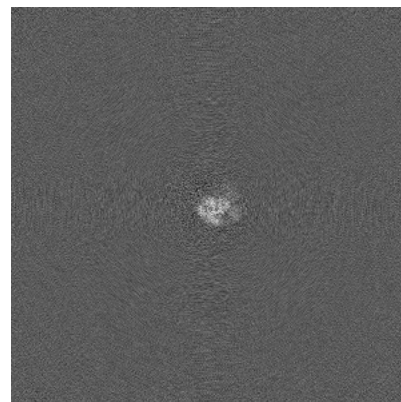
6.2.2 Raw map



X Index: 320



Y Index: 320



Z Index: 320

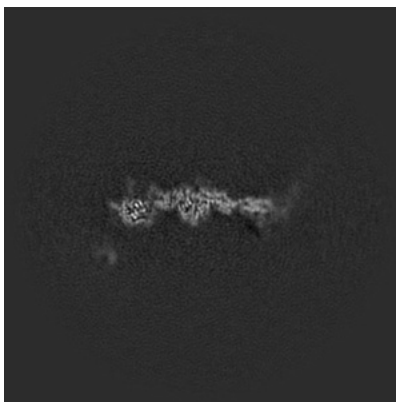
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

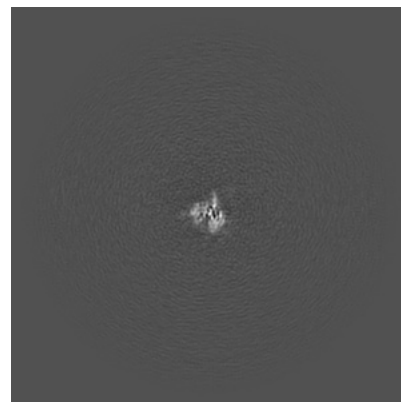
6.3.1 Primary map



X Index: 325



Y Index: 322

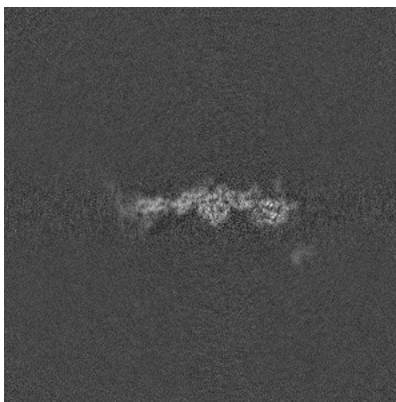


Z Index: 219

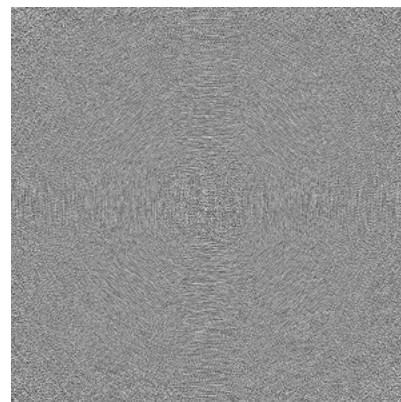
6.3.2 Raw map



X Index: 321



Y Index: 321



Z Index: 0

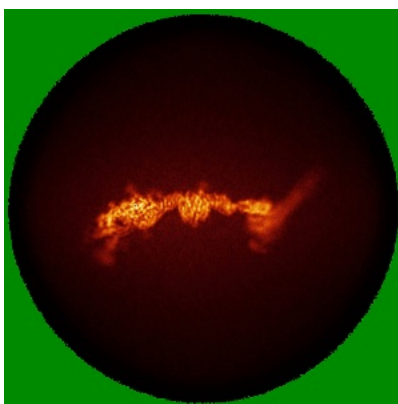
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



X

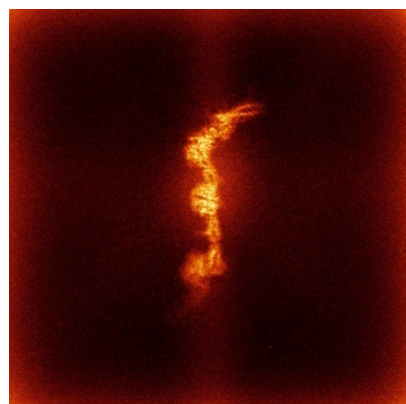


Y

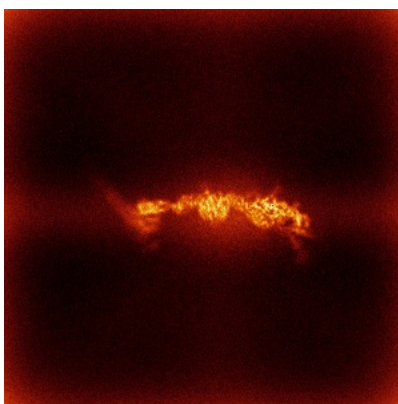


Z

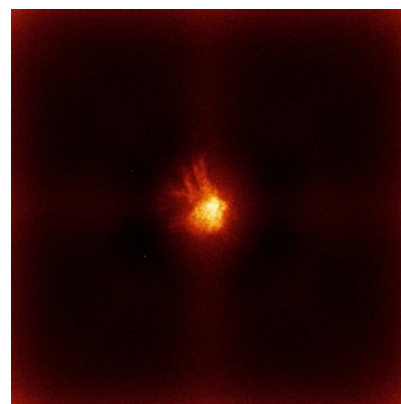
6.4.2 Raw map



X



Y

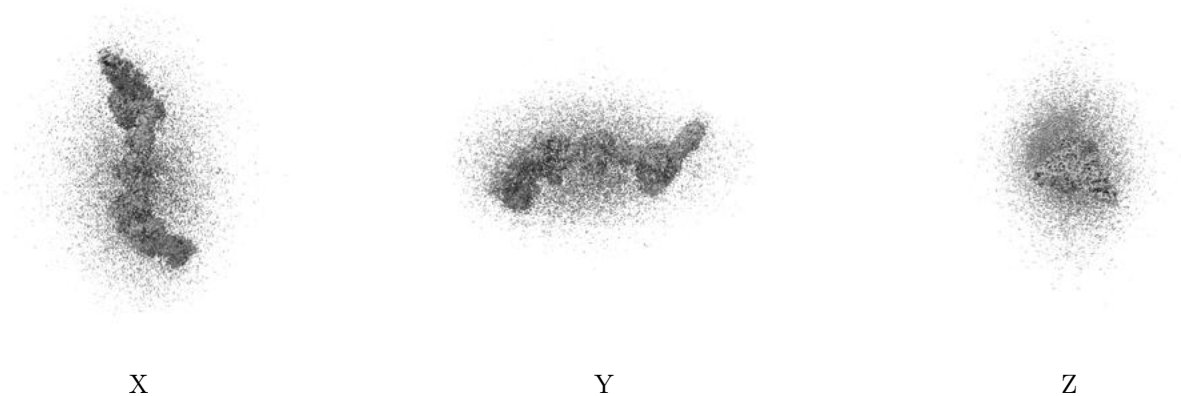


Z

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.

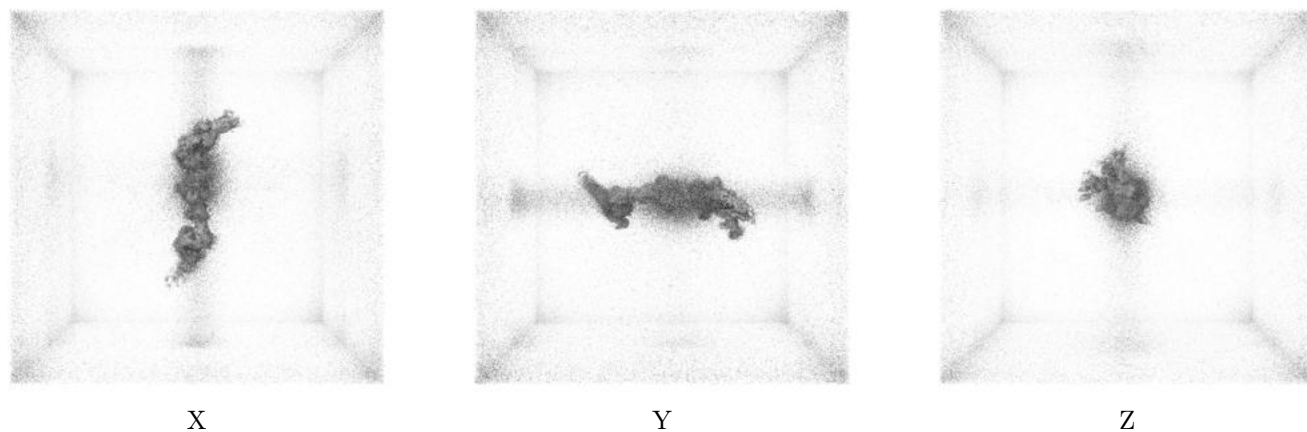
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0248. 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.

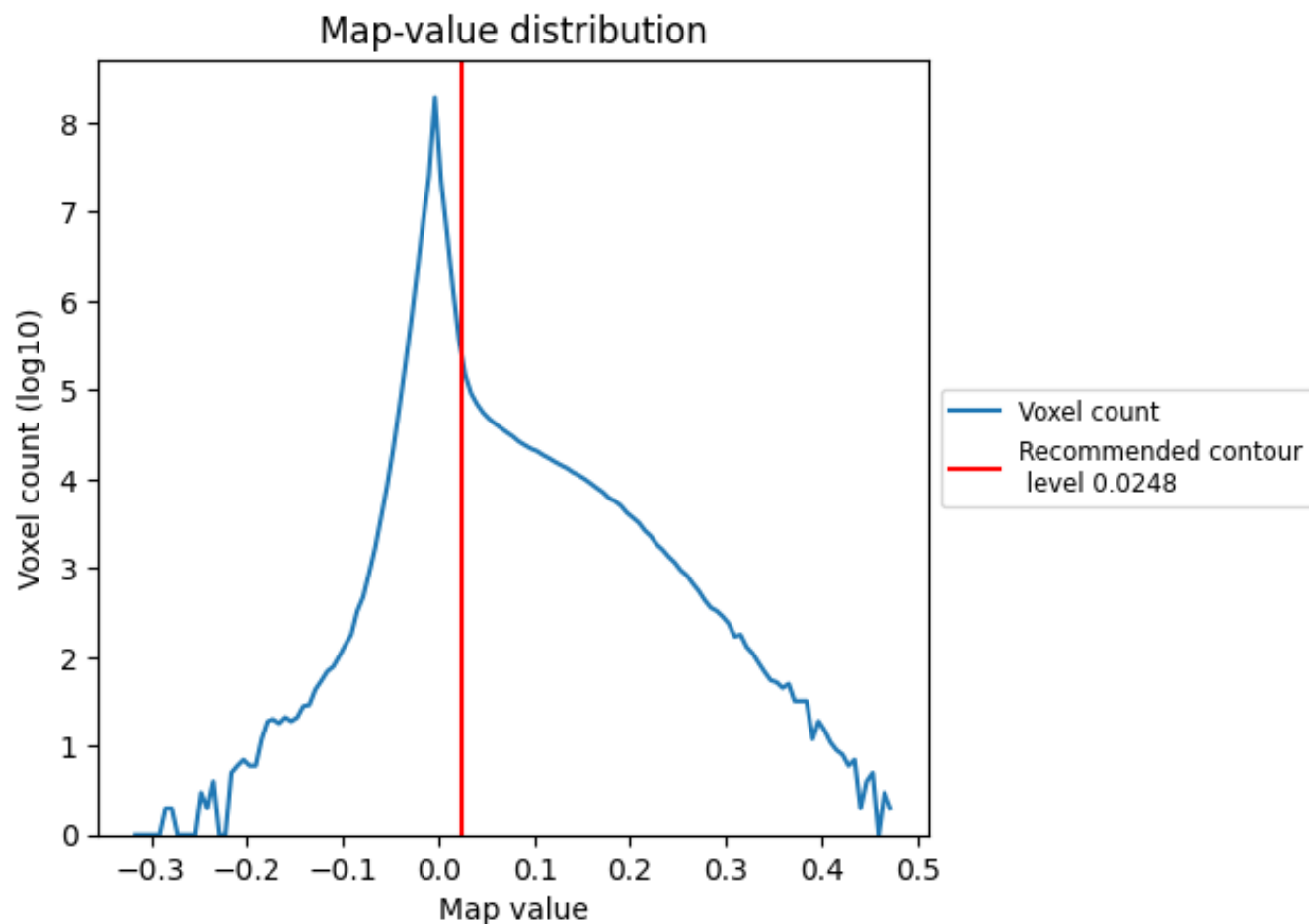
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

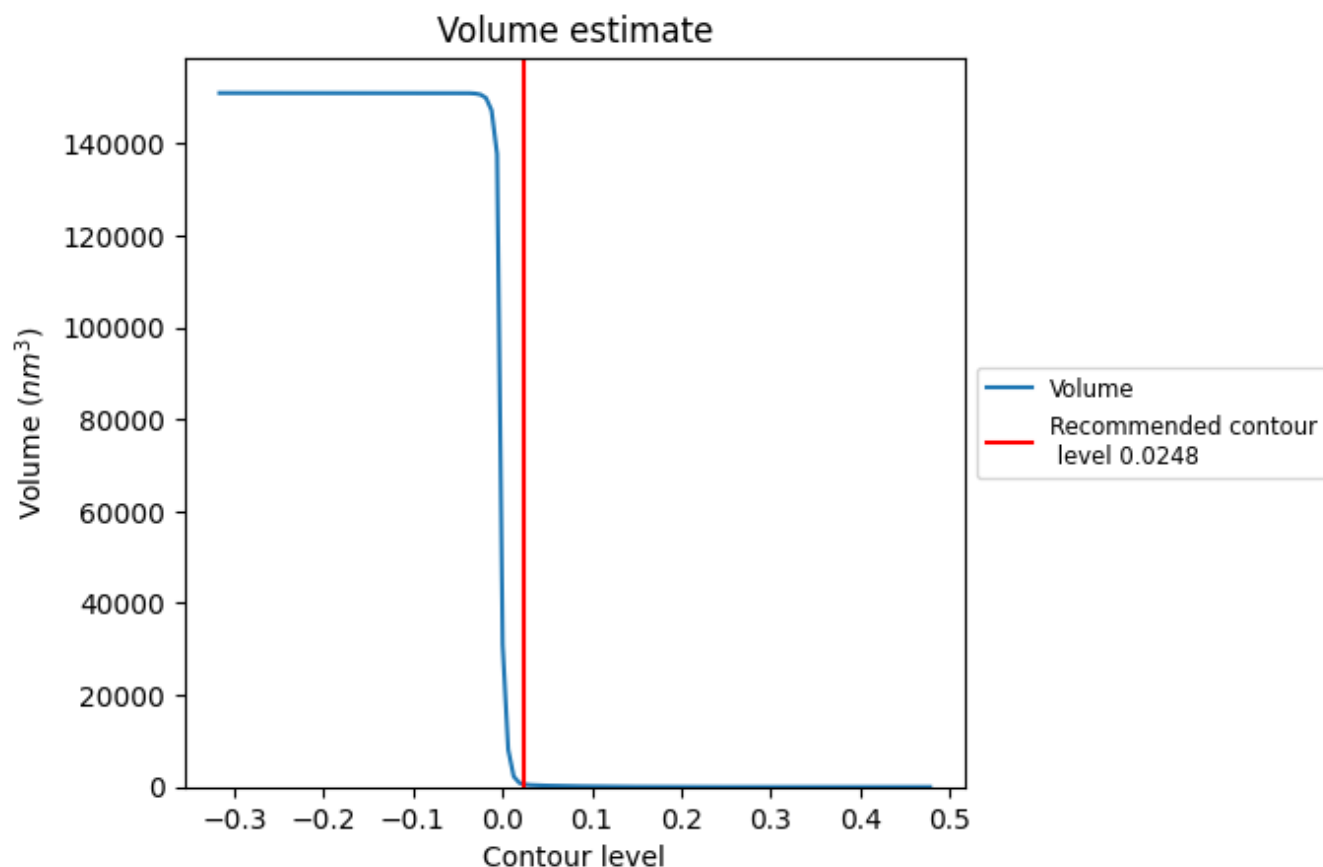
This section contains the results of statistical analysis of the map.

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.

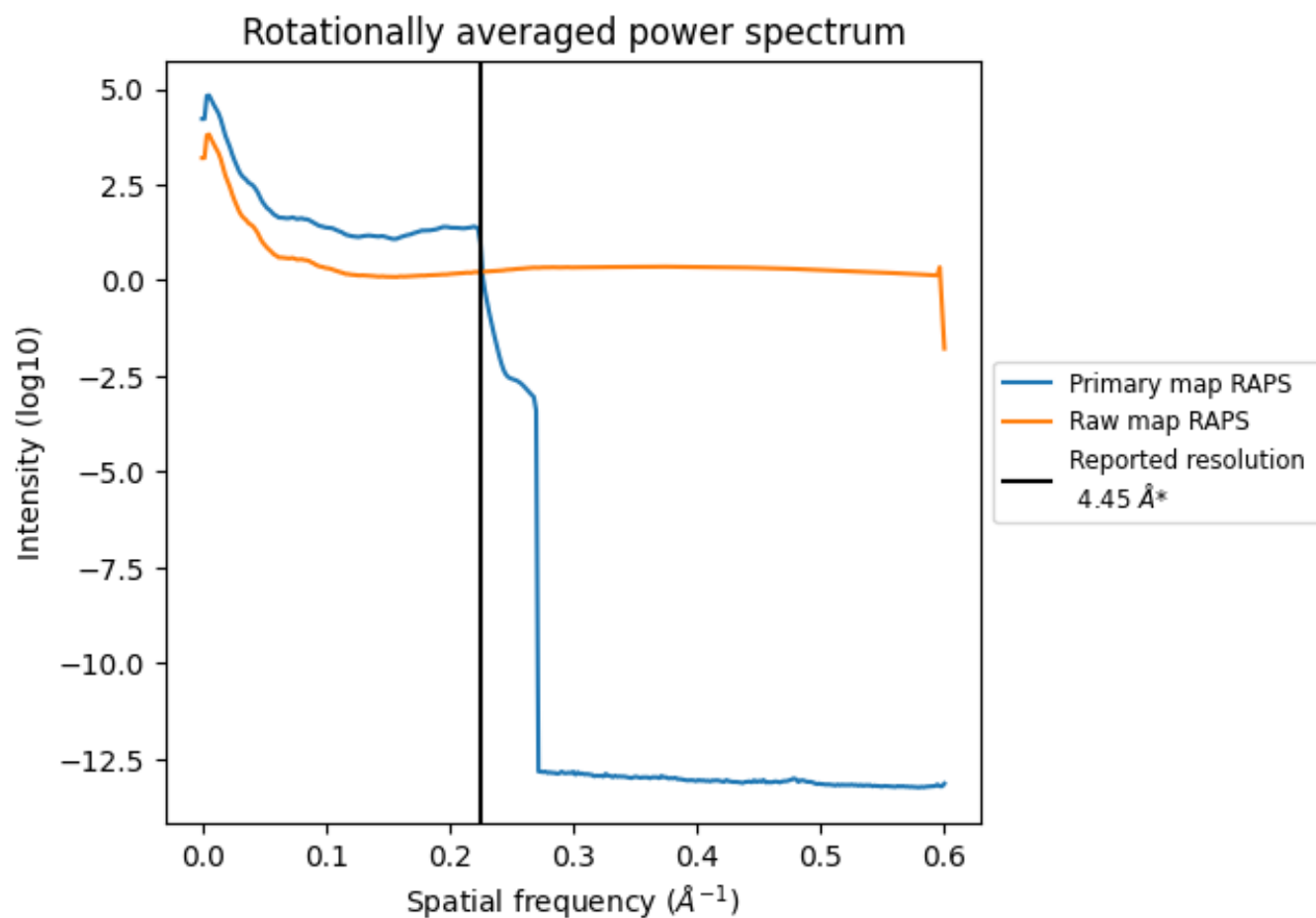
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 562 nm^3 ; this corresponds to an approximate mass of 508 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 ⓘ

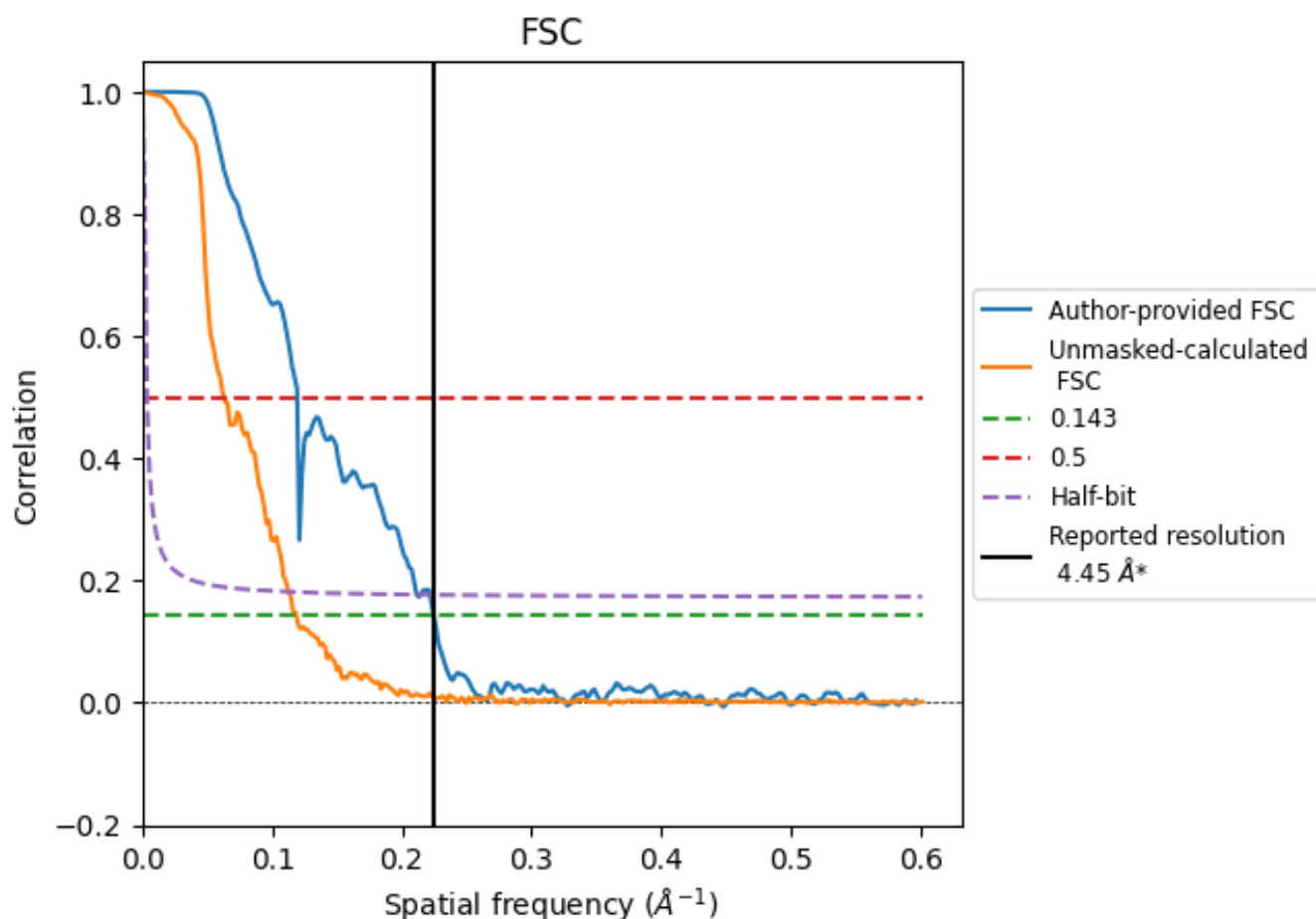


*Reported resolution corresponds to spatial frequency of 0.225 Å⁻¹

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 0.225 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

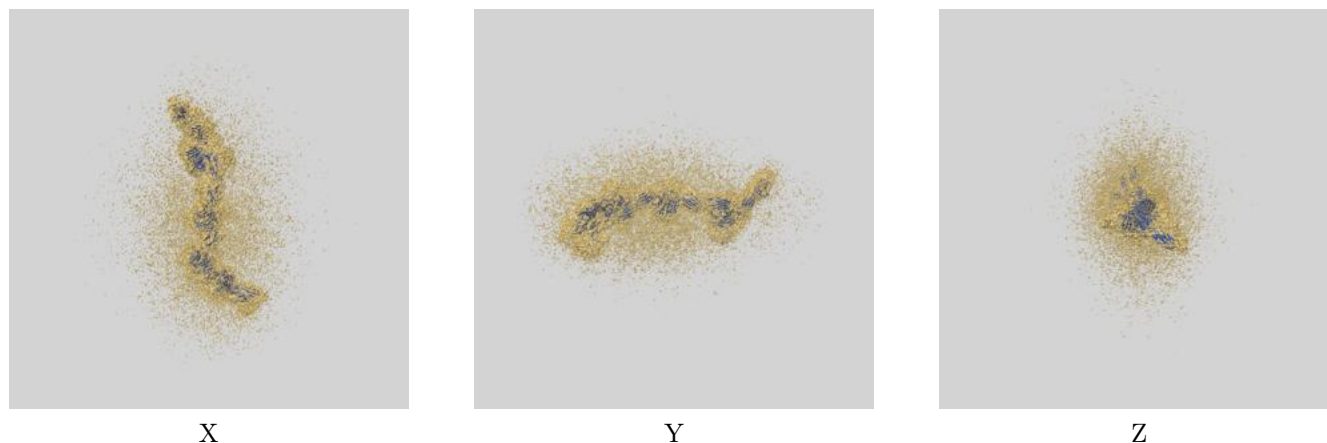
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.45	-	-
Author-provided FSC curve	4.45	8.38	4.73
Unmasked-calculated*	8.42	15.90	8.85

*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 8.42 differs from the reported value 4.45 by more than 10 %

9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-71938 and PDB model 9PWQ. Per-residue inclusion information can be found in section [3](#) on page [7](#).

9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 0.0248 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](#)



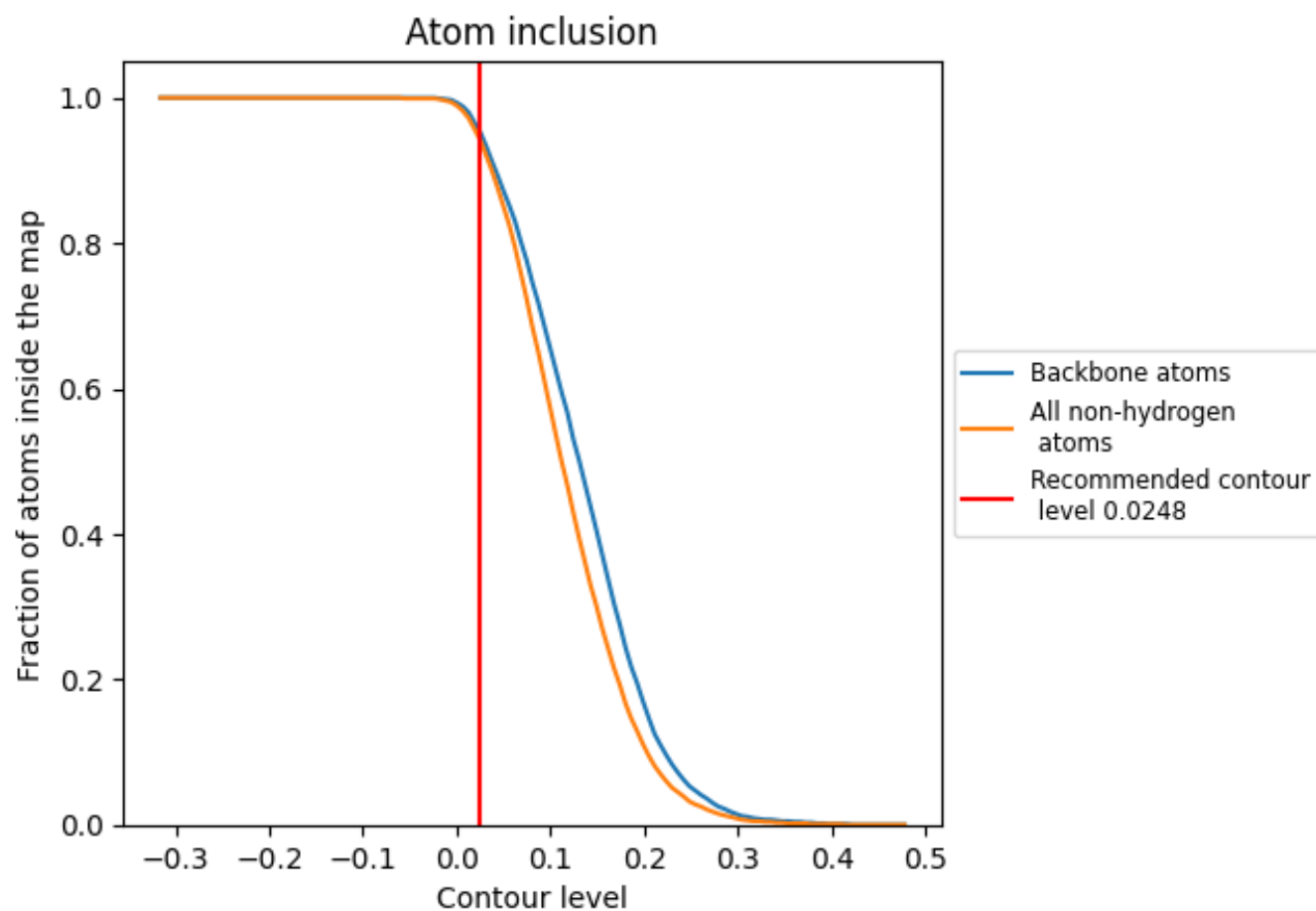
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0248).

9.4 Atom inclusion [i](#)



At the recommended contour level, 95% of all backbone atoms, 94% 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 (0.0248) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9430	0.1860
A	0.9400	0.1790
B	0.9620	0.2400

