wwPDB EM Validation Summary Report (i)

Aug 27, 2026 – 09:57 am BST

PDB ID	:	7OH5 / pdb_00007oh5
EMDB ID	:	EMD-12894
Title	:	Cryo-EM structure of Drs2p-Cdc50p in the E1-AlFx-ADP state
Authors	:	Timcenko, M.; Dieudonne, T.; Montigny, C.; Boesen, T.; Lyons, J.A.; Lenoir, G.; Nissen, P.
Deposited on	:	2021-05-09
Resolution	:	2.90 Å(reported)
Based on initial model	:	6ROJ

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 (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:

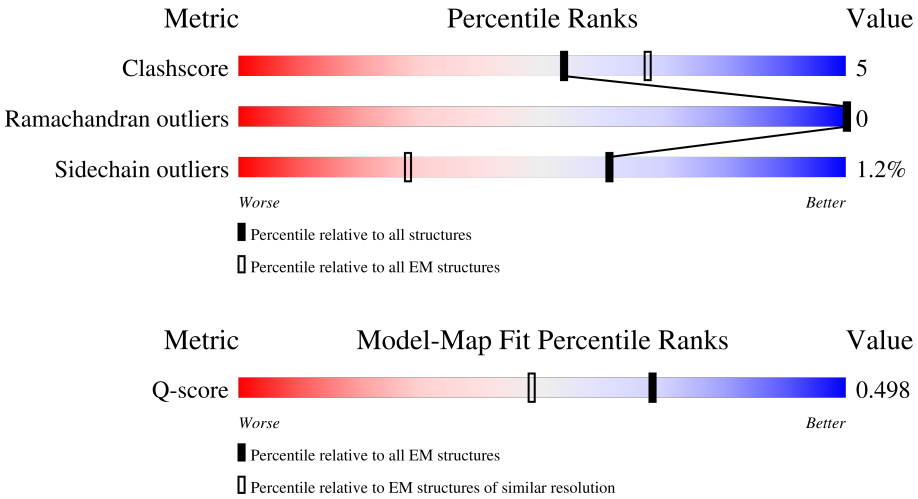
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

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 2.90 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	13054 (2.40 - 3.40)

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	1465	10% 61% 11% 27%
2	C	413	5% 75% 10% 14%
3	B	2	50% 50%
3	D	2	50% 100%

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Mol	Chain	Length	Quality of chain
4	E	4	50% 50%

2 Entry composition (i)

There are 10 unique types of molecules in this entry. The entry contains 11603 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,Probable p hospholipid-transporting ATPase DRS2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1064	Total	C	N	O	S	0	0
			8504	5499	1381	1588	36		

There are 110 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1247	SER	-	linker	UNP P39524
A	1248	LEU	-	linker	UNP P39524
A	1249	VAL	-	linker	UNP P39524
A	1250	PRO	-	linker	UNP P39524
A	1251	ARG	-	linker	UNP P39524
A	1252	GLY	-	linker	UNP P39524
A	1362	GLY	-	expression tag	UNP P39524
A	1363	GLY	-	expression tag	UNP P39524
A	1364	GLY	-	expression tag	UNP P39524
A	1365	GLY	-	expression tag	UNP P39524
A	1366	LEU	-	expression tag	UNP P39524
A	1367	VAL	-	expression tag	UNP P39524
A	1368	PRO	-	expression tag	UNP P39524
A	1369	ARG	-	expression tag	UNP P39524
A	1370	GLY	-	expression tag	UNP P39524
A	1371	SER	-	expression tag	UNP P39524
A	1372	GLY	-	expression tag	UNP P39524
A	1373	GLY	-	expression tag	UNP P39524
A	1374	THR	-	expression tag	UNP P39524
A	1375	ALA	-	expression tag	UNP P39524
A	1376	ALA	-	expression tag	UNP P39524
A	1377	ALA	-	expression tag	UNP P39524
A	1378	PRO	-	expression tag	UNP P39524
A	1379	GLY	-	expression tag	UNP P39524
A	1380	PRO	-	expression tag	UNP P39524
A	1381	ALA	-	expression tag	UNP P39524
A	1382	PRO	-	expression tag	UNP P39524

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1383	ALA	-	expression tag	UNP P39524
A	1384	PRO	-	expression tag	UNP P39524
A	1385	ALA	-	expression tag	UNP P39524
A	1386	PRO	-	expression tag	UNP P39524
A	1387	ALA	-	expression tag	UNP P39524
A	1388	SER	-	expression tag	UNP P39524
A	1389	ALA	-	expression tag	UNP P39524
A	1390	PRO	-	expression tag	UNP P39524
A	1391	ALA	-	expression tag	UNP P39524
A	1392	ALA	-	expression tag	UNP P39524
A	1393	ALA	-	expression tag	UNP P39524
A	1394	ALA	-	expression tag	UNP P39524
A	1395	PRO	-	expression tag	UNP P39524
A	1396	ALA	-	expression tag	UNP P39524
A	1397	GLY	-	expression tag	UNP P39524
A	1398	ALA	-	expression tag	UNP P39524
A	1399	GLY	-	expression tag	UNP P39524
A	1400	THR	-	expression tag	UNP P39524
A	1401	PRO	-	expression tag	UNP P39524
A	1402	VAL	-	expression tag	UNP P39524
A	1403	THR	-	expression tag	UNP P39524
A	1404	ALA	-	expression tag	UNP P39524
A	1405	PRO	-	expression tag	UNP P39524
A	1406	LEU	-	expression tag	UNP P39524
A	1407	ALA	-	expression tag	UNP P39524
A	1408	GLY	-	expression tag	UNP P39524
A	1409	THR	-	expression tag	UNP P39524
A	1410	ILE	-	expression tag	UNP P39524
A	1411	TRP	-	expression tag	UNP P39524
A	1412	LYS	-	expression tag	UNP P39524
A	1413	VAL	-	expression tag	UNP P39524
A	1414	LEU	-	expression tag	UNP P39524
A	1415	ALA	-	expression tag	UNP P39524
A	1416	SER	-	expression tag	UNP P39524
A	1417	GLU	-	expression tag	UNP P39524
A	1418	GLY	-	expression tag	UNP P39524
A	1419	GLN	-	expression tag	UNP P39524
A	1420	THR	-	expression tag	UNP P39524
A	1421	VAL	-	expression tag	UNP P39524
A	1422	ALA	-	expression tag	UNP P39524
A	1423	ALA	-	expression tag	UNP P39524
A	1424	GLY	-	expression tag	UNP P39524

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1425	GLU	-	expression tag	UNP P39524
A	1426	VAL	-	expression tag	UNP P39524
A	1427	LEU	-	expression tag	UNP P39524
A	1428	LEU	-	expression tag	UNP P39524
A	1429	ILE	-	expression tag	UNP P39524
A	1430	LEU	-	expression tag	UNP P39524
A	1431	GLU	-	expression tag	UNP P39524
A	1432	ALA	-	expression tag	UNP P39524
A	1433	MET	-	expression tag	UNP P39524
A	1434	LYS	-	expression tag	UNP P39524
A	1435	MET	-	expression tag	UNP P39524
A	1436	GLU	-	expression tag	UNP P39524
A	1437	THR	-	expression tag	UNP P39524
A	1438	GLU	-	expression tag	UNP P39524
A	1439	ILE	-	expression tag	UNP P39524
A	1440	ARG	-	expression tag	UNP P39524
A	1441	ALA	-	expression tag	UNP P39524
A	1442	ALA	-	expression tag	UNP P39524
A	1443	GLN	-	expression tag	UNP P39524
A	1444	ALA	-	expression tag	UNP P39524
A	1445	GLY	-	expression tag	UNP P39524
A	1446	THR	-	expression tag	UNP P39524
A	1447	VAL	-	expression tag	UNP P39524
A	1448	ARG	-	expression tag	UNP P39524
A	1449	GLY	-	expression tag	UNP P39524
A	1450	ILE	-	expression tag	UNP P39524
A	1451	ALA	-	expression tag	UNP P39524
A	1452	VAL	-	expression tag	UNP P39524
A	1453	LYS	-	expression tag	UNP P39524
A	1454	ALA	-	expression tag	UNP P39524
A	1455	GLY	-	expression tag	UNP P39524
A	1456	ASP	-	expression tag	UNP P39524
A	1457	ALA	-	expression tag	UNP P39524
A	1458	VAL	-	expression tag	UNP P39524
A	1459	ALA	-	expression tag	UNP P39524
A	1460	VAL	-	expression tag	UNP P39524
A	1461	GLY	-	expression tag	UNP P39524
A	1462	ASP	-	expression tag	UNP P39524
A	1463	THR	-	expression tag	UNP P39524
A	1464	LEU	-	expression tag	UNP P39524
A	1465	MET	-	expression tag	UNP P39524

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	355	Total	C	N	O	S	0	0
			2878	1860	477	529	12		

There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	392	GLY	-	expression tag	UNP A0A6L0Z5H3
C	393	GLY	-	expression tag	UNP A0A6L0Z5H3
C	394	GLY	-	expression tag	UNP A0A6L0Z5H3
C	395	GLY	-	expression tag	UNP A0A6L0Z5H3
C	396	LEU	-	expression tag	UNP A0A6L0Z5H3
C	397	VAL	-	expression tag	UNP A0A6L0Z5H3
C	398	PRO	-	expression tag	UNP A0A6L0Z5H3
C	399	ARG	-	expression tag	UNP A0A6L0Z5H3
C	400	GLY	-	expression tag	UNP A0A6L0Z5H3
C	401	SER	-	expression tag	UNP A0A6L0Z5H3
C	402	GLY	-	expression tag	UNP A0A6L0Z5H3
C	403	GLY	-	expression tag	UNP A0A6L0Z5H3
C	404	HIS	-	expression tag	UNP A0A6L0Z5H3
C	405	HIS	-	expression tag	UNP A0A6L0Z5H3
C	406	HIS	-	expression tag	UNP A0A6L0Z5H3
C	407	HIS	-	expression tag	UNP A0A6L0Z5H3
C	408	HIS	-	expression tag	UNP A0A6L0Z5H3
C	409	HIS	-	expression tag	UNP A0A6L0Z5H3
C	410	HIS	-	expression tag	UNP A0A6L0Z5H3
C	411	HIS	-	expression tag	UNP A0A6L0Z5H3
C	412	HIS	-	expression tag	UNP A0A6L0Z5H3
C	413	HIS	-	expression tag	UNP A0A6L0Z5H3

- 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
3	B	2	Total	C	N	O	0	0
			28	16	2	10		
3	D	2	Total	C	N	O	0	0
			28	16	2	10		

- 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.

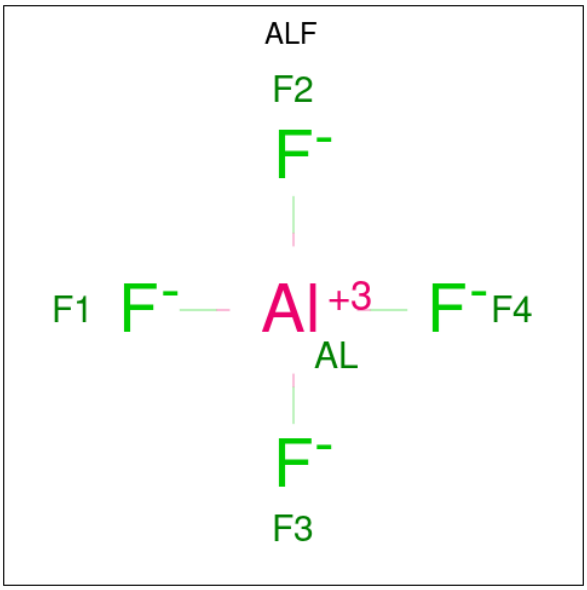


Mol	Chain	Residues	Atoms				AltConf	Trace
4	E	4	Total	C	N	O	0	0
			50	28	2	20		

- Molecule 5 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

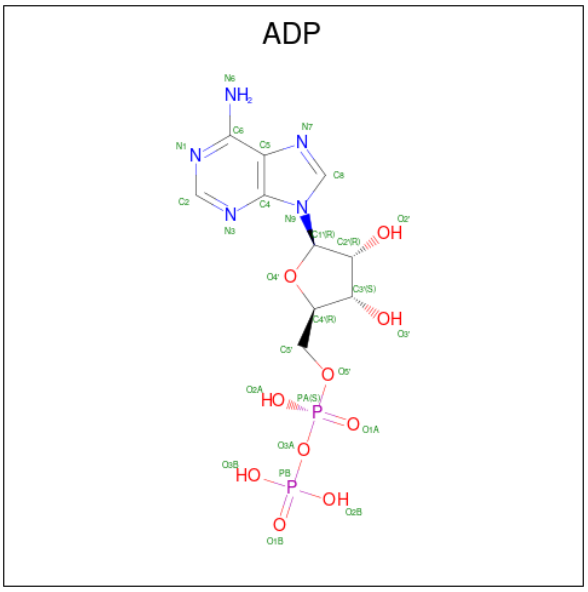
Mol	Chain	Residues	Atoms		AltConf
5	A	2	Total	Mg	0
			2	2	

- Molecule 6 is TETRAFLUOROALUMINATE ION (CCD ID: ALF) (formula: AlF_4).



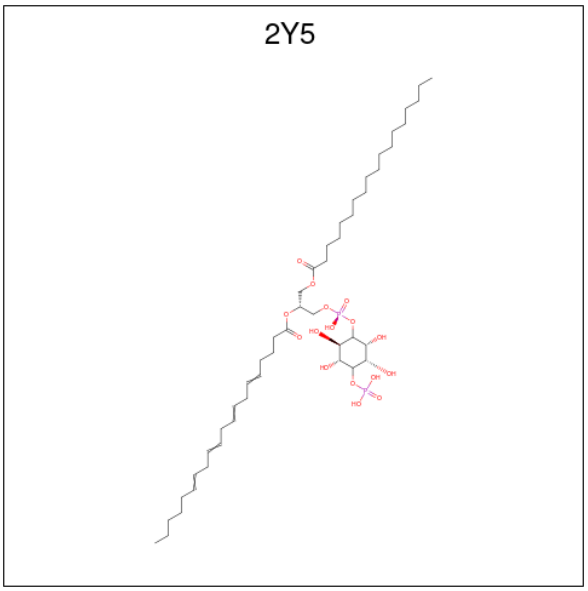
Mol	Chain	Residues	Atoms			AltConf
6	A	1	Total	Al	F	0
			5	1	4	

- Molecule 7 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



Mol	Chain	Residues	Atoms					AltConf
7	A	1	Total	C	N	O	P	0
			27	10	5	10	2	

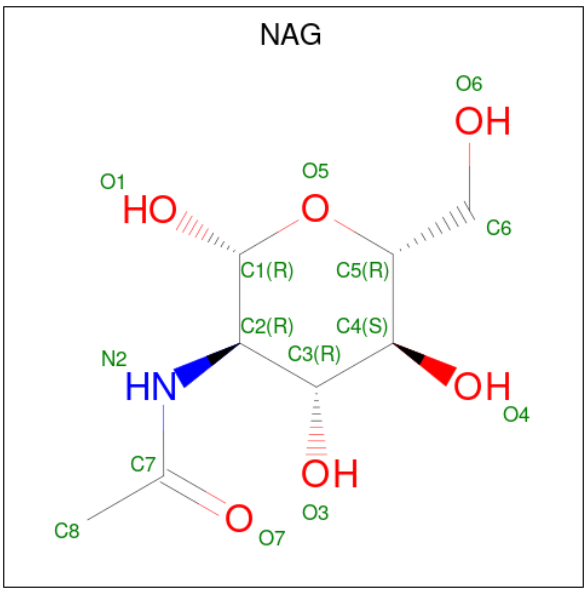
- Molecule 8 is (2R)-1-{[(R)-hydroxy{[(1R,2R,3R,4R,5S,6R)-2,3,5,6-tetrahydroxy-4-(phosphonooxy)cyclohexyl]oxy}phosphoryl]oxy}-3-(octadecanoyloxy)propan-2-yl (5Z,8Z,11Z,14Z)-icosa-5,8,11,14-tetraenoate (CCD ID: 2Y5) (formula: $C_{47}H_{84}O_{16}P_2$).



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

- Molecule 9 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula:

$C_8H_{15}NO_6$).



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

- Molecule 10 is water.

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

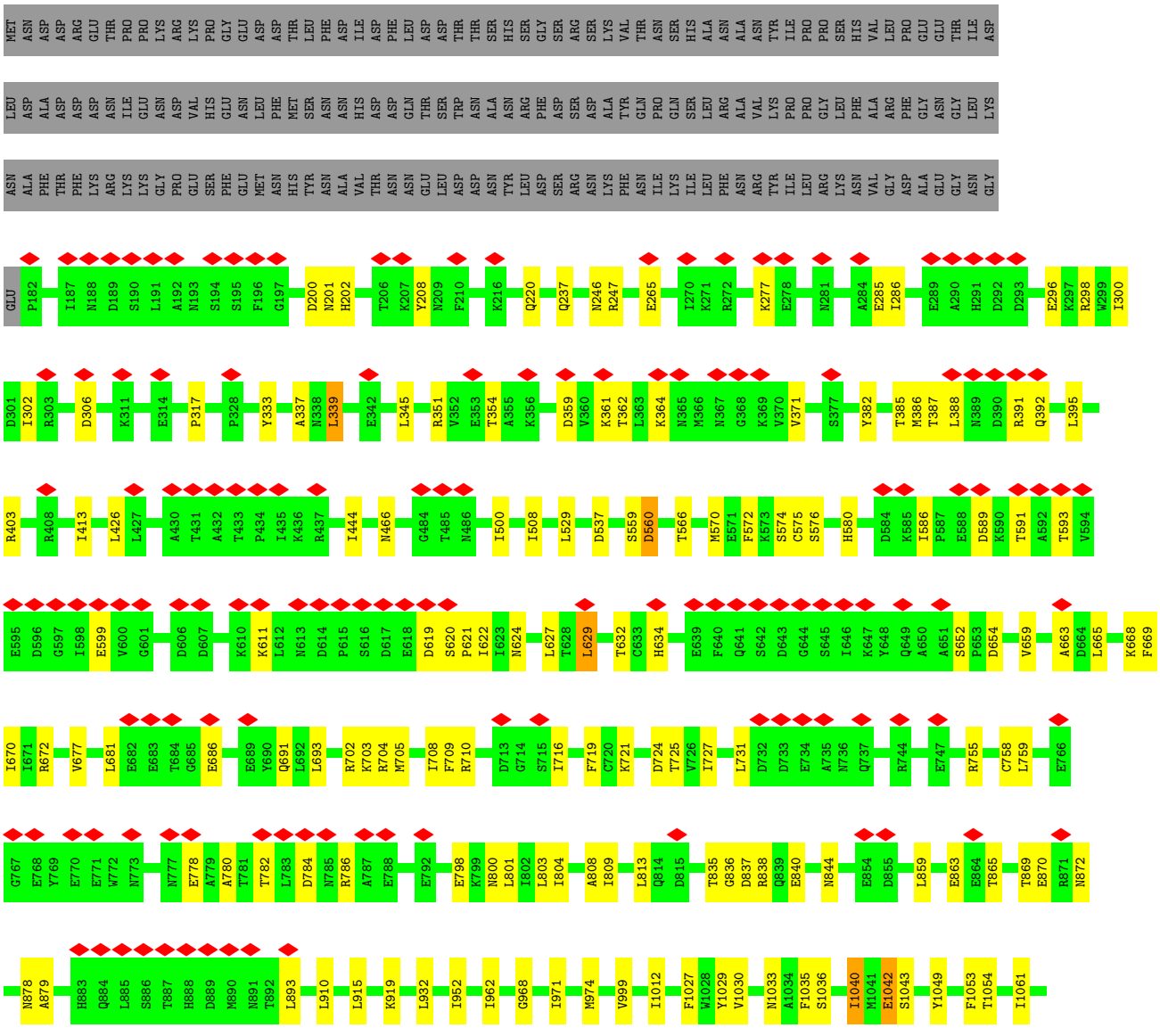
3 Residue-property plots (i)

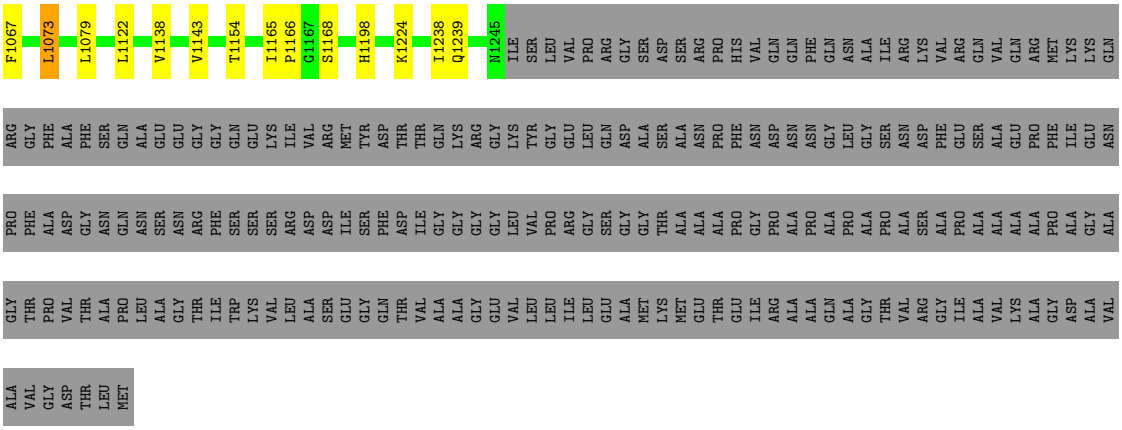
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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,Probable phospholipid-transporting ATPase DRS2

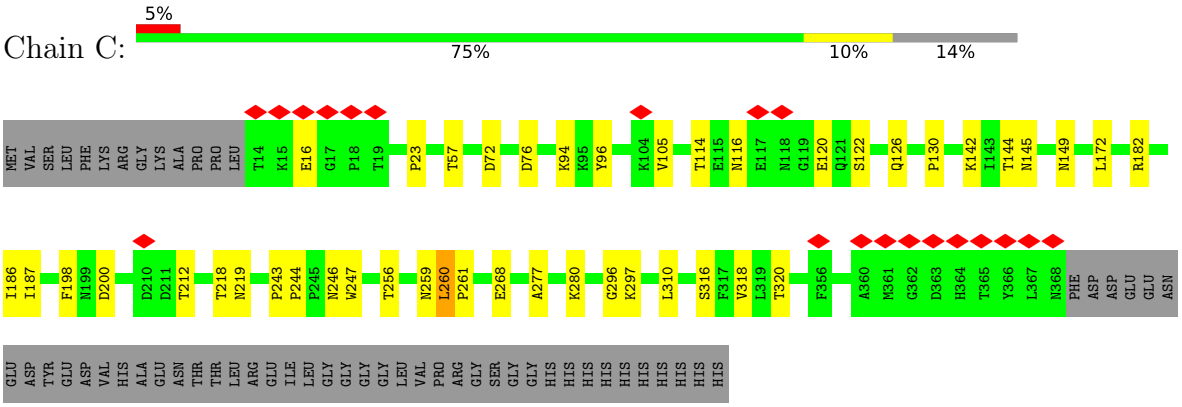
Chain A:







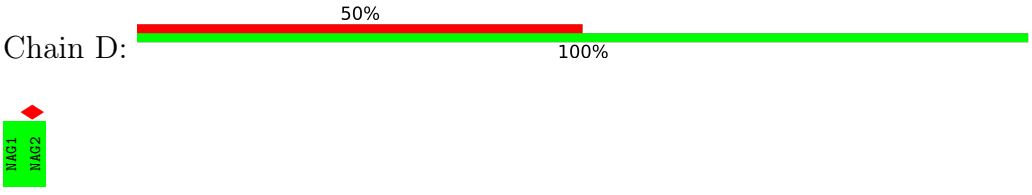
• Molecule 2: Cell division control protein 50



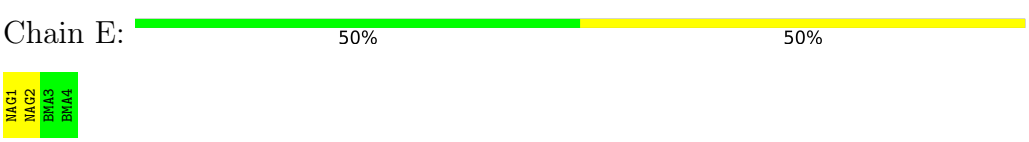
• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



• Molecule 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	256001	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	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 K3 (6k x 4k)	Depositor
Maximum map value	1.429	Depositor
Minimum map value	-0.840	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.033	Depositor
Recommended contour level	0.21	Depositor
Map size (Å)	263.9872, 263.9872, 263.9872	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.0312, 1.0312, 1.0312	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ALF, BMA, 2Y5, NAG, ADP, MG

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	0.09	0/8692	0.26	0/11790
2	C	0.09	0/2955	0.27	0/4007
All	All	0.09	0/11647	0.26	0/15797

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

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	8504	0	8516	95	0
2	C	2878	0	2865	25	0
3	B	28	0	25	1	0
3	D	28	0	25	0	0
4	E	50	0	43	2	0
5	A	2	0	0	0	0
6	A	5	0	0	0	0
7	A	27	0	12	1	0
8	A	65	0	81	2	0
9	C	14	0	13	0	0
10	A	2	0	0	0	0
All	All	11603	0	11580	120	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 120 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:708:ILE:HD11	1:A:716:ILE:HG22	1.68	0.74
1:A:835:THR:HG22	1:A:837:ASP:H	1.58	0.68
2:C:142:LYS:HB3	2:C:316:SER:HB2	1.77	0.65
1:A:870:GLU:HG2	1:A:910:LEU:HD21	1.78	0.65
1:A:580:HIS:ND1	1:A:599:GLU:OE1	2.32	0.62

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	1062/1465 (72%)	1020 (96%)	42 (4%)	0	100	100
2	C	353/413 (86%)	330 (94%)	23 (6%)	0	100	100
All	All	1415/1878 (75%)	1350 (95%)	65 (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	935/1257 (74%)	923 (99%)	12 (1%)	61	86
2	C	322/370 (87%)	319 (99%)	3 (1%)	70	90
All	All	1257/1627 (77%)	1242 (99%)	15 (1%)	61	86

5 of 15 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	725	THR
2	C	57	THR
1	A	865	THR
2	C	260	LEU
1	A	1073	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 6 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1038	GLN
2	C	305	ASN
2	C	368	ASN
1	A	486	ASN
1	A	193	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)

8 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	0.23	0	17,19,21	0.45	0
3	NAG	B	2	3	14,14,15	0.24	0	17,19,21	0.41	0
3	NAG	D	1	2,3	14,14,15	0.25	0	17,19,21	0.43	0
3	NAG	D	2	3	14,14,15	0.24	0	17,19,21	0.42	0
4	NAG	E	1	2,4	14,14,15	0.23	0	17,19,21	0.39	0
4	NAG	E	2	4	14,14,15	0.21	0	17,19,21	0.55	0
4	BMA	E	3	4	11,11,12	0.54	0	15,15,17	0.74	0
4	BMA	E	4	4	11,11,12	0.61	0	15,15,17	0.75	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
3	NAG	B	1	2,3	-	3/6/23/26	0/1/1/1
3	NAG	B	2	3	-	2/6/23/26	0/1/1/1
3	NAG	D	1	2,3	-	1/6/23/26	0/1/1/1
3	NAG	D	2	3	-	1/6/23/26	0/1/1/1
4	NAG	E	1	2,4	-	0/6/23/26	0/1/1/1
4	NAG	E	2	4	-	2/6/23/26	0/1/1/1
4	BMA	E	3	4	-	0/2/19/22	0/1/1/1
4	BMA	E	4	4	-	2/2/19/22	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 11 torsion outliers are listed below:

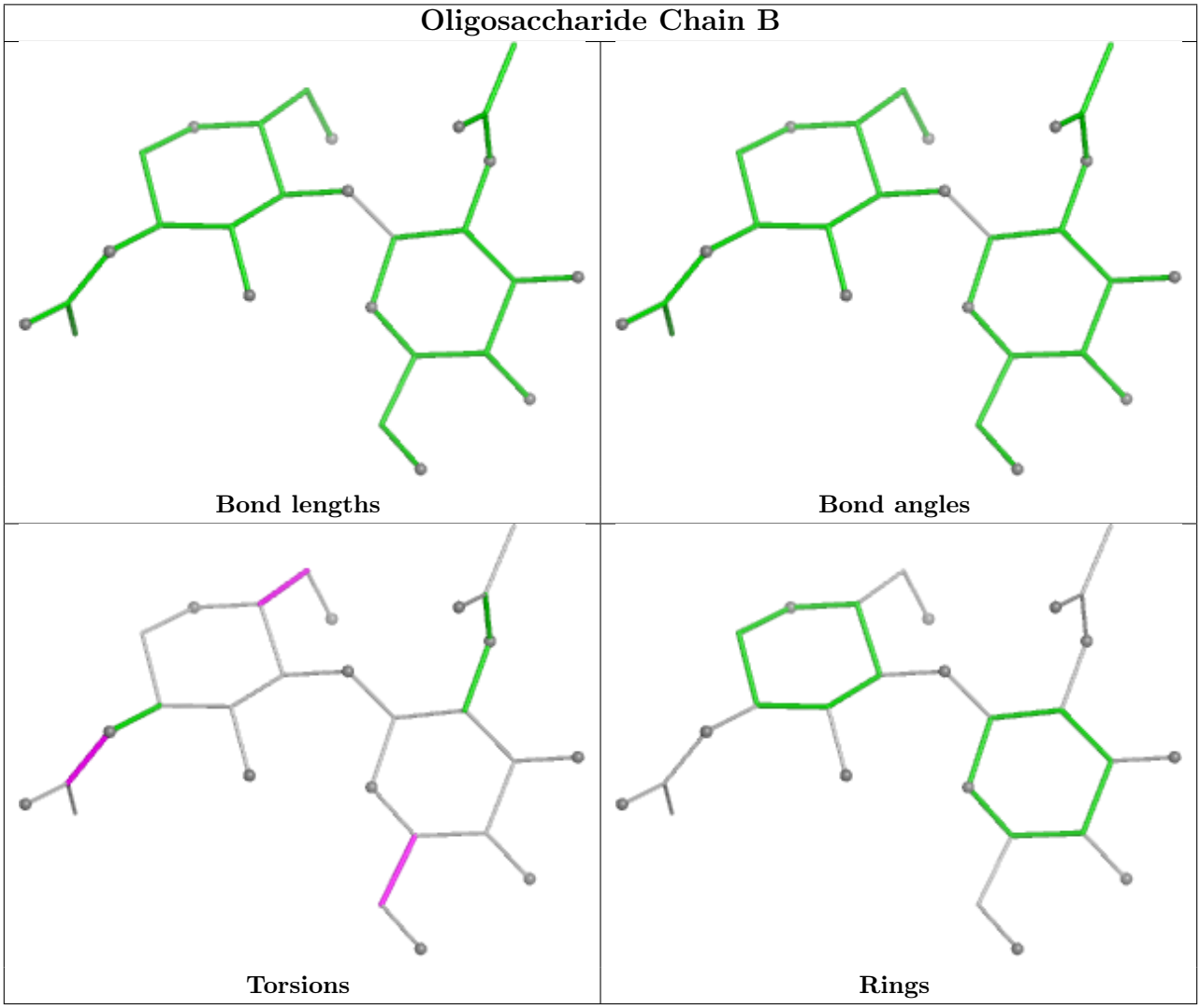
Mol	Chain	Res	Type	Atoms
3	B	2	NAG	C4-C5-C6-O6
3	B	2	NAG	O5-C5-C6-O6
3	B	1	NAG	C8-C7-N2-C2
3	B	1	NAG	O7-C7-N2-C2
4	E	2	NAG	C3-C2-N2-C7

There are no ring outliers.

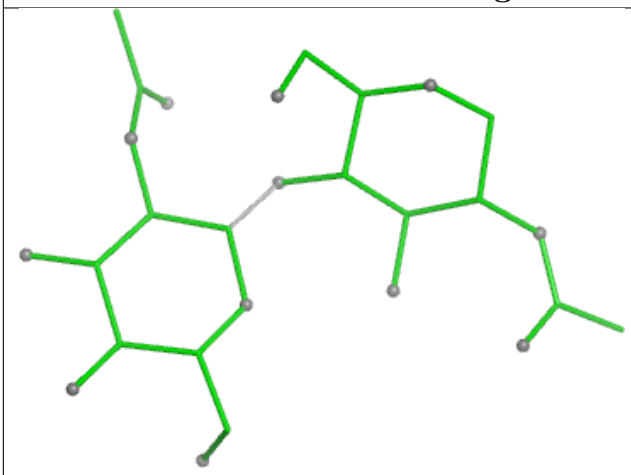
3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	1	NAG	1	0
4	E	2	NAG	1	0
4	E	1	NAG	1	0

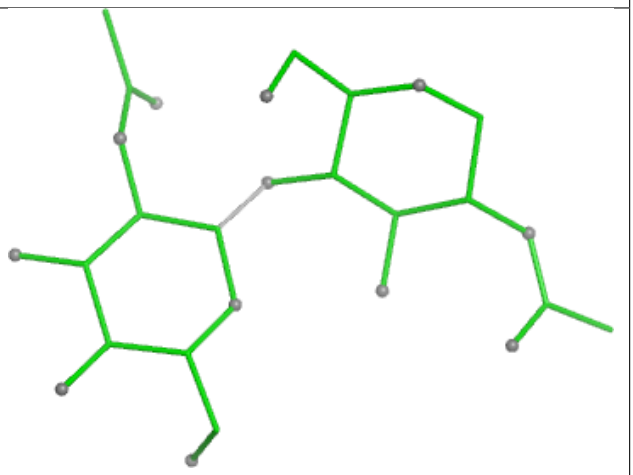
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.



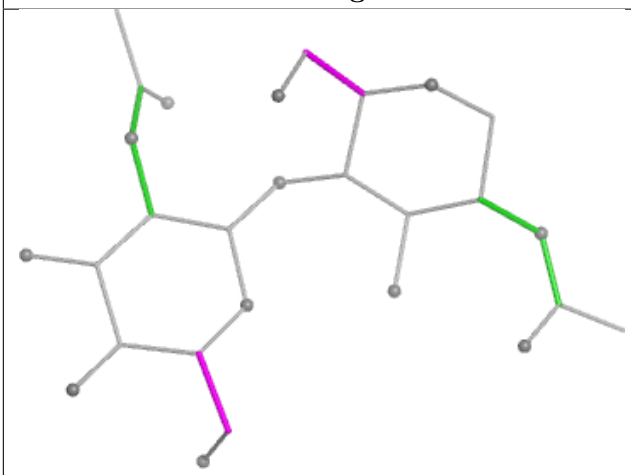
Oligosaccharide Chain D



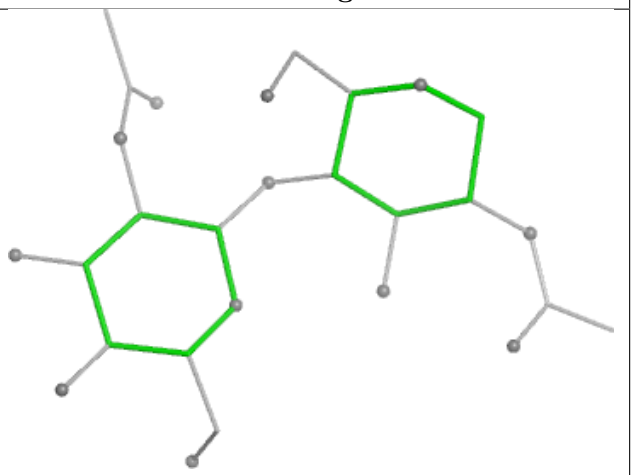
Bond lengths



Bond angles

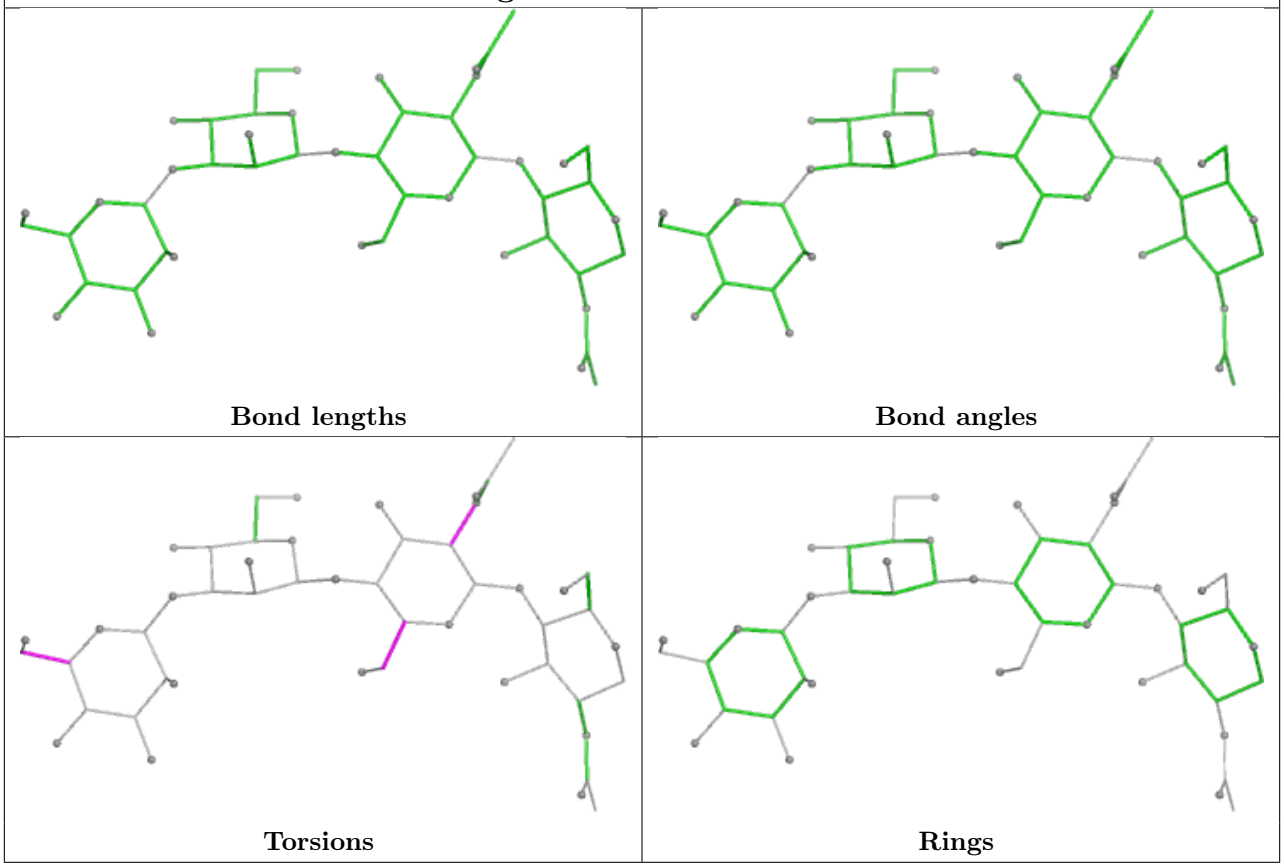


Torsions



Rings

Oligosaccharide Chain E



5.6 Ligand geometry (i)

Of 6 ligands modelled in this entry, 2 are monoatomic - leaving 4 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	ADP	A	1504	5,6	27,29,29	3.41	10 (37%)	42,45,45	2.41	14 (33%)
6	ALF	A	1502	7,1	0,4,4	-	-	-		
8	2Y5	A	1505	-	65,65,65	0.93	5 (7%)	77,80,80	1.07	5 (6%)
9	NAG	C	501	2	14,14,15	0.90	1 (7%)	17,19,21	1.31	1 (5%)

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	ADP	A	1504	5,6	-	7/16/32/32	0/3/3/3
8	2Y5	A	1505	-	-	26/61/85/85	0/1/1/1
9	NAG	C	501	2	-	2/6/23/26	0/1/1/1

The worst 5 of 16 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	1504	ADP	C3'-C4'	-9.70	1.28	1.53
7	A	1504	ADP	C2'-C1'	-7.70	1.28	1.53
7	A	1504	ADP	C6-N6	6.17	1.49	1.34
7	A	1504	ADP	O4'-C1'	5.48	1.55	1.42
7	A	1504	ADP	O4'-C4'	5.19	1.56	1.45

The worst 5 of 20 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	A	1504	ADP	N9-C8-N7	-5.75	106.05	113.91
7	A	1504	ADP	N3-C2-N1	-5.46	120.06	128.60
9	C	501	NAG	C1-O5-C5	4.98	118.93	112.19
7	A	1504	ADP	C4-N9-C1'	-4.90	114.93	126.59
7	A	1504	ADP	C5-C4-N3	-4.78	120.51	126.75

There are no chirality outliers.

5 of 35 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	1504	ADP	C5'-O5'-PA-O1A
7	A	1504	ADP	C5'-O5'-PA-O2A
8	A	1505	2Y5	C2-C1-O1-P1
8	A	1505	2Y5	C3-C4-O4-P4
8	A	1505	2Y5	C5-C4-O4-P4

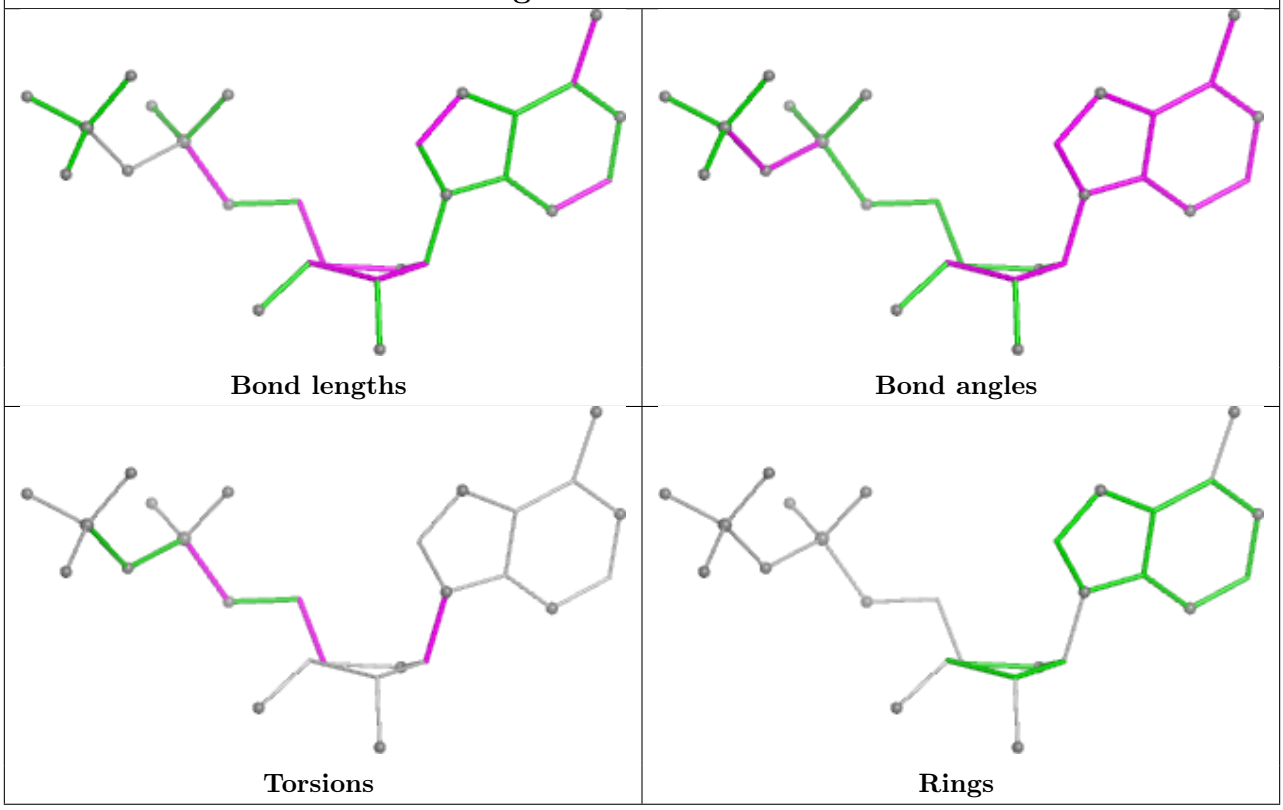
There are no ring outliers.

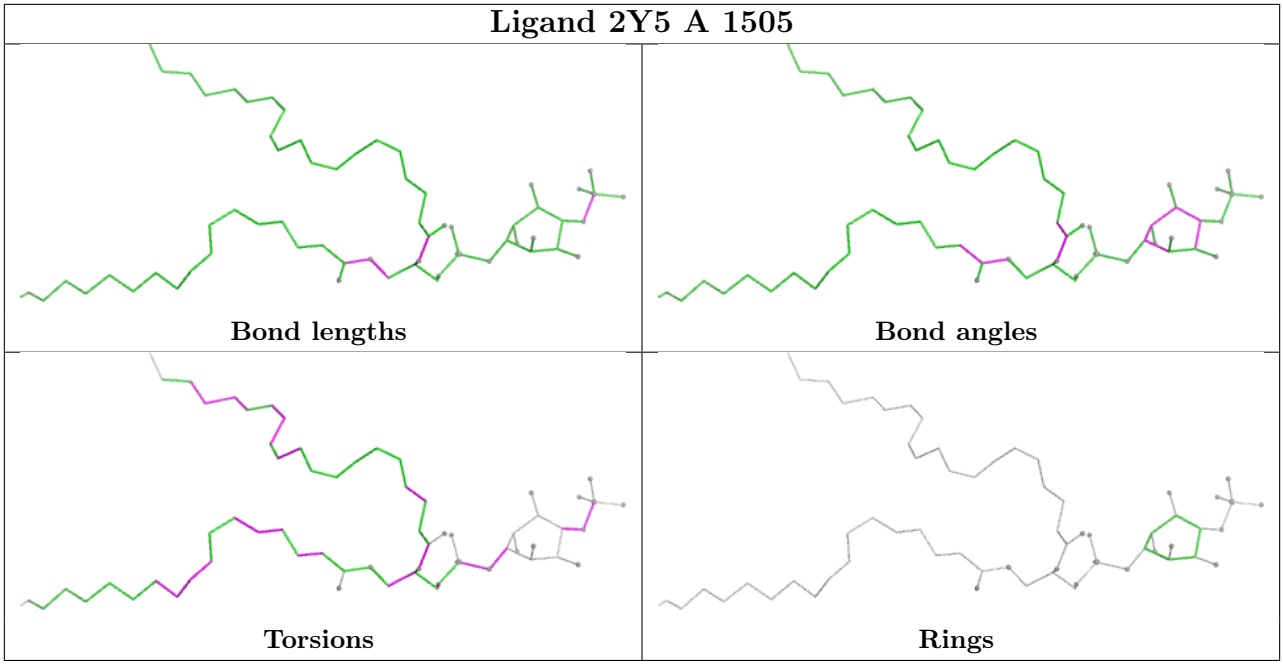
2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	1504	ADP	1	0
8	A	1505	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 ADP A 1504





5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

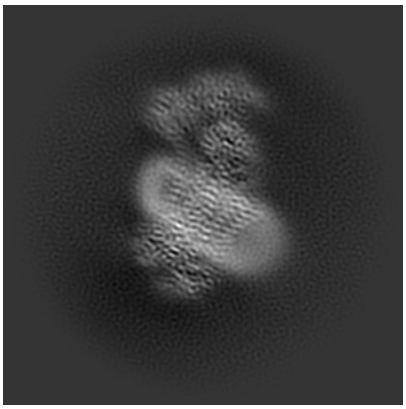
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-12894. These allow visual inspection of the internal detail of the map and identification of artifacts.

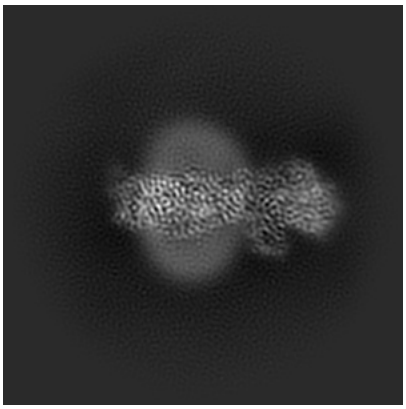
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

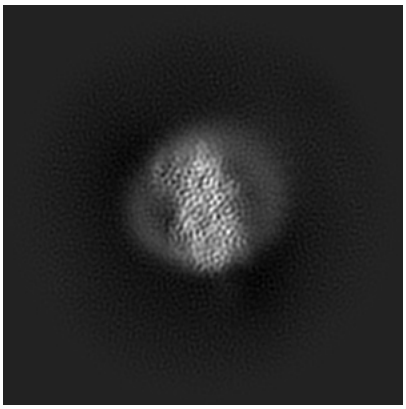
6.1.1 Primary map



X

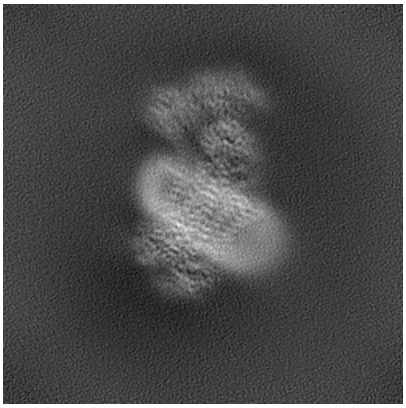


Y

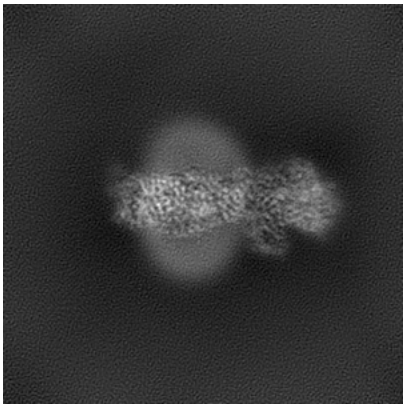


Z

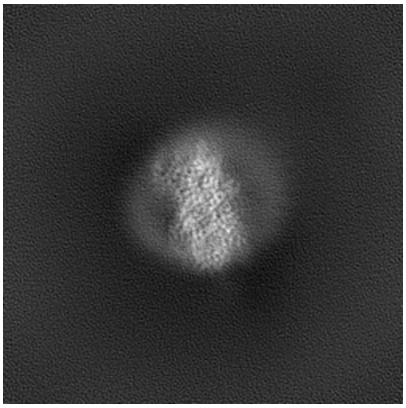
6.1.2 Raw map



X



Y

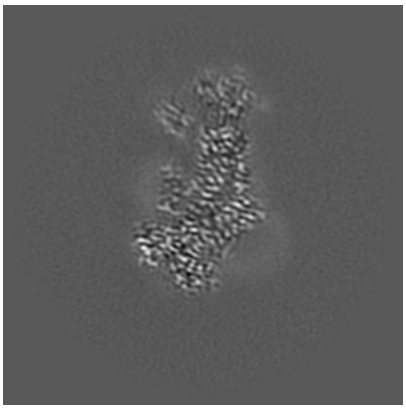


Z

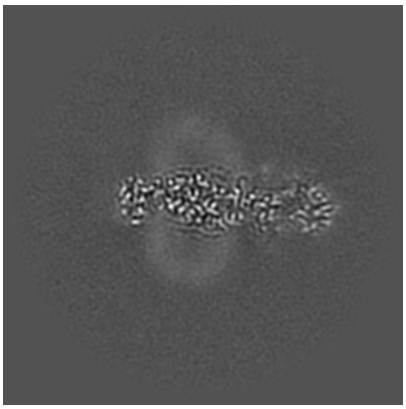
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

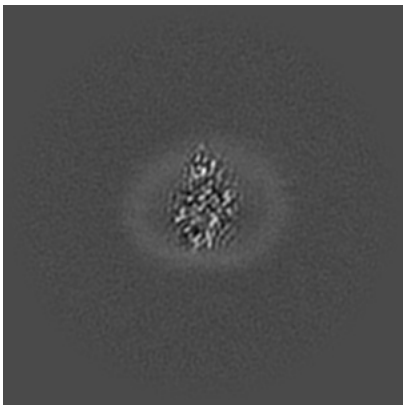
6.2.1 Primary map



X Index: 128

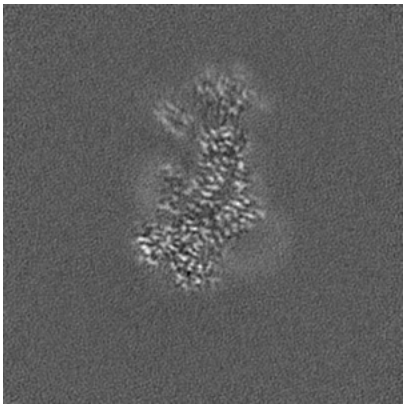


Y Index: 128

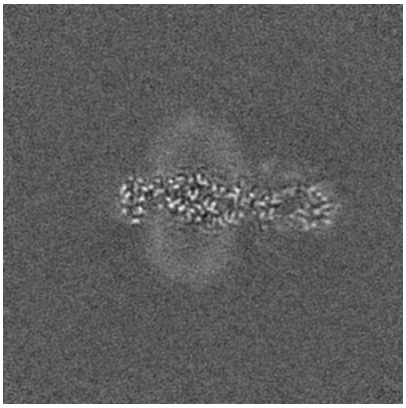


Z Index: 128

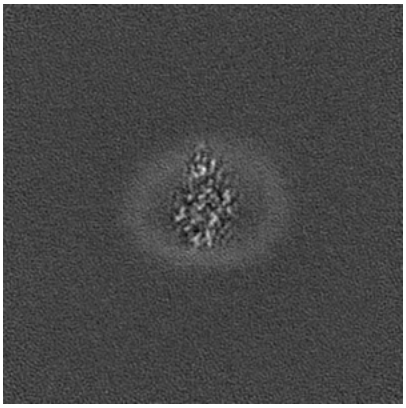
6.2.2 Raw map



X Index: 128



Y Index: 128

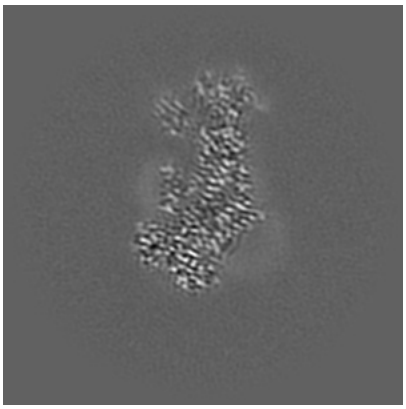


Z Index: 128

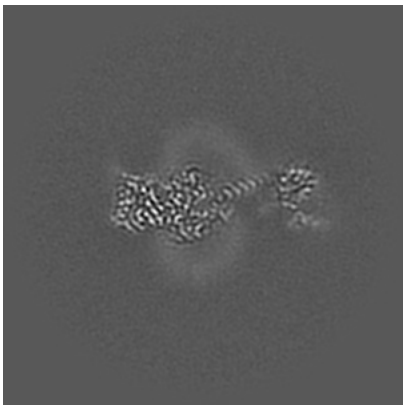
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

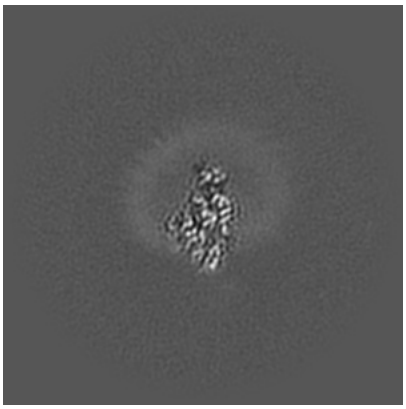
6.3.1 Primary map



X Index: 129

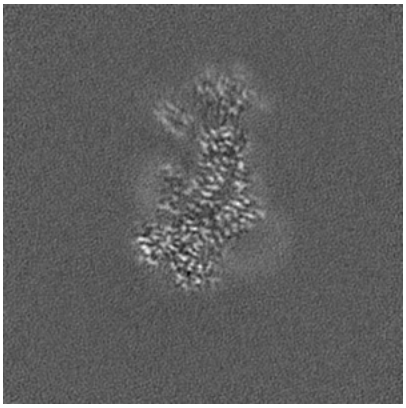


Y Index: 116

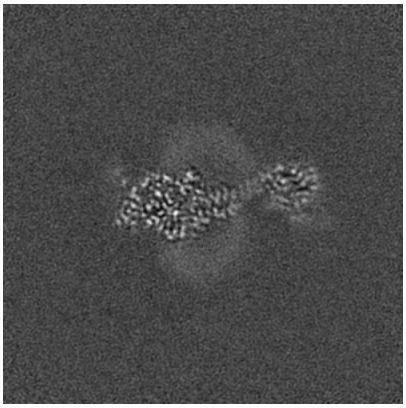


Z Index: 111

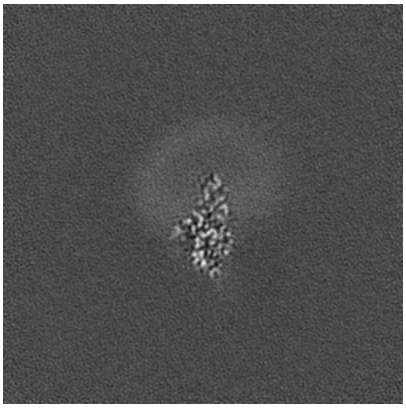
6.3.2 Raw map



X Index: 128



Y Index: 111

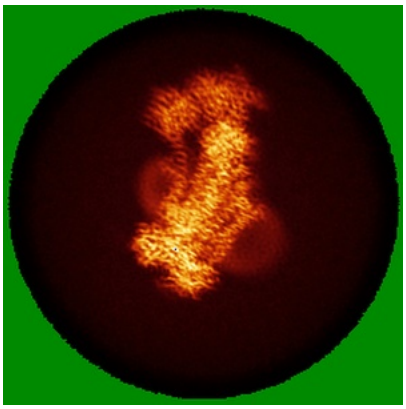


Z Index: 100

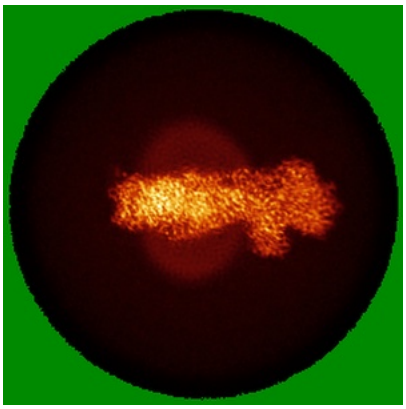
The images above show the largest variance slices of the map in three orthogonal directions.

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

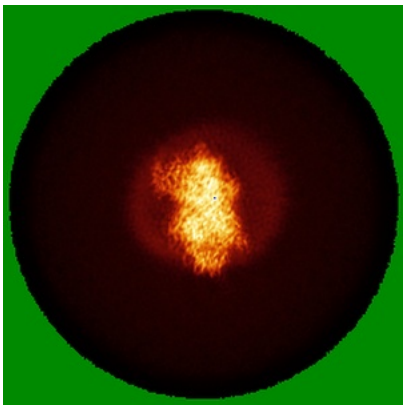
6.4.1 Primary map



X

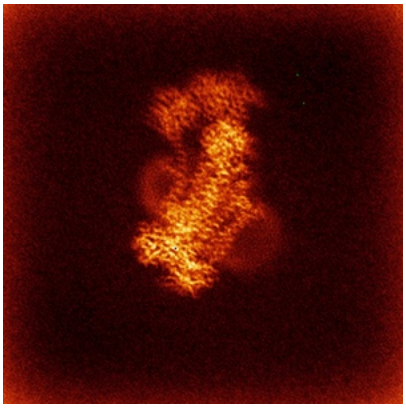


Y

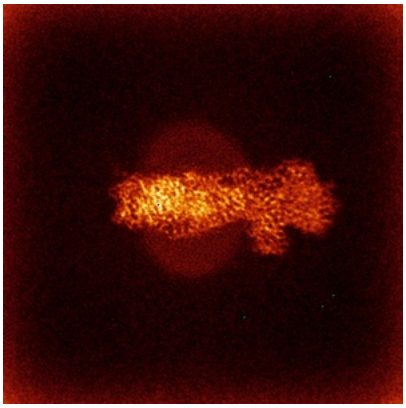


Z

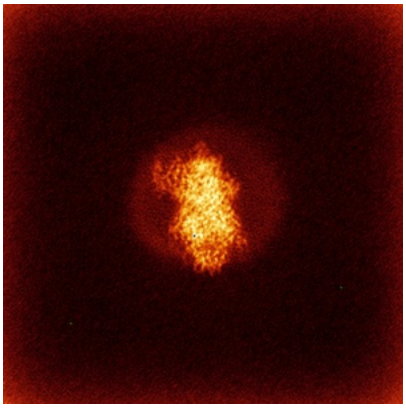
6.4.2 Raw map



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)

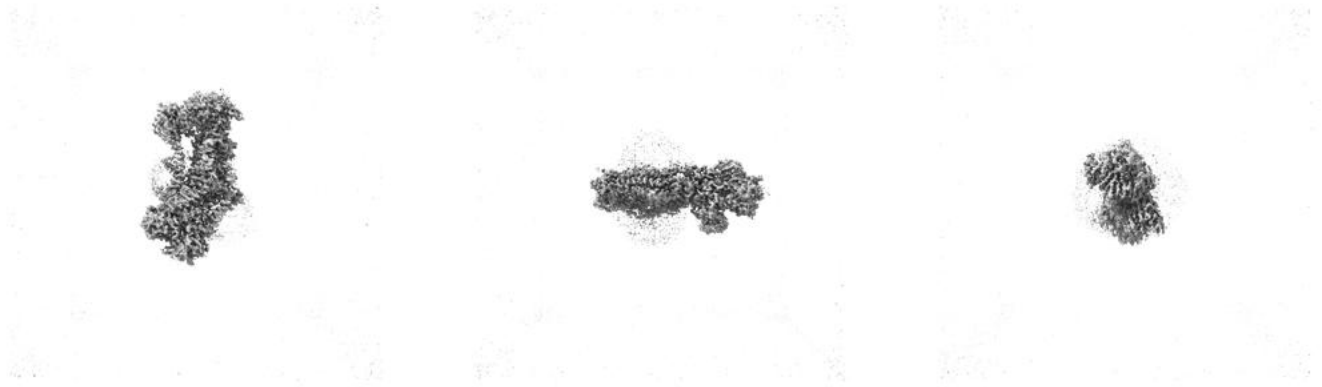
6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.21. 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.

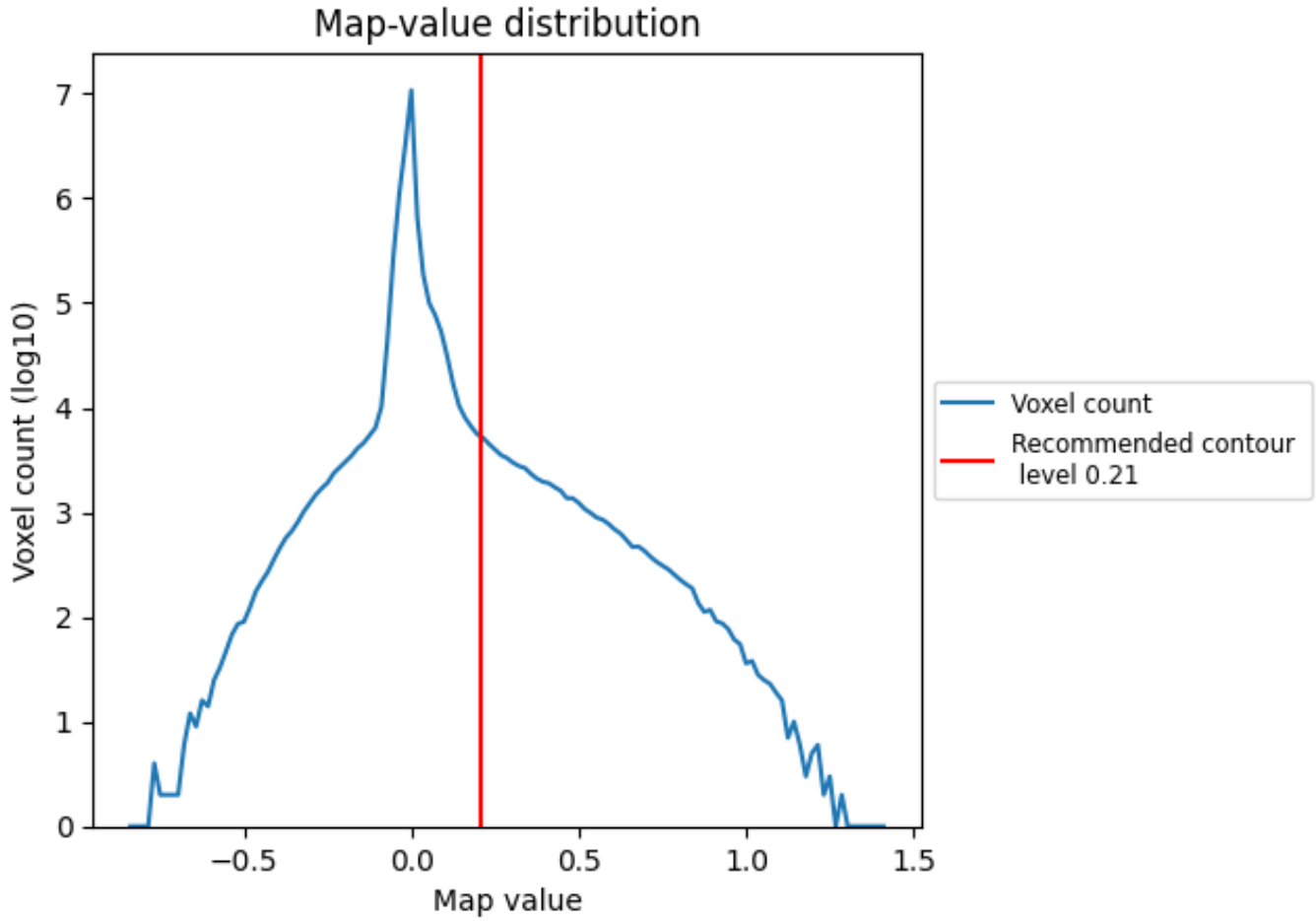
6.6 Mask visualisation (i)

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

7 Map analysis

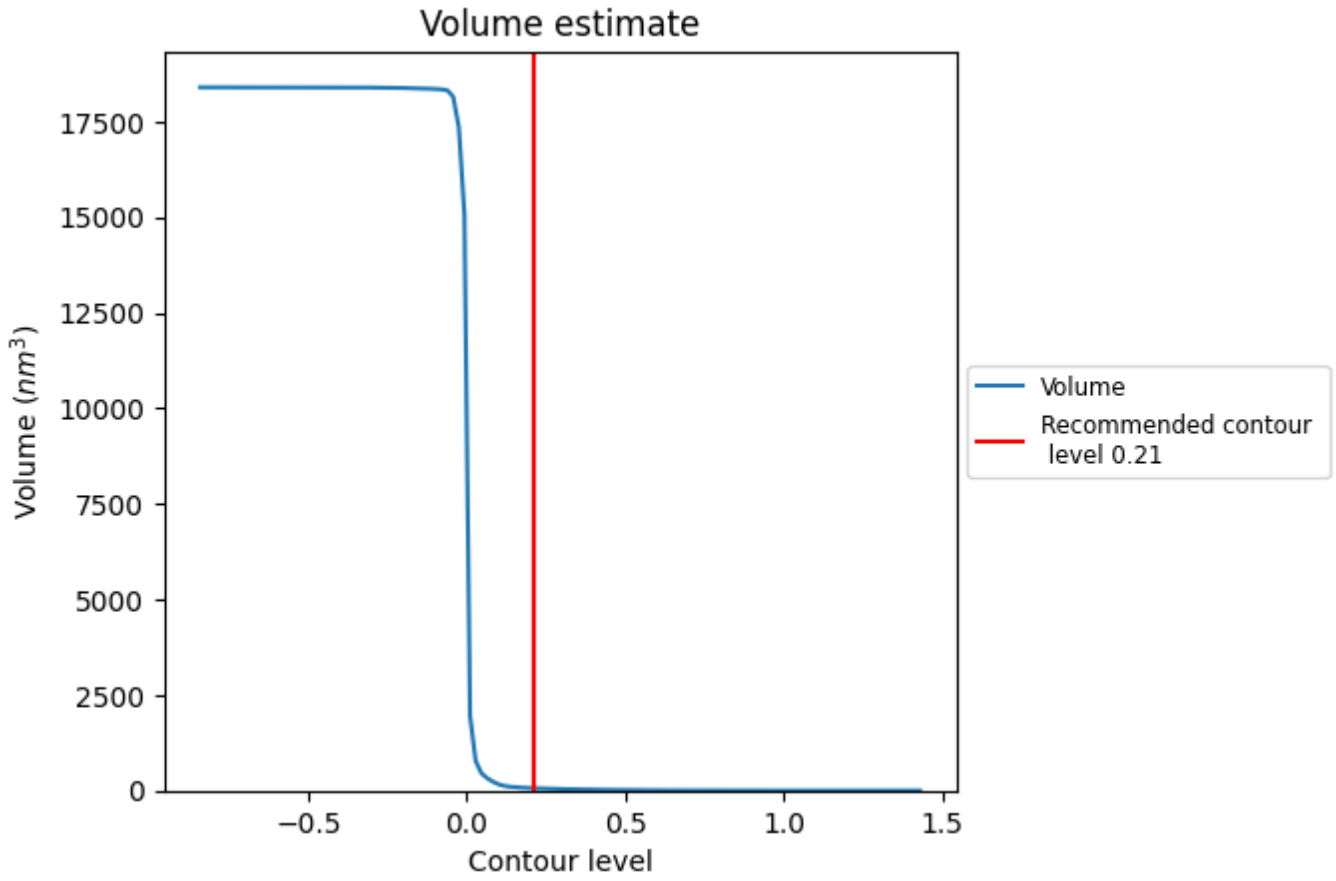
This section contains the results of statistical analysis of the map.

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.

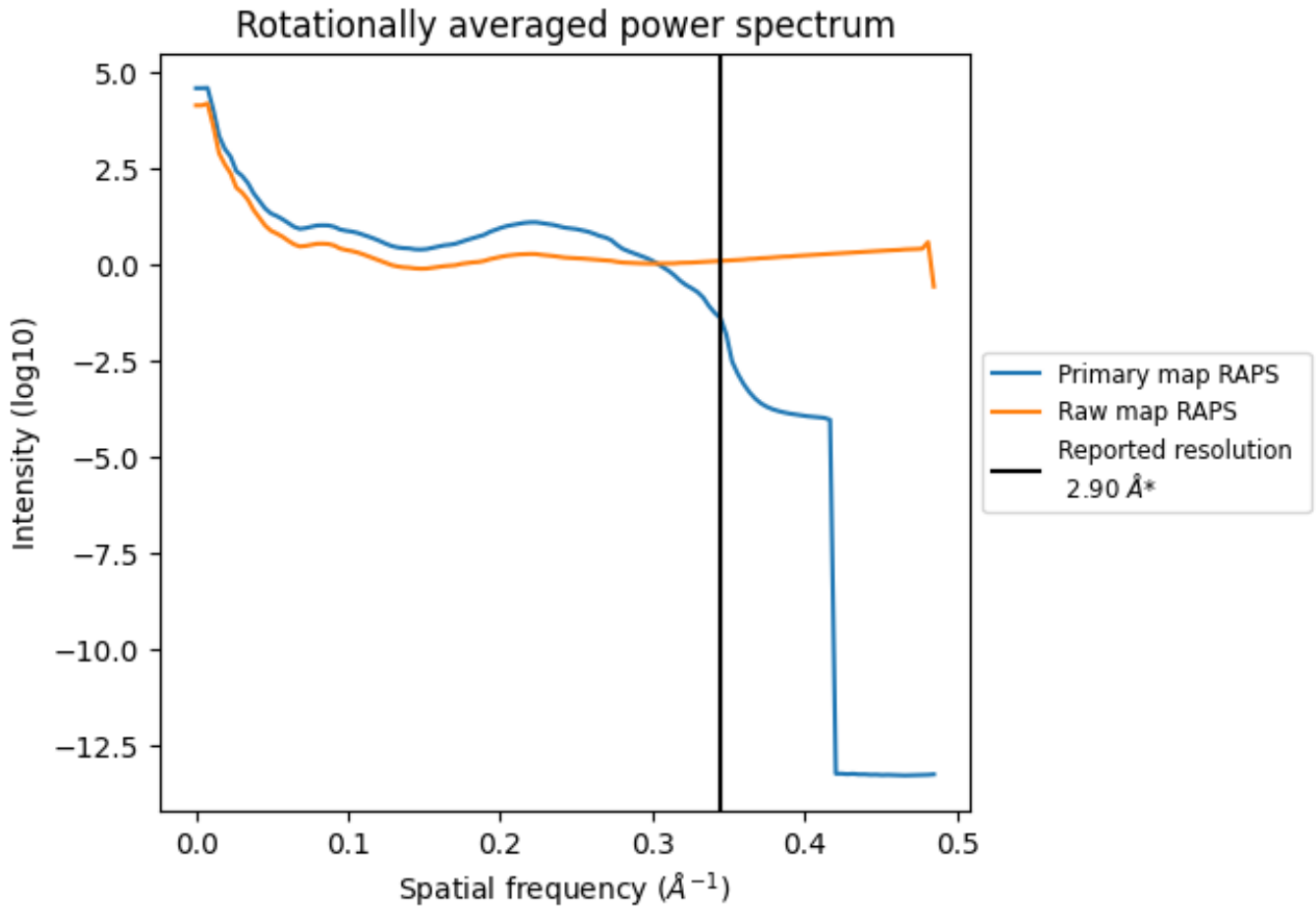
7.2 Volume estimate (i)



The volume at the recommended contour level is 62 nm^3; this corresponds to an approximate mass of 56 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)

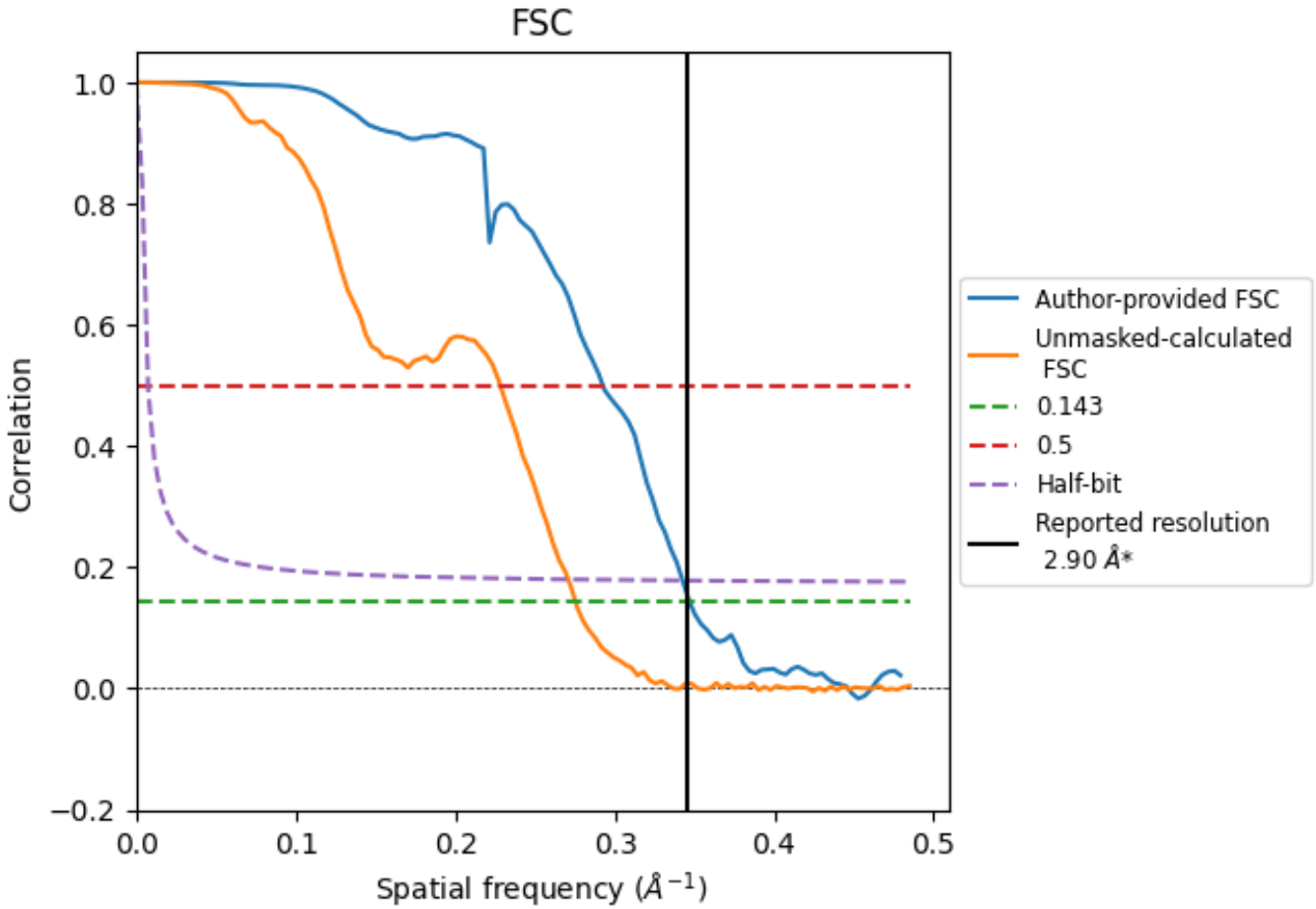


*Reported resolution corresponds to spatial frequency of 0.345 $Å^{-1}$

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 0.345 Å^{-1}

8.2 Resolution estimates (i)

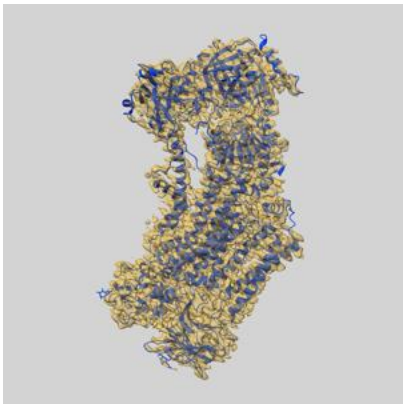
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.90	-	-
Author-provided FSC curve	2.88	3.42	2.92
Unmasked-calculated*	3.63	4.38	3.69

*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 3.63 differs from the reported value 2.9 by more than 10 %

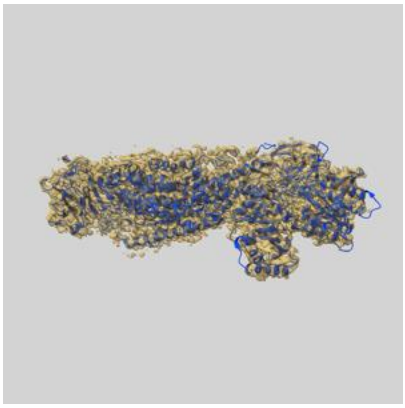
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-12894 and PDB model 7OH5. Per-residue inclusion information can be found in section 3 on page 11.

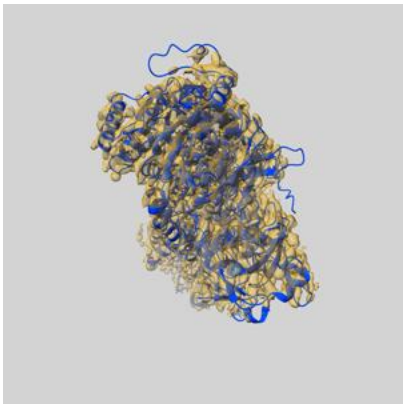
9.1 Map-model overlay



X



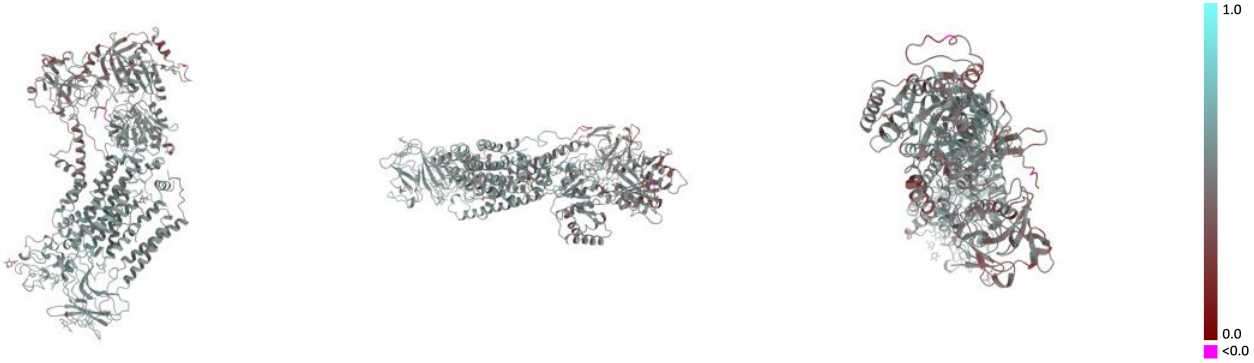
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.21 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.

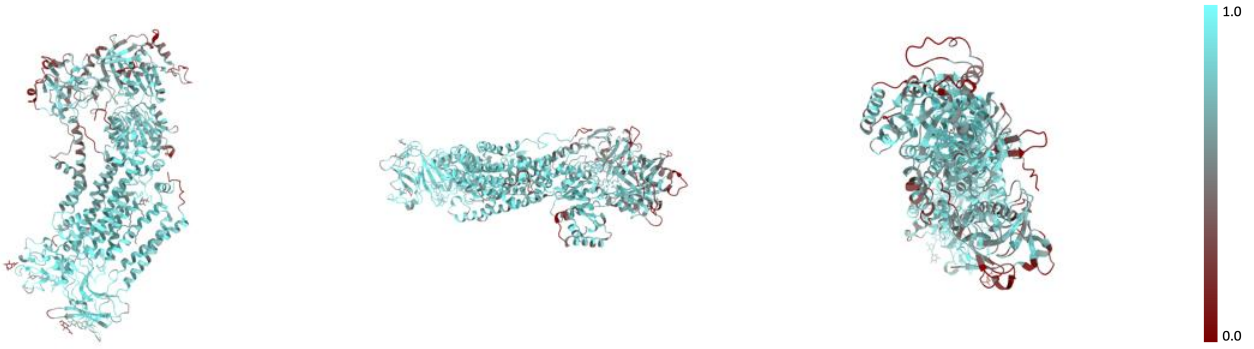
9.2 Q-score mapped to coordinate model (i)



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.

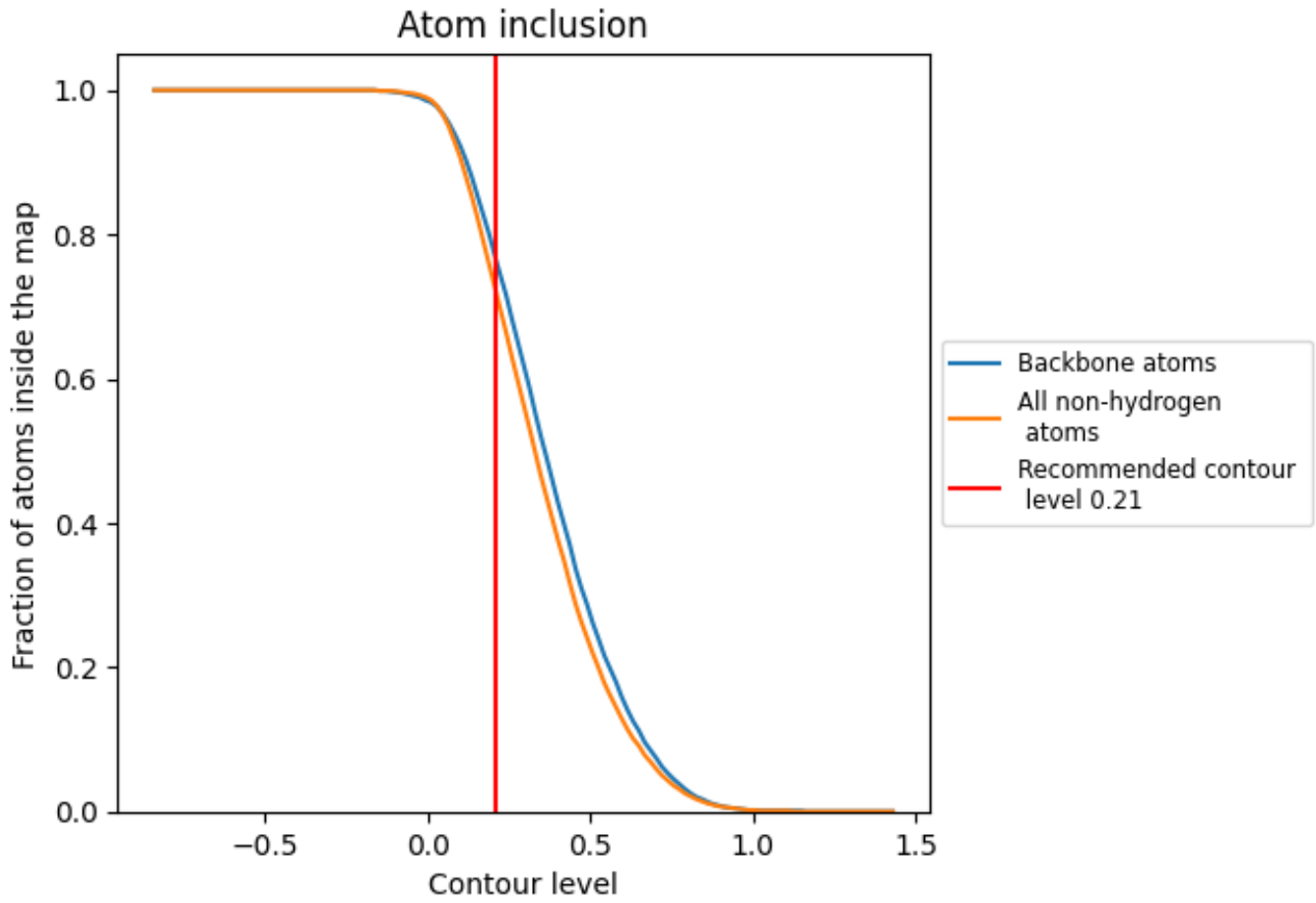
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.21).

9.4 Atom inclusion (i)



At the recommended contour level, 76% of all backbone atoms, 72% 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 (0.21) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7190	0.4980
A	0.6970	0.4900
B	0.6790	0.5530
C	0.7900	0.5220
D	0.3930	0.4770
E	0.8000	0.5050

