wwPDB EM Validation Summary Report (i)

Nov 4, 2023 – 10:11 AM EDT

PDB ID	:	6DW1
EMDB ID	:	EMD-8923
Title	:	Cryo-EM structure of the benzodiazepine-sensitive alpha1beta1gamma2S tri-heteromeric GABAA receptor in complex with GABA (ECD map)
Authors	:	Phulera, S.; Zhu, H.; Yu, J.; Yoshioka, C.; Gouaux, E.
Deposited on	:	2018-06-26
Resolution	:	3.10 Å(reported)

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:

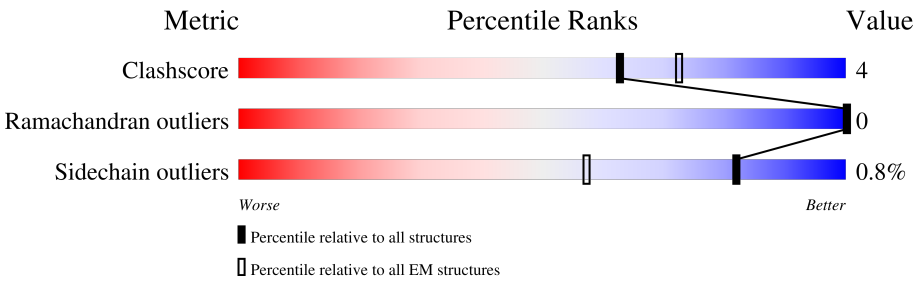
EMDB validation analysis	:	0.0.1.dev70
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.10 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	490	37% 5% 58%
2	A	402	45% 7% 48%
2	C	402	47% 5% 48%
3	B	384	45% 10% 45%
3	E	384	47% 7% 46%
4	F	4	75% 25% 75%
5	G	7	43% 29% 71%
6	H	3	33% 67% 33%

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Mol	Chain	Length	Quality of chain
6	J	3	33% / 100%
7	I	2	50% / 100%
7	K	2	50% / 100%

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 8595 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 Gamma-aminobutyric acid receptor subunit gamma-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	D	208	1612	1033	277	296	6	0	0

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	429	LEU	-	expression tag	UNP P18508
D	430	VAL	-	expression tag	UNP P18508
D	431	PRO	-	expression tag	UNP P18508
D	432	ARG	-	expression tag	UNP P18508
D	433	GLY	-	expression tag	UNP P18508
D	434	SER	-	expression tag	UNP P18508
D	435	ARG	-	expression tag	UNP P18508
D	436	HIS	-	expression tag	UNP P18508
D	437	HIS	-	expression tag	UNP P18508
D	438	HIS	-	expression tag	UNP P18508
D	439	HIS	-	expression tag	UNP P18508
D	440	HIS	-	expression tag	UNP P18508
D	441	HIS	-	expression tag	UNP P18508
D	442	HIS	-	expression tag	UNP P18508
D	443	HIS	-	expression tag	UNP P18508
D	444	THR	-	expression tag	UNP P18508
D	445	GLU	-	expression tag	UNP P18508
D	446	THR	-	expression tag	UNP P18508
D	447	SER	-	expression tag	UNP P18508
D	448	GLN	-	expression tag	UNP P18508
D	449	VAL	-	expression tag	UNP P18508
D	450	ALA	-	expression tag	UNP P18508
D	451	PRO	-	expression tag	UNP P18508
D	452	ALA	-	expression tag	UNP P18508

- Molecule 2 is a protein called Gamma-aminobutyric acid receptor subunit alpha-1,Gamma-aminobutyric acid receptor subunit alpha-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	C	210	1673	1062	296	306	9	0	0
2	A	210	1665	1059	291	305	10	0	0

There are 30 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	314	THR	-	linker	UNP P62813
C	362	LEU	-	expression tag	UNP P62813
C	363	VAL	-	expression tag	UNP P62813
C	364	PRO	-	expression tag	UNP P62813
C	365	ARG	-	expression tag	UNP P62813
C	366	GLY	-	expression tag	UNP P62813
C	367	SER	-	expression tag	UNP P62813
C	368	HIS	-	expression tag	UNP P62813
C	369	HIS	-	expression tag	UNP P62813
C	370	HIS	-	expression tag	UNP P62813
C	371	HIS	-	expression tag	UNP P62813
C	372	HIS	-	expression tag	UNP P62813
C	373	HIS	-	expression tag	UNP P62813
C	374	HIS	-	expression tag	UNP P62813
C	375	HIS	-	expression tag	UNP P62813
A	314	THR	-	linker	UNP P62813
A	362	LEU	-	expression tag	UNP P62813
A	363	VAL	-	expression tag	UNP P62813
A	364	PRO	-	expression tag	UNP P62813
A	365	ARG	-	expression tag	UNP P62813
A	366	GLY	-	expression tag	UNP P62813
A	367	SER	-	expression tag	UNP P62813
A	368	HIS	-	expression tag	UNP P62813
A	369	HIS	-	expression tag	UNP P62813
A	370	HIS	-	expression tag	UNP P62813
A	371	HIS	-	expression tag	UNP P62813
A	372	HIS	-	expression tag	UNP P62813
A	373	HIS	-	expression tag	UNP P62813
A	374	HIS	-	expression tag	UNP P62813
A	375	HIS	-	expression tag	UNP P62813

- Molecule 3 is a protein called Gamma-aminobutyric acid receptor subunit beta-1,Gamma-a minobutyric acid receptor subunit beta-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	E	208	1672	1068	278	316	10	0	0
3	B	210	1685	1077	286	312	10	0	0

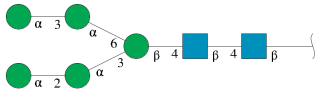
There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	309	GLY	-	linker	UNP P15431
E	310	THR	-	linker	UNP P15431
E	346	LEU	-	expression tag	UNP P15431
E	347	VAL	-	expression tag	UNP P15431
E	348	PRO	-	expression tag	UNP P15431
E	349	ARG	-	expression tag	UNP P15431
E	350	GLY	-	expression tag	UNP P15431
E	351	SER	-	expression tag	UNP P15431
E	352	HIS	-	expression tag	UNP P15431
E	353	HIS	-	expression tag	UNP P15431
E	354	HIS	-	expression tag	UNP P15431
E	355	HIS	-	expression tag	UNP P15431
E	356	HIS	-	expression tag	UNP P15431
E	357	HIS	-	expression tag	UNP P15431
E	358	HIS	-	expression tag	UNP P15431
E	359	HIS	-	expression tag	UNP P15431
B	309	GLY	-	linker	UNP P15431
B	310	THR	-	linker	UNP P15431
B	346	LEU	-	expression tag	UNP P15431
B	347	VAL	-	expression tag	UNP P15431
B	348	PRO	-	expression tag	UNP P15431
B	349	ARG	-	expression tag	UNP P15431
B	350	GLY	-	expression tag	UNP P15431
B	351	SER	-	expression tag	UNP P15431
B	352	HIS	-	expression tag	UNP P15431
B	353	HIS	-	expression tag	UNP P15431
B	354	HIS	-	expression tag	UNP P15431
B	355	HIS	-	expression tag	UNP P15431
B	356	HIS	-	expression tag	UNP P15431
B	357	HIS	-	expression tag	UNP P15431
B	358	HIS	-	expression tag	UNP P15431
B	359	HIS	-	expression tag	UNP P15431

- Molecule 4 is an oligosaccharide called alpha-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.

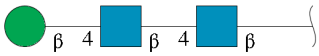
Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
4	F	4	50	28	2	20	0	0

- Molecule 5 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)]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
			Total	C	N	O		
5	G	7	83	46	2	35	0	0

- Molecule 6 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

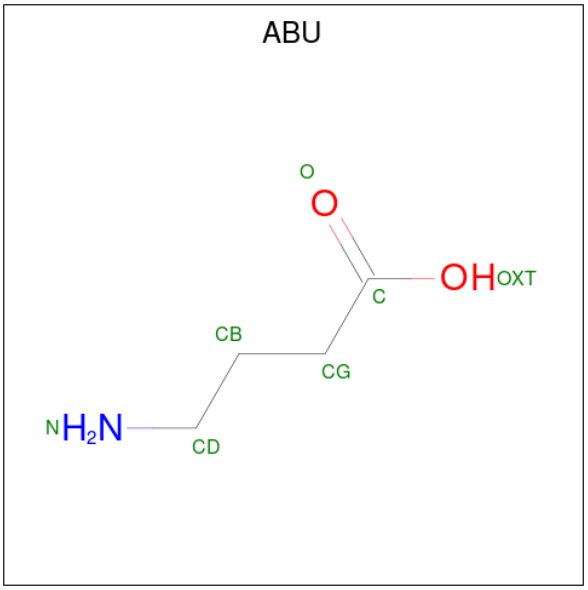


Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
6	H	3	39	22	2	15	0	0
6	J	3	39	22	2	15	0	0

- Molecule 7 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		
7	I	2	28	16	2	10	0	0
			Total	C	N	O		
7	K	2	28	16	2	10	0	0

- Molecule 8 is GAMMA-AMINO-BUTANOIC ACID (three-letter code: ABU) (formula: $C_4H_9NO_2$).



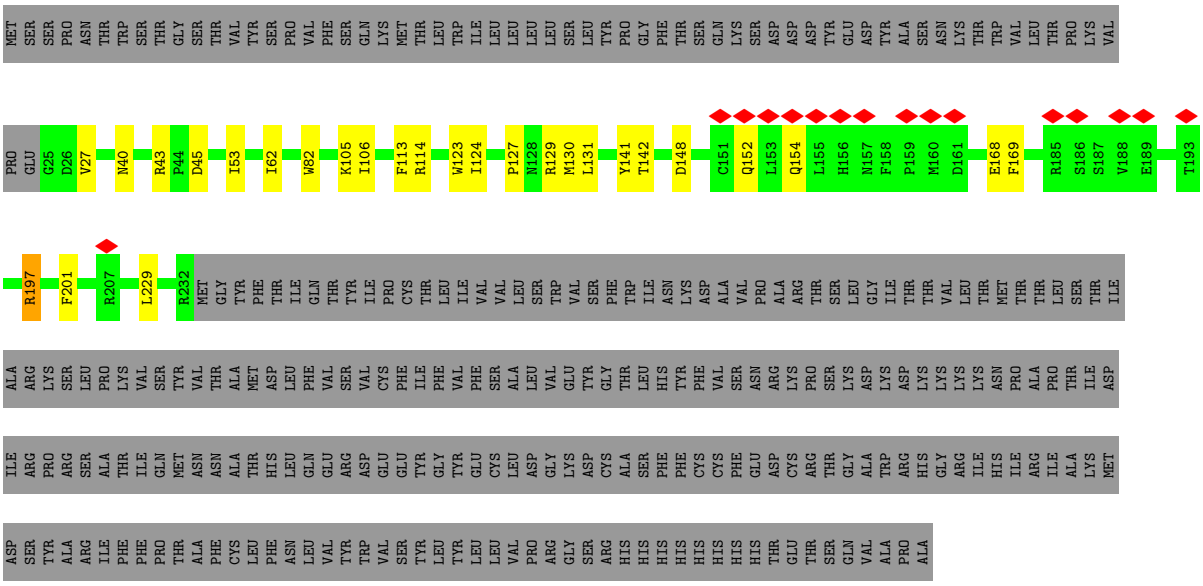
Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
8	C	1	7	4	1	2	0
			Total	C	N	O	
8	A	1	7	4	1	2	0
			Total	C	N	O	
8	A	1	7	4	1	2	0

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.

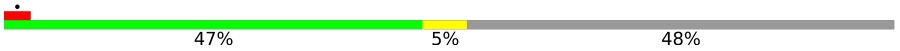
• Molecule 1: Gamma-aminobutyric acid receptor subunit gamma-2

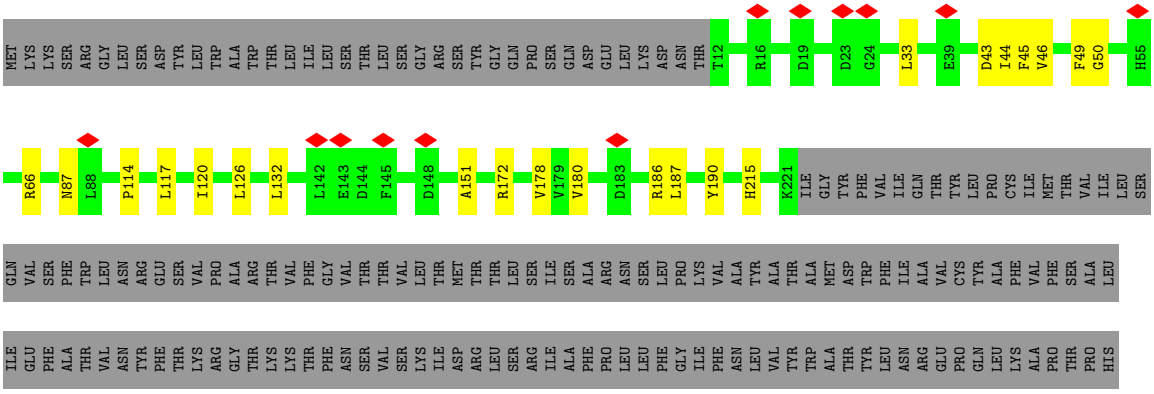
Chain D:



• Molecule 2: Gamma-aminobutyric acid receptor subunit alpha-1,Gamma-aminobutyric acid receptor subunit alpha-1

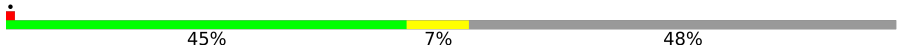
Chain C:

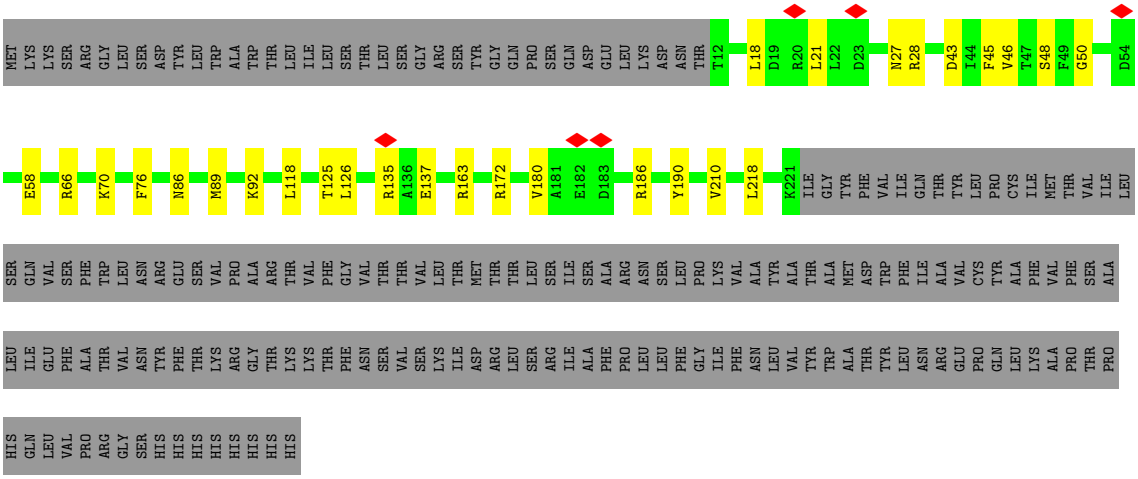




• Molecule 2: Gamma-aminobutyric acid receptor subunit alpha-1,Gamma-aminobutyric acid receptor subunit alpha-1

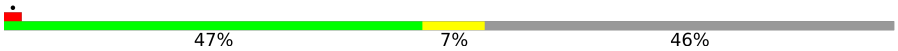
Chain A:

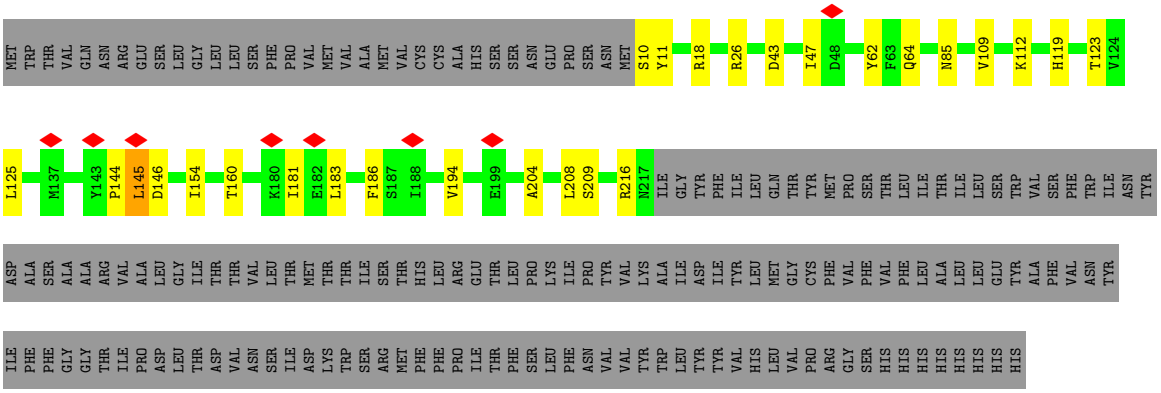




• Molecule 3: Gamma-aminobutyric acid receptor subunit beta-1,Gamma-aminobutyric acid receptor subunit beta-1

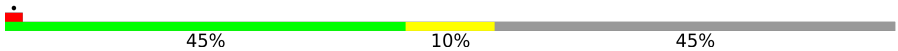
Chain E:

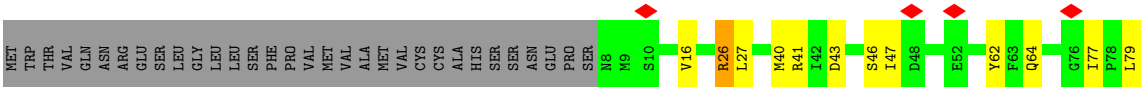


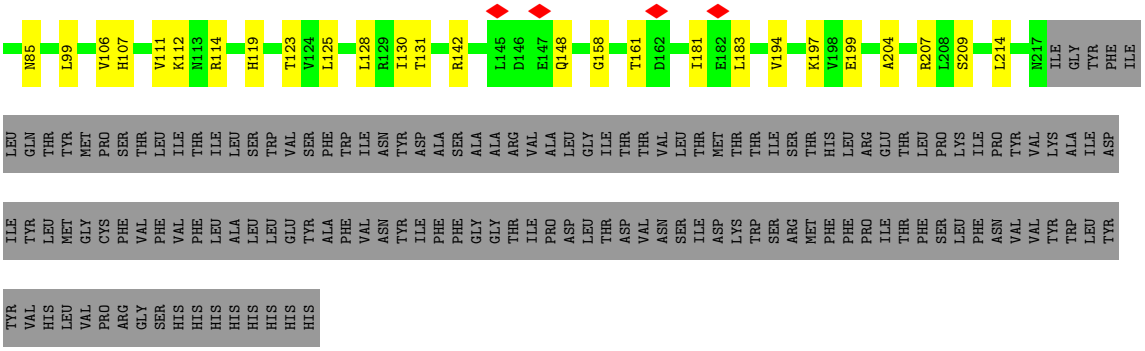


• Molecule 3: Gamma-aminobutyric acid receptor subunit beta-1,Gamma-aminobutyric acid receptor subunit beta-1

Chain B:







• Molecule 4: alpha-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

Chain F: 75% 25% 75%

• Molecule 5: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain G: 43% 29% 71%

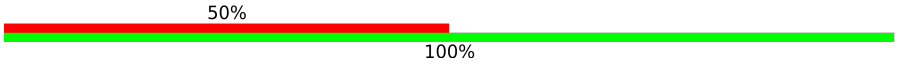
• Molecule 6: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain H: 33% 67% 33%

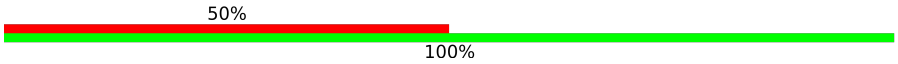
• Molecule 6: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain J: 33% 100%

• Molecule 7: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain I: 

• Molecule 7: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain K: 

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	68499	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 ($e^-/Å^2$)	37	Depositor
Minimum defocus (nm)	-1200	Depositor
Maximum defocus (nm)	-2500	Depositor
Magnification	120000	Depositor
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	32.438	Depositor
Minimum map value	-15.883	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	1.000	Depositor
Recommended contour level	7.68	Depositor
Map size (Å)	311.52, 311.52, 311.52	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.649, 0.649, 0.649	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, MAN, BMA, ABU

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	0.31	0/1652	0.60	0/2256
2	A	0.31	0/1703	0.54	0/2310
2	C	0.32	0/1712	0.57	0/2323
3	B	0.31	0/1722	0.55	0/2334
3	E	0.31	0/1709	0.55	1/2318 (0.0%)
All	All	0.31	0/8498	0.56	1/11541 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	E	145	LEU	CA-CB-CG	6.42	130.07	115.30

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	1494	17	0
2	A	1665	0	1631	16	0
2	C	1673	0	1635	13	0
3	B	1685	0	1665	21	0
3	E	1672	0	1641	14	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	F	50	0	43	0	0
5	G	83	0	70	0	0
6	H	39	0	34	0	0
6	J	39	0	34	0	0
7	I	28	0	25	0	0
7	K	28	0	25	0	0
8	A	14	0	0	0	0
8	C	7	0	0	0	0
All	All	8595	0	8297	75	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 4.

The worst 5 of 75 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)
3:B:107:HIS:HE2	3:B:131:THR:HG1	1.40	0.69
3:E:64:GLN:HE21	3:E:125:LEU:HD11	1.58	0.68
3:B:43:ASP:HB2	3:B:62:TYR:HB2	1.79	0.64
2:C:120:ILE:HG22	2:C:126:LEU:HD22	1.82	0.61
3:B:77:ILE:HG22	3:B:79:LEU:H	1.66	0.60

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	206/490 (42%)	187 (91%)	19 (9%)	0	100	100
2	A	208/402 (52%)	197 (95%)	11 (5%)	0	100	100
2	C	208/402 (52%)	197 (95%)	11 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	B	208/384 (54%)	200 (96%)	8 (4%)	0	100	100
3	E	206/384 (54%)	196 (95%)	10 (5%)	0	100	100
All	All	1036/2062 (50%)	977 (94%)	59 (6%)	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	D	164/449 (36%)	163 (99%)	1 (1%)	86	94
2	A	180/360 (50%)	179 (99%)	1 (1%)	86	94
2	C	181/360 (50%)	180 (99%)	1 (1%)	86	94
3	B	185/348 (53%)	182 (98%)	3 (2%)	62	84
3	E	185/348 (53%)	184 (100%)	1 (0%)	88	94
All	All	895/1865 (48%)	888 (99%)	7 (1%)	82	92

5 of 7 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	E	18	ARG
3	B	26	ARG
3	B	142	ARG
3	B	40	MET
2	A	172	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 8 such sidechains are listed below:

Mol	Chain	Res	Type
3	B	64	GLN
3	E	148	GLN
3	E	64	GLN

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Mol	Chain	Res	Type
2	A	101	HIS
3	E	65	GLN

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)

21 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	F	1	4,2	14,14,15	0.25	0	17,19,21	0.55	0
4	NAG	F	2	4	14,14,15	0.30	0	17,19,21	0.68	1 (5%)
4	BMA	F	3	4	11,11,12	0.75	0	15,15,17	1.12	1 (6%)
4	MAN	F	4	4	11,11,12	1.29	3 (27%)	15,15,17	1.21	2 (13%)
5	NAG	G	1	5,2	14,14,15	0.28	0	17,19,21	0.67	0
5	NAG	G	2	5	14,14,15	0.28	0	17,19,21	0.53	0
5	BMA	G	3	5	11,11,12	0.71	0	15,15,17	1.09	1 (6%)
5	MAN	G	4	5	11,11,12	1.06	0	15,15,17	1.77	4 (26%)
5	MAN	G	5	5	11,11,12	0.97	1 (9%)	15,15,17	0.88	1 (6%)
5	MAN	G	6	5	11,11,12	0.97	0	15,15,17	1.54	2 (13%)
5	MAN	G	7	5	11,11,12	0.85	1 (9%)	15,15,17	1.34	2 (13%)
6	NAG	H	1	3,6	14,14,15	0.44	0	17,19,21	0.39	0
6	NAG	H	2	6	14,14,15	0.44	0	17,19,21	0.41	0
6	BMA	H	3	6	11,11,12	0.91	1 (9%)	15,15,17	1.15	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
7	NAG	I	1	7,3	14,14,15	0.24	0	17,19,21	0.41	0
7	NAG	I	2	7	14,14,15	0.36	0	17,19,21	0.42	0
6	NAG	J	1	3,6	14,14,15	0.38	0	17,19,21	0.53	0
6	NAG	J	2	6	14,14,15	0.31	0	17,19,21	0.52	0
6	BMA	J	3	6	11,11,12	0.88	0	15,15,17	0.76	0
7	NAG	K	1	7,3	14,14,15	0.35	0	17,19,21	0.52	0
7	NAG	K	2	7	14,14,15	0.36	0	17,19,21	0.43	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	F	1	4,2	-	4/6/23/26	0/1/1/1
4	NAG	F	2	4	-	2/6/23/26	0/1/1/1
4	BMA	F	3	4	-	1/2/19/22	0/1/1/1
4	MAN	F	4	4	-	1/2/19/22	0/1/1/1
5	NAG	G	1	5,2	-	2/6/23/26	0/1/1/1
5	NAG	G	2	5	-	0/6/23/26	0/1/1/1
5	BMA	G	3	5	-	2/2/19/22	0/1/1/1
5	MAN	G	4	5	-	2/2/19/22	0/1/1/1
5	MAN	G	5	5	-	1/2/19/22	0/1/1/1
5	MAN	G	6	5	-	1/2/19/22	1/1/1/1
5	MAN	G	7	5	-	1/2/19/22	0/1/1/1
6	NAG	H	1	3,6	-	2/6/23/26	0/1/1/1
6	NAG	H	2	6	-	2/6/23/26	0/1/1/1
6	BMA	H	3	6	-	0/2/19/22	0/1/1/1
7	NAG	I	1	7,3	-	1/6/23/26	0/1/1/1
7	NAG	I	2	7	-	2/6/23/26	0/1/1/1
6	NAG	J	1	3,6	-	2/6/23/26	0/1/1/1
6	NAG	J	2	6	-	0/6/23/26	0/1/1/1
6	BMA	J	3	6	-	2/2/19/22	0/1/1/1
7	NAG	K	1	7,3	-	0/6/23/26	0/1/1/1
7	NAG	K	2	7	-	2/6/23/26	0/1/1/1

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	F	4	MAN	C2-C3	2.39	1.56	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	F	4	MAN	O5-C1	-2.30	1.40	1.43
4	F	4	MAN	C4-C3	2.19	1.57	1.52
5	G	7	MAN	C1-C2	2.14	1.57	1.52
5	G	5	MAN	O5-C1	-2.11	1.40	1.43

The worst 5 of 15 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	G	4	MAN	C1-O5-C5	4.42	118.18	112.19
5	G	6	MAN	C1-O5-C5	4.35	118.09	112.19
5	G	7	MAN	C1-O5-C5	3.60	117.06	112.19
5	G	4	MAN	O2-C2-C3	-2.98	104.17	110.14
5	G	4	MAN	C1-C2-C3	2.84	113.15	109.67

There are no chirality outliers.

5 of 30 torsion outliers are listed below:

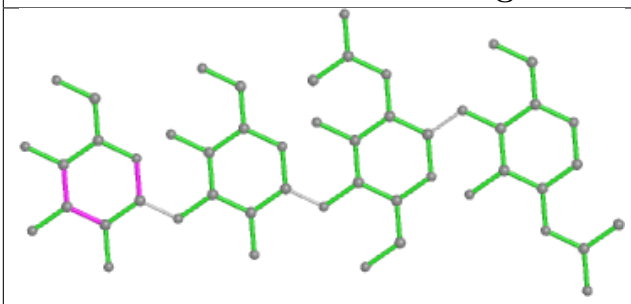
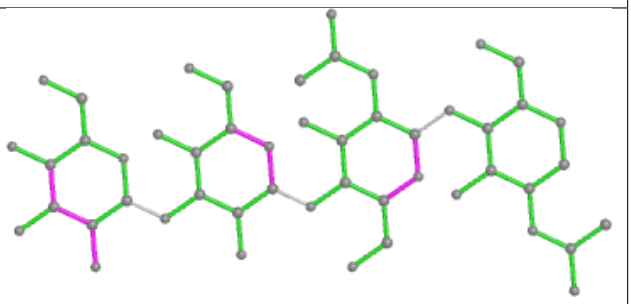
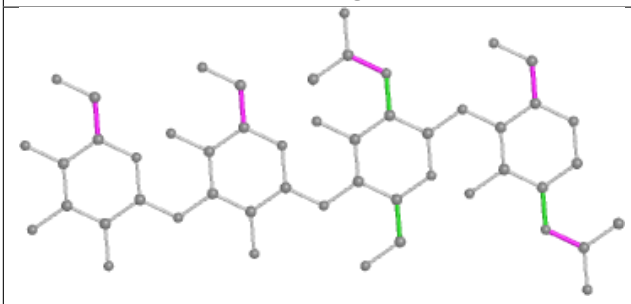
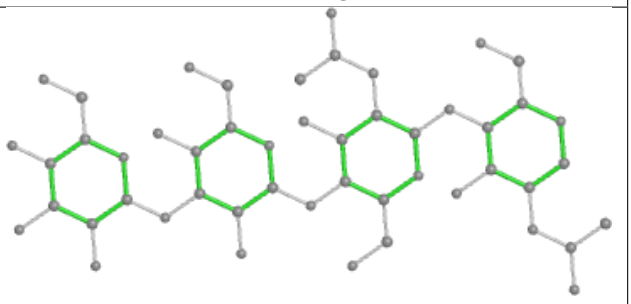
Mol	Chain	Res	Type	Atoms
6	J	1	NAG	O5-C5-C6-O6
6	H	2	NAG	O5-C5-C6-O6
5	G	4	MAN	O5-C5-C6-O6
7	K	2	NAG	O5-C5-C6-O6
4	F	1	NAG	O5-C5-C6-O6

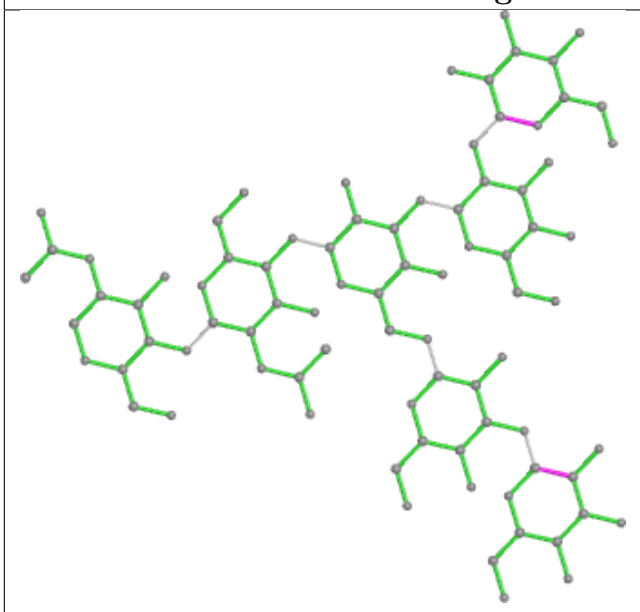
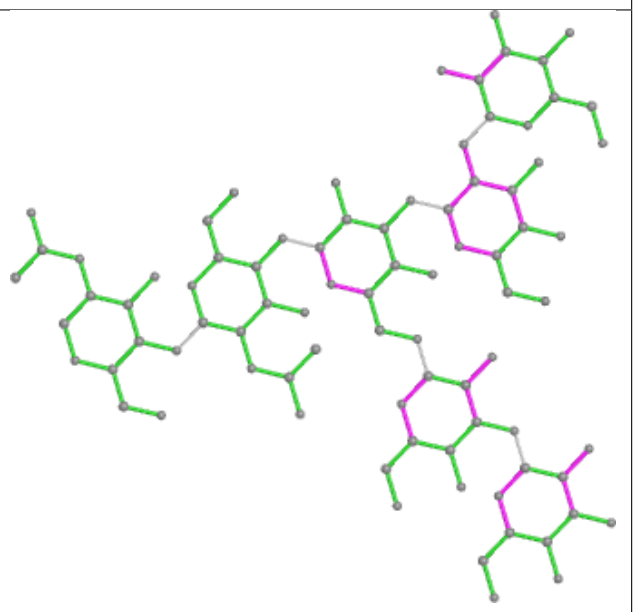
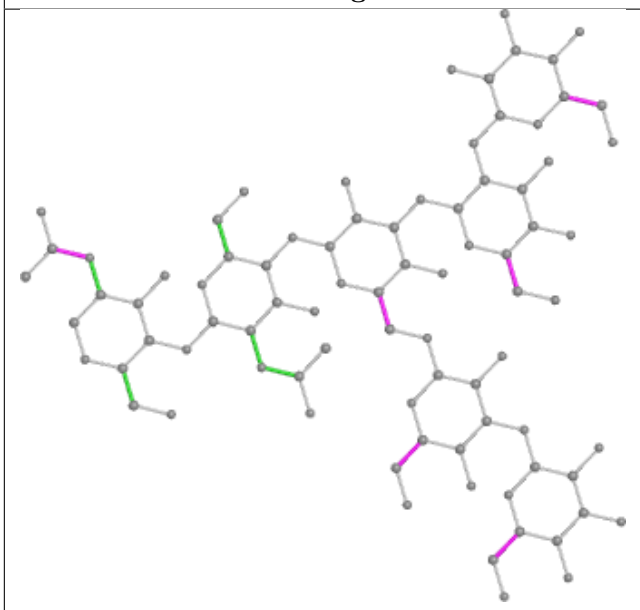
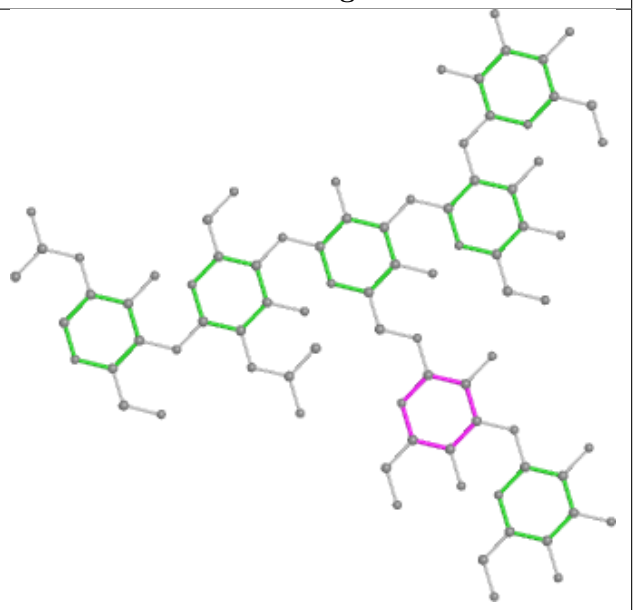
All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	G	6	MAN	C1-C2-C3-C4-C5-O5

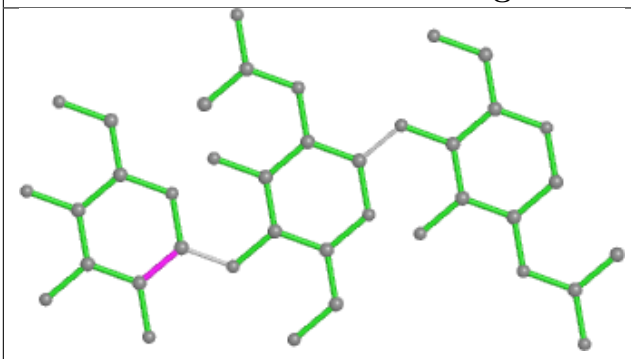
No monomer is involved in short contacts.

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

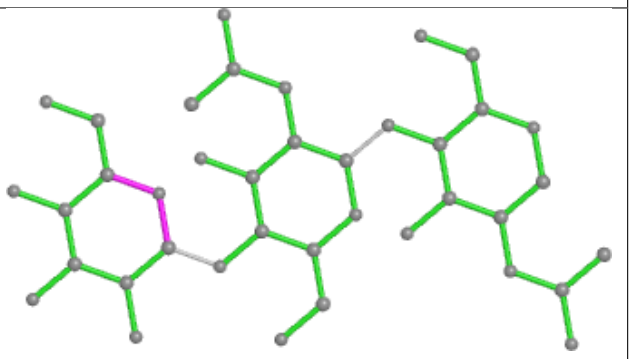
Oligosaccharide Chain F	
 Bond lengths	 Bond angles
 Torsions	 Rings

Oligosaccharide Chain G	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

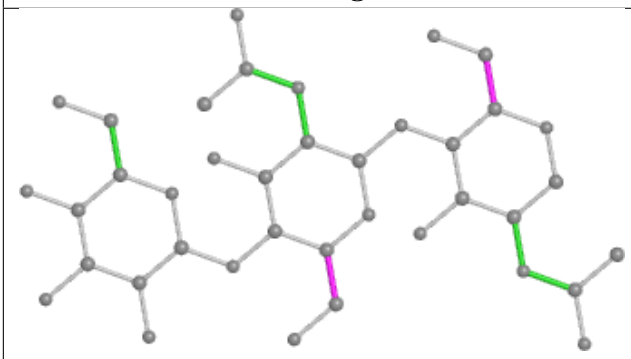
Oligosaccharide Chain H



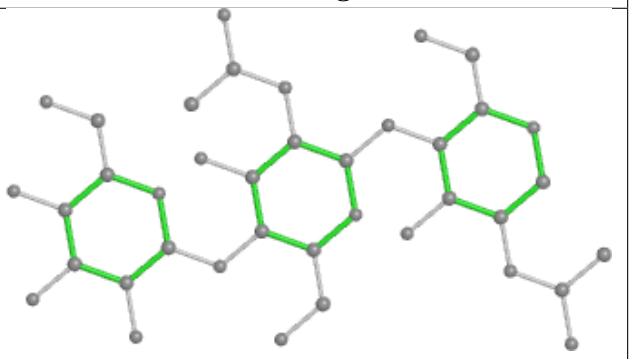
Bond lengths



Bond angles

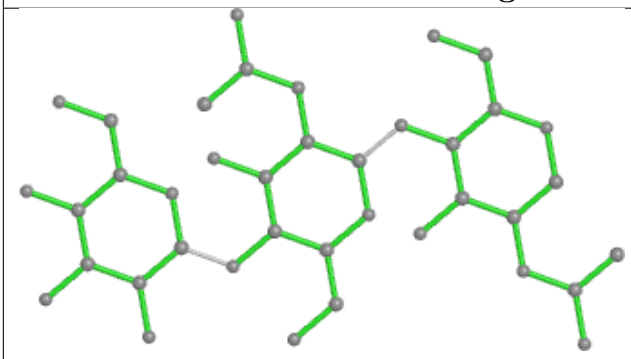


Torsions

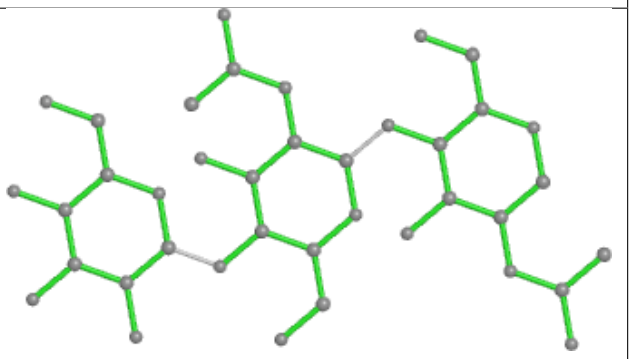


Rings

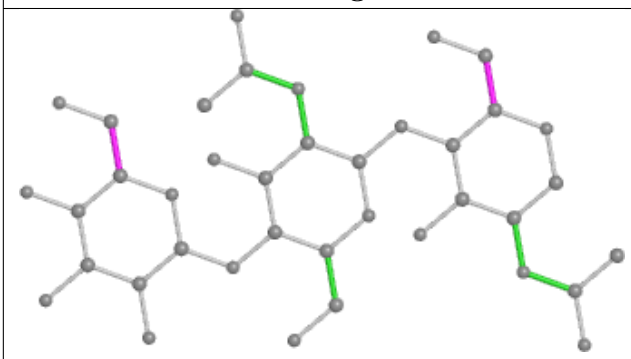
Oligosaccharide Chain J



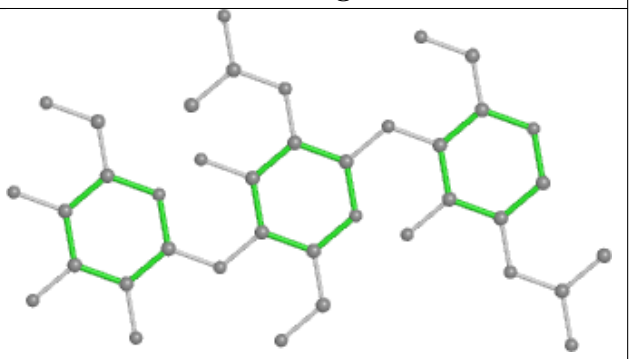
Bond lengths



Bond angles

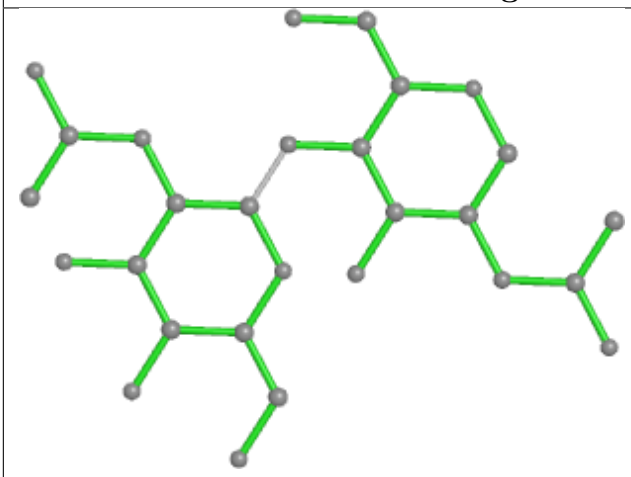


Torsions

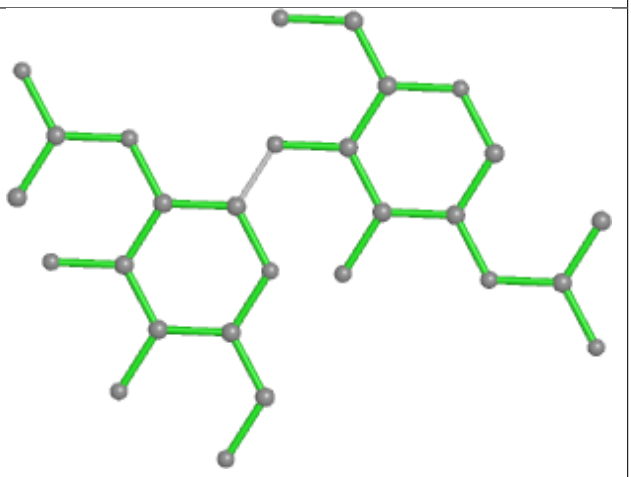


Rings

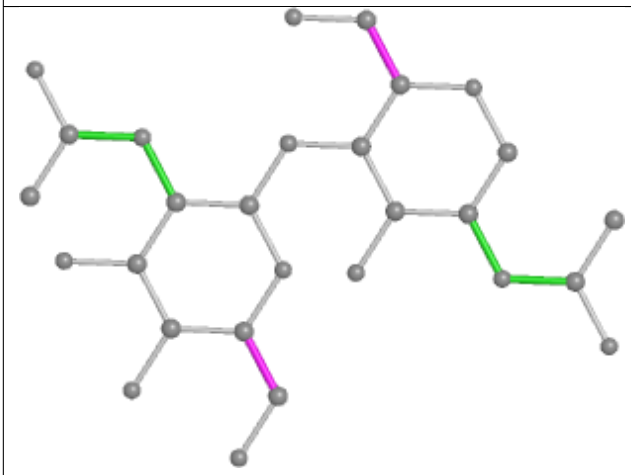
Oligosaccharide Chain I



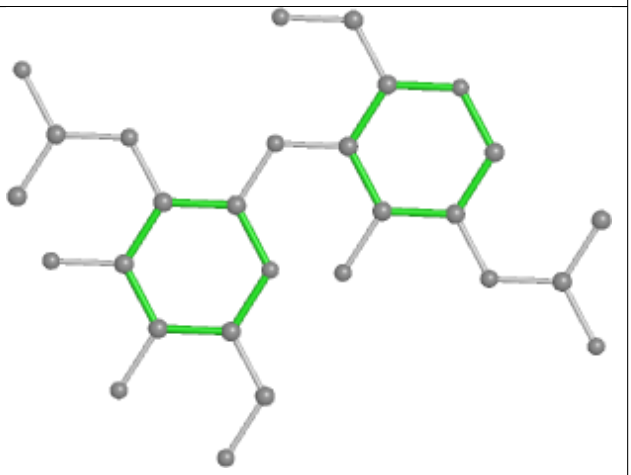
Bond lengths



Bond angles

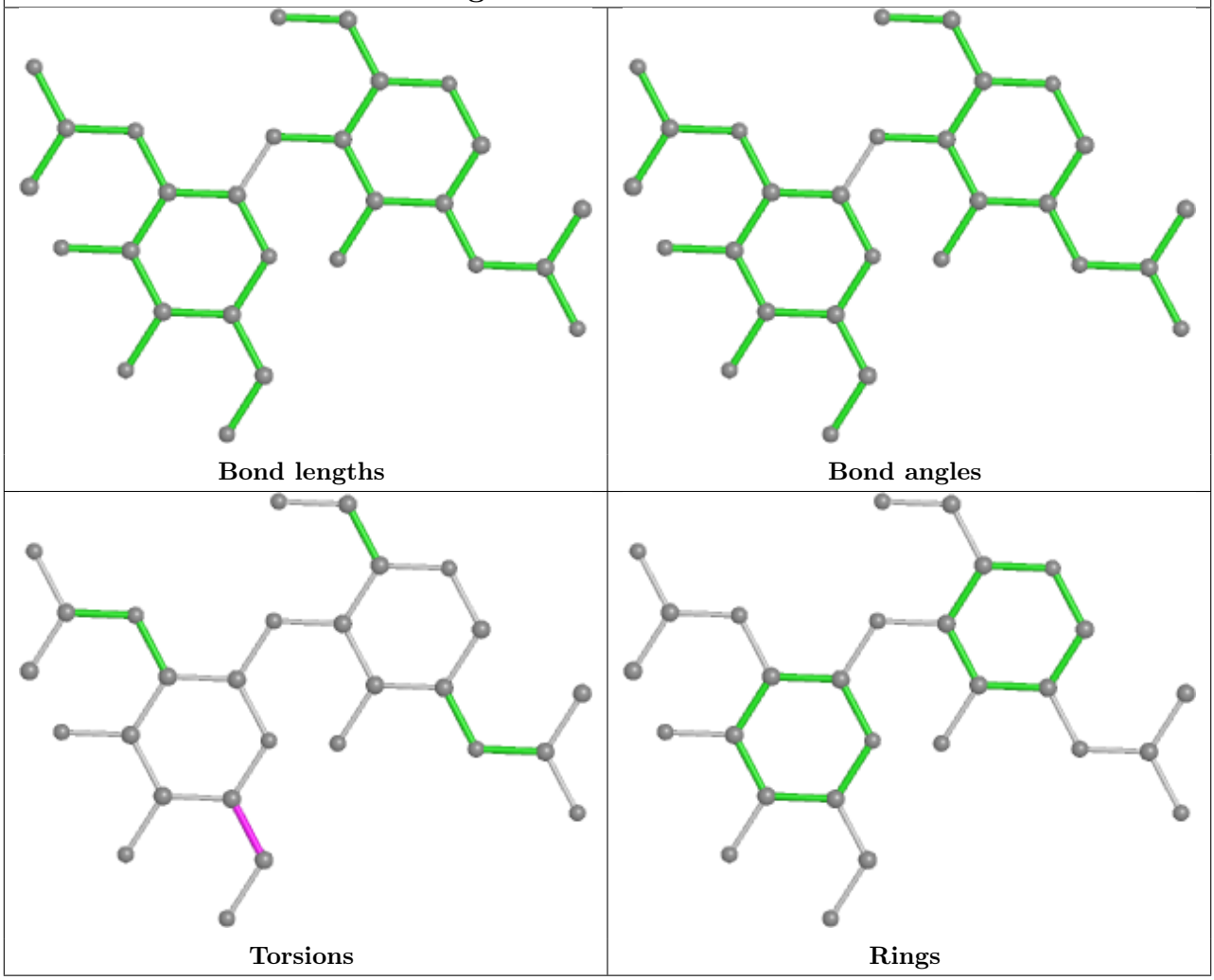


Torsions



Rings

Oligosaccharide Chain K



5.6 Ligand geometry (i)

3 ligands 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	$\#\|Z\| > 2$
8	ABU	A	409	-	6,6,6	0.93	0	6,6,6	1.28	0
8	ABU	C	405	-	6,6,6	0.86	0	6,6,6	1.43	0
8	ABU	A	408	-	6,6,6	0.85	0	6,6,6	1.45	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
8	ABU	A	409	-	-	3/4/4/4	-
8	ABU	C	405	-	-	2/4/4/4	-
8	ABU	A	408	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 7 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	A	409	ABU	CD-CB-CG-C
8	A	408	ABU	CD-CB-CG-C
8	C	405	ABU	O-C-CG-CB
8	C	405	ABU	OXT-C-CG-CB
8	A	409	ABU	OXT-C-CG-CB

There are no ring outliers.

No monomer is involved in short contacts.

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.

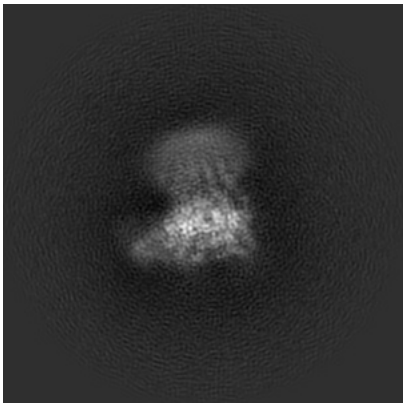
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-8923. These allow visual inspection of the internal detail of the map and identification of artifacts.

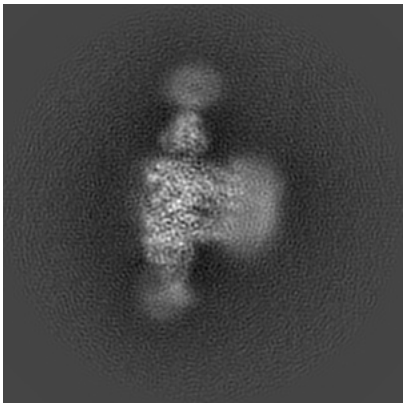
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

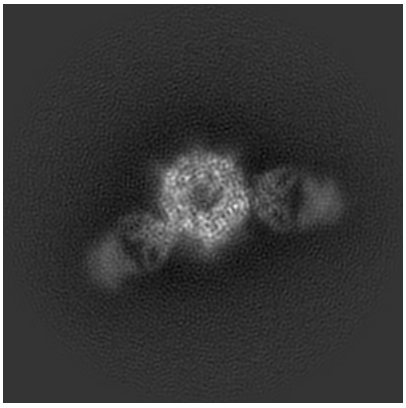
6.1.1 Primary map



X



Y

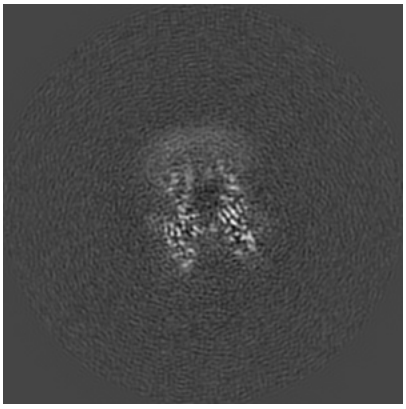


Z

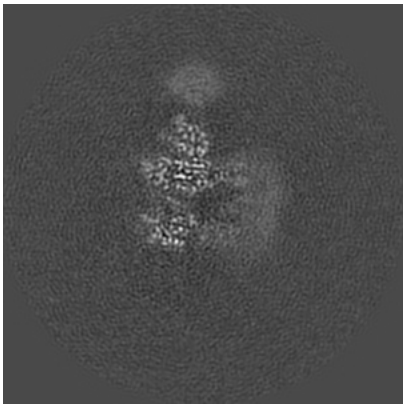
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

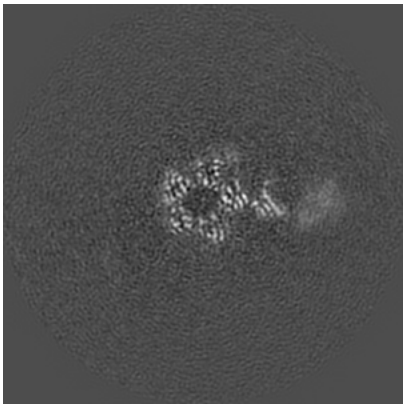
6.2.1 Primary map



X Index: 240



Y Index: 240

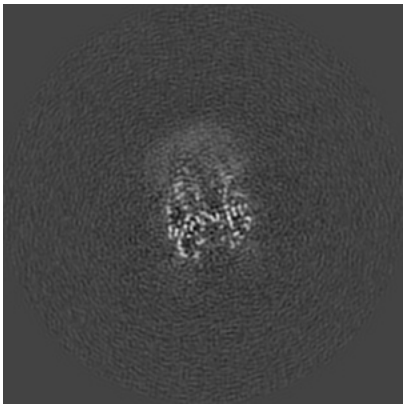


Z Index: 240

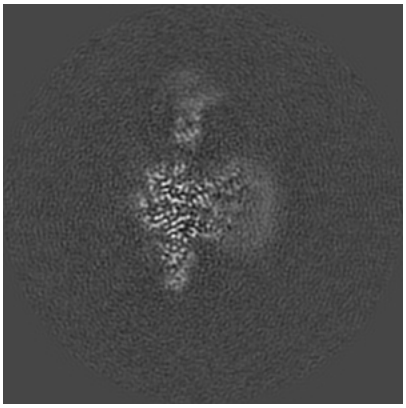
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

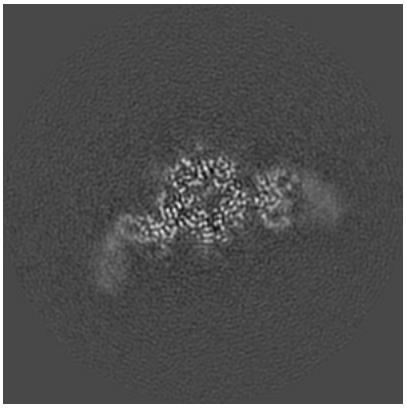
6.3.1 Primary map



X Index: 259



Y Index: 218

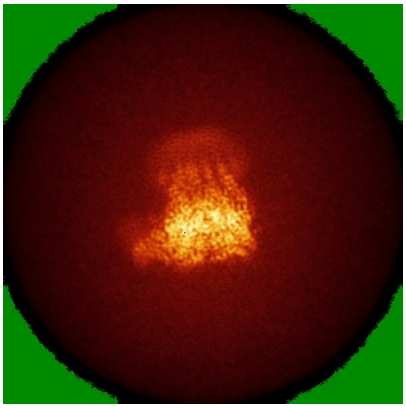


Z Index: 212

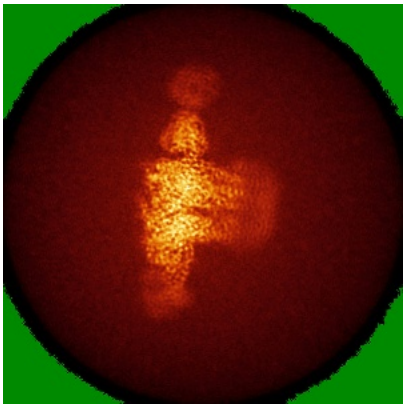
The images above show the largest variance slices of the map in three orthogonal directions.

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

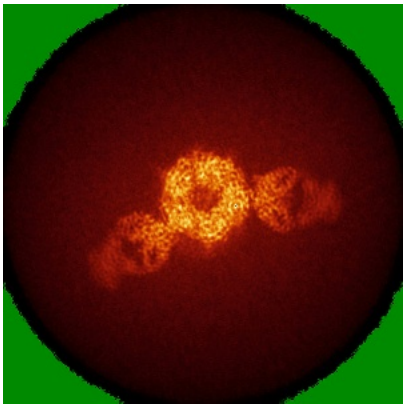
6.4.1 Primary map



X



Y



Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 7.68. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

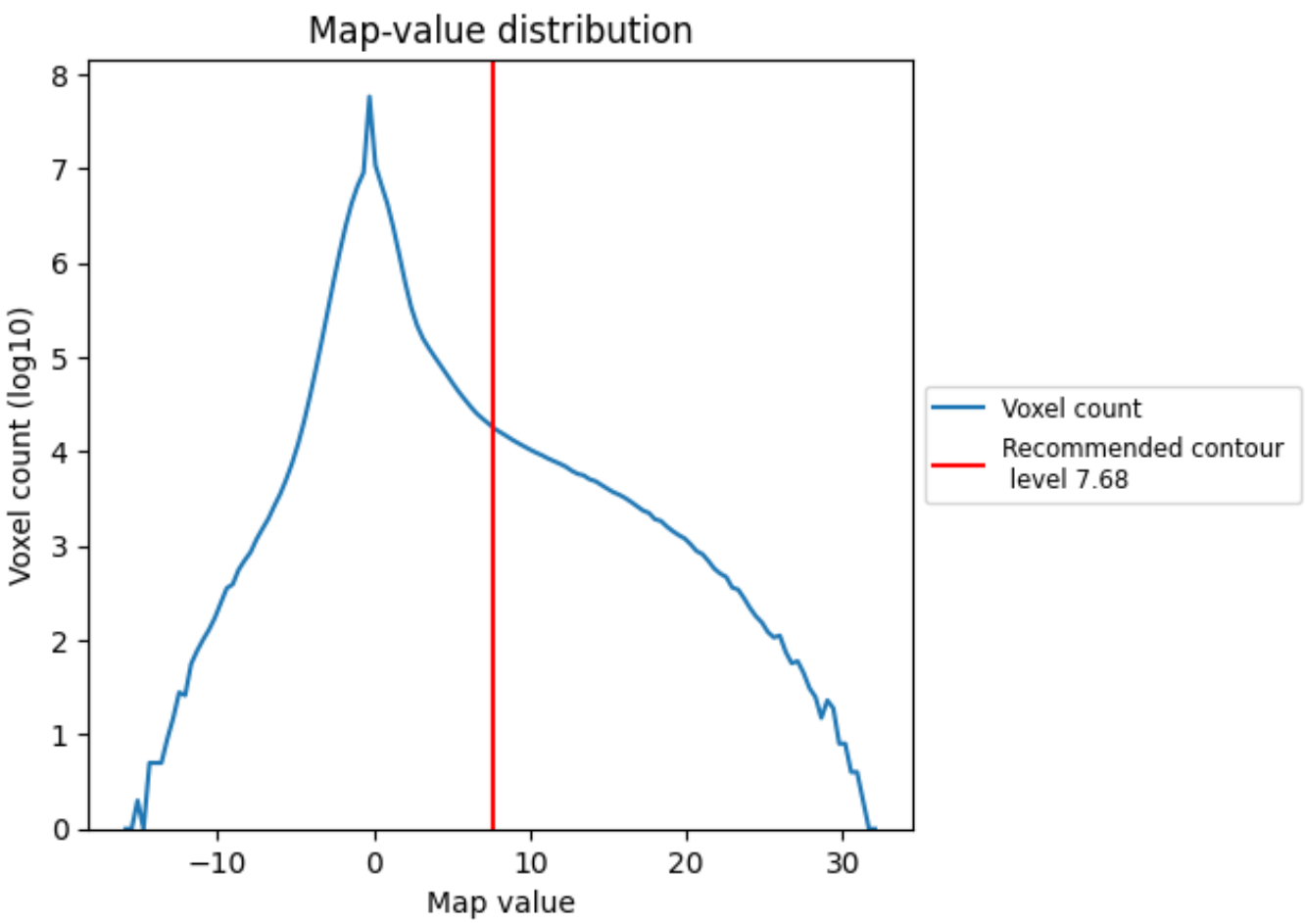
6.6 Mask visualisation (i)

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

7 Map analysis (i)

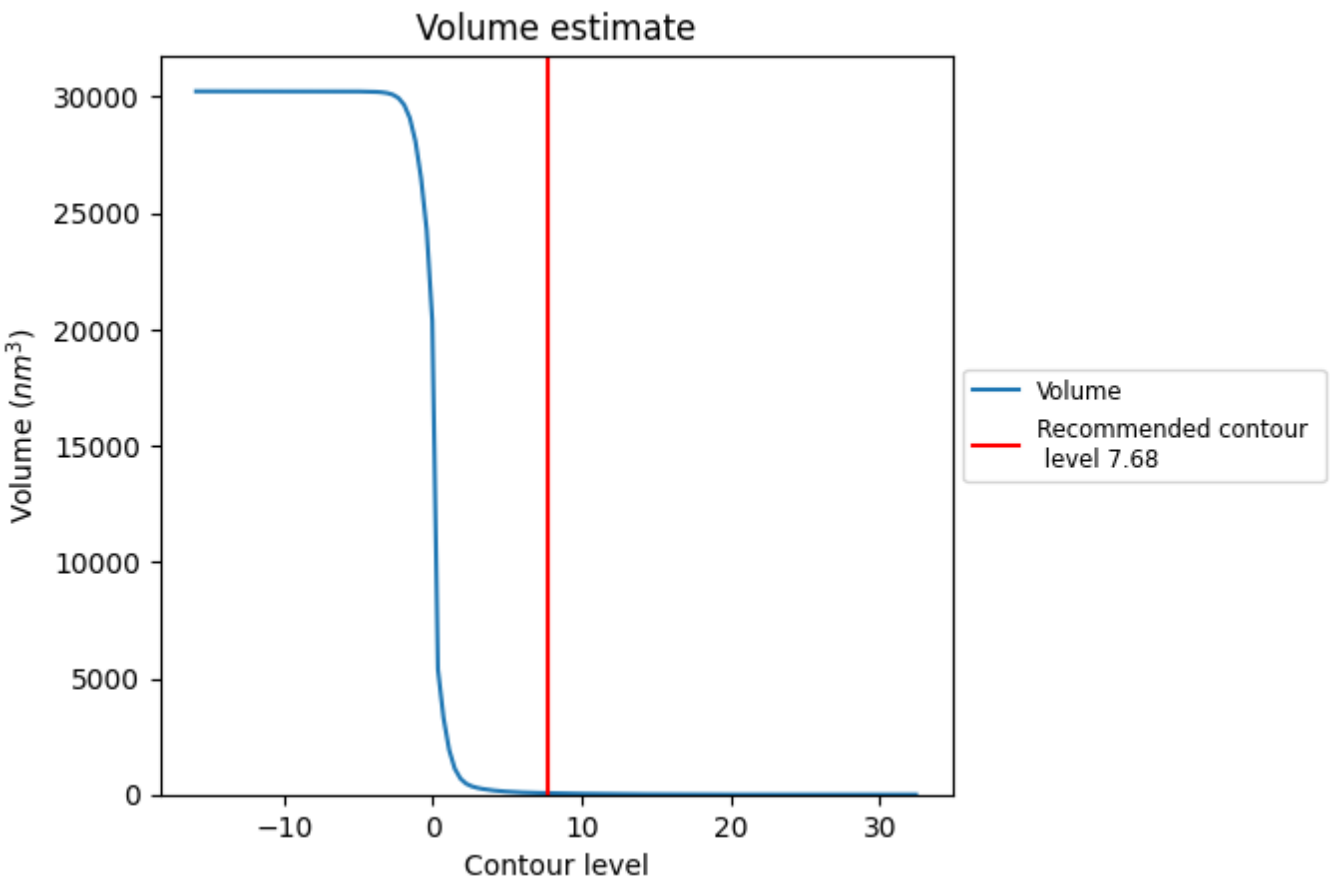
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution (i)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

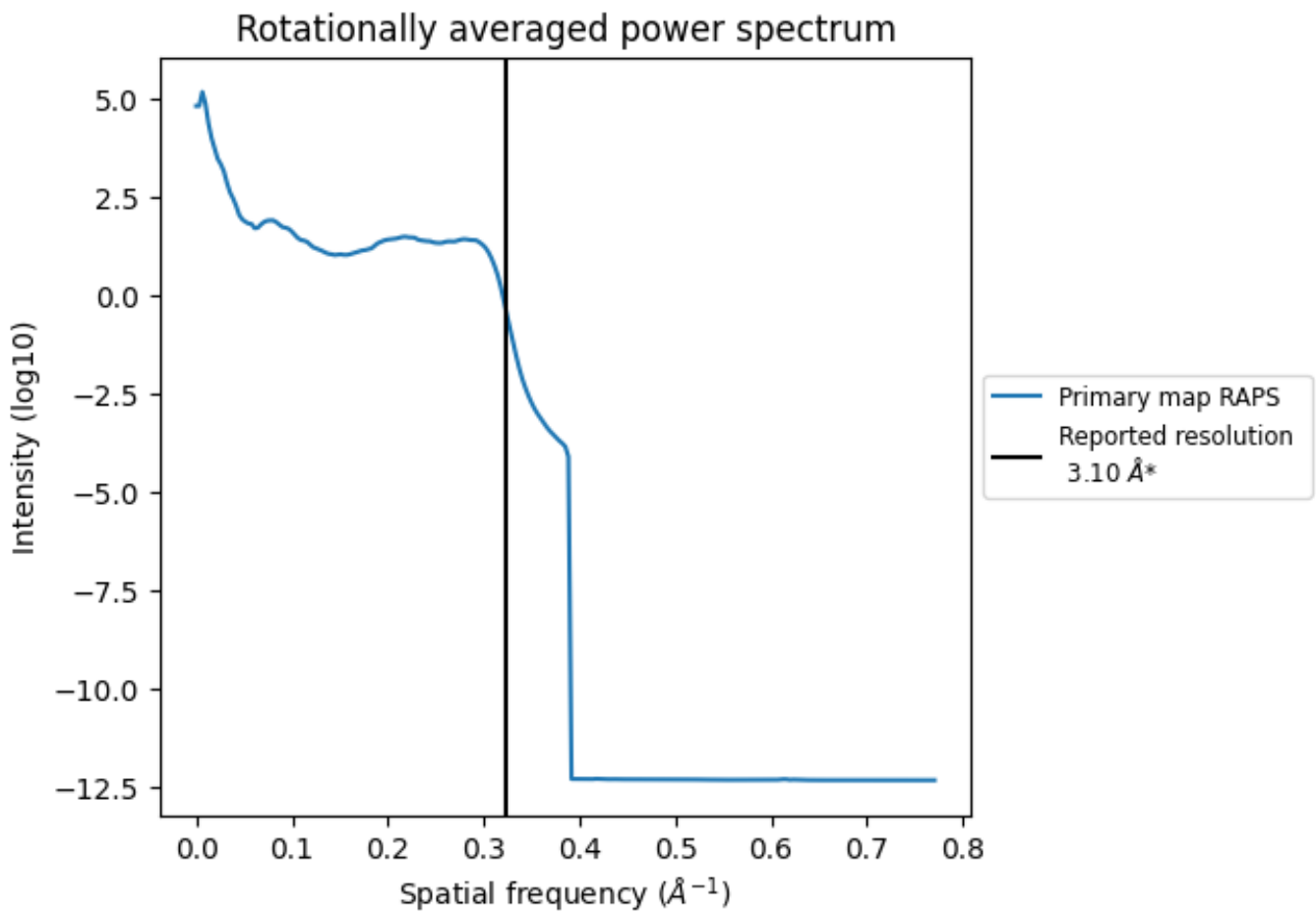
7.2 Volume estimate (i)



The volume at the recommended contour level is 60 nm^3; this corresponds to an approximate mass of 54 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 0.323 Å^{-1}

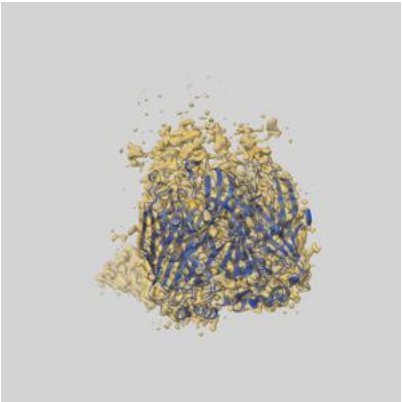
8 Fourier-Shell correlation (i)

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

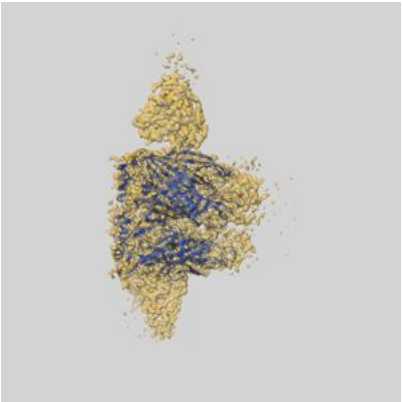
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-8923 and PDB model 6DW1. Per-residue inclusion information can be found in section 3 on page 9.

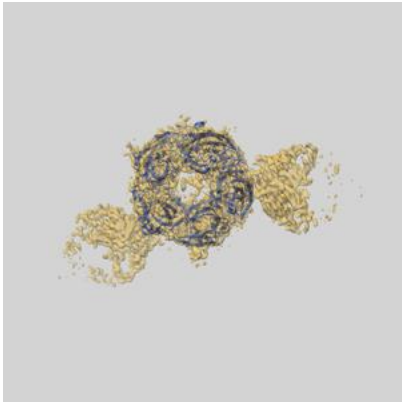
9.1 Map-model overlay (i)



X



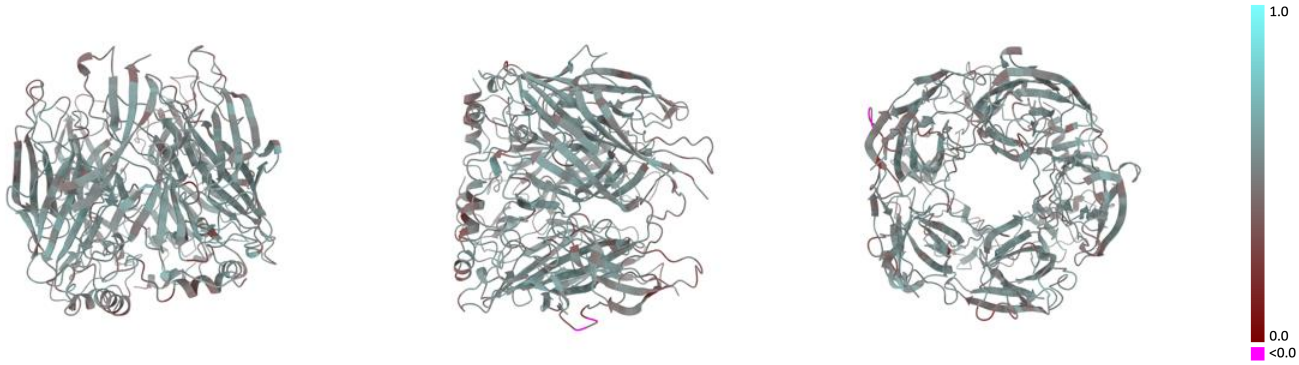
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 7.68 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.

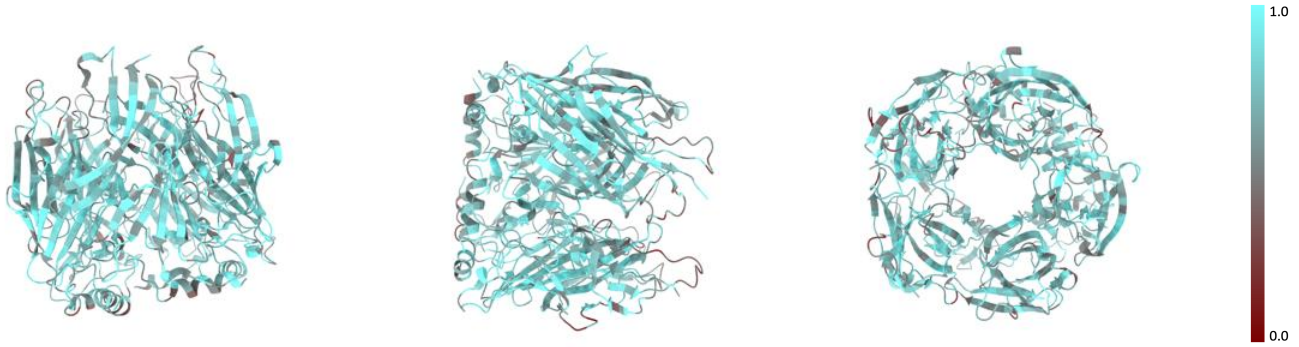
9.2 Q-score mapped to coordinate model (i)



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.

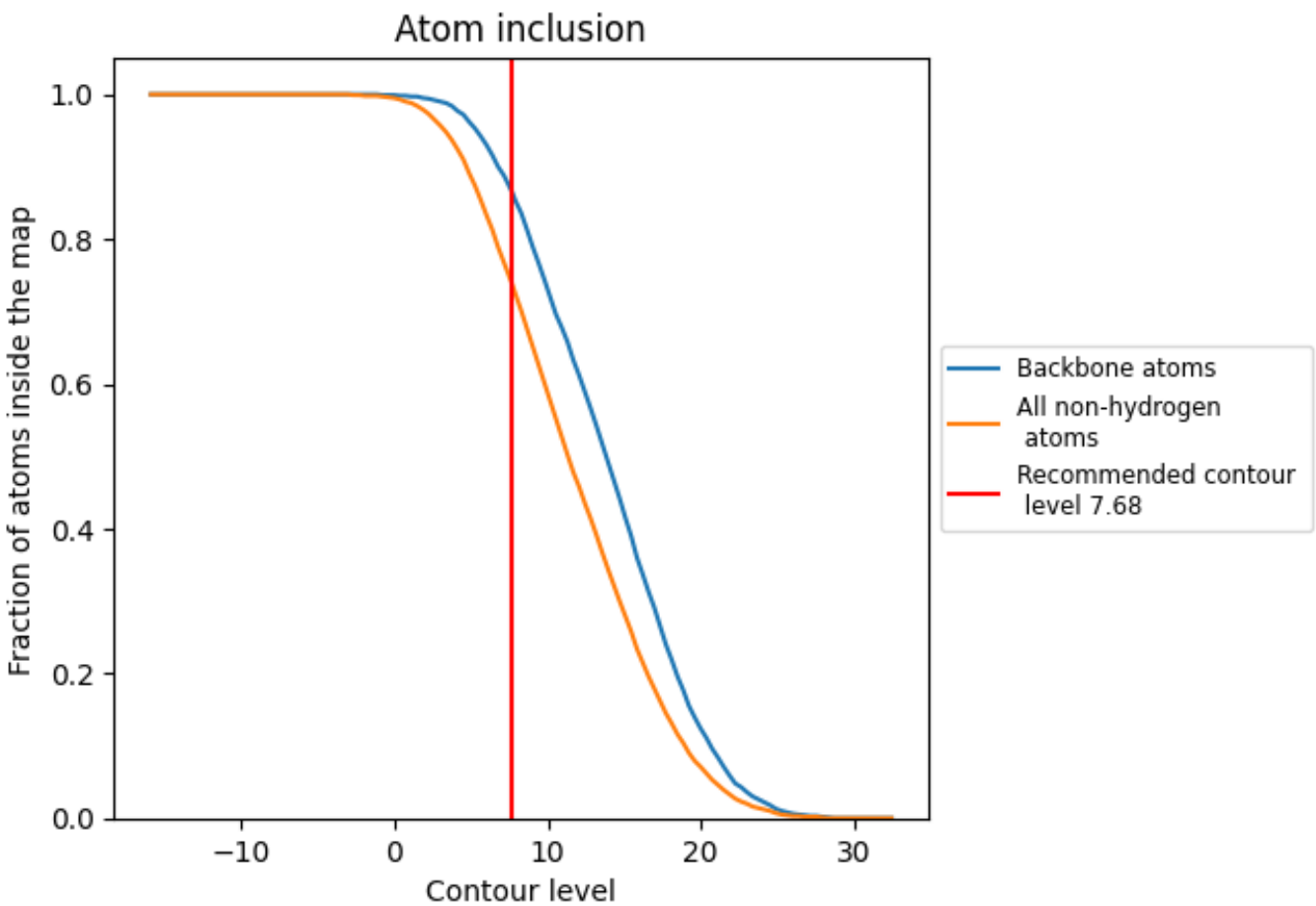
9.3 Atom inclusion mapped to coordinate model (i)



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 (7.68).

9.4 Atom inclusion (i)



At the recommended contour level, 86% of all backbone atoms, 74% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (7.68) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7380	0.5110
A	0.7520	0.5110
B	0.7470	0.5140
C	0.7460	0.5210
D	0.7480	0.4980
E	0.7470	0.5170
F	0.3800	0.4800
G	0.4700	0.4660
H	0.4100	0.4540
I	0.5000	0.4960
J	0.4100	0.4070
K	0.2860	0.4450