



wwPDB EM Validation Summary 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 wwPDB EM Validation Summary 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.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

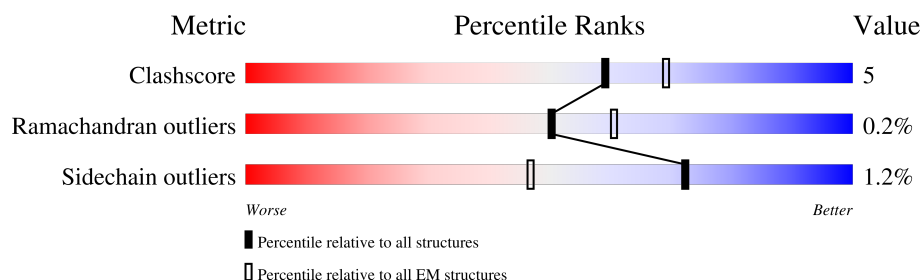
1 Overall quality at a glance

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 ≥ 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	
2	B	1451	

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		

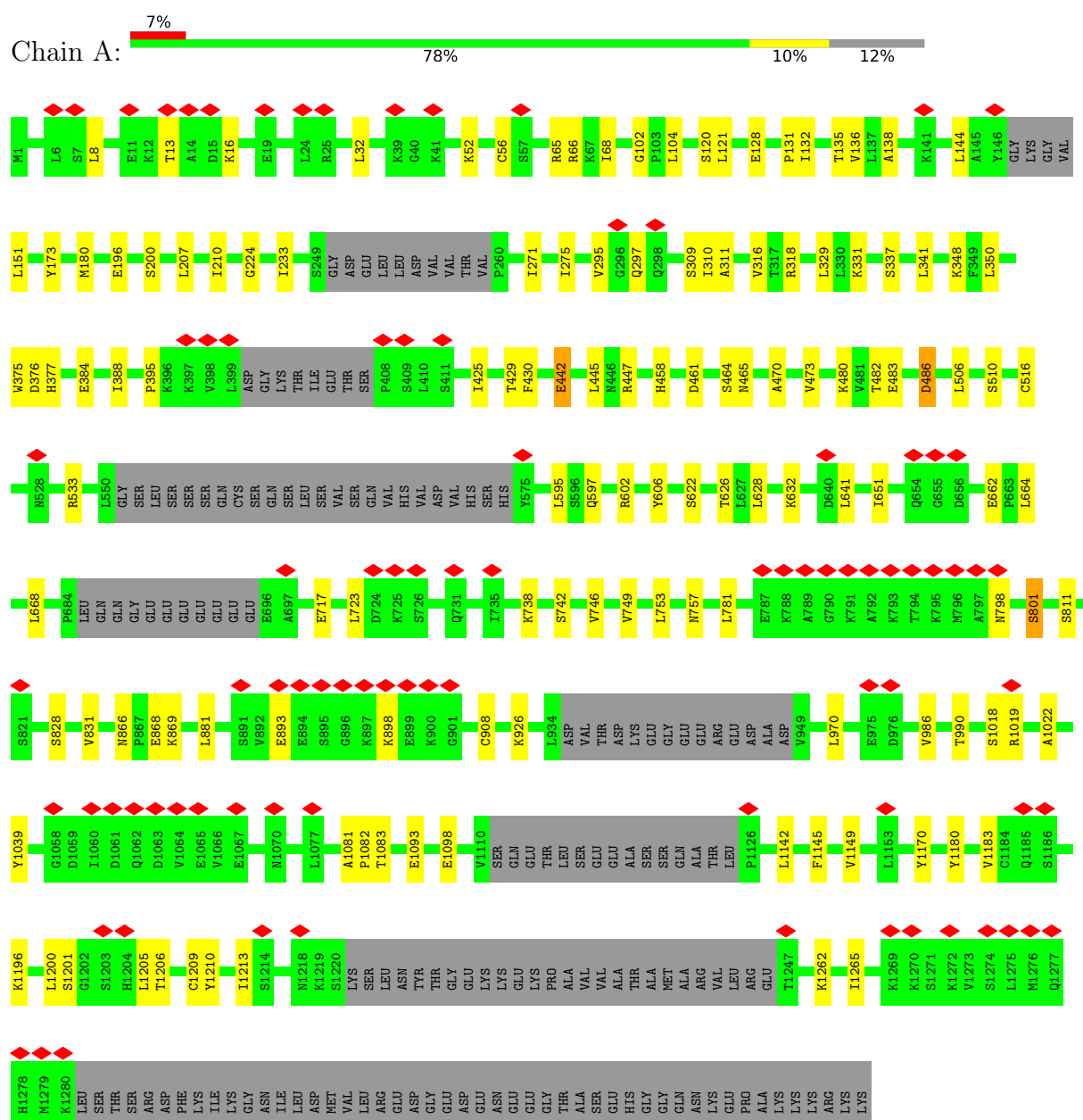
There are 2 discrepancies between the modelled and reference sequences:

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

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: Fanconi anemia, complementation group I



Chain B:



Lys	Cys	Arg	Glu	Asp	Ser	Phe	Trp	Leu	Gly	Asn	Leu	Lys	Arg	Asp	Leu	Gln	Gly	Glu	Glu	Leu	Lys	Ser	Gln	Glu	Ser	Glu	Asp	Asp	Met	Ser	Ser	Ser	Gln	Ala	Ala	Ser	Lys	Lys	Lys	Val	Ala	Gly	Glu																
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
Q1259	I1260	H1261	E1262	E1263	K1264	L1265	L1266	Y1267	W1268	M1269	M1270	A1271	V1272	R1273	D1274	F1275	S1276	I1277	L1278	I1279	N1280	L1281	I1282	K1283	V1284	F1285	D1286	S1287	H1288	P1289	V1290	L1291	H1292	V1293	C1294	L1295	K1296	Y1297	G1298	R1299	L1300	F1301	V1302	E1303	A1304	F1305	L1306	K1307	Q1308	C1309	M1310	P1311	L1312	L1313	D1314	F1315	S1316	F1317	R1318
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
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	M1176	I1177	S1178	M1179	D1180	Q1181	L1182	H1183	A1184	L1185	L1186	C1187	T1188	Y1189	L1190	E1191	H1192	T1193	E1194	S1195	T1196	L1197	K1198	

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

The worst 5 of 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

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.

5 of 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

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.

The worst 5 of 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

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	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

5 of 25 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	433	SER
2	B	729	CYS
2	B	1228	ARG
2	B	726	SER
2	B	774	MET

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

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
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

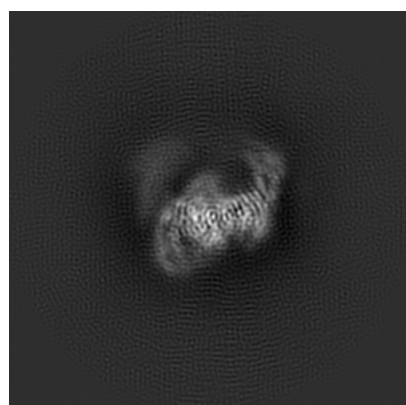
6 Map visualisation [i](#)

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.

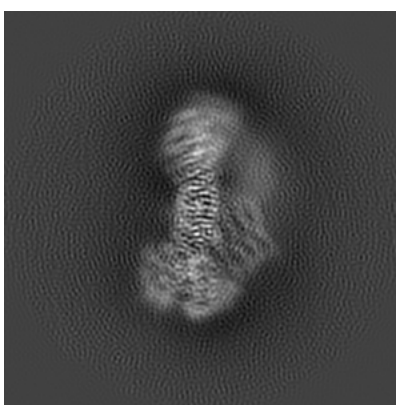
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

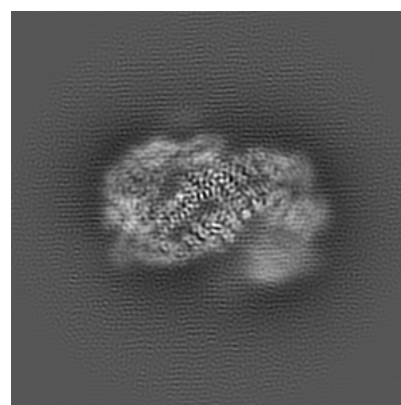
6.1.1 Primary map



X



Y

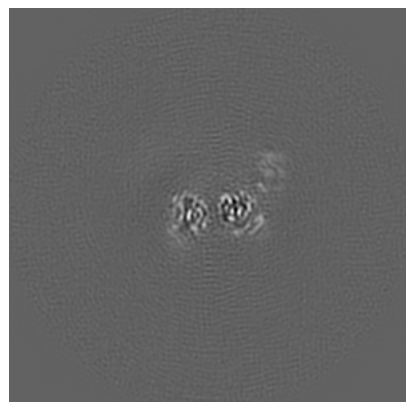


Z

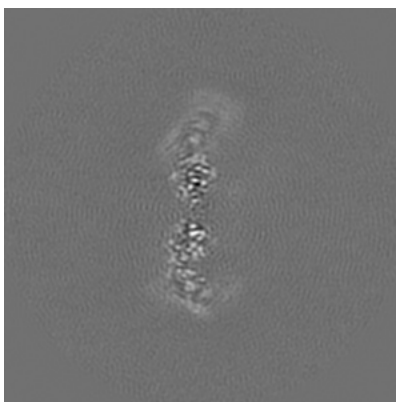
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

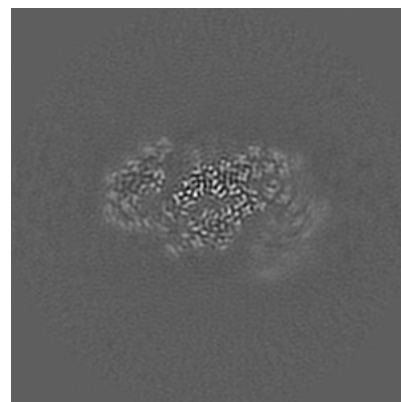
6.2.1 Primary map



X Index: 128



Y Index: 128

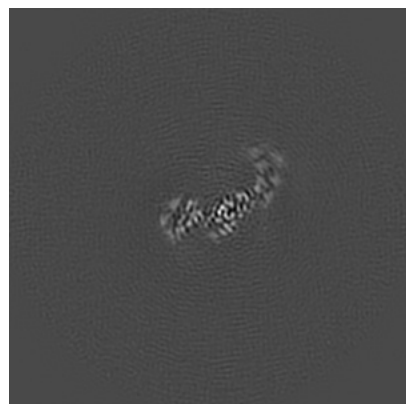


Z Index: 128

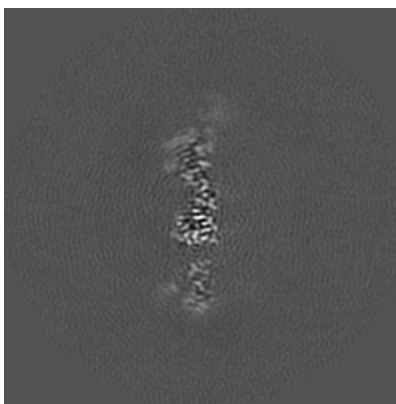
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

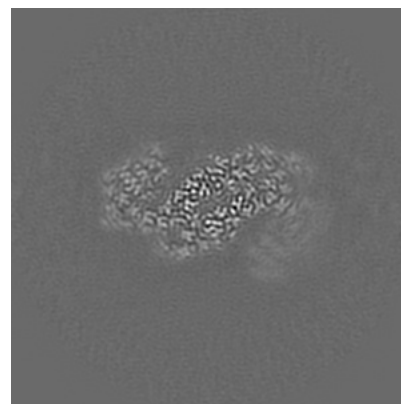
6.3.1 Primary map



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.

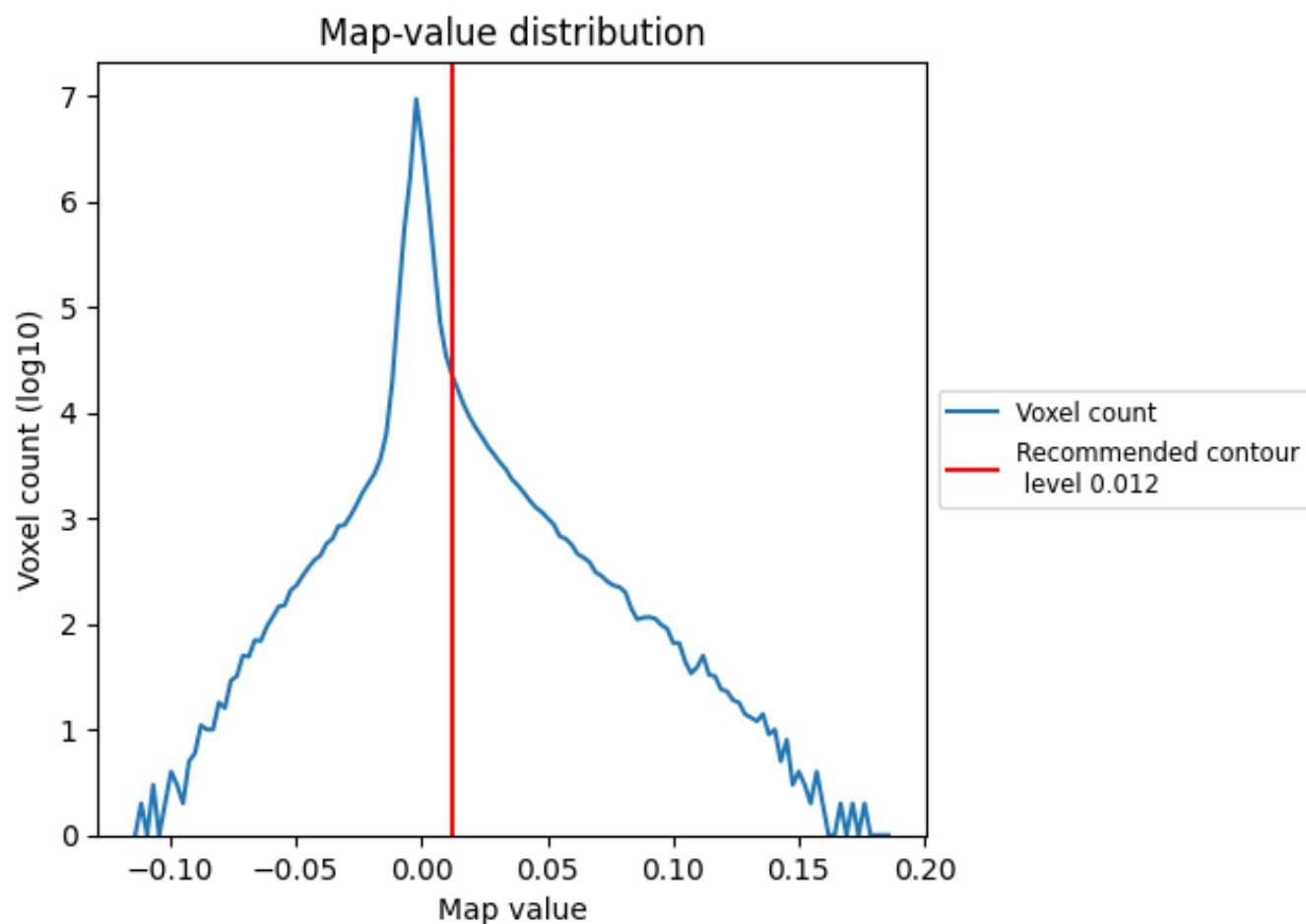
6.5 Mask visualisation

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

7 Map analysis [i](#)

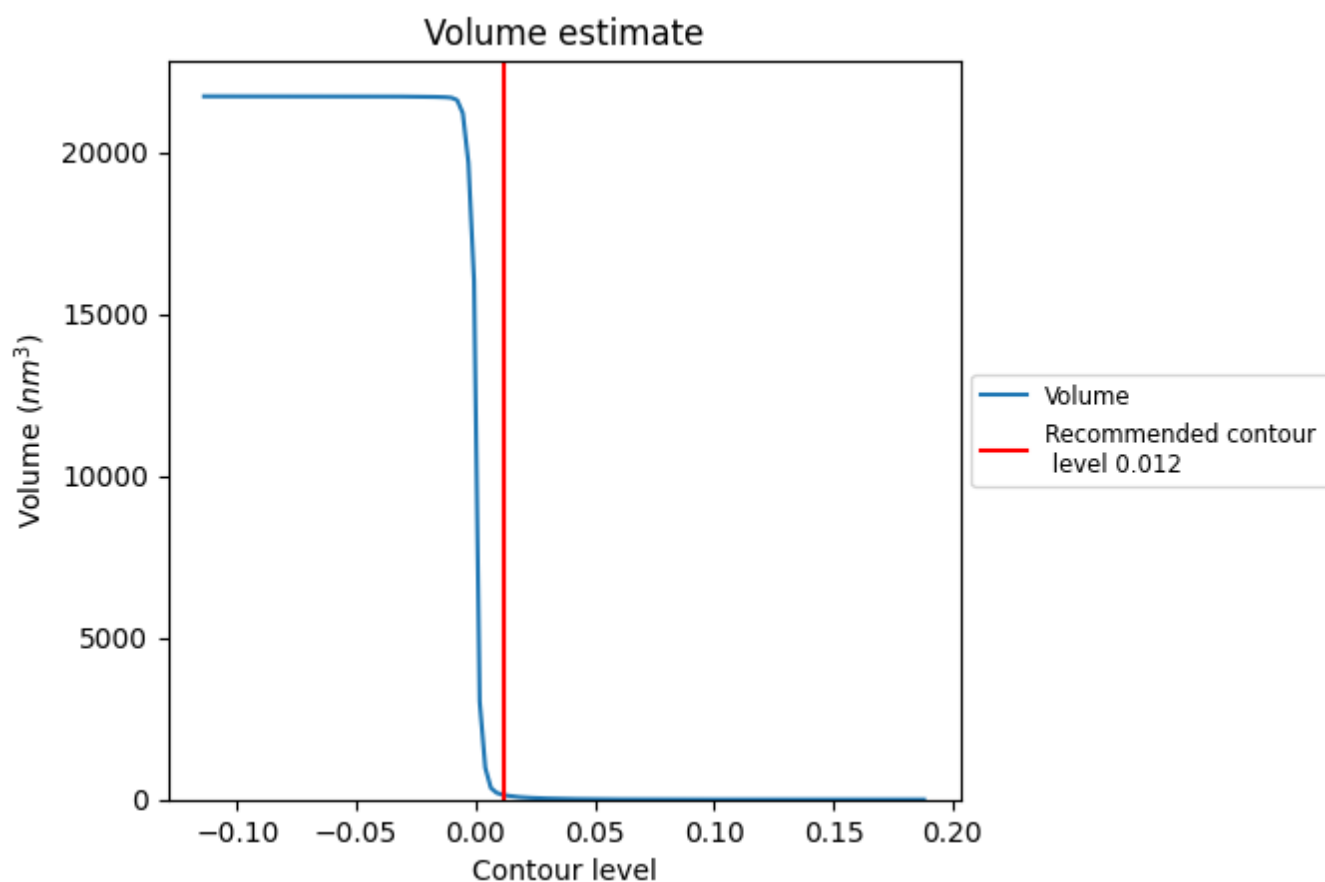
This section contains the results of statistical analysis of the map.

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.

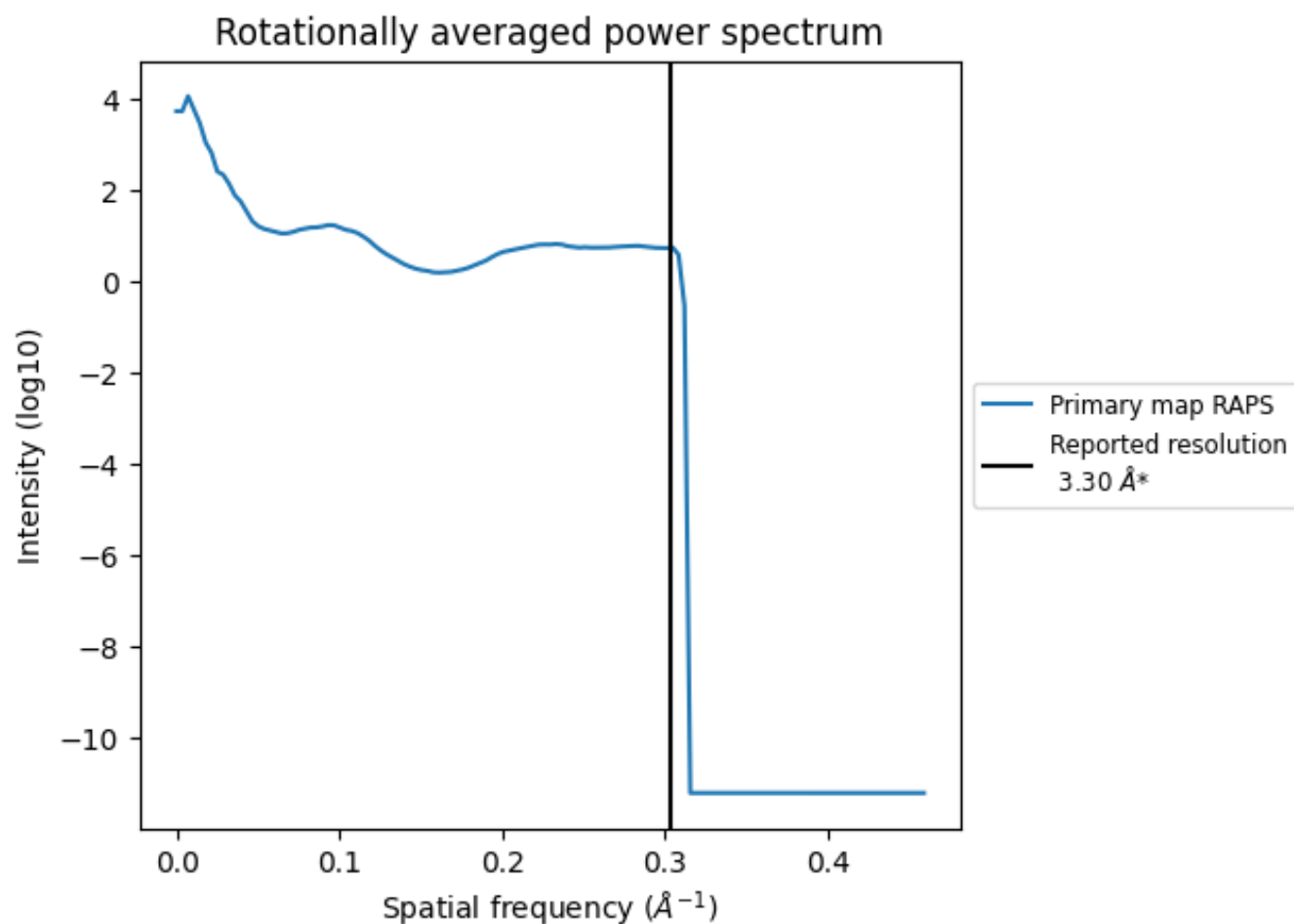
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 140 nm^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 ⓘ



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

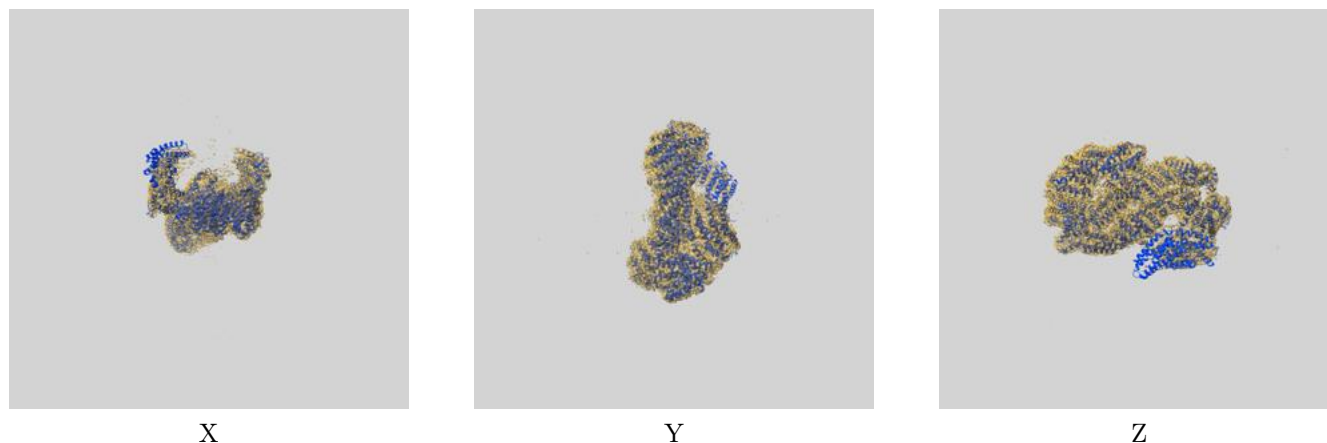
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

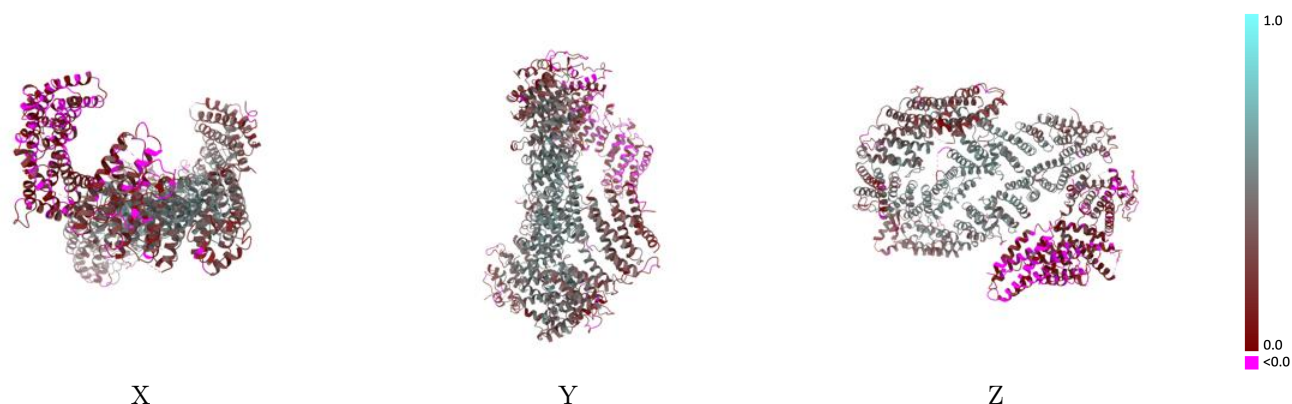
This section contains information regarding the fit between EMDB map EMD-21137 and PDB model 6VAD. Per-residue inclusion information can be found in [section 3](#) on [page 4](#).

9.1 Map-model overlay [i](#)



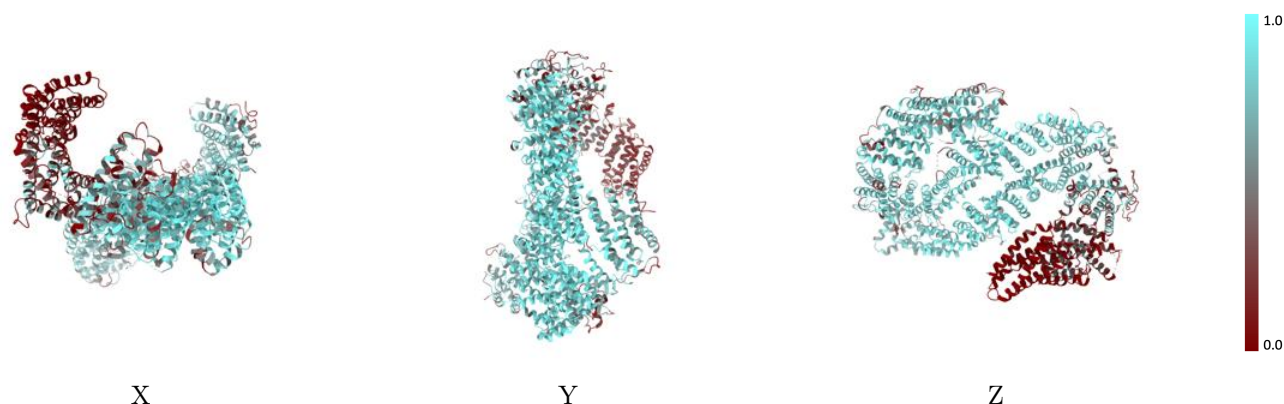
The images above show the 3D surface view of the map at the recommended contour level 0.012 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



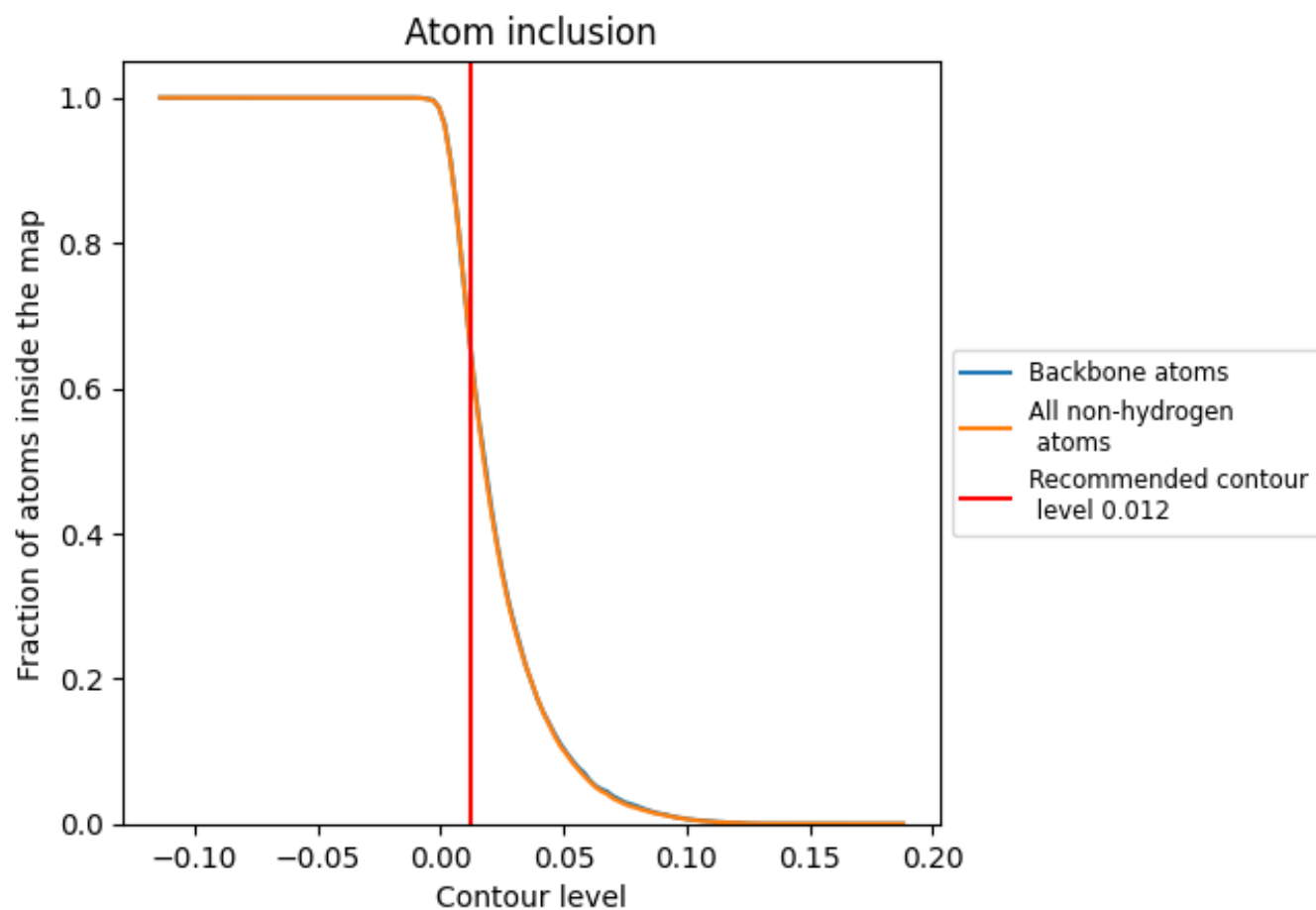
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

