Full wwPDB EM Validation Report (i)

Aug 28, 2022 – 07:08 am BST

PDB ID	:	7QTK
EMDB ID	:	EMD-14143
Title	:	SARS-CoV-2 S Omicron Spike B.1.1.529 - RBD down - 1-P2G3 Fab (Local)
Authors	:	Ni, D.; Lau, K.; Turelli, P.; Fenwick, C.; Perez, L.; Pojer, F.; Stahlberg, H.; Pantaleo, G.; Trono, D.
Deposited on	:	2022-01-14
Resolution	:	3.84 Å(reported)
Based on initial model	:	7QO7

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:

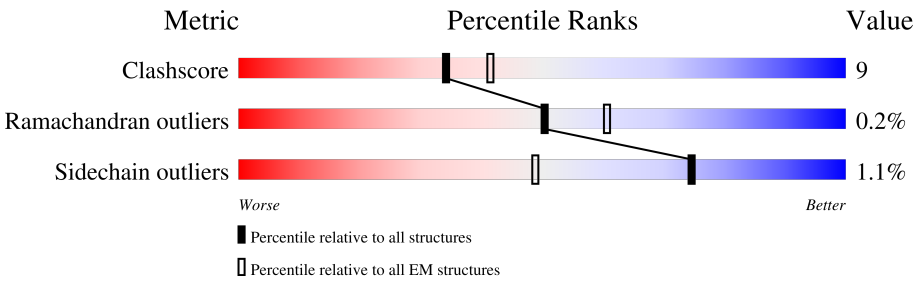
EMDB validation analysis	:	0.0.1.dev8
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.30

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 3.84 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	D	1285	12% 84%
2	B	228	33% 74% 26%
3	C	214	32% 81% 18%
4	A	2	100% 50% 50%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 5009 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 Surface glycoprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	D	201	1612	1039	273	292	8	0	0

There are 119 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	70	VAL	ALA	conflict	UNP A0A8A4XEV3
D	?	-	HIS	deletion	UNP A0A8A4XEV3
D	?	-	VAL	deletion	UNP A0A8A4XEV3
D	96	ILE	THR	conflict	UNP A0A8A4XEV3
D	?	-	ASN	deletion	UNP A0A8A4XEV3
D	209	ILE	LEU	conflict	UNP A0A8A4XEV3
D	212	GLU	-	insertion	UNP A0A8A4XEV3
D	213	PRO	-	insertion	UNP A0A8A4XEV3
D	214	GLU	-	insertion	UNP A0A8A4XEV3
D	339	ASP	GLY	conflict	UNP A0A8A4XEV3
D	371	LEU	SER	conflict	UNP A0A8A4XEV3
D	373	PRO	SER	conflict	UNP A0A8A4XEV3
D	375	PHE	SER	conflict	UNP A0A8A4XEV3
D	417	ASN	LYS	conflict	UNP A0A8A4XEV3
D	440	LYS	ASN	conflict	UNP A0A8A4XEV3
D	446	SER	GLY	conflict	UNP A0A8A4XEV3
D	477	ASN	SER	conflict	UNP A0A8A4XEV3
D	478	LYS	THR	conflict	UNP A0A8A4XEV3
D	484	ALA	ARG	conflict	UNP A0A8A4XEV3
D	493	ARG	GLN	conflict	UNP A0A8A4XEV3
D	496	SER	GLY	conflict	UNP A0A8A4XEV3
D	498	ARG	GLN	conflict	UNP A0A8A4XEV3
D	501	TYR	ASN	conflict	UNP A0A8A4XEV3
D	505	HIS	TYR	conflict	UNP A0A8A4XEV3
D	547	LYS	THR	conflict	UNP A0A8A4XEV3
D	655	TYR	HIS	conflict	UNP A0A8A4XEV3
D	679	LYS	ASN	conflict	UNP A0A8A4XEV3
D	681	HIS	PRO	conflict	UNP A0A8A4XEV3

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Chain	Residue	Modelled	Actual	Comment	Reference
D	682	GLY	ARG	conflict	UNP A0A8A4XEV3
D	683	SER	ARG	conflict	UNP A0A8A4XEV3
D	685	SER	ARG	conflict	UNP A0A8A4XEV3
D	764	LYS	ASN	conflict	UNP A0A8A4XEV3
D	796	TYR	ASP	conflict	UNP A0A8A4XEV3
D	856	LYS	ASN	conflict	UNP A0A8A4XEV3
D	954	HIS	GLN	conflict	UNP A0A8A4XEV3
D	969	LYS	ASN	conflict	UNP A0A8A4XEV3
D	981	PHE	LEU	conflict	UNP A0A8A4XEV3
D	986	PRO	LYS	conflict	UNP A0A8A4XEV3
D	987	PRO	VAL	conflict	UNP A0A8A4XEV3
D	1209	GLY	-	expression tag	UNP A0A8A4XEV3
D	1210	SER	-	expression tag	UNP A0A8A4XEV3
D	1211	GLY	-	expression tag	UNP A0A8A4XEV3
D	1212	TYR	-	expression tag	UNP A0A8A4XEV3
D	1213	ILE	-	expression tag	UNP A0A8A4XEV3
D	1214	PRO	-	expression tag	UNP A0A8A4XEV3
D	1215	GLU	-	expression tag	UNP A0A8A4XEV3
D	1216	ALA	-	expression tag	UNP A0A8A4XEV3
D	1217	PRO	-	expression tag	UNP A0A8A4XEV3
D	1218	ARG	-	expression tag	UNP A0A8A4XEV3
D	1219	ASP	-	expression tag	UNP A0A8A4XEV3
D	1220	GLY	-	expression tag	UNP A0A8A4XEV3
D	1221	GLN	-	expression tag	UNP A0A8A4XEV3
D	1222	ALA	-	expression tag	UNP A0A8A4XEV3
D	1223	TYR	-	expression tag	UNP A0A8A4XEV3
D	1224	VAL	-	expression tag	UNP A0A8A4XEV3
D	1225	ARG	-	expression tag	UNP A0A8A4XEV3
D	1226	LYS	-	expression tag	UNP A0A8A4XEV3
D	1227	ASP	-	expression tag	UNP A0A8A4XEV3
D	1228	GLY	-	expression tag	UNP A0A8A4XEV3
D	1229	GLU	-	expression tag	UNP A0A8A4XEV3
D	1230	TRP	-	expression tag	UNP A0A8A4XEV3
D	1231	VAL	-	expression tag	UNP A0A8A4XEV3
D	1232	LEU	-	expression tag	UNP A0A8A4XEV3
D	1233	LEU	-	expression tag	UNP A0A8A4XEV3
D	1234	SER	-	expression tag	UNP A0A8A4XEV3
D	1235	THR	-	expression tag	UNP A0A8A4XEV3
D	1236	PHE	-	expression tag	UNP A0A8A4XEV3
D	1237	LEU	-	expression tag	UNP A0A8A4XEV3
D	1238	GLY	-	expression tag	UNP A0A8A4XEV3
D	1239	ARG	-	expression tag	UNP A0A8A4XEV3

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Chain	Residue	Modelled	Actual	Comment	Reference
D	1240	SER	-	expression tag	UNP A0A8A4XEV3
D	1241	LEU	-	expression tag	UNP A0A8A4XEV3
D	1242	GLU	-	expression tag	UNP A0A8A4XEV3
D	1243	VAL	-	expression tag	UNP A0A8A4XEV3
D	1244	LEU	-	expression tag	UNP A0A8A4XEV3
D	1245	PHE	-	expression tag	UNP A0A8A4XEV3
D	1246	GLN	-	expression tag	UNP A0A8A4XEV3
D	1247	GLY	-	expression tag	UNP A0A8A4XEV3
D	1248	PRO	-	expression tag	UNP A0A8A4XEV3
D	1249	GLY	-	expression tag	UNP A0A8A4XEV3
D	1250	HIS	-	expression tag	UNP A0A8A4XEV3
D	1251	HIS	-	expression tag	UNP A0A8A4XEV3
D	1252	HIS	-	expression tag	UNP A0A8A4XEV3
D	1253	HIS	-	expression tag	UNP A0A8A4XEV3
D	1254	HIS	-	expression tag	UNP A0A8A4XEV3
D	1255	HIS	-	expression tag	UNP A0A8A4XEV3
D	1256	HIS	-	expression tag	UNP A0A8A4XEV3
D	1257	HIS	-	expression tag	UNP A0A8A4XEV3
D	1258	SER	-	expression tag	UNP A0A8A4XEV3
D	1259	ALA	-	expression tag	UNP A0A8A4XEV3
D	1260	TRP	-	expression tag	UNP A0A8A4XEV3
D	1261	SER	-	expression tag	UNP A0A8A4XEV3
D	1262	HIS	-	expression tag	UNP A0A8A4XEV3
D	1263	PRO	-	expression tag	UNP A0A8A4XEV3
D	1264	GLN	-	expression tag	UNP A0A8A4XEV3
D	1265	PHE	-	expression tag	UNP A0A8A4XEV3
D	1266	GLU	-	expression tag	UNP A0A8A4XEV3
D	1267	LYS	-	expression tag	UNP A0A8A4XEV3
D	1268	GLY	-	expression tag	UNP A0A8A4XEV3
D	1269	GLY	-	expression tag	UNP A0A8A4XEV3
D	1270	GLY	-	expression tag	UNP A0A8A4XEV3
D	1271	SER	-	expression tag	UNP A0A8A4XEV3
D	1272	GLY	-	expression tag	UNP A0A8A4XEV3
D	1273	GLY	-	expression tag	UNP A0A8A4XEV3
D	1274	GLY	-	expression tag	UNP A0A8A4XEV3
D	1275	GLY	-	expression tag	UNP A0A8A4XEV3
D	1276	SER	-	expression tag	UNP A0A8A4XEV3
D	1277	GLY	-	expression tag	UNP A0A8A4XEV3
D	1278	GLY	-	expression tag	UNP A0A8A4XEV3
D	1279	SER	-	expression tag	UNP A0A8A4XEV3
D	1280	ALA	-	expression tag	UNP A0A8A4XEV3
D	1281	TRP	-	expression tag	UNP A0A8A4XEV3

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Chain	Residue	Modelled	Actual	Comment	Reference
D	1282	SER	-	expression tag	UNP A0A8A4XEV3
D	1283	HIS	-	expression tag	UNP A0A8A4XEV3
D	1284	PRO	-	expression tag	UNP A0A8A4XEV3
D	1285	GLN	-	expression tag	UNP A0A8A4XEV3
D	1286	PHE	-	expression tag	UNP A0A8A4XEV3
D	1287	GLU	-	expression tag	UNP A0A8A4XEV3
D	1288	LYS	-	expression tag	UNP A0A8A4XEV3

- Molecule 2 is a protein called P2G3 Heavy Chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	228	1729	1090	296	337	6	0	0

- Molecule 3 is a protein called P2G3 Light Chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	214	1640	1026	274	335	5	0	0

- Molecule 4 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

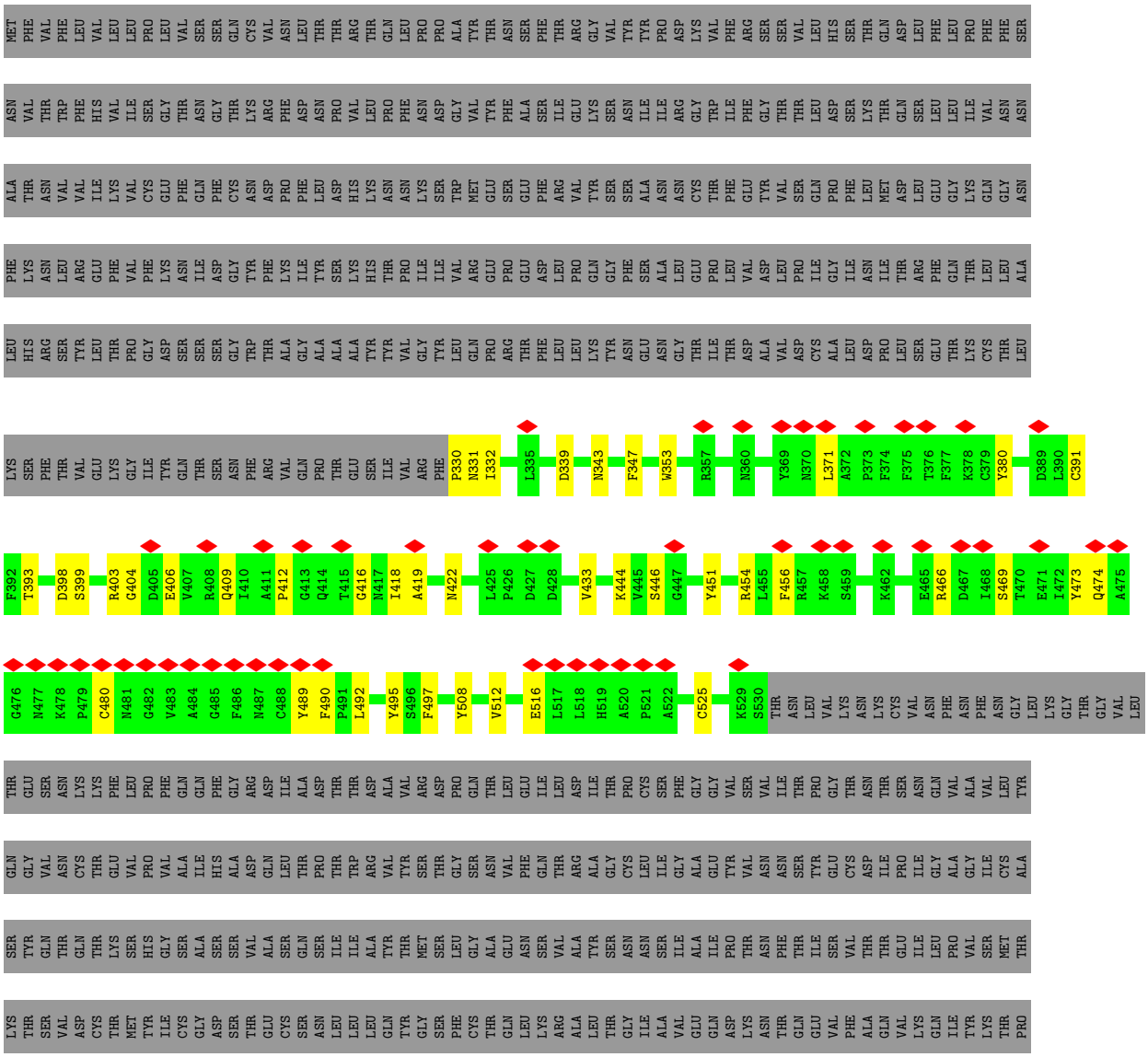
Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
4	A	2	28	16	2	10	0	0

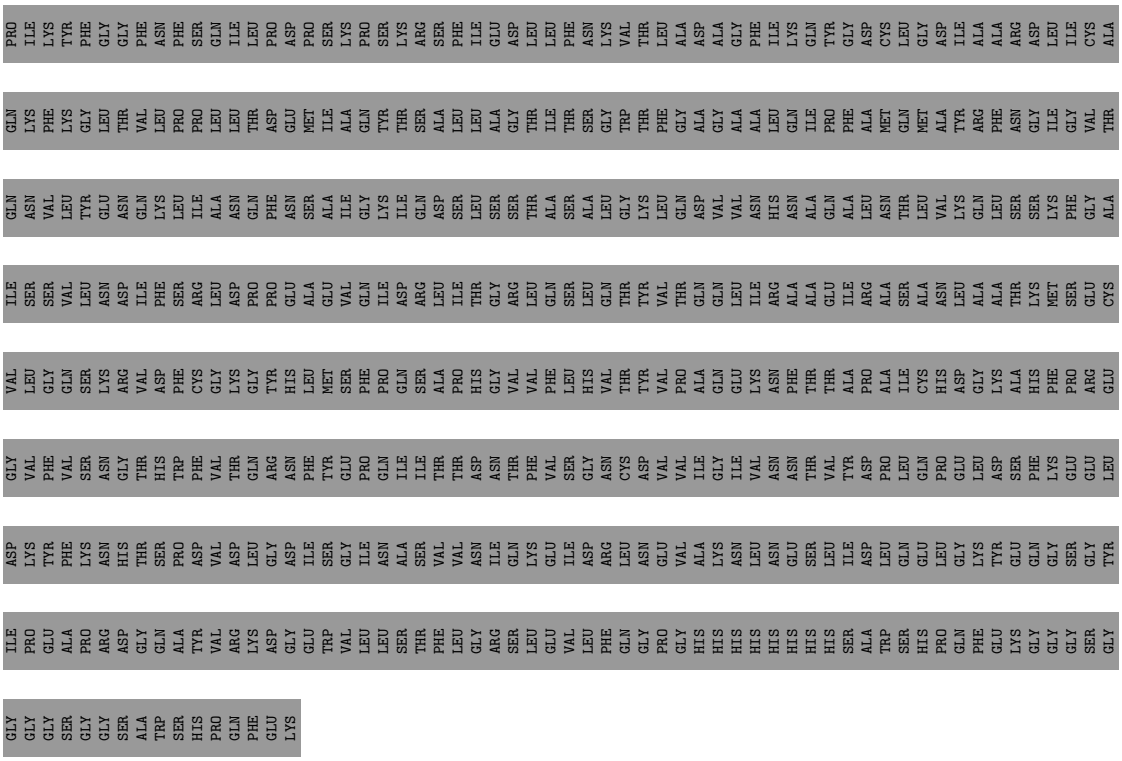
3 Residue-property plots (i)

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: Surface glycoprotein

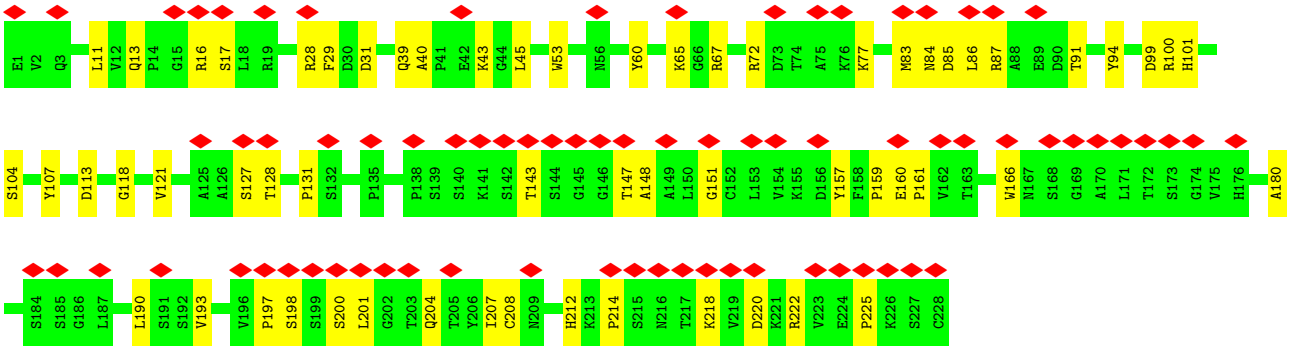
Chain D:





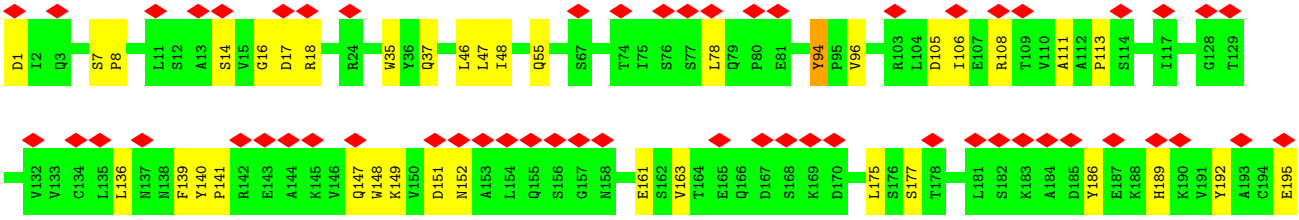
- Molecule 2: P2G3 Heavy Chain

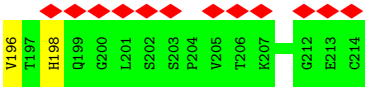
Chain B:



- Molecule 3: P2G3 Light Chain

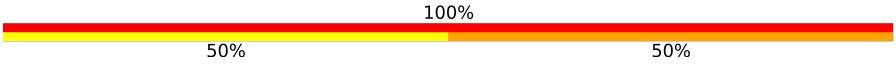
Chain C:





• Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain A:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	21672	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	60	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	1.919	Depositor
Minimum map value	-1.722	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.029	Depositor
Recommended contour level	0.256	Depositor
Map size (Å)	414.99, 414.99, 414.99	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.3833, 1.3833, 1.3833	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: NAG

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	D	0.26	0/1660	0.53	0/2258
2	B	0.29	0/1771	0.54	0/2409
3	C	0.31	0/1675	0.53	0/2278
All	All	0.28	0/5106	0.54	0/6945

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	D	1612	0	1549	28	0
2	B	1729	0	1684	40	0
3	C	1640	0	1585	22	0
4	A	28	0	25	3	0
All	All	5009	0	4843	88	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 9.

All (88) 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)
2:B:99:ASP:OD1	2:B:100:ARG:N	2.18	0.77
3:C:147:GLN:HB3	3:C:195:GLU:HB2	1.70	0.72
1:D:404:GLY:HA2	1:D:508:TYR:HD2	1.54	0.70
2:B:147:THR:HA	2:B:197:PRO:HA	1.75	0.69
2:B:198:SER:HA	2:B:201:LEU:HD23	1.74	0.68
1:D:406:GLU:OE2	1:D:409:GLN:NE2	2.28	0.66
2:B:94:TYR:O	2:B:118:GLY:HA2	1.96	0.65
2:B:17:SER:OG	2:B:84:ASN:ND2	2.30	0.64
2:B:39:GLN:HB2	2:B:45:LEU:HD23	1.82	0.61
1:D:454:ARG:NH2	1:D:469:SER:O	2.33	0.61
1:D:371:LEU:HD13	4:A:1:NAG:H83	1.83	0.59
1:D:409:GLN:OE1	1:D:419:ALA:N	2.34	0.59
2:B:218:LYS:NZ	2:B:220:ASP:OD1	2.35	0.59
3:C:149:LYS:HE2	3:C:152:ASN:HA	1.83	0.59
2:B:131:PRO:HB3	2:B:157:TYR:HB3	1.85	0.58
2:B:201:LEU:HD12	2:B:225:PRO:HG3	1.85	0.58
1:D:353:TRP:O	1:D:466:ARG:NH1	2.36	0.57
1:D:371:LEU:HD12	4:A:2:NAG:H3	1.86	0.56
3:C:37:GLN:HB2	3:C:47:LEU:HD11	1.87	0.56
1:D:456:PHE:HE2	1:D:473:TYR:HB3	1.71	0.56
1:D:404:GLY:HA2	1:D:508:TYR:CD2	2.40	0.56
2:B:94:TYR:O	2:B:118:GLY:CA	2.54	0.55
2:B:104:SER:HB2	3:C:94:TYR:CZ	2.42	0.55
2:B:128:THR:HG23	2:B:159:PRO:HG3	1.89	0.55
3:C:163:VAL:HG22	3:C:175:LEU:HD13	1.89	0.54
3:C:14:SER:OG	3:C:17:ASP:OD2	2.21	0.54
1:D:398:ASP:HB2	1:D:512:VAL:HG22	1.90	0.53
3:C:113:PRO:HB3	3:C:139:PHE:HB3	1.90	0.53
3:C:7:SER:HB2	3:C:8:PRO:HD3	1.91	0.52
3:C:35:TRP:HB2	3:C:48:ILE:HG22	1.92	0.51
2:B:151:GLY:HA3	2:B:193:VAL:HG12	1.92	0.51
1:D:418:ILE:HA	1:D:422:ASN:HB2	1.92	0.51
1:D:409:GLN:NE2	1:D:416:GLY:HA3	2.27	0.50
3:C:113:PRO:HB2	3:C:136:LEU:HD12	1.95	0.49
2:B:40:ALA:HB3	2:B:43:LYS:HB2	1.95	0.48
1:D:380:TYR:HE2	1:D:412:PRO:HD2	1.78	0.48
2:B:67:ARG:HG3	2:B:67:ARG:HH11	1.79	0.48
2:B:29:PHE:CD2	2:B:77:LYS:HA	2.49	0.48
1:D:454:ARG:NH2	1:D:469:SER:OG	2.47	0.47
2:B:85:ASP:O	2:B:87:ARG:NH1	2.47	0.47
3:C:186:TYR:O	3:C:192:TYR:OH	2.31	0.47
2:B:67:ARG:O	2:B:84:ASN:HB2	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:136:LEU:HD11	3:C:196:VAL:HG11	1.97	0.47
1:D:433:VAL:HG12	1:D:512:VAL:HG12	1.97	0.46
2:B:212:HIS:CD2	2:B:214:PRO:HD2	2.50	0.46
3:C:18:ARG:NH1	3:C:18:ARG:HB3	2.31	0.46
1:D:456:PHE:CZ	1:D:489:TYR:HB2	2.51	0.46
4:A:1:NAG:H83	4:A:1:NAG:H3	1.98	0.46
3:C:111:ALA:HB3	3:C:140:TYR:H	1.80	0.46
3:C:16:GLY:H	3:C:78:LEU:HB2	1.81	0.45
1:D:393:THR:HB	1:D:516:GLU:HG3	1.98	0.45
1:D:391:CYS:HA	1:D:525:CYS:CB	2.46	0.45
3:C:46:LEU:HD23	3:C:55:GLN:HG3	1.99	0.45
2:B:85:ASP:OD1	2:B:87:ARG:NH1	2.48	0.45
1:D:444:LYS:HB2	2:B:107:TYR:HE1	1.80	0.45
2:B:180:ALA:HB2	2:B:190:LEU:HD23	1.99	0.45
1:D:391:CYS:HA	1:D:525:CYS:HB3	1.99	0.44
2:B:67:ARG:CZ	2:B:87:ARG:HH22	2.31	0.44
2:B:101:HIS:ND1	2:B:107:TYR:HD2	2.14	0.44
3:C:151:ASP:OD2	3:C:189:HIS:ND1	2.49	0.44
1:D:339:ASP:O	1:D:343:ASN:HB2	2.18	0.44
2:B:157:TYR:HE2	2:B:161:PRO:HA	1.82	0.44
2:B:13:GLN:OE1	2:B:13:GLN:N	2.51	0.43
2:B:180:ALA:HA	2:B:190:LEU:HB3	2.00	0.43
2:B:91:THR:HA	2:B:121:VAL:O	2.18	0.43
1:D:451:TYR:HD2	1:D:497:PHE:HE2	1.67	0.43
2:B:207:ILE:HG12	2:B:222:ARG:HA	2.00	0.43
2:B:53:TRP:HA	2:B:72:ARG:HH12	1.84	0.43
1:D:330:PRO:HB2	1:D:331:ASN:H	1.70	0.43
2:B:60:TYR:HB2	2:B:65:LYS:HG3	2.00	0.43
3:C:148:TRP:HE1	3:C:177:SER:HG	1.65	0.43
2:B:100:ARG:HB3	2:B:113:ASP:OD2	2.19	0.42
2:B:200:SER:HB2	2:B:204:GLN:HG3	2.01	0.42
3:C:105:ASP:OD1	3:C:106:ILE:N	2.51	0.42
1:D:444:LYS:HE3	1:D:446:SER:HB3	2.02	0.42
3:C:161:GLU:HB2	3:C:175:LEU:HD11	2.02	0.42
1:D:347:PHE:CE2	1:D:399:SER:HB2	2.55	0.42
1:D:403:ARG:HE	1:D:495:TYR:HE1	1.68	0.41
2:B:83:MET:HB3	2:B:86:LEU:HD21	2.02	0.41
1:D:490:PHE:CE2	1:D:492:LEU:HB2	2.55	0.41
2:B:104:SER:HB2	3:C:94:TYR:OH	2.20	0.41
2:B:160:GLU:HB2	2:B:214:PRO:HG2	2.02	0.41
2:B:166:TRP:CZ3	2:B:208:CYS:HB3	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:141:PRO:HD2	3:C:198:HIS:CE1	2.55	0.41
1:D:474:GLN:OE1	1:D:480:CYS:N	2.54	0.41
2:B:28:ARG:NH1	2:B:31:ASP:OD2	2.53	0.41
2:B:143:THR:HA	2:B:148:ALA:HA	2.03	0.40
2:B:11:LEU:H	2:B:11:LEU:HD23	1.87	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	D	199/1285 (16%)	186 (94%)	12 (6%)	1 (0%)	29	66
2	B	226/228 (99%)	219 (97%)	7 (3%)	0	100	100
3	C	212/214 (99%)	200 (94%)	12 (6%)	0	100	100
All	All	637/1727 (37%)	605 (95%)	31 (5%)	1 (0%)	50	78

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	332	ILE

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	D	176/1113 (16%)	176 (100%)	0	100	100
2	B	192/192 (100%)	190 (99%)	2 (1%)	76	86
3	C	187/187 (100%)	183 (98%)	4 (2%)	53	73
All	All	555/1492 (37%)	549 (99%)	6 (1%)	74	85

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	16	ARG
2	B	127	SER
3	C	1	ASP
3	C	94	TYR
3	C	96	VAL
3	C	108	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	84	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)

2 monosaccharides are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	NAG	A	1	4,1	14,14,15	0.73	0	17,19,21	1.50	3 (17%)
4	NAG	A	2	4	14,14,15	0.25	0	17,19,21	0.48	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	A	1	4,1	-	5/6/23/26	0/1/1/1
4	NAG	A	2	4	-	4/6/23/26	0/1/1/1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	1	NAG	C2-N2-C7	4.28	129.00	122.90
4	A	1	NAG	C1-O5-C5	2.53	115.62	112.19
4	A	1	NAG	C1-C2-N2	2.26	114.35	110.49

There are no chirality outliers.

All (9) torsion outliers are listed below:

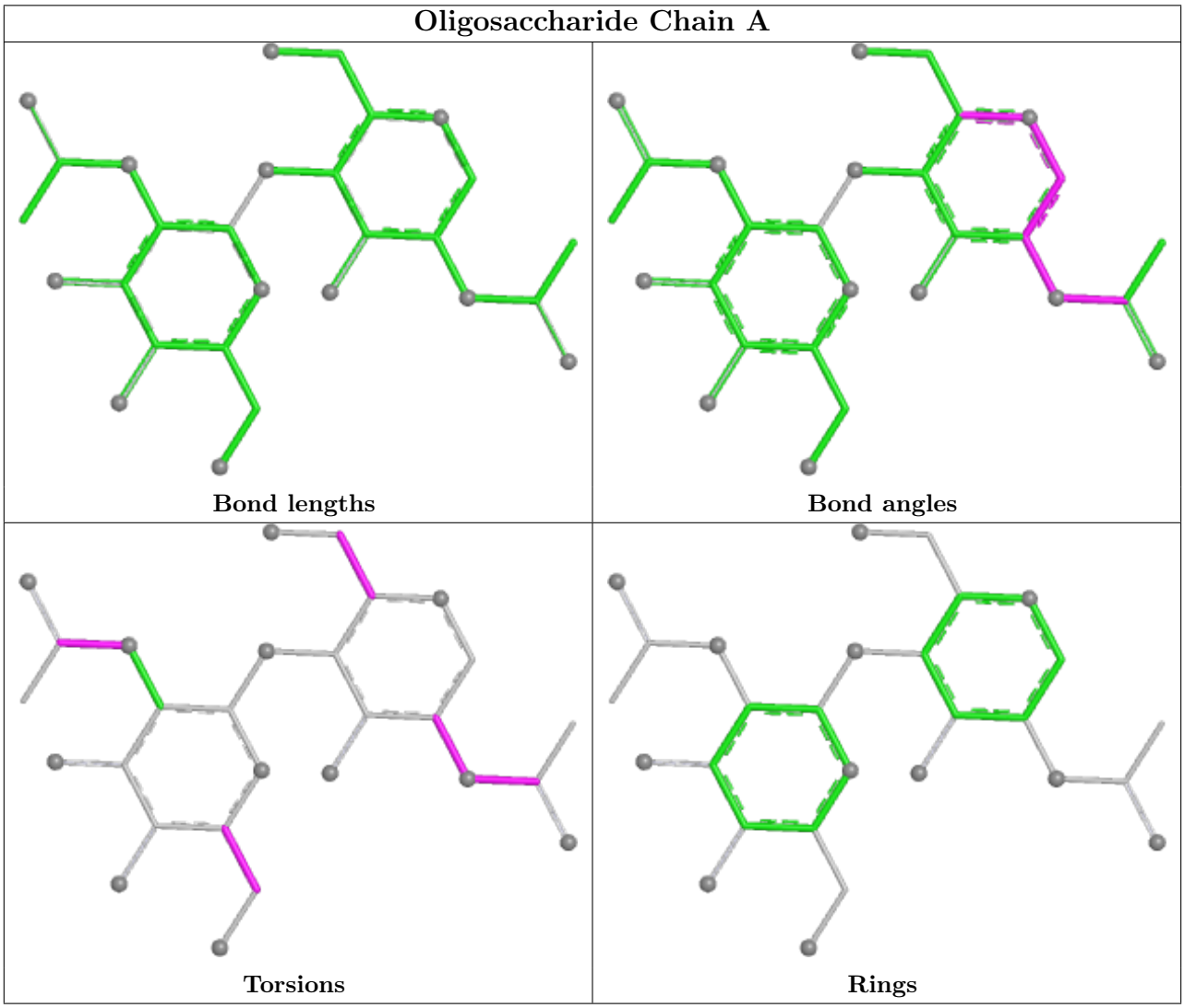
Mol	Chain	Res	Type	Atoms
4	A	2	NAG	C4-C5-C6-O6
4	A	1	NAG	O5-C5-C6-O6
4	A	2	NAG	O5-C5-C6-O6
4	A	1	NAG	C4-C5-C6-O6
4	A	1	NAG	C8-C7-N2-C2
4	A	1	NAG	O7-C7-N2-C2
4	A	2	NAG	C8-C7-N2-C2
4	A	2	NAG	O7-C7-N2-C2
4	A	1	NAG	C3-C2-N2-C7

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	2	NAG	1	0
4	A	1	NAG	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.



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.

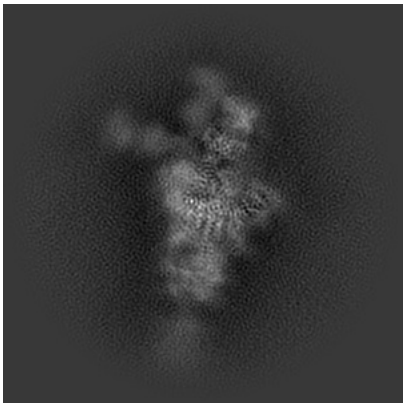
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-14143. These allow visual inspection of the internal detail of the map and identification of artifacts.

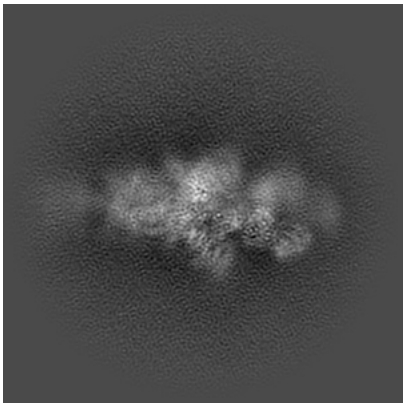
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

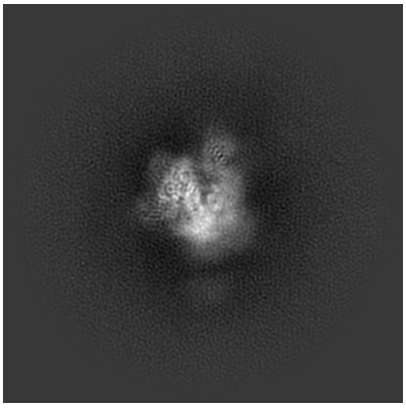
6.1.1 Primary map



X



Y

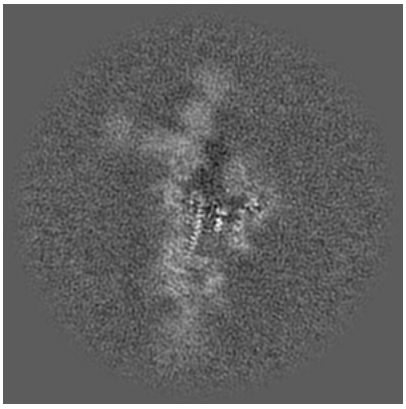


Z

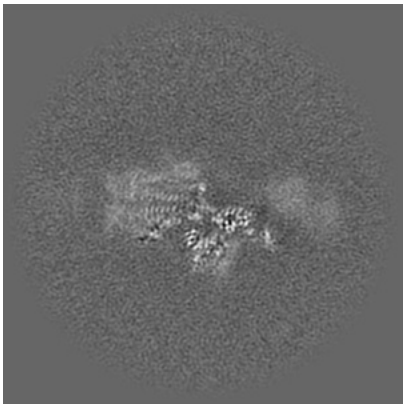
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

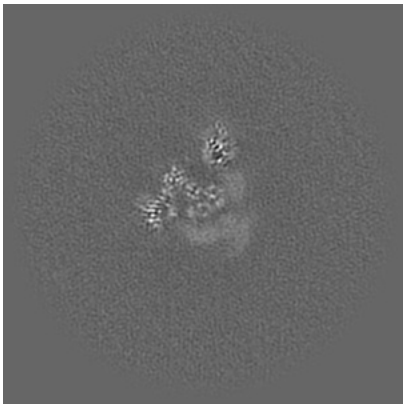
6.2.1 Primary map



X Index: 150



Y Index: 150

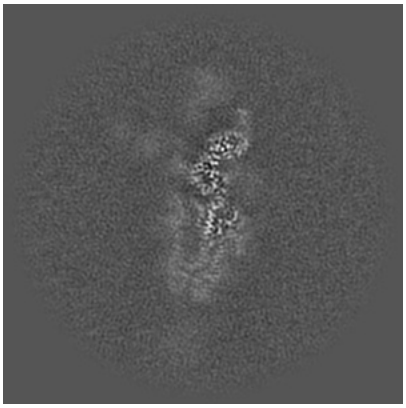


Z Index: 150

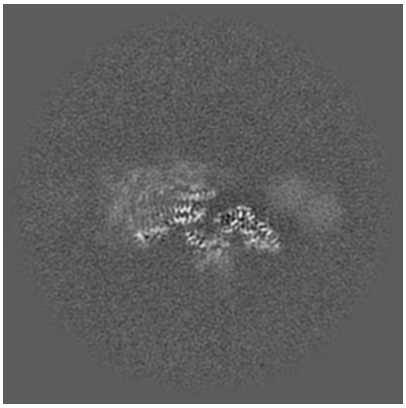
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

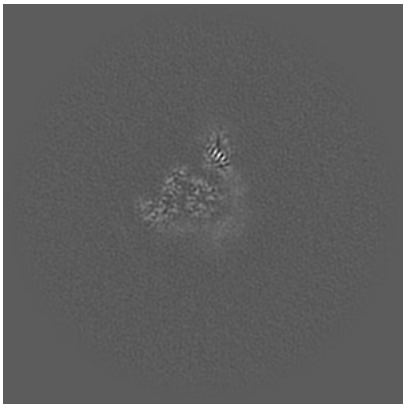
6.3.1 Primary map



X Index: 138



Y Index: 154



Z Index: 145

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

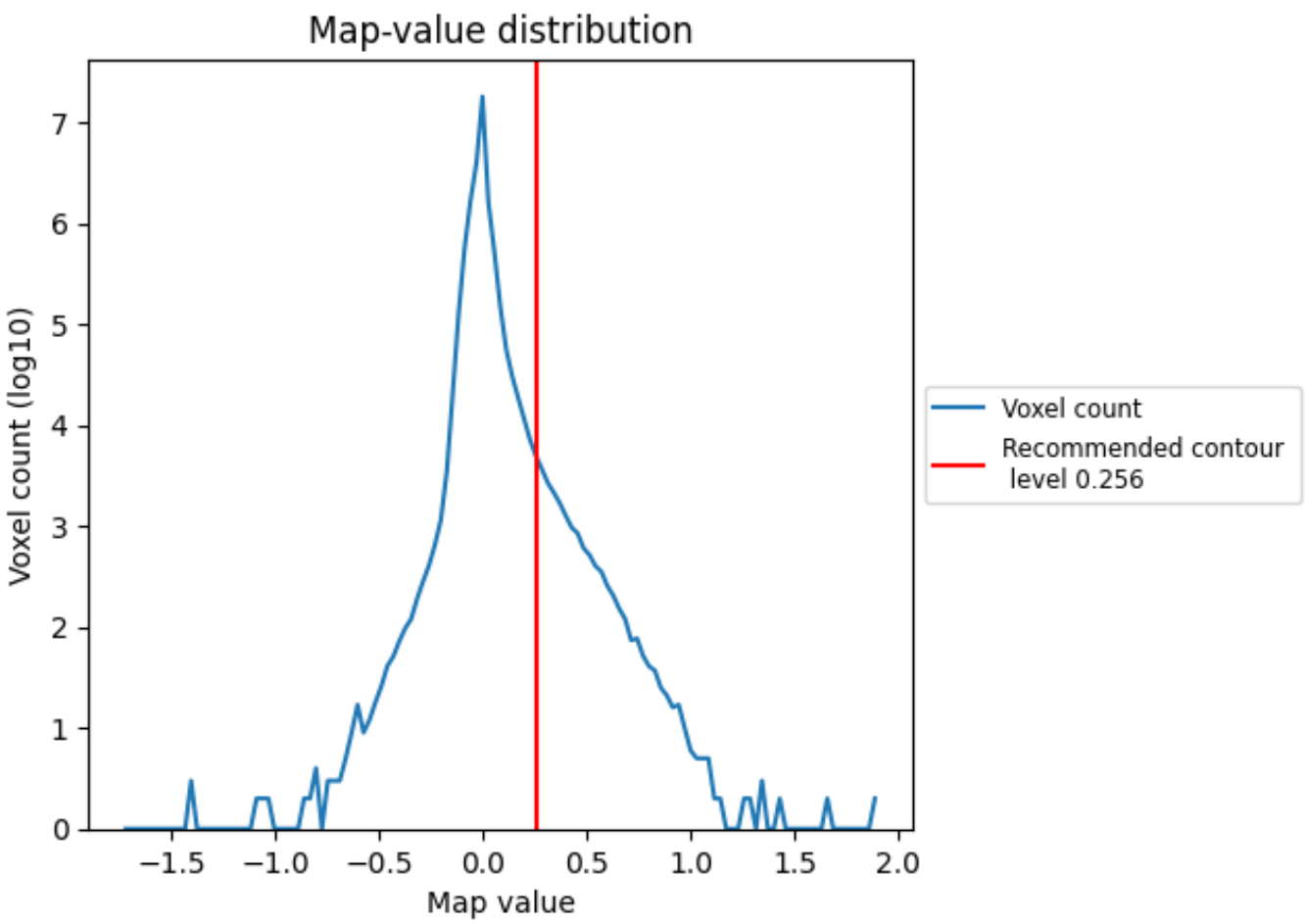
6.5 Mask visualisation (i)

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

7 Map analysis (i)

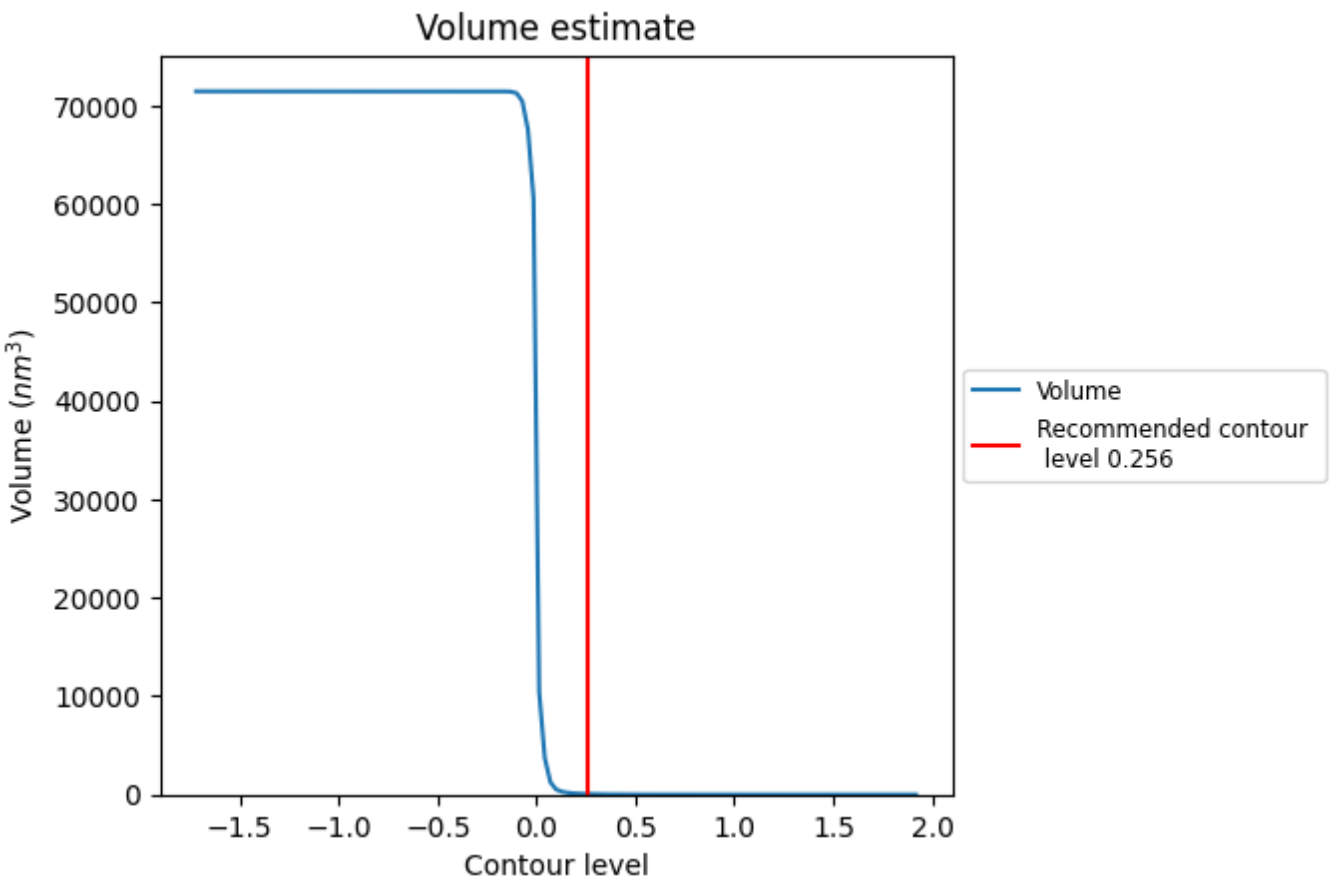
This section contains the results of statistical analysis of the map.

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.

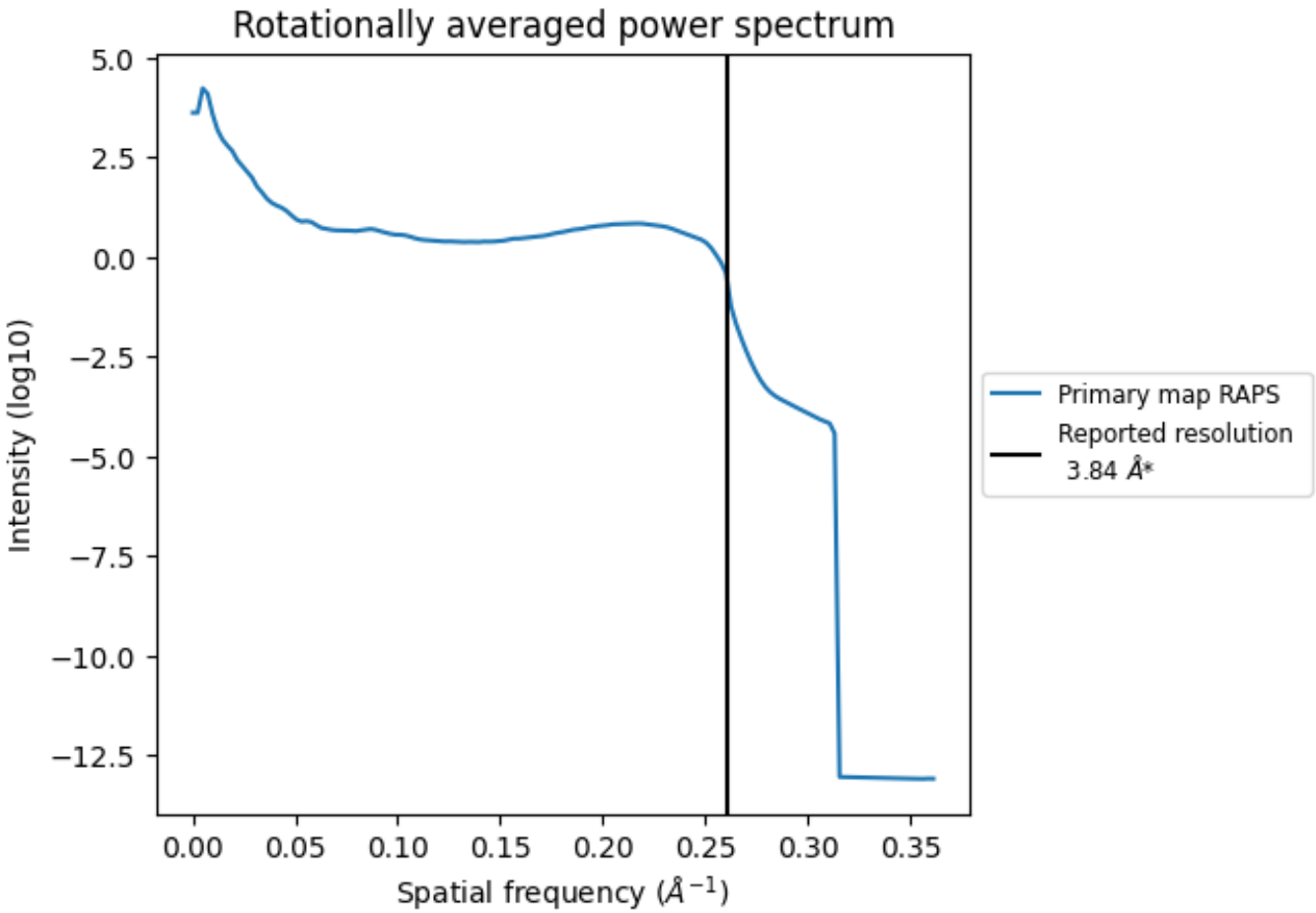
7.2 Volume estimate (i)



The volume at the recommended contour level is 57 nm^3; this corresponds to an approximate mass of 51 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)

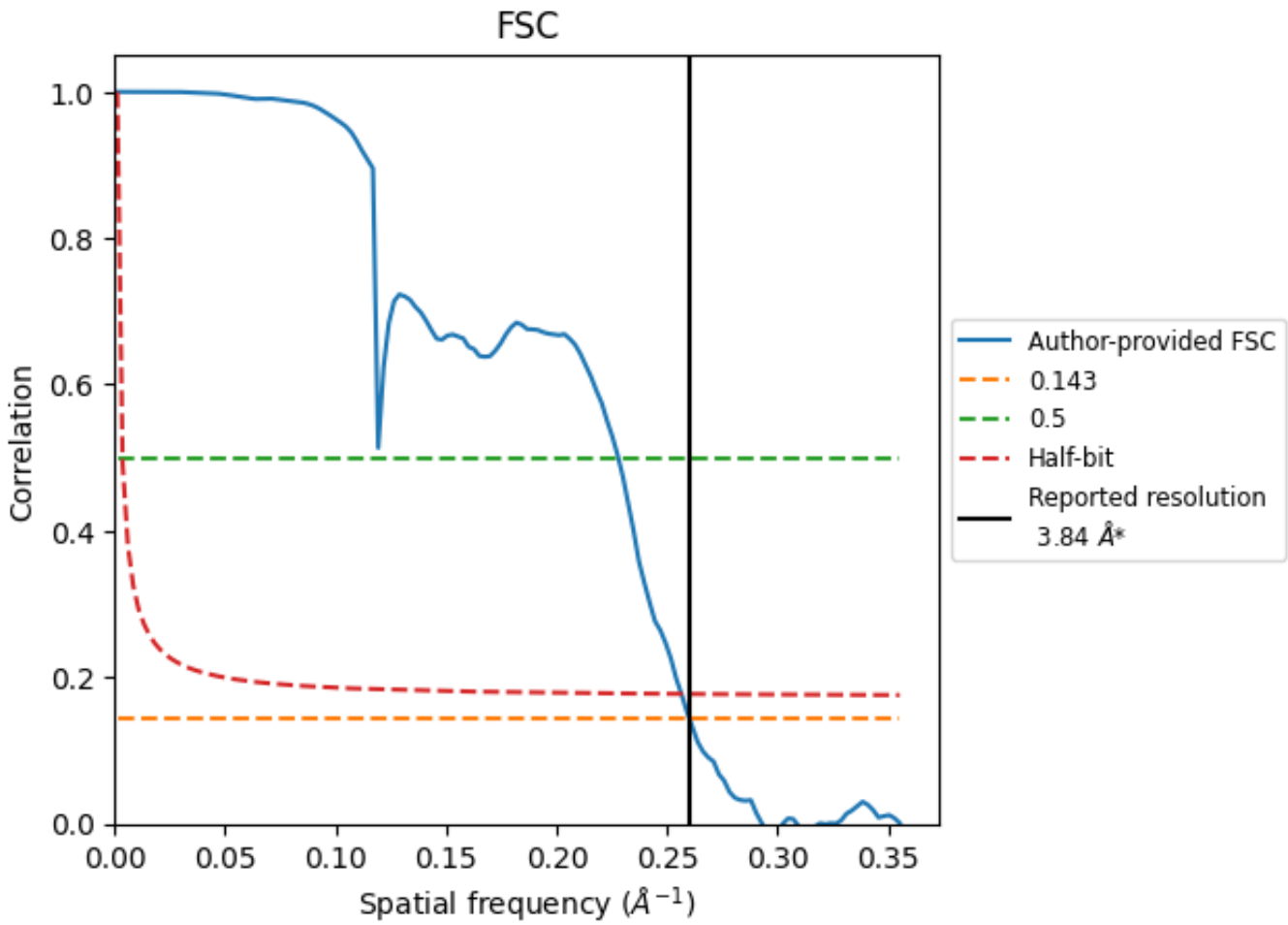


*Reported resolution corresponds to spatial frequency of 0.260 Å^{-1}

8 Fourier-Shell correlation (i)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC (i)



*Reported resolution corresponds to spatial frequency of 0.260 Å^{-1}

8.2 Resolution estimates (i)

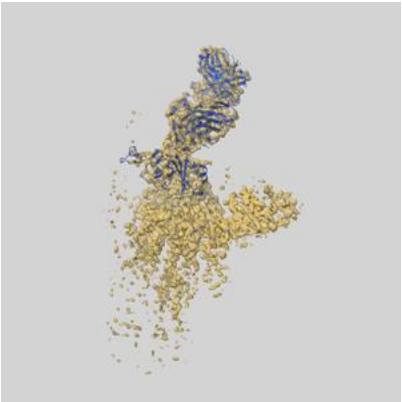
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.84	-	-
Author-provided FSC curve	3.84	4.39	3.90
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

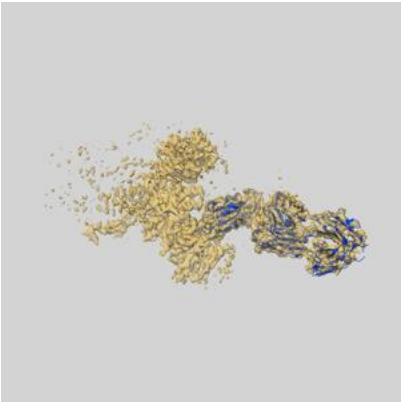
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-14143 and PDB model 7QTK. Per-residue inclusion information can be found in section 3 on page 7.

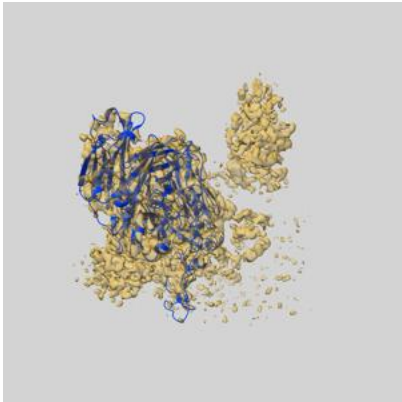
9.1 Map-model overlay (i)



X



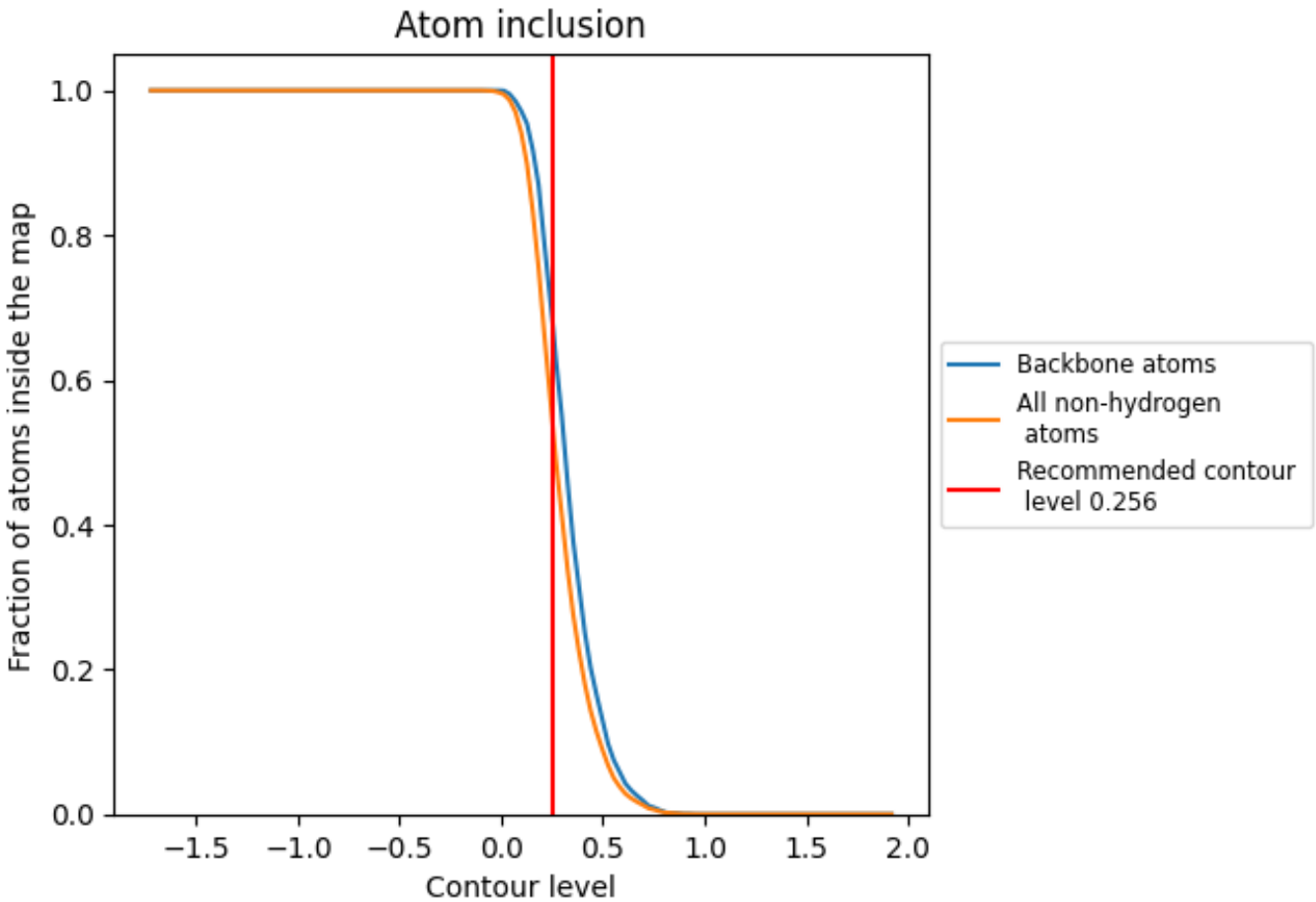
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.256 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 Atom inclusion (i)



At the recommended contour level, 67% of all backbone atoms, 53% of all non-hydrogen atoms, are inside the map.