Full wwPDB EM Validation Report ⓘ

Apr 1, 2025 – 09:55 pm BST

PDB ID	:	6ROI / pdb_00006roi
EMDB ID	:	EMD-4973
Title	:	Cryo-EM structure of the partially activated Drs2p-Cdc50p
Authors	:	Timcenko, M.; Lyons, J.A.; Januliene, D.; Ulstrup, J.J.; Dieudonne, T.; Montigny, C.; Ash, M.R.; Karlsen, J.L.; Boesen, T.; Kuhlbrandt, W.; Lenoir, G.; Moeller, A.; Nissen, P.
Deposited on	:	2019-05-13
Resolution	:	3.70 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

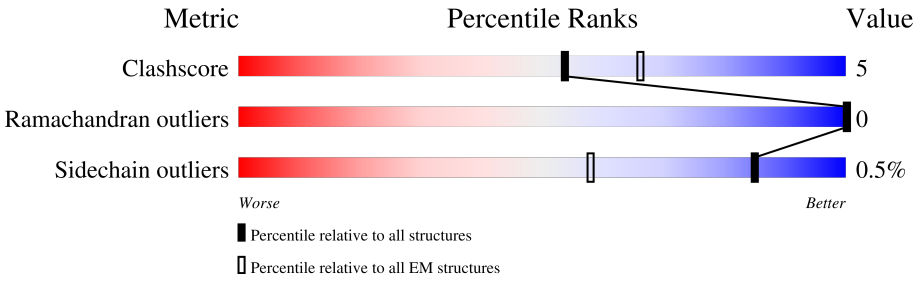
EMDB validation analysis	:	0.0.1.dev117
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.42

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 3.70 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	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	1460	9% 64% 12% 24%
2	C	413	75% 7% 18%
3	B	2	50% 50% 50%
4	D	4	25% 100%

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 11775 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 Probable phospholipid-transporting ATPase DRS2.

Mol	Chain	Residues	Atoms							AltConf	Trace
			Total	Be	C	F	N	O	S		
1	A	1108	8861	1	5715	3	1448	1656	38	0	0

There are 105 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1356	GLY	-	expression tag	UNP P39524
A	1357	GLY	-	expression tag	UNP P39524
A	1358	GLY	-	expression tag	UNP P39524
A	1359	GLY	-	expression tag	UNP P39524
A	1360	LEU	-	expression tag	UNP P39524
A	1361	VAL	-	expression tag	UNP P39524
A	1362	PRO	-	expression tag	UNP P39524
A	1363	ARG	-	expression tag	UNP P39524
A	1364	GLY	-	expression tag	UNP P39524
A	1365	SER	-	expression tag	UNP P39524
A	1366	GLY	-	expression tag	UNP P39524
A	1367	GLY	-	expression tag	UNP P39524
A	1368	THR	-	expression tag	UNP P39524
A	1369	ALA	-	expression tag	UNP P39524
A	1370	ALA	-	expression tag	UNP P39524
A	1371	ALA	-	expression tag	UNP P39524
A	1372	PRO	-	expression tag	UNP P39524
A	1373	GLY	-	expression tag	UNP P39524
A	1374	PRO	-	expression tag	UNP P39524
A	1375	ALA	-	expression tag	UNP P39524
A	1376	PRO	-	expression tag	UNP P39524
A	1377	ALA	-	expression tag	UNP P39524
A	1378	PRO	-	expression tag	UNP P39524
A	1379	ALA	-	expression tag	UNP P39524
A	1380	PRO	-	expression tag	UNP P39524
A	1381	ALA	-	expression tag	UNP P39524
A	1382	SER	-	expression tag	UNP P39524
A	1383	ALA	-	expression tag	UNP P39524

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1384	PRO	-	expression tag	UNP P39524
A	1385	ALA	-	expression tag	UNP P39524
A	1386	ALA	-	expression tag	UNP P39524
A	1387	ALA	-	expression tag	UNP P39524
A	1388	ALA	-	expression tag	UNP P39524
A	1389	PRO	-	expression tag	UNP P39524
A	1390	ALA	-	expression tag	UNP P39524
A	1391	GLY	-	expression tag	UNP P39524
A	1392	ALA	-	expression tag	UNP P39524
A	1393	GLY	-	expression tag	UNP P39524
A	1394	THR	-	expression tag	UNP P39524
A	1395	PRO	-	expression tag	UNP P39524
A	1396	VAL	-	expression tag	UNP P39524
A	1397	THR	-	expression tag	UNP P39524
A	1398	ALA	-	expression tag	UNP P39524
A	1399	PRO	-	expression tag	UNP P39524
A	1400	LEU	-	expression tag	UNP P39524
A	1401	ALA	-	expression tag	UNP P39524
A	1402	GLY	-	expression tag	UNP P39524
A	1403	THR	-	expression tag	UNP P39524
A	1404	ILE	-	expression tag	UNP P39524
A	1405	TRP	-	expression tag	UNP P39524
A	1406	LYS	-	expression tag	UNP P39524
A	1407	VAL	-	expression tag	UNP P39524
A	1408	LEU	-	expression tag	UNP P39524
A	1409	ALA	-	expression tag	UNP P39524
A	1410	SER	-	expression tag	UNP P39524
A	1411	GLU	-	expression tag	UNP P39524
A	1412	GLY	-	expression tag	UNP P39524
A	1413	GLN	-	expression tag	UNP P39524
A	1414	THR	-	expression tag	UNP P39524
A	1415	VAL	-	expression tag	UNP P39524
A	1416	ALA	-	expression tag	UNP P39524
A	1417	ALA	-	expression tag	UNP P39524
A	1418	GLY	-	expression tag	UNP P39524
A	1419	GLU	-	expression tag	UNP P39524
A	1420	VAL	-	expression tag	UNP P39524
A	1421	LEU	-	expression tag	UNP P39524
A	1422	LEU	-	expression tag	UNP P39524
A	1423	ILE	-	expression tag	UNP P39524
A	1424	LEU	-	expression tag	UNP P39524
A	1425	GLU	-	expression tag	UNP P39524

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1426	ALA	-	expression tag	UNP P39524
A	1427	MET	-	expression tag	UNP P39524
A	1428	LYS	-	expression tag	UNP P39524
A	1429	MET	-	expression tag	UNP P39524
A	1430	GLU	-	expression tag	UNP P39524
A	1431	THR	-	expression tag	UNP P39524
A	1432	GLU	-	expression tag	UNP P39524
A	1433	ILE	-	expression tag	UNP P39524
A	1434	ARG	-	expression tag	UNP P39524
A	1435	ALA	-	expression tag	UNP P39524
A	1436	ALA	-	expression tag	UNP P39524
A	1437	GLN	-	expression tag	UNP P39524
A	1438	ALA	-	expression tag	UNP P39524
A	1439	GLY	-	expression tag	UNP P39524
A	1440	THR	-	expression tag	UNP P39524
A	1441	VAL	-	expression tag	UNP P39524
A	1442	ARG	-	expression tag	UNP P39524
A	1443	GLY	-	expression tag	UNP P39524
A	1444	ILE	-	expression tag	UNP P39524
A	1445	ALA	-	expression tag	UNP P39524
A	1446	VAL	-	expression tag	UNP P39524
A	1447	LYS	-	expression tag	UNP P39524
A	1448	ALA	-	expression tag	UNP P39524
A	1449	GLY	-	expression tag	UNP P39524
A	1450	ASP	-	expression tag	UNP P39524
A	1451	ALA	-	expression tag	UNP P39524
A	1452	VAL	-	expression tag	UNP P39524
A	1453	ALA	-	expression tag	UNP P39524
A	1454	VAL	-	expression tag	UNP P39524
A	1455	GLY	-	expression tag	UNP P39524
A	1456	ASP	-	expression tag	UNP P39524
A	1457	THR	-	expression tag	UNP P39524
A	1458	LEU	-	expression tag	UNP P39524
A	1459	MET	-	expression tag	UNP P39524
A	1460	THR	-	expression tag	UNP P39524

- Molecule 2 is a protein called Cell division control protein 50.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	339	Total	C	N	O	S	0	0
			2754	1785	454	504	11		

There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	392	GLY	-	expression tag	UNP P25656
C	393	GLY	-	expression tag	UNP P25656
C	394	GLY	-	expression tag	UNP P25656
C	395	GLY	-	expression tag	UNP P25656
C	396	LEU	-	expression tag	UNP P25656
C	397	VAL	-	expression tag	UNP P25656
C	398	PRO	-	expression tag	UNP P25656
C	399	ARG	-	expression tag	UNP P25656
C	400	GLY	-	expression tag	UNP P25656
C	401	SER	-	expression tag	UNP P25656
C	402	GLY	-	expression tag	UNP P25656
C	403	GLY	-	expression tag	UNP P25656
C	404	HIS	-	expression tag	UNP P25656
C	405	HIS	-	expression tag	UNP P25656
C	406	HIS	-	expression tag	UNP P25656
C	407	HIS	-	expression tag	UNP P25656
C	408	HIS	-	expression tag	UNP P25656
C	409	HIS	-	expression tag	UNP P25656
C	410	HIS	-	expression tag	UNP P25656
C	411	HIS	-	expression tag	UNP P25656
C	412	HIS	-	expression tag	UNP P25656
C	413	HIS	-	expression tag	UNP P25656

- Molecule 3 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		
3	B	2	28	16	2	10	0	0

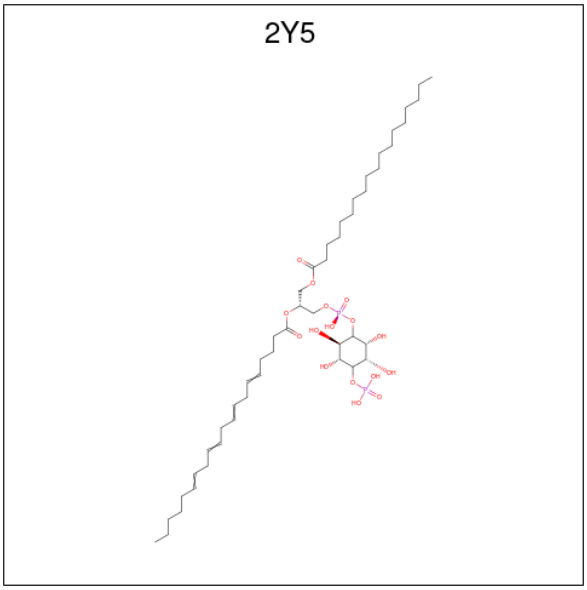
- Molecule 4 is an oligosaccharide called beta-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

Mol	Chain	Residues	Atoms				AltConf	Trace
4	D	4	Total	C	N	O	0	0
			50	28	2	20		

- Molecule 5 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

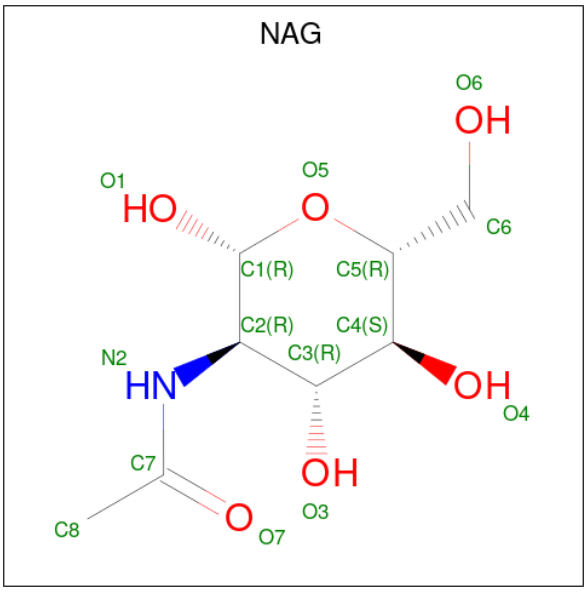
Mol	Chain	Residues	Atoms		AltConf
5	A	1	Total	Mg	0
			1	1	

- Molecule 6 is (2R)-1-{[(R)-hydroxy{[(1R,2R,3R,4R,5S,6R)-2,3,5,6-tetrahydroxy-4-(phosphonooxy)cyclohexyl]oxy}phosphoryl]oxy}-3-(octadecanoyloxy)propan-2-yl (5Z,8Z,11Z,14Z)-icosa-5,8,11,14-tetraenoate (CCD ID: 2Y5) (formula: $C_{47}H_{84}O_{16}P_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
6	A	1	Total	C	O	P	0
			65	47	16	2	

- Molecule 7 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				AltConf
7	C	1	Total	C	N	O	0
			14	8	1	5	

- Molecule 8 is water.

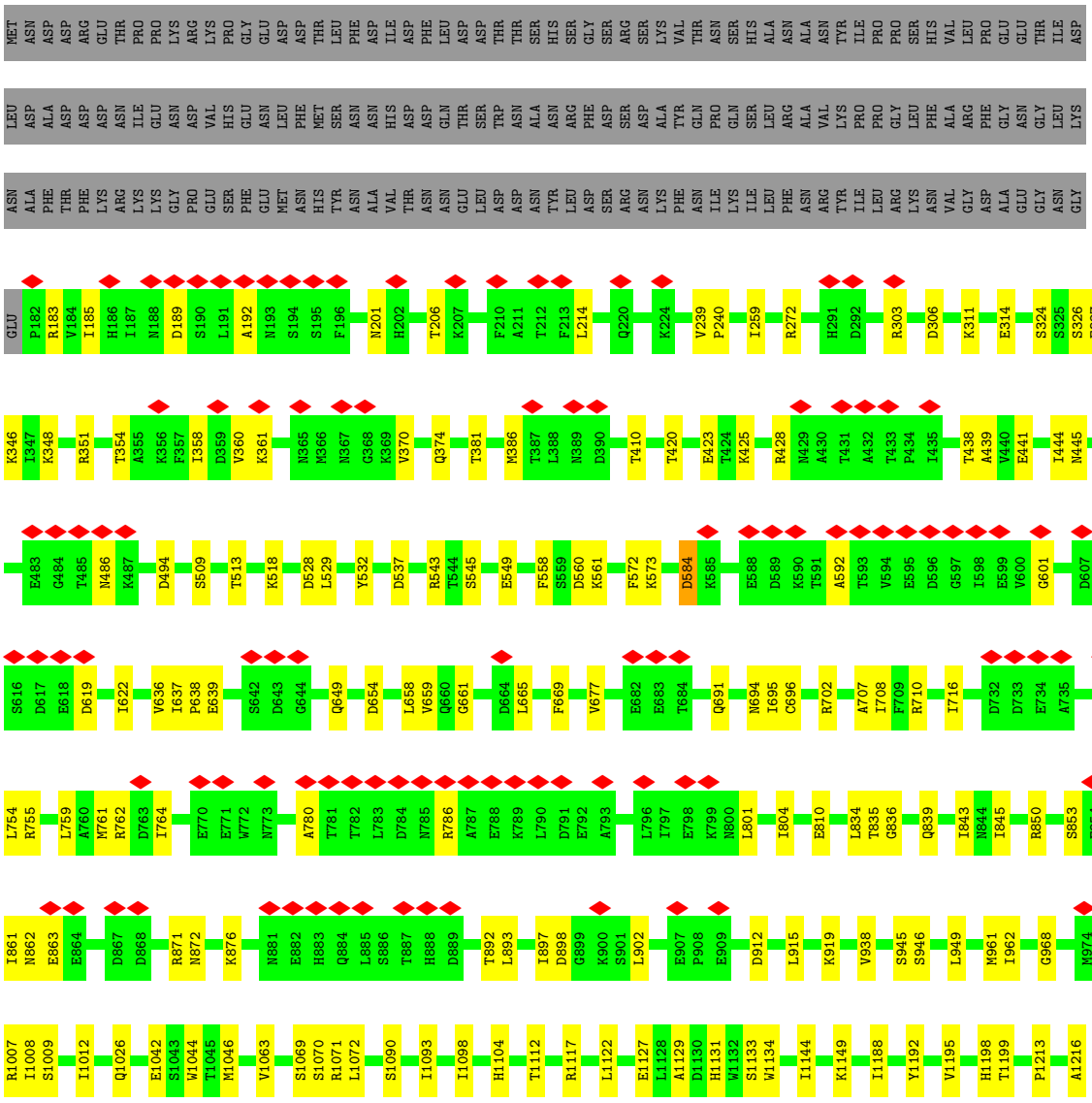
Mol	Chain	Residues	Atoms		AltConf
8	A	2	Total	O	0
			2	2	

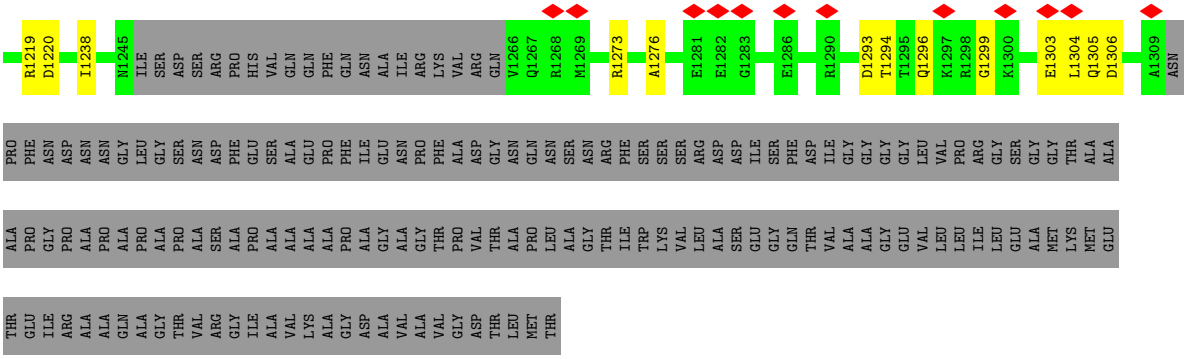
3 Residue-property plots (i)

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.

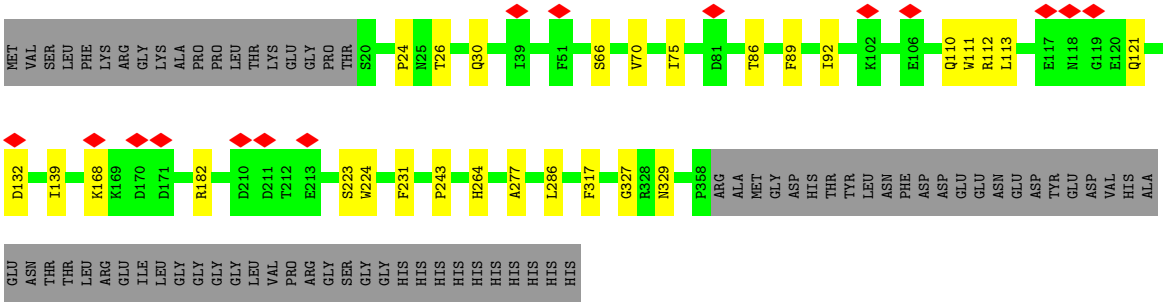
• Molecule 1: Probable phospholipid-transporting ATPase DRS2

Chain A:





• Molecule 2: Cell division control protein 50



• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

• Molecule 4: beta-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	78981	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 ($e^-/Å^2$)	60	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	0.201	Depositor
Minimum map value	-0.128	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.025	Depositor
Map size (Å)	275.712, 275.712, 275.712	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.077, 1.077, 1.077	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: BFD, BMA, MG, 2Y5, 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	A	0.42	0/9039	0.57	2/12245 (0.0%)
2	C	0.42	0/2828	0.56	0/3835
All	All	0.42	0/11867	0.56	2/16080 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	214	LEU	CA-CB-CG	5.86	128.77	115.30
1	A	1192	TYR	CA-CB-CG	5.18	123.25	113.40

There are no chirality outliers.

There are no planarity outliers.

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	8861	0	8865	102	0
2	C	2754	0	2749	17	0
3	B	28	0	25	0	0
4	D	50	0	43	0	0
5	A	1	0	0	0	0
6	A	65	0	79	2	0
7	C	14	0	13	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	A	2	0	0	0	0
All	All	11775	0	11774	117	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 (117) 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:183:ARG:H	1:A:374:GLN:HE22	1.45	0.63
1:A:423:GLU:HA	1:A:428:ARG:HD3	1.82	0.61
1:A:938:VAL:HG13	1:A:949:LEU:HD11	1.81	0.61
1:A:1026:GLN:NE2	1:A:1046:MET:SD	2.73	0.61
1:A:716:ILE:HG13	1:A:764:ILE:HG23	1.84	0.60
1:A:529:LEU:H	2:C:30:GLN:HE22	1.50	0.59
1:A:441:GLU:OE2	1:A:445:ASN:ND2	2.36	0.59
1:A:444:ILE:HD11	1:A:1012:ILE:HD13	1.84	0.59
1:A:861:ILE:HB	1:A:897:ILE:HG22	1.84	0.58
1:A:1149:LYS:NZ	1:A:1220:ASP:OD2	2.36	0.58
1:A:856:MET:HG2	1:A:892:THR:HA	1.86	0.57
1:A:201:ASN:OD1	1:A:420:THR:OG1	2.23	0.57
1:A:370:VAL:HG22	1:A:386:MET:HG2	1.87	0.57
1:A:185:ILE:HB	1:A:370:VAL:HB	1.87	0.56
1:A:561:LYS:HD3	1:A:845:ILE:HG13	1.88	0.56
1:A:334:ILE:HD11	1:A:348:LYS:HE3	1.88	0.56
1:A:1303:GLU:OE2	1:A:1305:GLN:NE2	2.38	0.56
1:A:381:THR:O	1:A:425:LYS:NZ	2.38	0.56
1:A:691:GLN:HB2	1:A:710:ARG:HB3	1.88	0.55
1:A:863:GLU:HG3	1:A:872:ASN:HD22	1.71	0.55
2:C:223:SER:OG	2:C:224:TRP:N	2.39	0.54
2:C:182:ARG:NH2	2:C:243:PRO:O	2.40	0.54
1:A:839:GLN:HE21	1:A:843:ILE:HD11	1.74	0.53
1:A:466:ASN:ND2	1:A:494:ASP:OD2	2.41	0.53
1:A:945:SER:OG	1:A:946:SER:N	2.41	0.53
1:A:1069:SER:OG	1:A:1070:SER:N	2.41	0.53
1:A:592:ALA:HA	1:A:601:GLY:HA3	1.92	0.52
1:A:695:ILE:HA	1:A:707:ALA:HA	1.92	0.52
1:A:853:SER:OG	1:A:856:MET:SD	2.68	0.51
1:A:780:ALA:O	1:A:786:ARG:NH1	2.43	0.51
1:A:835:THR:OG1	1:A:836:GLY:N	2.42	0.51
1:A:1044:TRP:HE1	1:A:1188:ILE:HD11	1.77	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:86:THR:O	2:C:112:ARG:NH1	2.45	0.50
1:A:342:GLU:OE1	1:A:346:LYS:NZ	2.40	0.50
1:A:639:GLU:OE2	1:A:649:GLN:NE2	2.45	0.50
1:A:912:ASP:N	1:A:912:ASP:OD1	2.45	0.50
1:A:438:THR:OG1	1:A:439:ALA:N	2.39	0.50
1:A:206:THR:HA	1:A:272:ARG:HD2	1.94	0.49
1:A:654:ASP:OD2	1:A:755:ARG:NH1	2.44	0.49
1:A:755:ARG:HB3	1:A:1276:ALA:HB3	1.94	0.49
1:A:1299:GLY:HA3	1:A:1304:LEU:HG	1.94	0.49
1:A:189:ASP:OD2	1:A:192:ALA:N	2.40	0.49
1:A:324:SER:OG	1:A:354:THR:O	2.30	0.49
1:A:862:ASN:N	1:A:862:ASN:OD1	2.45	0.49
1:A:558:PHE:HD2	1:A:834:LEU:HD11	1.78	0.49
1:A:532:TYR:OH	1:A:537:ASP:OD1	2.29	0.49
1:A:528:ASP:OD2	1:A:995:LYS:NZ	2.43	0.48
1:A:696:CYS:HB3	1:A:702:ARG:HH12	1.78	0.48
1:A:637:ILE:HD12	1:A:638:PRO:HD2	1.95	0.48
1:A:1007:ARG:NH1	1:A:1063:VAL:O	2.46	0.48
1:A:326:SER:HB2	1:A:1303:GLU:HB3	1.96	0.48
1:A:518:LYS:O	1:A:545:SER:OG	2.32	0.47
1:A:754:LEU:HG	1:A:810:GLU:HB3	1.97	0.47
1:A:1090:SER:H	1:A:1093:ILE:HG22	1.80	0.47
1:A:584:ASP:N	1:A:584:ASP:OD1	2.46	0.47
1:A:694:ASN:O	1:A:708:ILE:N	2.47	0.47
1:A:1122:LEU:HD13	1:A:1129:ALA:HB2	1.96	0.47
1:A:1131:HIS:HA	2:C:277:ALA:HB2	1.96	0.47
2:C:89:PHE:HB3	2:C:110:GLN:HB3	1.97	0.47
1:A:327:GLU:HG2	1:A:410:THR:HG23	1.96	0.47
1:A:1127:GLU:OE1	1:A:1198:HIS:NE2	2.44	0.47
1:A:1296:GLN:NE2	1:A:1306:ASP:OD1	2.47	0.47
2:C:139:ILE:HB	2:C:286:LEU:HB2	1.97	0.47
1:A:619:ASP:OD1	1:A:619:ASP:N	2.46	0.46
1:A:1133:SER:O	1:A:1133:SER:OG	2.30	0.46
1:A:1144:ILE:HG23	1:A:1213:PRO:HG3	1.97	0.46
1:A:545:SER:OG	1:A:545:SER:O	2.32	0.46
2:C:92:ILE:HG13	2:C:111:TRP:CD1	2.50	0.46
1:A:762:ARG:HB3	1:A:801:LEU:HD23	1.97	0.46
1:A:549:GLU:HB3	1:A:1008:ILE:HD12	1.97	0.46
1:A:1104:HIS:HD2	1:A:1216:ALA:HB1	1.81	0.46
2:C:231:PHE:O	2:C:264:HIS:ND1	2.47	0.46
1:A:360:VAL:HG23	1:A:361:LYS:HE2	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:351:ARG:HD3	1:A:351:ARG:HA	1.76	0.46
1:A:1293:ASP:OD1	1:A:1294:THR:N	2.49	0.46
1:A:573:LYS:HD3	1:A:810:GLU:HG2	1.98	0.45
2:C:113:LEU:HD11	2:C:121:GLN:HB3	1.99	0.45
1:A:572:PHE:HB3	1:A:661:GLY:HA3	1.98	0.45
1:A:1117:ARG:NH1	2:C:329:ASN:OD1	2.50	0.44
2:C:70:VAL:HG11	2:C:327:GLY:HA2	1.99	0.44
1:A:324:SER:HB3	1:A:358:ILE:HG22	1.99	0.44
1:A:1009:SER:O	1:A:1009:SER:OG	2.30	0.44
1:A:669:PHE:HE1	1:A:677:VAL:HB	1.83	0.44
1:A:839:GLN:OE1	1:A:862:ASN:ND2	2.51	0.44
1:A:509:SER:O	1:A:513:THR:OG1	2.34	0.44
1:A:1219:ARG:NH1	6:A:1502:2Y5:O18	2.51	0.44
1:A:1112:THR:HB	1:A:1134:TRP:HE1	1.84	0.43
1:A:486:ASN:N	1:A:486:ASN:OD1	2.52	0.43
1:A:1195:VAL:O	1:A:1199:THR:N	2.51	0.43
2:C:168:LYS:HD2	2:C:168:LYS:HA	1.87	0.43
1:A:897:ILE:HD12	1:A:902:LEU:HD13	2.00	0.43
1:A:859:LEU:HD22	1:A:893:LEU:HD21	2.00	0.43
1:A:259:ILE:HD13	1:A:259:ILE:HA	1.88	0.43
1:A:915:LEU:O	1:A:919:LYS:N	2.50	0.43
1:A:915:LEU:HD12	1:A:919:LYS:HE3	2.00	0.42
2:C:75:ILE:HB	2:C:317:PHE:HD2	1.84	0.42
2:C:66:SER:O	2:C:66:SER:OG	2.36	0.42
1:A:303:ARG:N	1:A:306:ASP:OD2	2.52	0.42
1:A:1042:GLU:OE1	1:A:1044:TRP:N	2.51	0.42
1:A:239:VAL:HA	1:A:240:PRO:HD3	1.90	0.42
1:A:622:ILE:HG23	1:A:804:ILE:HG23	2.01	0.42
1:A:1072:LEU:HD23	1:A:1238:ILE:HG22	2.02	0.42
2:C:132:ASP:OD1	2:C:132:ASP:N	2.52	0.42
1:A:938:VAL:HG21	1:A:961:MET:HG3	2.02	0.41
1:A:761:MET:HG2	1:A:804:ILE:HD11	2.03	0.41
2:C:24:PRO:HB2	2:C:26:THR:HG23	2.02	0.41
1:A:636:VAL:HG11	1:A:659:VAL:HG21	2.02	0.41
1:A:665:LEU:HA	1:A:665:LEU:HD23	1.88	0.41
1:A:872:ASN:O	1:A:876:LYS:HG2	2.21	0.41
1:A:272:ARG:HE	1:A:543:ARG:HB3	1.86	0.41
1:A:311:LYS:N	1:A:314:GLU:OE1	2.44	0.40
1:A:658:LEU:HD23	1:A:658:LEU:HA	1.93	0.40
1:A:1098:ILE:HD13	1:A:1098:ILE:HA	1.94	0.40
6:A:1502:2Y5:H39	6:A:1502:2Y5:H45	1.84	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:456:ILE:HD13	1:A:456:ILE:HA	1.87	0.40
1:A:759:LEU:HD23	1:A:759:LEU:HA	1.87	0.40
1:A:962:ILE:HG23	1:A:968:GLY:HA3	2.04	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	1103/1460 (76%)	1046 (95%)	57 (5%)	0	100	100
2	C	337/413 (82%)	321 (95%)	16 (5%)	0	100	100
All	All	1440/1873 (77%)	1367 (95%)	73 (5%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	969/1252 (77%)	963 (99%)	6 (1%)	84	90
2	C	309/370 (84%)	309 (100%)	0	100	100
All	All	1278/1622 (79%)	1272 (100%)	6 (0%)	85	92

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

Mol	Chain	Res	Type
1	A	584	ASP
1	A	850	ARG
1	A	871	ARG
1	A	898	ASP
1	A	1071	ARG
1	A	1273	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	374	GLN
1	A	409	ASN
1	A	613	ASN
1	A	660	GLN
1	A	694	ASN
1	A	872	ASN
1	A	1019	ASN
1	A	1050	ASN
2	C	30	GLN
2	C	116	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)

1 non-standard protein/DNA/RNA residue is 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	$\#\|Z\| > 2$
1	BFD	A	560	1,5	8,11,12	0.95	0	3,15,17	2.43	2 (66%)

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
1	BFD	A	560	1,5	-	2/5/11/13	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	560	BFD	OD2-CG-CB	-3.58	116.83	124.73
1	A	560	BFD	CB-CA-C	2.20	115.60	111.47

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	560	BFD	N-CA-CB-CG
1	A	560	BFD	C-CA-CB-CG

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

6 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	$\#\|Z\| > 2$
3	NAG	B	1	2,3	14,14,15	0.38	0	17,19,21	0.73	1 (5%)
3	NAG	B	2	3	14,14,15	0.38	0	17,19,21	0.36	0
4	NAG	D	1	2,4	14,14,15	1.02	1 (7%)	17,19,21	0.75	0
4	NAG	D	2	4	14,14,15	0.22	0	17,19,21	1.16	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	BMA	D	3	4	11,11,12	1.01	0	15,15,17	1.02	2 (13%)
4	BMA	D	4	4	11,11,12	0.94	1 (9%)	15,15,17	1.22	1 (6%)

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
3	NAG	B	1	2,3	-	4/6/23/26	0/1/1/1
3	NAG	B	2	3	-	1/6/23/26	0/1/1/1
4	NAG	D	1	2,4	-	2/6/23/26	0/1/1/1
4	NAG	D	2	4	-	3/6/23/26	0/1/1/1
4	BMA	D	3	4	-	0/2/19/22	0/1/1/1
4	BMA	D	4	4	-	2/2/19/22	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	1	NAG	O5-C1	-3.51	1.38	1.43
4	D	4	BMA	C1-C2	2.06	1.56	1.52

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	D	2	NAG	C2-N2-C7	3.16	127.40	122.90
4	D	4	BMA	C1-O5-C5	2.89	116.11	112.19
3	B	1	NAG	C1-O5-C5	2.38	115.42	112.19
4	D	3	BMA	C2-C3-C4	2.10	114.52	110.89
4	D	3	BMA	O2-C2-C3	-2.05	106.03	110.14
4	D	2	NAG	C1-O5-C5	2.01	114.92	112.19

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	D	4	BMA	O5-C5-C6-O6
4	D	4	BMA	C4-C5-C6-O6
3	B	1	NAG	C8-C7-N2-C2
3	B	1	NAG	O7-C7-N2-C2

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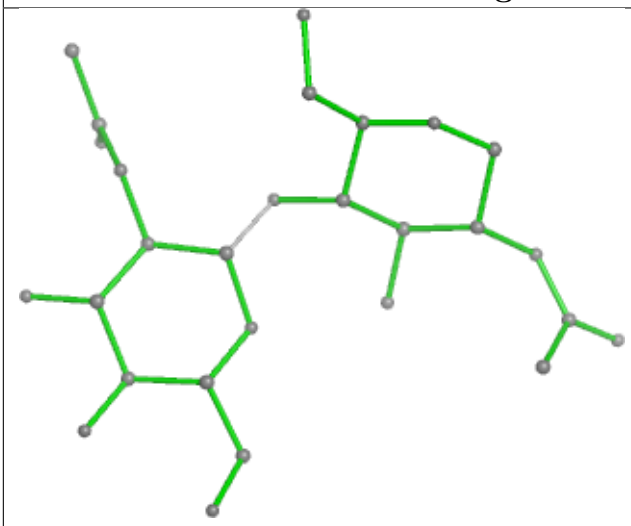
Mol	Chain	Res	Type	Atoms
4	D	1	NAG	O5-C5-C6-O6
4	D	1	NAG	C4-C5-C6-O6
3	B	2	NAG	O5-C5-C6-O6
3	B	1	NAG	C4-C5-C6-O6
3	B	1	NAG	O5-C5-C6-O6
4	D	2	NAG	C3-C2-N2-C7
4	D	2	NAG	C4-C5-C6-O6
4	D	2	NAG	O5-C5-C6-O6

There are no ring outliers.

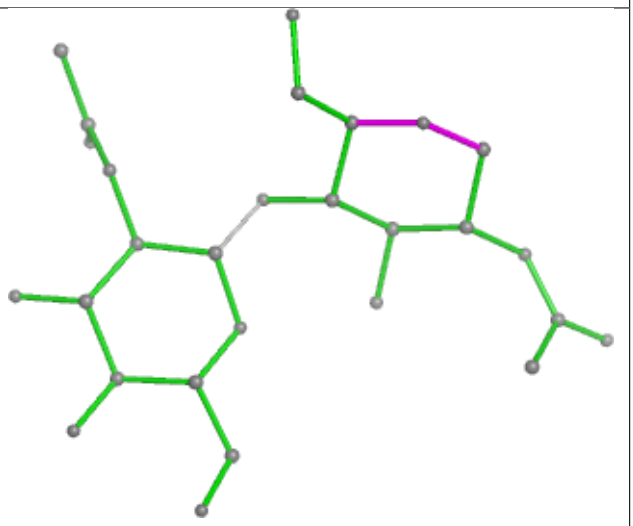
No monomer is involved in short contacts.

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

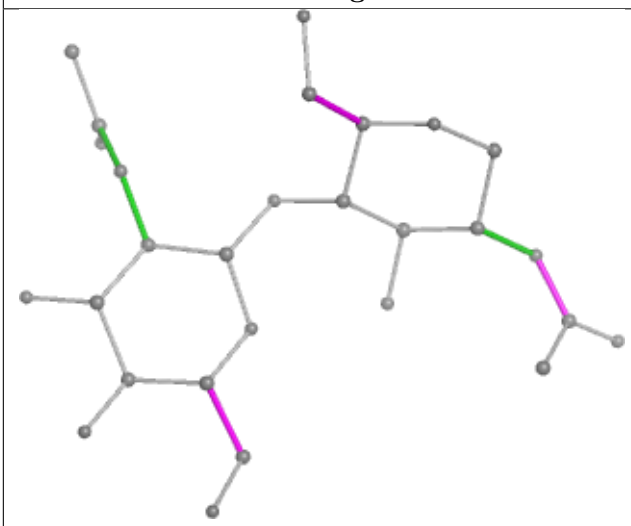
Oligosaccharide Chain B



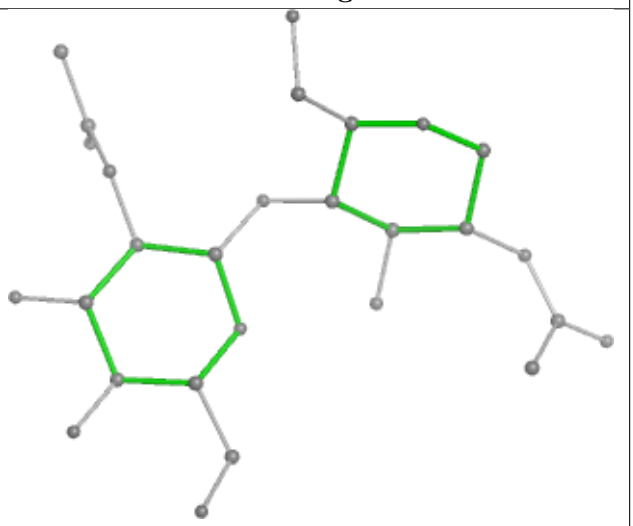
Bond lengths



Bond angles

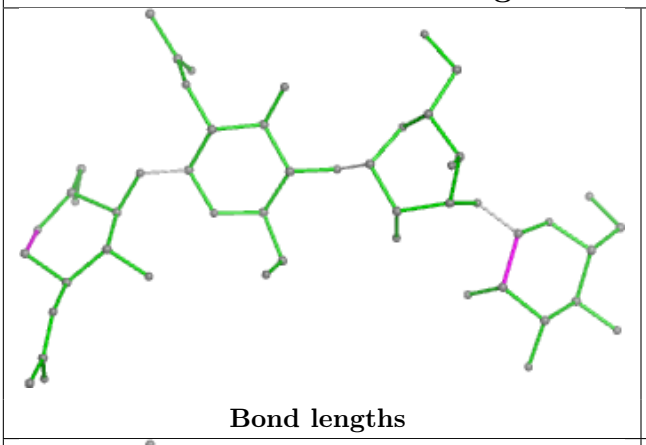


Torsions

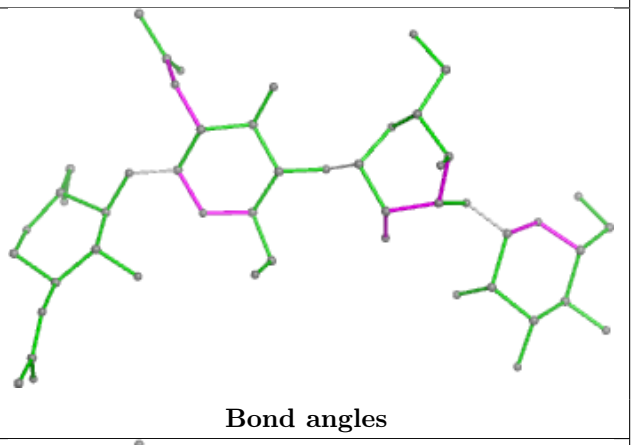


Rings

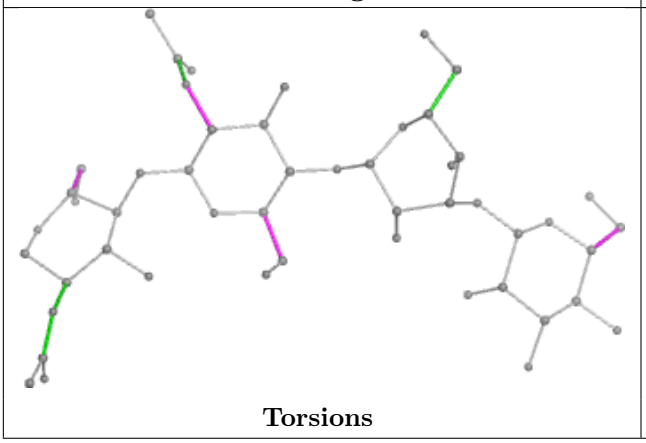
Oligosaccharide Chain D



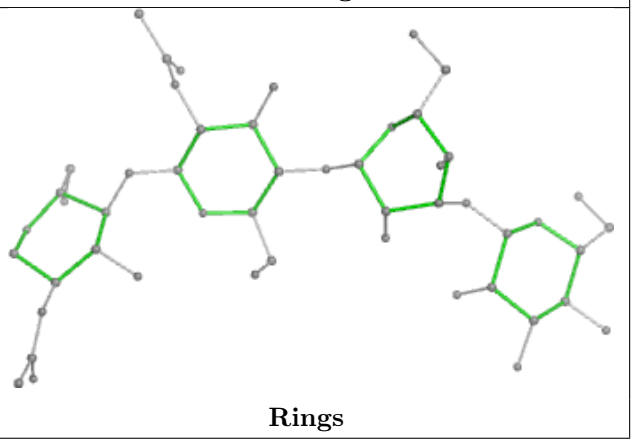
Bond lengths



Bond angles



Torsions



Rings

5.6 Ligand geometry (i)

Of 3 ligands modelled in this entry, 1 is monoatomic - leaving 2 for Mogul analysis.

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	$\#\|Z\| > 2$
7	NAG	C	503	2	14,14,15	0.38	0	17,19,21	0.57	0
6	2Y5	A	1502	1	65,65,65	0.94	5 (7%)	77,80,80	1.14	5 (6%)

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
7	NAG	C	503	2	-	2/6/23/26	0/1/1/1
6	2Y5	A	1502	1	-	27/61/85/85	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	1502	2Y5	P4-O4	3.02	1.65	1.59
6	A	1502	2Y5	O18-C11	2.54	1.40	1.33
6	A	1502	2Y5	O16-C8	-2.45	1.40	1.46
6	A	1502	2Y5	O16-C10	2.31	1.40	1.34
6	A	1502	2Y5	O18-C9	-2.13	1.40	1.45

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	A	1502	2Y5	C5-C4-C3	3.76	116.27	110.85
6	A	1502	2Y5	O16-C10-C12	3.75	119.58	111.50
6	A	1502	2Y5	C3-C2-C1	3.19	116.97	109.68
6	A	1502	2Y5	C2-C3-C4	3.06	116.68	109.68
6	A	1502	2Y5	O18-C11-C31	2.90	121.02	111.91

There are no chirality outliers.

All (29) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	1502	2Y5	C4-O4-P4-O43
6	A	1502	2Y5	O19-C11-O18-C9
6	A	1502	2Y5	O17-C10-O16-C8
6	A	1502	2Y5	C31-C11-O18-C9
6	A	1502	2Y5	C12-C10-O16-C8
7	C	503	NAG	C4-C5-C6-O6
6	A	1502	2Y5	C31-C32-C33-C34
6	A	1502	2Y5	C43-C44-C45-C46
6	A	1502	2Y5	C10-C12-C13-C14
6	A	1502	2Y5	C34-C35-C36-C37
6	A	1502	2Y5	C11-C31-C32-C33
7	C	503	NAG	O5-C5-C6-O6
6	A	1502	2Y5	C7-C8-C9-O18
6	A	1502	2Y5	C38-C39-C40-C41
6	A	1502	2Y5	C41-C42-C43-C44
6	A	1502	2Y5	C16-C17-C18-C19
6	A	1502	2Y5	C33-C34-C35-C36

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Mol	Chain	Res	Type	Atoms
6	A	1502	2Y5	C8-C7-O13-P1
6	A	1502	2Y5	O16-C8-C9-O18
6	A	1502	2Y5	C3-C4-O4-P4
6	A	1502	2Y5	C42-C43-C44-C45
6	A	1502	2Y5	C19-C20-C21-C22
6	A	1502	2Y5	C44-C45-C46-C47
6	A	1502	2Y5	C32-C33-C34-C35
6	A	1502	2Y5	O16-C10-C12-C13
6	A	1502	2Y5	C27-C28-C29-C30
6	A	1502	2Y5	C12-C13-C14-C15
6	A	1502	2Y5	O17-C10-C12-C13
6	A	1502	2Y5	O18-C11-C31-C32

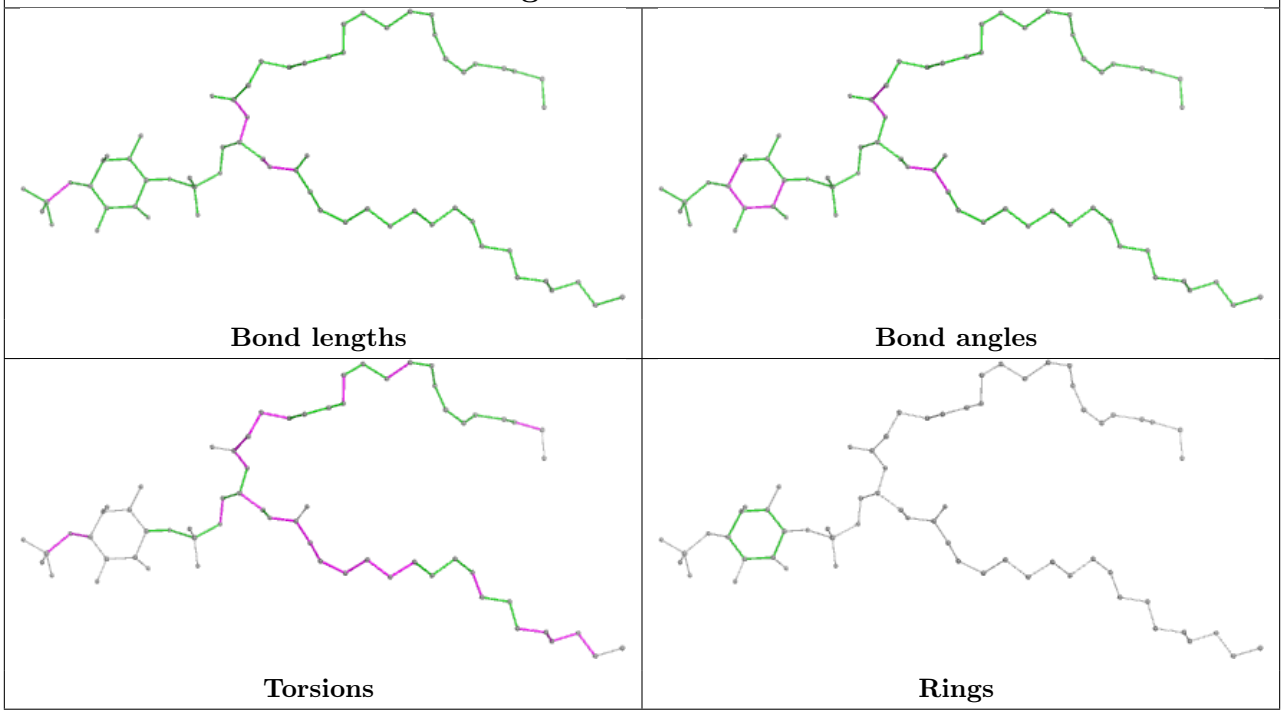
There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	1502	2Y5	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 all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand 2Y5 A 1502



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

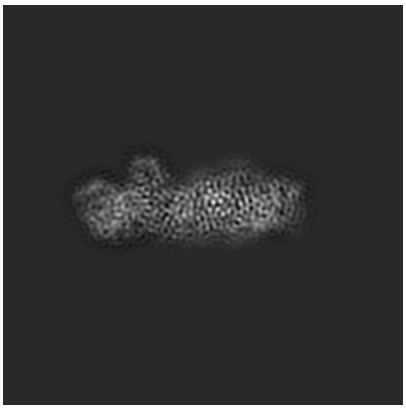
This section contains visualisations of the EMDB entry EMD-4973. These allow visual inspection of the internal detail of the map and identification of artifacts.

Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

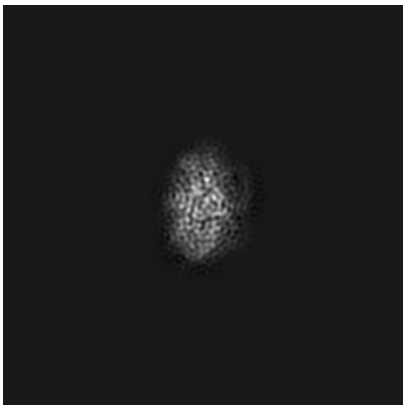
6.1 Orthogonal projections

6.1.1 Primary map

X

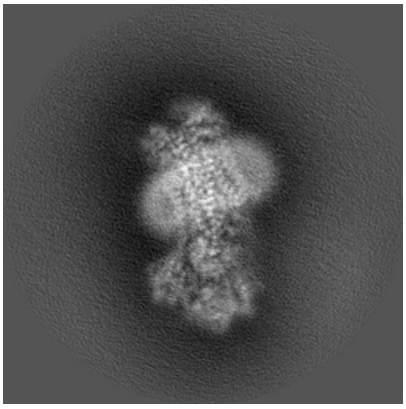


Y

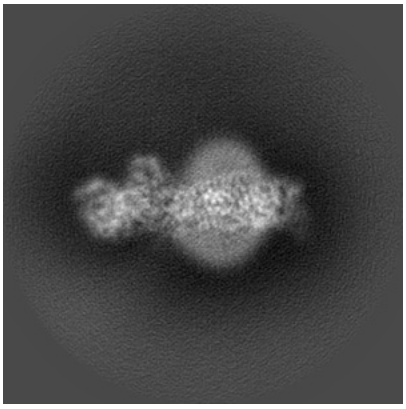


Z

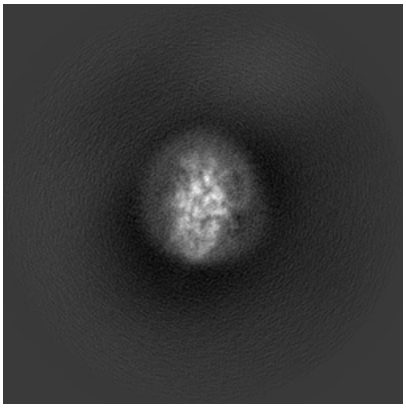
6.1.2 Raw map



X



Y



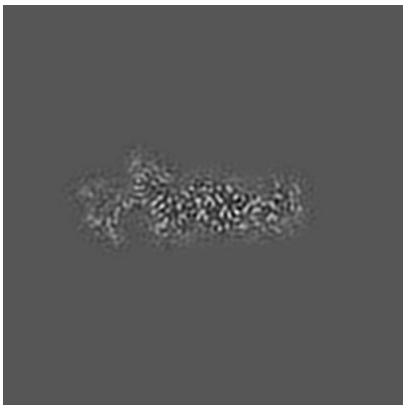
Z

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

6.2 Central slices (i)

6.2.1 Primary map

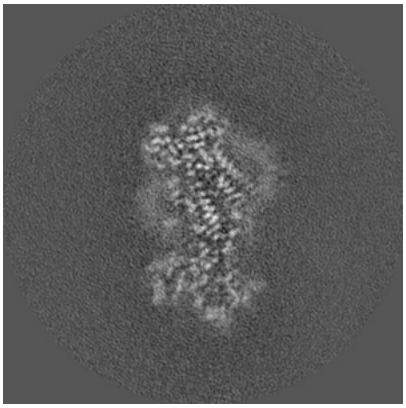
X Index: 128



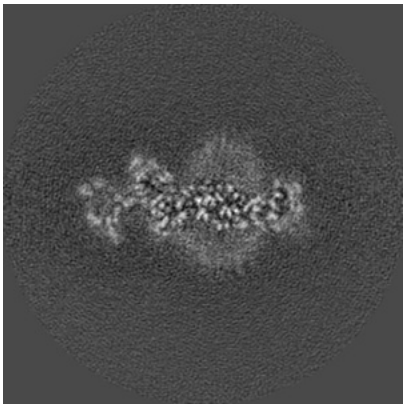
Y Index: 128

Z Index: 128

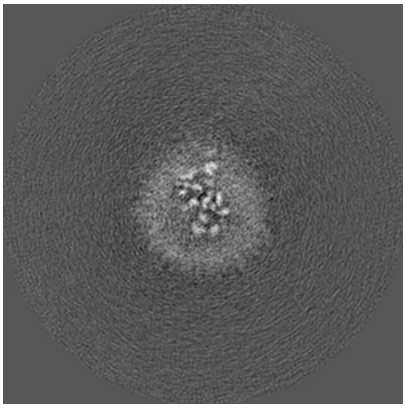
6.2.2 Raw map



X Index: 128



Y Index: 128



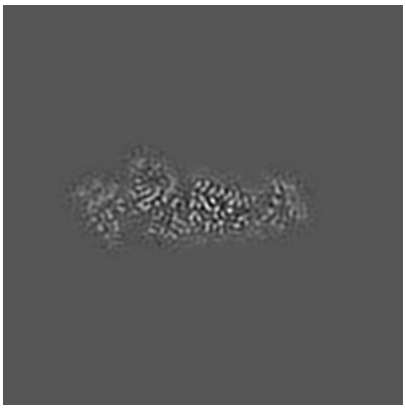
Z Index: 128

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

6.3 Largest variance slices (i)

6.3.1 Primary map

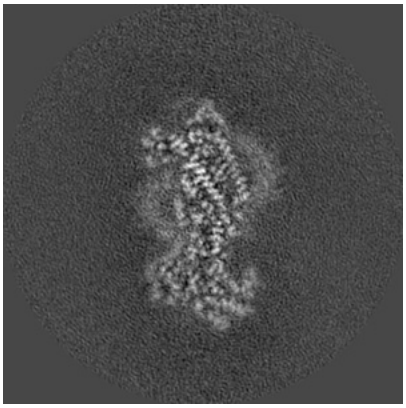
X Index: 125



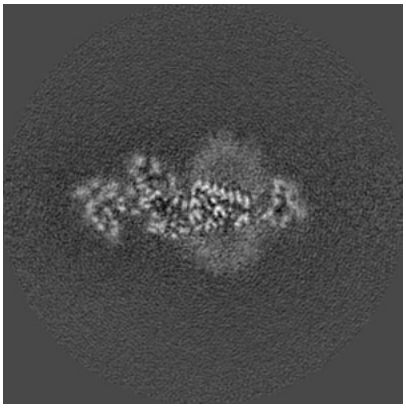
Y Index: 131

Z Index: 151

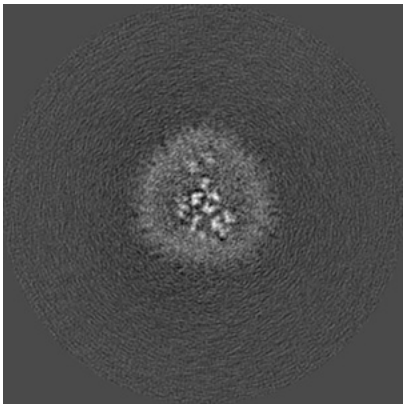
6.3.2 Raw map



X Index: 123



Y Index: 132

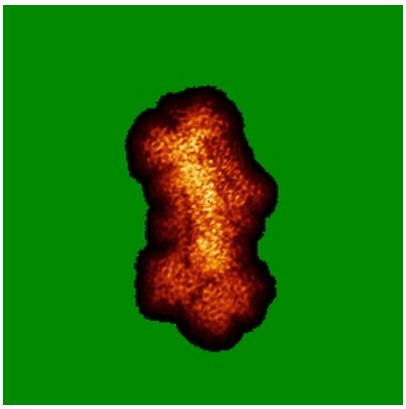


Z Index: 140

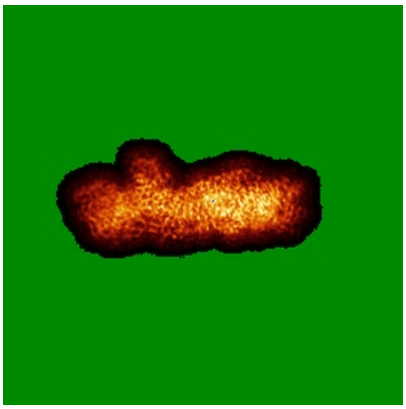
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

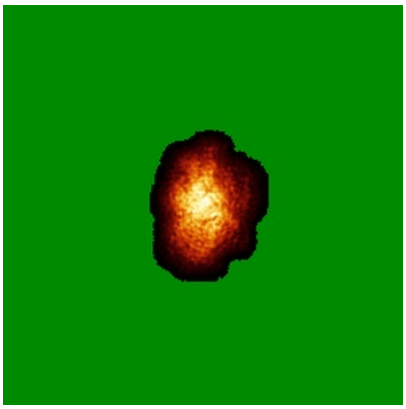
6.4.1 Primary map



X

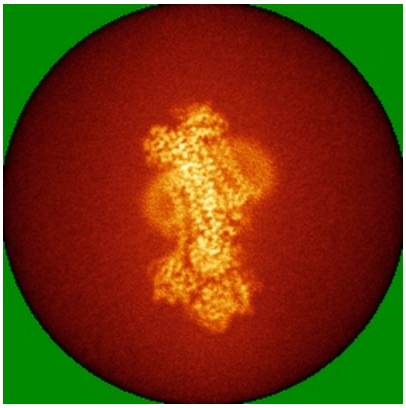


Y

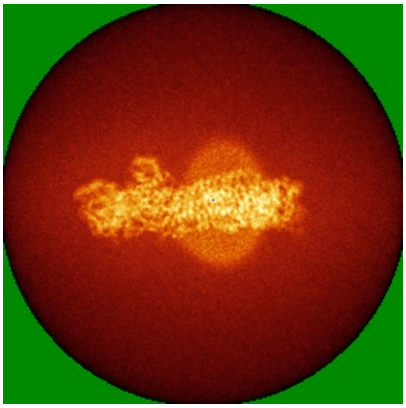


Z

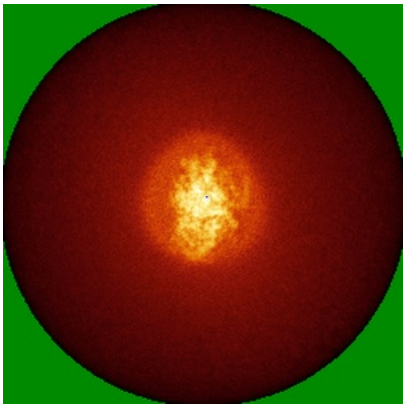
6.4.2 Raw map



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.

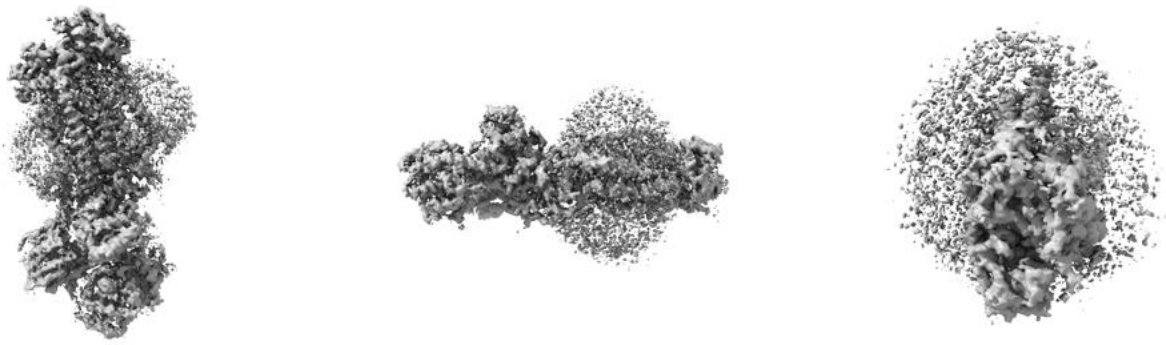
6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.025. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X Y Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

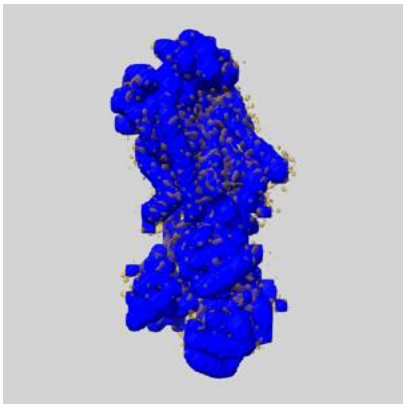
6.6 Mask visualisation (i)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

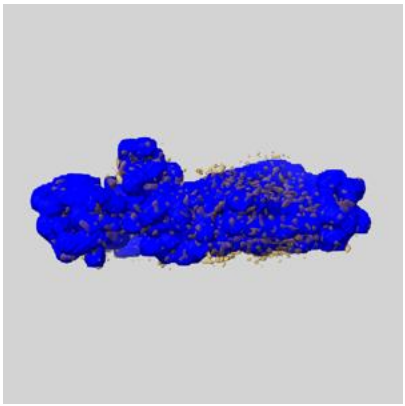
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

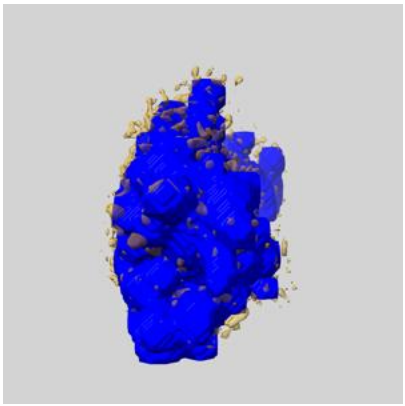
6.6.1 emd_4973_msk_1.map (i)



X



Y

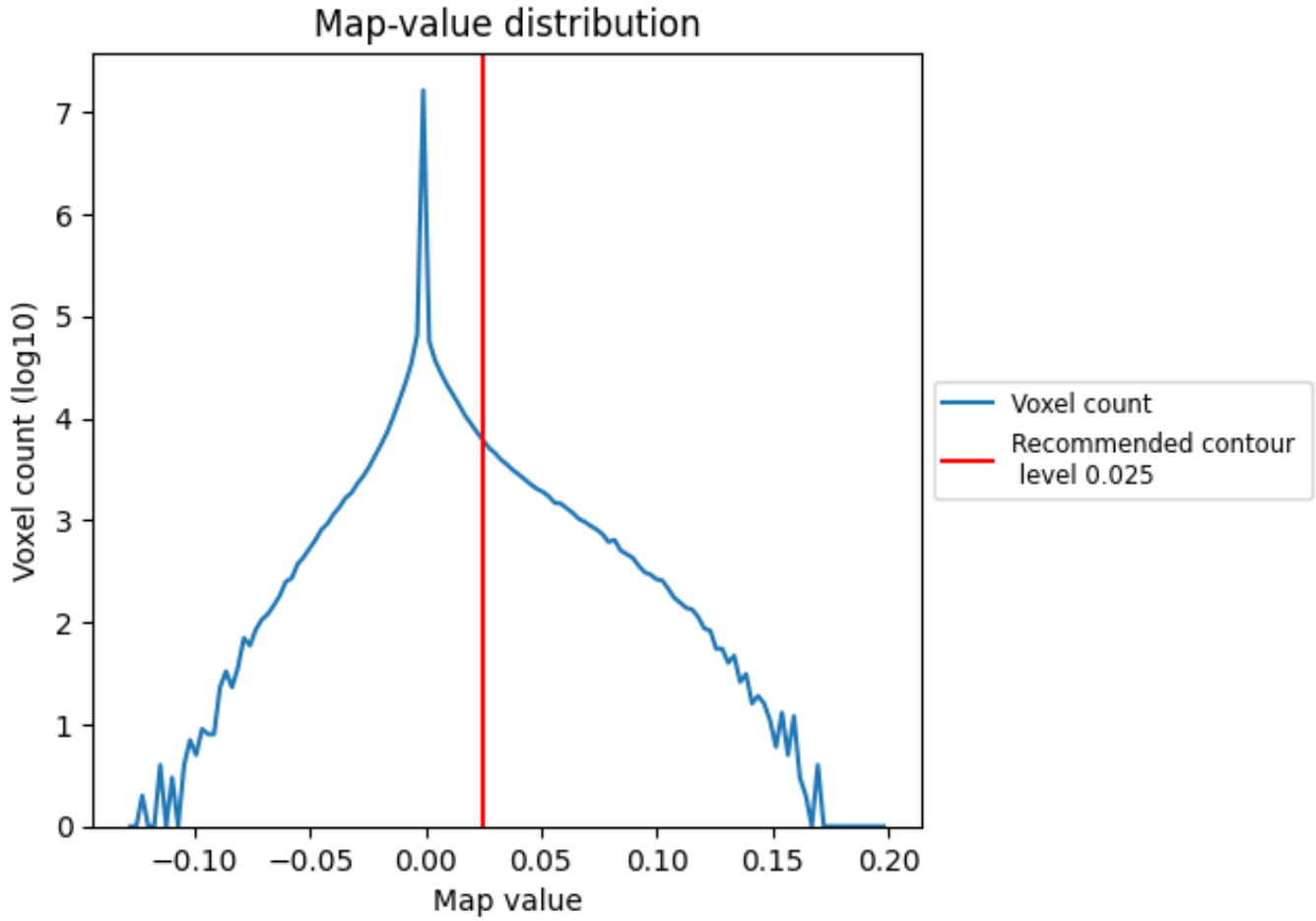


Z

7 Map analysis

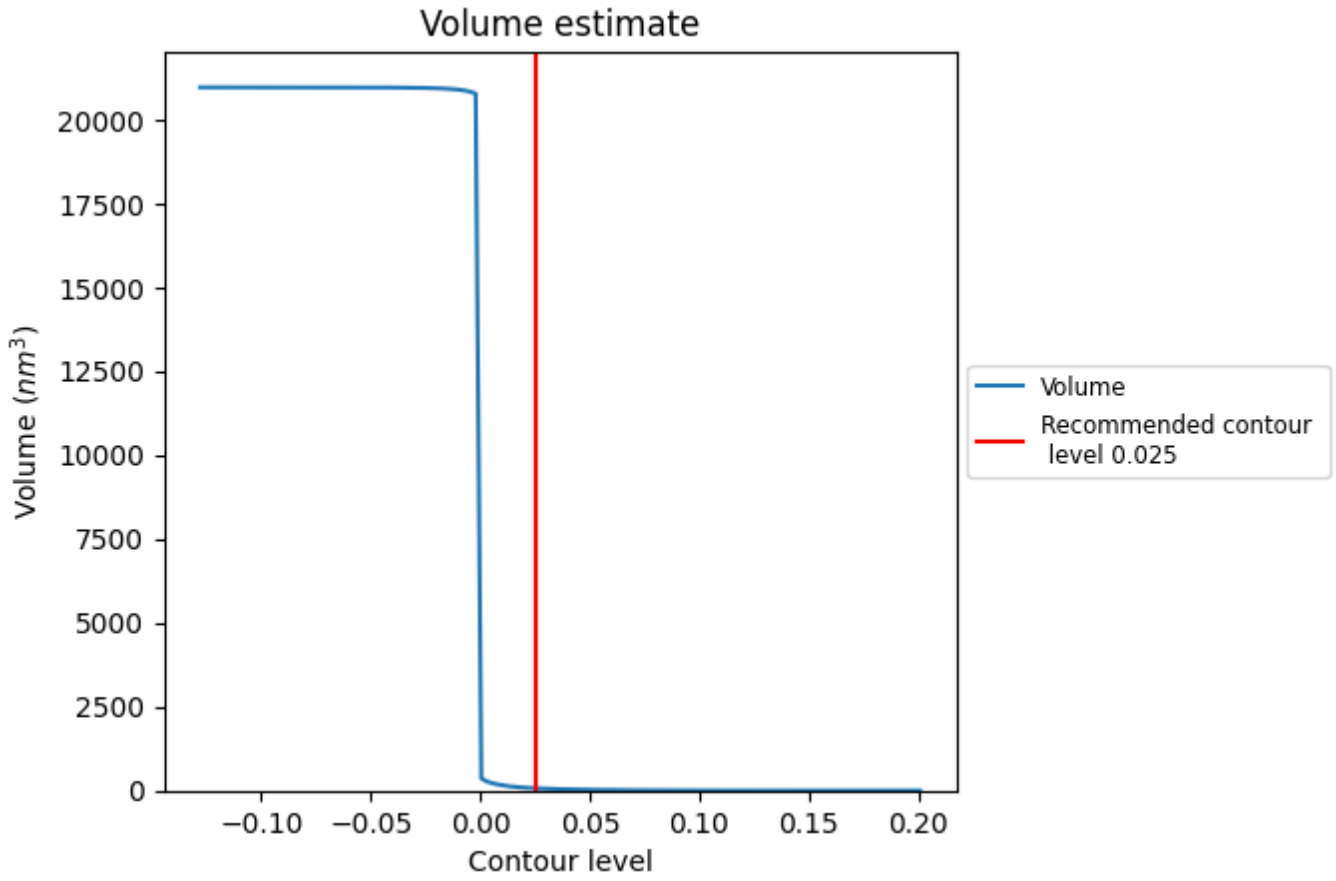
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

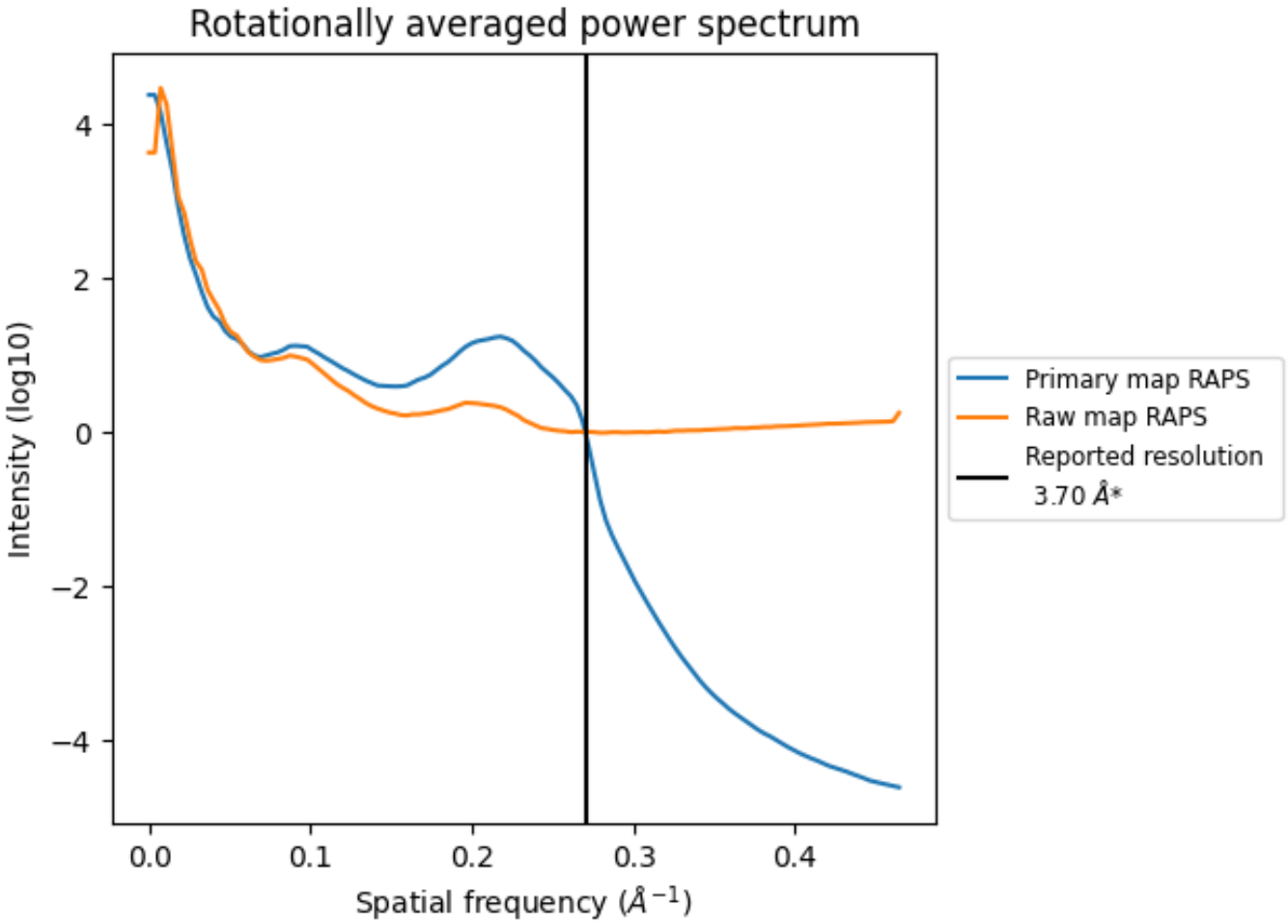
7.2 Volume estimate (i)



The volume at the recommended contour level is 68 nm^3; this corresponds to an approximate mass of 62 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)

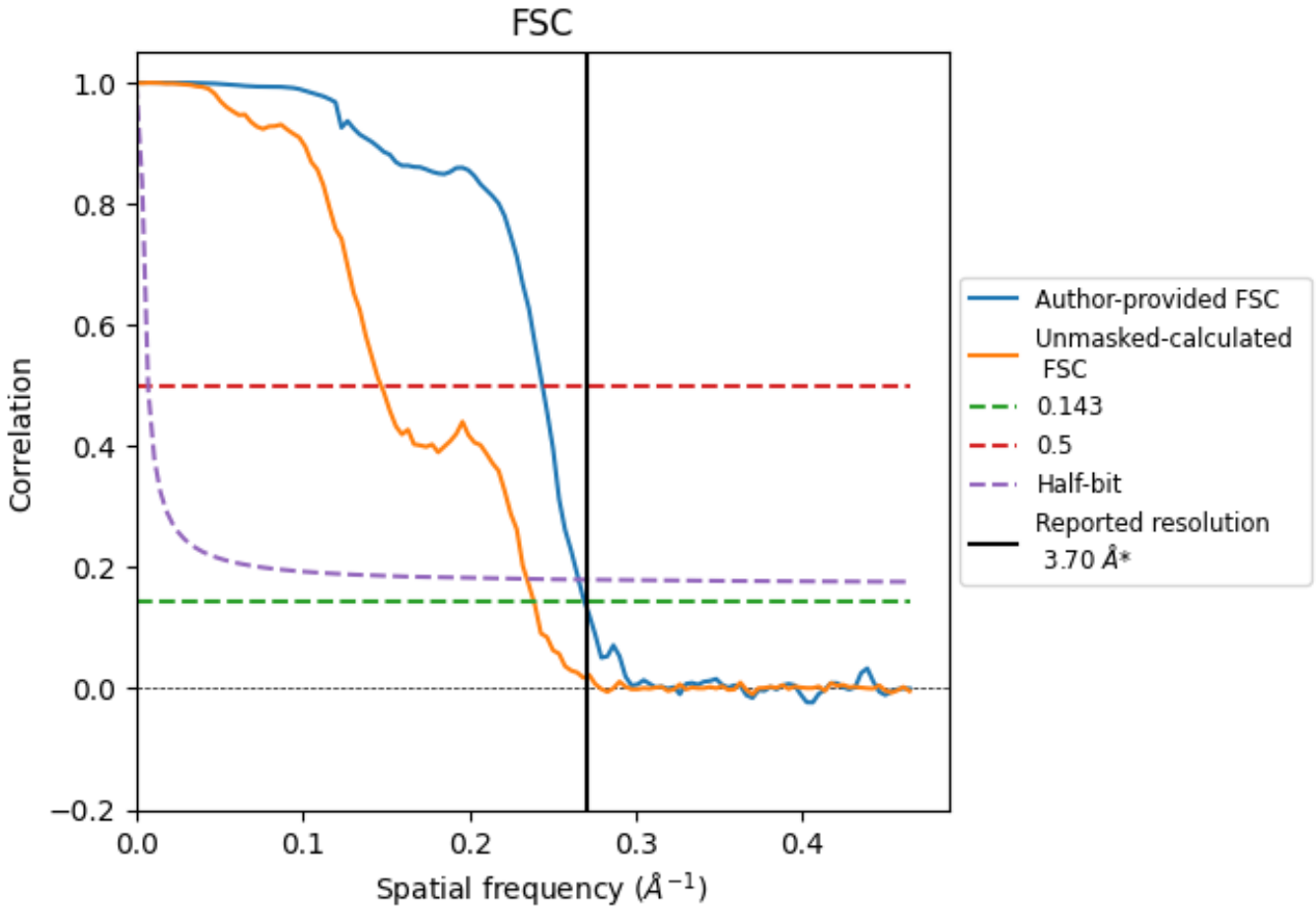


*Reported resolution corresponds to spatial frequency of 0.270 $Å^{-1}$

8 Fourier-Shell correlation

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



*Reported resolution corresponds to spatial frequency of 0.270 Å^{-1}

8.2 Resolution estimates (i)

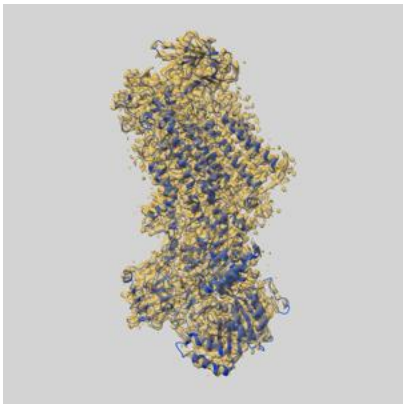
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.70	-	-
Author-provided FSC curve	3.71	4.10	3.77
Unmasked-calculated*	4.19	6.80	4.26

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.19 differs from the reported value 3.7 by more than 10 %

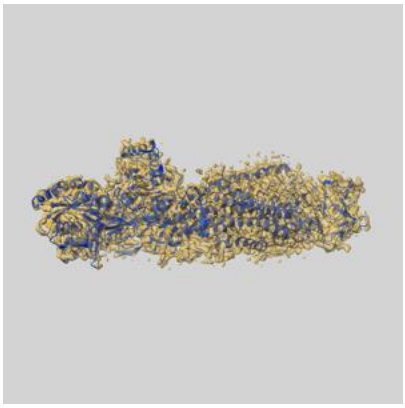
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-4973 and PDB model 6ROI. Per-residue inclusion information can be found in section 3 on page 9.

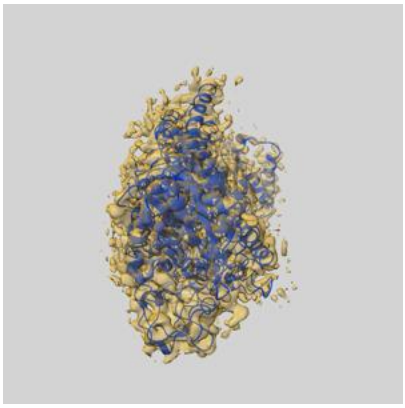
9.1 Map-model overlay



X



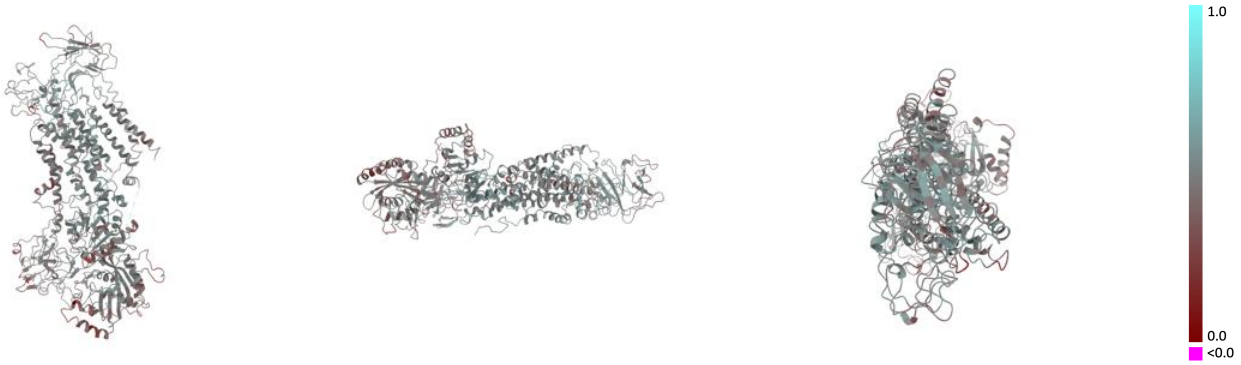
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.025 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.

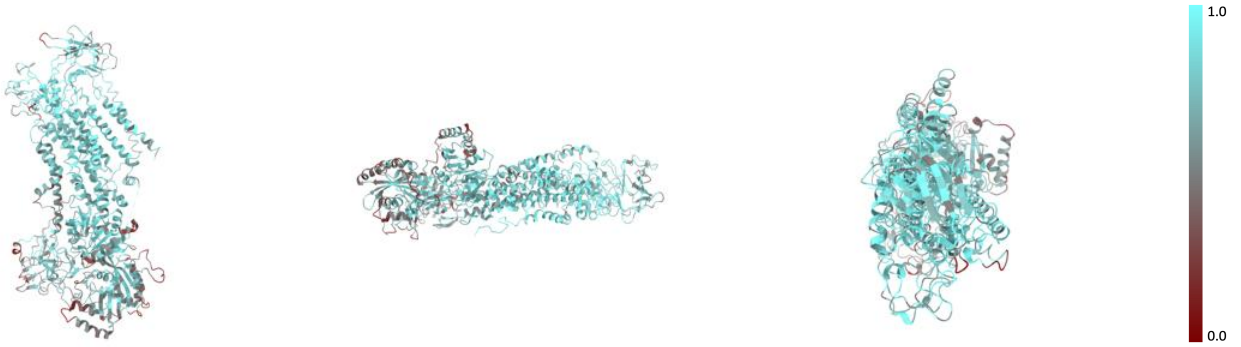
9.2 Q-score mapped to coordinate model (i)



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.

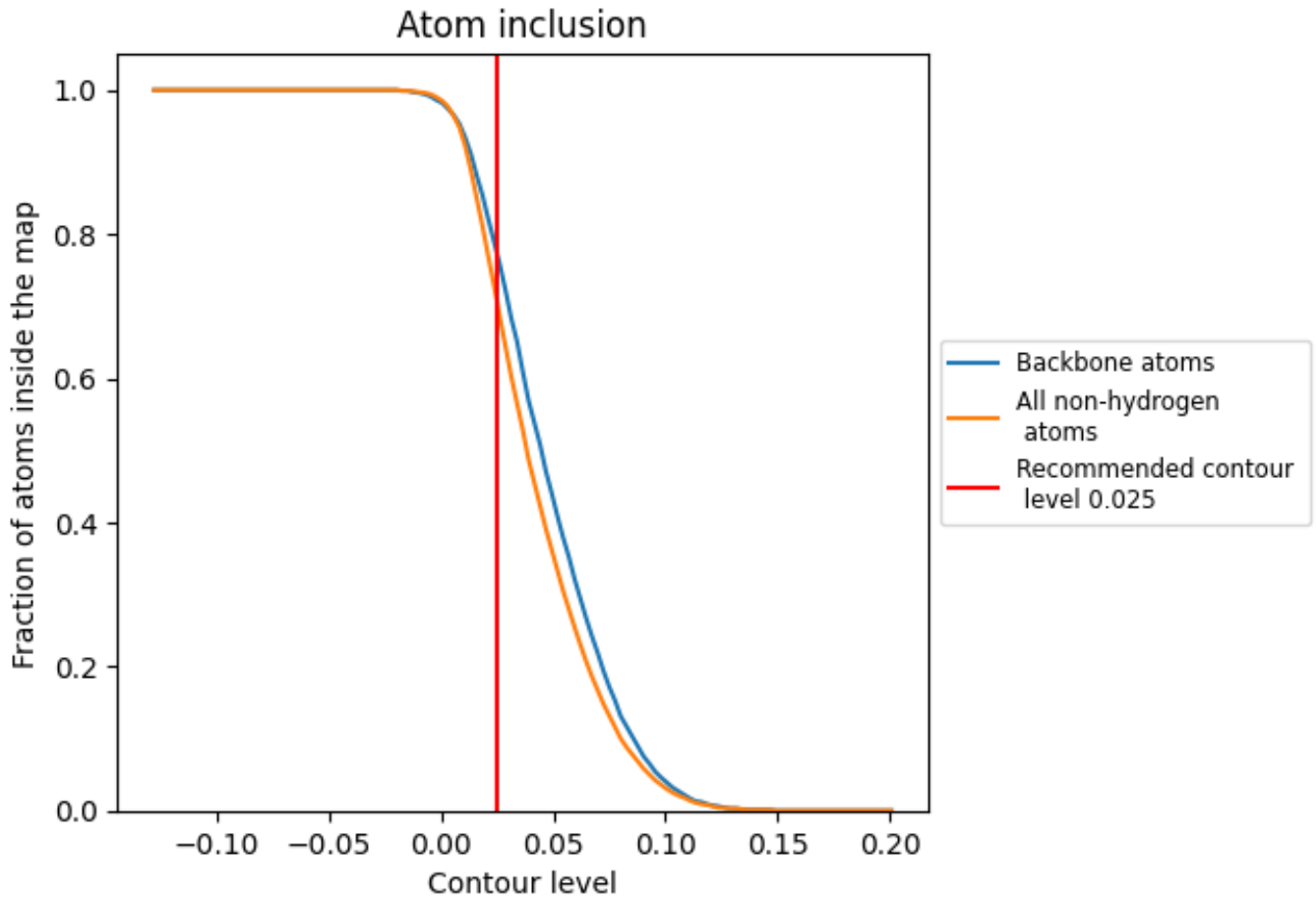
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.025).

9.4 Atom inclusion (i)



At the recommended contour level, 77% of all backbone atoms, 71% 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 (0.025) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7070	0.4720
A	0.6930	0.4670
B	0.5000	0.4220
C	0.7620	0.4860
D	0.6400	0.4800