wwPDB EM Validation Summary Report

Nov 8, 2022 – 02:02 AM EST

PDB ID	:	6D03
EMDB ID	:	EMD-7783
Title	:	Cryo-EM structure of a Plasmodium vivax invasion complex essential for entry into human reticulocytes; one molecule of parasite ligand.
Authors	:	Gruszczyk, J.; Huang, R.K.; Hong, C.; Yu, Z.; Tham, W.H.
Deposited on	:	2018-04-10
Resolution	:	3.68 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 ⓘ symbol.

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

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

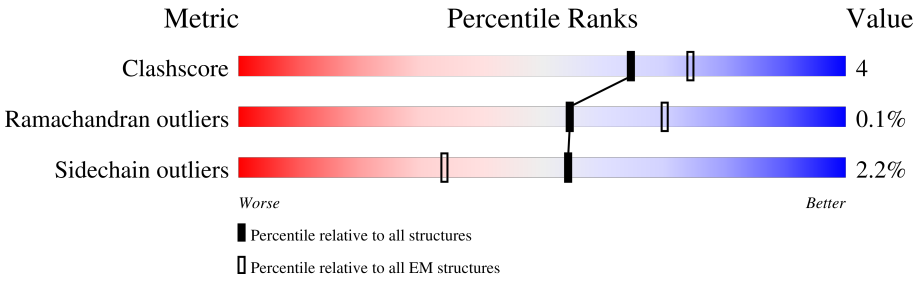
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

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 3.68 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	A	659	83% 14%
1	B	659	87% 10%
2	C	698	10% 83% 14%
2	D	698	11% 86% 11%
3	E	820	17% 47% 9% 43%
4	F	2	50% 50%
4	G	2	100%
4	H	2	100%

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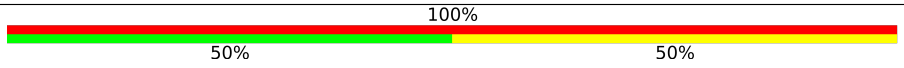
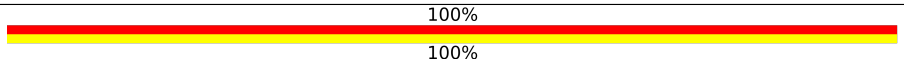
Mol	Chain	Length	Quality of chain
4	I	2	
4	K	2	
5	J	2	

2 Entry composition (i)

There are 9 unique types of molecules in this entry. The entry contains 24844 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 Transferrin receptor protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	641	Total	C	N	O	S	0	0
			5081	3260	855	952	14		
1	B	641	Total	C	N	O	S	0	0
			5081	3260	855	952	14		

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	102	ALA	-	expression tag	UNP P02786
A	103	ASP	-	expression tag	UNP P02786
A	104	PRO	-	expression tag	UNP P02786
A	105	HIS	-	expression tag	UNP P02786
A	106	HIS	-	expression tag	UNP P02786
A	107	HIS	-	expression tag	UNP P02786
A	108	HIS	-	expression tag	UNP P02786
A	109	HIS	-	expression tag	UNP P02786
A	110	HIS	-	expression tag	UNP P02786
A	111	SER	-	expression tag	UNP P02786
A	112	SER	-	expression tag	UNP P02786
A	113	GLY	-	expression tag	UNP P02786
A	114	ILE	-	expression tag	UNP P02786
A	115	GLU	-	expression tag	UNP P02786
A	116	GLY	-	expression tag	UNP P02786
A	117	ARG	-	expression tag	UNP P02786
A	118	GLY	-	expression tag	UNP P02786
A	119	GLU	-	expression tag	UNP P02786
A	120	PHE	-	expression tag	UNP P02786
A	142	SER	GLY	variant	UNP P02786
B	102	ALA	-	expression tag	UNP P02786
B	103	ASP	-	expression tag	UNP P02786
B	104	PRO	-	expression tag	UNP P02786
B	105	HIS	-	expression tag	UNP P02786
B	106	HIS	-	expression tag	UNP P02786
B	107	HIS	-	expression tag	UNP P02786

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Chain	Residue	Modelled	Actual	Comment	Reference
B	108	HIS	-	expression tag	UNP P02786
B	109	HIS	-	expression tag	UNP P02786
B	110	HIS	-	expression tag	UNP P02786
B	111	SER	-	expression tag	UNP P02786
B	112	SER	-	expression tag	UNP P02786
B	113	GLY	-	expression tag	UNP P02786
B	114	ILE	-	expression tag	UNP P02786
B	115	GLU	-	expression tag	UNP P02786
B	116	GLY	-	expression tag	UNP P02786
B	117	ARG	-	expression tag	UNP P02786
B	118	GLY	-	expression tag	UNP P02786
B	119	GLU	-	expression tag	UNP P02786
B	120	PHE	-	expression tag	UNP P02786
B	142	SER	GLY	variant	UNP P02786

- Molecule 2 is a protein called Serotransferrin.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	679	Total	C	N	O	S	0	0
			5266	3305	912	1002	47		
2	D	679	Total	C	N	O	S	0	0
			5266	3305	912	1002	47		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	429	VAL	ILE	variant	UNP P02787
D	429	VAL	ILE	variant	UNP P02787

- Molecule 3 is a protein called Reticulocyte binding protein 2, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	E	466	Total	C	N	O	S	0	0
			3904	2495	650	749	10		

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	150	GLY	-	expression tag	UNP A5K736
E	151	ALA	-	expression tag	UNP A5K736
E	152	MET	-	expression tag	UNP A5K736
E	153	GLY	-	expression tag	UNP A5K736

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Chain	Residue	Modelled	Actual	Comment	Reference
E	154	SER	-	expression tag	UNP A5K736
E	155	MET	-	expression tag	UNP A5K736
E	168	SER	ILE	variant	UNP A5K736

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

Mol	Chain	Residues	Atoms	AltConf	Trace
4	F	2	Total C N O 28 16 2 10	0	0
4	G	2	Total C N O 28 16 2 10	0	0
4	H	2	Total C N O 28 16 2 10	0	0
4	I	2	Total C N O 28 16 2 10	0	0
4	K	2	Total C N O 28 16 2 10	0	0

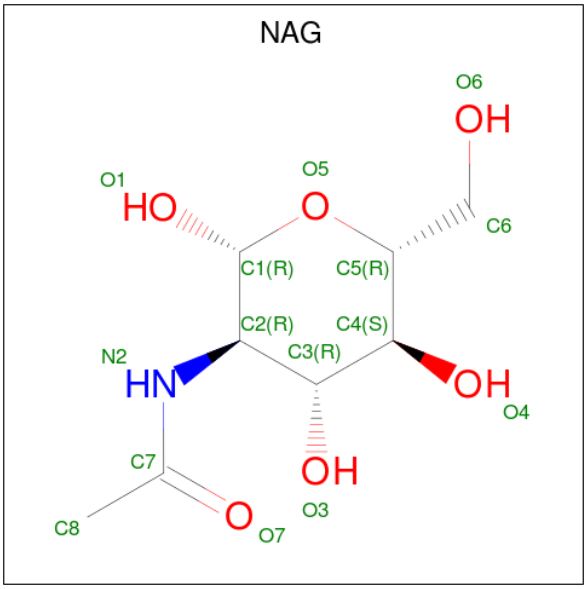
- Molecule 5 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(2-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

Mol	Chain	Residues	Atoms	AltConf	Trace
5	J	2	Total C N O 28 16 2 10	0	0

- Molecule 6 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	AltConf
6	A	1	Total Ca 1 1	0
6	B	1	Total Ca 1 1	0

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

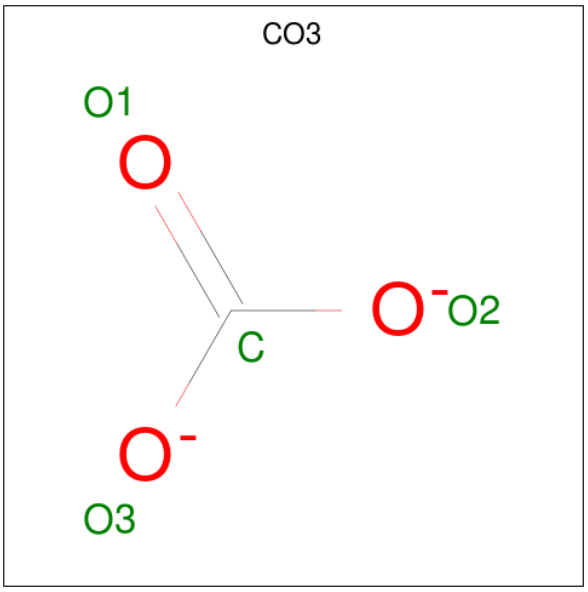


Mol	Chain	Residues	Atoms				AltConf
7	A	1	Total	C	N	O	0
			14	8	1	5	
7	B	1	Total	C	N	O	0
			14	8	1	5	
7	C	1	Total	C	N	O	0
			14	8	1	5	
7	D	1	Total	C	N	O	0
			14	8	1	5	

- Molecule 8 is FE (III) ION (three-letter code: FE) (formula: Fe).

Mol	Chain	Residues	Atoms		AltConf
8	C	2	Total	Fe	0
			2	2	
8	D	2	Total	Fe	0
			2	2	

- Molecule 9 is CARBONATE ION (three-letter code: CO3) (formula: CO_3).



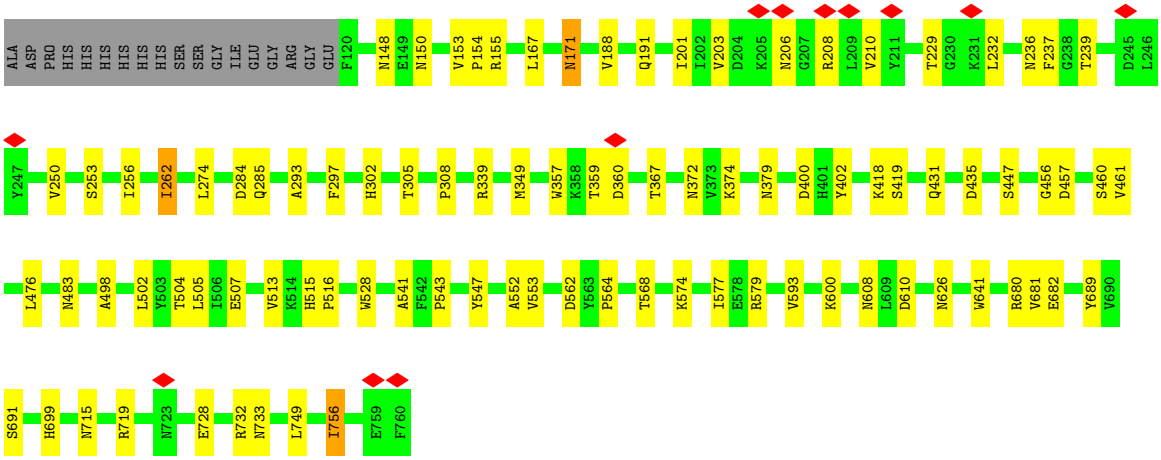
Mol	Chain	Residues	Atoms			AltConf
9	C	1	Total	C	O	0
			8	2	6	
9	C	1	Total	C	O	0
			8	2	6	
9	D	1	Total	C	O	0
			8	2	6	
9	D	1	Total	C	O	0
			8	2	6	

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.

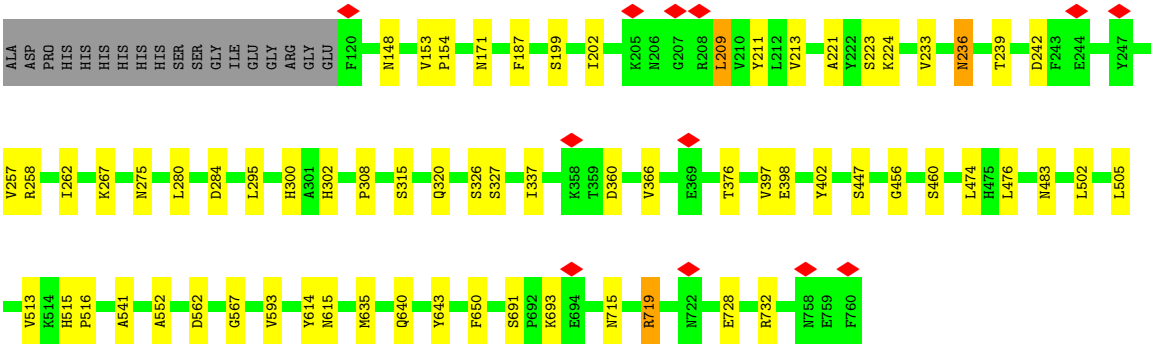
• Molecule 1: Transferrin receptor protein 1

Chain A:



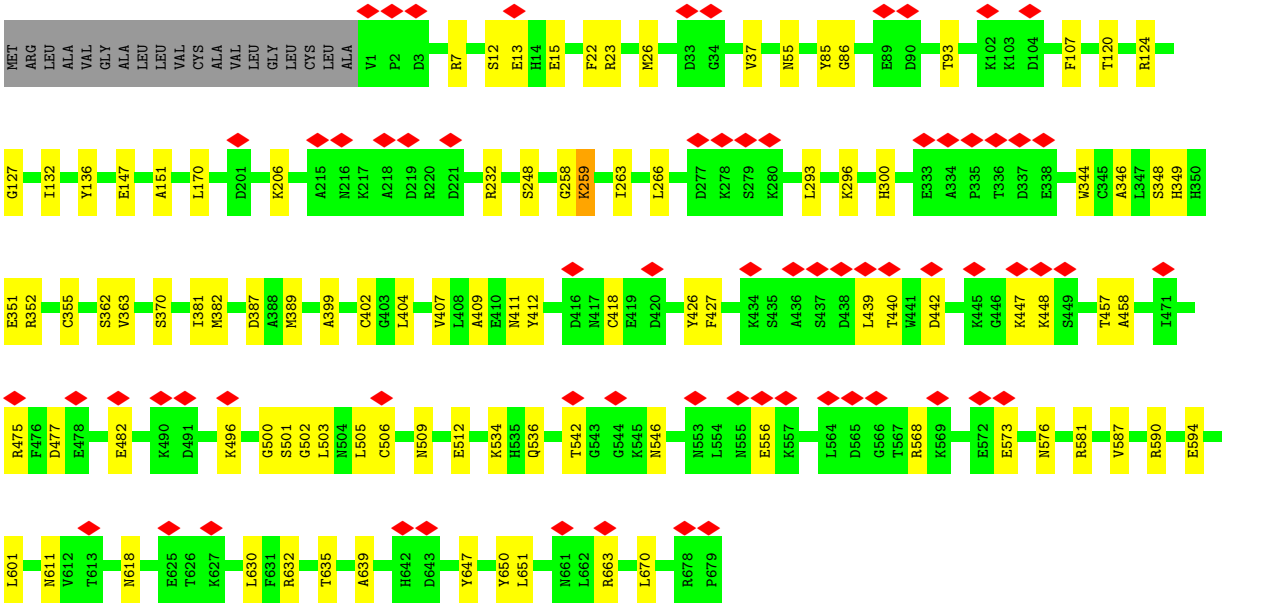
• Molecule 1: Transferrin receptor protein 1

Chain B:



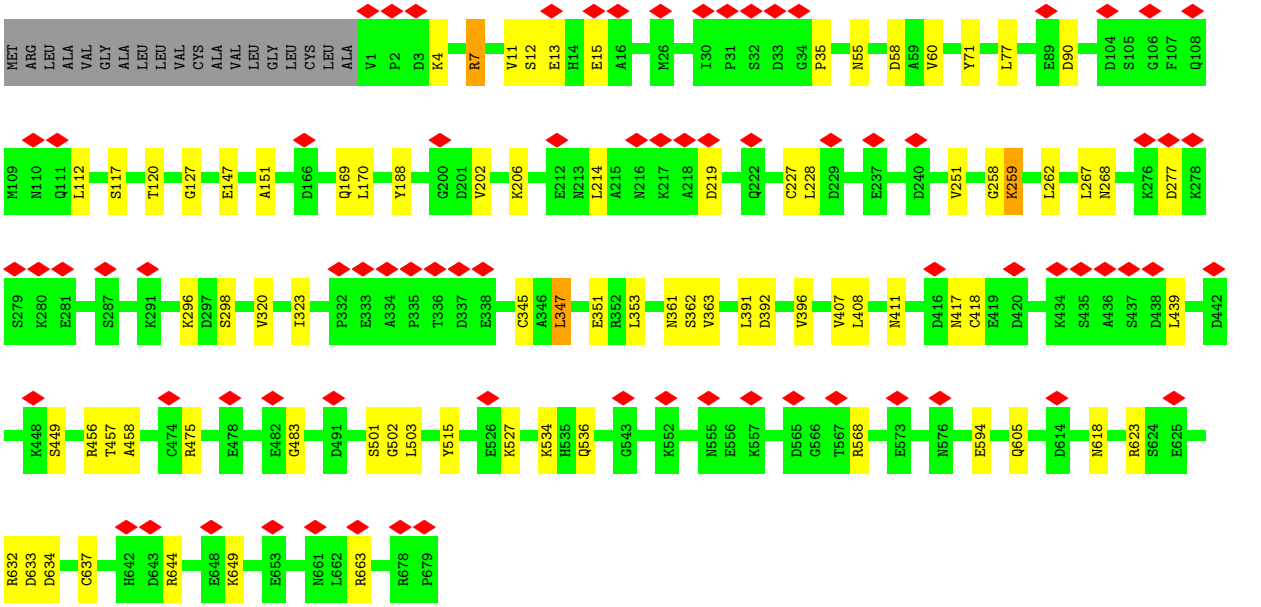
• Molecule 2: Serotransferrin

Chain C:



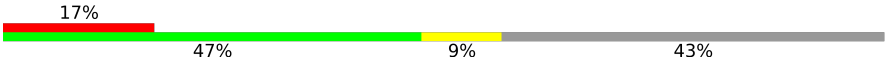
• Molecule 2: Serotransferrin

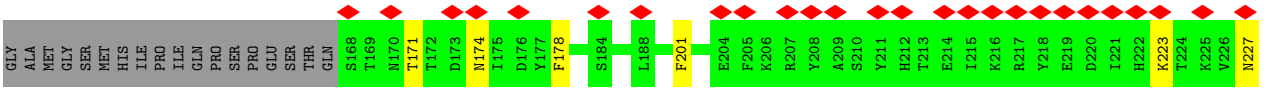
Chain D:

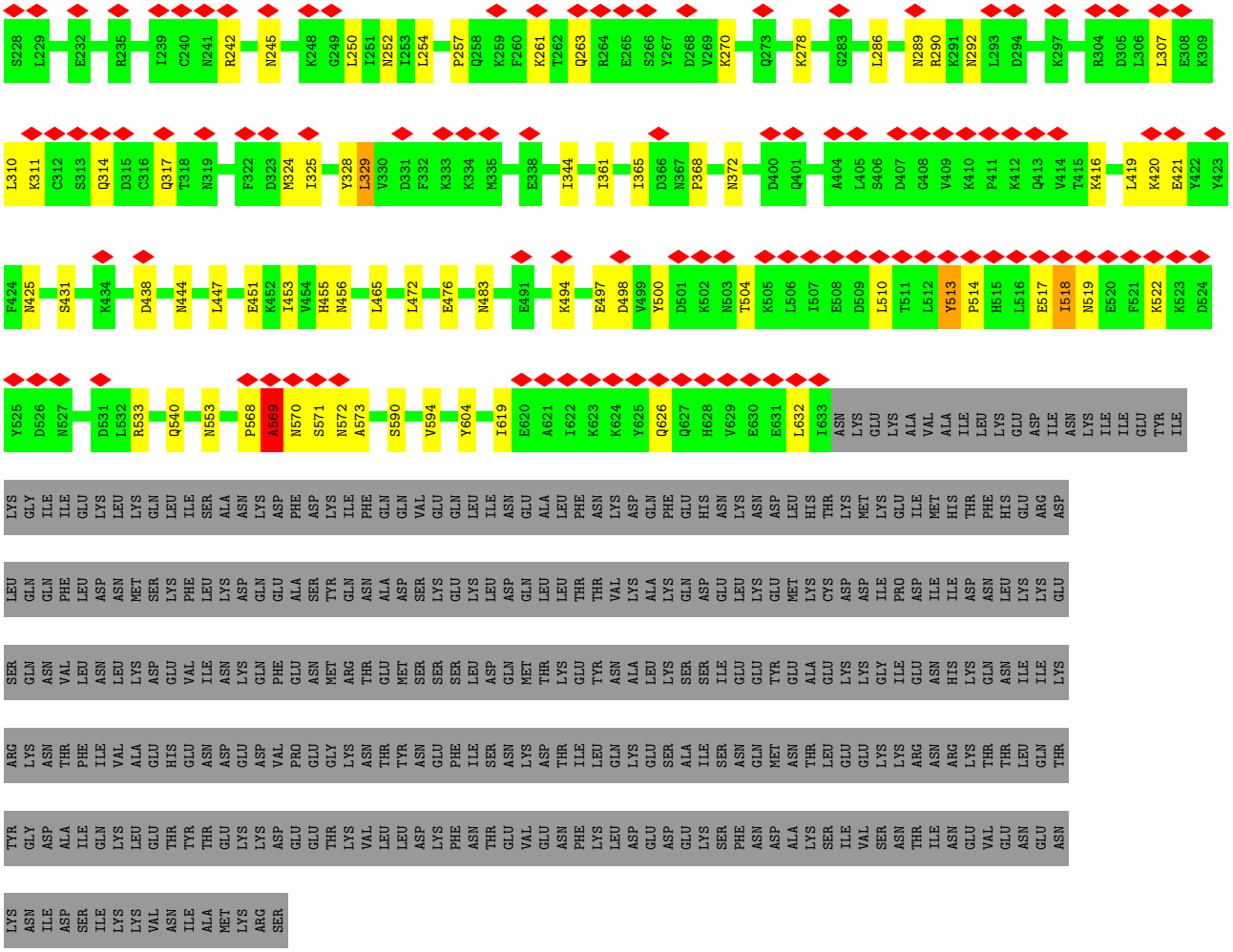


• Molecule 3: Reticulocyte binding protein 2, putative

Chain E:





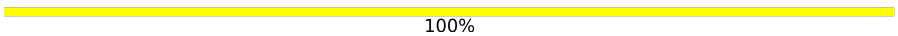


• Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain F:

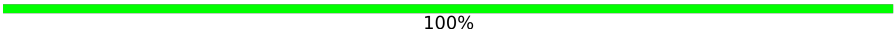
• Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain G:



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

Chain H:

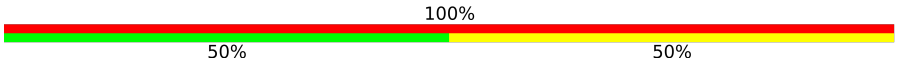


• Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain I:

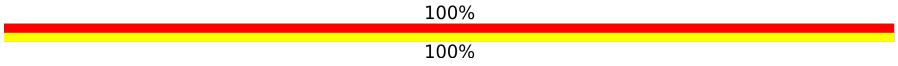
• Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain K:



• Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(2-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain J:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	637649	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 ($e^-/Å^2$)	80	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	37037	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.462	Depositor
Minimum map value	-0.349	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.017	Depositor
Recommended contour level	0.081	Depositor
Map size (Å)	243.0, 243.0, 243.0	wwPDB
Map dimensions	180, 180, 180	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.35, 1.35, 1.35	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NAG, CA, CO3, FE

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	0.49	0/5203	0.64	2/7053 (0.0%)
1	B	0.50	0/5203	0.62	3/7053 (0.0%)
2	C	0.43	0/5386	0.61	3/7280 (0.0%)
2	D	0.42	0/5386	0.62	6/7280 (0.1%)
3	E	0.40	0/3973	0.60	3/5337 (0.1%)
All	All	0.45	0/25151	0.62	17/34003 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
3	E	0	2
All	All	0	4

There are no bond length outliers.

The worst 5 of 17 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	476	LEU	CA-CB-CG	6.79	130.92	115.30
1	B	209	LEU	CA-CB-CG	6.55	130.37	115.30
2	D	112	LEU	CA-CB-CG	6.22	129.61	115.30
2	D	347	LEU	CA-CB-CG	6.12	129.38	115.30
2	C	503	LEU	CA-CB-CG	6.04	129.19	115.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	756	ILE	Peptide
1	B	567	GLY	Peptide
3	E	513	TYR	Peptide
3	E	569	ALA	Peptide

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5081	0	5009	47	0
1	B	5081	0	5010	32	0
2	C	5266	0	5086	56	0
2	D	5266	0	5085	38	0
3	E	3904	0	3918	39	0
4	F	28	0	25	0	0
4	G	28	0	25	0	0
4	H	28	0	25	0	0
4	I	28	0	25	0	0
4	K	28	0	25	0	0
5	J	28	0	24	0	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
7	A	14	0	13	0	0
7	B	14	0	13	0	0
7	C	14	0	13	0	0
7	D	14	0	13	0	0
8	C	2	0	0	0	0
8	D	2	0	0	0	0
9	C	8	0	0	2	0
9	D	8	0	0	1	0
All	All	24844	0	24309	208	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 208 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:543:PRO:O	1:A:547:TYR:HB3	1.77	0.84
2:C:132:ILE:O	2:C:136:TYR:HB2	1.82	0.79
1:A:203:VAL:O	1:A:372:ASN:HB3	1.82	0.79
2:D:449:SER:O	2:D:483:GLY:HA2	1.90	0.71
3:E:421:GLU:O	3:E:425:ASN:HB2	1.91	0.70

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	639/659 (97%)	606 (95%)	33 (5%)	0	100	100
1	B	639/659 (97%)	608 (95%)	31 (5%)	0	100	100
2	C	677/698 (97%)	633 (94%)	44 (6%)	0	100	100
2	D	677/698 (97%)	632 (93%)	45 (7%)	0	100	100
3	E	464/820 (57%)	450 (97%)	12 (3%)	2 (0%)	34	69
All	All	3096/3534 (88%)	2929 (95%)	165 (5%)	2 (0%)	54	83

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	E	519	ASN
3	E	518	ILE

5.3.2 Protein sidechains (i)

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

The Analysed column shows the number of residues for which the sidechain conformation was

analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	550/564 (98%)	539 (98%)	11 (2%)	55	74
1	B	550/564 (98%)	540 (98%)	10 (2%)	59	77
2	C	572/585 (98%)	562 (98%)	10 (2%)	60	79
2	D	572/585 (98%)	559 (98%)	13 (2%)	50	71
3	E	442/775 (57%)	428 (97%)	14 (3%)	39	64
All	All	2686/3073 (87%)	2628 (98%)	58 (2%)	54	72

5 of 58 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	C	546	ASN
3	E	456	ASN
2	D	268	ASN
3	E	453	ILE
3	E	311	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 38 such sidechains are listed below:

Mol	Chain	Res	Type
2	D	618	ASN
3	E	428	ASN
3	E	174	ASN
3	E	289	ASN
3	E	483	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)

12 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	1,4	14,14,15	0.27	0	17,19,21	1.52	2 (11%)
4	NAG	F	2	4	14,14,15	0.23	0	17,19,21	0.52	0
4	NAG	G	1	1,4	14,14,15	0.54	0	17,19,21	1.06	1 (5%)
4	NAG	G	2	4	14,14,15	0.69	1 (7%)	17,19,21	0.66	0
4	NAG	H	1	1,4	14,14,15	0.61	0	17,19,21	0.56	0
4	NAG	H	2	4	14,14,15	0.41	0	17,19,21	0.39	0
4	NAG	I	1	1,4	14,14,15	0.57	0	17,19,21	1.08	1 (5%)
4	NAG	I	2	4	14,14,15	0.40	0	17,19,21	0.43	0
5	NAG	J	1	2,5	14,14,15	0.42	0	17,19,21	0.88	1 (5%)
5	NAG	J	2	5	14,14,15	0.60	0	17,19,21	0.92	1 (5%)
4	NAG	K	1	4,2	14,14,15	0.41	0	17,19,21	0.67	0
4	NAG	K	2	4	14,14,15	1.36	1 (7%)	17,19,21	1.48	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
4	NAG	F	1	1,4	-	1/6/23/26	0/1/1/1
4	NAG	F	2	4	-	0/6/23/26	0/1/1/1
4	NAG	G	1	1,4	-	1/6/23/26	0/1/1/1
4	NAG	G	2	4	-	4/6/23/26	0/1/1/1
4	NAG	H	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	H	2	4	-	2/6/23/26	0/1/1/1
4	NAG	I	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	I	2	4	-	2/6/23/26	0/1/1/1
5	NAG	J	1	2,5	-	2/6/23/26	0/1/1/1
5	NAG	J	2	5	-	3/6/23/26	0/1/1/1
4	NAG	K	1	4,2	-	4/6/23/26	0/1/1/1
4	NAG	K	2	4	-	2/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	K	2	NAG	O5-C1	4.87	1.51	1.43
4	G	2	NAG	C1-C2	2.37	1.55	1.52

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	K	2	NAG	C1-O5-C5	5.74	119.97	112.19
4	F	1	NAG	C1-O5-C5	4.83	118.74	112.19
4	I	1	NAG	C2-N2-C7	3.22	127.48	122.90
5	J	2	NAG	C2-N2-C7	3.18	127.43	122.90
4	G	1	NAG	C2-N2-C7	3.14	127.38	122.90

There are no chirality outliers.

5 of 25 torsion outliers are listed below:

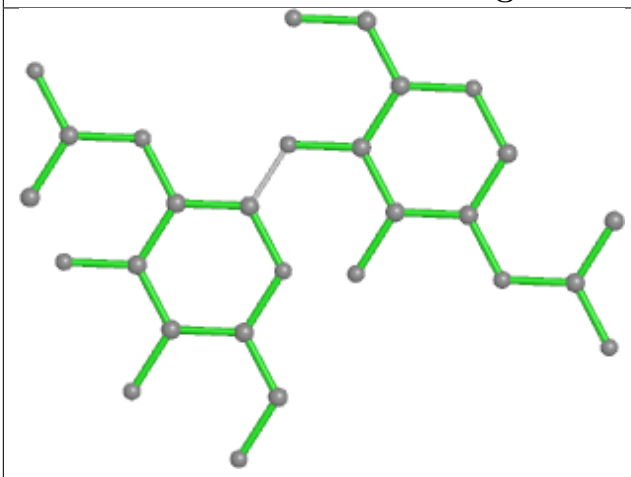
Mol	Chain	Res	Type	Atoms
4	I	2	NAG	O5-C5-C6-O6
5	J	2	NAG	O5-C5-C6-O6
4	I	2	NAG	C4-C5-C6-O6
4	G	2	NAG	C8-C7-N2-C2
4	G	2	NAG	O7-C7-N2-C2

There are no ring outliers.

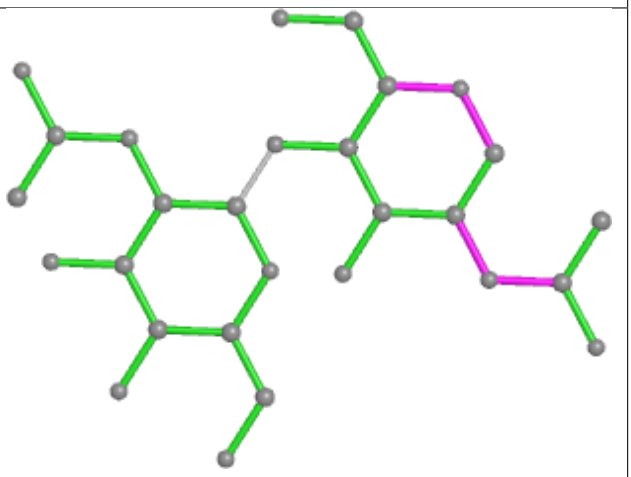
No monomer is involved in short contacts.

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

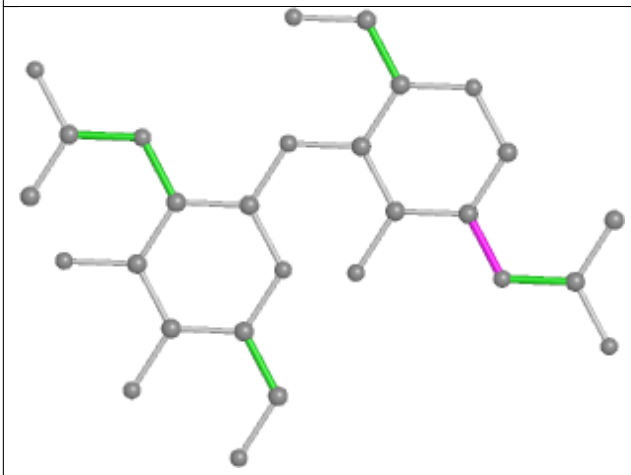
Oligosaccharide Chain F



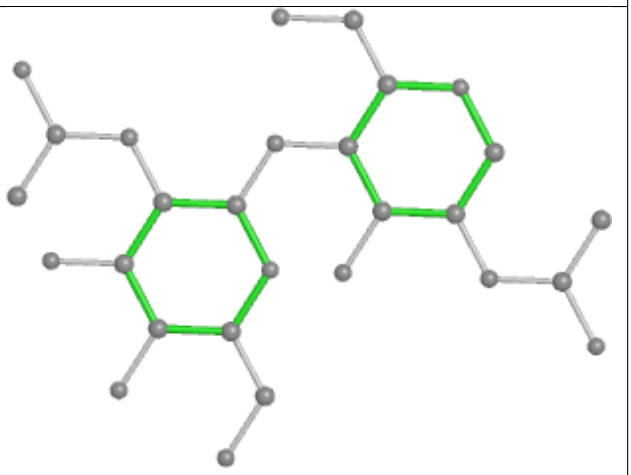
Bond lengths



Bond angles

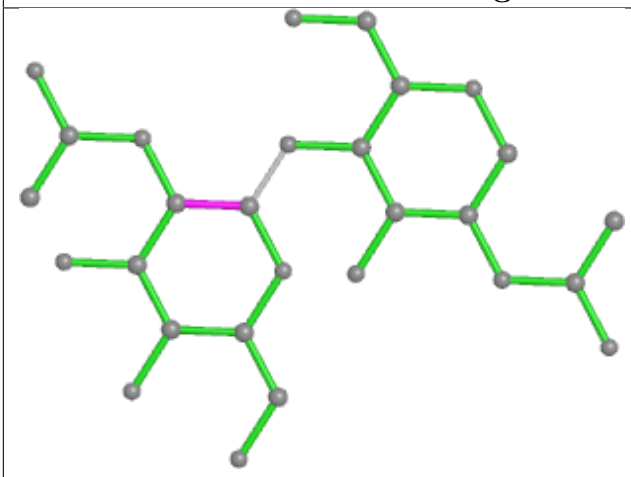


Torsions

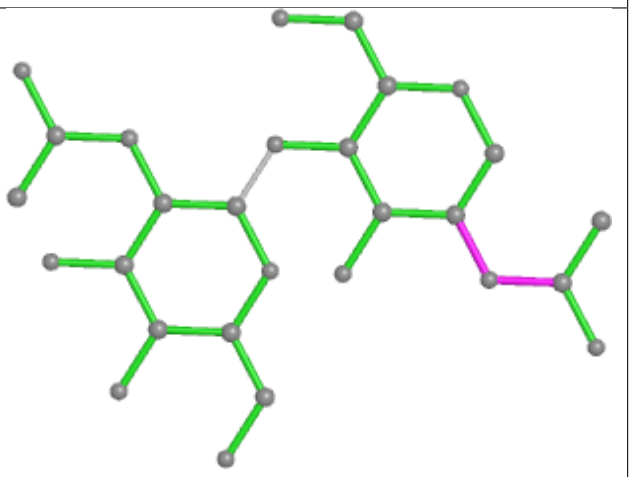


Rings

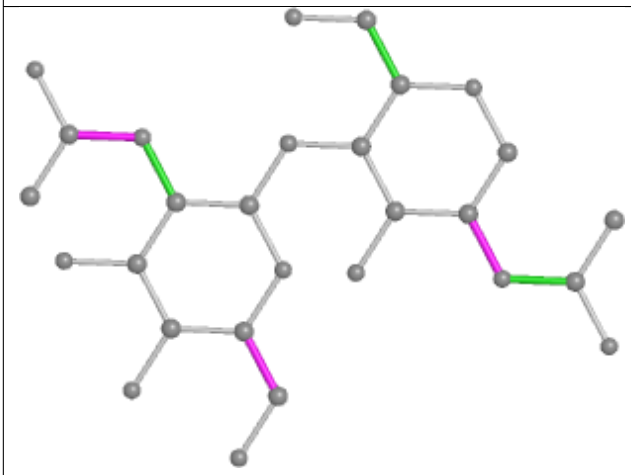
Oligosaccharide Chain G



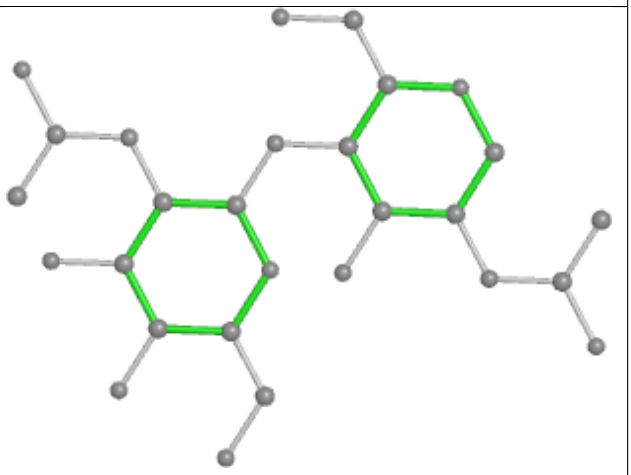
Bond lengths



Bond angles

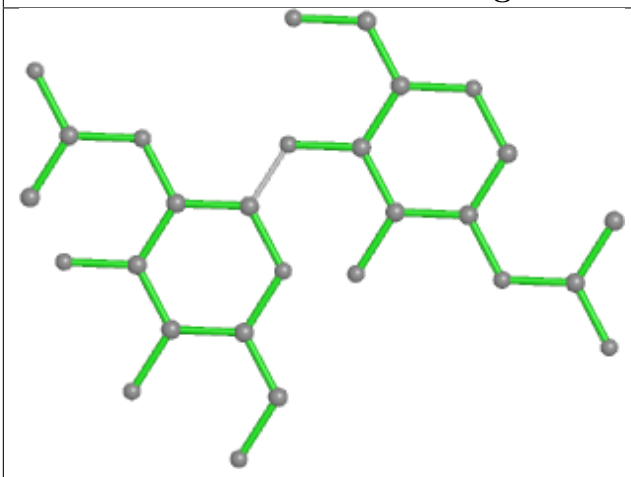


Torsions

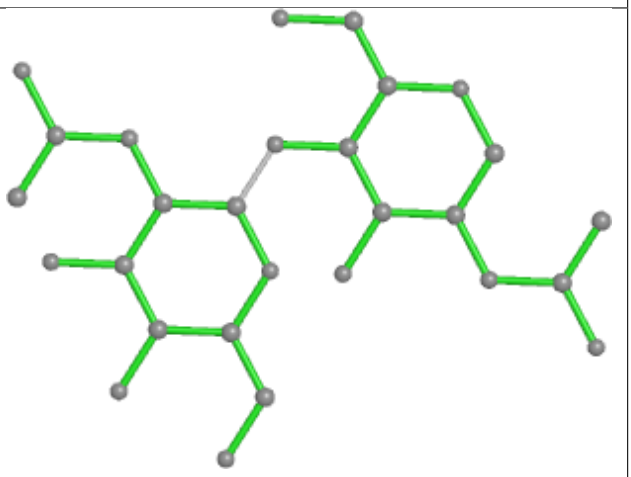


Rings

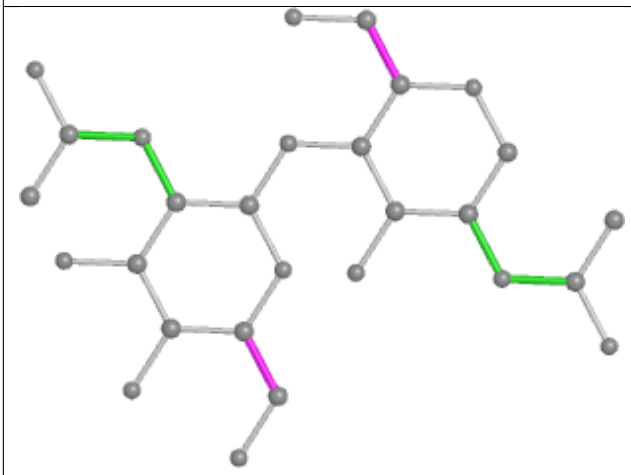
Oligosaccharide Chain H



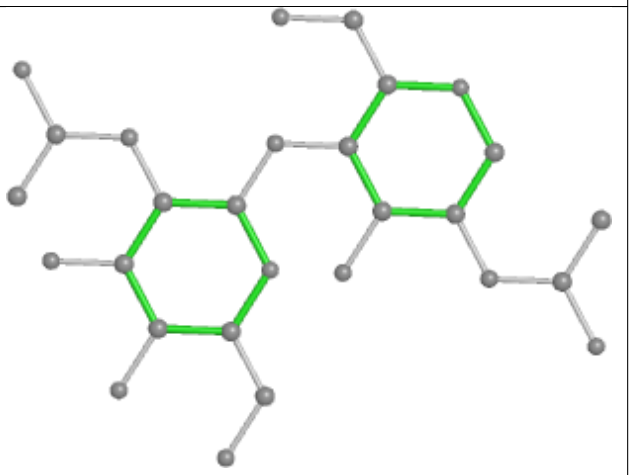
Bond lengths



Bond angles

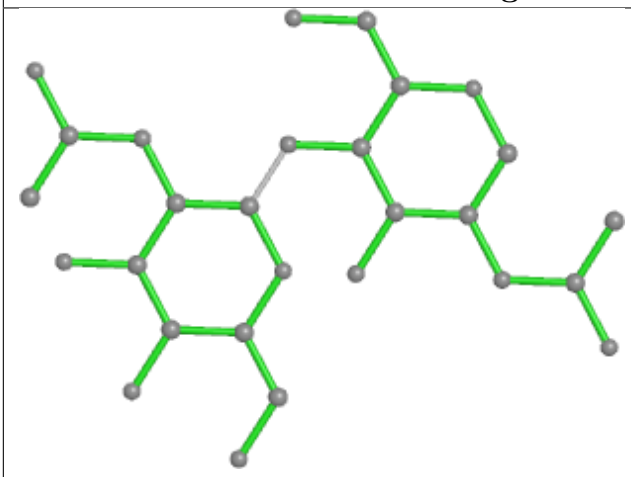


Torsions

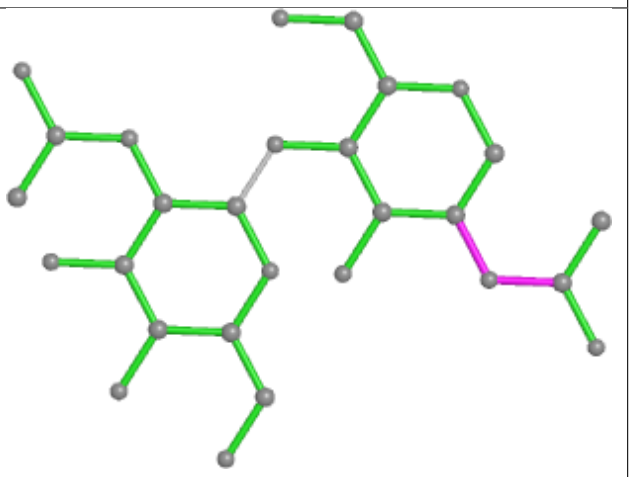


Rings

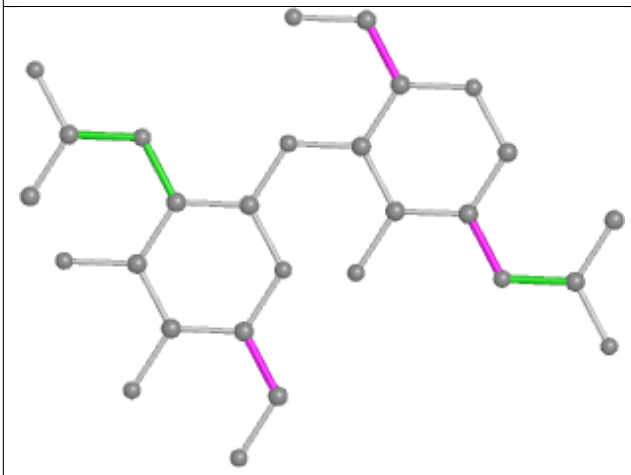
Oligosaccharide Chain I



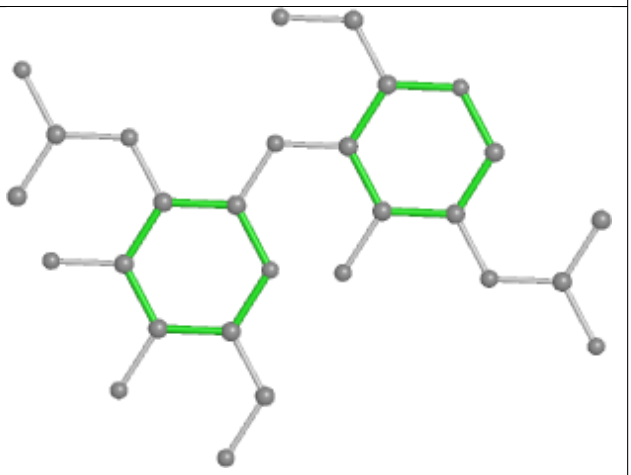
Bond lengths



Bond angles

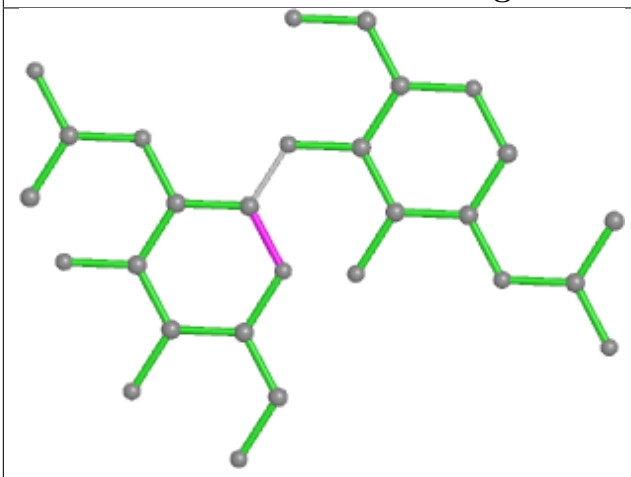


Torsions

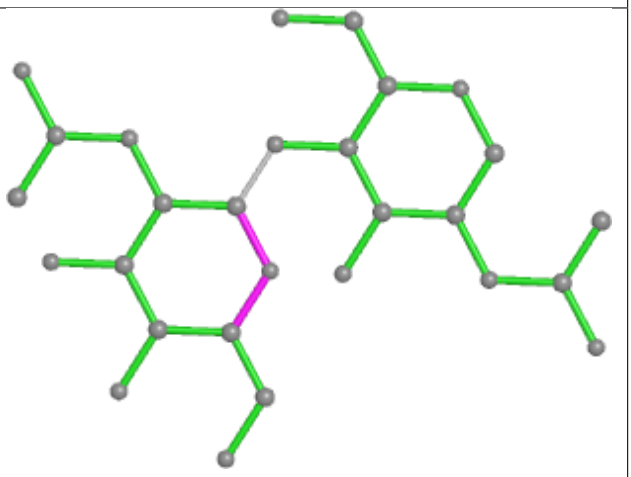


Rings

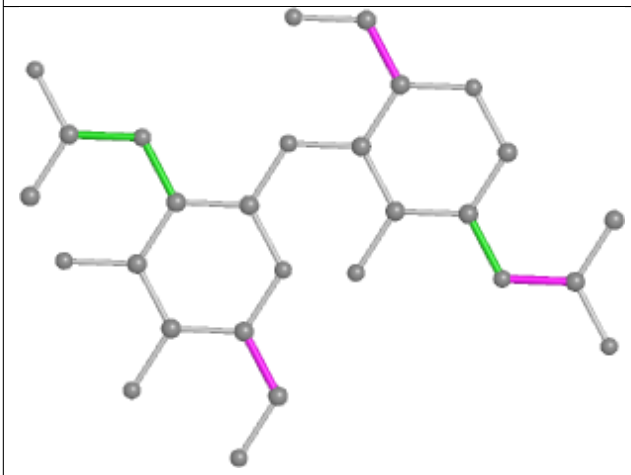
Oligosaccharide Chain K



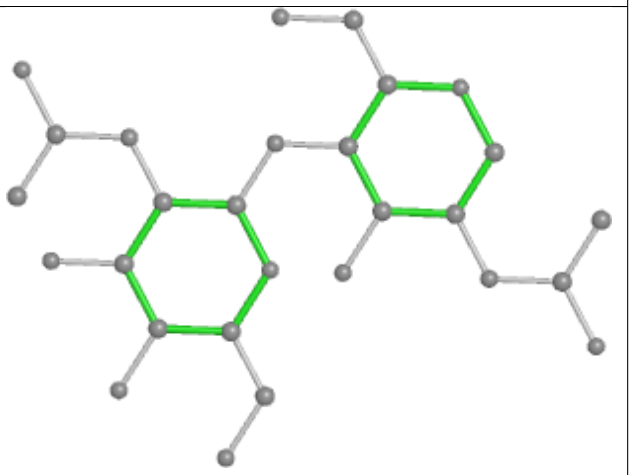
Bond lengths



Bond angles

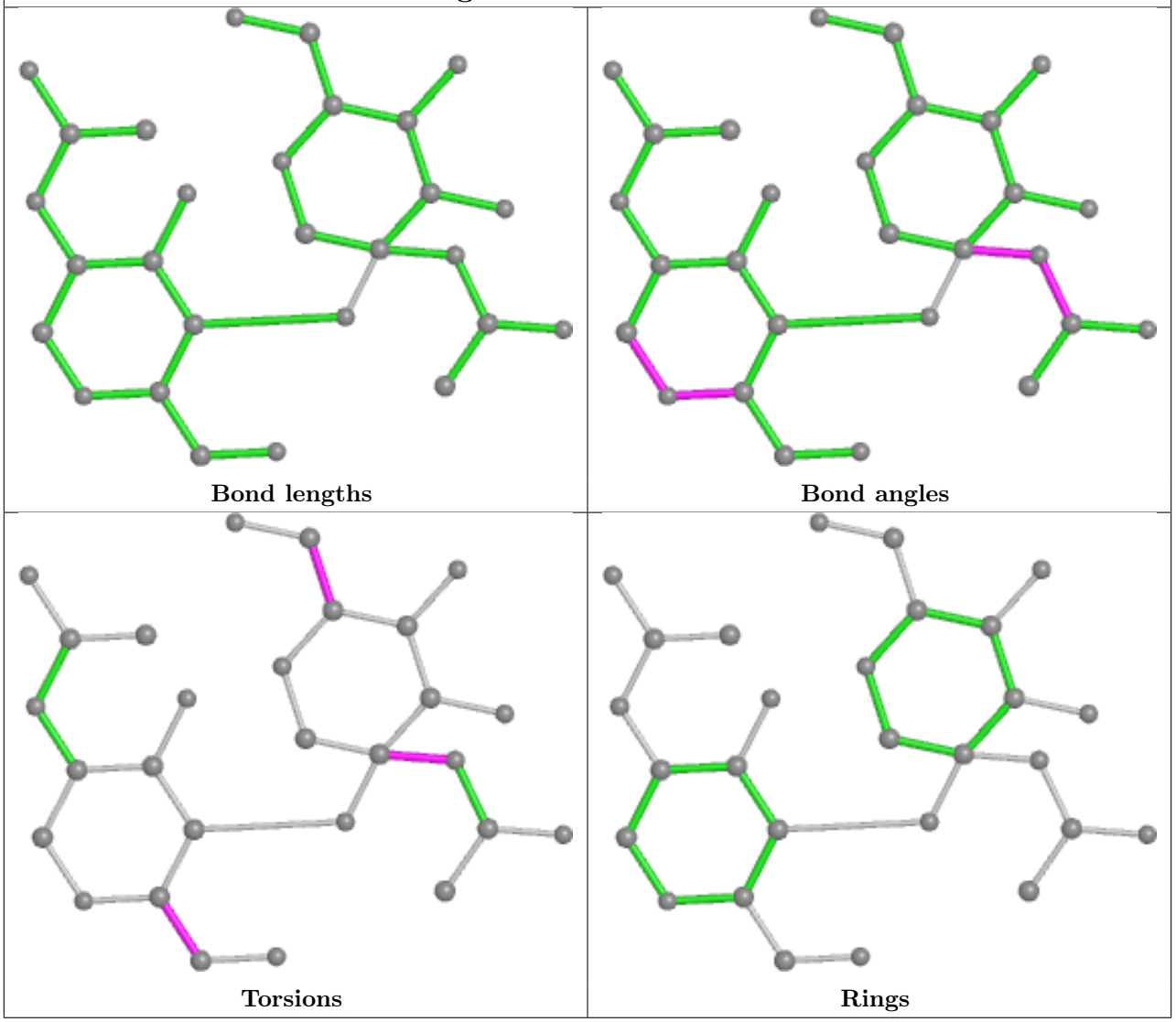


Torsions



Rings

Oligosaccharide Chain J



5.6 Ligand geometry (i)

Of 14 ligands modelled in this entry, 6 are monoatomic - leaving 8 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	B	802	1	14,14,15	0.51	0	17,19,21	0.64	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
9	CO3	C	704	8	2,3,3	0.44	0	2,3,3	0.16	0
9	CO3	D	704	8	2,3,3	0.42	0	2,3,3	0.46	0
9	CO3	D	702	8	2,3,3	0.53	0	2,3,3	0.20	0
7	NAG	A	802	1	14,14,15	0.50	0	17,19,21	0.57	0
7	NAG	D	707	2	14,14,15	1.23	1 (7%)	17,19,21	1.31	1 (5%)
9	CO3	C	702	8	2,3,3	0.45	0	2,3,3	0.17	0
7	NAG	C	707	2	14,14,15	0.37	0	17,19,21	0.65	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	NAG	C	707	2	-	2/6/23/26	0/1/1/1
7	NAG	A	802	1	-	2/6/23/26	0/1/1/1
7	NAG	B	802	1	-	2/6/23/26	0/1/1/1
7	NAG	D	707	2	-	0/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	D	707	NAG	O5-C1	4.18	1.50	1.43

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	D	707	NAG	C1-O5-C5	5.12	119.13	112.19
7	C	707	NAG	C1-O5-C5	2.29	115.30	112.19
7	B	802	NAG	C1-O5-C5	2.13	115.08	112.19

There are no chirality outliers.

5 of 6 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	802	NAG	O5-C5-C6-O6
7	A	802	NAG	C4-C5-C6-O6
7	B	802	NAG	O5-C5-C6-O6
7	C	707	NAG	O5-C5-C6-O6
7	C	707	NAG	C4-C5-C6-O6

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	C	704	CO3	1	0
9	D	702	CO3	1	0
9	C	702	CO3	1	0

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.

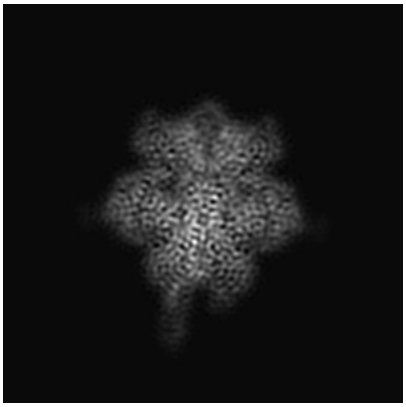
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-7783. These allow visual inspection of the internal detail of the map and identification of artifacts.

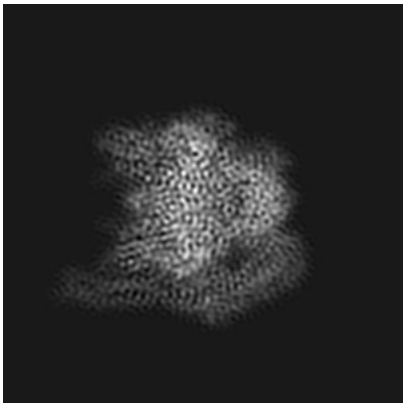
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

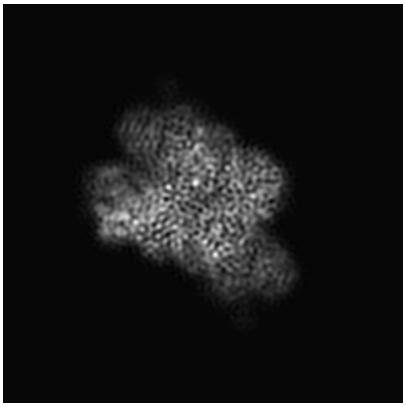
6.1.1 Primary map



X



Y



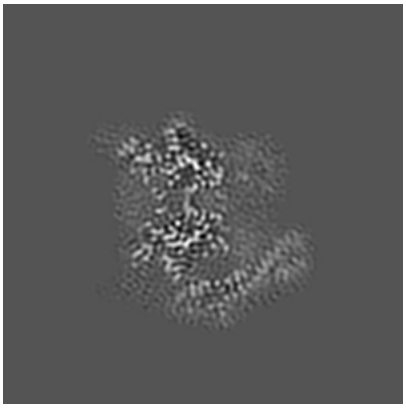
Z

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

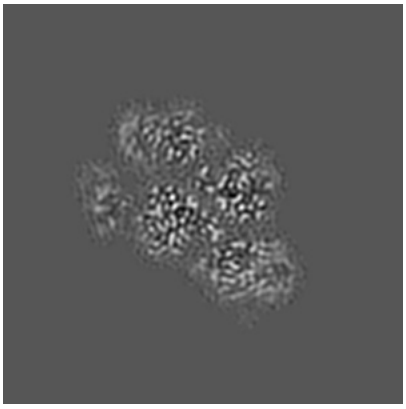
6.2 Central slices

6.2.1 Primary map

X Index: 90



Y Index: 90

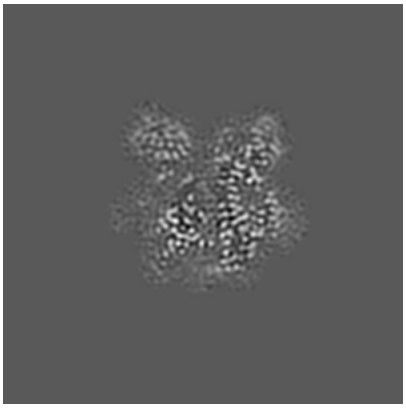


Z Index: 90

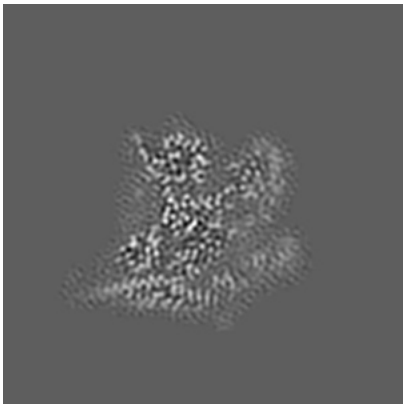
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

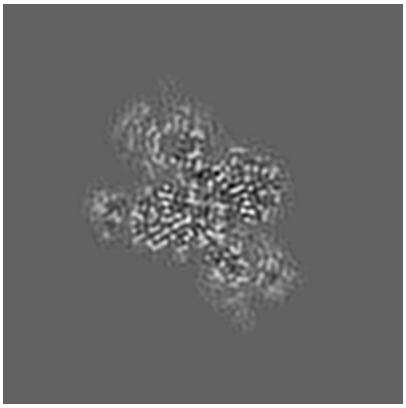
6.3.1 Primary map



X Index: 88



Y Index: 84

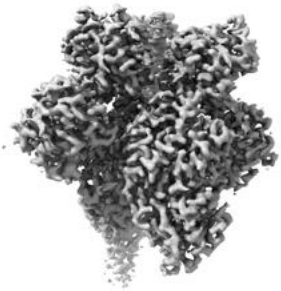


Z Index: 83

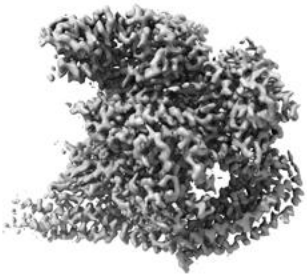
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views (i)

6.4.1 Primary map



X



Y

Z

The images above show the 3D surface view of the map at the recommended contour level 0.081. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

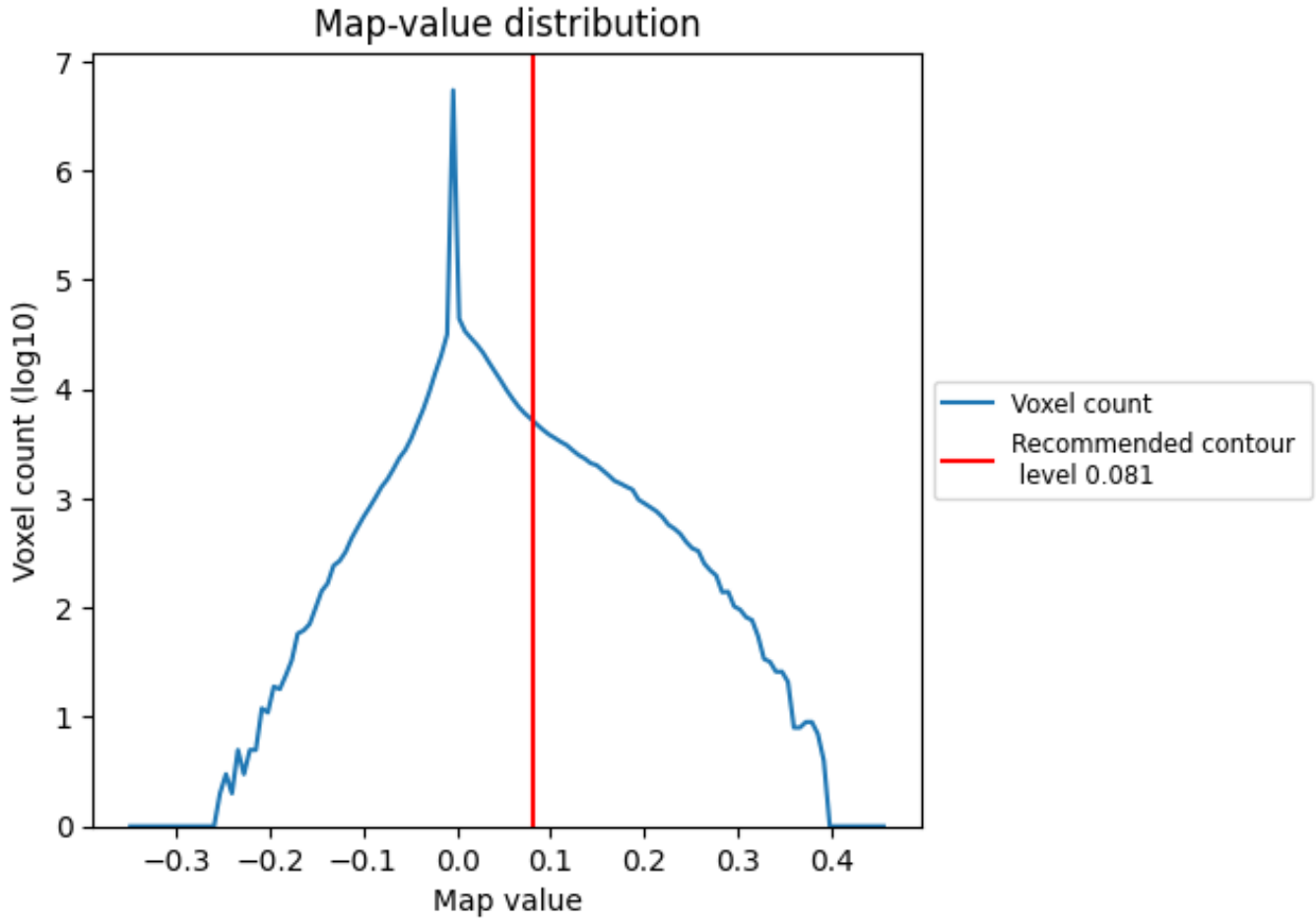
6.5 Mask visualisation (i)

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

7 Map analysis

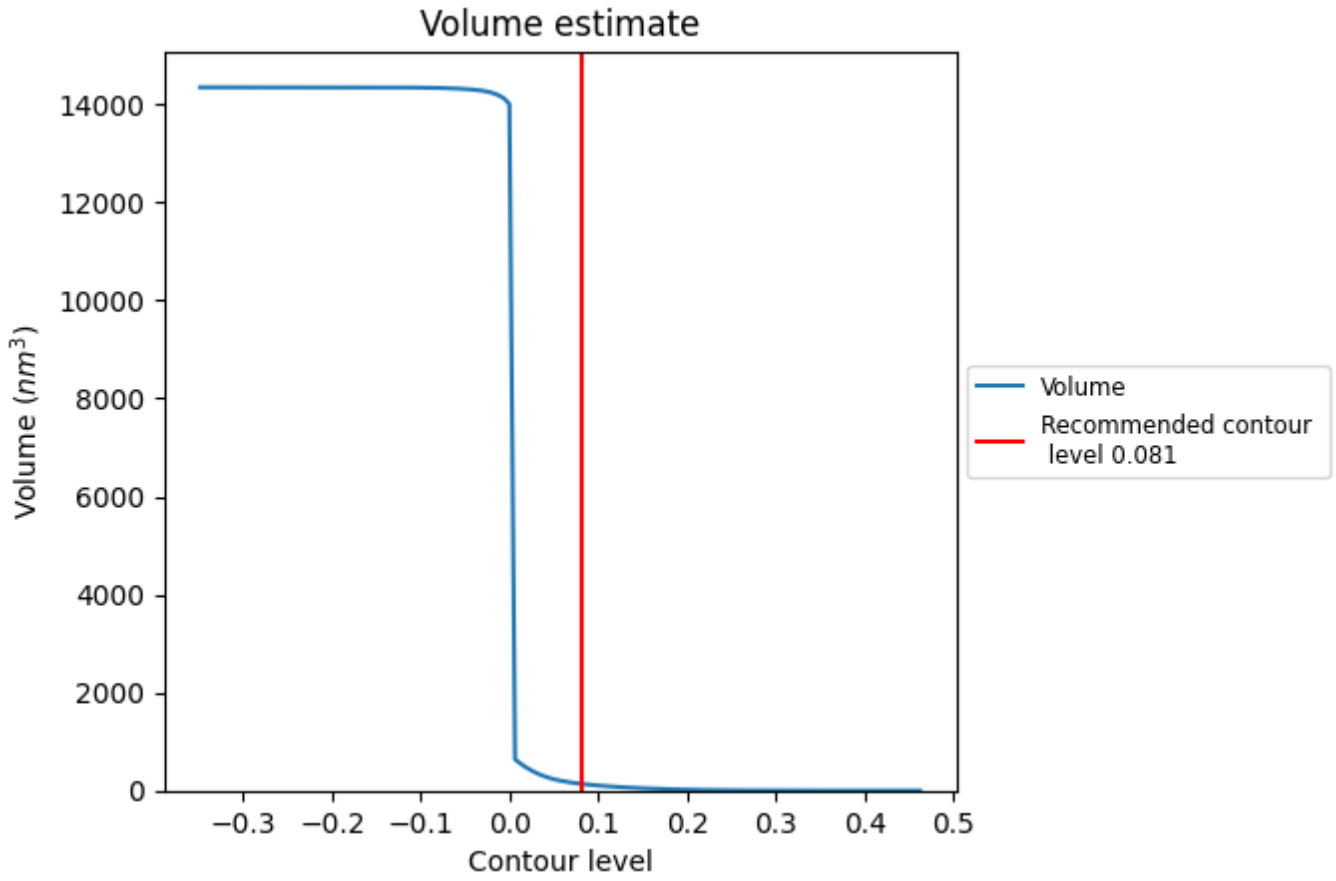
This section contains the results of statistical analysis of the map.

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.

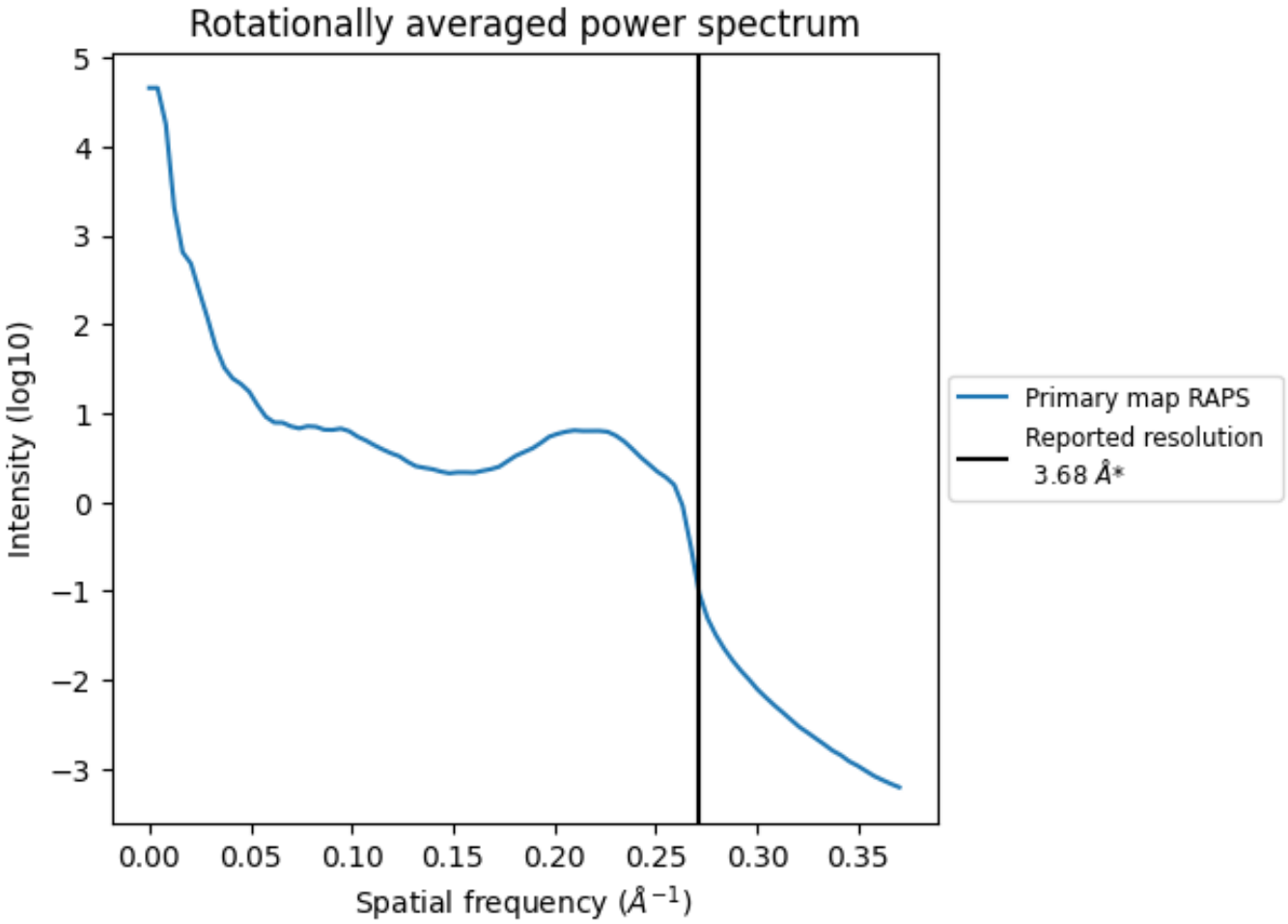
7.2 Volume estimate (i)



The volume at the recommended contour level is 136 nm^3; this corresponds to an approximate mass of 123 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 0.272 Å^{-1}

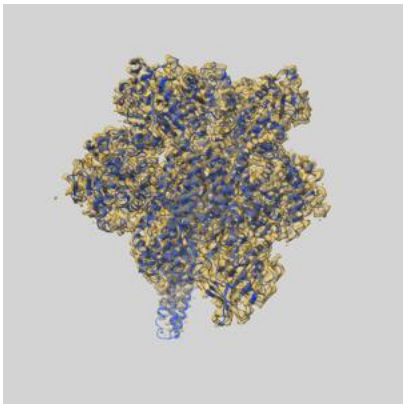
8 Fourier-Shell correlation (i)

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

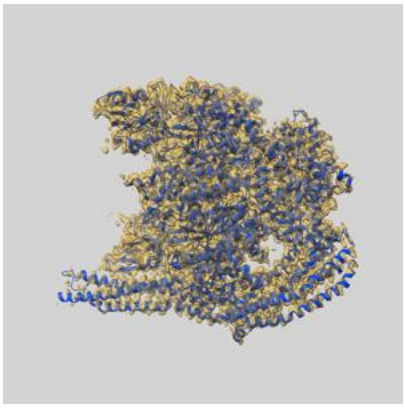
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-7783 and PDB model 6D03. Per-residue inclusion information can be found in section 3 on page 9.

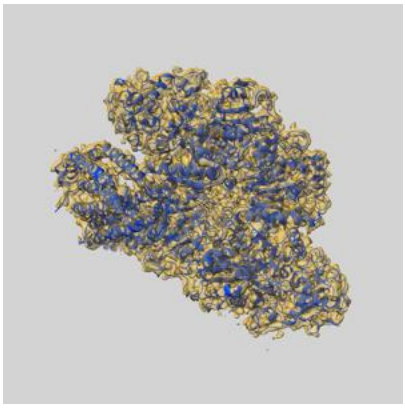
9.1 Map-model overlay



X



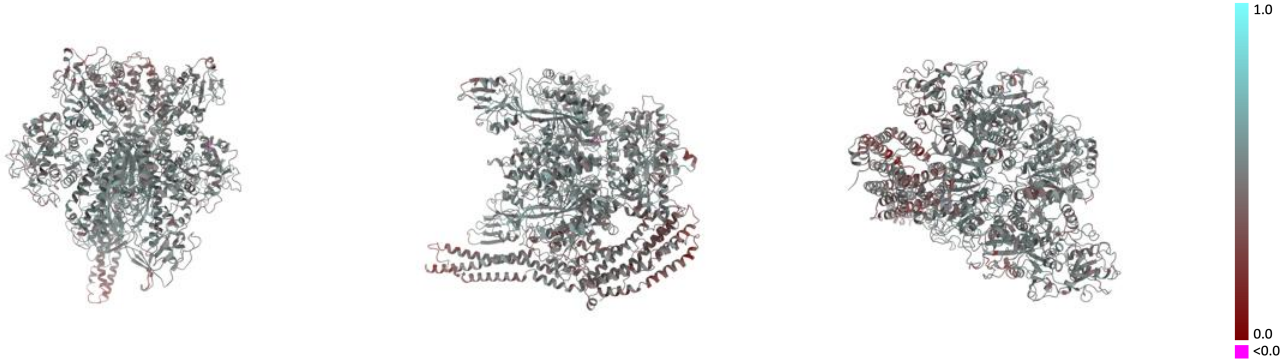
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.081 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.

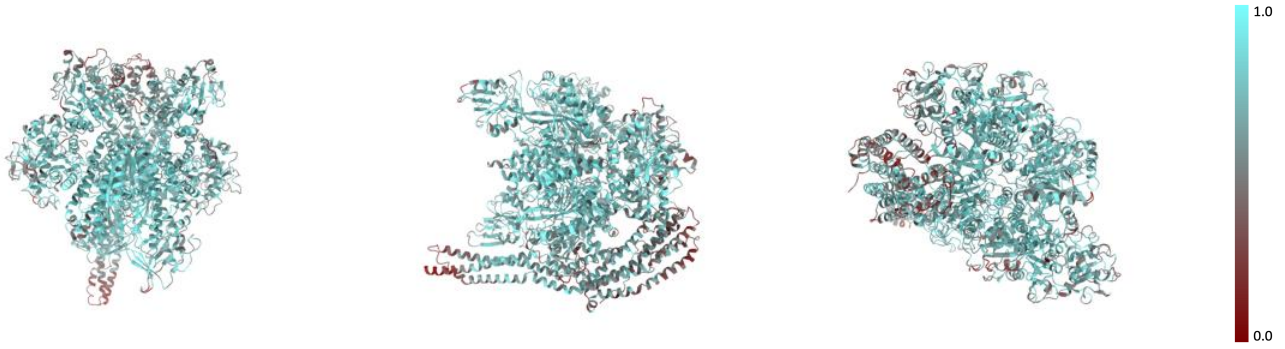
9.2 Q-score mapped to coordinate model



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.

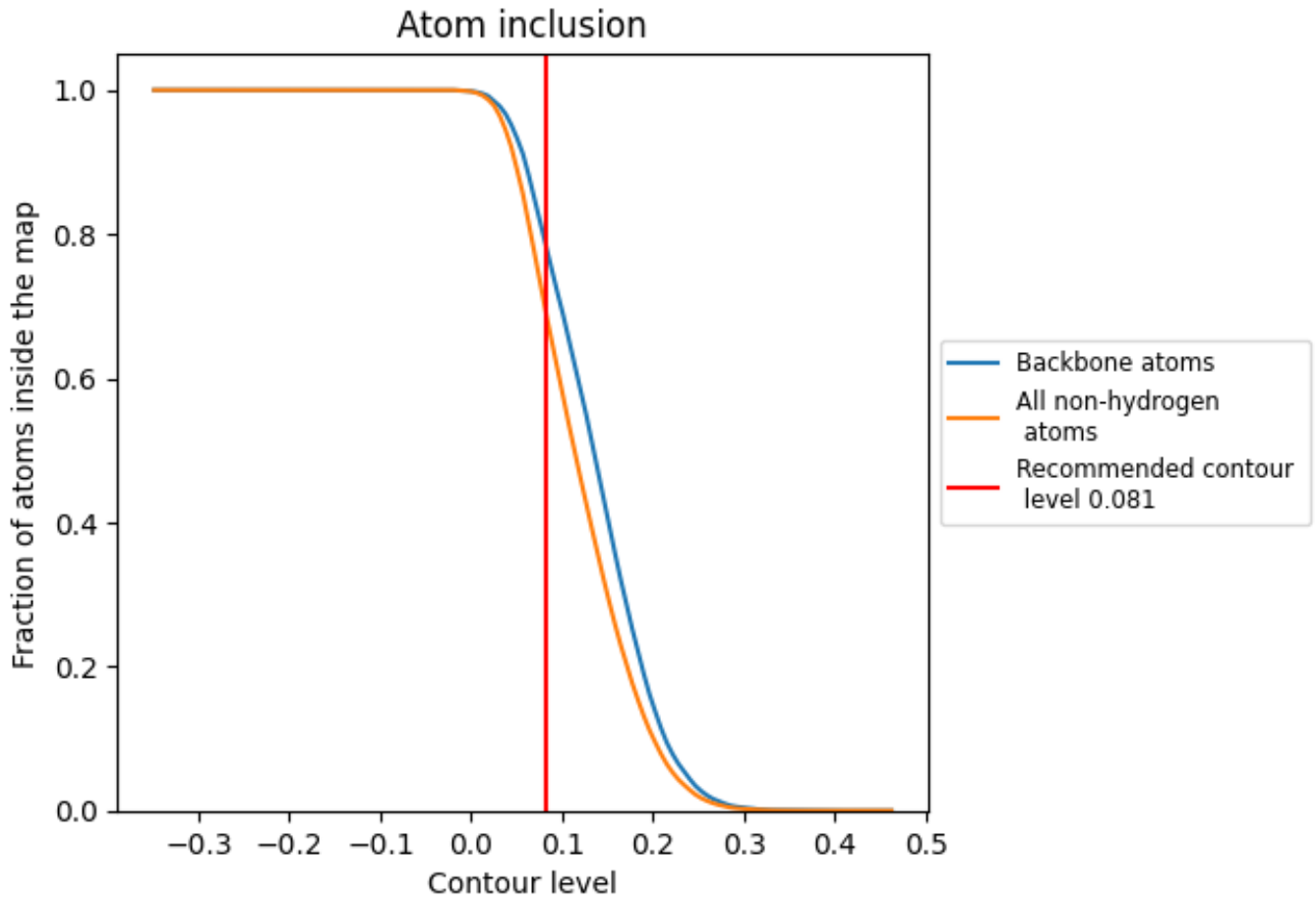
9.3 Atom inclusion mapped to coordinate model



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 (0.081).

9.4 Atom inclusion (i)



At the recommended contour level, 79% of all backbone atoms, 70% 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 (0.081) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6970	0.4820
A	0.7782	0.5130
B	0.8002	0.5190
C	0.6781	0.4770
D	0.6678	0.4810
E	0.5366	0.4070
F	0.5714	0.5070
G	0.5000	0.4310
H	0.5714	0.5150
I	0.3214	0.3420
J	0.1429	0.3400
K	0.0357	0.1940