



## Full wwPDB EM Validation Report ⓘ

Nov 12, 2022 – 06:55 PM EST

PDB ID : 6VAD  
EMDB ID : EMD-21137  
Title : Fanconi Anemia ID complex  
Authors : Pavletich, N.P.  
Deposited on : 2019-12-17  
Resolution : 3.35 Å(reported)  
Based on initial model : 3S4W

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

We welcome your comments at [validation@mail.wwpdb.org](mailto: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>.

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

EMDB validation analysis : 0.0.1.dev43  
MolProbity : 4.02b-467  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.9  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.31.2

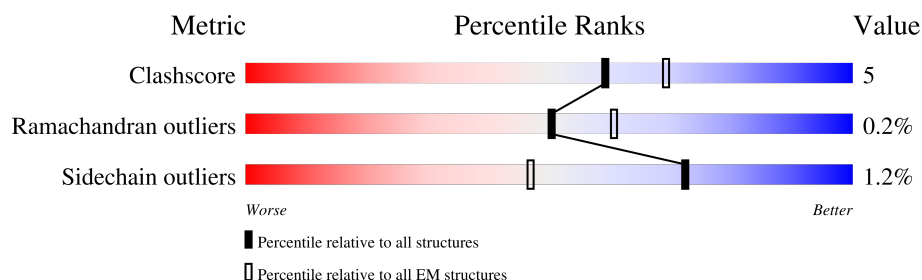
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.35 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	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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  $\geq 3$ , 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	1328	<div> <div>7%</div> <div>78%</div> <div>10%</div> <div>12%</div> </div>
2	B	1451	<div> <div>31%</div> <div>65%</div> <div>14%</div> <div>21%</div> </div>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 37613 atoms, of which 19096 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 Fanconi anemia, complementation group I.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	1168	Total	C	H	N	O	S	0	0
			18879	5934	9619	1549	1723	54		

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	136	VAL	ALA	conflict	UNP B7ZMF2
A	476	ASN	SER	conflict	UNP B7ZMF2
A	638	GLU	LYS	conflict	UNP B7ZMF2
A	657	GLN	LYS	conflict	UNP B7ZMF2
A	877	LEU	ILE	conflict	UNP B7ZMF2
A	1235	VAL	ALA	conflict	UNP B7ZMF2
A	1274	SER	ASN	conflict	UNP B7ZMF2

- Molecule 2 is a protein called Fanconi anemia group D2 protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	B	1153	Total	C	H	N	O	S	0	0
			18734	5969	9477	1527	1709	52		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	654	GLN	HIS	conflict	UNP Q9BXW9
B	693	ASN	ASP	conflict	UNP Q9BXW9



Chain B:



LYS GLU GLN ASP SER ASP GLU GLU SER LEU TYR ASP ASP SER ASP ASP	ASN	K1319	Q1259	A1199	L1137
	CYS	H1320	I1260	I1200	L1138
	ARG	R1321	H1261	E1201	M1139
	GLU	E1322	E1262	E1202	V1140
	ALA	D1323	E1263	I1203	I1141
	PHE	D1323	K1264	A1204	L1142
	TRP	V1324	L1265	G1205	E1143
	LEU	L1325	L1266	G1206	K1144
	GLY	S1326	L1267	V1207	S1145
	LEU	L1327	W1268	G1207	THR
LYS ASN ASP ARG ASP LEU GLN GLY GLU GLU ILE LYS SER SER GLN ASN SER GLN GLU SER GLU ASP ASP ASP MET SER SER SER GLN ALA SER LYS LYS ALA THR ALA GLU SER GLU SER ASP ASP ASP MET SER SER SER GLN ALA SER	LYS	L1328	W1269	P1209	ALA
	ASN	E1329	M1270	V1208	SER
	ASP	L1330	A1271	L1211	ALA
	LEU	Q1332	V1272	I1212	SER
	GLN	L1333	R1273	G1213	ALA
	GLY	D1334	D1274	S1214	ALA
	GLU	T1335	F1275	P1215	ALA
	GLU	R1336	S1276	LVS	ALA
	GLN	L1337	I1277	ALA	ALA
	ASN	L1338	L1278	SER	SER
LYS ASN ASP ARG ASP LEU GLN GLY GLU GLU ILE LYS SER SER SER SER GLN ALA SER LYS LYS ALA THR ALA GLU SER GLU SER ASP ASP ASP MET SER SER SER GLN ALA SER LYS LYS ALA THR ALA GLU SER GLU SER ASP ASP ASP MET SER SER SER GLN ALA SER	LYS	K1319	Q1259	A1199	L1137
	ASN	H1320	I1260	I1200	L1138
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	LEU	V1324	K1264	A1204	L1142
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	GLY	S1326	L1266	G1206	K1144
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LYS ASN ASP ARG ASP LEU GLN GLY GLU GLU ILE LYS SER SER SER SER GLN ALA SER LYS LYS ALA THR ALA GLU SER GLU SER ASP ASP ASP MET SER SER SER GLN ALA SER LYS LYS ALA THR ALA GLU SER GLU SER ASP ASP ASP MET SER SER SER GLN ALA SER	LYS	K1319	Q1259	A1199	L1137
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	THR	L1327	W1268	G1207	S1145
	ASP	L1328	W1269	P1209	THR
LYS ASN ASP ARG ASP LEU GLN GLY GLU GLU ILE LYS SER SER SER SER GLN ALA SER LYS LYS ALA THR ALA GLU SER GLU SER ASP ASP ASP MET SER SER SER GLN ALA SER LYS LYS ALA THR ALA GLU SER GLU SER ASP ASP ASP MET SER SER SER GLN ALA SER	LYS	K1319	Q1259	A1199	L1137
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LYS ASN ASP ARG ASP LEU GLN GLY GLU GLU ILE LYS SER SER SER SER GLN ALA SER LYS LYS ALA THR ALA GLU SER GLU SER ASP ASP ASP MET SER SER SER GLN ALA SER LYS LYS ALA THR ALA GLU SER GLU SER ASP ASP ASP MET SER SER SER GLN ALA SER	LYS	K1319	Q1259	A1199	L1137
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	GLY	S1326	L1266	G1206	K1144
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	ASP	L1328	W1269	P1209	THR
LYS ASN ASP ARG ASP LEU GLN 					

## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	251271	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 ( $e^-/\text{\AA}^2$ )	51	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.188	Depositor
Minimum map value	-0.114	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.012	Depositor
Map size (Å)	279.04, 279.04, 279.04	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.09, 1.09, 1.09	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	0.77	7/9403 (0.1%)	0.85	4/12681 (0.0%)
2	B	0.63	0/9427	0.79	1/12745 (0.0%)
All	All	0.70	7/18830 (0.0%)	0.82	5/25426 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	4
2	B	0	4
All	All	0	8

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	384	GLU	CD-OE2	11.21	1.38	1.25
1	A	384	GLU	CD-OE1	9.65	1.36	1.25
1	A	309	SER	CA-CB	-6.99	1.42	1.52
1	A	442	GLU	CD-OE2	6.83	1.33	1.25
1	A	483	GLU	CD-OE2	6.79	1.33	1.25
1	A	464	SER	CA-CB	-6.77	1.42	1.52
1	A	329	LEU	C-O	5.35	1.33	1.23

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	430	PHE	CB-CG-CD1	-5.92	116.66	120.80
2	B	356	TYR	CB-CG-CD2	5.69	124.42	121.00
1	A	430	PHE	CB-CG-CD2	5.45	124.62	120.80
1	A	447	ARG	NE-CZ-NH1	5.29	122.95	120.30
1	A	318	ARG	NE-CZ-NH2	-5.21	117.70	120.30



There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	224	GLY	Peptide
1	A	641	LEU	Peptide
1	A	717	GLU	Peptide
1	A	801	SER	Peptide
2	B	222	SER	Peptide
2	B	375	SER	Peptide
2	B	484	GLY	Peptide
2	B	485	ASN	Peptide

## 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	9260	9619	9587	64	0
2	B	9257	9477	9421	116	0
All	All	18517	19096	19008	179	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 (179) 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:425:ILE:O	1:A:429:THR:OG1	1.97	0.79
1:A:1170:TYR:OH	1:A:1209:CYS:SG	2.40	0.79
2:B:1122:HIS:O	2:B:1165:ARG:NH1	2.16	0.78
2:B:1279:ILE:HG23	2:B:1341:LEU:HD11	1.64	0.78
1:A:622:SER:O	1:A:626:THR:OG1	2.04	0.74
1:A:486:ASP:N	1:A:486:ASP:OD1	2.19	0.74
1:A:723:LEU:HD13	1:A:781:LEU:HD21	1.73	0.71
1:A:128:GLU:OE1	2:B:560:ARG:NH1	2.25	0.69
2:B:787:PHE:O	2:B:791:ASN:ND2	2.26	0.68
2:B:1077:GLY:O	2:B:1083:ASN:ND2	2.27	0.67
1:A:121:LEU:O	1:A:173:TYR:OH	2.10	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:533:PHE:O	2:B:537:SER:OG	2.11	0.66
2:B:1117:TYR:O	2:B:1120:ASN:ND2	2.29	0.66
2:B:621:SER:O	2:B:624:SER:N	2.32	0.62
2:B:196:ILE:HD12	2:B:215:LEU:HD21	1.82	0.62
2:B:793:PHE:HA	2:B:796:ILE:HD12	1.81	0.62
1:A:1022:ALA:HB1	1:A:1083:THR:HG21	1.83	0.61
2:B:1328:LEU:HD13	2:B:1375:LEU:HD13	1.83	0.61
2:B:371:THR:O	2:B:406:LYS:NZ	2.34	0.60
2:B:1056:HIS:O	2:B:1059:SER:OG	2.15	0.60
2:B:391:THR:OG1	2:B:392:ASN:N	2.35	0.59
2:B:1203:ILE:O	2:B:1207:GLY:N	2.36	0.59
2:B:1236:ARG:HA	2:B:1293:VAL:HG21	1.83	0.59
2:B:965:LEU:HD23	2:B:1061:CYS:SG	2.42	0.59
1:A:144:LEU:O	1:A:151:LEU:N	2.36	0.59
1:A:595:LEU:O	1:A:602:ARG:NE	2.36	0.58
2:B:756:LEU:O	2:B:815:ARG:NH2	2.36	0.58
2:B:235:LEU:HD11	2:B:242:THR:HG22	1.83	0.58
2:B:637:ASN:ND2	2:B:844:ASP:OD2	2.37	0.57
1:A:506:LEU:O	1:A:510:SER:OG	2.16	0.57
2:B:456:LEU:HD12	2:B:460:TYR:CE1	2.39	0.57
2:B:1208:VAL:HG23	2:B:1209:PRO:HD3	1.87	0.56
1:A:395:PRO:HD2	1:A:458:HIS:ND1	2.21	0.56
2:B:1187:CYS:SG	2:B:1237:VAL:HG23	2.46	0.56
1:A:1210:TYR:HA	1:A:1213:ILE:HD12	1.88	0.55
2:B:417:LEU:HD13	2:B:453:PHE:CZ	2.41	0.55
2:B:185:ARG:NH1	2:B:186:VAL:O	2.40	0.55
2:B:1078:PHE:O	2:B:1084:GLN:NE2	2.40	0.54
1:A:316:VAL:HG12	1:A:316:VAL:O	2.06	0.54
2:B:684:TYR:HE1	2:B:765:LEU:HD12	1.72	0.54
1:A:442:GLU:HB3	1:A:480:LYS:HD2	1.88	0.54
2:B:783:CYS:SG	2:B:784:SER:N	2.81	0.54
2:B:428:LEU:O	2:B:431:MET:HG2	2.08	0.53
1:A:132:ILE:O	1:A:136:VAL:HG23	2.07	0.53
1:A:375:TRP:O	1:A:377:HIS:N	2.40	0.53
1:A:828:SER:O	1:A:831:VAL:HG22	2.09	0.53
1:A:316:VAL:O	1:A:316:VAL:CG1	2.57	0.53
1:A:8:LEU:HD22	1:A:16:LYS:HD3	1.91	0.53
2:B:811:LYS:O	2:B:814:THR:OG1	2.24	0.52
2:B:931:GLU:N	2:B:931:GLU:OE1	2.43	0.52
2:B:144:ILE:HG13	2:B:145:LEU:HD12	1.92	0.52
1:A:66:ARG:HG3	1:A:104:LEU:HD22	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:970:LEU:O	1:A:1019:ARG:NH2	2.43	0.51
2:B:801:CYS:SG	2:B:802:GLN:N	2.84	0.51
2:B:364:TRP:CE2	2:B:384:MET:HG2	2.45	0.51
2:B:1269:ASN:HA	2:B:1327:LEU:HD11	1.92	0.51
2:B:243:VAL:HG13	2:B:244:PRO:HD3	1.92	0.51
2:B:945:ILE:HD12	2:B:1034:PHE:CD1	2.46	0.51
2:B:1182:LEU:HB3	2:B:1233:VAL:HG11	1.93	0.51
2:B:263:ARG:NH2	2:B:288:SER:O	2.44	0.50
2:B:1274:ASP:O	2:B:1278:LEU:HD23	2.11	0.50
1:A:881:LEU:HD22	1:A:908:CYS:SG	2.51	0.50
2:B:928:LEU:HD23	2:B:932:VAL:HG11	1.92	0.50
2:B:197:MET:CE	2:B:227:VAL:HG13	2.41	0.50
1:A:651:ILE:HD13	1:A:738:LYS:HA	1.92	0.50
2:B:749:LEU:HD22	2:B:800:PHE:CE2	2.46	0.50
1:A:461:ASP:O	1:A:465:ASN:OD1	2.30	0.50
2:B:613:LEU:O	2:B:617:VAL:HG23	2.12	0.50
2:B:132:SER:OG	2:B:133:LYS:N	2.45	0.49
2:B:1201:GLU:OE2	2:B:1277:ILE:HD11	2.12	0.49
1:A:986:VAL:O	1:A:990:THR:OG1	2.30	0.49
2:B:579:VAL:HG21	2:B:634:GLU:HG3	1.95	0.49
2:B:668:SER:N	2:B:694:GLY:O	2.45	0.49
2:B:684:TYR:CZ	2:B:822:LEU:HD21	2.48	0.49
2:B:1235:PHE:CD2	2:B:1290:VAL:HG13	2.48	0.49
2:B:1247:LYS:HE2	2:B:1304:ALA:HB2	1.94	0.49
2:B:1017:PHE:CE2	2:B:1072:LEU:HD11	2.48	0.49
1:A:1142:LEU:CD2	1:A:1205:LEU:HD22	2.44	0.48
1:A:331:LYS:HD3	1:A:388:ILE:CG2	2.43	0.48
2:B:586:ALA:HB1	2:B:644:LEU:HB2	1.96	0.48
2:B:623:GLN:O	2:B:624:SER:N	2.46	0.48
2:B:1223:PHE:O	2:B:1226:LEU:HD23	2.14	0.48
2:B:200:ILE:HD11	2:B:212:ILE:HD12	1.94	0.47
2:B:583:GLY:HA3	2:B:638:LEU:HD11	1.96	0.47
2:B:606:GLN:O	2:B:610:VAL:HG23	2.13	0.47
1:A:1262:LYS:HA	1:A:1265:ILE:HD12	1.96	0.47
1:A:1081:ALA:HB3	1:A:1082:PRO:HD3	1.97	0.46
2:B:605:GLU:OE1	2:B:605:GLU:N	2.43	0.46
2:B:1261:HIS:CE1	2:B:1265:LEU:HD22	2.50	0.46
2:B:391:THR:O	2:B:392:ASN:C	2.52	0.46
2:B:1243:GLU:OE1	2:B:1300:LEU:HD13	2.16	0.46
1:A:470:ALA:HB3	1:A:473:VAL:HG22	1.97	0.46
1:A:295:VAL:O	1:A:297:GLN:N	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:233:ILE:HG21	1:A:271:ILE:HG21	1.98	0.46
2:B:244:PRO:O	2:B:248:VAL:HG23	2.15	0.46
2:B:1279:ILE:HG23	2:B:1341:LEU:CD1	2.42	0.45
2:B:629:ALA:HB1	2:B:843:PHE:CD2	2.51	0.45
1:A:196:GLU:O	1:A:200:SER:OG	2.30	0.45
1:A:628:LEU:HD11	1:A:632:LYS:HE3	1.97	0.45
2:B:1098:LEU:HD11	2:B:1117:TYR:HA	1.98	0.45
1:A:32:LEU:HD11	1:A:68:ILE:CG1	2.47	0.45
2:B:933:PHE:HZ	2:B:971:ASP:OD2	2.00	0.45
1:A:1180:TYR:HA	1:A:1183:VAL:HG12	1.98	0.45
2:B:1017:PHE:O	2:B:1021:THR:OG1	2.34	0.45
1:A:135:THR:O	1:A:138:ALA:HB3	2.17	0.45
2:B:491:THR:O	2:B:495:VAL:HG23	2.17	0.45
1:A:1145:PHE:O	1:A:1149:VAL:HG23	2.17	0.45
1:A:866:ASN:ND2	1:A:869:LYS:HG2	2.32	0.45
2:B:480:HIS:ND1	2:B:488:GLU:OE1	2.40	0.45
2:B:104:ILE:O	2:B:156:LYS:NZ	2.50	0.44
2:B:495:VAL:O	2:B:499:LEU:HG	2.17	0.44
1:A:102:GLY:HA3	1:A:144:LEU:HD21	2.00	0.44
1:A:1196:LYS:O	1:A:1200:LEU:HD23	2.18	0.44
2:B:235:LEU:CD1	2:B:242:THR:HG22	2.48	0.44
2:B:1227:THR:N	2:B:1230:THR:OG1	2.45	0.44
1:A:868:GLU:OE1	1:A:926:LYS:NZ	2.51	0.44
2:B:68:LEU:N	2:B:118:GLU:O	2.51	0.44
2:B:385:LEU:HD22	2:B:399:ILE:HG23	2.00	0.44
2:B:654:GLN:O	2:B:658:ASN:ND2	2.51	0.44
2:B:792:TRP:CE2	2:B:796:ILE:HD11	2.52	0.44
1:A:348:LYS:HG2	1:A:1039:TYR:O	2.18	0.43
2:B:435:ILE:HG23	2:B:457:LEU:HD22	1.99	0.43
2:B:1302:VAL:HG21	2:B:1367:LEU:HD22	2.00	0.43
2:B:1186:LEU:HB2	2:B:1237:VAL:HG21	1.99	0.43
1:A:668:LEU:HD12	1:A:749:VAL:HG22	1.99	0.43
1:A:56:CYS:SG	1:A:65:ARG:NH1	2.91	0.43
2:B:462:PHE:CD2	2:B:499:LEU:HD22	2.52	0.43
2:B:212:ILE:HD11	2:B:231:LEU:HD22	2.00	0.43
1:A:1018:SER:OG	1:A:1019:ARG:N	2.52	0.43
2:B:734:PHE:CD1	2:B:792:TRP:HZ3	2.37	0.43
2:B:1182:LEU:CB	2:B:1233:VAL:HG11	2.49	0.43
1:A:310:ILE:O	1:A:311:ALA:C	2.54	0.43
2:B:270:LEU:HD12	2:B:273:ILE:HD12	2.00	0.43
1:A:533:ARG:HD3	1:A:597:GLN:HE22	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:113:CYS:O	2:B:134:SER:OG	2.37	0.43
2:B:665:VAL:HG13	2:B:695:ILE:HG23	2.01	0.43
2:B:1086:LEU:O	2:B:1090:ALA:N	2.46	0.43
1:A:798:ASN:HA	1:A:801:SER:HB3	2.01	0.42
1:A:606:TYR:OH	1:A:662:GLU:OE2	2.25	0.42
2:B:197:MET:HA	2:B:200:ILE:HG22	2.00	0.42
2:B:517:ILE:HG21	2:B:532:LEU:HD11	2.01	0.42
2:B:531:LYS:O	2:B:535:VAL:HG23	2.19	0.42
2:B:759:PRO:O	2:B:760:ILE:HD13	2.19	0.42
2:B:1346:LYS:O	2:B:1349:GLN:NE2	2.52	0.42
2:B:929:ASP:O	2:B:932:VAL:HG23	2.19	0.42
2:B:1122:HIS:HB2	2:B:1162:PHE:CE2	2.55	0.42
2:B:1292:HIS:HD2	2:B:1353:LEU:HD23	1.84	0.42
2:B:1213:ASN:OD1	2:B:1214:SER:N	2.50	0.42
2:B:1302:VAL:HG21	2:B:1367:LEU:CD2	2.50	0.41
1:A:131:PRO:HD3	1:A:180:MET:HG3	2.01	0.41
2:B:196:ILE:HD12	2:B:215:LEU:CD2	2.50	0.41
2:B:1272:VAL:HG11	2:B:1327:LEU:HD12	2.02	0.41
1:A:350:LEU:HD11	1:A:1098:GLU:HB3	2.02	0.41
1:A:742:SER:O	1:A:746:VAL:HG23	2.20	0.41
2:B:524:ILE:HG22	2:B:529:ILE:HG13	2.02	0.41
1:A:866:ASN:HD22	1:A:869:LYS:HG2	1.85	0.41
2:B:578:ALA:HB1	2:B:613:LEU:CD2	2.51	0.41
1:A:753:LEU:O	1:A:757:ASN:ND2	2.53	0.41
2:B:1108:GLU:OE2	2:B:1145:SER:OG	2.37	0.41
1:A:271:ILE:O	1:A:275:ILE:HG13	2.20	0.41
2:B:351:LYS:O	2:B:354:ILE:HG12	2.21	0.41
2:B:462:PHE:HB2	2:B:473:VAL:HG11	2.03	0.41
2:B:506:ALA:O	2:B:510:ASN:ND2	2.53	0.41
2:B:777:LYS:O	2:B:780:SER:OG	2.33	0.41
1:A:482:THR:HB	1:A:516:CYS:SG	2.61	0.41
2:B:699:LEU:HD23	2:B:785:LEU:HD12	2.03	0.41
1:A:207:LEU:HD23	1:A:210:ILE:HD12	2.02	0.41
2:B:578:ALA:HB1	2:B:613:LEU:HD21	2.03	0.41
1:A:13:THR:HG22	1:A:52:LYS:HE2	2.03	0.40
1:A:32:LEU:HD11	1:A:68:ILE:HG13	2.03	0.40
1:A:445:LEU:HA	1:A:445:LEU:HD23	1.88	0.40
2:B:1033:TYR:O	2:B:1037:LEU:HD23	2.21	0.40
2:B:365:ILE:HG21	2:B:398:TYR:CE2	2.56	0.40
1:A:13:THR:HG22	1:A:52:LYS:CE	2.51	0.40
1:A:1201:SER:O	1:A:1206:THR:HG23	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:197:MET:HE3	2:B:227:VAL:HG13	2.03	0.40
2:B:1017:PHE:HE2	2:B:1072:LEU:HD11	1.86	0.40
2:B:738:ARG:HD3	2:B:799:ALA:HB2	2.03	0.40
2:B:1186:LEU:CB	2:B:1237:VAL:HG11	2.51	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1149/1328 (86%)	1075 (94%)	72 (6%)	2 (0%)	47	78
2	B	1123/1451 (77%)	1050 (94%)	70 (6%)	3 (0%)	41	73
All	All	2272/2779 (82%)	2125 (94%)	142 (6%)	5 (0%)	50	78

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	376	ASP
1	A	120	SER
2	B	391	THR
2	B	767	PRO
2	B	220	GLY

### 5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	1067/1205 (88%)	1059 (99%)	8 (1%)	84	92
2	B	1065/1324 (80%)	1048 (98%)	17 (2%)	62	81
All	All	2132/2529 (84%)	2107 (99%)	25 (1%)	72	85

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	337	SER
1	A	341	LEU
1	A	486	ASP
1	A	664	LEU
1	A	811	SER
1	A	893	GLU
1	A	898	LYS
1	A	1093	GLU
2	B	185	ARG
2	B	247	ASP
2	B	302	ARG
2	B	342	CYS
2	B	391	THR
2	B	392	ASN
2	B	433	SER
2	B	643	LYS
2	B	726	SER
2	B	729	CYS
2	B	774	MET
2	B	943	LYS
2	B	1021	THR
2	B	1028	GLU
2	B	1208	VAL
2	B	1211	LEU
2	B	1228	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	657	GLN
1	A	757	ASN
1	A	865	GLN
2	B	72	GLN
2	B	1176	ASN

### 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 monosaccharides 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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	B	4
1	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	773:SER	C	774:MET	N	3.97
1	B	187:VAL	C	188:ASP	N	3.61
1	B	623:GLN	C	624:SER	N	3.18
1	B	643:LYS	C	644:LEU	N	3.18
1	A	260:PRO	C	261:SER	N	3.11



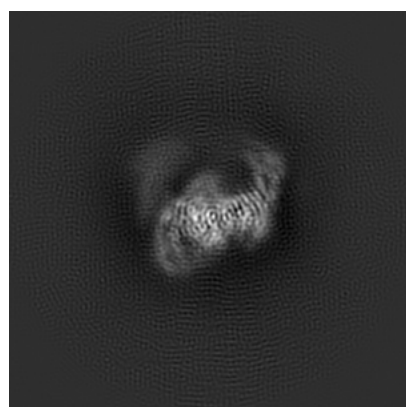
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-21137. These allow visual inspection of the internal detail of the map and identification of artifacts.

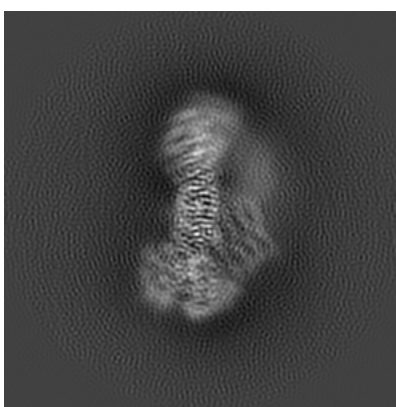
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

### 6.1 Orthogonal projections [i](#)

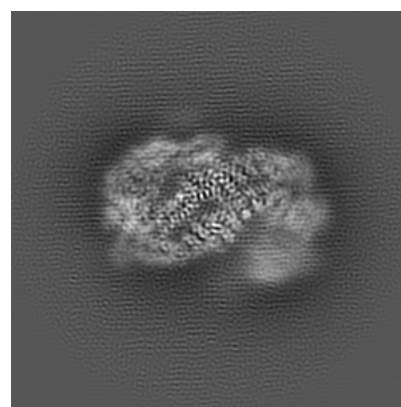
#### 6.1.1 Primary map



X



Y

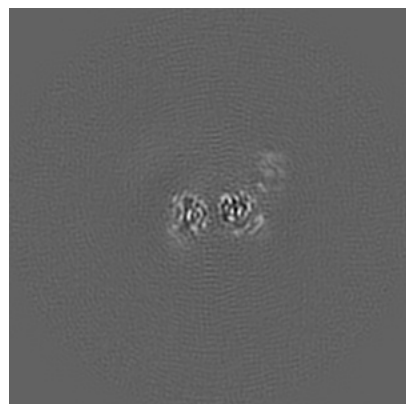


Z

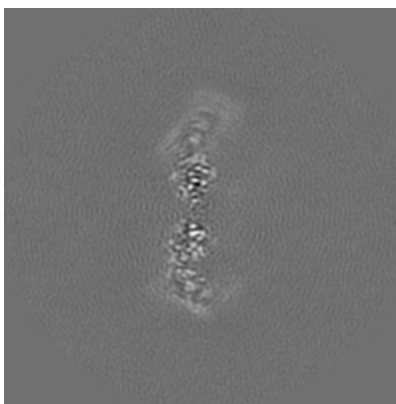
The images above show the map projected in three orthogonal directions.

### 6.2 Central slices [i](#)

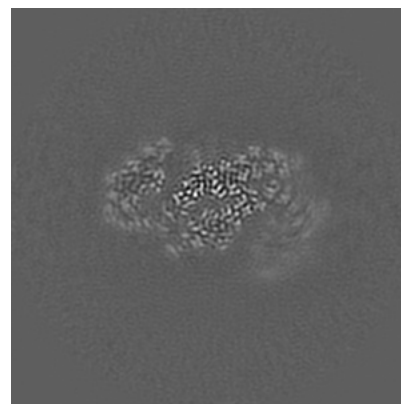
#### 6.2.1 Primary map



X Index: 128



Y Index: 128



Z Index: 128

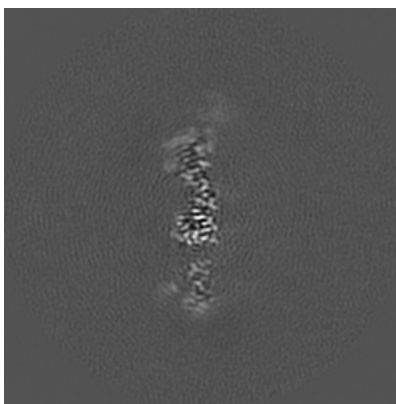
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

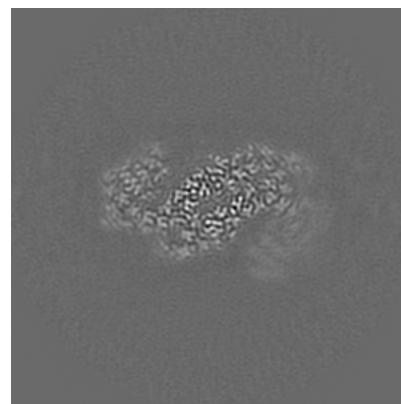
### 6.3.1 Primary map



X Index: 117



Y Index: 137



Z Index: 123

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

## 6.4 Orthogonal surface views [i](#)

### 6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.012. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

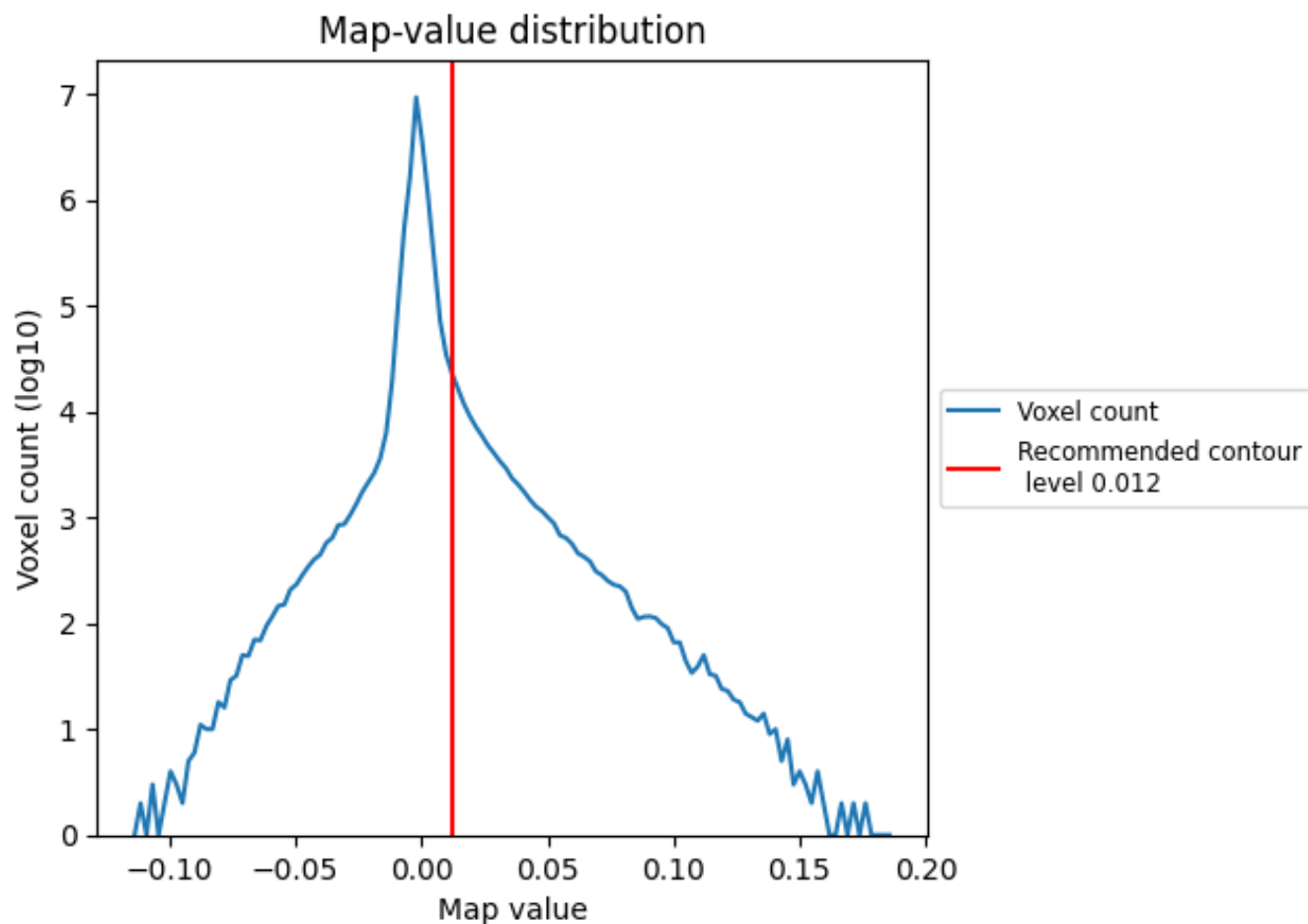
## 6.5 Mask visualisation

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

## 7 Map analysis [i](#)

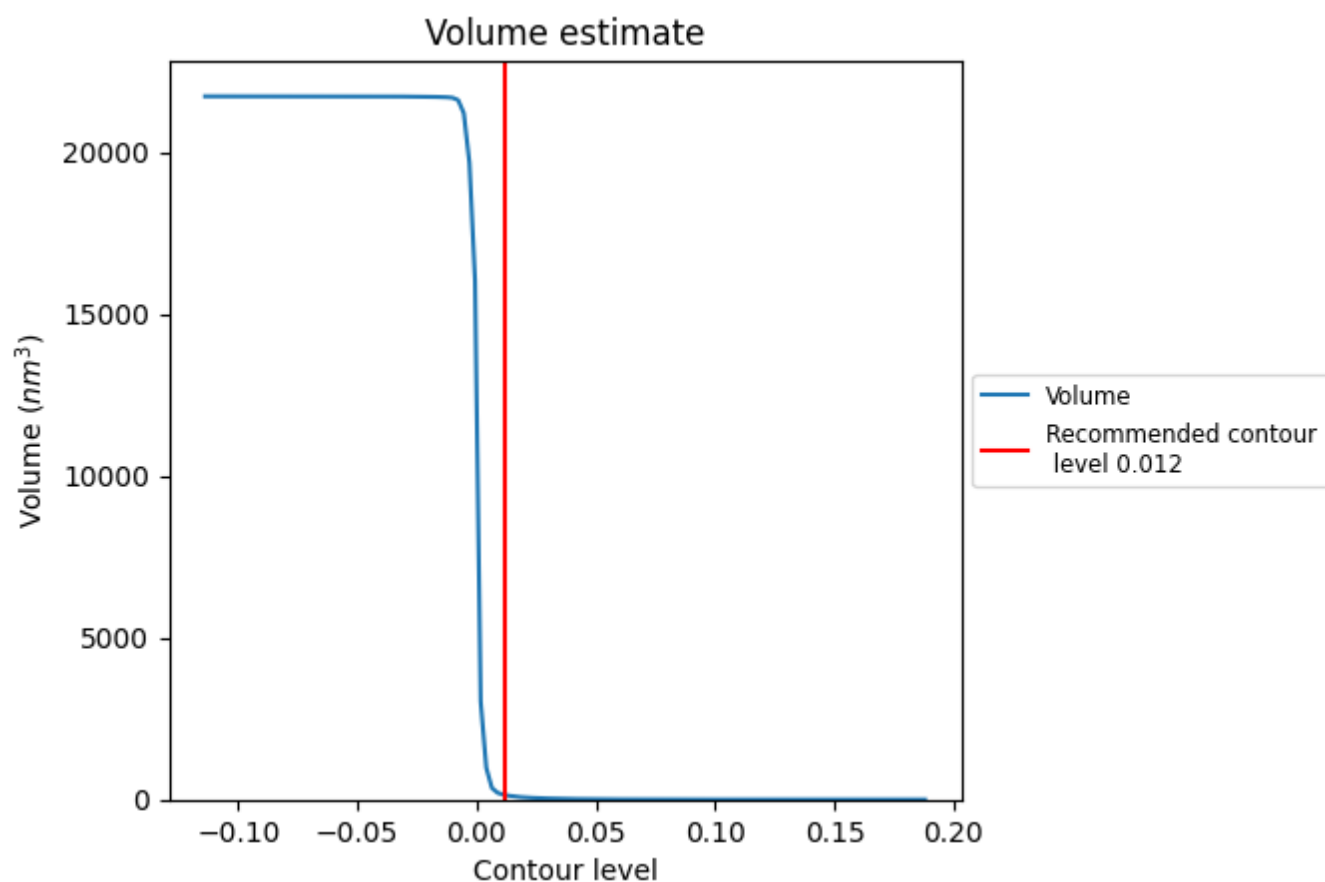
This section contains the results of statistical analysis of the map.

### 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.

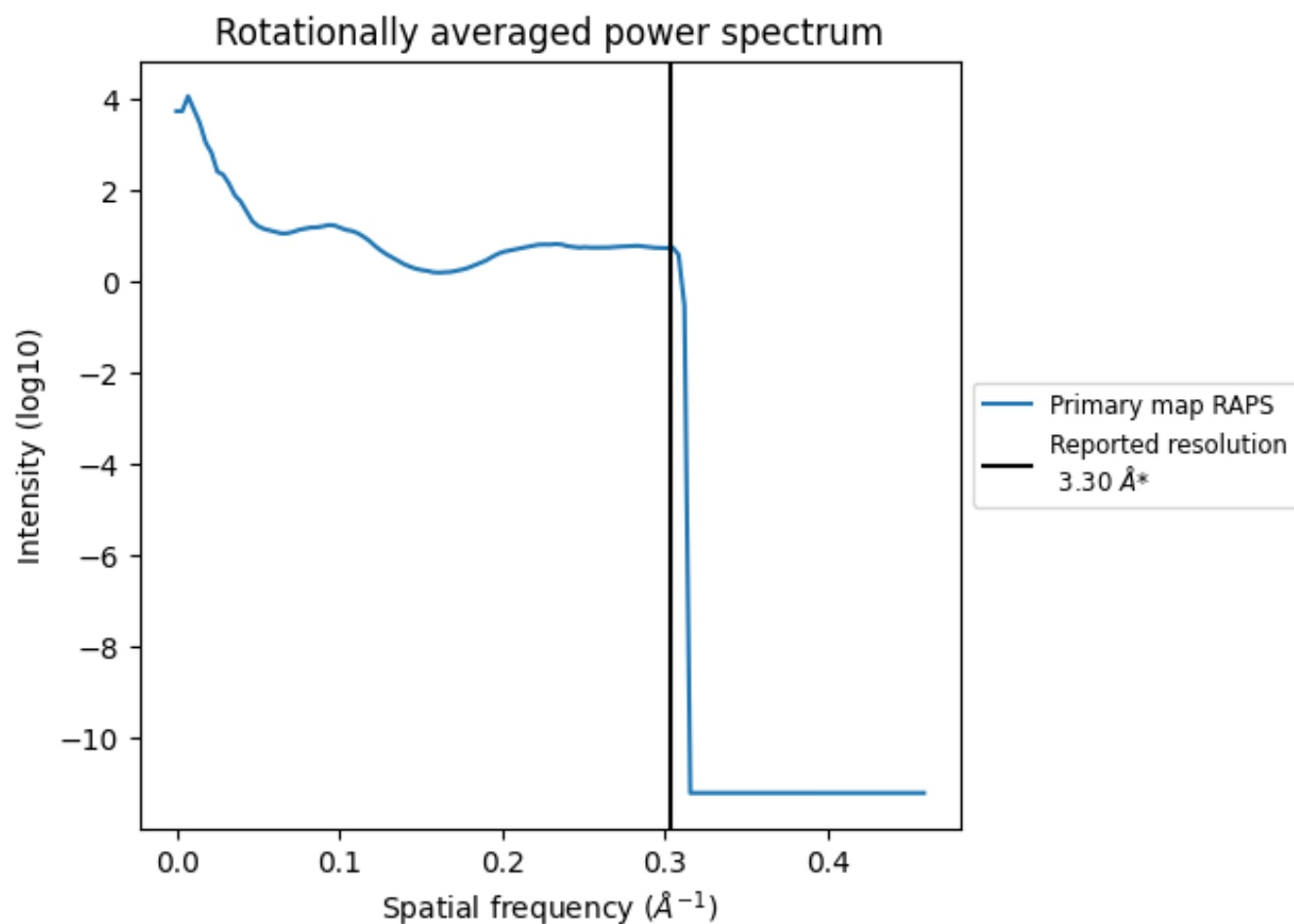
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 140 nm<sup>3</sup>; this corresponds to an approximate mass of 127 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 0.303 Å<sup>-1</sup>

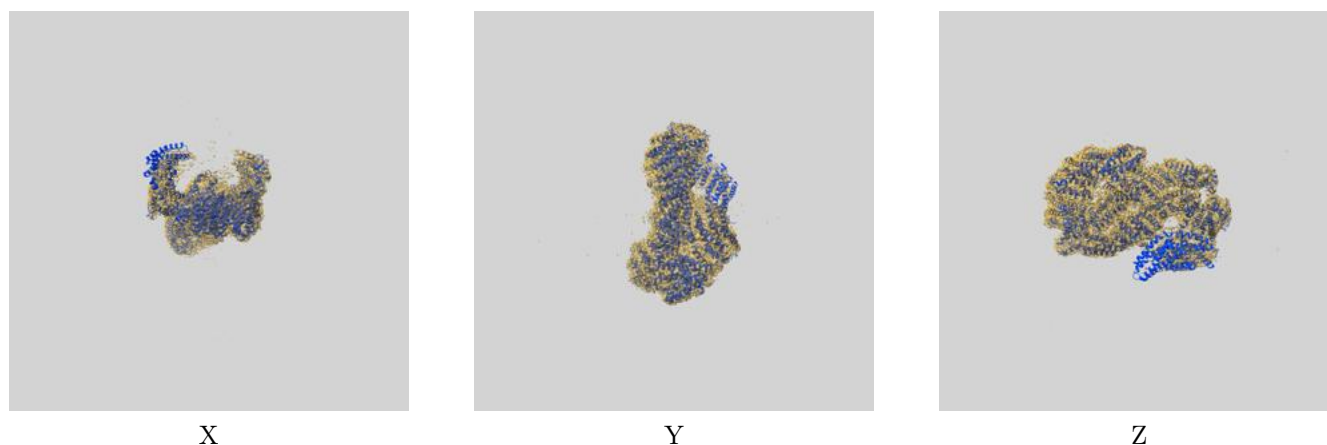
## 8 Fourier-Shell correlation

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-21137 and PDB model 6VAD. Per-residue inclusion information can be found in section 3 on page 4.

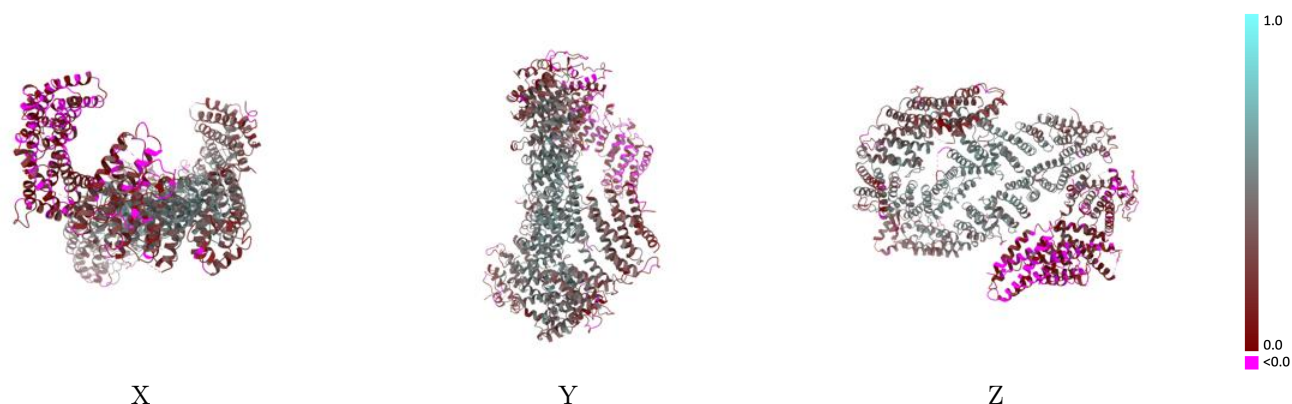
### 9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 0.012 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

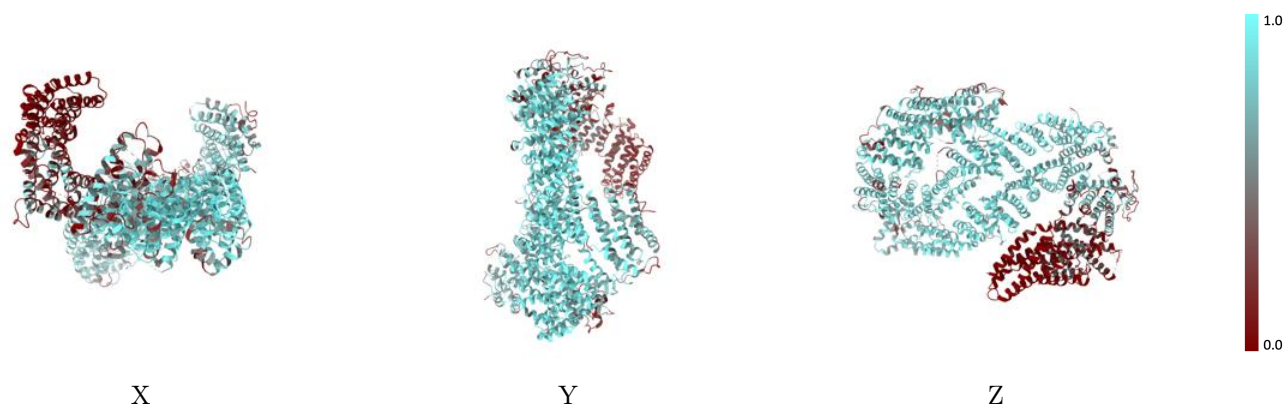


## 9.2 Q-score mapped to coordinate model [i](#)



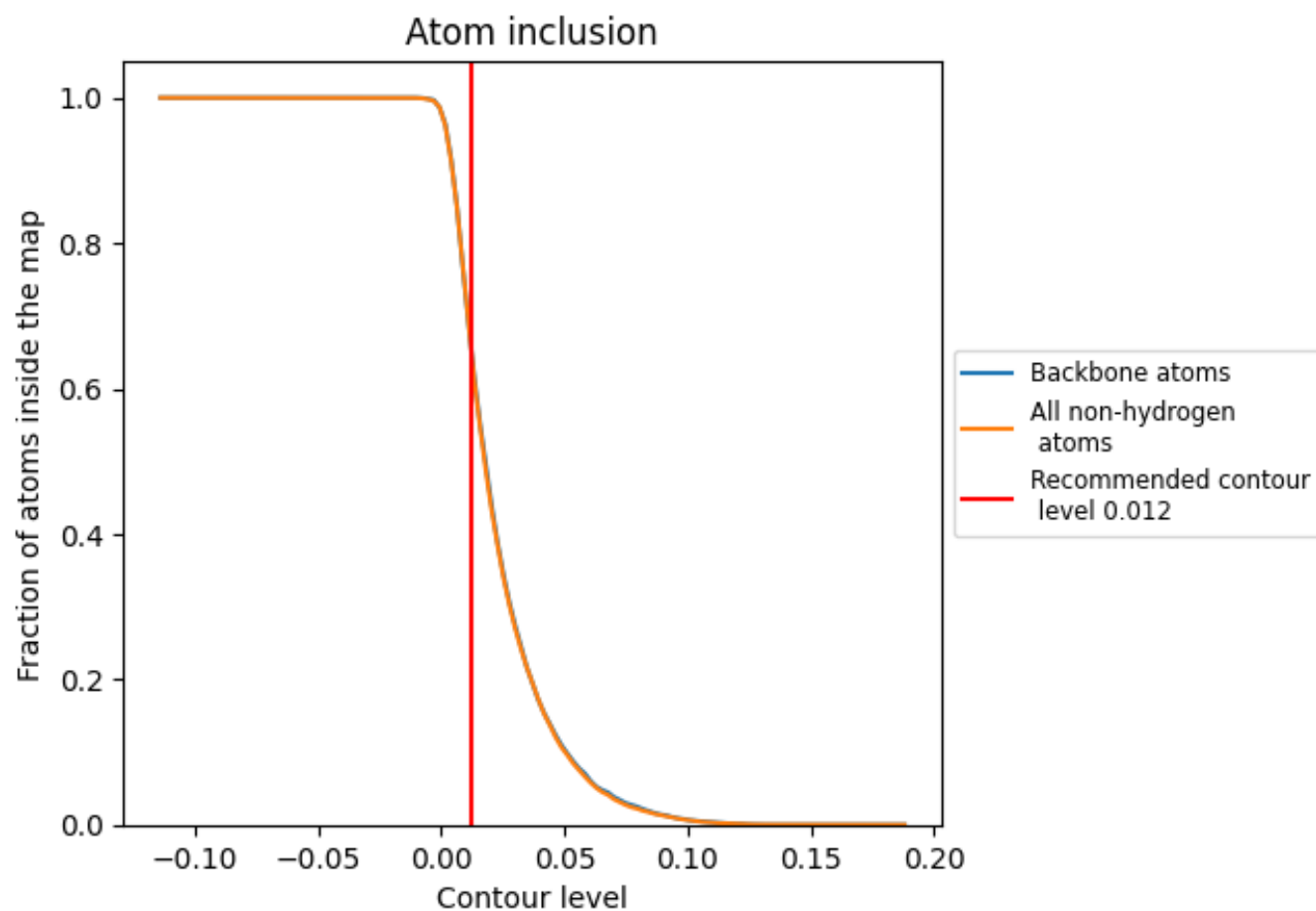
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

## 9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.012).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 66% of all backbone atoms, 66% 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 (0.012) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.6583	<div></div> 0.3190
A	<div></div> 0.7960	<div></div> 0.4010
B	<div></div> 0.5282	<div></div> 0.2360

