Full wwPDB EM Validation Report ⓘ

Jan 2, 2025 – 03:13 pm GMT

PDB ID	:	8P1J
EMDB ID	:	EMD-17351
Title	:	Structure of hantaan orthohantavirus (HTNV) polymerase - Apo core
Authors	:	Keown, J.R.; Carrique, L.; Grimes, J.M.
Deposited on	:	2023-05-12
Resolution	:	2.78 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:

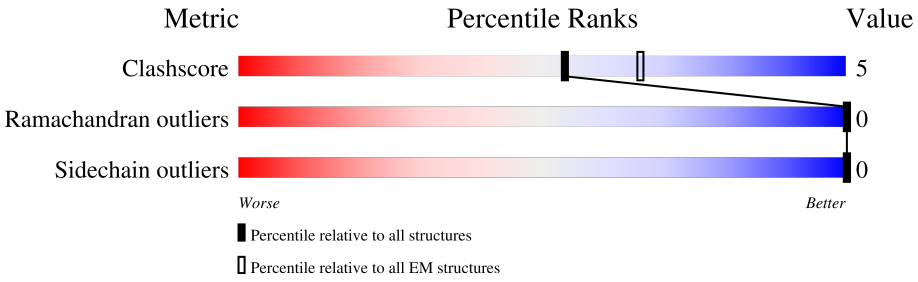
EMDB validation analysis	:	0.0.1.dev113
MolProbity	:	4.02b-467
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.40

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 2.78 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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 <=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	2196	51% 8% 41%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 10435 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 RNA-directed RNA polymerase L.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	1293	10435	6714	1752	1913	56	1	0

There are 46 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-44	MET	-	initiating methionine	UNP P23456
A	-43	TRP	-	expression tag	UNP P23456
A	-42	SER	-	expression tag	UNP P23456
A	-41	HIS	-	expression tag	UNP P23456
A	-40	PRO	-	expression tag	UNP P23456
A	-39	GLN	-	expression tag	UNP P23456
A	-38	PHE	-	expression tag	UNP P23456
A	-37	GLU	-	expression tag	UNP P23456
A	-36	LYS	-	expression tag	UNP P23456
A	-35	GLY	-	expression tag	UNP P23456
A	-34	GLY	-	expression tag	UNP P23456
A	-33	GLY	-	expression tag	UNP P23456
A	-32	SER	-	expression tag	UNP P23456
A	-31	GLY	-	expression tag	UNP P23456
A	-30	GLY	-	expression tag	UNP P23456
A	-29	GLY	-	expression tag	UNP P23456
A	-28	SER	-	expression tag	UNP P23456
A	-27	GLY	-	expression tag	UNP P23456
A	-26	GLY	-	expression tag	UNP P23456
A	-25	SER	-	expression tag	UNP P23456
A	-24	SER	-	expression tag	UNP P23456
A	-23	ALA	-	expression tag	UNP P23456
A	-22	TRP	-	expression tag	UNP P23456
A	-21	SER	-	expression tag	UNP P23456
A	-20	HIS	-	expression tag	UNP P23456
A	-19	PRO	-	expression tag	UNP P23456
A	-18	GLN	-	expression tag	UNP P23456
A	-17	PHE	-	expression tag	UNP P23456

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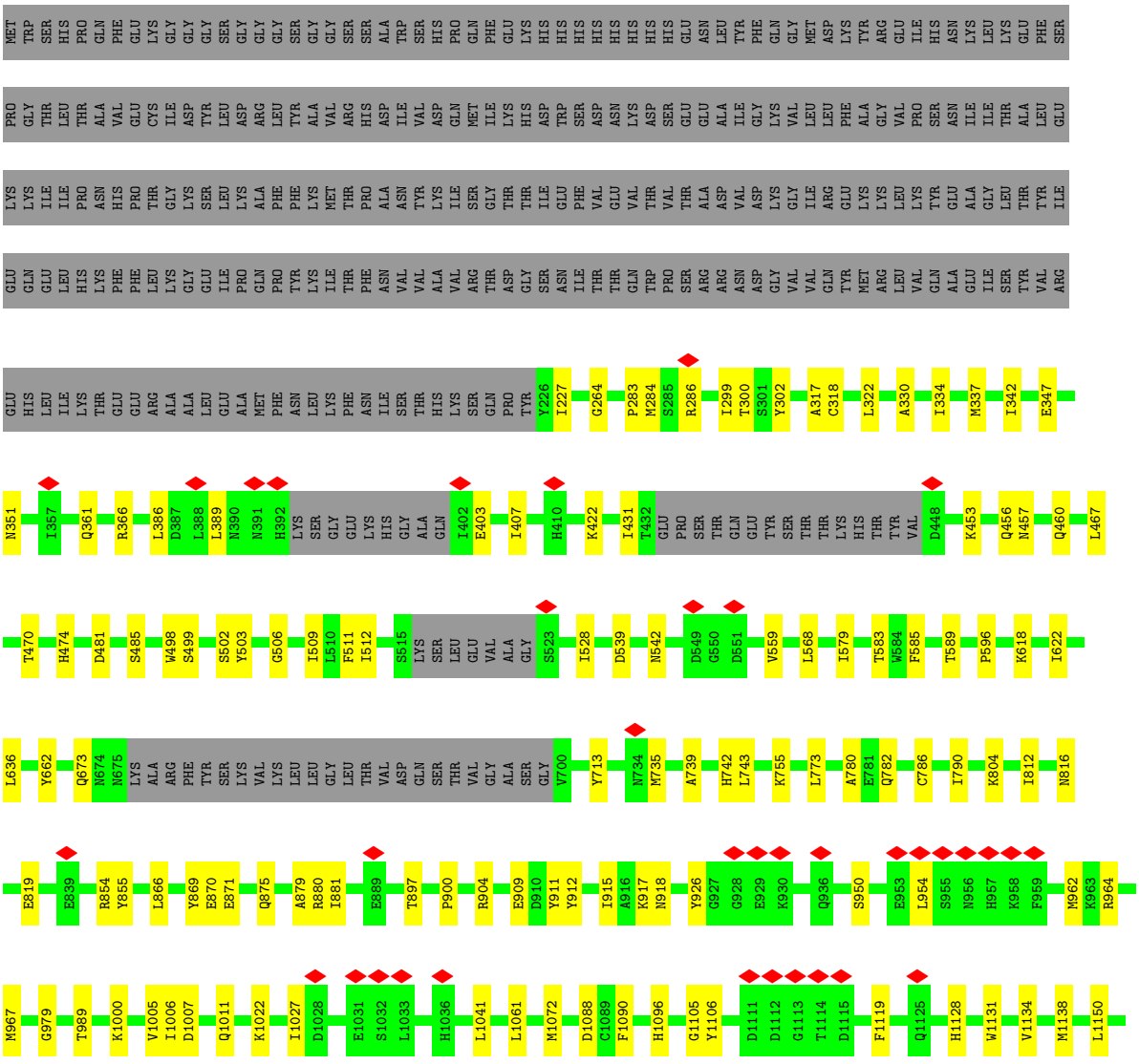
Chain	Residue	Modelled	Actual	Comment	Reference
A	-16	GLU	-	expression tag	UNP P23456
A	-15	LYS	-	expression tag	UNP P23456
A	-14	HIS	-	expression tag	UNP P23456
A	-13	HIS	-	expression tag	UNP P23456
A	-12	HIS	-	expression tag	UNP P23456
A	-11	HIS	-	expression tag	UNP P23456
A	-10	HIS	-	expression tag	UNP P23456
A	-9	HIS	-	expression tag	UNP P23456
A	-8	HIS	-	expression tag	UNP P23456
A	-7	HIS	-	expression tag	UNP P23456
A	-6	GLU	-	expression tag	UNP P23456
A	-5	ASN	-	expression tag	UNP P23456
A	-4	LEU	-	expression tag	UNP P23456
A	-3	TYR	-	expression tag	UNP P23456
A	-2	PHE	-	expression tag	UNP P23456
A	-1	GLN	-	expression tag	UNP P23456
A	0	GLY	-	expression tag	UNP P23456
A	97	ALA	ASP	engineered mutation	UNP P23456

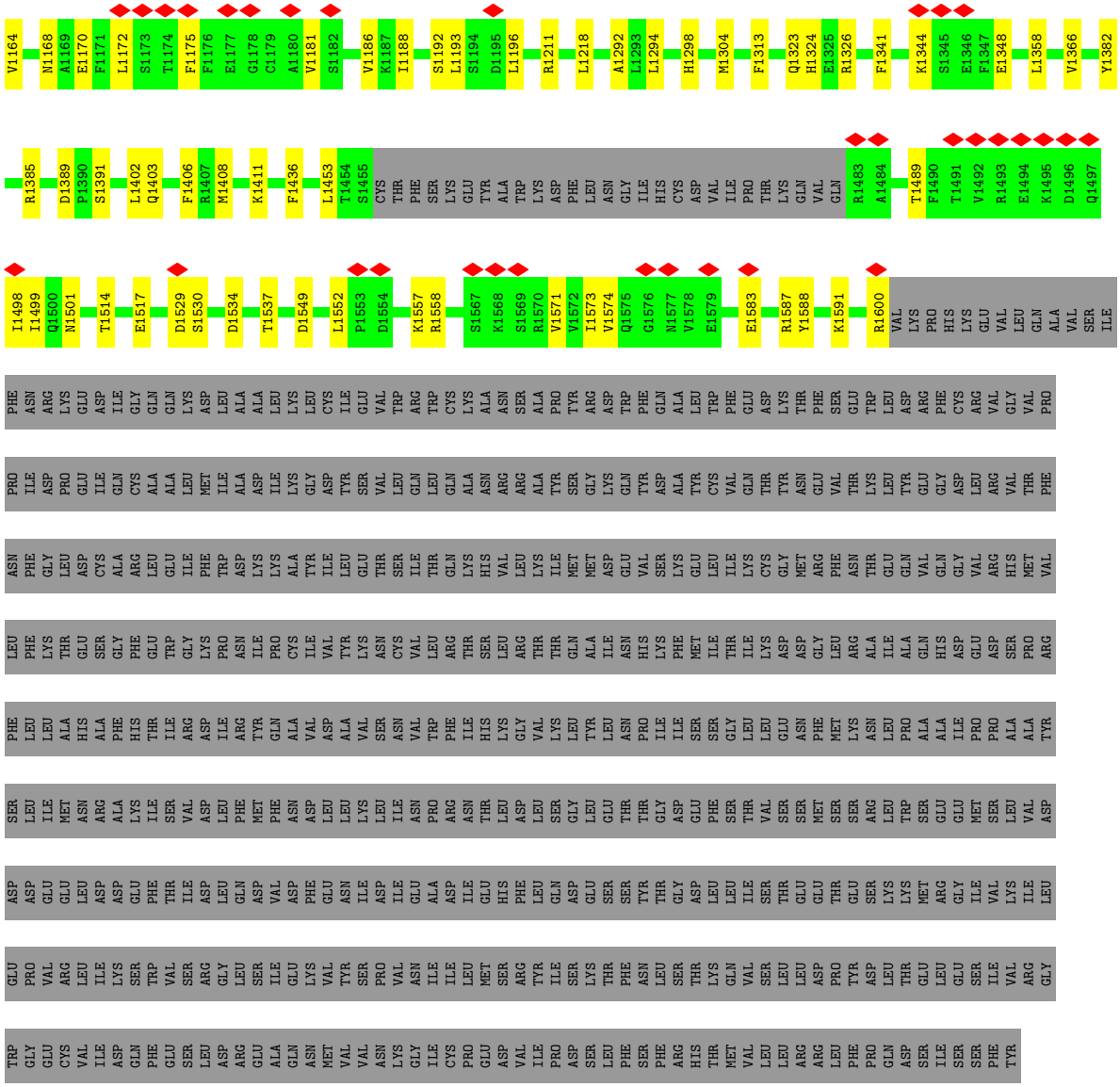
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: RNA-directed RNA polymerase L

Chain A:




V1164 N1168 A1169 E1170 F1171 L1172 S1173 T1174 F1175 F1176 E1177 G1178 C1179 A1180 V1181 S1182 V1186 K1187 I1188 S1192 L1193 S1194 D1195 L1196 R1211 L1218 A1292 L1293 L1294 H1298 M1304 F1313 Q1323 H1324 E1325 R1326 F1341 K1344 S1345 E1346 F1347 E1348 L1358 V1366 Y1382
R1385 D1389 P1390 S1391 L1402 Q1403 F1406 R1407 M1408 K1411 F1436 L1453 T1454 S1455 CYS THR PHE SER LYS GLU TYR ALA TRP LYS ASP PHE LEU ASN GLY ILE HIS CYS ASP VAL ILE PRO THR LYS GLN VAL GLN R1483 A1484 T1489 F1490 T1491 V1492 R1493 E1494 K1495 D1496 Q1497
I1498 I1499 Q1500 N1501 T1514 E1517 D1529 S1530 D1534 T1537 D1549 L1552 P1553 D1554 K1557 R1558 S1567 K1568 S1569 R1570 V1571 V1572 I1573 V1574 Q1575 G1576 N1577 V1578 E1579 E1583 R1587 Y1588 K1591 R1600 VAL LYS PRO HIS LYS GLU VAL LEU GLN ALA VAL SER ILE
PHE ASN ARG LYS GLU ASP ILE GLY GLN GLN LYS ASP LEU ALA ALA LEU LYS LEU CYS ILE GLU VAL TRP ARG TRP CYS LYS ALA ASN SER ALA PRO TYR ARG ASP TRP PHE GLN ALA LEU TRP PHE GLU ASP LYS THR PHE SER GLU TRP LEU ASP ARG PHE CYS ARG VAL GLY VAL PRO
PRO ILE ASP PRO GLU ILE GLN CYS ALA ALA LEU MET ILE ALA ASP ILE LYS GLY ASP TYR SER VAL LEU GLN LEU GLN ALA ASN ARG ARG ALA TYR SER GLY LYS GLN TYR ASP ALA TYR CYS VAL GLN THR THR TYR ASN GLU VAL THR LYS LEU TYR GLU GLY ASP LEU ARG VAL THR PHE
ASN PHE GLY LEU ASP CYS ALA ARG LEU GLU GLU ILE PHE TRP ASP LYS LYS ALA TYR ILE LEU GLU THR SER ILE THR GLN LYS HIS VAL LEU LYS ILE MET MET ASP GLU VAL SER LYS GLU LEU ILE LYS CYS GLY MET ARG PHE ASN THR GLU GLN VAL GLN GLY VAL ARG HIS MET VAL
LEU PHE LYS THR GLU SER GLY PHE GLU TRP GLY LYS PRO ASN ILE PRO CYS ILE VAL TYR LYS ASN CYS VAL LEU ARG THR SER LEU LYS ARG THR THR GLN ALA ILE ASN HIS LYS PHE MET ILE THR ILE LYS ASP ASP GLY LEU ARG ALA ILE ALA GLN HIS ASP GLU ASP SER PRO ARG
PHE LEU LEU ALA HIS ALA PHE HIS THR ILE ARG ARG ASP ILE ARG TYR GLN ALA VAL ASP ALA VAL SER ASN VAL TRP PHE ILE HIS LYS GLY VAL LYS LEU TYR LEU ASN VAL PRO ILE ILE SER SER GLY LEU ILE ASN PRO ILE ILE SER GLY LEU GLU ASN PHE MET LYS ASN LEU PRO ALA ALA ILE PRO PRO ALA TYR
SER LEU LEU ALA LYS ILE SER VAL ASP LEU PHE MET PHE ASN ASP LEU LEU LYS LEU ILE ASN PRO ARG ASN THR LEU ASP LEU SER GLY LEU GLU THR THR GLY ASP GLU PHE SER THR VAL SER SER MET SER SER ARG LEU TRP SER GLU GLU MET SER LEU VAL ASP
ASP ASP GLU GLU LEU ASP ASP GLU PHE THR ILE ASP LEU GLN ASP VAL ASP PHE GLU ASN ILE ASP ILE GLU ALA ASP ILE GLU HIS PHE LEU GLN ASP GLU SER SER TYR THR GLY ASP LEU LEU ILE SER THR GLU GLU THR GLU SER LYS LYS MET ARG GLY ILE VAL LYS LEU ILE LEU
GLU PRO VAL ARG LEU ILE LYS SER TRP VAL SER ARG GLY LEU SER ILE GLU LYS VAL TYR SER PRO VAL ASN ILE ILE LEU MET SER ARG TYR ILE SER LYS THR PHE ASN LEU SER THR LYS GLN VAL SER LEU LEU ASP PRO TYR ASP LEU THR GLU GLU GLU SER ILE VAL ARG GLY
TRP GLY GLU CYS VAL ILE ASP GLN PHE GLU SER LEU ASP ARG GLU ALA GLN ASN MET VAL VAL ASN LYS GLY ILE CYS PRO GLU ASP VAL ILE PRO ASP SER LEU PHE SER PHE ARG HIS THR MET VAL LEU LEU LEU ARG ARG LEU PHE PRO GLN ASP SER ILE SER SER PHE TYR

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	500000	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 ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	1400	Depositor
Maximum defocus (nm)	2600	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	3.316	Depositor
Minimum map value	-2.391	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.074	Depositor
Recommended contour level	0.356	Depositor
Map size (Å)	279.6, 279.6, 279.6	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.93200004, 0.93200004, 0.93200004	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	0.27	0/10668	0.47	0/14413

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	10435	0	10453	104	0
All	All	10435	0	10453	104	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 5.

All (104) 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:917:LYS:HA	1:A:926:TYR:HE2	1.47	0.79
1:A:568:LEU:HB2	1:A:1408:MET:HE2	1.65	0.76
1:A:869:TYR:OH	1:A:1007:ASP:OD2	2.08	0.70
1:A:583:THR:HG21	1:A:1186:VAL:HG22	1.78	0.66
1:A:755:LYS:NZ	1:A:782:GLN:O	2.27	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:227:ILE:HB	1:A:1000:LYS:HE2	1.78	0.65
1:A:337:MET:HE2	1:A:511:PHE:HD2	1.62	0.63
1:A:1344:LYS:HE3	1:A:1402:LEU:HD11	1.79	0.63
1:A:1591:LYS:HE2	1:A:1600:ARG:HG3	1.81	0.63
1:A:1027:ILE:HG21	1:A:1041:LEU:HD21	1.81	0.62
1:A:1323:GLN:HB3	1:A:1326:ARG:HG3	1.81	0.61
1:A:855:TYR:OH	1:A:871:GLU:OE1	2.18	0.61
1:A:1196:LEU:HD23	1:A:1211:ARG:HH12	1.65	0.61
1:A:283:PRO:HB2	1:A:403:GLU:HG2	1.84	0.60
1:A:636:LEU:HD23	1:A:967:MET:HE1	1.85	0.59
1:A:854:ARG:NH2	1:A:1348:GLU:OE1	2.35	0.59
1:A:1181:VAL:HG12	1:A:1573:ILE:HD11	1.84	0.58
1:A:299:ILE:HG13	1:A:300:THR:HG23	1.85	0.58
1:A:1498:ILE:HB	1:A:1537:THR:HG21	1.85	0.58
1:A:485:SER:OG	1:A:503:TYR:OH	2.15	0.58
1:A:389:LEU:HD11	1:A:559:VAL:HG21	1.86	0.58
1:A:909:GLU:OE2	1:A:1061:LEU:HA	2.03	0.58
1:A:1294:LEU:O	1:A:1298:HIS:ND1	2.37	0.57
1:A:485:SER:HG	1:A:503:TYR:HH	1.49	0.57
1:A:875:GLN:O	1:A:904:ARG:NH2	2.35	0.57
1:A:302:TYR:OH	1:A:481:ASP:OD2	2.19	0.57
1:A:585:PHE:O	1:A:589:THR:HG23	2.05	0.56
1:A:786:CYS:O	1:A:790:ILE:HG12	2.06	0.56
1:A:579:ILE:HD12	1:A:1193:LEU:HD11	1.88	0.55
1:A:618:LYS:HE3	1:A:622:ILE:HD11	1.89	0.55
1:A:1358:LEU:HD22	1:A:1385:ARG:HB2	1.89	0.54
1:A:1514:THR:HB	1:A:1517:GLU:HG3	1.90	0.54
1:A:880:ARG:NH1	1:A:881:ILE:O	2.41	0.53
1:A:361:GLN:OE1	1:A:366:ARG:NH2	2.41	0.53
1:A:742:HIS:CE1	1:A:881:ILE:HG13	2.44	0.53
1:A:318:CYS:HB2	1:A:342:ILE:HD11	1.90	0.53
1:A:1292:ALA:HA	1:A:1304:MET:SD	2.49	0.53
1:A:453:LYS:O	1:A:457:ASN:ND2	2.42	0.52
1:A:407:ILE:O	1:A:662[B]:TYR:OH	2.23	0.52
1:A:1549:ASP:HB3	1:A:1552:LEU:HD23	1.92	0.52
1:A:1583:GLU:O	1:A:1587:ARG:HG2	2.09	0.51
1:A:900:PRO:O	1:A:904:ARG:HG3	2.11	0.51
1:A:1529:ASP:OD1	1:A:1530:SER:N	2.44	0.51
1:A:816:ASN:HB3	1:A:819:GLU:HB2	1.92	0.50
1:A:330:ALA:O	1:A:334:ILE:HG12	2.12	0.50
1:A:917:LYS:HA	1:A:926:TYR:CE2	2.38	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1090:PHE:HB3	1:A:1105:GLY:HA3	1.94	0.49
1:A:1489:THR:HG22	1:A:1571:VAL:HG13	1.95	0.49
1:A:735:MET:SD	1:A:1022:LYS:HG2	2.53	0.49
1:A:539:ASP:OD2	1:A:542:ASN:ND2	2.36	0.49
1:A:1326:ARG:NH1	1:A:1389:ASP:OD1	2.46	0.48
1:A:1406:PHE:O	1:A:1411:LYS:NZ	2.38	0.48
1:A:1389:ASP:OD2	1:A:1391:SER:OG	2.30	0.48
1:A:386:LEU:HD11	1:A:498:TRP:HH2	1.77	0.48
1:A:1341:PHE:CD2	1:A:1403:GLN:HB2	2.49	0.48
1:A:264:GLY:HA3	1:A:673:GLN:HG3	1.95	0.48
1:A:284:MET:HB3	1:A:286:ARG:HH12	1.78	0.48
1:A:912:TYR:OH	1:A:989:THR:HB	2.14	0.47
1:A:739:ALA:O	1:A:743:LEU:HD23	2.15	0.47
1:A:1324:HIS:NE2	1:A:1382:TYR:OH	2.46	0.47
1:A:499:SER:HB3	1:A:512:ILE:HB	1.96	0.47
1:A:347:GLU:O	1:A:351:ASN:ND2	2.46	0.47
1:A:782:GLN:HG2	1:A:979:GLY:O	2.15	0.47
1:A:317:ALA:HB1	1:A:509:ILE:HG12	1.97	0.47
1:A:334:ILE:HG23	1:A:511:PHE:CZ	2.50	0.47
1:A:964:ARG:NH2	1:A:1088:ASP:OD2	2.43	0.46
1:A:1499:ILE:HA	1:A:1534:ASP:OD1	2.15	0.46
1:A:1501:ASN:ND2	1:A:1534:ASP:OD2	2.48	0.46
1:A:422:LYS:HE3	1:A:422:LYS:HB3	1.71	0.46
1:A:954:LEU:HD12	1:A:1119:PHE:HB2	1.97	0.45
1:A:1366:VAL:HG21	1:A:1557:LYS:HE3	1.98	0.45
1:A:1192:SER:HA	1:A:1211:ARG:HD2	1.99	0.45
1:A:911:TYR:CG	1:A:1005:VAL:HG21	2.52	0.45
1:A:456:GLN:HA	1:A:460:GLN:HB3	1.98	0.45
1:A:1168:ASN:HB2	1:A:1172:LEU:HD23	2.00	0.44
1:A:950:SER:HB2	1:A:962:MET:HB2	1.99	0.44
1:A:812:ILE:HD11	1:A:915:ILE:HG12	1.99	0.44
1:A:1131:TRP:HA	1:A:1134:VAL:HG12	2.00	0.44
1:A:585:PHE:CE1	1:A:596:PRO:HD2	2.53	0.44
1:A:1188:ILE:HG13	1:A:1218:LEU:HD12	2.00	0.44
1:A:804:LYS:HD3	1:A:918:ASN:HB3	2.01	0.43
1:A:334:ILE:HD12	1:A:511:PHE:CD1	2.53	0.43
1:A:1106:TYR:HB2	1:A:1138:MET:HB3	2.00	0.43
1:A:1453:LEU:HD21	1:A:1558:ARG:HD2	2.01	0.43
1:A:467:LEU:O	1:A:470:THR:OG1	2.34	0.42
1:A:866:LEU:O	1:A:870:GLU:HG3	2.20	0.42
1:A:713:TYR:CZ	1:A:1170:GLU:HG3	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:528:ILE:HD11	1:A:559:VAL:HG22	2.01	0.42
1:A:1007:ASP:O	1:A:1011:GLN:HG2	2.20	0.42
1:A:470:THR:O	1:A:474:HIS:HD2	2.03	0.41
1:A:911:TYR:O	1:A:915:ILE:HG13	2.20	0.41
1:A:989:THR:HG23	1:A:1006:ILE:HG12	2.02	0.41
1:A:1128:HIS:HB3	1:A:1131:TRP:CD1	2.56	0.41
1:A:1313:PHE:HB2	1:A:1436:PHE:CD1	2.56	0.41
1:A:773:LEU:HD11	1:A:780:ALA:HB2	2.03	0.41
1:A:967:MET:HE3	1:A:1164:VAL:HG12	2.03	0.41
1:A:879:ALA:HB2	1:A:897:THR:HG22	2.03	0.41
1:A:1574:VAL:HG12	1:A:1588:TYR:CD2	2.56	0.41
1:A:502:SER:OG	1:A:506:GLY:HA2	2.21	0.40
1:A:431:ILE:HG21	1:A:474:HIS:CD2	2.57	0.40
1:A:1072:MET:HB3	1:A:1150:LEU:HD23	2.04	0.40
1:A:1096:HIS:HB2	1:A:1175:PHE:CE2	2.57	0.40
1:A:318:CYS:O	1:A:322:LEU:HG	2.21	0.40
1:A:904:ARG:HD3	1:A:1011:GLN:HB2	2.02	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	1282/2196 (58%)	1250 (98%)	32 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	1148/1955 (59%)	1148 (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. There are no such sidechains identified.

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.

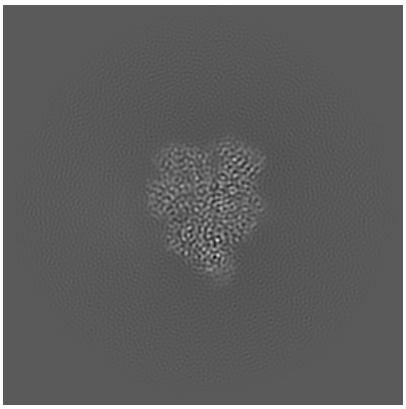
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-17351. These allow visual inspection of the internal detail of the map and identification of artifacts.

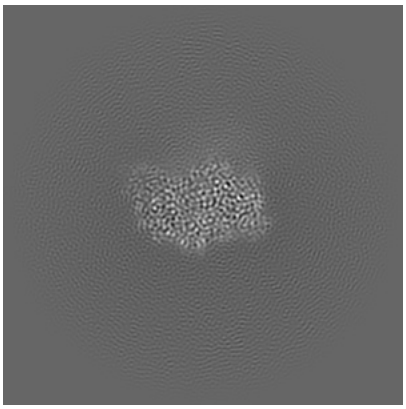
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

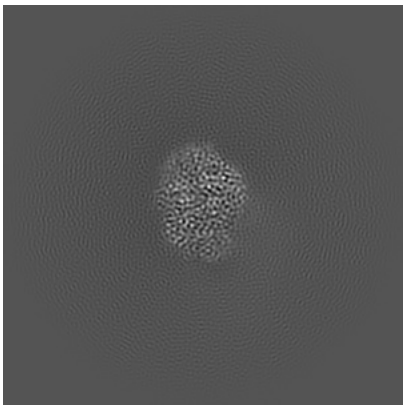
6.1.1 Primary map



X

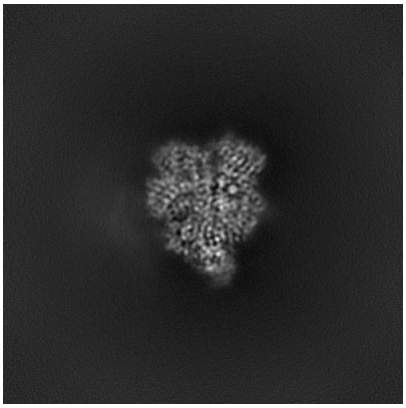


Y

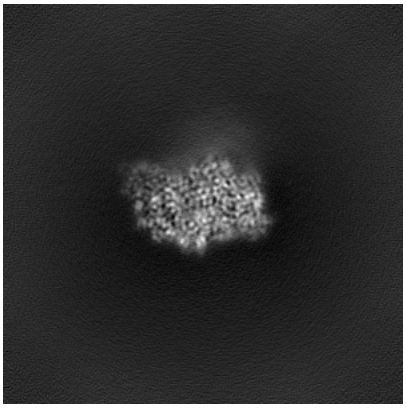


Z

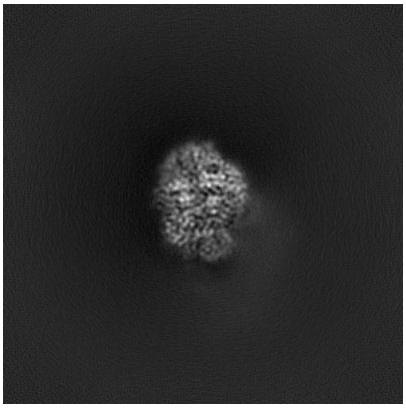
6.1.2 Raw map



X



Y

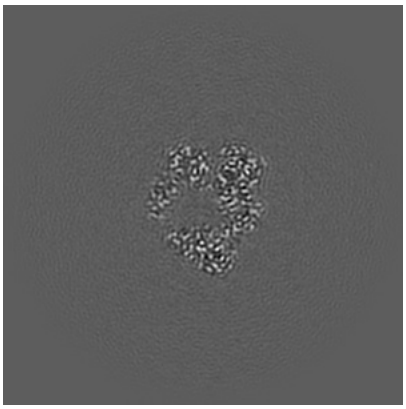


Z

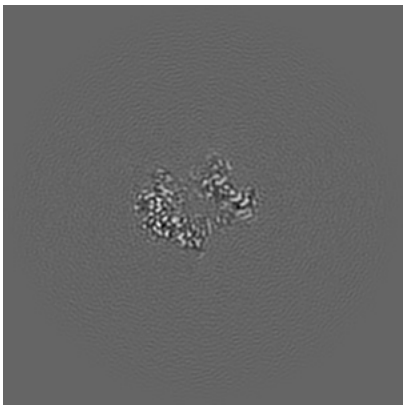
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

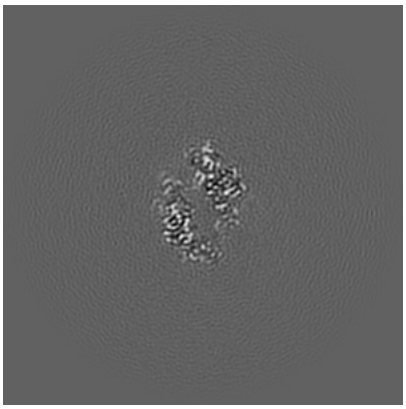
6.2.1 Primary map



X Index: 150

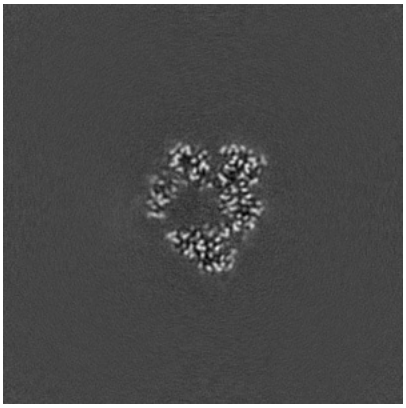


Y Index: 150

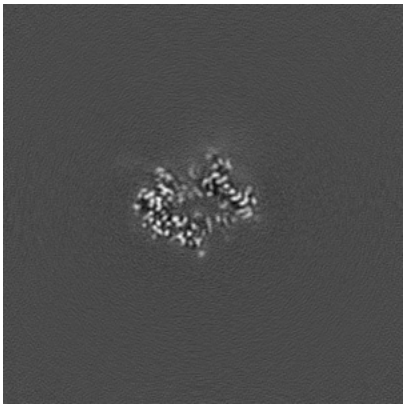


Z Index: 150

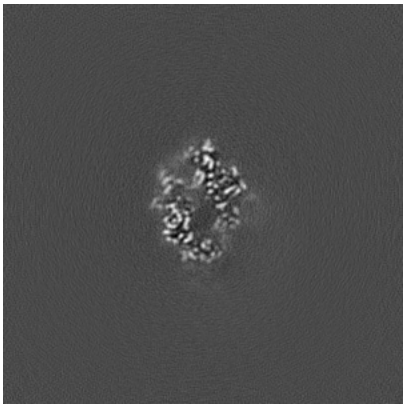
6.2.2 Raw map



X Index: 150



Y Index: 150

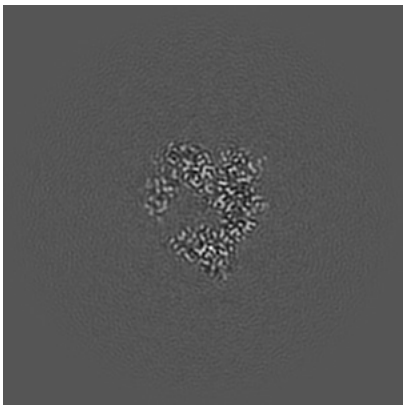


Z Index: 150

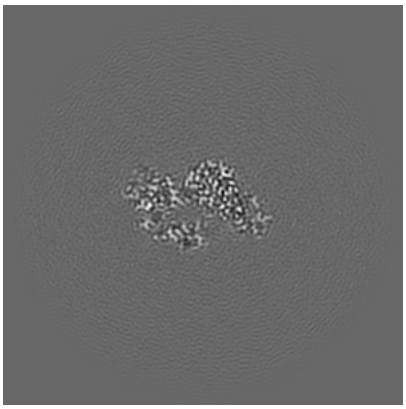
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

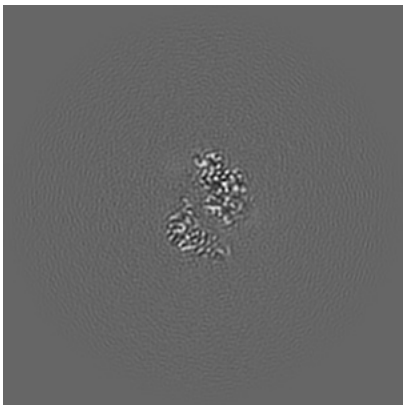
6.3.1 Primary map



X Index: 154

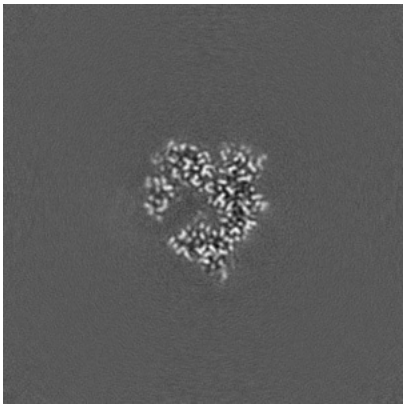


Y Index: 164

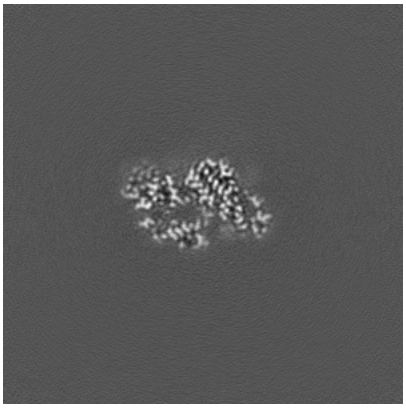


Z Index: 160

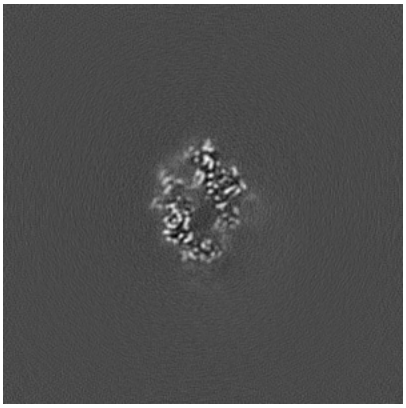
6.3.2 Raw map



X Index: 154



Y Index: 164

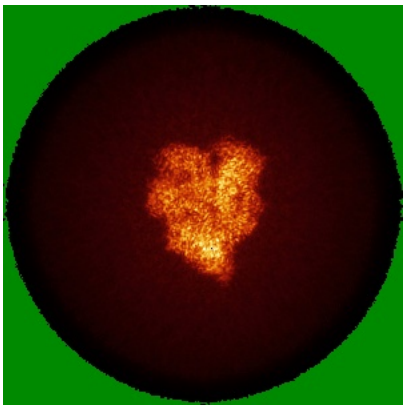


Z Index: 150

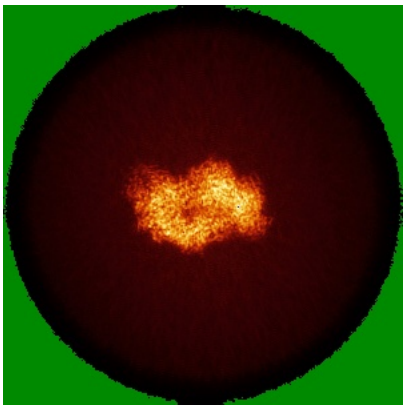
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

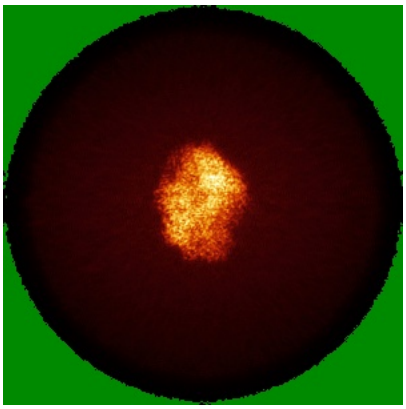
6.4.1 Primary map



X

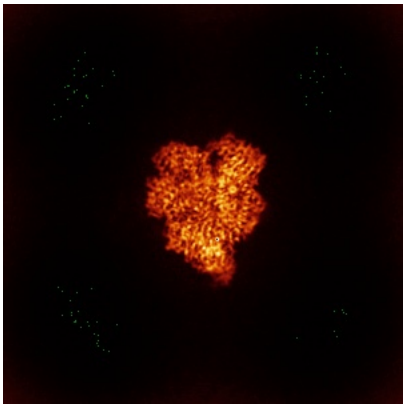


Y

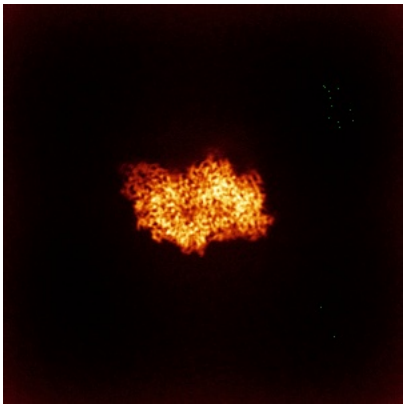


Z

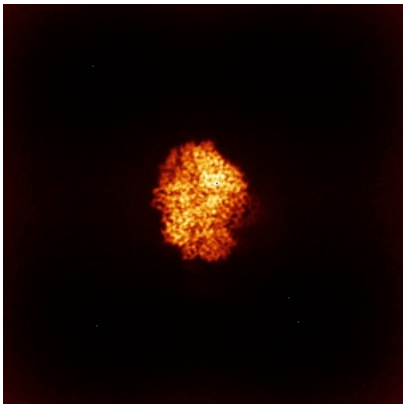
6.4.2 Raw map



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

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.356. 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

X Y Z

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.

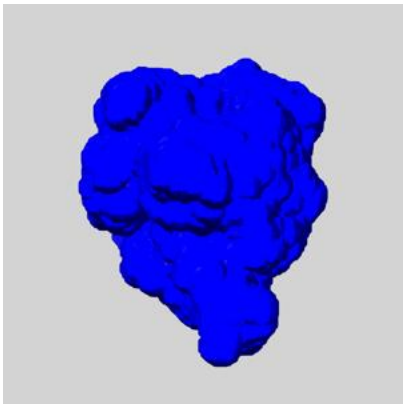
6.6 Mask visualisation (i)

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

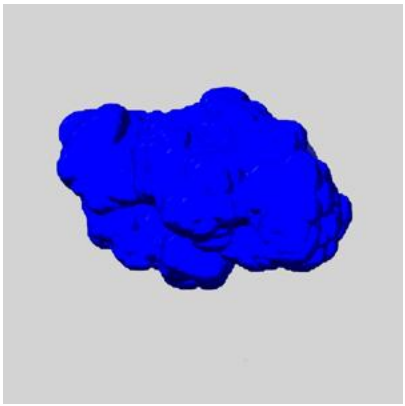
A mask typically either:

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

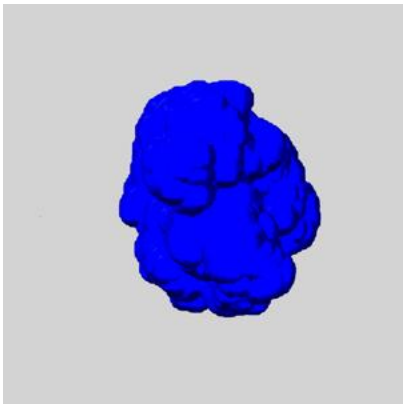
6.6.1 emd_17351_msk_1.map (i)



X



Y

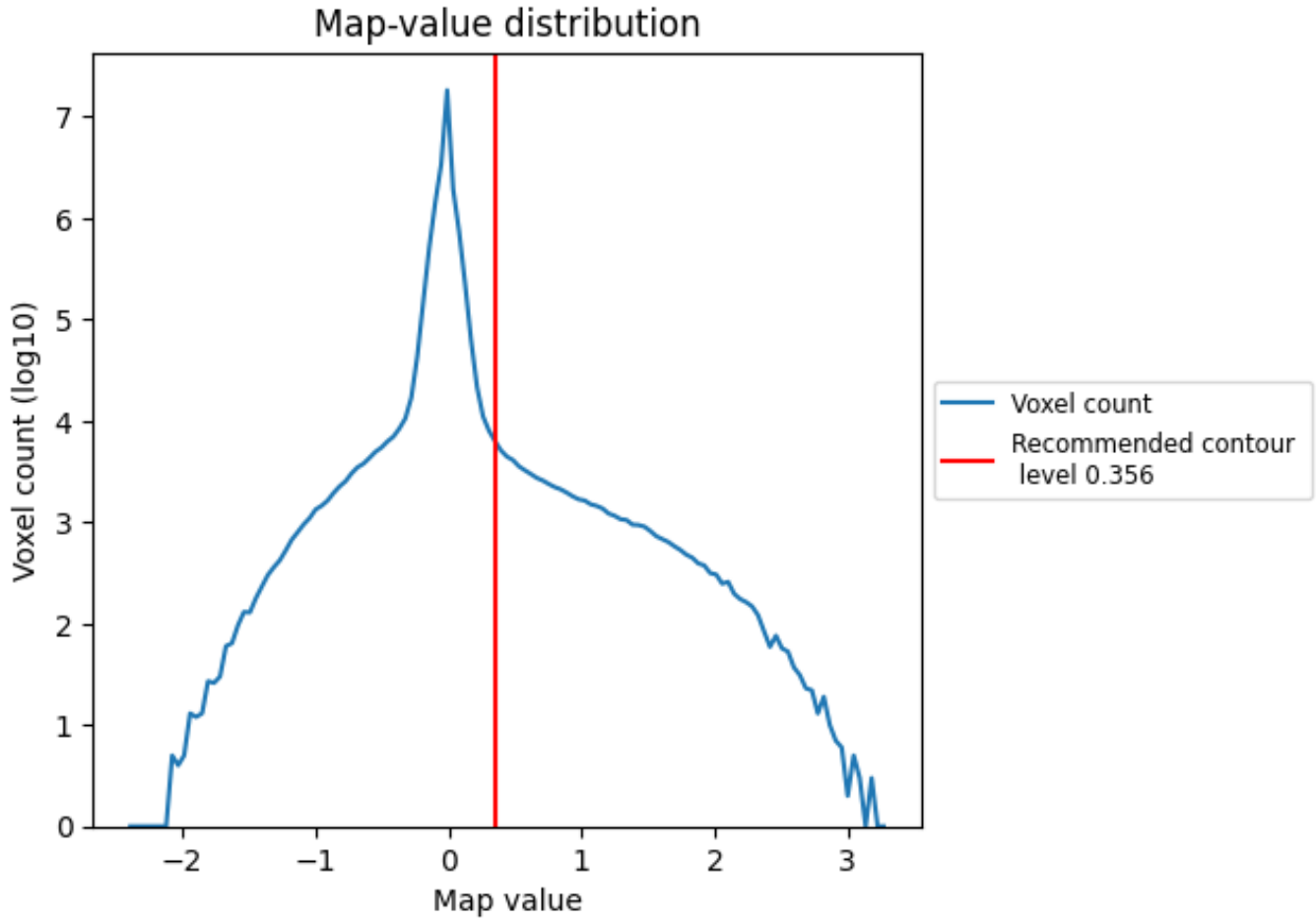


Z

7 Map analysis

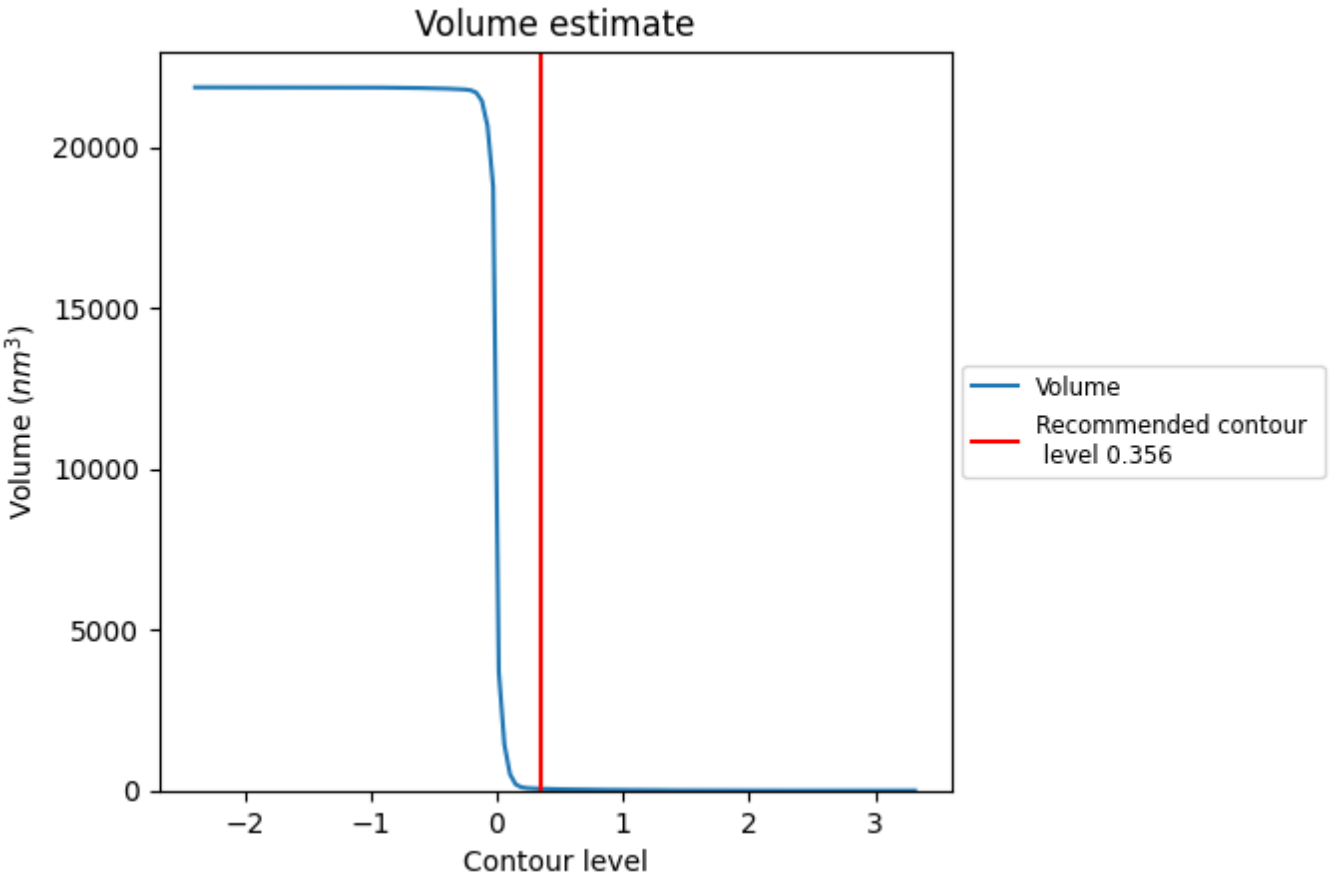
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

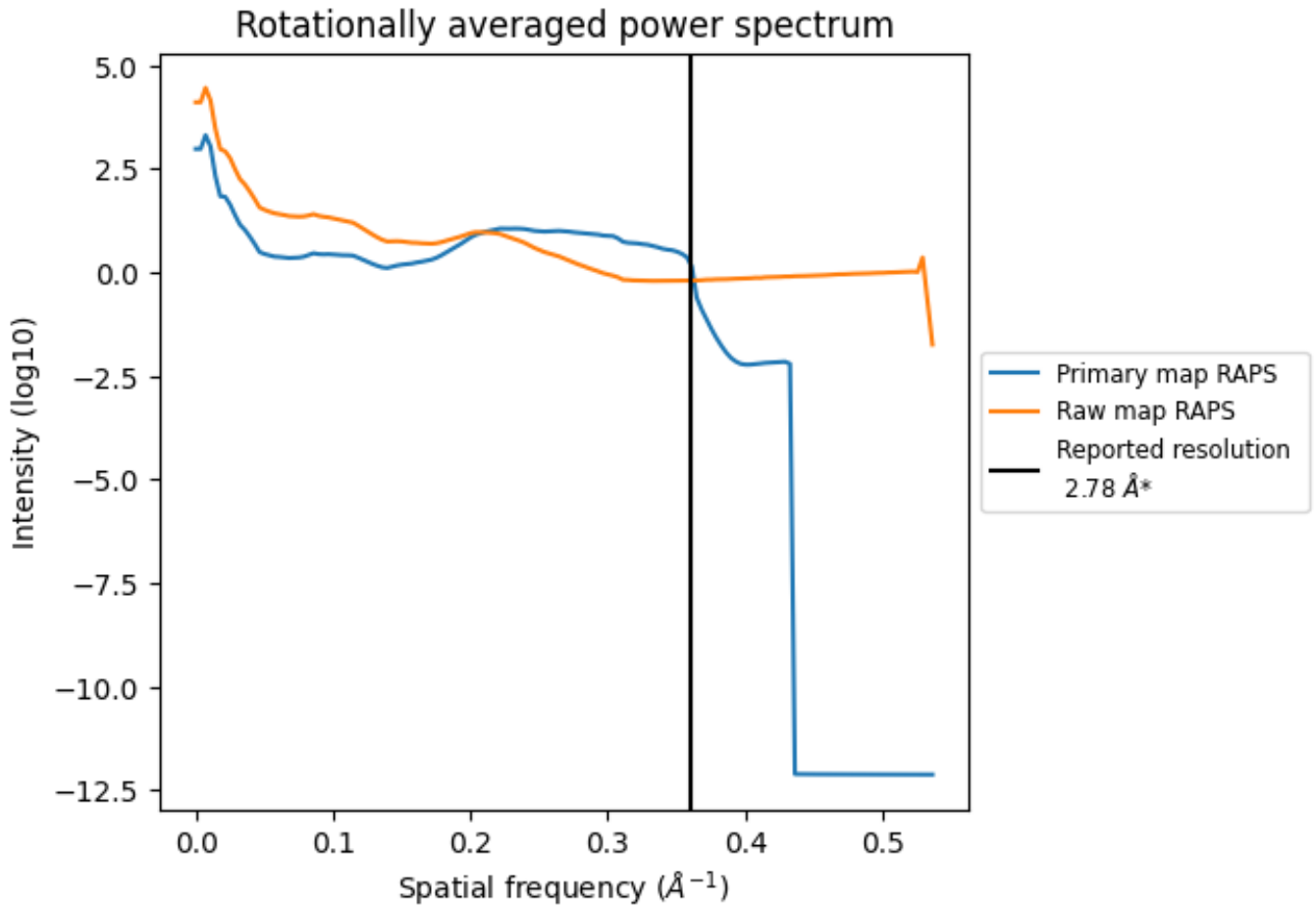
7.2 Volume estimate



The volume at the recommended contour level is 55 nm^3; this corresponds to an approximate mass of 50 kDa.

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

7.3 Rotationally averaged power spectrum (i)

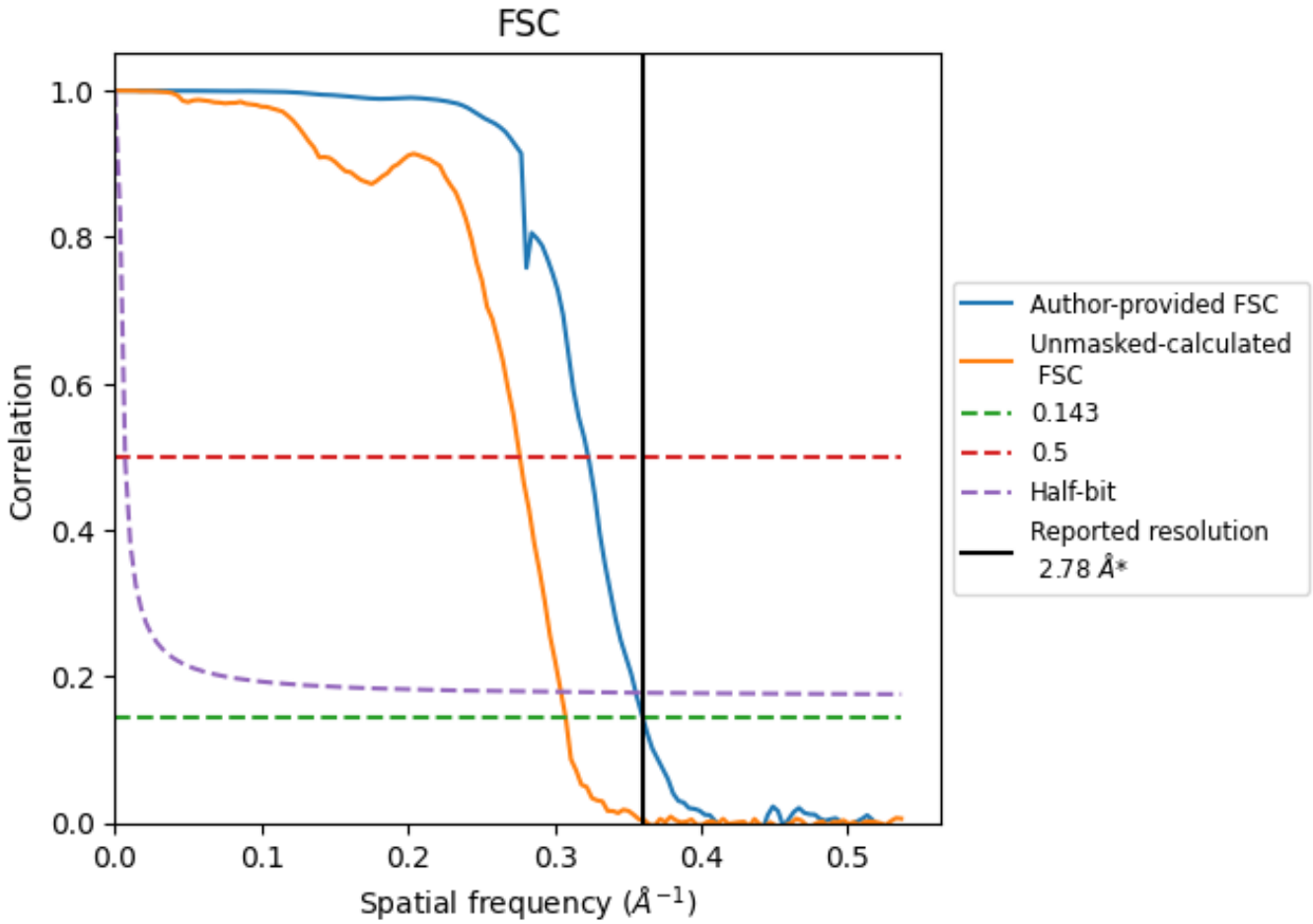


*Reported resolution corresponds to spatial frequency of 0.360 $Å^{-1}$

8 Fourier-Shell correlation

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



*Reported resolution corresponds to spatial frequency of 0.360 Å^{-1}

8.2 Resolution estimates (i)

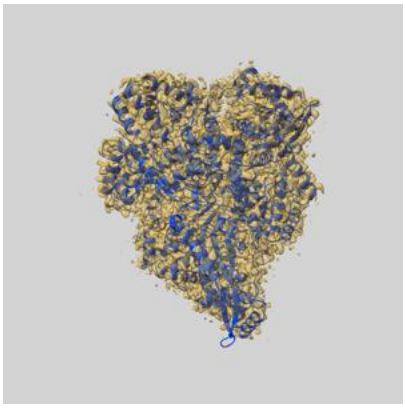
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.78	-	-
Author-provided FSC curve	2.78	3.10	2.81
Unmasked-calculated*	3.25	3.62	3.29

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.25 differs from the reported value 2.78 by more than 10 %

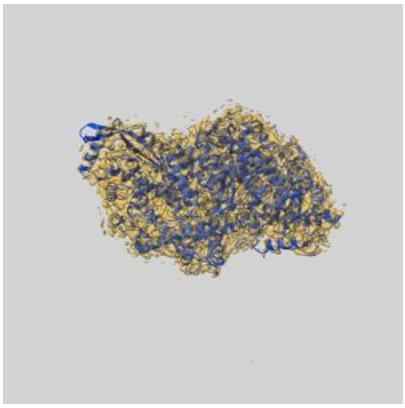
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-17351 and PDB model 8P1J. Per-residue inclusion information can be found in section 3 on page 5.

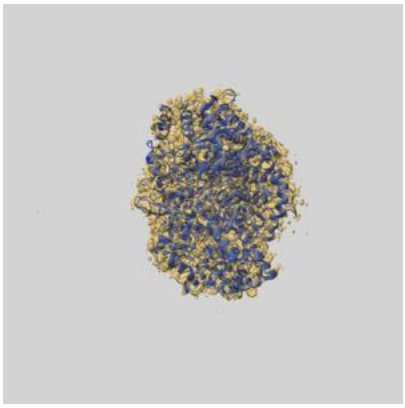
9.1 Map-model overlay



X



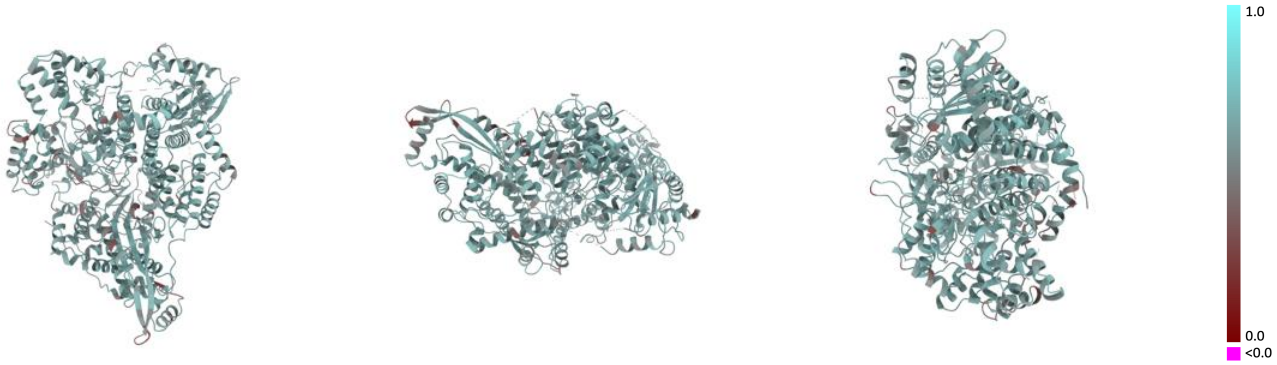
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.356 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.

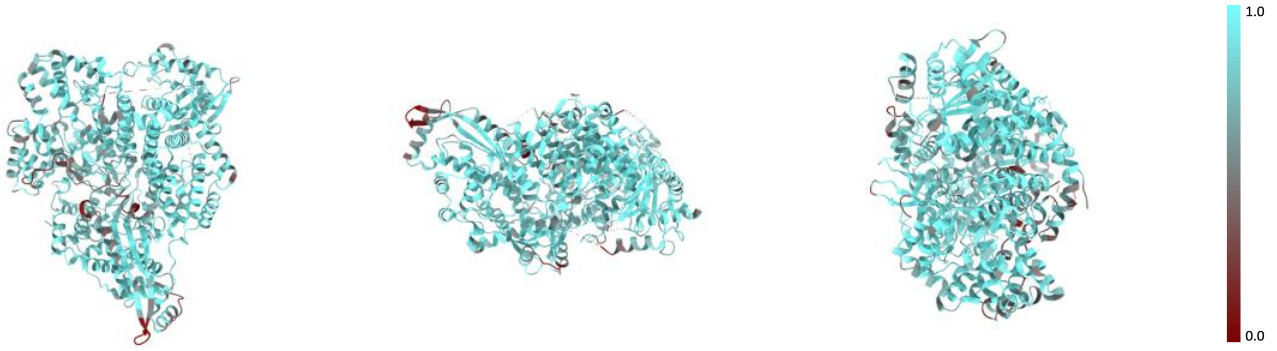
9.2 Q-score mapped to coordinate model (i)



X Y Z

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.

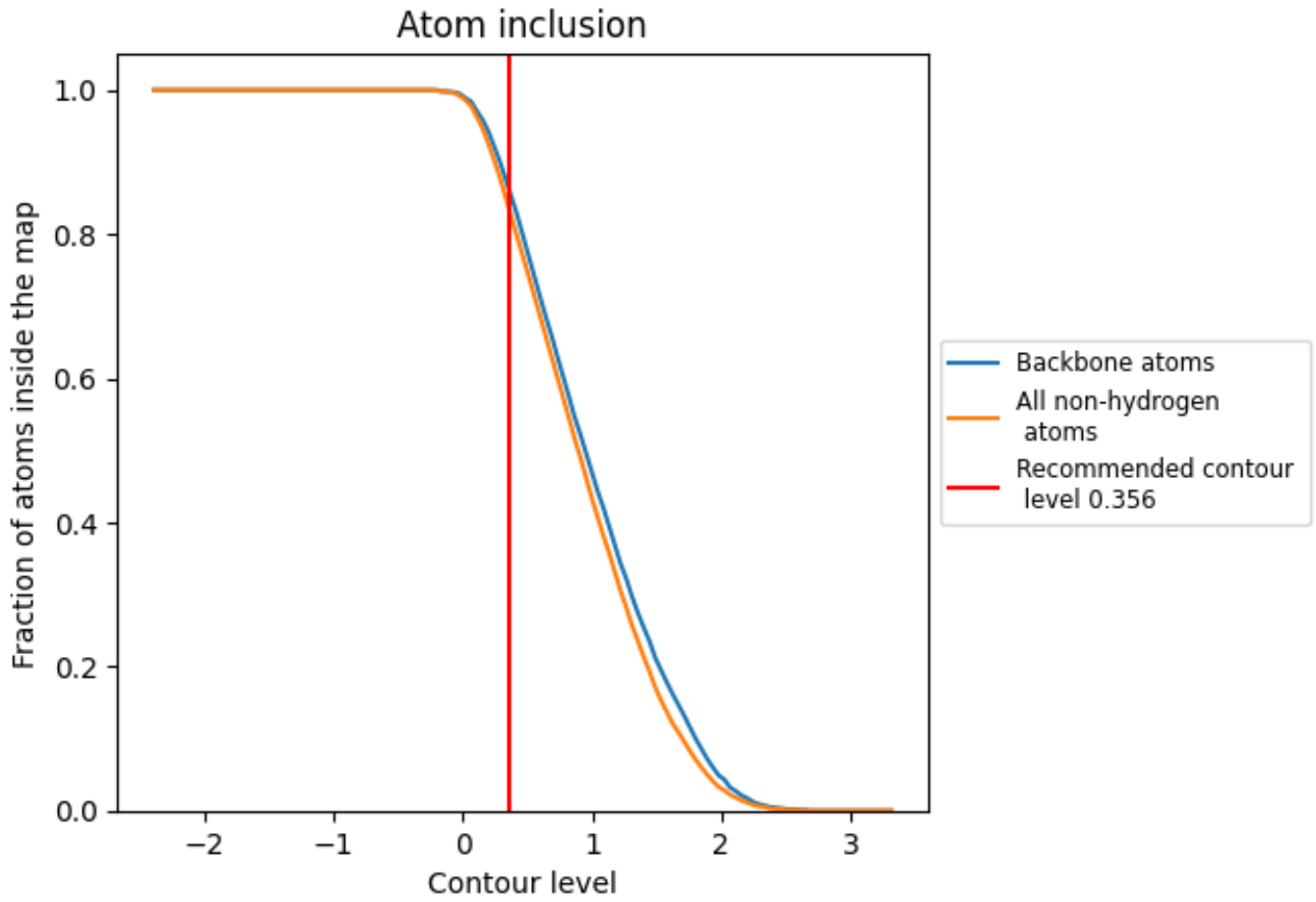
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

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 (0.356).

9.4 Atom inclusion (i)



At the recommended contour level, 86% of all backbone atoms, 84% 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 (0.356) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8350	0.6010
A	0.8350	0.6010