



Full wwPDB EM Validation Report ⓘ

Mar 20, 2026 – 11:25 AM UTC

PDB ID : 8HGG / pdb_00008hgg
EMDB ID : EMD-34738
Title : Structure of 2:2 PAPP-A.ProMBP complex
Authors : Zhong, Q.H.; Chu, H.L.; Wang, G.P.; Zhang, C.; Wei, Y.; Qiao, J.; Hang, J.
Deposited on : 2022-11-14
Resolution : 3.64 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

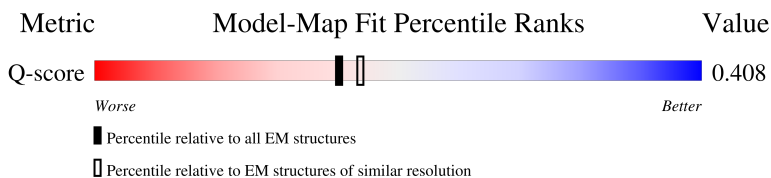
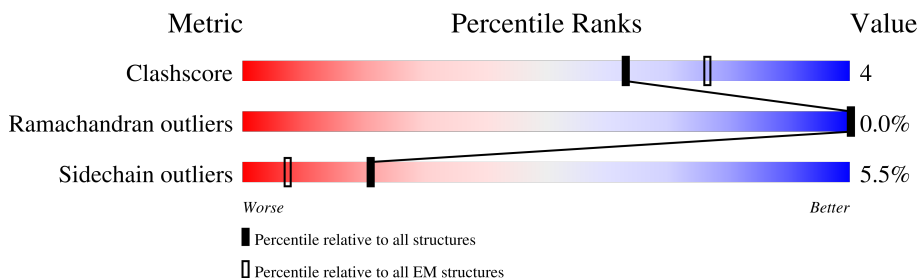
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.64 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	11633 (3.14 - 4.14)

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	222	
1	B	222	
2	C	1627	
2	D	1627	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 25404 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 Bone marrow proteoglycan.

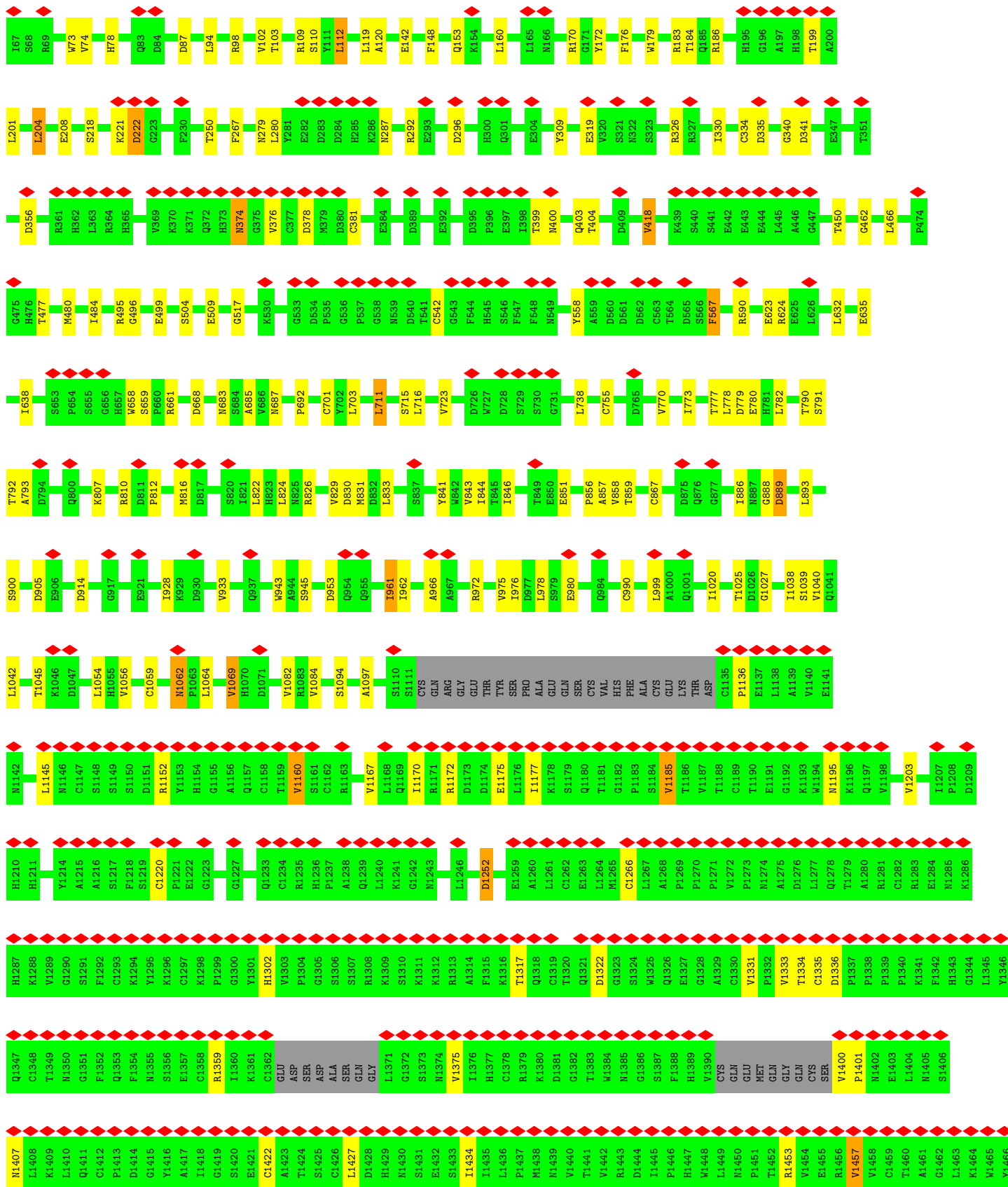
Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	135	Total	C	N	O	S	0	0
			1101	691	218	181	11		
1	B	135	Total	C	N	O	S	0	0
			1101	691	218	181	11		

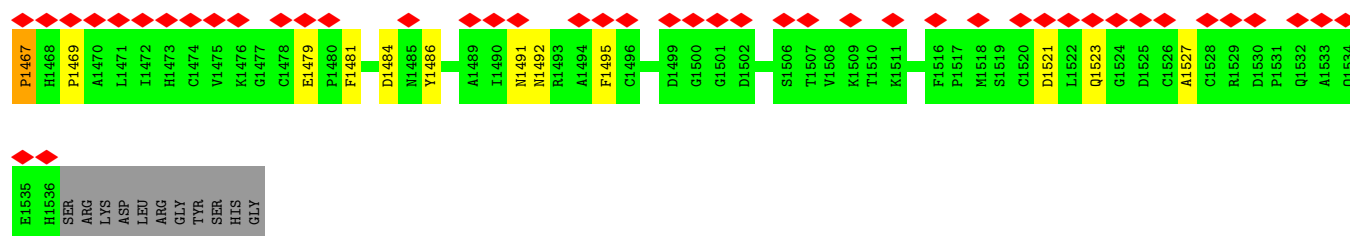
- Molecule 2 is a protein called Pappalysin-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	1484	Total	C	N	O	S	0	0
			11600	7267	2009	2225	99		
2	D	1484	Total	C	N	O	S	0	0
			11600	7267	2009	2225	99		

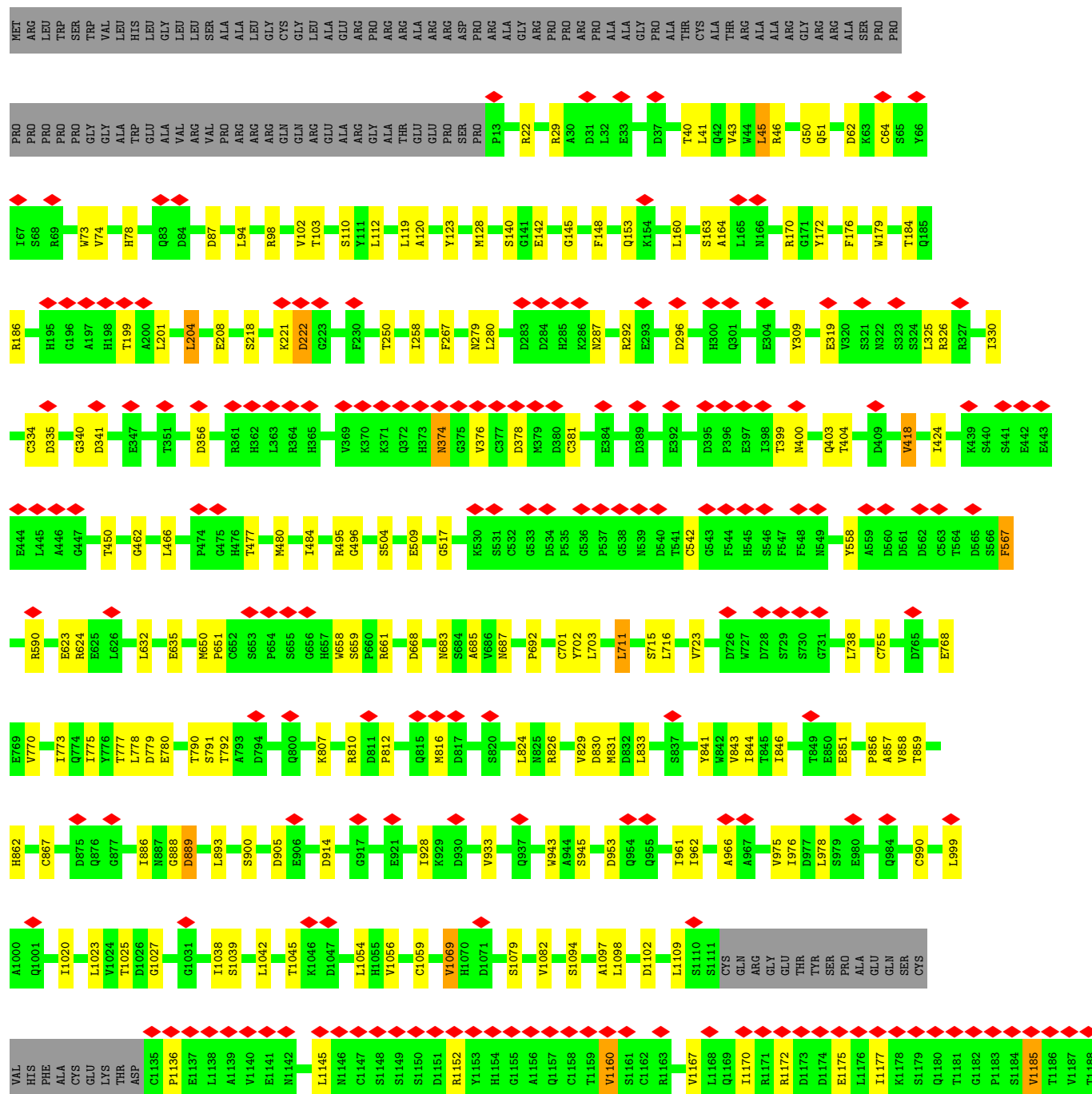
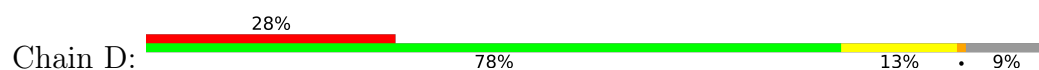
- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
3	C	1	Total	Zn	0
			1	1	
3	D	1	Total	Zn	0
			1	1	





• Molecule 2: Pappalysin-1



D1521	V1454	E1455	R1456	V1457	V1458	C1459	T1460	A1461	G1462	L1463	K1464	W1465	Y1466	P1467	H1468	P1469	A1470	L1471	I1472	H1473	C1474	V1475	K1476	G1477	C1478	E1479	P1480	F1481	D1484	N1485	Y1486	A1489	I1490	N1491	N1492	R1493	A1494	F1495	C1496	D1499	G1500	G1501	D1502	C1503	S1506	T1507	V1508	K1509	T1510	K1511	F1516	P1517	M1518	S1519	C1520
L1522	E1455	R1456	V1457	V1458	C1459	T1460	A1461	G1462	L1463	K1464	W1465	Y1466	P1467	H1468	P1469	A1470	L1471	I1472	H1473	C1474	V1475	K1476	G1477	C1478	E1479	P1480	F1481	D1484	N1485	Y1486	A1489	I1490	N1491	N1492	R1493	A1494	F1495	C1496	D1499	G1500	G1501	D1502	C1503	S1506	T1507	V1508	K1509	T1510	K1511	F1516	P1517	M1518	S1519	C1520	
Q1523	E1455	R1456	V1457	V1458	C1459	T1460	A1461	G1462	L1463	K1464	W1465	Y1466	P1467	H1468	P1469	A1470	L1471	I1472	H1473	C1474	V1475	K1476	G1477	C1478	E1479	P1480	F1481	D1484	N1485	Y1486	A1489	I1490	N1491	N1492	R1493	A1494	F1495	C1496	D1499	G1500	G1501	D1502	C1503	S1506	T1507	V1508	K1509	T1510	K1511	F1516	P1517	M1518	S1519	C1520	
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SER	E1455	R1456	V1457	V1458	C1459	T1460	A1461	G1462	L1463	K1464	W1465	Y1466	P1467	H1468	P1469	A1470	L1471	I1472	H1473	C1474	V1475	K1476	G1477	C1478	E1479	P1480	F1481	D1484	N1485	Y1486	A1489	I1490	N1491	N1492	R1493	A1494	F1495	C1496	D1499	G1500	G1501	D1502	C1503	S1506	T1507	V1508	K1509	T1510	K1511	F1516	P1517	M1518	S1519	C1520	
ARG	E1455	R1456	V1457	V1458	C1459	T1460	A1461	G1462	L1463	K1464	W1465	Y1466	P1467	H1468	P1469	A1470	L1471	I1472	H1473	C1474	V1475	K1476	G1477	C1478	E1479	P1480	F1481	D1484	N1485	Y1486	A1489	I1490	N1491	N1492	R1493	A1494	F1495	C1496	D1499	G1500	G1501	D1502	C1503	S1506	T1507	V1508	K1509	T1510	K1511	F1516	P1517	M1518	S1519	C1520	
LYS	E1455	R1456	V1457	V1458	C1459	T1460	A1461	G1462	L1463	K1464	W1465	Y1466	P1467	H1468	P1469	A1470	L1471	I1472	H1473	C1474	V1475	K1476	G1477	C1478	E1479	P1480	F1481	D1484	N1485	Y1486	A1489	I1490	N1491	N1492	R1493	A1494	F1495	C1496	D1499	G1500	G1501	D1502	C1503	S1506	T1507	V1508	K1509	T1510	K1511	F1516	P1517	M1518	S1519	C1520	
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ARG	E1455	R1456	V1457	V1458	C1459	T1460	A1461	G1462	L1463	K1464	W1465	Y1466	P1467	H1468	P1469	A1470	L1471	I1472	H1473	C1474	V1475	K1476	G1477	C1478	E1479	P1480	F1481	D1484	N1485	Y1486	A1489	I1490	N1491	N1492	R1493	A1494	F1495	C1496	D1499	G1500	G1501	D1502	C1503	S1506	T1507	V1508	K1509	T1510	K1511	F1516	P1517	M1518	S1519	C1520	
GLY	E1455	R1456	V1457	V1458	C1459	T1460	A1461	G1462	L1463	K1464	W1465	Y1466	P1467	H1468	P1469	A1470	L1471	I1472	H1473	C1474	V1475	K1476	G1477	C1478	E1479	P1480	F1481	D1484	N1485	Y1486	A1489	I1490	N1491	N1492	R1493	A1494	F1495	C1496	D1499	G1500	G1501	D1502	C1503	S1506	T1507	V1508	K1509	T1510	K1511	F1516	P1517	M1518	S1519	C1520	
TYR	E1455	R1456	V1457	V1458	C1459	T1460	A1461	G1462	L1463	K1464	W1465	Y1466	P1467	H1468	P1469	A1470	L1471	I1472	H1473	C1474	V1475	K1476	G1477	C1478	E1479	P1480	F1481	D1484	N1485	Y1486	A1489	I1490	N1491	N1492	R1493	A1494	F1495	C1496	D1499	G1500	G1501	D1502	C1503	S1506	T1507	V1508	K1509	T1510	K1511	F1516	P1517	M1518	S1519	C1520	
SER	E1455	R1456	V1457	V1458	C1459	T1460	A1461	G1462	L1463	K1464	W1465	Y1466	P1467	H1468	P1469	A1470	L1471	I1472	H1473	C1474	V1475	K1476	G1477	C1478	E1479	P1480	F1481	D1484	N1485	Y1486	A1489	I1490	N1491	N1492	R1493	A1494	F1495</																		

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	261371	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	60.1	Depositor
Minimum defocus (nm)	700	Depositor
Maximum defocus (nm)	1200	Depositor
Magnification	Not provided	
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	0.207	Depositor
Minimum map value	-0.128	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.0262	Depositor
Map size (Å)	269.312, 269.312, 269.312	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.052, 1.052, 1.052	Depositor

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.14	0/1134	0.37	0/1535
1	B	0.14	0/1134	0.37	0/1535
2	C	0.18	0/11914	0.37	0/16222
2	D	0.18	0/11914	0.36	0/16222
All	All	0.18	0/26096	0.36	0/35514

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	1101	0	1051	15	0
1	B	1101	0	1051	15	0
2	C	11600	0	10964	101	0
2	D	11600	0	10964	94	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
All	All	25404	0	24030	208	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 4.

All (208) 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:D:777:THR:HG22	2:D:779:ASP:H	1.56	0.70
2:C:777:THR:HG22	2:C:779:ASP:H	1.56	0.69
1:A:214:ARG:HH21	2:C:1481:PHE:HB3	1.59	0.68
2:C:1020:ILE:HB	2:C:1097:ALA:HB3	1.79	0.63
1:B:214:ARG:HH21	2:D:1481:PHE:HB3	1.63	0.63
2:C:29:ARG:HE	2:C:218:SER:HB3	1.64	0.62
1:B:123:PHE:HB3	1:B:127:ARG:HH21	1.66	0.60
1:A:123:PHE:HB3	1:A:127:ARG:HH21	1.66	0.60
2:D:29:ARG:HE	2:D:218:SER:HB3	1.66	0.60
2:C:1335:CYS:SG	2:C:1336:ASP:N	2.74	0.60
2:C:41:LEU:O	2:C:120:ALA:HA	2.04	0.58
2:D:1020:ILE:HB	2:D:1097:ALA:HB3	1.86	0.58
2:D:50:GLY:O	2:D:170:ARG:NH1	2.36	0.57
1:B:98:VAL:HG23	1:B:144:ARG:HH21	1.69	0.57
1:A:98:VAL:HG23	1:A:144:ARG:HH21	1.70	0.57
2:C:403:GLN:HG3	2:C:404:THR:HG23	1.88	0.56
2:D:41:LEU:O	2:D:120:ALA:HA	2.05	0.56
2:C:1401:PRO:HB3	2:C:1469:PRO:HG2	1.88	0.56
2:D:403:GLN:HG3	2:D:404:THR:HG23	1.88	0.55
2:D:816:MET:SD	2:D:816:MET:N	2.80	0.55
1:A:179:ARG:HH21	2:D:340:GLY:HA3	1.72	0.55
1:B:179:ARG:HH21	2:C:340:GLY:HA3	1.72	0.55
2:D:846:ILE:HG12	2:D:851:GLU:HG2	1.88	0.55
2:C:50:GLY:O	2:C:170:ARG:NH1	2.36	0.54
2:C:1172:ARG:HB2	2:C:1175:GLU:HB3	1.90	0.54
1:B:214:ARG:NH2	2:D:1484:ASP:OD2	2.40	0.54
2:C:846:ILE:HG12	2:C:851:GLU:HG2	1.89	0.54
2:C:45:LEU:HD21	2:C:119:LEU:HD12	1.89	0.54
1:A:214:ARG:NH2	2:C:1484:ASP:OD2	2.41	0.53
1:B:181:ASN:ND2	2:C:341:ASP:OD1	2.41	0.53
2:C:816:MET:SD	2:C:816:MET:N	2.81	0.53
2:D:1172:ARG:HB2	2:D:1175:GLU:HB3	1.91	0.53
2:D:45:LEU:HD21	2:D:119:LEU:HD12	1.89	0.52
2:C:1136:PRO:O	2:C:1152:ARG:NH1	2.42	0.52
2:C:148:PHE:HE2	2:C:153:GLN:HG3	1.75	0.52
2:D:1145:LEU:HD12	2:D:1160:VAL:HB	1.90	0.52
2:C:738:LEU:HD23	2:C:770:VAL:HG21	1.93	0.51
2:C:1172:ARG:HH12	2:C:1195:ASN:HB2	1.75	0.51
2:C:1359:ARG:HG2	2:C:1375:VAL:HG22	1.92	0.51
2:D:889:ASP:N	2:D:889:ASP:OD1	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:1136:PRO:O	2:D:1152:ARG:NH1	2.44	0.51
2:D:1359:ARG:HG2	2:D:1375:VAL:HG22	1.92	0.51
1:A:181:ASN:ND2	2:D:341:ASP:OD1	2.43	0.51
2:C:1025:THR:HG22	2:C:1027:GLY:H	1.76	0.51
2:C:1453:ARG:NH2	2:C:1495:PHE:O	2.44	0.51
2:D:683:ASN:ND2	2:D:780:GLU:O	2.44	0.50
2:C:1145:LEU:HD12	2:C:1160:VAL:HB	1.93	0.50
2:D:635:GLU:OE1	2:D:826:ARG:NH1	2.43	0.50
2:C:40:THR:HB	2:C:179:TRP:HB2	1.94	0.50
2:D:148:PHE:HE2	2:D:153:GLN:HG3	1.76	0.50
2:C:683:ASN:ND2	2:C:780:GLU:O	2.45	0.50
2:C:830:ASP:N	2:C:830:ASP:OD1	2.44	0.50
2:D:87:ASP:OD1	2:D:110:SER:OG	2.30	0.50
2:C:287:ASN:O	2:C:326:ARG:NH1	2.45	0.50
2:D:287:ASN:O	2:D:326:ARG:NH1	2.45	0.50
2:D:1172:ARG:HH12	2:D:1195:ASN:HB2	1.77	0.50
2:C:378:ASP:HB2	2:C:381:CYS:HB2	1.93	0.49
2:D:1521:ASP:OD1	2:D:1523:GLN:NE2	2.45	0.49
2:C:399:THR:OG1	2:C:400:ASN:N	2.45	0.49
2:C:841:TYR:O	2:C:857:ALA:HA	2.12	0.49
2:D:222:ASP:N	2:D:222:ASP:OD1	2.45	0.49
2:C:1252:ASP:OD1	2:D:98:ARG:NH2	2.45	0.49
2:D:830:ASP:N	2:D:830:ASP:OD1	2.44	0.49
1:B:190:PRO:HB2	2:C:692:PRO:HD2	1.95	0.49
2:C:292:ARG:NH1	2:C:296:ASP:OD1	2.45	0.49
2:D:292:ARG:NH1	2:D:296:ASP:OD1	2.46	0.49
2:D:399:THR:OG1	2:D:400:ASN:N	2.45	0.49
2:D:738:LEU:HD23	2:D:770:VAL:HG21	1.93	0.49
2:D:933:VAL:HG21	2:D:943:TRP:HZ2	1.77	0.49
2:C:966:ALA:H	2:C:1094:SER:HB3	1.78	0.49
2:C:889:ASP:N	2:C:889:ASP:OD1	2.43	0.49
2:D:966:ALA:H	2:D:1094:SER:HB3	1.78	0.49
2:D:1025:THR:HG22	2:D:1027:GLY:H	1.77	0.49
2:D:73:TRP:HB3	2:D:94:LEU:HD13	1.95	0.48
2:C:1521:ASP:OD1	2:C:1523:GLN:NE2	2.45	0.48
2:D:1453:ARG:NH2	2:D:1495:PHE:O	2.47	0.48
2:D:40:THR:HB	2:D:179:TRP:HB2	1.94	0.48
2:D:841:TYR:O	2:D:857:ALA:HA	2.13	0.48
2:C:280:LEU:O	2:C:326:ARG:NH1	2.47	0.48
1:B:97:LYS:HG3	1:B:108:ARG:HD3	1.96	0.48
2:C:87:ASP:OD1	2:C:110:SER:OG	2.30	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:97:LYS:HG3	1:A:108:ARG:HD3	1.95	0.48
2:D:378:ASP:HB2	2:D:381:CYS:HB2	1.95	0.48
2:D:280:LEU:O	2:D:326:ARG:NH1	2.47	0.48
1:A:148:SER:HA	2:D:999:LEU:HD22	1.96	0.47
2:C:945:SER:HA	2:C:962:ILE:HG23	1.96	0.47
2:C:1302:HIS:NE2	2:C:1334:THR:OG1	2.47	0.47
2:C:711:LEU:HD13	2:C:791:SER:HB2	1.97	0.47
2:D:186:ARG:NH2	2:D:905:ASP:OD2	2.47	0.47
1:A:190:PRO:HB2	2:D:692:PRO:HD2	1.97	0.47
2:C:933:VAL:HG21	2:C:943:TRP:HZ2	1.79	0.47
2:D:504:SER:HB3	2:D:1059:CYS:H	1.79	0.47
2:C:186:ARG:NH2	2:C:905:ASP:OD2	2.48	0.46
2:D:496:GLY:HA3	2:D:509:GLU:HG2	1.97	0.46
2:D:886:ILE:HG22	2:D:888:GLY:H	1.80	0.46
2:D:900:SER:HB2	2:D:914:ASP:HB2	1.97	0.46
2:C:73:TRP:HB3	2:C:94:LEU:HD13	1.95	0.46
2:C:659:SER:OG	2:C:661:ARG:NH2	2.49	0.46
2:D:810:ARG:HG2	2:D:812:PRO:HD2	1.96	0.46
2:D:945:SER:HA	2:D:962:ILE:HG23	1.96	0.46
2:C:222:ASP:N	2:C:222:ASP:OD1	2.45	0.46
2:C:635:GLU:OE1	2:C:826:ARG:NH1	2.43	0.46
2:D:791:SER:OG	2:D:792:THR:N	2.49	0.46
1:B:148:SER:HA	2:C:999:LEU:HD22	1.97	0.46
2:C:374:ASN:OD1	2:C:374:ASN:N	2.49	0.46
2:C:1069:VAL:HG12	2:D:1069:VAL:HG12	1.98	0.46
1:B:98:VAL:HG13	1:B:109:TYR:HB2	1.98	0.46
2:C:807:LYS:HB3	2:C:844:ILE:HG13	1.98	0.46
1:A:117:THR:OG1	1:A:120:GLN:OE1	2.33	0.45
2:D:374:ASN:OD1	2:D:374:ASN:N	2.49	0.45
2:C:900:SER:HB2	2:C:914:ASP:HB2	1.97	0.45
2:C:1160:VAL:HG13	2:C:1185:VAL:HG13	1.98	0.45
2:D:711:LEU:HD13	2:D:791:SER:HB2	1.97	0.45
1:B:194:GLY:HA2	2:D:1484:ASP:HA	1.98	0.45
2:D:450:THR:HG21	2:D:462:GLY:HA2	1.99	0.45
2:C:496:GLY:HA3	2:C:509:GLU:HG2	1.99	0.45
2:C:450:THR:HG21	2:C:462:GLY:HA2	1.98	0.45
1:A:115:LEU:HB3	1:A:215:ARG:HB3	1.97	0.45
2:D:807:LYS:HB3	2:D:844:ILE:HG13	1.99	0.45
2:C:791:SER:OG	2:C:792:THR:N	2.50	0.45
2:C:495:ARG:NH1	2:C:517:GLY:O	2.44	0.45
2:C:542:CYS:HB3	2:C:1056:VAL:HG21	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:668:ASP:N	2:D:668:ASP:OD1	2.51	0.45
2:C:668:ASP:N	2:C:668:ASP:OD1	2.50	0.44
2:C:1040:VAL:HG22	2:C:1084:VAL:HG22	1.98	0.44
1:B:117:THR:OG1	1:B:120:GLN:OE1	2.35	0.44
2:C:810:ARG:HG2	2:C:812:PRO:HD2	1.99	0.44
2:D:267:PHE:HZ	2:D:856:PRO:HD3	1.83	0.44
2:C:886:ILE:HG22	2:C:888:GLY:H	1.82	0.44
2:D:1160:VAL:HG13	2:D:1185:VAL:HG13	2.00	0.44
2:D:1403:GLU:O	2:D:1469:PRO:HB2	2.18	0.44
2:D:1422:CYS:HB2	2:D:1457:VAL:HG23	1.99	0.44
2:C:309:TYR:CZ	2:C:567:PHE:HB2	2.53	0.44
2:C:715:SER:HB3	2:C:790:THR:HB	2.00	0.44
2:D:495:ARG:NH1	2:D:517:GLY:O	2.46	0.44
1:B:120:GLN:O	1:B:124:THR:OG1	2.35	0.43
2:C:267:PHE:HZ	2:C:856:PRO:HD3	1.83	0.43
2:D:659:SER:OG	2:D:661:ARG:NH2	2.50	0.43
1:A:98:VAL:HG13	1:A:109:TYR:HB2	1.99	0.43
2:C:334:CYS:SG	2:C:335:ASP:N	2.91	0.43
2:C:1322:ASP:OD1	2:C:1322:ASP:N	2.49	0.43
2:D:334:CYS:SG	2:D:335:ASP:N	2.91	0.43
2:C:466:LEU:HD11	2:C:480:MET:HG3	2.01	0.43
2:C:1457:VAL:HA	2:C:1467:PRO:HG2	2.00	0.43
2:C:400:ASN:O	2:C:404:THR:OG1	2.33	0.43
2:C:1422:CYS:HB2	2:C:1457:VAL:HG23	1.99	0.43
2:D:309:TYR:CZ	2:D:567:PHE:HB2	2.53	0.43
2:D:590:ARG:NH2	2:D:624:ARG:O	2.52	0.43
2:C:98:ARG:NH2	2:D:1252:ASP:OD1	2.51	0.43
2:C:590:ARG:NH2	2:C:624:ARG:O	2.52	0.43
2:D:103:THR:HG21	2:D:142:GLU:HB2	2.00	0.43
2:D:716:LEU:HD11	2:D:773:ILE:HD13	2.01	0.43
2:C:504:SER:HB3	2:C:1059:CYS:H	1.84	0.43
2:D:542:CYS:HB3	2:D:1056:VAL:HG21	2.01	0.42
2:C:716:LEU:HD11	2:C:773:ILE:HD13	2.01	0.42
2:D:466:LEU:HD11	2:D:480:MET:HG3	2.00	0.42
2:C:103:THR:HG21	2:C:142:GLU:HB2	2.01	0.42
2:D:768:GLU:H	2:D:768:GLU:HG2	1.62	0.42
2:C:183:ARG:H	2:C:183:ARG:HG2	1.65	0.42
2:C:62:ASP:OD1	2:C:62:ASP:N	2.52	0.42
2:C:112:LEU:HD13	2:C:112:LEU:HA	1.90	0.42
2:C:1434:ILE:HG22	2:C:1453:ARG:HA	2.01	0.42
2:D:325:LEU:HD11	2:D:424:ILE:HG21	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:687:ASN:N	2:C:687:ASN:OD1	2.52	0.42
2:C:1059:CYS:O	2:C:1062:ASN:ND2	2.52	0.42
2:C:495:ARG:HA	2:C:499:GLU:HB2	2.02	0.42
1:A:193:ARG:HD2	1:A:193:ARG:HA	1.94	0.42
2:C:109:ARG:HH22	2:C:112:LEU:HD21	1.85	0.42
2:D:62:ASP:OD1	2:D:62:ASP:N	2.52	0.42
2:C:1039:SER:HB3	2:C:1054:LEU:HD23	2.02	0.41
2:C:1407:ASN:O	2:C:1427:LEU:N	2.48	0.41
2:D:176:PHE:HB3	2:D:208:GLU:HB2	2.02	0.41
2:D:658:TRP:CE2	2:D:685:ALA:HB2	2.55	0.41
1:A:120:GLN:O	1:A:124:THR:OG1	2.35	0.41
1:A:194:GLY:HA2	2:C:1484:ASP:HA	2.02	0.41
1:B:115:LEU:HB3	1:B:215:ARG:HB3	2.01	0.41
2:C:658:TRP:CE2	2:C:685:ALA:HB2	2.55	0.41
2:C:1400:VAL:HA	2:C:1401:PRO:HD3	1.94	0.41
2:C:1492:ASN:ND2	2:C:1527:ALA:O	2.49	0.41
2:D:687:ASN:OD1	2:D:687:ASN:N	2.52	0.41
2:C:176:PHE:HB3	2:C:208:GLU:HB2	2.02	0.41
2:C:1479:GLU:HB2	2:C:1491:ASN:HD21	1.85	0.41
2:D:199:THR:HA	2:D:204:LEU:HD12	2.01	0.41
2:C:330:ILE:HG22	2:C:418:VAL:HG22	2.02	0.41
2:D:46:ARG:HB3	2:D:172:TYR:HB2	2.03	0.41
2:C:199:THR:HA	2:C:204:LEU:HD12	2.02	0.41
2:C:638:ILE:HG22	2:C:793:ALA:HA	2.03	0.41
2:D:1102:ASP:OD1	2:D:1102:ASP:N	2.54	0.41
2:D:1274:ASN:HA	2:D:1298:LYS:HE3	2.03	0.41
2:C:1042:LEU:HD23	2:C:1082:VAL:HG22	2.02	0.41
2:D:650:MET:HA	2:D:651:PRO:HD3	1.95	0.40
2:D:702:TYR:HA	2:D:775:ILE:O	2.21	0.40
2:D:1042:LEU:HD23	2:D:1082:VAL:HG22	2.02	0.40
2:D:1109:LEU:HD12	2:D:1109:LEU:HA	1.94	0.40
2:D:123:TYR:OH	2:D:145:GLY:O	2.35	0.40
2:D:163:SER:OG	2:D:164:ALA:N	2.54	0.40
2:D:330:ILE:HG22	2:D:418:VAL:HG22	2.03	0.40
2:D:1039:SER:HB3	2:D:1054:LEU:HD23	2.02	0.40
1:B:149:VAL:HG11	1:B:219:ILE:HD11	2.03	0.40
2:C:46:ARG:HB3	2:C:172:TYR:HB2	2.04	0.40
2:C:972:ARG:HH12	2:C:980:GLU:HB3	1.86	0.40
2:D:128:MET:HG3	2:D:140:SER:HB3	2.03	0.40
2:D:715:SER:HB3	2:D:790:THR:HB	2.03	0.40
2:D:1079:SER:HB2	2:D:1098:LEU:HD21	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:326:ARG:HA	2:C:326:ARG:HD2	1.90	0.40
2:C:961:ILE:H	2:C:961:ILE:HG13	1.64	0.40
2:D:258:ILE:HD12	2:D:258:ILE:HA	1.94	0.40
2:D:1492:ASN:ND2	2:D:1527:ALA:O	2.49	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	133/222 (60%)	128 (96%)	5 (4%)	0	100	100
1	B	133/222 (60%)	128 (96%)	5 (4%)	0	100	100
2	C	1476/1627 (91%)	1426 (97%)	49 (3%)	1 (0%)	48	78
2	D	1476/1627 (91%)	1425 (96%)	51 (4%)	0	100	100
All	All	3218/3698 (87%)	3107 (97%)	110 (3%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	1467	PRO

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	115/191 (60%)	109 (95%)	6 (5%)	21	45
1	B	115/191 (60%)	109 (95%)	6 (5%)	21	45
2	C	1304/1414 (92%)	1232 (94%)	72 (6%)	19	44
2	D	1304/1414 (92%)	1233 (95%)	71 (5%)	20	44
All	All	2838/3210 (88%)	2683 (94%)	155 (6%)	21	44

All (155) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	98	VAL
1	A	125	CYS
1	A	134	VAL
1	A	145	ILE
1	A	156	GLN
1	A	215	ARG
1	B	98	VAL
1	B	125	CYS
1	B	134	VAL
1	B	145	ILE
1	B	156	GLN
1	B	215	ARG
2	C	22	ARG
2	C	43	VAL
2	C	45	LEU
2	C	51	GLN
2	C	64	CYS
2	C	74	VAL
2	C	78	HIS
2	C	102	VAL
2	C	112	LEU
2	C	160	LEU
2	C	184	THR
2	C	201	LEU
2	C	204	LEU
2	C	221	LYS
2	C	222	ASP
2	C	250	THR
2	C	279	ASN
2	C	319	GLU
2	C	356	ASP
2	C	374	ASN
2	C	376	VAL

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Mol	Chain	Res	Type
2	C	418	VAL
2	C	477	THR
2	C	484	ILE
2	C	558	TYR
2	C	567	PHE
2	C	623	GLU
2	C	632	LEU
2	C	701	CYS
2	C	703	LEU
2	C	711	LEU
2	C	723	VAL
2	C	755	CYS
2	C	778	LEU
2	C	782	LEU
2	C	822	LEU
2	C	824	LEU
2	C	829	VAL
2	C	831	MET
2	C	833	LEU
2	C	843	VAL
2	C	858	VAL
2	C	859	THR
2	C	867	CYS
2	C	889	ASP
2	C	893	LEU
2	C	928	ILE
2	C	953	ASP
2	C	961	ILE
2	C	975	VAL
2	C	976	ILE
2	C	978	LEU
2	C	990	CYS
2	C	1038	ILE
2	C	1045	THR
2	C	1062	ASN
2	C	1064	LEU
2	C	1069	VAL
2	C	1160	VAL
2	C	1167	VAL
2	C	1170	ILE
2	C	1177	ILE
2	C	1185	VAL

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Mol	Chain	Res	Type
2	C	1203	VAL
2	C	1220	CYS
2	C	1252	ASP
2	C	1266	CYS
2	C	1317	THR
2	C	1331	VAL
2	C	1333	VAL
2	C	1457	VAL
2	C	1486	TYR
2	D	22	ARG
2	D	43	VAL
2	D	45	LEU
2	D	51	GLN
2	D	64	CYS
2	D	74	VAL
2	D	78	HIS
2	D	102	VAL
2	D	112	LEU
2	D	160	LEU
2	D	184	THR
2	D	201	LEU
2	D	204	LEU
2	D	221	LYS
2	D	222	ASP
2	D	250	THR
2	D	279	ASN
2	D	319	GLU
2	D	356	ASP
2	D	374	ASN
2	D	376	VAL
2	D	418	VAL
2	D	477	THR
2	D	484	ILE
2	D	558	TYR
2	D	567	PHE
2	D	623	GLU
2	D	632	LEU
2	D	701	CYS
2	D	703	LEU
2	D	711	LEU
2	D	723	VAL
2	D	755	CYS

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Mol	Chain	Res	Type
2	D	778	LEU
2	D	824	LEU
2	D	829	VAL
2	D	831	MET
2	D	833	LEU
2	D	843	VAL
2	D	858	VAL
2	D	859	THR
2	D	862	HIS
2	D	867	CYS
2	D	889	ASP
2	D	893	LEU
2	D	928	ILE
2	D	953	ASP
2	D	961	ILE
2	D	975	VAL
2	D	976	ILE
2	D	978	LEU
2	D	990	CYS
2	D	1023	LEU
2	D	1038	ILE
2	D	1045	THR
2	D	1069	VAL
2	D	1160	VAL
2	D	1167	VAL
2	D	1170	ILE
2	D	1177	ILE
2	D	1185	VAL
2	D	1203	VAL
2	D	1252	ASP
2	D	1266	CYS
2	D	1317	THR
2	D	1331	VAL
2	D	1333	VAL
2	D	1334	THR
2	D	1336	ASP
2	D	1457	VAL
2	D	1486	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (38) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	116	GLN
1	A	142	ASN
1	A	188	HIS
1	A	211	HIS
1	B	116	GLN
1	B	188	HIS
1	B	211	HIS
2	C	25	GLN
2	C	78	HIS
2	C	168	ASN
2	C	403	GLN
2	C	467	ASN
2	C	492	HIS
2	C	521	ASN
2	C	570	ASN
2	C	913	HIS
2	C	942	GLN
2	C	1146	ASN
2	C	1285	ASN
2	C	1287	HIS
2	C	1402	ASN
2	C	1491	ASN
2	C	1523	GLN
2	D	25	GLN
2	D	78	HIS
2	D	403	GLN
2	D	467	ASN
2	D	492	HIS
2	D	521	ASN
2	D	587	GLN
2	D	913	HIS
2	D	1062	ASN
2	D	1146	ASN
2	D	1239	GLN
2	D	1285	ASN
2	D	1287	HIS
2	D	1402	ASN
2	D	1523	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

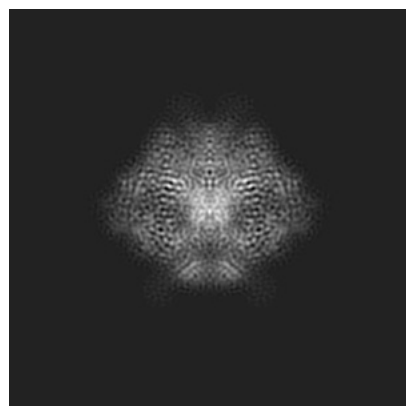
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-34738. These allow visual inspection of the internal detail of the map and identification of artifacts.

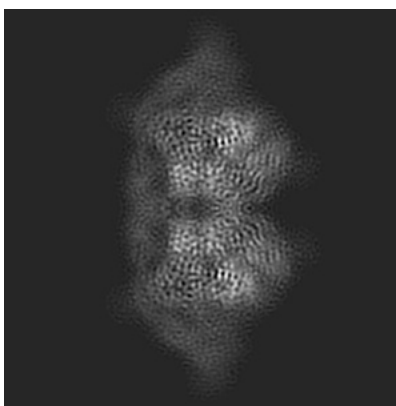
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

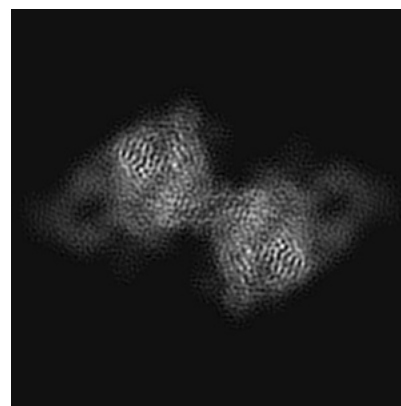
6.1.1 Primary map



X

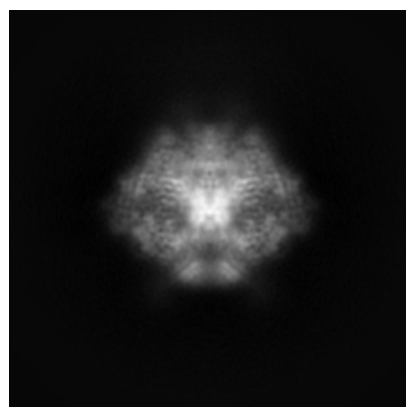


Y

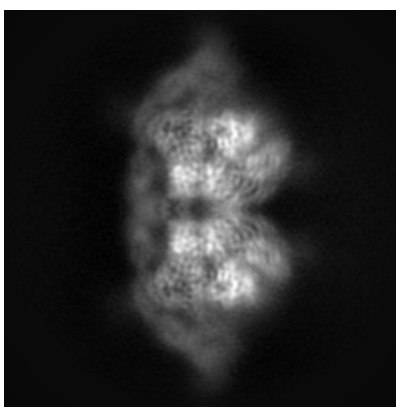


Z

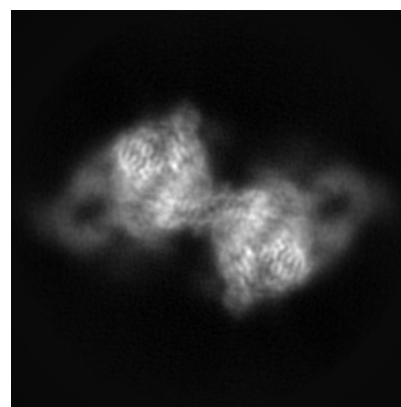
6.1.2 Raw map



X



Y



Z

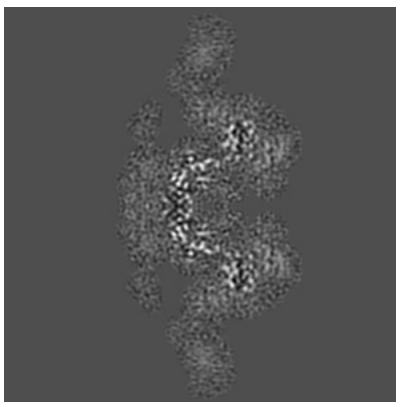
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

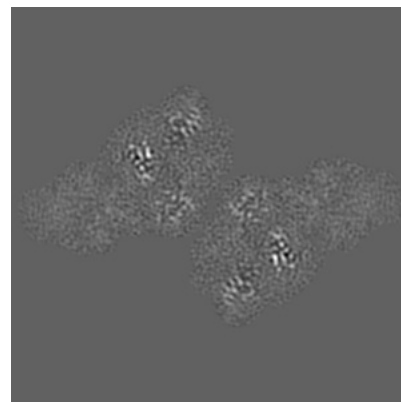
6.2.1 Primary map



X Index: 128

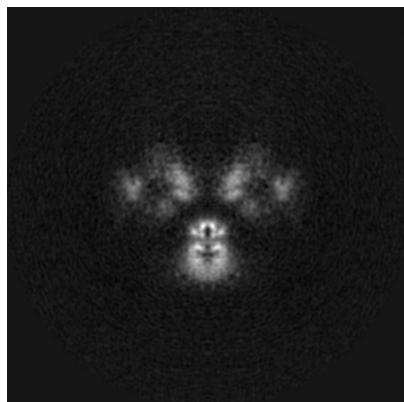


Y Index: 128

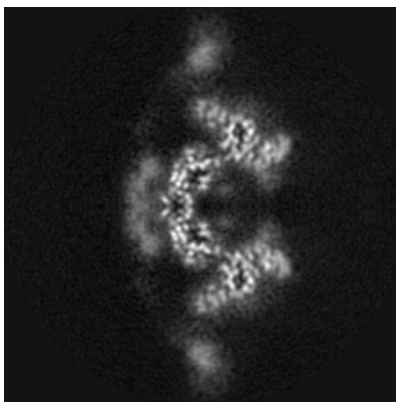


Z Index: 128

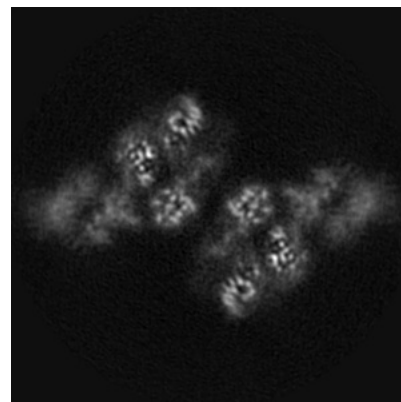
6.2.2 Raw map



X Index: 128



Y Index: 128



Z Index: 128

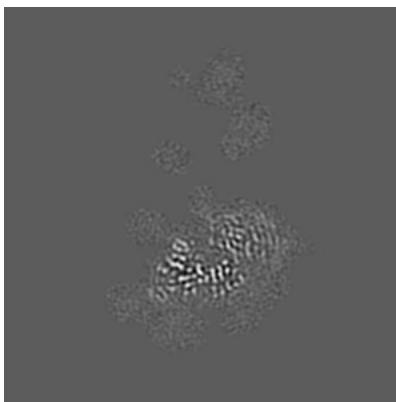
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

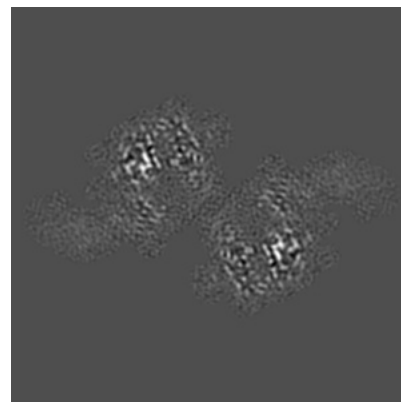
6.3.1 Primary map



X Index: 85

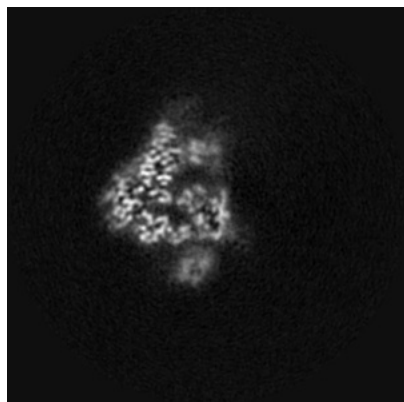


Y Index: 157

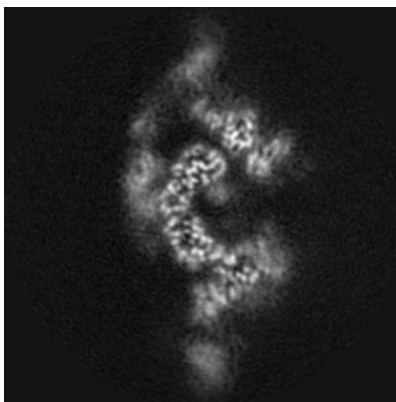


Z Index: 142

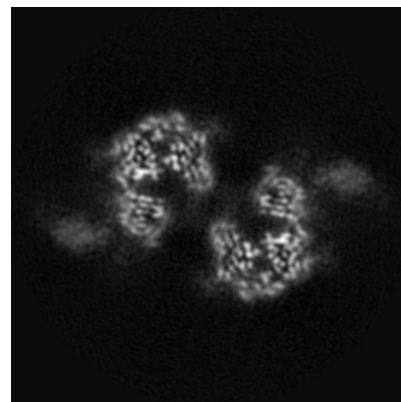
6.3.2 Raw map



X Index: 151



Y Index: 123

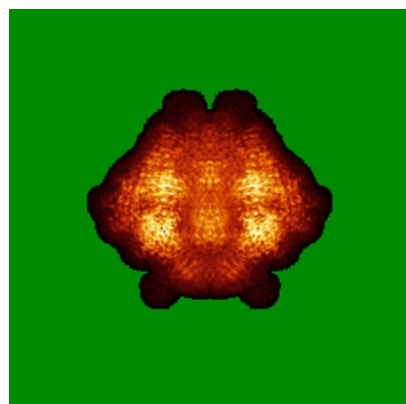


Z Index: 146

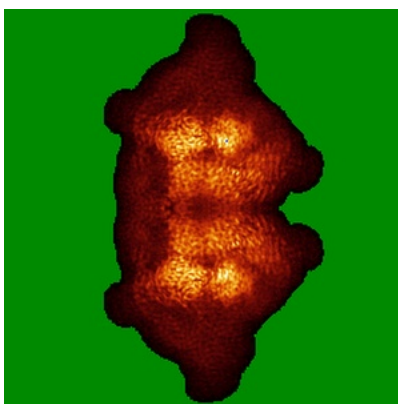
The images above show the largest variance slices of the map in three orthogonal directions.

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

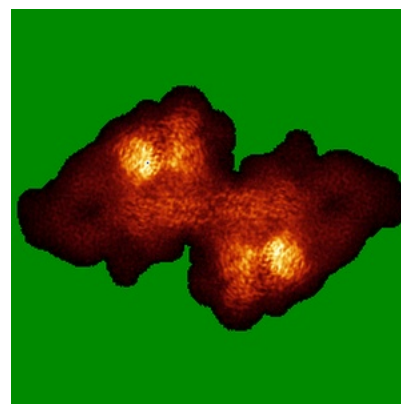
6.4.1 Primary map



X

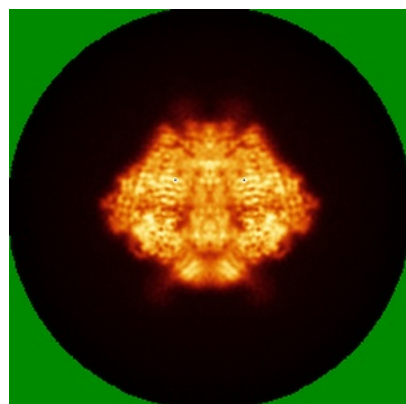


Y

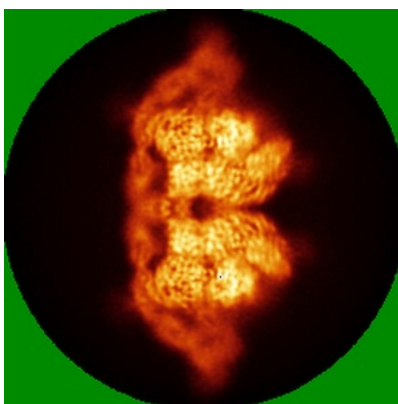


Z

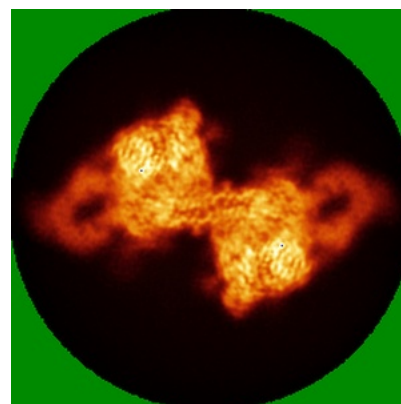
6.4.2 Raw map



X



Y

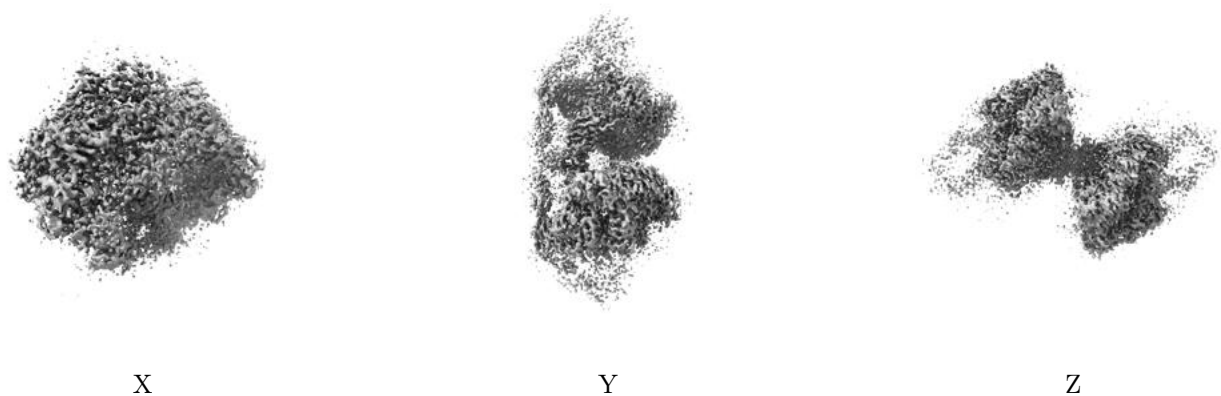


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

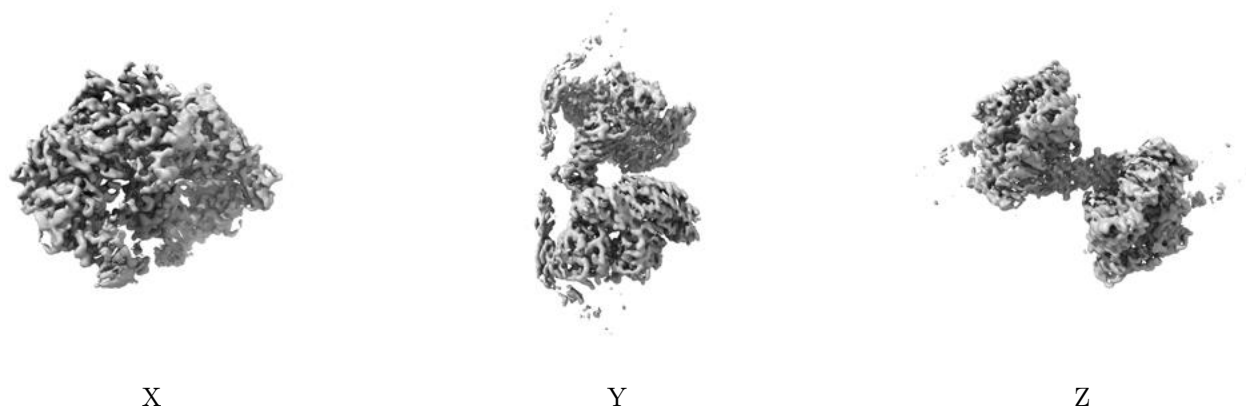
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0262. 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.

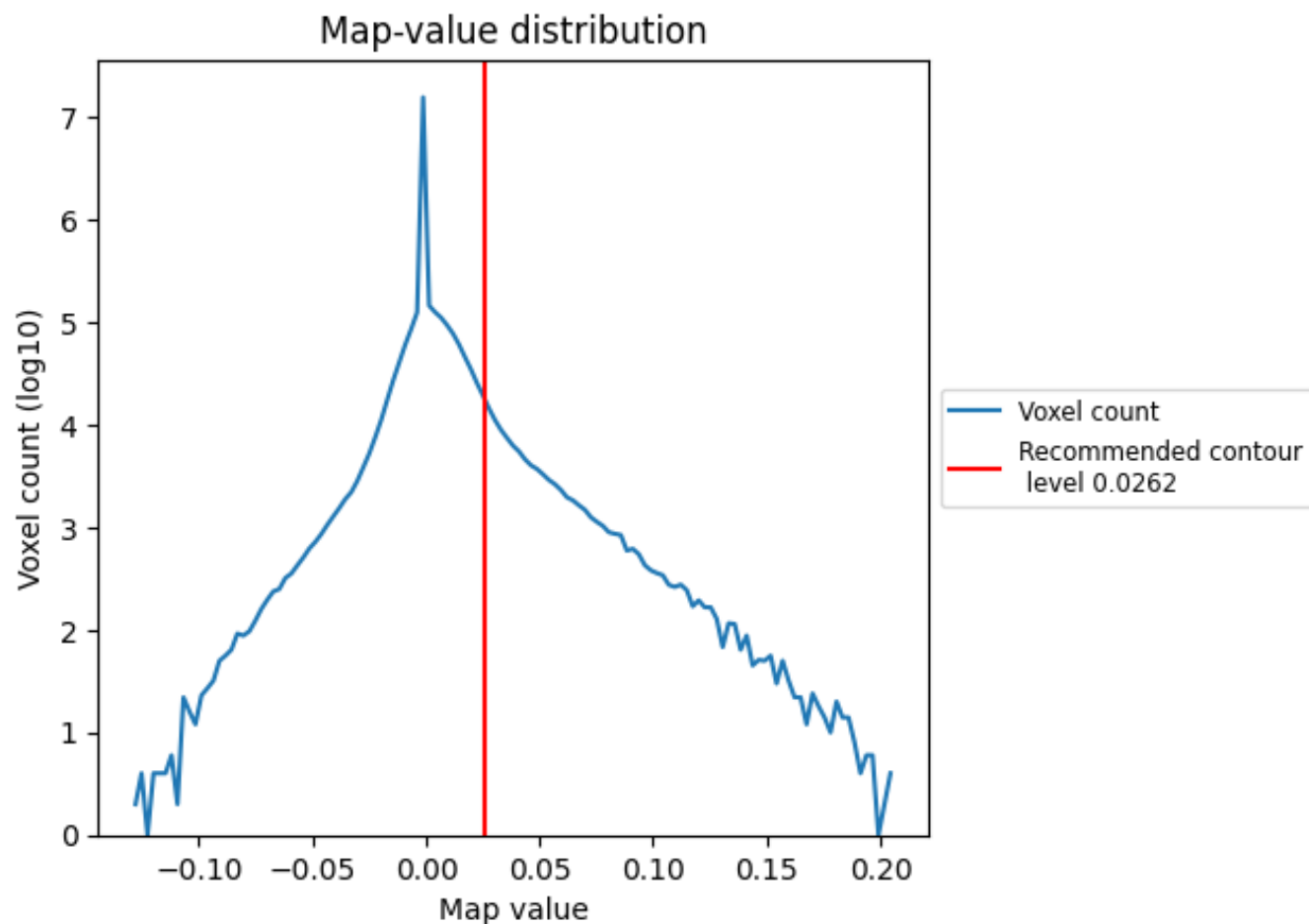
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

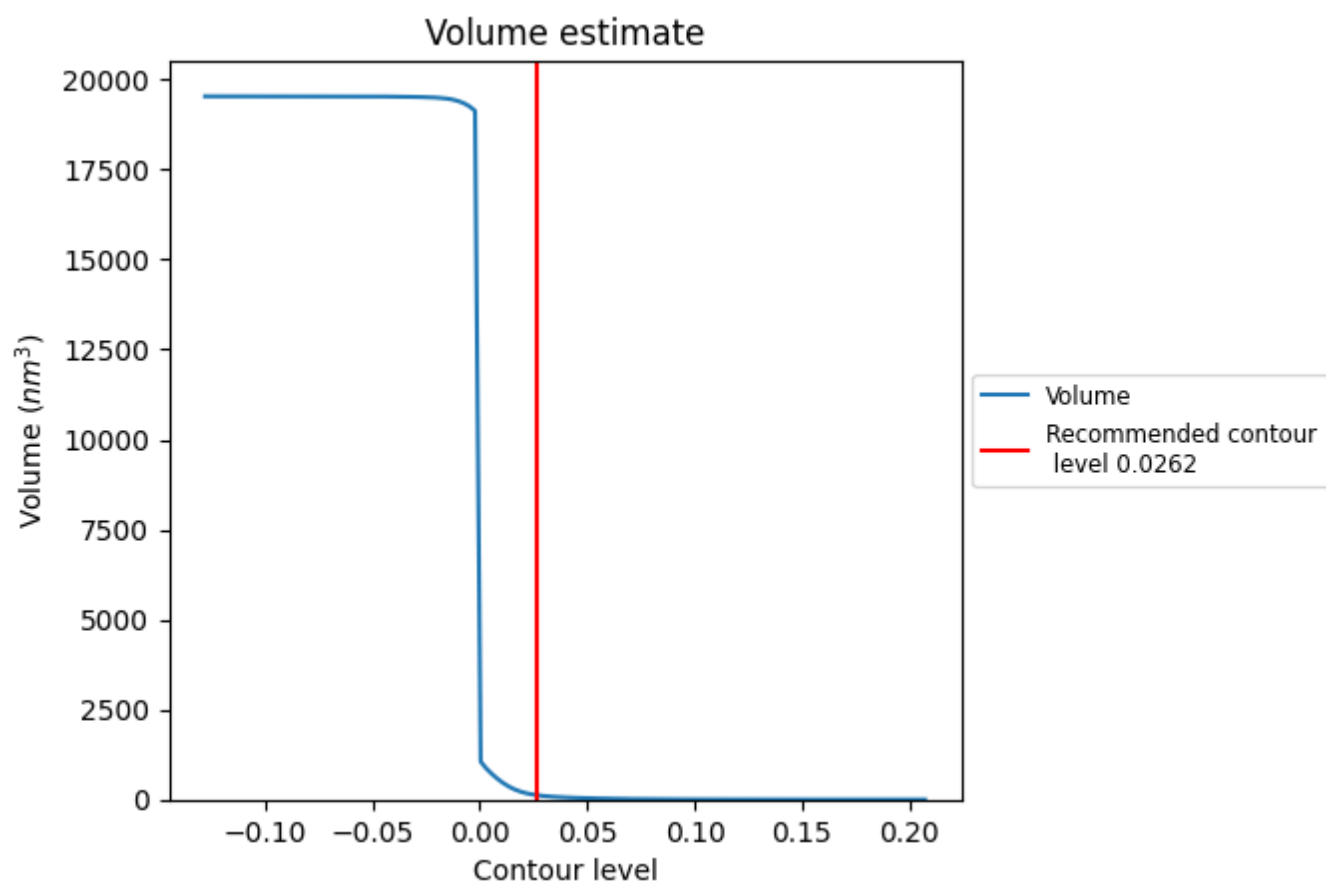
This section contains the results of statistical analysis of the map.

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.

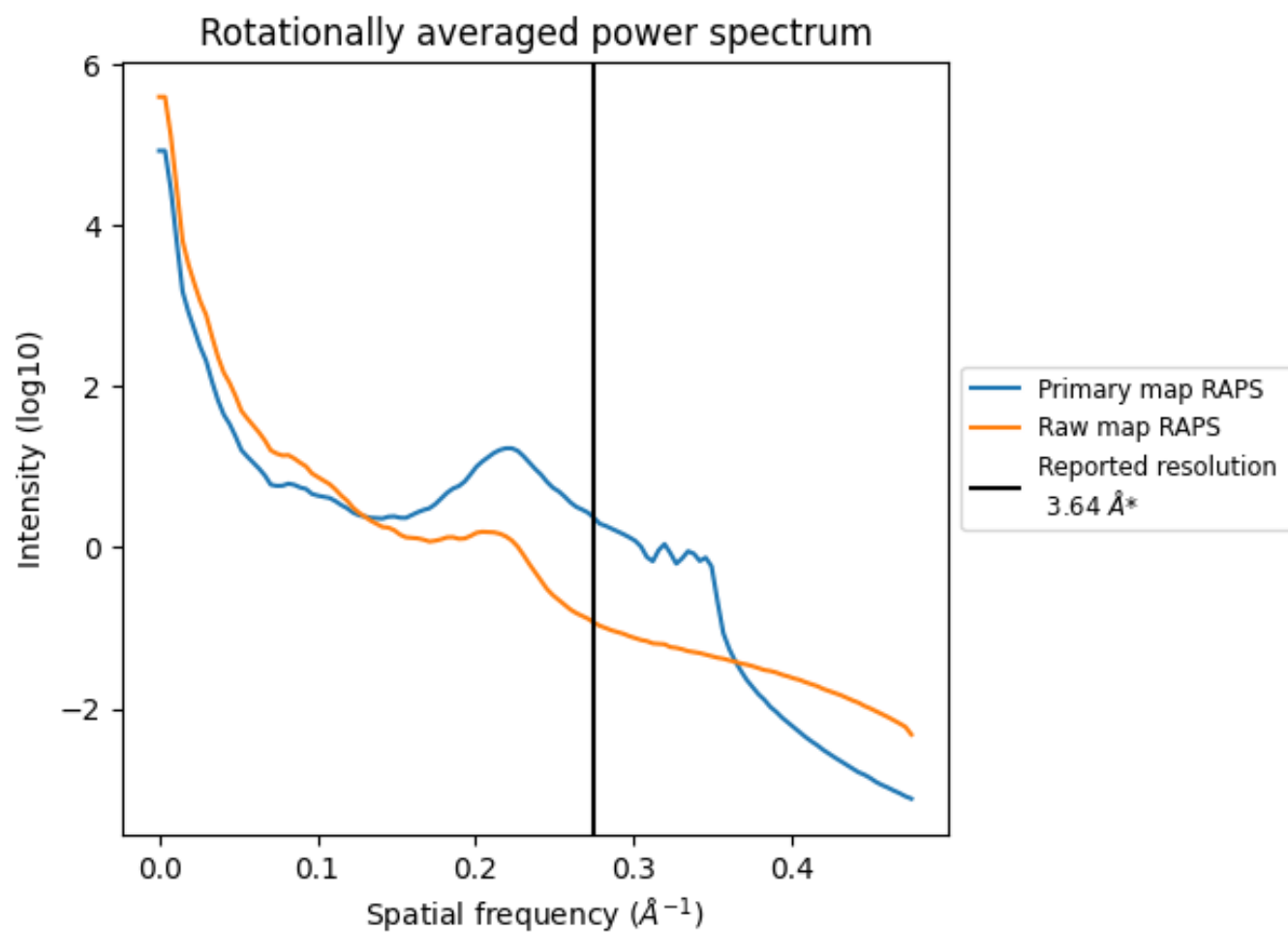
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 125 nm³; this corresponds to an approximate mass of 112 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 ⓘ

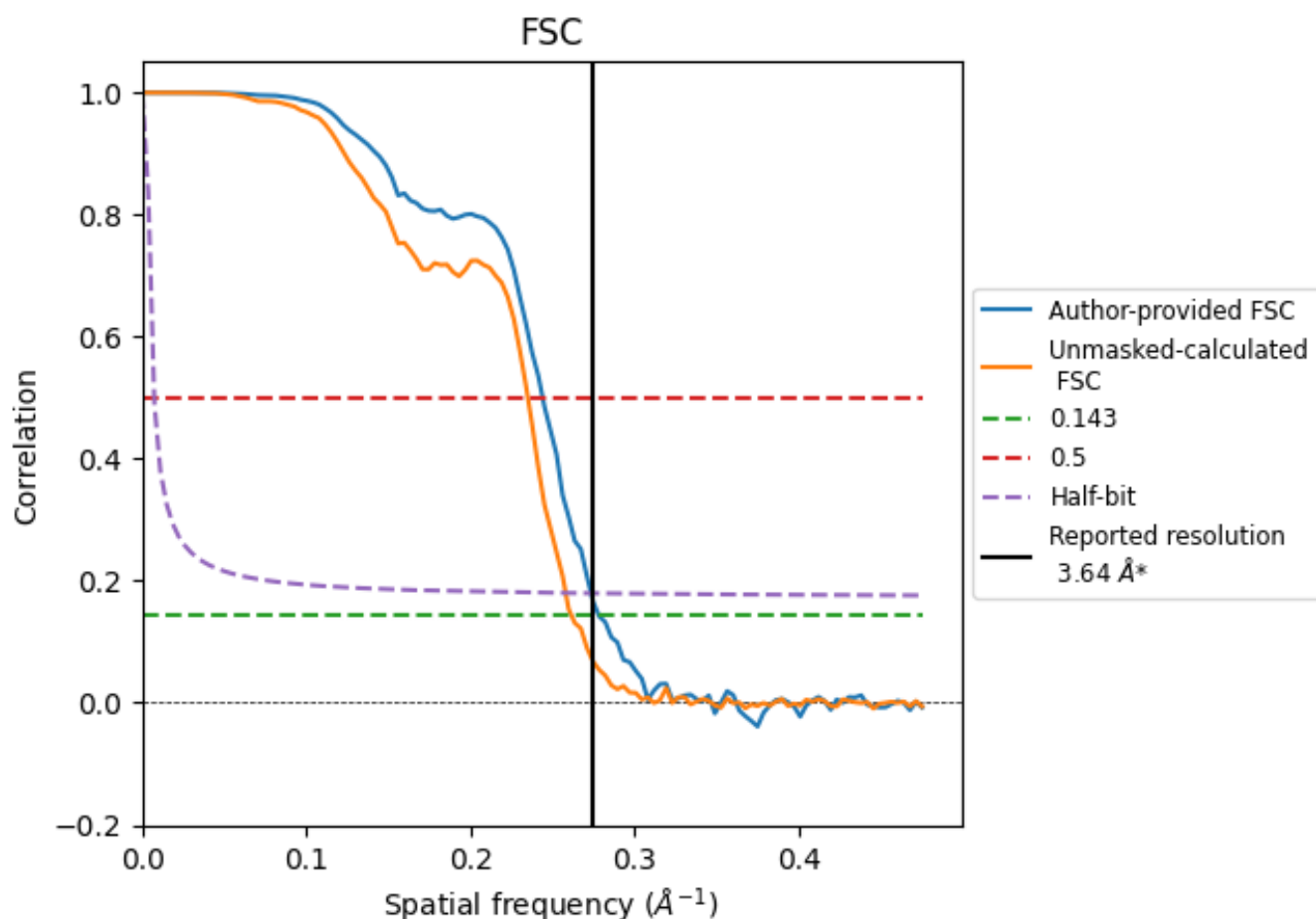


*Reported resolution corresponds to spatial frequency of $0.275 \text{ \AA}^{-1}$

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.275 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.64	-	-
Author-provided FSC curve	3.59	4.10	3.66
Unmasked-calculated*	3.82	4.25	3.87

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

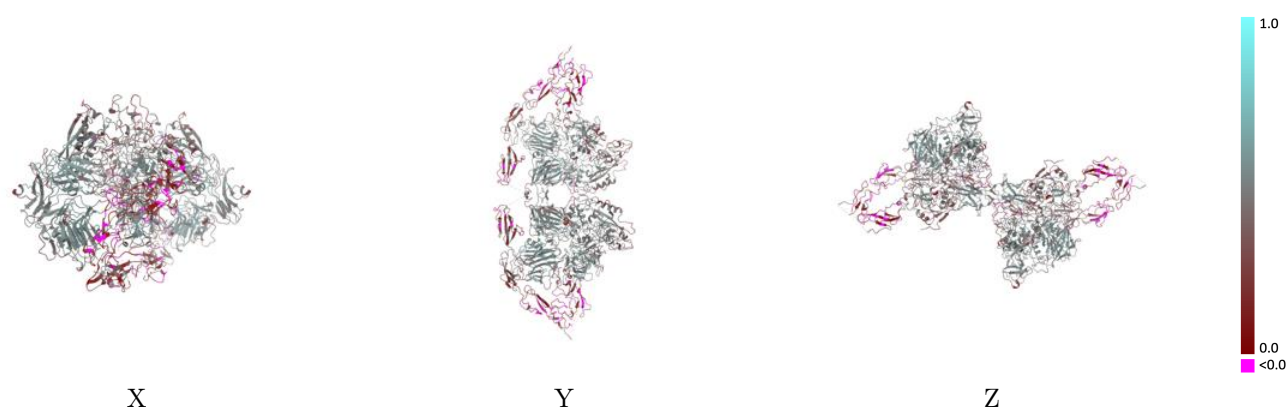
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-34738 and PDB model 8HGG. Per-residue inclusion information can be found in section [3](#) on page [4](#).

9.1 Map-model overlay [i](#)

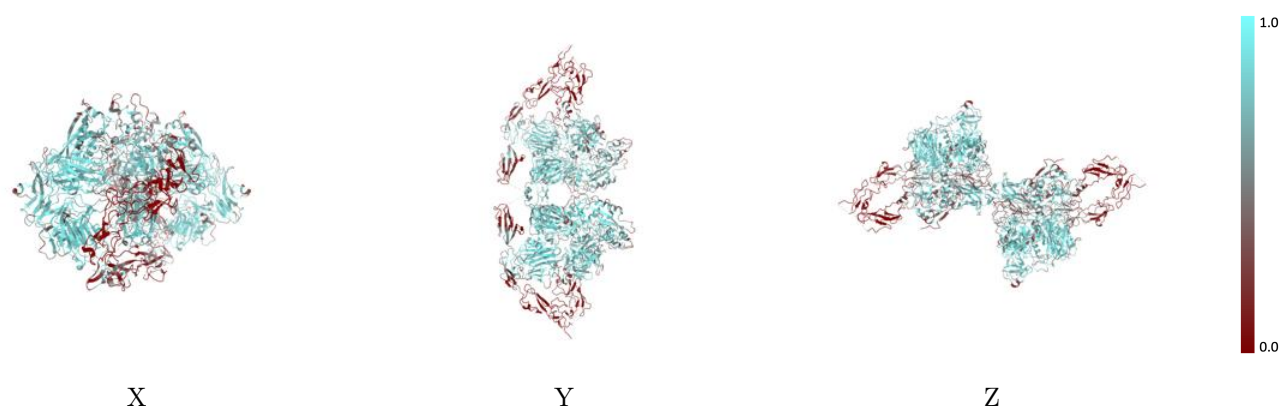
This section was not generated.

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



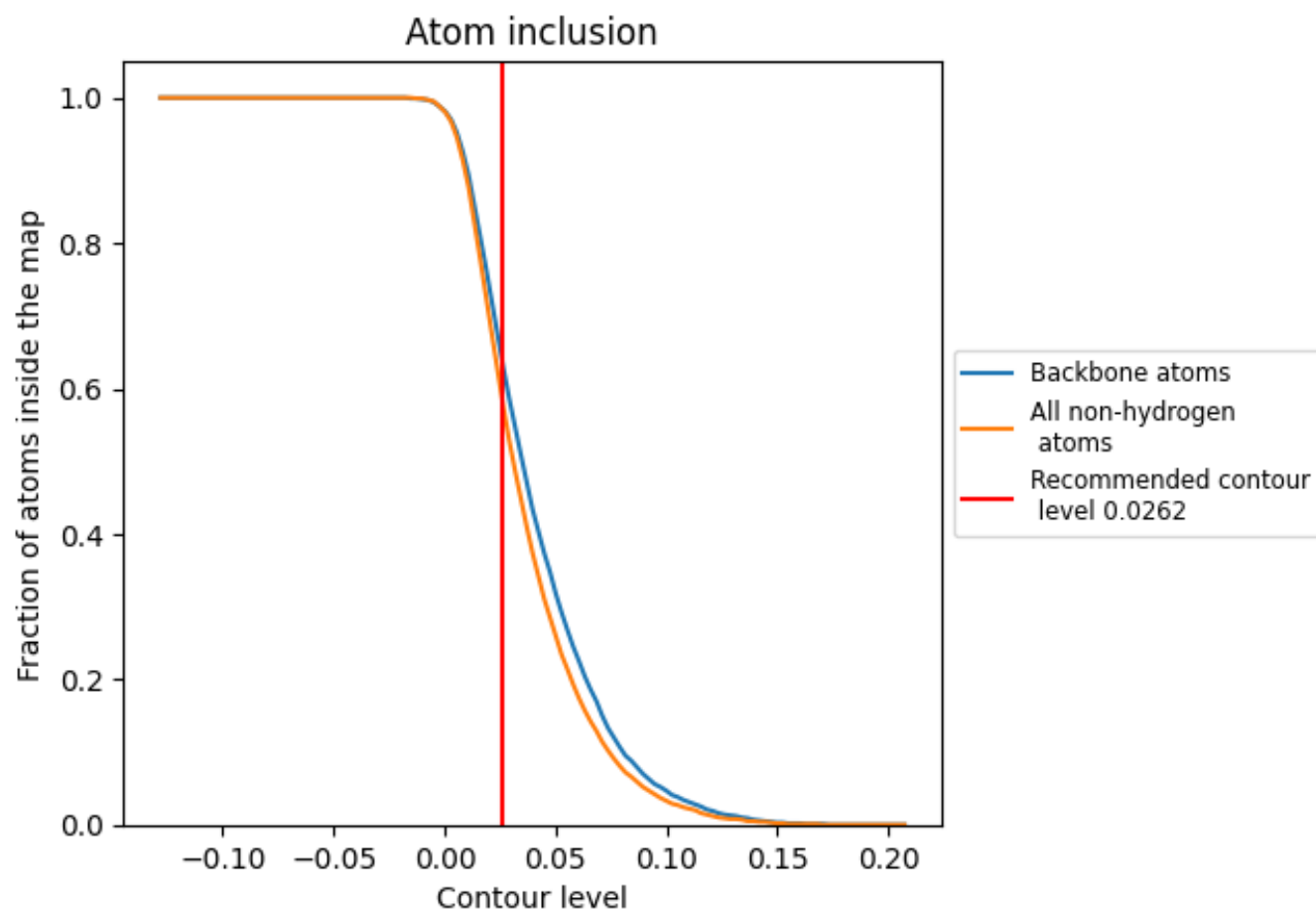
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0262).

9.4 Atom inclusion [i](#)



At the recommended contour level, 63% of all backbone atoms, 58% 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 (0.0262) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5800	0.4080
A	0.6200	0.4430
B	0.6230	0.4420
C	0.5770	0.4060
D	0.5760	0.4030

