Full wwPDB EM Validation Report (i)

Feb 27, 2024 – 10:54 AM EST

PDB ID	:	6VAD
EMDB ID	:	EMD-21137
Title	:	Fanconi Anemia ID complex
Authors	:	Pavletich, N.P.
Deposited on	:	2019-12-17
Resolution	:	3.30 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*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the (i) 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 (i)) were used in the production of this report:

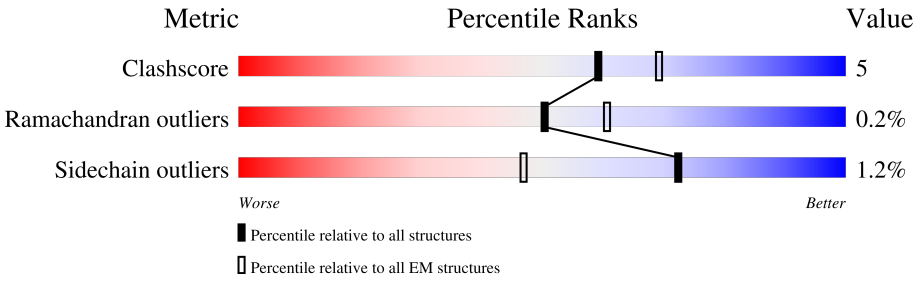
EMDB validation analysis	:	0.0.1.dev70
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 3.30 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)
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 >=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	1328	7% 78% 10% 12%
2	B	1451	31% 65% 14% 21%

2 Entry composition (i)

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
			Total	C	H	N	O	S		
1	A	1168	18879	5934	9619	1549	1723	54	0	0

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
			Total	C	H	N	O	S		
2	B	1153	18734	5969	9477	1527	1709	52	0	0

There are 2 discrepancies between the modelled and reference sequences:

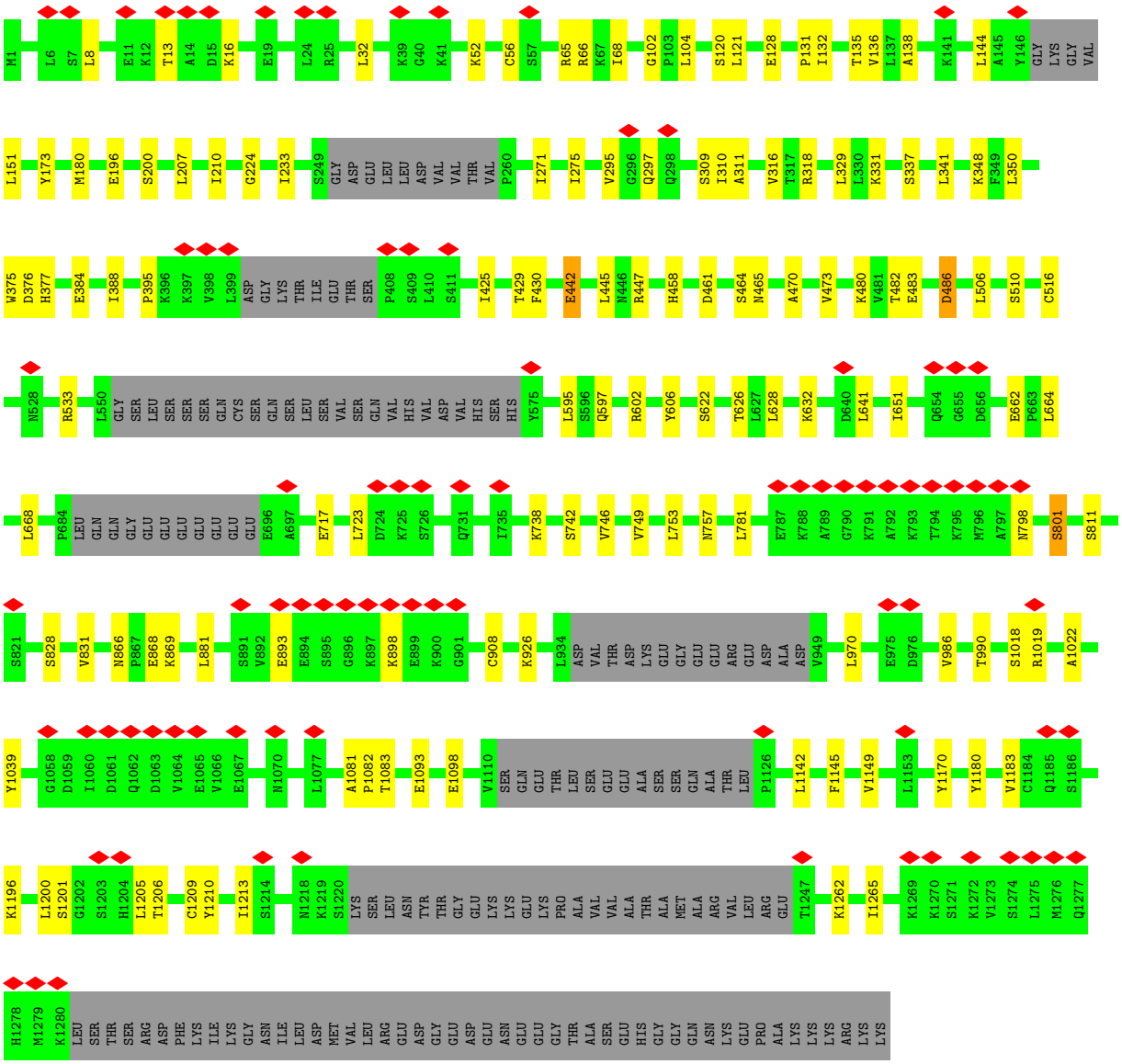
Chain	Residue	Modelled	Actual	Comment	Reference
B	654	GLN	HIS	conflict	UNP Q9BXW9
B	693	ASN	ASP	conflict	UNP Q9BXW9

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.

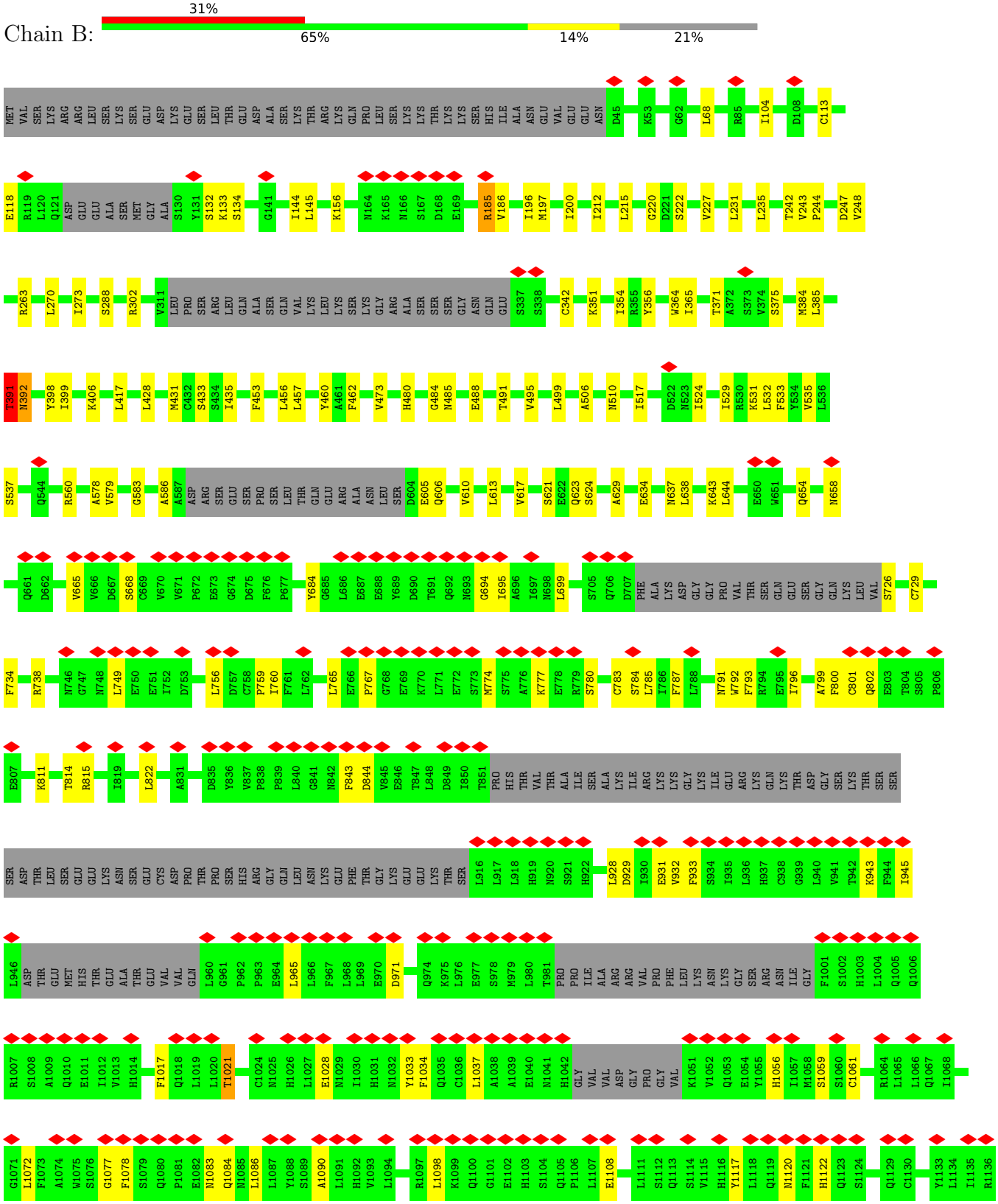
- Molecule 1: Fanconi anemia, complementation group I

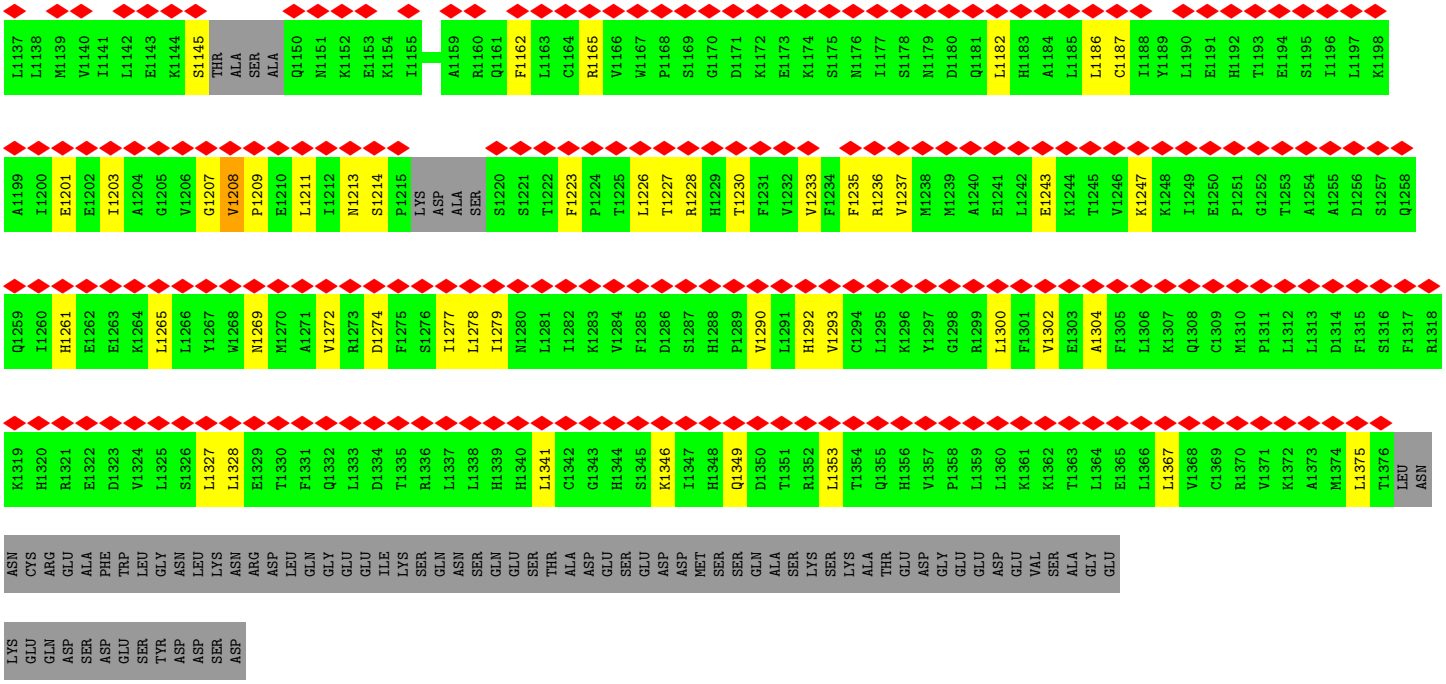
Chain A: 7% 78% 10% 12%



- Molecule 2: Fanconi anemia group D2 protein

Chain B:




L1137
L1138
M1139
V1140
I1141
L1142
E1143
K1144
S1145
THR
ALA
SER
ALA
Q1150
N1151
K1152
E1153
K1154
I1155
A1159
R1160
Q1161
F1162
L1163
C1164
R1165
V1166
W1167
P1168
S1169
G1170
D1171
K1172
E1173
K1174
S1175
N1176
I1177
S1178
N1179
D1180
Q1181
L1182
H1183
A1184
L1185
L1186
C1187
I1188
Y1189
L1190
E1191
H1192
T1193
E1194
S1195
I1196
L1197
K1198
A1199
I1200
E1201
E1202
I1203
A1204
G1205
V1206
G1207
V1208
P1209
E1210
L1211
I1212
N1213
S1214
P1215
LYS
ASP
ALA
SER
S1220
S1221
T1222
F1223
P1224
T1225
L1226
T1227
R1228
H1229
T1230
F1231
V1232
V1233
F1234
F1235
R1236
V1237
M1238
M1239
A1240
E1241
L1242
E1243
K1244
T1245
V1246
K1247
K1248
I1249
E1250
P1251
G1252
T1253
A1254
A1255
D1256
S1257
Q1258
Q1259
I1260
H1261
E1262
E1263
K1264
L1265
L1266
Y1267
W1268
N1269
M1270
A1271
V1272
R1273
D1274
F1275
S1276
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I1279
N1280
L1281
I1282
K1283
V1284
F1285
D1286
S1287
H1288
P1289
V1290
L1291
H1292
V1293
C1294
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Y1297
G1298
R1299
L1300
F1301
V1302
E1303
A1304
F1305
L1306
K1307
Q1308
C1309
M1310
P1311
L1312
L1313
D1314
F1315
S1316
F1317
R1318
K1319
H1320
R1321
E1322
D1323
V1324
L1325
S1326
L1327
L1328
E1329
T1330
F1331
Q1332
L1333
D1334
T1335
R1336
L1337
L1338
H1339
H1340
L1341
C1342
G1343
H1344
S1345
K1346
I1347
H1348
Q1349
D1350
T1351
R1352
L1353
T1354
Q1355
H1356
V1357
P1358
L1359
L1360
K1361
K1362
T1363
L1364
E1365
L1366
L1367
V1368
C1369
R1370
V1371
K1372
A1373
M1374
L1375
T1376
LEU
ASN
ASN
CYS
ARG
GLU
ALA
PHE
TRP
LEU
GLY
ASN
LEU
LYS
ASN
ARG
ASP
LEU
GLN
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GLU
GLN
ASP
SER
ASP
GLU
SER
TYR
ASP
ASP
SER
ASP

4 Experimental information (i)

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 ($e^-/Å^2$)	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 (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	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(^{o})	Ideal(^{o})
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 (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	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 (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	1149/1328 (86%)	1075 (94%)	72 (6%)	2 (0%)	47	77
2	B	1123/1451 (77%)	1050 (94%)	70 (6%)	3 (0%)	41	71
All	All	2272/2779 (82%)	2125 (94%)	142 (6%)	5 (0%)	50	77

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 (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	1067/1205 (88%)	1059 (99%)	8 (1%)	84	90
2	B	1065/1324 (80%)	1048 (98%)	17 (2%)	62	79
All	All	2132/2529 (84%)	2107 (99%)	25 (1%)	72	83

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

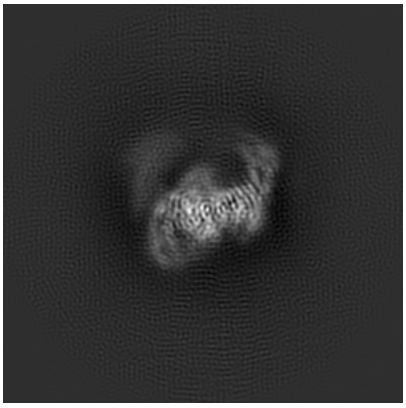
6 Map visualisation (i)

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.

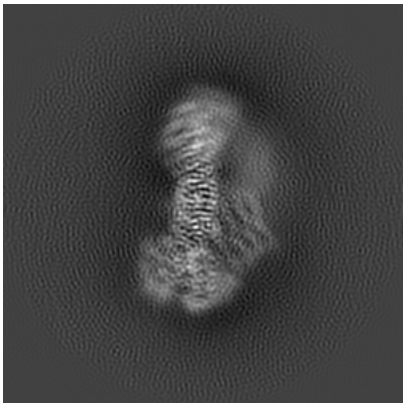
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

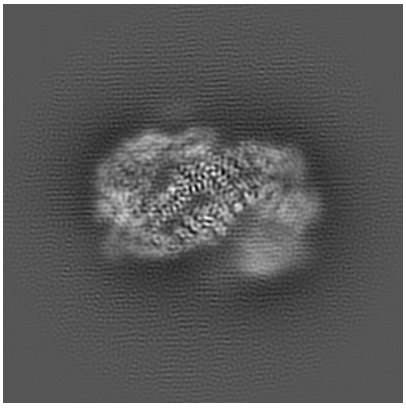
6.1.1 Primary map



X



Y

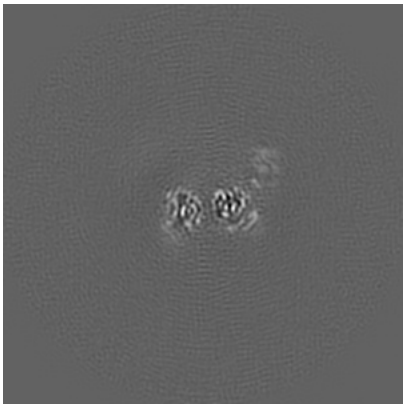


Z

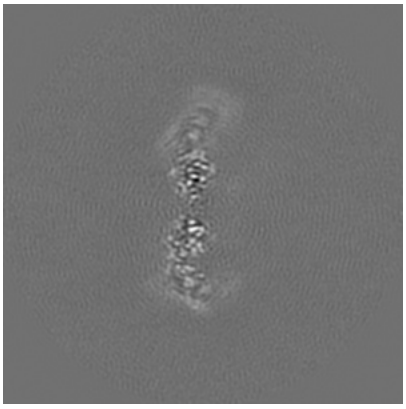
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

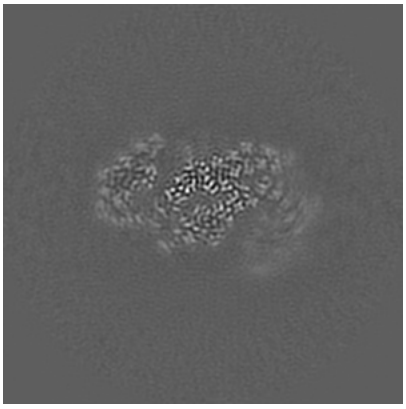
6.2.1 Primary map



X Index: 128



Y Index: 128

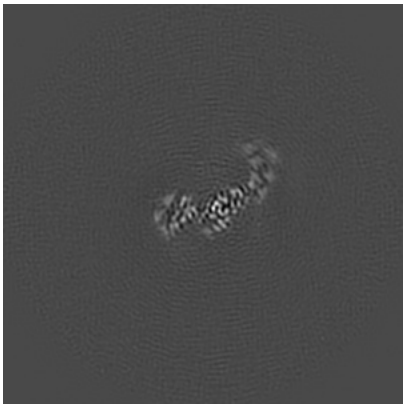


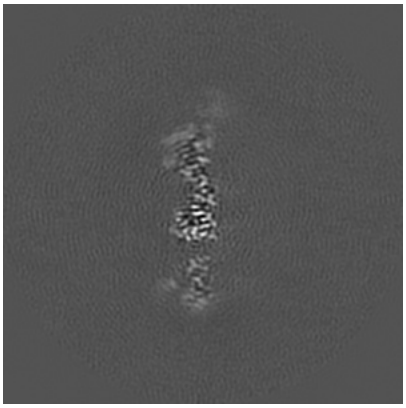
Z Index: 128

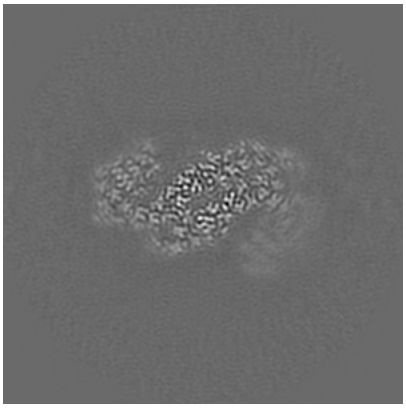
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

6.3.1 Primary map


X Index: 117

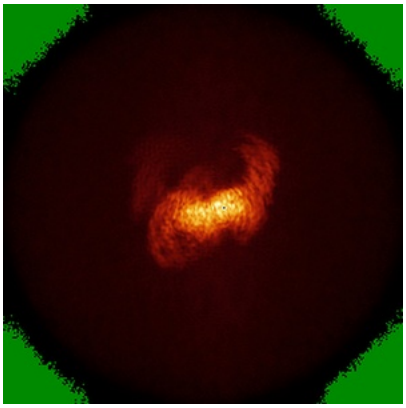

Y Index: 137

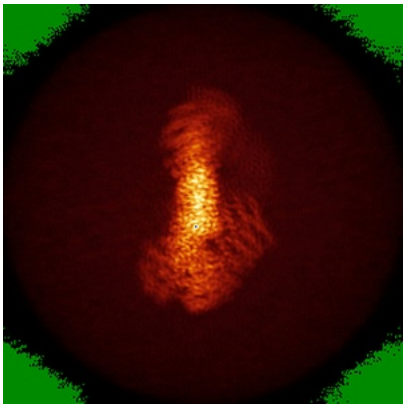

Z Index: 123

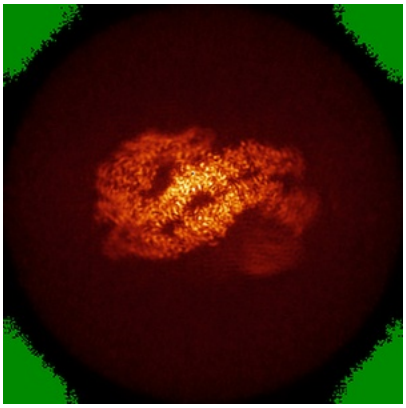
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal 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

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.

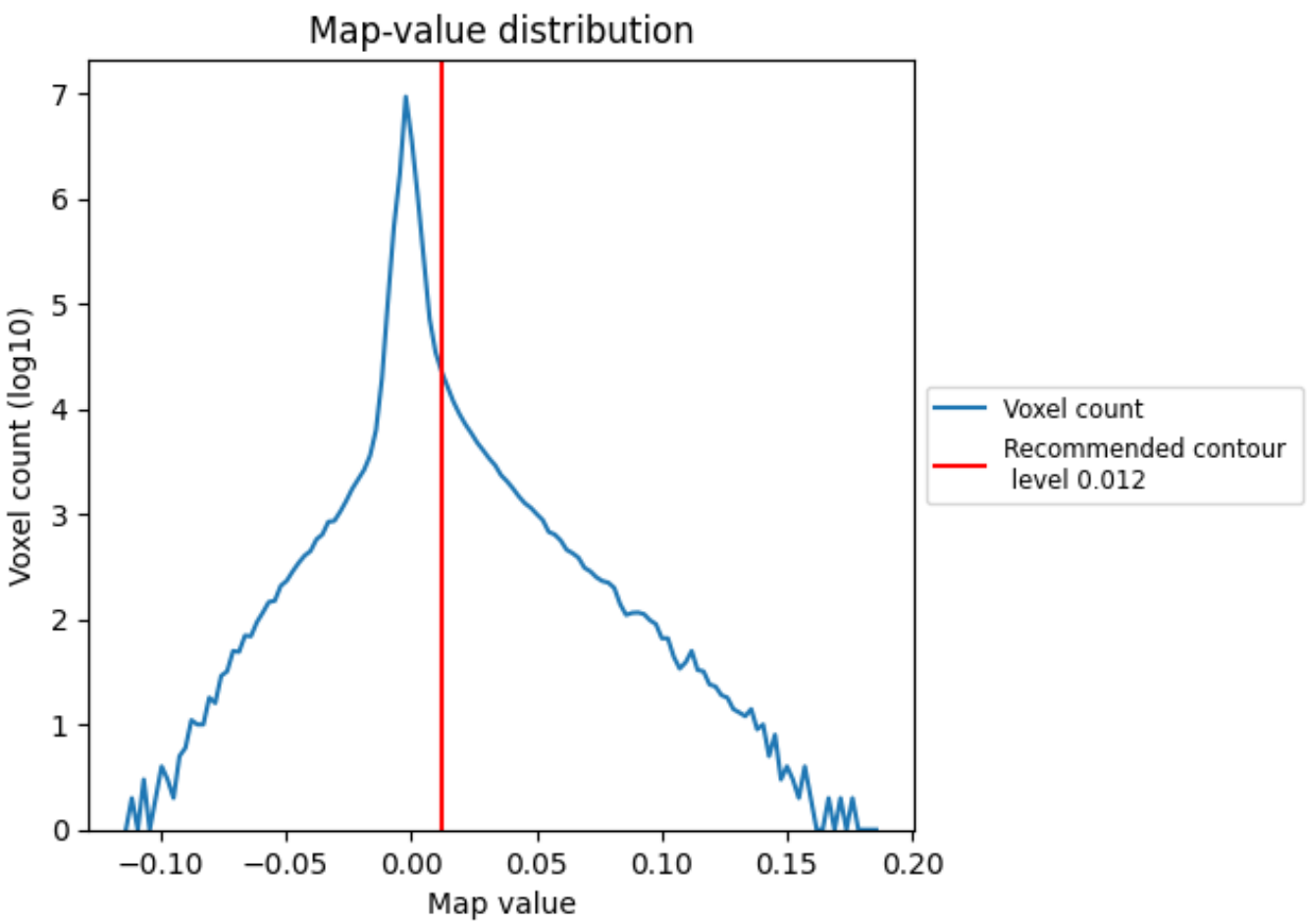
6.6 Mask visualisation (i)

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

7 Map analysis (i)

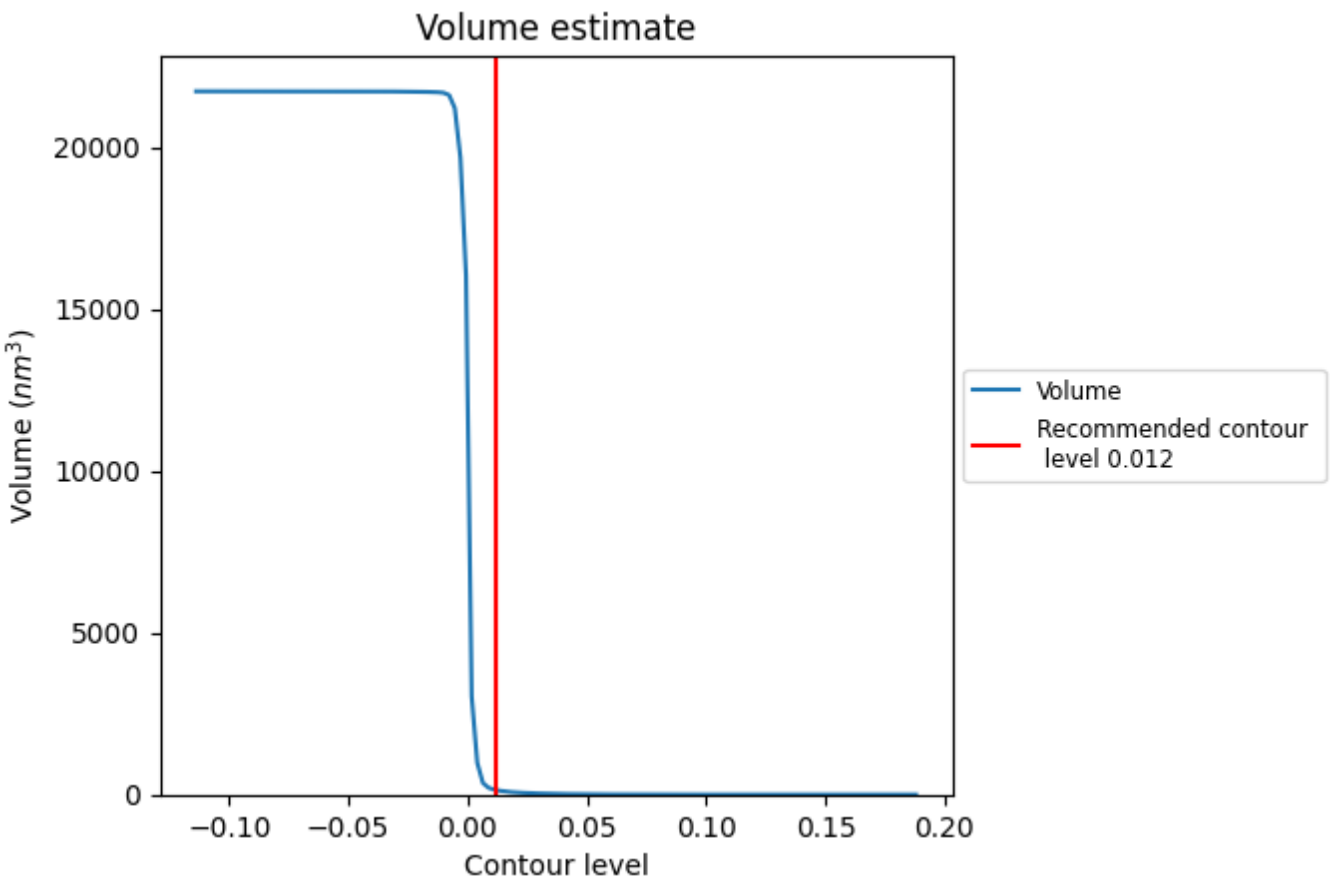
This section contains the results of statistical analysis of the map.

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.

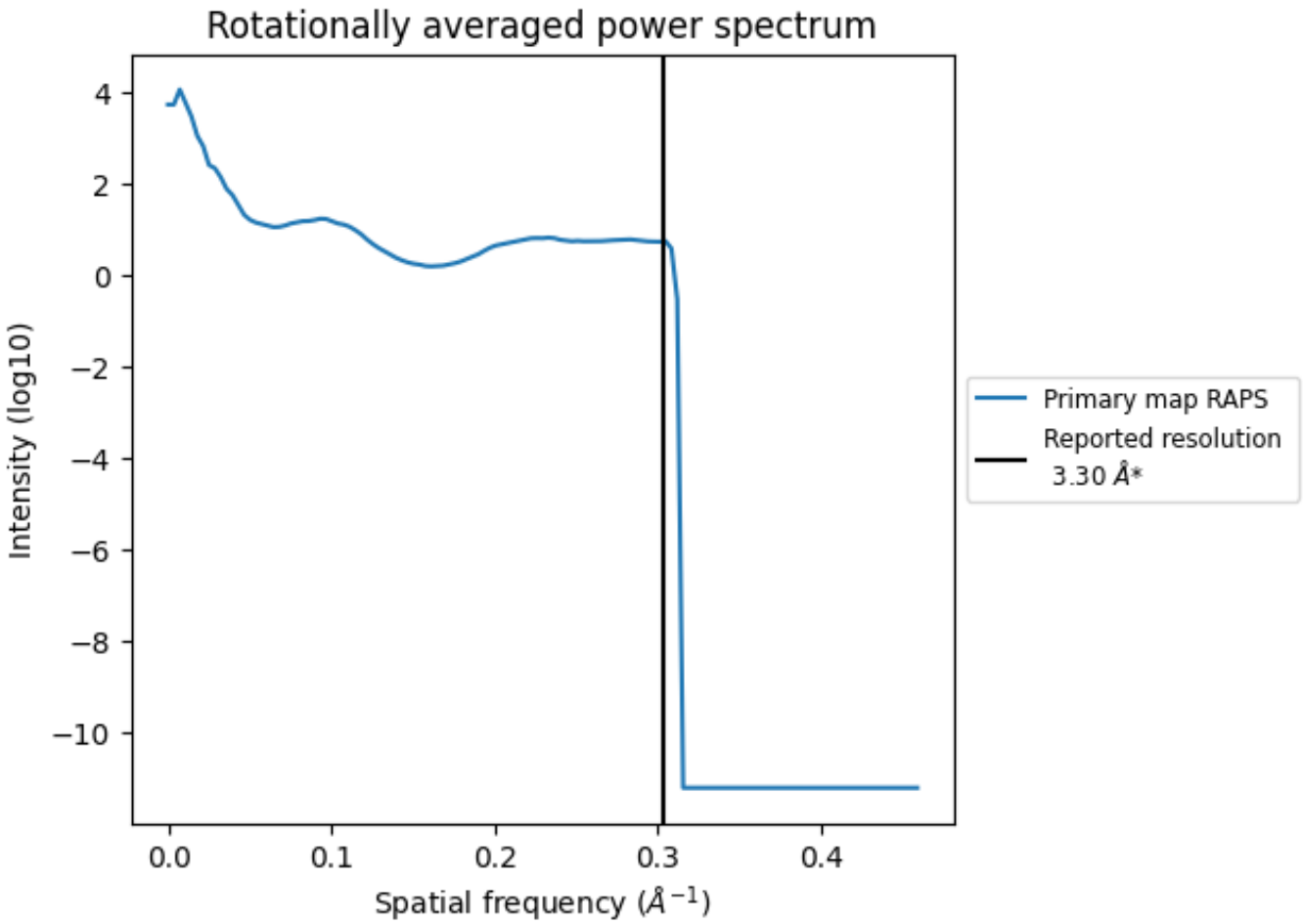
7.2 Volume estimate (i)



The volume at the recommended contour level is 140 nm^3; 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 (i)



*Reported resolution corresponds to spatial frequency of 0.303 Å^{-1}

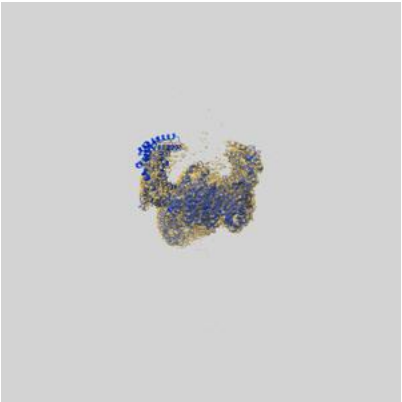
8 Fourier-Shell correlation (i)

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

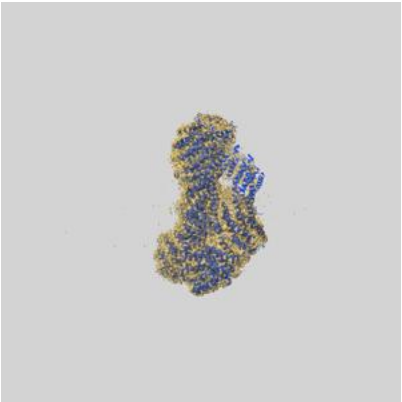
9 Map-model fit (i)

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.

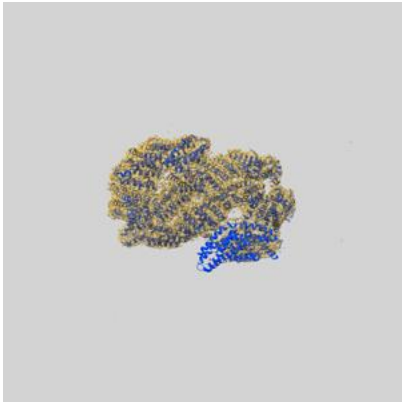
9.1 Map-model overlay (i)



X



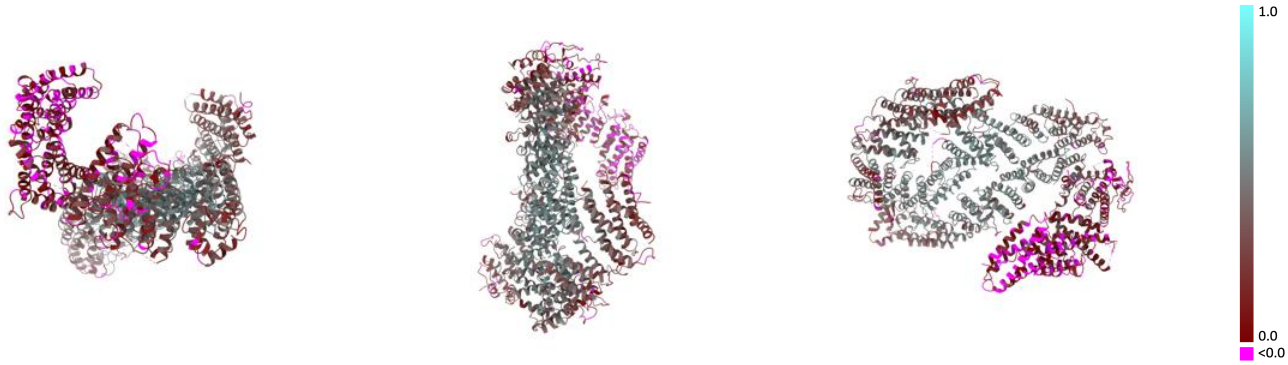
Y



Z

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.

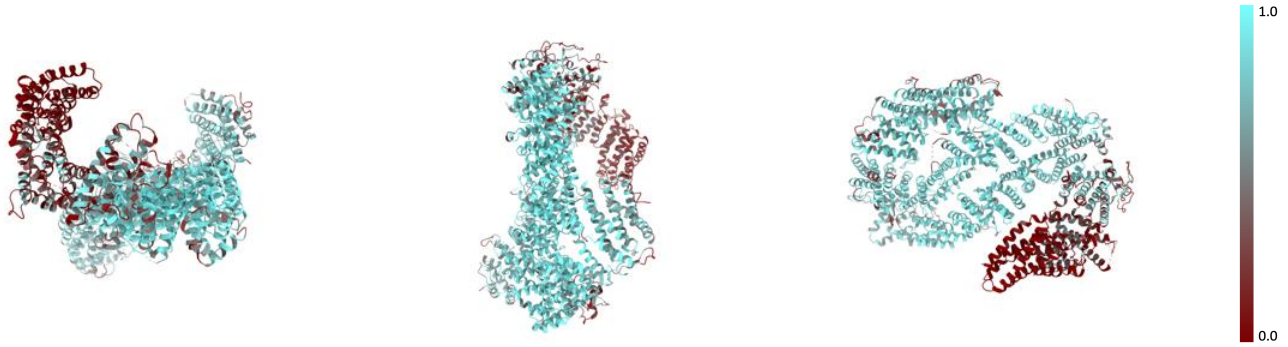
9.2 Q-score mapped to coordinate model (i)



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.

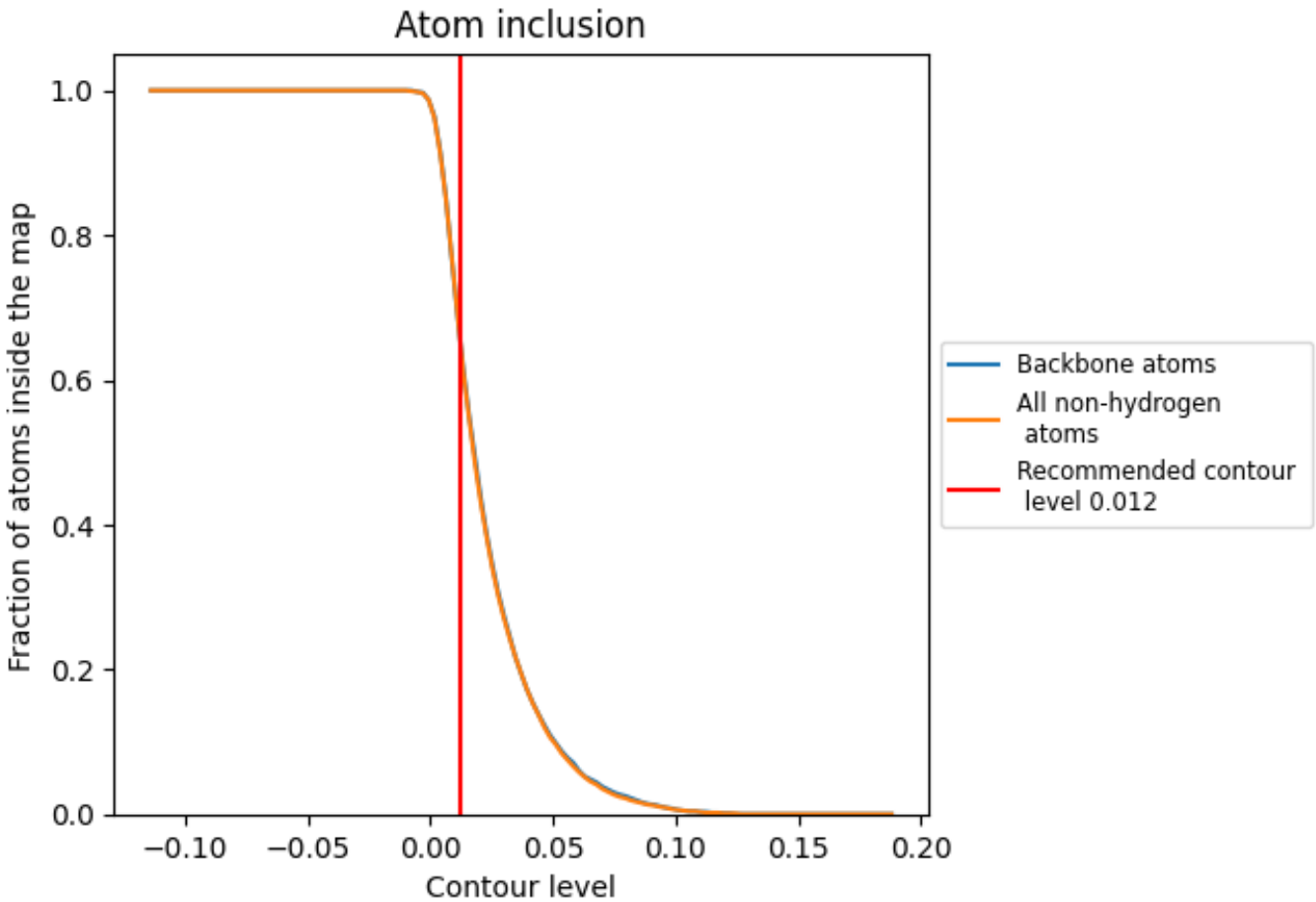
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.012).

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 (i)

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	0.6580	0.3190
A	0.7960	0.4010
B	0.5280	0.2360