



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 11:51 AM UTC

PDB ID : 6VJY / pdb_00006vjy
EMDB ID : EMD-21220
Title : Cryo-EM structure of Hrd1/Hrd3 monomer
Authors : Wu, X.; Rapoport, T.A.
Deposited on : 2020-01-18
Resolution : 4.30 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

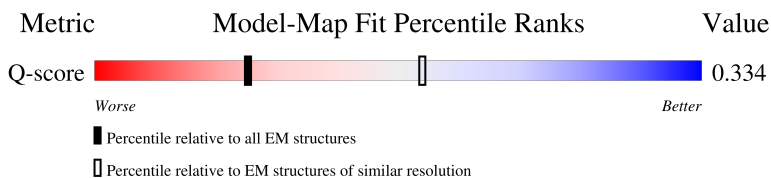
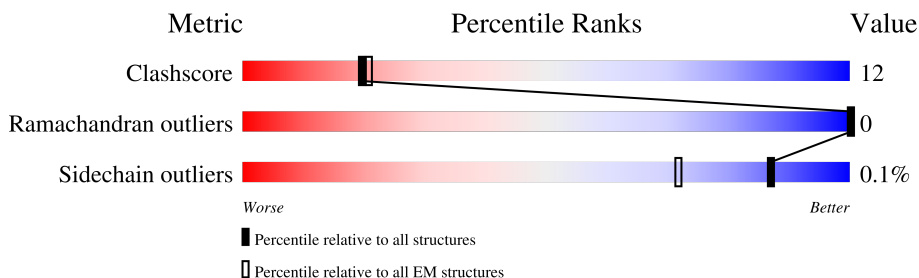
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

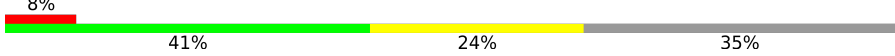
The reported resolution of this entry is 4.30 Å.

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	4585 (3.80 - 4.80)

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	B	430	
2	A	767	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 7266 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 ERAD-associated E3 ubiquitin-protein ligase HRD1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	B	280	Total	C	N	O	S	0	0
			2343	1565	368	396	14		

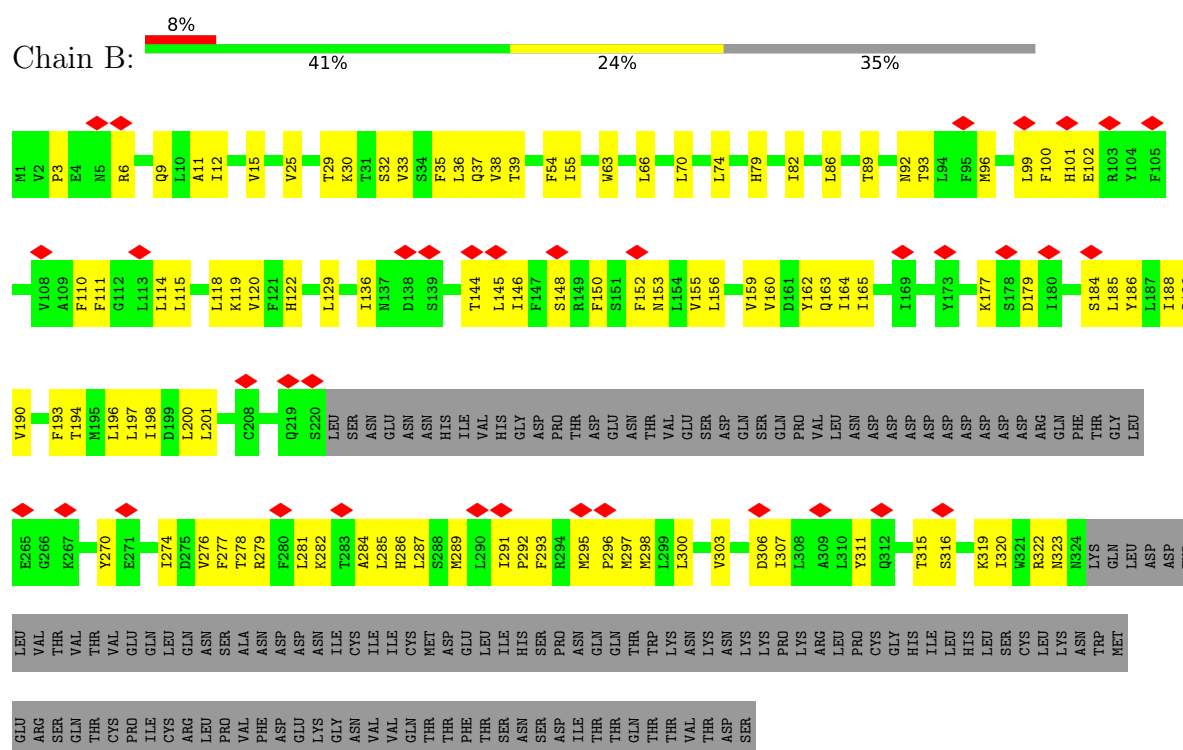
- Molecule 2 is a protein called ERAD-associated E3 ubiquitin-protein ligase component HRD3.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A	603	Total	C	N	O	S	0	0
			4923	3151	836	916	20		

3 Residue-property plots

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: ERAD-associated E3 ubiquitin-protein ligase HRD1



THR	Y587	I434	R321
SER	T588	K439	I322
TRP			Q336
LYS	I628	N447	R342
LEU	L634	Q448	L346
THR	G635	I449	
LYS	Y636	Q453	L349
ILE	M637	E464	T350
LEU	H638	K465	Y351
GLN	E639	I466	K352
ARG	H640		E353
MET	G641	N471	
ARG	L642		L361
HIS	G643	E474	D362
LYS	V644		P363
GLU		F481	L364
ASP	L650	I482	Q365
ASP		P483	V366
LYS	R653		F367
ALA	V658	G495	Y368
ALA		MET	Y369
GLU	D662	N497	V370
ASP	H663		R371
SER	R664	N504	C372
HIS	F665		L373
LYS	Y666	L508	Q374
HIS	L667	F509	
ARG	A668	N516	H378
THR	S669	E517	
VAL	R670	M520	N390
VAL	V673		I391
GLN		F528	H392
ASN		I532	M393
GLY	T686		A394
ALA	ARG	A547	E395
ASN	GLU	E548	E396
HIS	LYS	Q549	I397
ARG	VAL		L398
GLY	ASN	Q555	T399
ASP	TYR	V556	T400
ASP	TRP	S557	
GLN	LYS	A558	I404
GLU	PRO	A559	S405
GLU	ALA		R406
GLU	SER	LEU	R414
ILE	LEU	ASN	A415
LEU	PRO	PRO	
GLY	GLU	T576	D418
PHE	PHE	D577	L419
GLN	GLN	Q578	
MET	MET	R579	I422
GLU	GLU	K580	I426
ASP	ASP	T581	
		I584	I430

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	197173	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	47.7	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.105	Depositor
Minimum map value	-0.061	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.013	Depositor
Map size ($\text{\AA}$)	226.0, 226.0, 226.0	wwPDB
Map dimensions	200, 200, 200	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.13, 1.13, 1.13	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	B	0.16	0/2399	0.41	0/3249
2	A	0.19	0/5046	0.39	0/6829
All	All	0.18	0/7445	0.40	0/10078

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 [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	B	2343	0	2425	89	0
2	A	4923	0	4784	95	0
All	All	7266	0	7209	181	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 12.

All (181) 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:B:3:PRO:HD2	1:B:6:ARG:HD2	1.25	1.19
1:B:184:SER:HB2	1:B:293:PHE:CZ	1.89	1.05

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3:PRO:CD	1:B:6:ARG:HD2	1.89	1.03
1:B:184:SER:HB2	1:B:293:PHE:CE2	2.05	0.89
2:A:637:MET:HB2	2:A:642:LEU:HD11	1.68	0.75
1:B:3:PRO:HD2	1:B:6:ARG:CD	2.12	0.75
2:A:374:GLN:HE21	2:A:415:ALA:H	1.33	0.75
1:B:184:SER:HB2	1:B:293:PHE:HZ	1.50	0.74
1:B:184:SER:CB	1:B:293:PHE:CZ	2.69	0.73
1:B:285:LEU:HD12	1:B:286:HIS:N	2.03	0.72
2:A:367:PHE:HE1	2:A:371:ARG:HH21	1.38	0.70
1:B:184:SER:CB	1:B:293:PHE:CE2	2.76	0.69
2:A:639:GLU:OE2	2:A:640:HIS:ND1	2.25	0.68
2:A:361:LEU:HB3	2:A:365:GLN:HB2	1.76	0.68
2:A:83:THR:H	2:A:86:GLN:HE21	1.43	0.67
1:B:185:LEU:HA	1:B:188:ILE:HD12	1.76	0.67
2:A:638:HIS:ND1	2:A:644:VAL:HG21	2.12	0.65
1:B:279:ARG:HA	1:B:282:LYS:HE2	1.78	0.64
2:A:398:LEU:HB3	2:A:419:LEU:HD21	1.78	0.64
2:A:448:GLY:HA3	2:A:481:PHE:HB2	1.79	0.63
1:B:278:THR:O	1:B:282:LYS:HG3	1.98	0.63
1:B:282:LYS:O	1:B:285:LEU:HG	1.99	0.63
1:B:118:LEU:O	1:B:122:HIS:ND1	2.22	0.61
1:B:144:THR:O	1:B:148:SER:CB	2.49	0.61
2:A:109:LEU:HA	2:A:112:ILE:HD12	1.83	0.61
1:B:9:GLN:HA	1:B:12:ILE:HD12	1.82	0.61
1:B:39:THR:HG21	2:A:668:ALA:HB2	1.81	0.61
1:B:144:THR:O	1:B:148:SER:HB2	2.01	0.60
1:B:319:LYS:HA	1:B:322:ARG:HD3	1.83	0.60
2:A:155:THR:HG23	2:A:157:GLY:H	1.67	0.59
1:B:188:ILE:HD13	1:B:298:MET:HE1	1.84	0.59
2:A:187:LEU:HB3	2:A:520:MET:HE1	1.84	0.59
1:B:185:LEU:O	1:B:189:GLN:HG2	2.03	0.59
2:A:374:GLN:HE21	2:A:415:ALA:N	2.01	0.59
2:A:576:THR:HG23	2:A:579:ARG:H	1.67	0.58
2:A:48:ALA:HA	2:A:336:GLN:HE21	1.69	0.58
2:A:482:ILE:HB	2:A:483:PRO:HD3	1.85	0.58
2:A:239:SER:OG	2:A:265:ARG:NH1	2.37	0.58
1:B:153:ASN:HA	1:B:156:LEU:HD12	1.86	0.57
2:A:90:TYR:O	2:A:94:VAL:HG23	2.04	0.57
1:B:186:TYR:O	1:B:190:VAL:HG23	2.04	0.57
1:B:160:VAL:O	1:B:164:ILE:HG12	2.04	0.57
2:A:547:ALA:HB1	2:A:555:GLN:HG2	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:84:ASP:HA	2:A:87:ARG:HD3	1.87	0.57
1:B:89:THR:O	1:B:93:THR:HG23	2.06	0.56
1:B:30:LYS:NZ	2:A:568:GLU:O	2.39	0.56
1:B:111:PHE:HA	1:B:114:LEU:HD12	1.88	0.56
2:A:669:SER:O	2:A:673:VAL:HG23	2.06	0.56
1:B:289:MET:C	1:B:292:PRO:HD2	2.31	0.55
1:B:3:PRO:CG	1:B:6:ARG:HD2	2.37	0.55
2:A:43:PRO:HG2	2:A:532:ILE:HD11	1.88	0.55
2:A:516:ASN:OD1	2:A:517:GLU:N	2.40	0.55
2:A:395:GLU:O	2:A:399:THR:HG23	2.06	0.55
2:A:650:LEU:HD13	2:A:653:ARG:HD2	1.87	0.55
1:B:316:SER:O	1:B:320:ILE:HG12	2.06	0.55
1:B:188:ILE:CD1	1:B:298:MET:HE1	2.38	0.54
1:B:270:TYR:O	1:B:274:ILE:HG12	2.07	0.54
2:A:88:HIS:O	2:A:91:GLU:HG2	2.07	0.54
1:B:114:LEU:O	1:B:118:LEU:HG	2.08	0.54
1:B:145:LEU:HD12	1:B:146:ILE:HG23	1.89	0.54
1:B:74:LEU:HD13	1:B:79:HIS:HB2	1.88	0.54
2:A:107:TYR:HB2	2:A:134:PHE:CE2	2.43	0.54
1:B:115:LEU:HB3	1:B:193:PHE:HE1	1.73	0.53
2:A:662:ASP:OD1	2:A:663:HIS:N	2.33	0.53
1:B:79:HIS:HA	1:B:82:ILE:HD12	1.90	0.53
2:A:370:VAL:HA	2:A:373:LEU:HD12	1.90	0.53
1:B:274:ILE:O	1:B:278:THR:HG23	2.09	0.53
1:B:315:THR:O	1:B:319:LYS:HG2	2.09	0.53
2:A:636:TYR:O	2:A:639:GLU:HG3	2.09	0.53
1:B:129:LEU:HB2	1:B:150:PHE:HZ	1.74	0.52
2:A:430:ILE:O	2:A:434:ILE:HG12	2.09	0.52
1:B:66:LEU:O	1:B:70:LEU:HG	2.08	0.52
1:B:177:LYS:HE2	1:B:179:ASP:HB3	1.91	0.52
2:A:140:PHE:O	2:A:180:ARG:NH1	2.35	0.52
2:A:171:SER:OG	2:A:202:ASN:ND2	2.30	0.52
1:B:193:PHE:O	1:B:197:LEU:HG	2.10	0.52
2:A:239:SER:H	2:A:265:ARG:HH12	1.56	0.52
1:B:303:VAL:HA	1:B:306:ASP:HB2	1.92	0.52
2:A:391:ILE:HG21	2:A:426:ILE:HG21	1.92	0.52
1:B:36:LEU:HD11	2:A:665:PHE:HD2	1.75	0.51
1:B:152:PHE:HA	1:B:155:VAL:HG22	1.92	0.51
1:B:194:THR:O	1:B:198:ILE:HG12	2.10	0.51
1:B:311:TYR:O	1:B:315:THR:HG23	2.09	0.51
2:A:362:ASP:OD1	2:A:362:ASP:N	2.36	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:197:LEU:O	1:B:201:LEU:HG	2.10	0.51
2:A:42:ASP:OD1	2:A:42:ASP:N	2.44	0.51
2:A:346:LEU:O	2:A:350:THR:HG23	2.11	0.51
2:A:214:TYR:HB3	2:A:509:PHE:HB3	1.92	0.50
1:B:35:PHE:O	1:B:38:VAL:HG12	2.11	0.50
1:B:291:ILE:N	1:B:292:PRO:CD	2.75	0.50
1:B:25:VAL:O	1:B:29:THR:OG1	2.25	0.50
1:B:300:LEU:HA	1:B:303:VAL:HG22	1.94	0.50
2:A:481:PHE:CE2	2:A:483:PRO:HD2	2.46	0.49
2:A:578:GLN:HA	2:A:581:THR:HG22	1.93	0.49
2:A:396:GLU:O	2:A:400:THR:HG23	2.12	0.49
2:A:107:TYR:HB2	2:A:134:PHE:HE2	1.76	0.49
2:A:131:LEU:HB3	2:A:149:LEU:HD13	1.95	0.49
2:A:191:GLN:NE2	2:A:549:GLN:HB3	2.27	0.49
2:A:628:ILE:HG23	2:A:658:VAL:HG23	1.96	0.48
1:B:196:LEU:O	1:B:200:LEU:HG	2.13	0.48
2:A:128:HIS:HB2	2:A:152:MET:HE1	1.95	0.48
1:B:63:TRP:HZ2	1:B:120:VAL:HG11	1.77	0.48
1:B:285:LEU:HD12	1:B:285:LEU:C	2.38	0.48
2:A:400:THR:O	2:A:404:ILE:HG12	2.13	0.48
2:A:322:ILE:HG13	2:A:346:LEU:HD21	1.96	0.48
2:A:113:HIS:CE1	2:A:126:LEU:HD13	2.49	0.48
1:B:101:HIS:CD2	1:B:102:GLU:H	2.32	0.48
2:A:406:ARG:HA	2:A:406:ARG:HD2	1.70	0.47
1:B:115:LEU:O	1:B:119:LYS:HG2	2.14	0.47
2:A:140:PHE:HD2	2:A:180:ARG:HG2	1.79	0.47
2:A:390:ASN:ND2	2:A:393:MET:SD	2.87	0.47
1:B:33:VAL:N	1:B:37:GLN:OE1	2.38	0.47
1:B:156:LEU:O	1:B:160:VAL:HG22	2.15	0.47
2:A:374:GLN:NE2	2:A:415:ALA:H	2.07	0.47
1:B:129:LEU:HB2	1:B:150:PHE:CZ	2.50	0.47
2:A:634:LEU:O	2:A:637:MET:HG3	2.15	0.46
2:A:349:LEU:O	2:A:353:GLU:HG2	2.15	0.46
2:A:418:ASP:O	2:A:422:ILE:HG13	2.15	0.46
2:A:83:THR:H	2:A:86:GLN:NE2	2.10	0.46
2:A:369:TYR:O	2:A:373:LEU:HG	2.16	0.46
2:A:666:TYR:CE1	2:A:670:LYS:HG3	2.50	0.46
2:A:313:ASP:N	2:A:316:GLU:OE1	2.49	0.45
1:B:276:VAL:HA	1:B:279:ARG:HD2	1.97	0.45
2:A:86:GLN:HA	2:A:89:ILE:HG12	1.99	0.45
2:A:244:ILE:HG22	2:A:557:SER:HA	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:320:ILE:HA	1:B:323:ASN:ND2	2.31	0.45
2:A:176:LEU:HD23	2:A:176:LEU:HA	1.82	0.45
2:A:666:TYR:CE2	2:A:670:LYS:HE3	2.51	0.45
1:B:289:MET:O	1:B:292:PRO:HD2	2.16	0.45
2:A:39:LYS:HB3	2:A:117:GLN:HB2	1.98	0.45
2:A:471:ASN:HA	2:A:474:GLU:OE1	2.17	0.44
2:A:481:PHE:CD2	2:A:483:PRO:HD2	2.53	0.44
1:B:277:PHE:O	1:B:281:LEU:HG	2.17	0.44
1:B:303:VAL:O	1:B:307:ILE:HG12	2.17	0.44
2:A:584:ILE:O	2:A:588:THR:OG1	2.32	0.44
2:A:269:THR:OG1	2:A:270:ARG:N	2.51	0.44
2:A:449:ILE:O	2:A:453:GLN:HG2	2.18	0.44
2:A:112:ILE:HA	2:A:117:GLN:HG2	1.98	0.44
2:A:464:GLU:HB2	2:A:466:ILE:HG12	1.98	0.44
2:A:559:ALA:HB1	2:A:587:TYR:CE2	2.54	0.43
2:A:73:ASN:O	2:A:77:ILE:HG12	2.18	0.43
1:B:11:ALA:O	1:B:15:VAL:HG23	2.19	0.43
2:A:192:VAL:HG23	2:A:548:GLU:O	2.18	0.43
2:A:361:LEU:O	2:A:366:VAL:HG13	2.18	0.43
2:A:365:GLN:H	2:A:365:GLN:CD	2.25	0.43
1:B:155:VAL:O	1:B:159:VAL:HG12	2.18	0.43
1:B:100:PHE:HE2	1:B:185:LEU:HD13	1.84	0.43
1:B:101:HIS:CG	1:B:102:GLU:H	2.37	0.43
1:B:30:LYS:HD2	1:B:30:LYS:HA	1.74	0.42
1:B:110:PHE:O	1:B:114:LEU:HG	2.19	0.42
1:B:159:VAL:O	1:B:163:GLN:HG2	2.19	0.42
2:A:68:ARG:HA	2:A:68:ARG:HD3	1.86	0.42
2:A:352:LYS:NZ	2:A:353:GLU:OE2	2.49	0.42
2:A:378:HIS:CD2	2:A:414:ARG:HH22	2.37	0.42
2:A:230:TRP:CH2	2:A:483:PRO:HB3	2.54	0.42
1:B:188:ILE:HG12	1:B:298:MET:SD	2.60	0.42
1:B:194:THR:HA	1:B:197:LEU:HD12	2.02	0.42
1:B:54:PHE:CD2	1:B:55:ILE:HD13	2.55	0.42
2:A:150:ALA:HB2	2:A:177:TYR:HB3	2.02	0.42
1:B:82:ILE:O	1:B:86:LEU:HG	2.19	0.42
1:B:99:LEU:CD2	1:B:298:MET:HE3	2.49	0.42
1:B:136:ILE:HD12	1:B:136:ILE:HA	1.90	0.42
1:B:284:ALA:O	1:B:287:LEU:HG	2.19	0.42
2:A:123:ASN:HD22	2:A:126:LEU:HD12	1.85	0.42
1:B:291:ILE:HB	1:B:292:PRO:HD3	2.02	0.41
2:A:447:ASN:OD1	2:A:448:GLY:N	2.49	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:504:ASN:O	2:A:508:LEU:HD23	2.20	0.41
1:B:92:ASN:O	1:B:96:MET:HG2	2.20	0.41
1:B:320:ILE:HD13	1:B:323:ASN:HD21	1.86	0.41
2:A:229:GLU:HB3	2:A:235:PRO:HD3	2.03	0.41
1:B:99:LEU:HD11	1:B:297:MET:HE1	2.02	0.41
1:B:162:TYR:HA	1:B:165:ILE:HG22	2.04	0.40
1:B:295:MET:HA	1:B:296:PRO:HD3	1.95	0.40
2:A:45:LYS:HE3	2:A:45:LYS:HB2	1.86	0.40
2:A:48:ALA:O	2:A:342:ARG:NH2	2.53	0.40
1:B:3:PRO:HG2	1:B:6:ARG:HD2	2.03	0.40
1:B:32:SER:HA	1:B:37:GLN:NE2	2.36	0.40
2:A:316:GLU:O	2:A:320:ILE:HD12	2.20	0.40
2:A:364:LEU:HD12	2:A:364:LEU:HA	1.89	0.40
2:A:439:LYS:HB3	2:A:439:LYS:HE2	1.79	0.40
1:B:189:GLN:HG2	1:B:189:GLN:H	1.70	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	B	276/430 (64%)	268 (97%)	8 (3%)	0	100	100
2	A	593/767 (77%)	565 (95%)	28 (5%)	0	100	100
All	All	869/1197 (73%)	833 (96%)	36 (4%)	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	B	266/412 (65%)	266 (100%)	0	100	100
2	A	523/666 (78%)	522 (100%)	1 (0%)	87	85
All	All	789/1078 (73%)	788 (100%)	1 (0%)	87	88

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	A	528	PHE

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

Mol	Chain	Res	Type
1	B	58	ASN
1	B	81	HIS
1	B	101	HIS
1	B	153	ASN
1	B	163	GLN
1	B	286	HIS
1	B	323	ASN
2	A	73	ASN
2	A	86	GLN
2	A	111	GLN
2	A	113	HIS
2	A	123	ASN
2	A	179	GLN
2	A	191	GLN
2	A	202	ASN
2	A	336	GLN
2	A	374	GLN
2	A	429	ASN

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](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

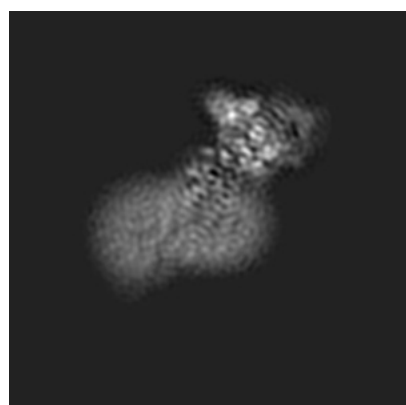
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-21220. These allow visual inspection of the internal detail of the map and identification of artifacts.

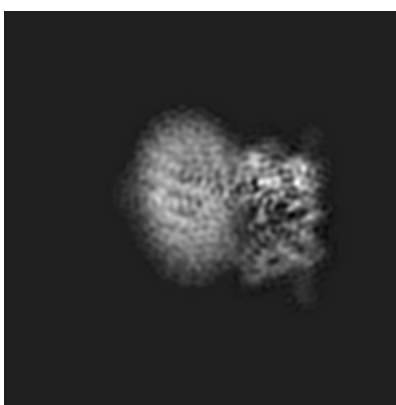
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

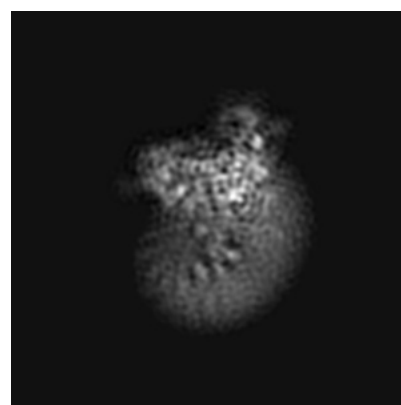
6.1.1 Primary map



X



Y

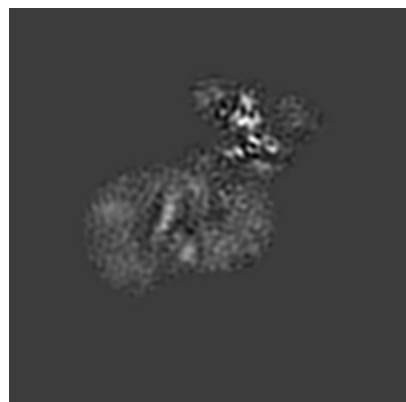


Z

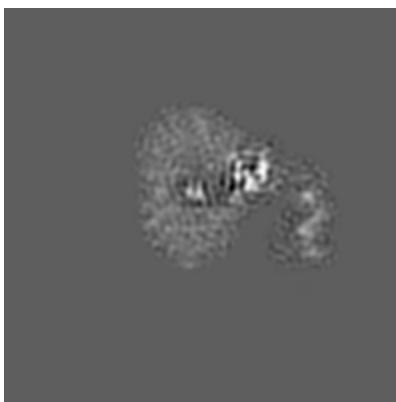
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

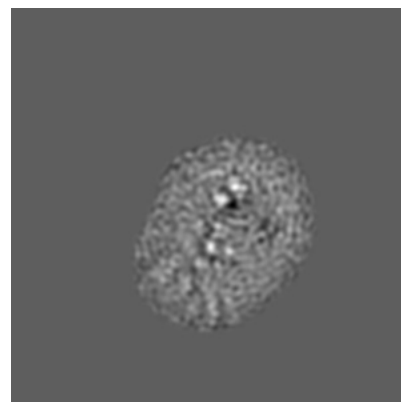
6.2.1 Primary map



X Index: 100



Y Index: 100

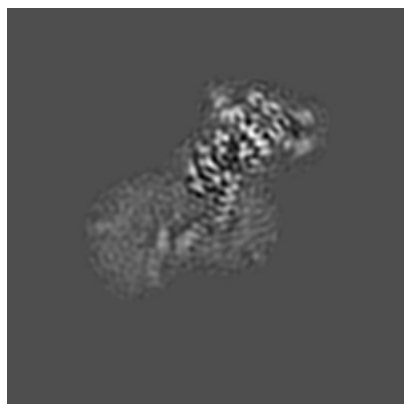


Z Index: 100

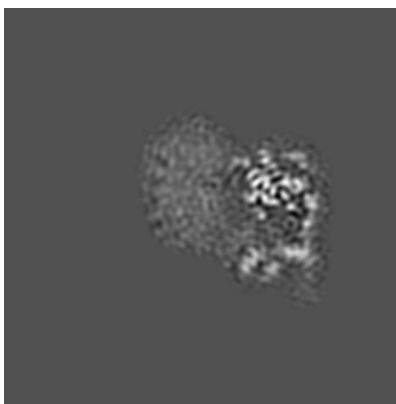
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

6.3.1 Primary map



X Index: 113



Y Index: 117

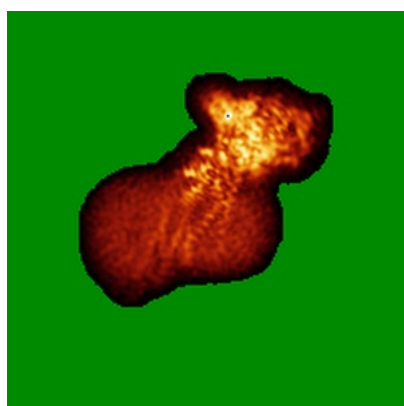


Z Index: 128

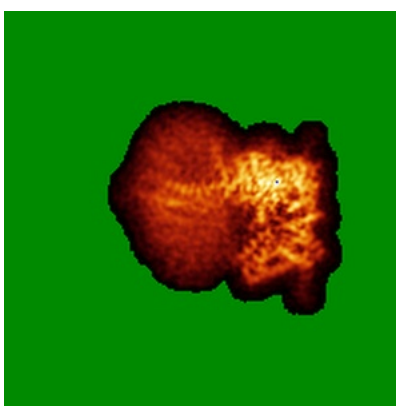
The images above show the largest variance slices of the map in three orthogonal directions.

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

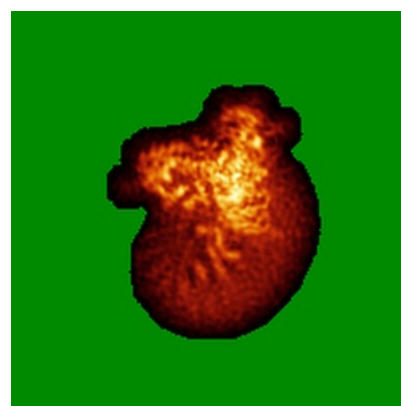
6.4.1 Primary map



X



Y

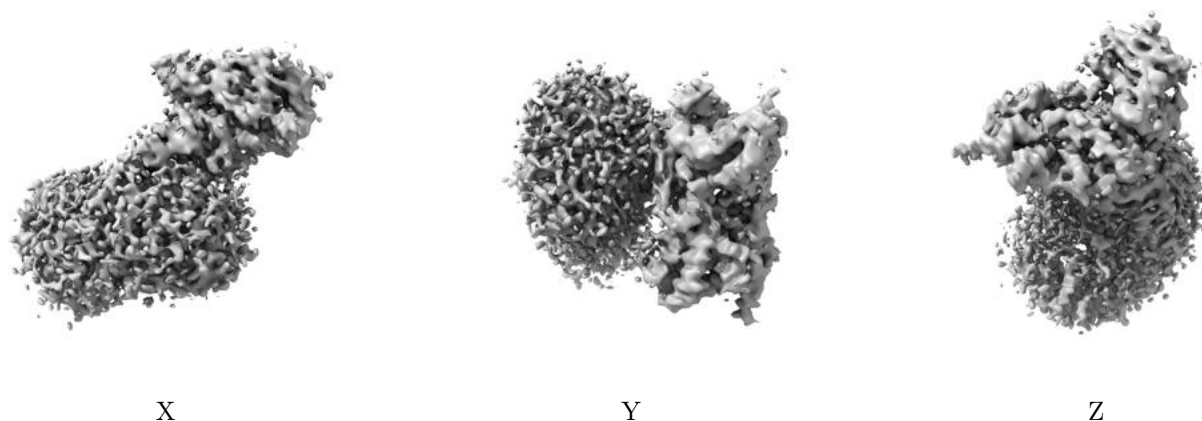


Z

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 0.013. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

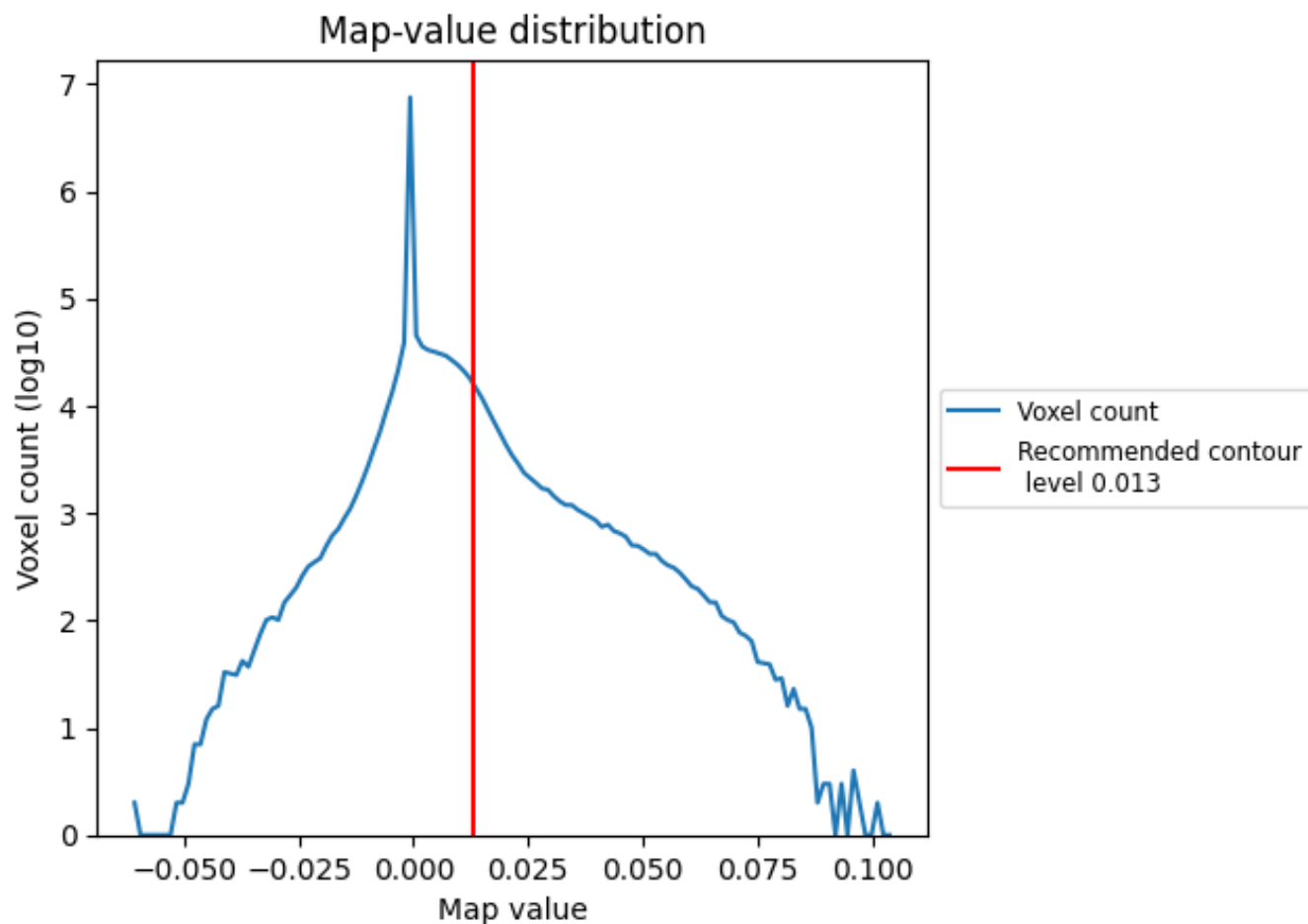
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

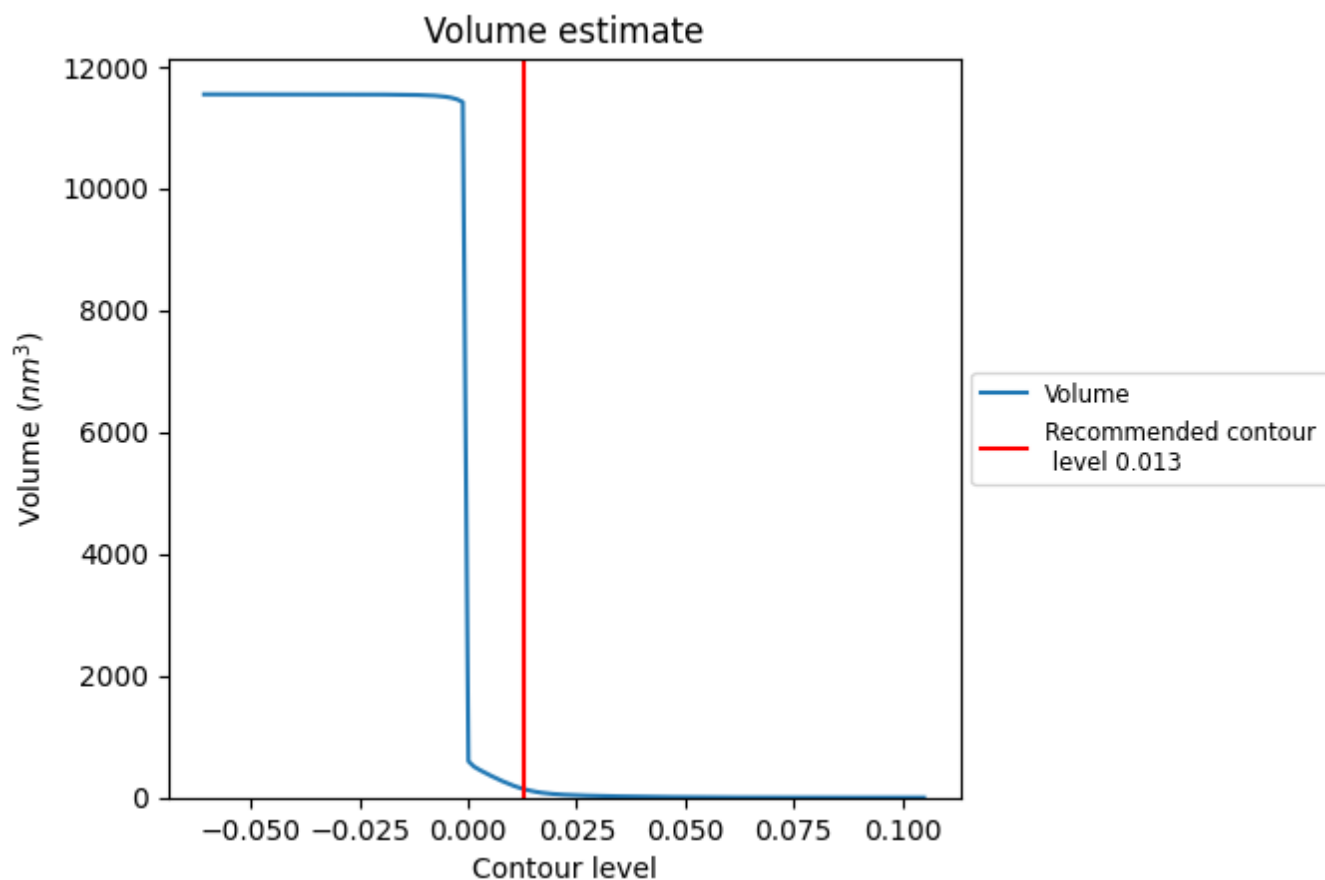
This section contains the results of statistical analysis of the map.

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.

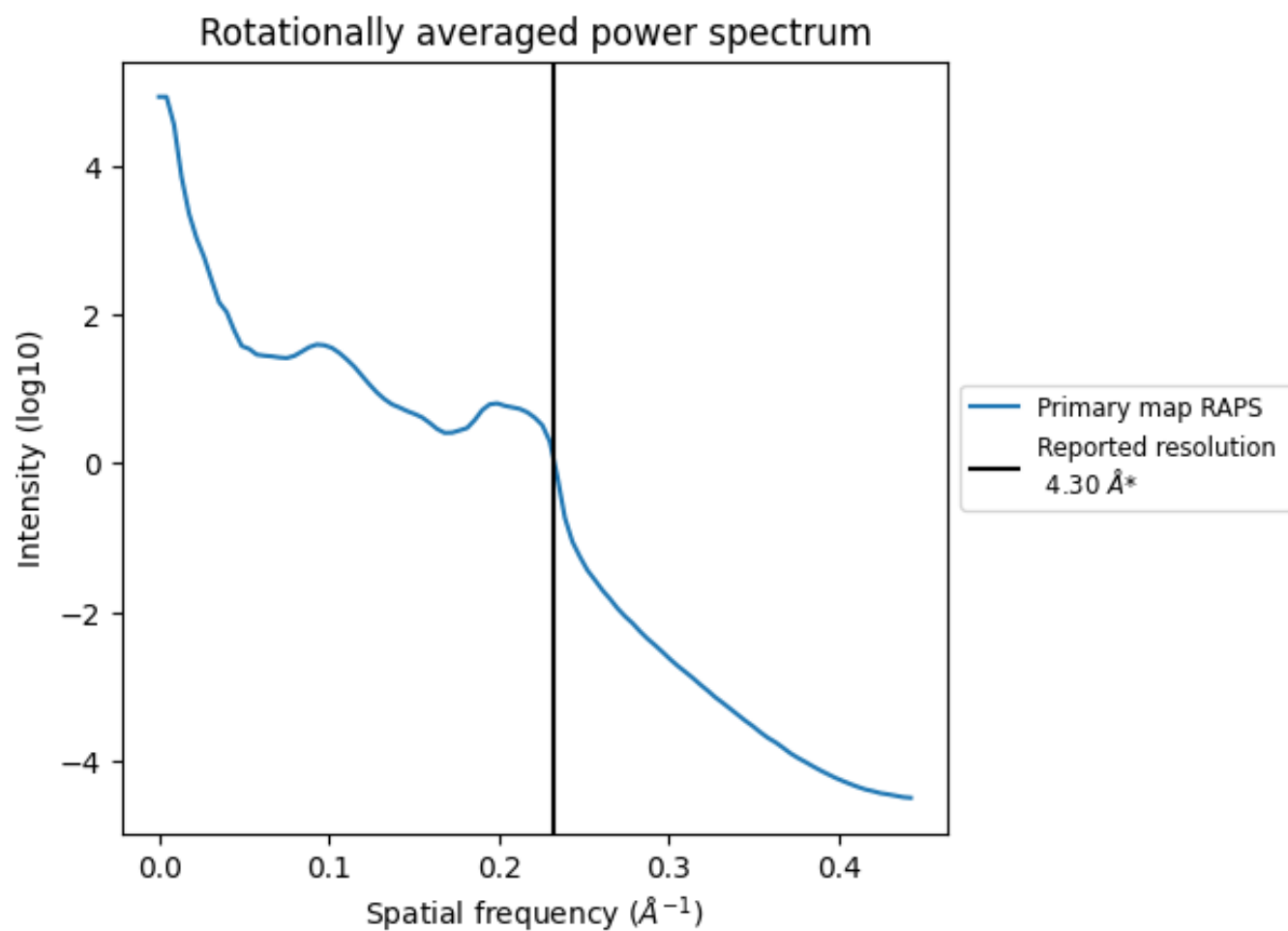
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 137 nm³; this corresponds to an approximate mass of 124 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 0.233 $\text{\AA}^{-1}$

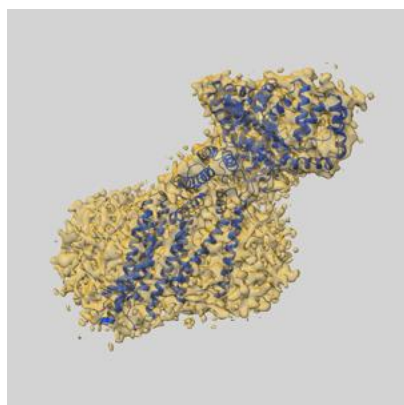
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

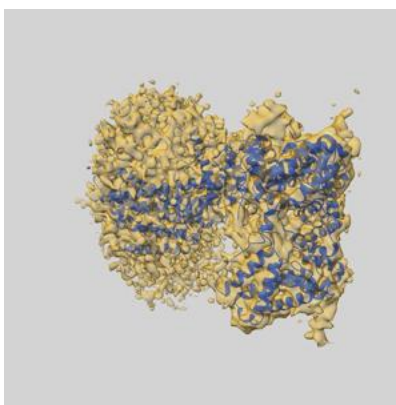
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-21220 and PDB model 6VJY. Per-residue inclusion information can be found in [section 3](#) on [page 4](#).

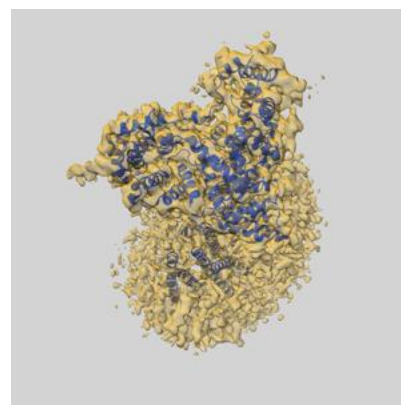
9.1 Map-model overlay [i](#)



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.013 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](#)

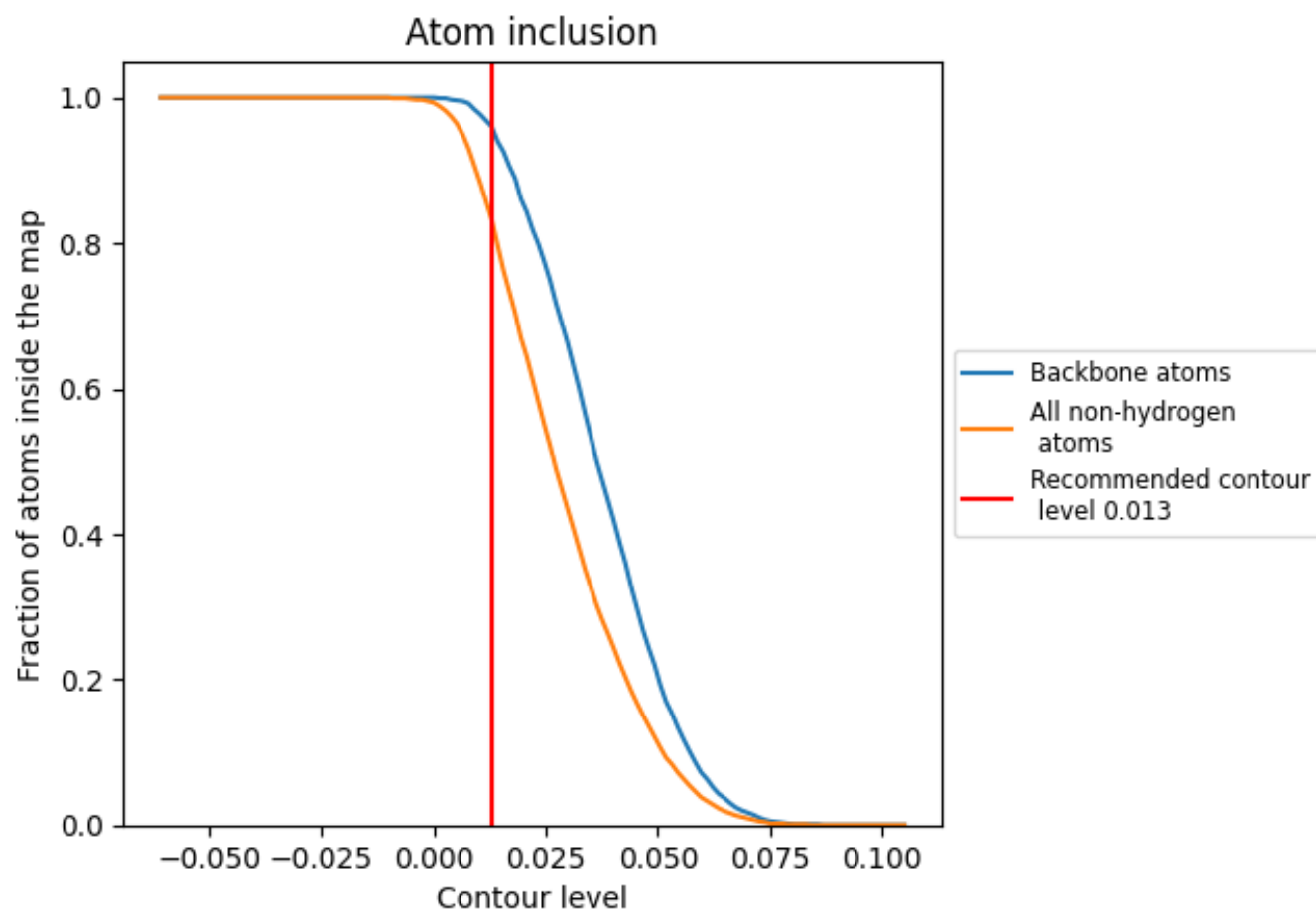


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

This section was not generated.

9.4 Atom inclusion [i](#)



At the recommended contour level, 96% of all backbone atoms, 83% 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 (0.013) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8330	0.3340
A	0.9080	0.3840
B	0.6770	0.2280

