wwPDB EM Validation Summary Report (i)

Nov 20, 2022 – 12:50 PM EST

PDB ID	:	7TY0
EMDB ID	:	EMD-26163
Title	:	Nipah Virus attachment (G) glycoprotein ectodomain in complex with nAH1.3 neutralizing antibody Fab fragment (local refinement of the stalk region)
Authors	:	Wang, Z.Q.; Seattle Structural Genomics Center for Infectious Disease (SSGCID); Veesler, D.
Deposited on	:	2022-02-10
Resolution	:	3.50 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:

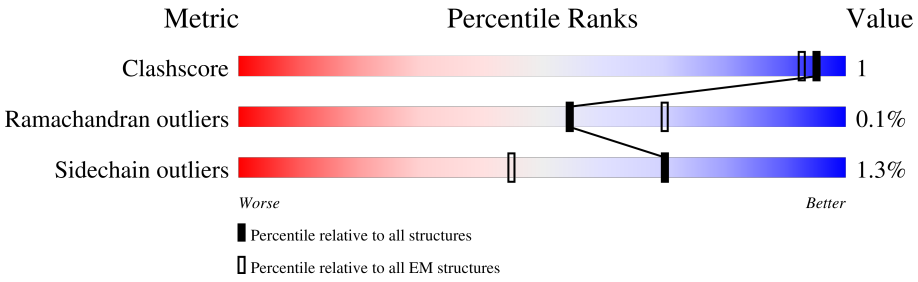
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

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 3.50 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	539	14% 86%
1	B	539	13% 87%
1	C	539	8% 88% 9%
1	D	539	87% 10%
2	J	458	22% 78%
2	K	458	21% 78%
3	N	218	7% 47% 52%
3	O	218	12% 44% 56%

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Mol	Chain	Length	Quality of chain
4	E	2	50% 100%
4	F	2	100% 100%
4	G	2	100% 100%
4	H	2	50% 50% 50%
4	M	2	50% 100%
4	P	2	50% 100%
5	I	3	67% 100%
6	L	3	100% 100%

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 10640 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 Glycoprotein G.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	77	Total	C	N	O	S	0	0
			458	284	86	85	3		
1	B	68	Total	C	N	O	S	0	0
			414	256	76	79	3		
1	D	485	Total	C	N	O	S	0	0
			3380	2189	598	569	24		
1	C	488	Total	C	N	O	S	0	0
			3389	2203	595	567	24		

There are 28 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	64	HIS	-	expression tag	UNP Q9IH62
A	65	HIS	-	expression tag	UNP Q9IH62
A	66	HIS	-	expression tag	UNP Q9IH62
A	67	HIS	-	expression tag	UNP Q9IH62
A	68	HIS	-	expression tag	UNP Q9IH62
A	69	HIS	-	expression tag	UNP Q9IH62
A	602	TYR	-	expression tag	UNP Q9IH62
B	64	HIS	-	expression tag	UNP Q9IH62
B	65	HIS	-	expression tag	UNP Q9IH62
B	66	HIS	-	expression tag	UNP Q9IH62
B	67	HIS	-	expression tag	UNP Q9IH62
B	68	HIS	-	expression tag	UNP Q9IH62
B	69	HIS	-	expression tag	UNP Q9IH62
B	602	TYR	-	expression tag	UNP Q9IH62
D	64	HIS	-	expression tag	UNP Q9IH62
D	65	HIS	-	expression tag	UNP Q9IH62
D	66	HIS	-	expression tag	UNP Q9IH62
D	67	HIS	-	expression tag	UNP Q9IH62
D	68	HIS	-	expression tag	UNP Q9IH62
D	69	HIS	-	expression tag	UNP Q9IH62
D	602	TYR	-	expression tag	UNP Q9IH62
C	64	HIS	-	expression tag	UNP Q9IH62

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Chain	Residue	Modelled	Actual	Comment	Reference
C	65	HIS	-	expression tag	UNP Q9IH62
C	66	HIS	-	expression tag	UNP Q9IH62
C	67	HIS	-	expression tag	UNP Q9IH62
C	68	HIS	-	expression tag	UNP Q9IH62
C	69	HIS	-	expression tag	UNP Q9IH62
C	602	TYR	-	expression tag	UNP Q9IH62

- Molecule 2 is a protein called Igh protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	J	103	Total	C	N	O	S	0	0
			704	457	126	117	4		
2	K	99	Total	C	N	O	S	0	0
			657	428	116	110	3		

There are 122 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
J	3	LYS	ASN	conflict	UNP I6L985
J	5	GLU	VAL	conflict	UNP I6L985
J	18	MET	LEU	conflict	UNP I6L985
J	19	LYS	ARG	conflict	UNP I6L985
J	23	VAL	ALA	conflict	UNP I6L985
J	28	SER	THR	conflict	UNP I6L985
J	30	SER	THR	conflict	UNP I6L985
J	31	TYR	ASP	conflict	UNP I6L985
J	33	TRP	TYR	conflict	UNP I6L985
J	35	ASN	SER	conflict	UNP I6L985
J	40	SER	PRO	conflict	UNP I6L985
J	42	GLU	GLY	conflict	UNP I6L985
J	44	GLY	ALA	conflict	UNP I6L985
J	48	VAL	LEU	conflict	UNP I6L985
J	49	ALA	GLY	conflict	UNP I6L985
J	50	GLU	PHE	conflict	UNP I6L985
J	53	LEU	ASN	conflict	UNP I6L985
J	55	SER	ALA	conflict	UNP I6L985
J	57	ASN	GLY	conflict	UNP I6L985
J	59	GLY	THR	conflict	UNP I6L985
J	61	HIS	GLU	conflict	UNP I6L985
J	63	ALA	SER	conflict	UNP I6L985
J	64	GLU	ALA	conflict	UNP I6L985
J	76	ASP	ASN	conflict	UNP I6L985

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Chain	Residue	Modelled	Actual	Comment	Reference
J	78	LYS	GLN	conflict	UNP I6L985
J	80	SER	ILE	conflict	UNP I6L985
J	81	VAL	LEU	conflict	UNP I6L985
J	87	ASN	ALA	conflict	UNP I6L985
J	90	PRO	ALA	conflict	UNP I6L985
J	93	THR	SER	conflict	UNP I6L985
J	94	GLY	ALA	conflict	UNP I6L985
J	95	ILE	THR	conflict	UNP I6L985
J	99	THR	ALA	conflict	UNP I6L985
J	?	-	ASP	deletion	UNP I6L985
J	?	-	ARG	deletion	UNP I6L985
J	?	-	ARG	deletion	UNP I6L985
J	?	-	SER	deletion	UNP I6L985
J	?	-	SER	deletion	UNP I6L985
J	?	-	TYR	deletion	UNP I6L985
J	?	-	TYR	deletion	UNP I6L985
J	101	VAL	TYR	conflict	UNP I6L985
J	102	ILE	SER	conflict	UNP I6L985
J	103	THR	GLY	conflict	UNP I6L985
J	105	VAL	SER	conflict	UNP I6L985
J	197	GLU	GLN	conflict	UNP I6L985
J	286	GLN	LYS	conflict	UNP I6L985
J	444	GLY	-	expression tag	UNP I6L985
J	445	GLY	-	expression tag	UNP I6L985
J	446	SER	-	expression tag	UNP I6L985
J	447	GLY	-	expression tag	UNP I6L985
J	448	GLY	-	expression tag	UNP I6L985
J	449	GLY	-	expression tag	UNP I6L985
J	450	SER	-	expression tag	UNP I6L985
J	451	TRP	-	expression tag	UNP I6L985
J	452	SER	-	expression tag	UNP I6L985
J	453	HIS	-	expression tag	UNP I6L985
J	454	PRO	-	expression tag	UNP I6L985
J	455	GLN	-	expression tag	UNP I6L985
J	456	PHE	-	expression tag	UNP I6L985
J	457	GLU	-	expression tag	UNP I6L985
J	458	LYS	-	expression tag	UNP I6L985
K	3	LYS	ASN	conflict	UNP I6L985
K	5	GLU	VAL	conflict	UNP I6L985
K	18	MET	LEU	conflict	UNP I6L985
K	19	LYS	ARG	conflict	UNP I6L985
K	23	VAL	ALA	conflict	UNP I6L985

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Chain	Residue	Modelled	Actual	Comment	Reference
K	28	SER	THR	conflict	UNP I6L985
K	30	SER	THR	conflict	UNP I6L985
K	31	TYR	ASP	conflict	UNP I6L985
K	33	TRP	TYR	conflict	UNP I6L985
K	35	ASN	SER	conflict	UNP I6L985
K	40	SER	PRO	conflict	UNP I6L985
K	42	GLU	GLY	conflict	UNP I6L985
K	44	GLY	ALA	conflict	UNP I6L985
K	48	VAL	LEU	conflict	UNP I6L985
K	49	ALA	GLY	conflict	UNP I6L985
K	50	GLU	PHE	conflict	UNP I6L985
K	53	LEU	ASN	conflict	UNP I6L985
K	55	SER	ALA	conflict	UNP I6L985
K	57	ASN	GLY	conflict	UNP I6L985
K	59	GLY	THR	conflict	UNP I6L985
K	61	HIS	GLU	conflict	UNP I6L985
K	63	ALA	SER	conflict	UNP I6L985
K	64	GLU	ALA	conflict	UNP I6L985
K	76	ASP	ASN	conflict	UNP I6L985
K	78	LYS	GLN	conflict	UNP I6L985
K	80	SER	ILE	conflict	UNP I6L985
K	81	VAL	LEU	conflict	UNP I6L985
K	87	ASN	ALA	conflict	UNP I6L985
K	90	PRO	ALA	conflict	UNP I6L985
K	93	THR	SER	conflict	UNP I6L985
K	94	GLY	ALA	conflict	UNP I6L985
K	95	ILE	THR	conflict	UNP I6L985
K	99	THR	ALA	conflict	UNP I6L985
K	?	-	ASP	deletion	UNP I6L985
K	?	-	ARG	deletion	UNP I6L985
K	?	-	ARG	deletion	UNP I6L985
K	?	-	SER	deletion	UNP I6L985
K	?	-	SER	deletion	UNP I6L985
K	?	-	TYR	deletion	UNP I6L985
K	?	-	TYR	deletion	UNP I6L985
K	101	VAL	TYR	conflict	UNP I6L985
K	102	ILE	SER	conflict	UNP I6L985
K	103	THR	GLY	conflict	UNP I6L985
K	105	VAL	SER	conflict	UNP I6L985
K	197	GLU	GLN	conflict	UNP I6L985
K	286	GLN	LYS	conflict	UNP I6L985
K	444	GLY	-	expression tag	UNP I6L985

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Chain	Residue	Modelled	Actual	Comment	Reference
K	445	GLY	-	expression tag	UNP I6L985
K	446	SER	-	expression tag	UNP I6L985
K	447	GLY	-	expression tag	UNP I6L985
K	448	GLY	-	expression tag	UNP I6L985
K	449	GLY	-	expression tag	UNP I6L985
K	450	SER	-	expression tag	UNP I6L985
K	451	TRP	-	expression tag	UNP I6L985
K	452	SER	-	expression tag	UNP I6L985
K	453	HIS	-	expression tag	UNP I6L985
K	454	PRO	-	expression tag	UNP I6L985
K	455	GLN	-	expression tag	UNP I6L985
K	456	PHE	-	expression tag	UNP I6L985
K	457	GLU	-	expression tag	UNP I6L985
K	458	LYS	-	expression tag	UNP I6L985

- Molecule 3 is a protein called nAH Fab light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	N	105	Total	C	N	O	S	0	0
			688	439	125	121	3		
3	O	97	Total	C	N	O	S	0	0
			621	400	110	109	2		

- 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	E	2	Total	C	N	O	0	0
			28	16	2	10		
4	F	2	Total	C	N	O	0	0
			28	16	2	10		
4	G	2	Total	C	N	O	0	0
			28	16	2	10		
4	H	2	Total	C	N	O	0	0
			28	16	2	10		
4	M	2	Total	C	N	O	0	0
			28	16	2	10		

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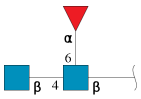
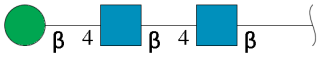
Mol	Chain	Residues	Atoms				AltConf	Trace
4	P	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 5 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.



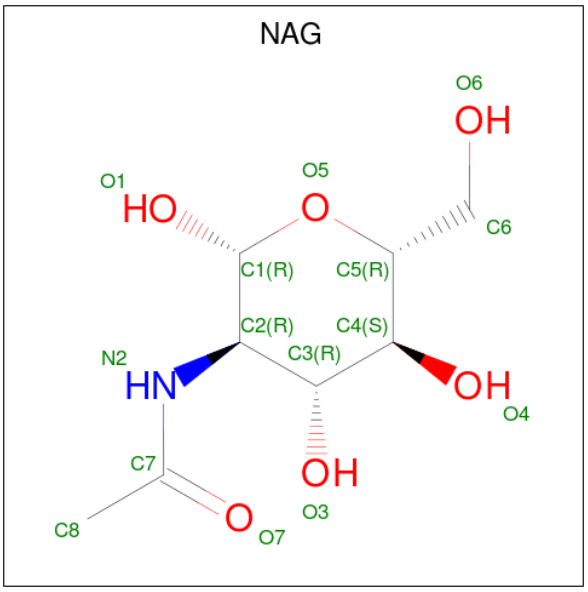
Mol	Chain	Residues	Atoms				AltConf	Trace
5	I	3	Total	C	N	O	0	0
			38	22	2	14		

- 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
6	L	3	Total	C	N	O	0	0
			39	22	2	15		

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



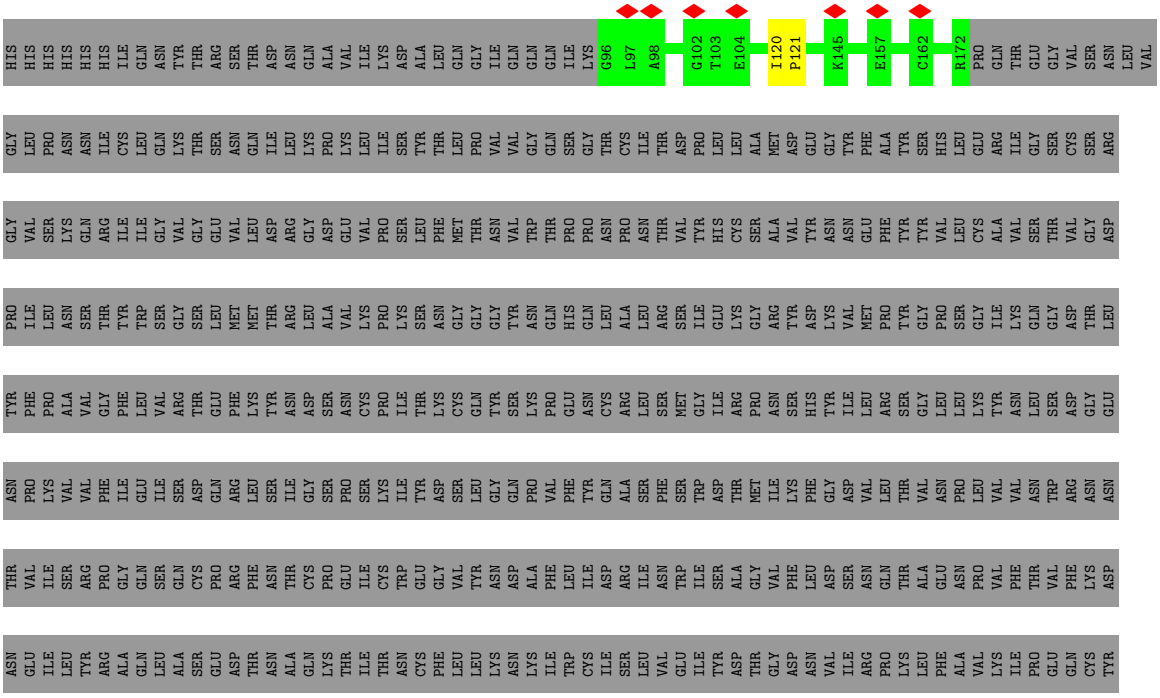
Mol	Chain	Residues	Atoms				AltConf
7	D	1	Total	C	N	O	0
			42	24	3	15	
7	D	1	Total	C	N	O	0
			42	24	3	15	
7	D	1	Total	C	N	O	0
			42	24	3	15	
7	C	1	Total	C	N	O	0
			42	24	3	15	
7	C	1	Total	C	N	O	0
			42	24	3	15	
7	C	1	Total	C	N	O	0
			42	24	3	15	

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.

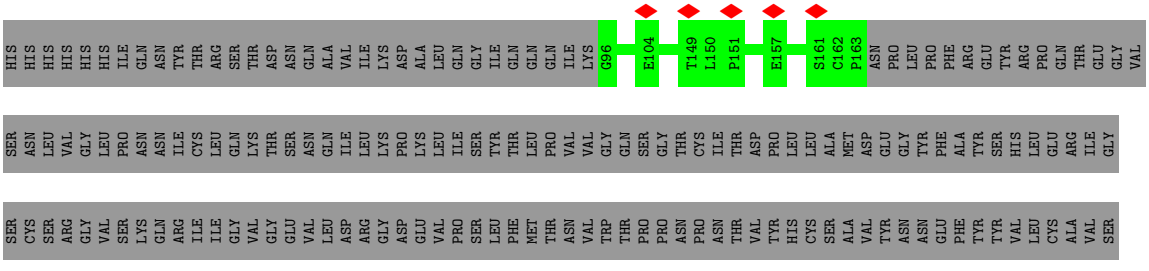
• Molecule 1: Glycoprotein G

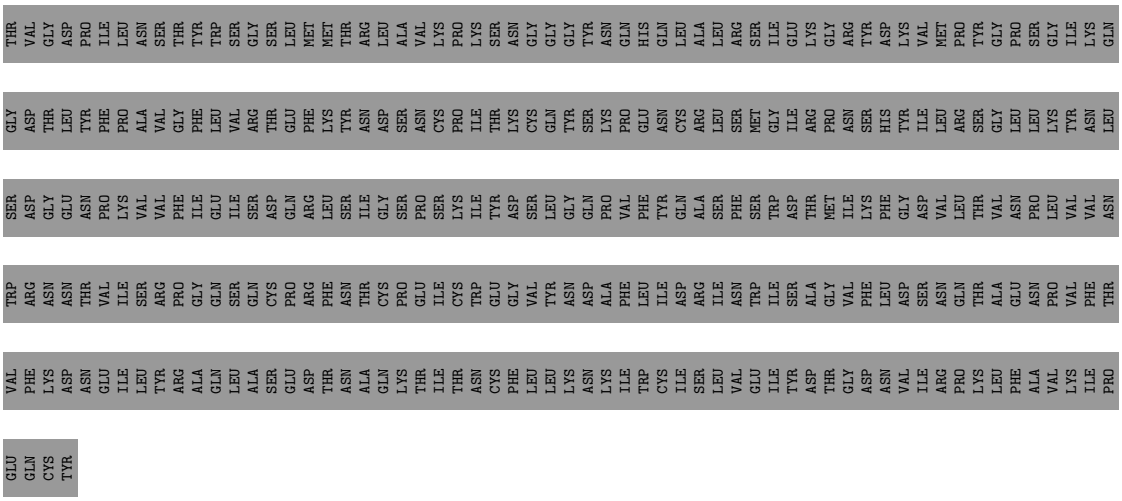
Chain A:



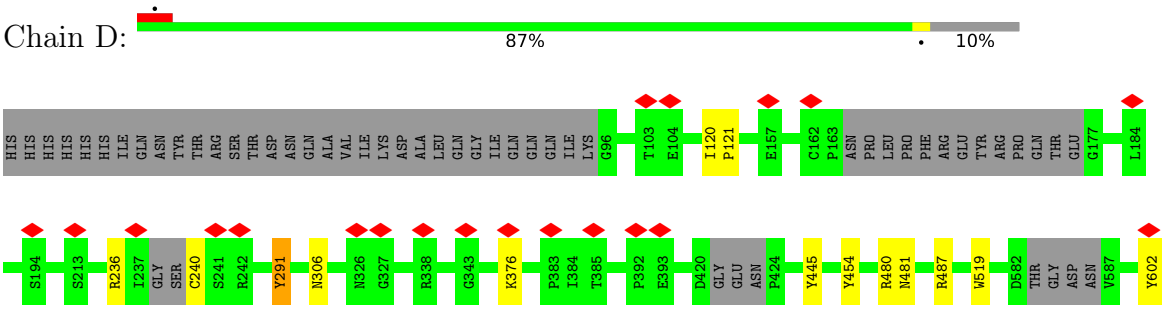
• Molecule 1: Glycoprotein G

Chain B:

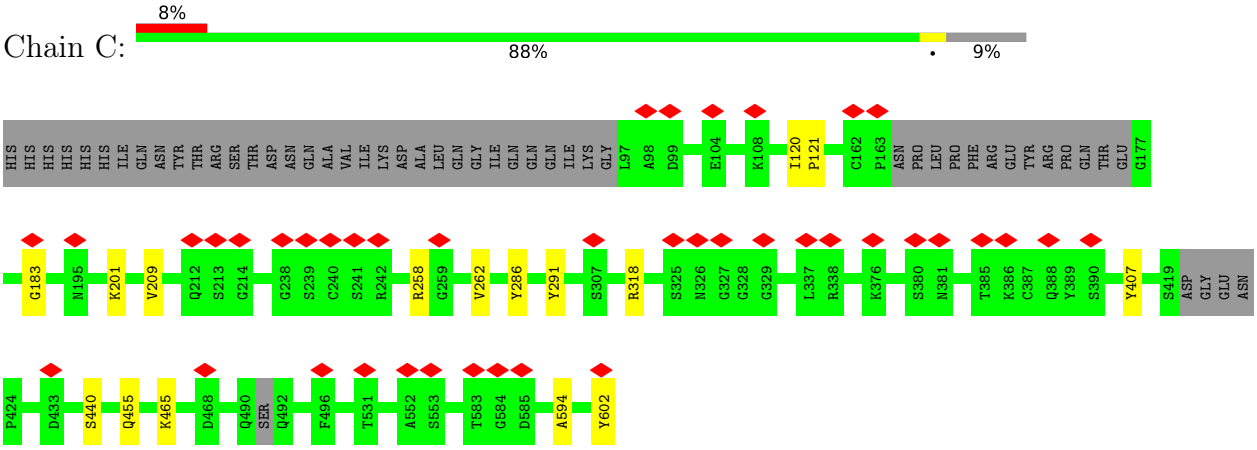




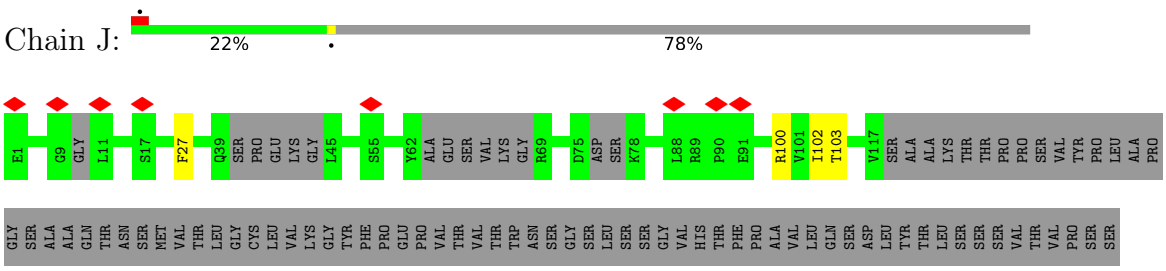
• Molecule 1: Glycoprotein G

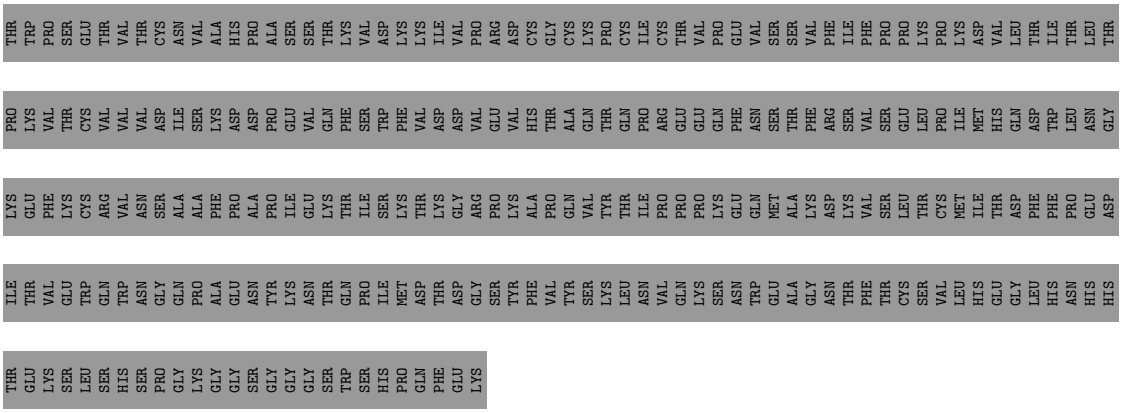


• Molecule 1: Glycoprotein G



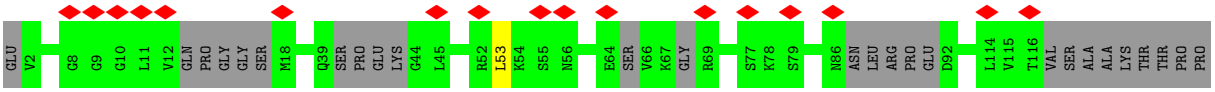
• Molecule 2: Igh protein





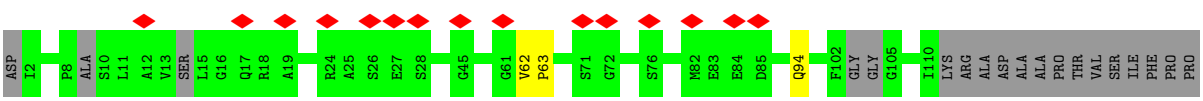
• Molecule 2: Igh protein

Chain K:



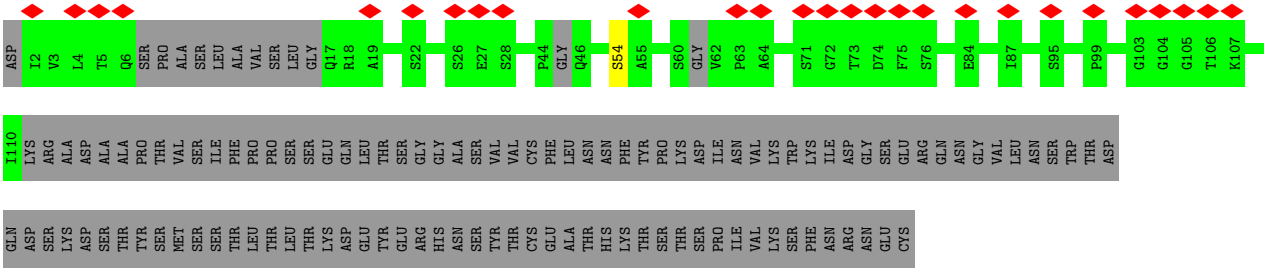
• Molecule 3: nAH Fab light chain

Chain N:



• Molecule 3: nAH Fab light chain

Chain O:

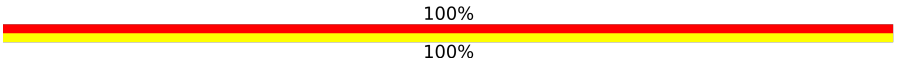


• Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

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

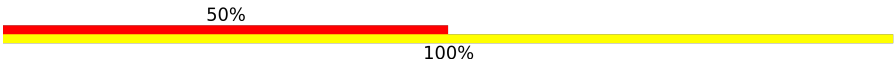
Chain G:

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

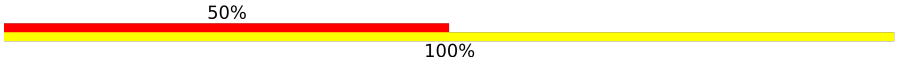
Chain H:

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

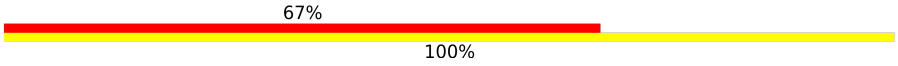
Chain M:



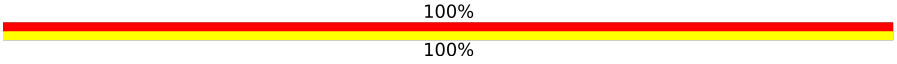
• Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain P: 

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

Chain I: 

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

Chain L: 

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	168035	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 ($e^-/Å^2$)	70	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	12.855	Depositor
Minimum map value	-4.996	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.062	Depositor
Recommended contour level	0.6	Depositor
Map size (Å)	482.99997, 482.99997, 482.99997	wwPDB
Map dimensions	460, 460, 460	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.05, 1.05, 1.05	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, BMA, FUC

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.42	0/464	0.55	0/641
1	B	0.43	0/418	0.57	0/575
1	C	0.65	3/3471 (0.1%)	0.75	4/4755 (0.1%)
1	D	0.65	3/3460 (0.1%)	0.70	2/4736 (0.0%)
2	J	0.66	0/722	0.75	0/984
2	K	0.68	0/671	0.74	0/913
3	N	0.52	0/704	0.68	0/962
3	O	0.55	0/636	0.68	0/870
All	All	0.63	6/10546 (0.1%)	0.71	6/14436 (0.0%)

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	602	TYR	CG-CD2	5.39	1.46	1.39
1	C	602	TYR	CG-CD1	5.37	1.46	1.39
1	D	602	TYR	CG-CD1	5.26	1.46	1.39
1	D	602	TYR	CG-CD2	5.25	1.46	1.39
1	C	602	TYR	CE1-CZ	5.25	1.45	1.38

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	209	VAL	CG1-CB-CG2	12.53	130.94	110.90
1	D	445	TYR	CB-CG-CD2	-7.71	116.38	121.00
1	C	209	VAL	CA-CB-CG2	-5.49	102.67	110.90
1	C	286	TYR	CB-CG-CD2	-5.30	117.82	121.00
1	D	291	TYR	CB-CG-CD2	-5.29	117.83	121.00

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	A	458	0	358	1	0
1	B	414	0	340	0	0
1	C	3389	0	2970	8	0
1	D	3380	0	2977	7	0
2	J	704	0	514	2	0
2	K	657	0	458	0	0
3	N	688	0	510	1	0
3	O	621	0	439	0	0
4	E	28	0	25	0	0
4	F	28	0	25	0	0
4	G	28	0	25	0	0
4	H	28	0	25	4	0
4	M	28	0	25	0	0
4	P	28	0	25	0	0
5	I	38	0	34	0	0
6	L	39	0	34	0	0
7	C	42	0	39	0	0
7	D	42	0	39	0	0
All	All	10640	0	8862	19	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 1.

The worst 5 of 19 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:D:480:ARG:HA	4:H:1:NAG:H82	1.14	1.11
1:D:480:ARG:CA	4:H:1:NAG:H82	2.07	0.80
1:D:480:ARG:HA	4:H:1:NAG:C8	2.08	0.73
1:C:201:LYS:HE2	1:C:262:VAL:CG2	2.30	0.62
1:D:480:ARG:HD2	4:H:1:NAG:C8	2.37	0.54

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	75/539 (14%)	74 (99%)	1 (1%)	0	100 100
1	B	66/539 (12%)	65 (98%)	1 (2%)	0	100 100
1	C	480/539 (89%)	468 (98%)	11 (2%)	1 (0%)	47 81
1	D	475/539 (88%)	463 (98%)	12 (2%)	0	100 100
2	J	93/458 (20%)	91 (98%)	2 (2%)	0	100 100
2	K	87/458 (19%)	87 (100%)	0	0	100 100
3	N	97/218 (44%)	94 (97%)	3 (3%)	0	100 100
3	O	89/218 (41%)	87 (98%)	1 (1%)	1 (1%)	14 52
All	All	1462/3508 (42%)	1429 (98%)	31 (2%)	2 (0%)	54 84

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	O	54	SER
1	C	183	GLY

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	31/483 (6%)	31 (100%)	0	100 100
1	B	31/483 (6%)	31 (100%)	0	100 100
1	C	277/483 (57%)	275 (99%)	2 (1%)	84 93

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	D	282/483 (58%)	276 (98%)	6 (2%)	53 79
2	J	41/408 (10%)	41 (100%)	0	100 100
2	K	33/408 (8%)	32 (97%)	1 (3%)	41 71
3	N	43/191 (22%)	42 (98%)	1 (2%)	50 77
3	O	35/191 (18%)	35 (100%)	0	100 100
All	All	773/3130 (25%)	763 (99%)	10 (1%)	70 86

5 of 10 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	519	TRP
1	C	291	TYR
1	C	318	ARG
1	D	306	ASN
1	D	376	LYS

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

Mol	Chain	Res	Type
1	B	133	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)

18 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	E	1	4,1	14,14,15	1.64	2 (14%)	17,19,21	0.96	1 (5%)
4	NAG	E	2	4	14,14,15	1.43	2 (14%)	17,19,21	0.87	1 (5%)
4	NAG	F	1	4,1	14,14,15	1.58	2 (14%)	17,19,21	0.91	1 (5%)
4	NAG	F	2	4	14,14,15	1.49	2 (14%)	17,19,21	0.99	1 (5%)
4	NAG	G	1	4,1	14,14,15	1.54	2 (14%)	17,19,21	1.01	1 (5%)
4	NAG	G	2	4	14,14,15	1.46	2 (14%)	17,19,21	0.89	1 (5%)
4	NAG	H	1	4,1	14,14,15	1.65	3 (21%)	17,19,21	1.25	3 (17%)
4	NAG	H	2	4	14,14,15	1.45	2 (14%)	17,19,21	0.83	0
5	NAG	I	1	5,1	14,14,15	1.24	2 (14%)	17,19,21	0.96	0
5	NAG	I	2	5	14,14,15	1.57	3 (21%)	17,19,21	0.90	1 (5%)
5	FUC	I	3	5	10,10,11	1.60	4 (40%)	14,14,16	0.73	0
6	NAG	L	1	1,6	14,14,15	1.53	2 (14%)	17,19,21	0.90	1 (5%)
6	NAG	L	2	6	14,14,15	1.53	2 (14%)	17,19,21	0.87	1 (5%)
6	BMA	L	3	6	11,11,12	1.43	3 (27%)	15,15,17	0.70	0
4	NAG	M	1	4,1	14,14,15	1.55	2 (14%)	17,19,21	0.87	0
4	NAG	M	2	4	14,14,15	1.42	2 (14%)	17,19,21	0.89	1 (5%)
4	NAG	P	1	4,1	14,14,15	1.54	3 (21%)	17,19,21	1.05	0
4	NAG	P	2	4	14,14,15	1.56	2 (14%)	17,19,21	0.94	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	E	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	E	2	4	-	0/6/23/26	0/1/1/1
4	NAG	F	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	F	2	4	-	0/6/23/26	0/1/1/1
4	NAG	G	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	G	2	4	-	0/6/23/26	0/1/1/1
4	NAG	H	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	H	2	4	-	0/6/23/26	0/1/1/1
5	NAG	I	1	5,1	-	2/6/23/26	0/1/1/1
5	NAG	I	2	5	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	FUC	I	3	5	-	-	0/1/1/1
6	NAG	L	1	1,6	-	0/6/23/26	0/1/1/1
6	NAG	L	2	6	-	0/6/23/26	0/1/1/1
6	BMA	L	3	6	-	0/2/19/22	0/1/1/1
4	NAG	M	1	4,1	-	1/6/23/26	0/1/1/1
4	NAG	M	2	4	-	0/6/23/26	0/1/1/1
4	NAG	P	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	P	2	4	-	0/6/23/26	0/1/1/1

The worst 5 of 42 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	G	1	NAG	C1-C2	4.21	1.58	1.52
4	E	1	NAG	C1-C2	4.17	1.58	1.52
4	F	1	NAG	C1-C2	4.09	1.58	1.52
4	H	1	NAG	C1-C2	4.06	1.58	1.52
4	M	1	NAG	C1-C2	4.06	1.58	1.52

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	F	2	NAG	C8-C7-N2	2.69	120.65	116.10
4	H	1	NAG	C1-O5-C5	2.58	115.69	112.19
5	I	2	NAG	C8-C7-N2	2.53	120.38	116.10
4	P	2	NAG	C8-C7-N2	2.49	120.31	116.10
4	E	1	NAG	C8-C7-N2	2.42	120.19	116.10

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	P	1	NAG	O5-C5-C6-O6
5	I	1	NAG	O5-C5-C6-O6
5	I	1	NAG	C4-C5-C6-O6
4	P	1	NAG	C4-C5-C6-O6
4	M	1	NAG	O5-C5-C6-O6

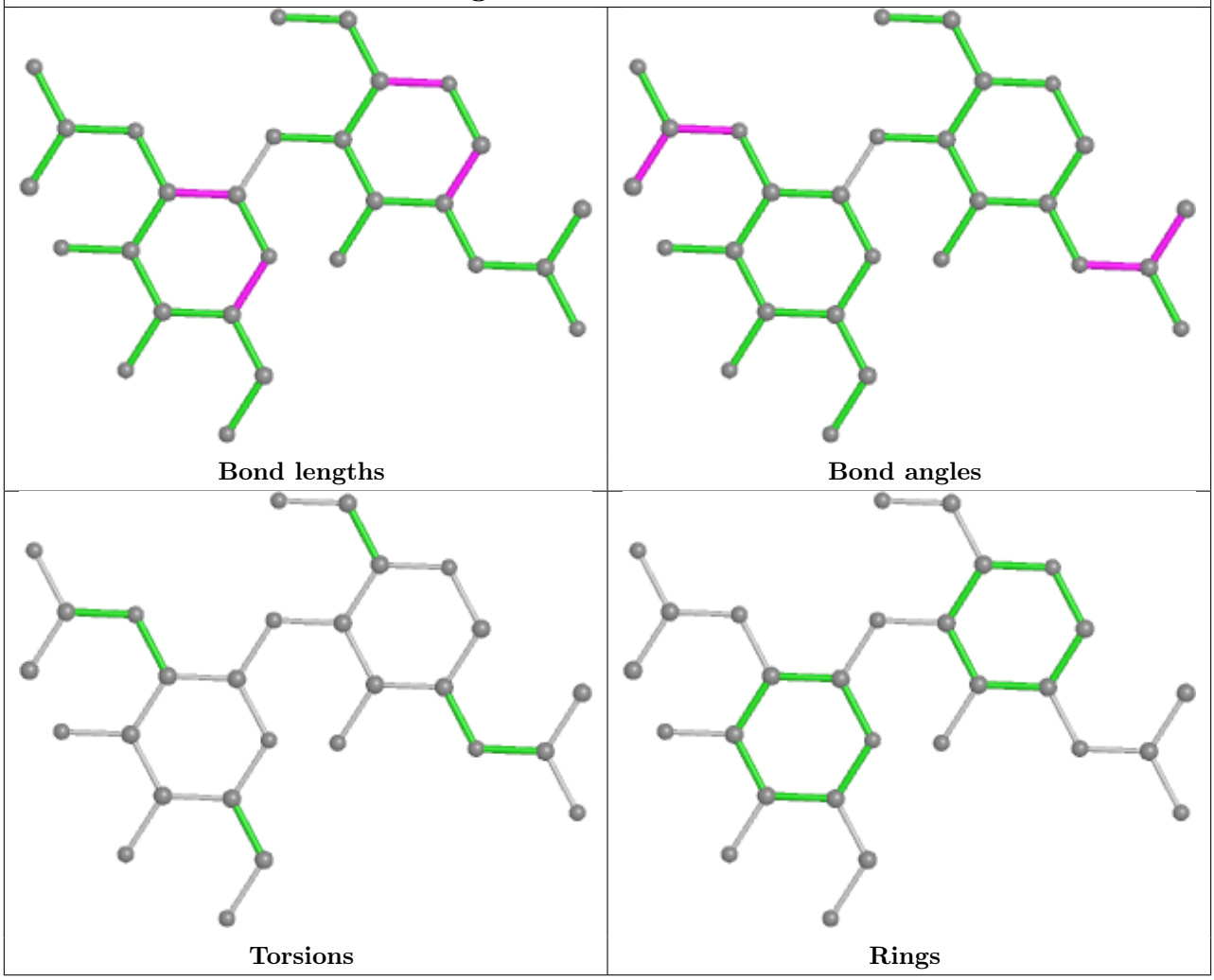
There are no ring outliers.

1 monomer is involved in 4 short contacts:

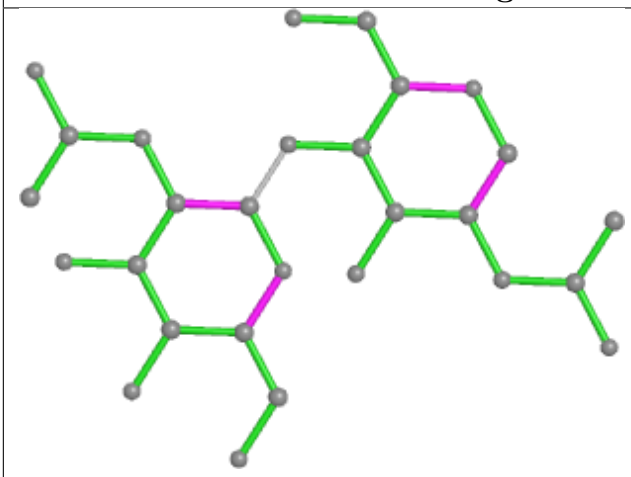
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	H	1	NAG	4	0

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

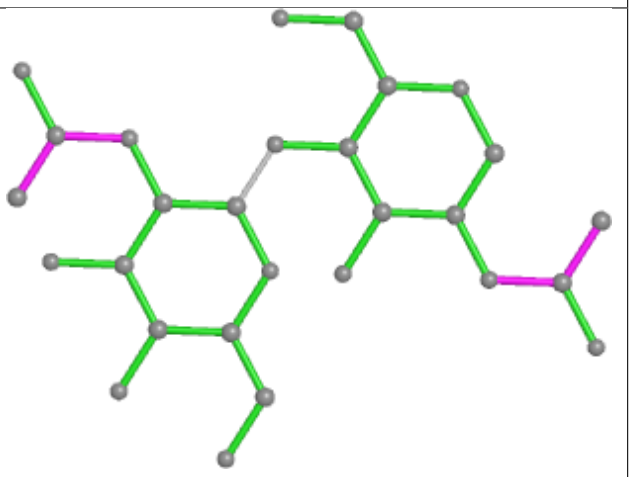
Oligosaccharide Chain E



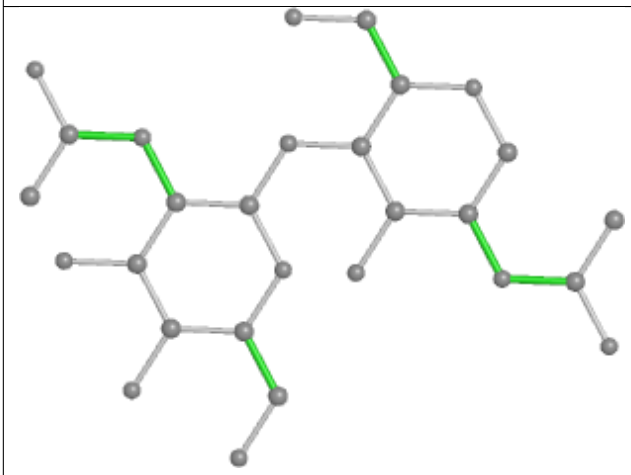
Oligosaccharide Chain F



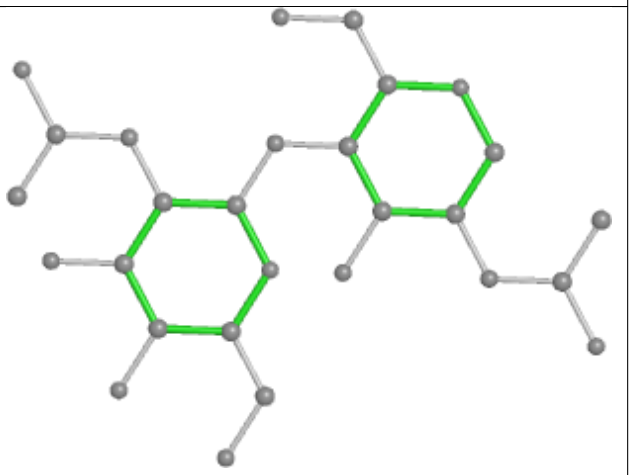
Bond lengths



Bond angles

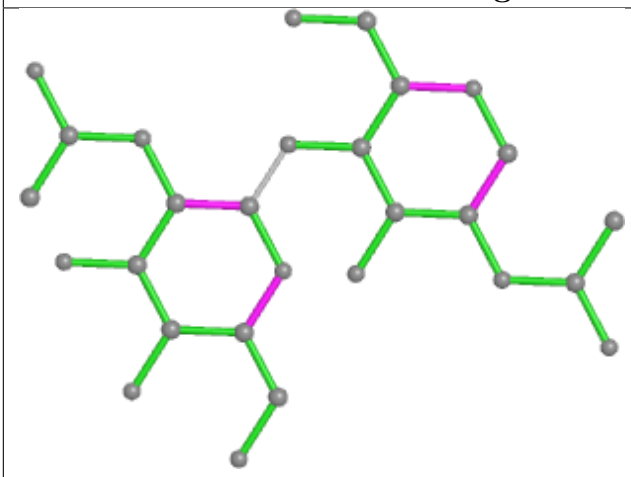


Torsions

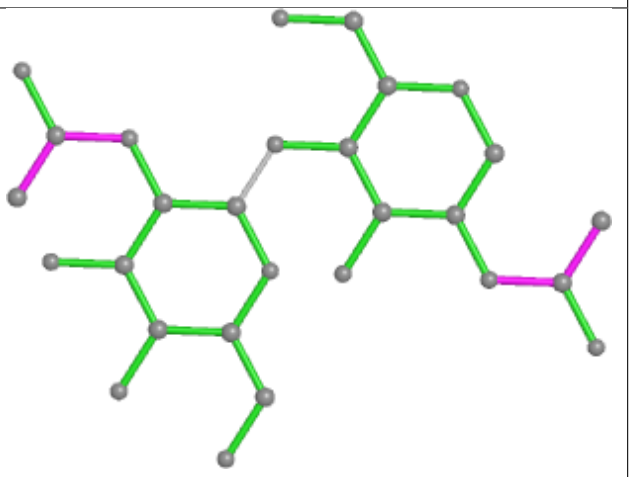


Rings

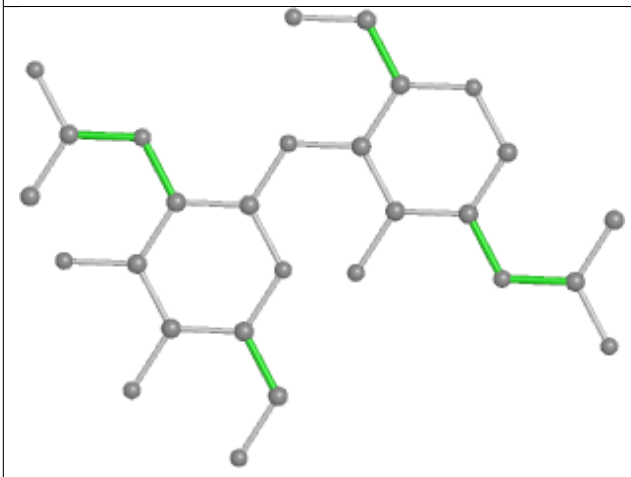
Oligosaccharide Chain G



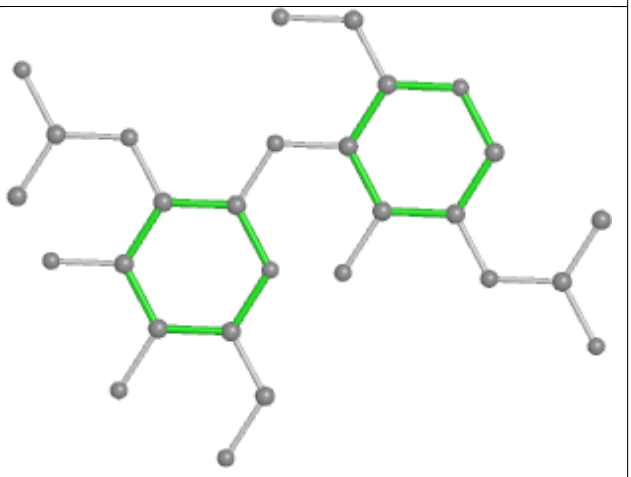
Bond lengths



Bond angles

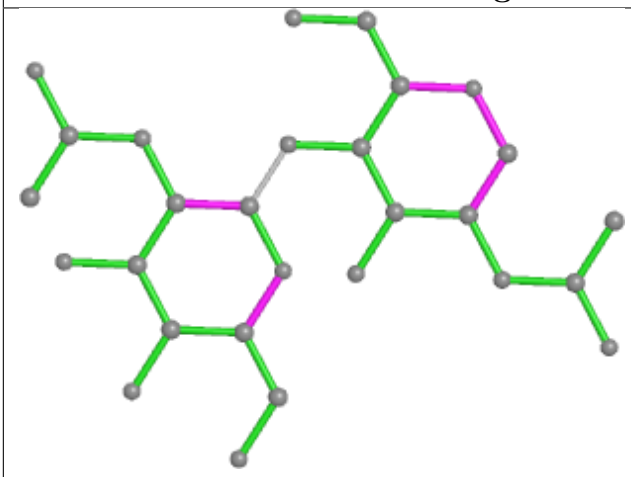


Torsions

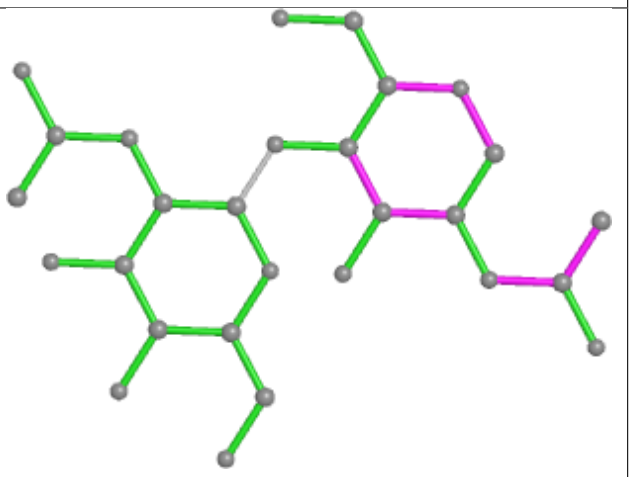


Rings

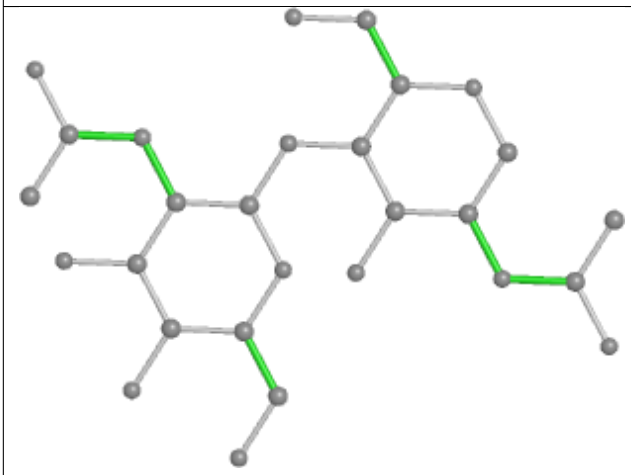
Oligosaccharide Chain H



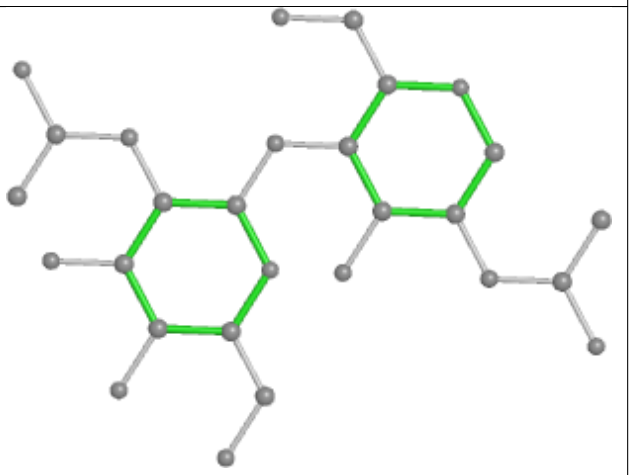
Bond lengths



Bond angles

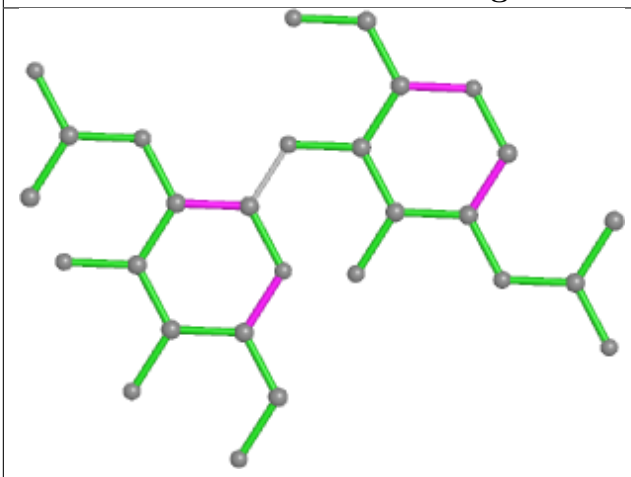


Torsions

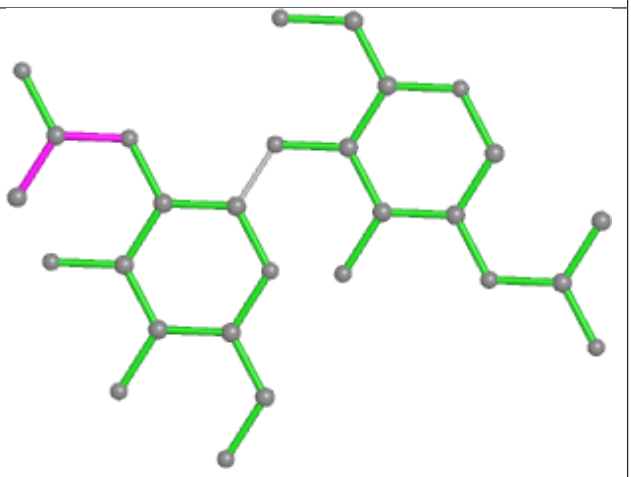


Rings

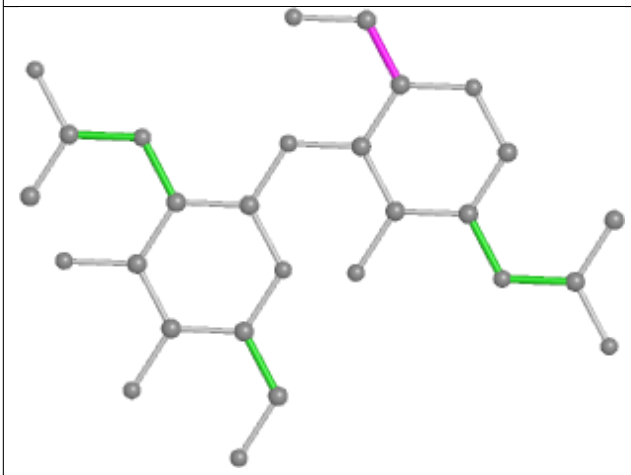
Oligosaccharide Chain M



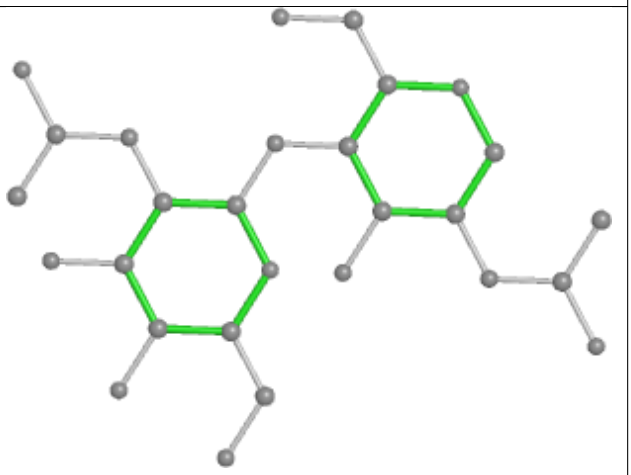
Bond lengths



Bond angles

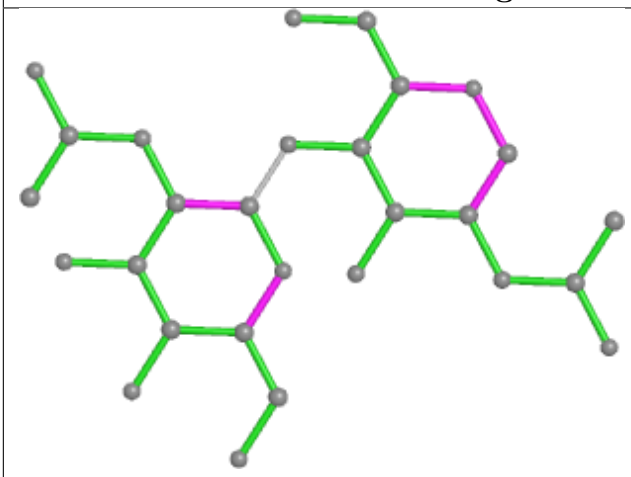


Torsions

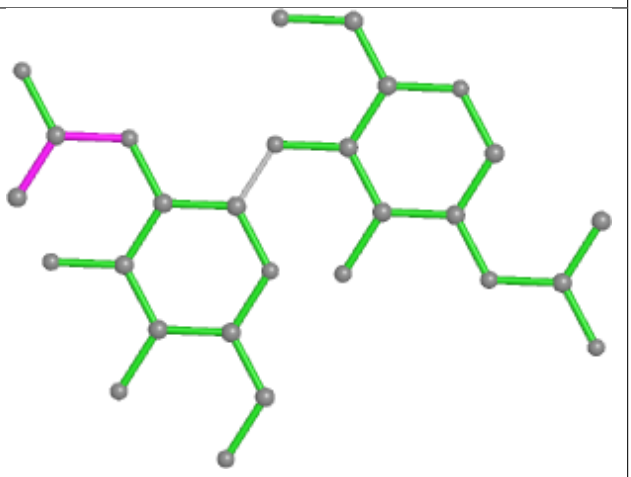


Rings

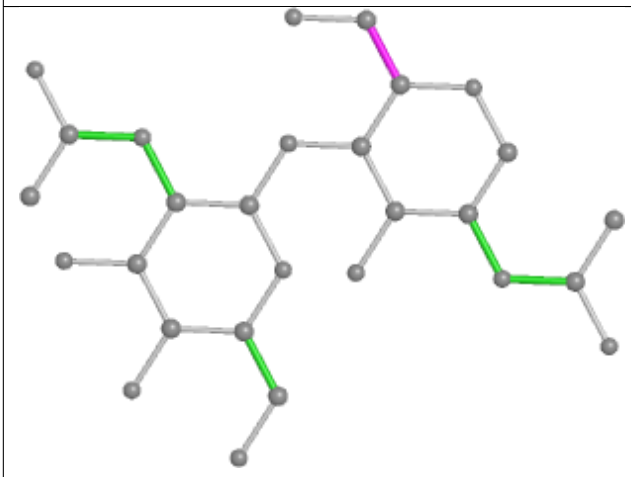
Oligosaccharide Chain P



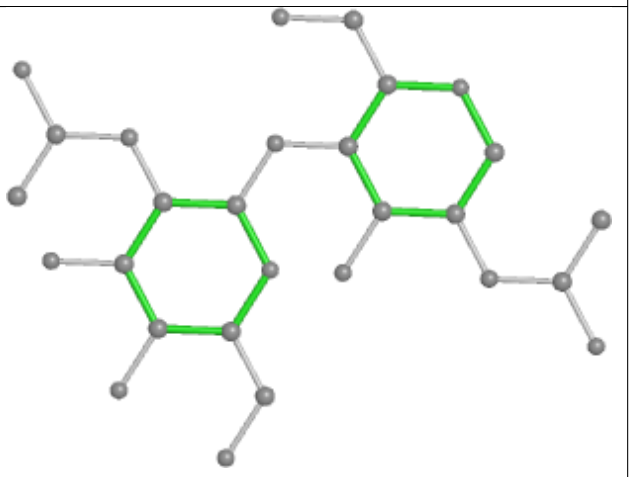
Bond lengths



Bond angles

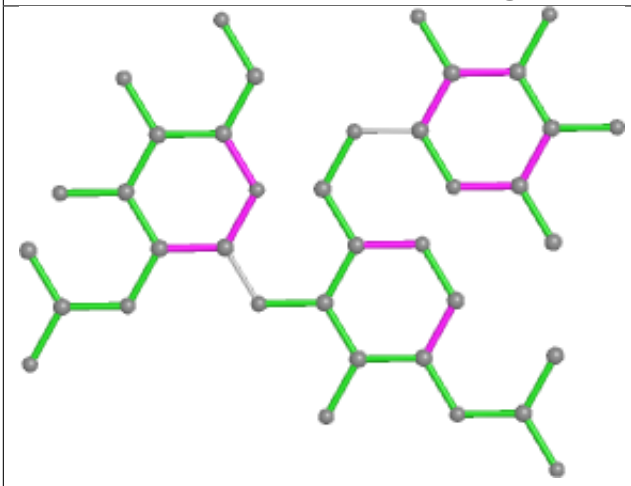


Torsions

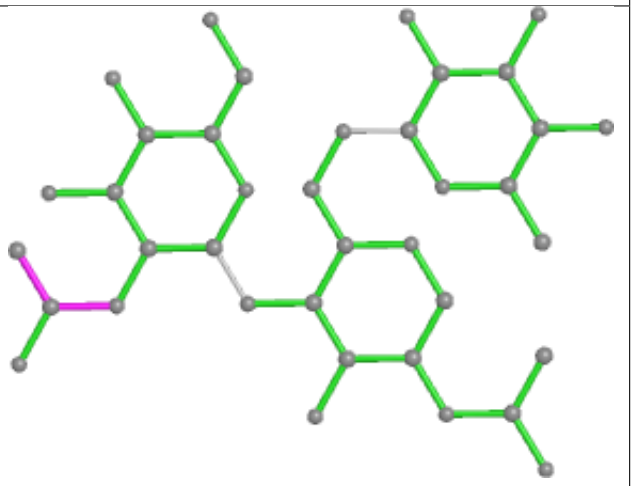


Rings

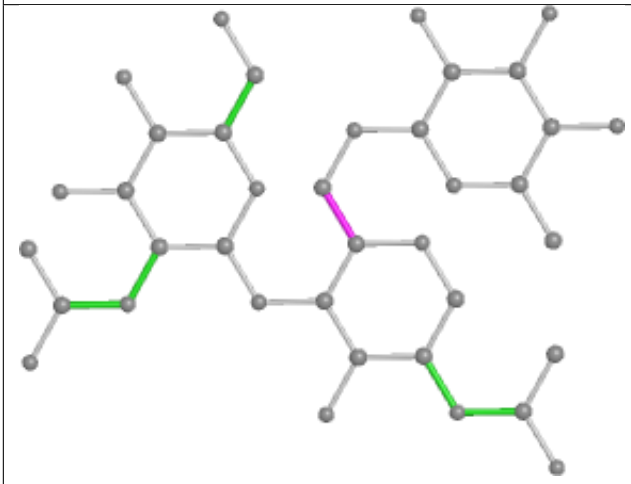
Oligosaccharide Chain I



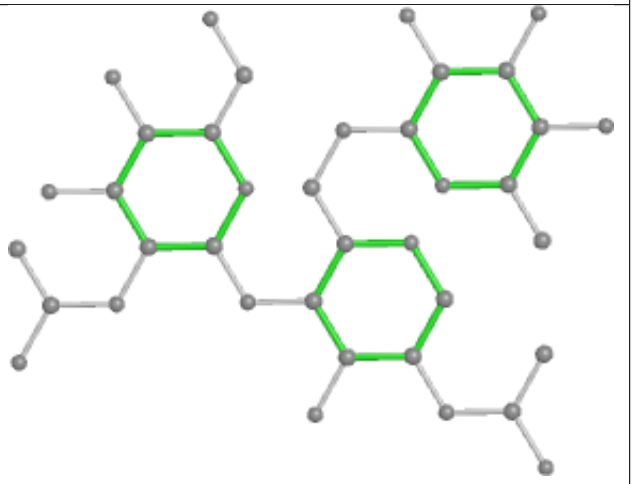
Bond lengths



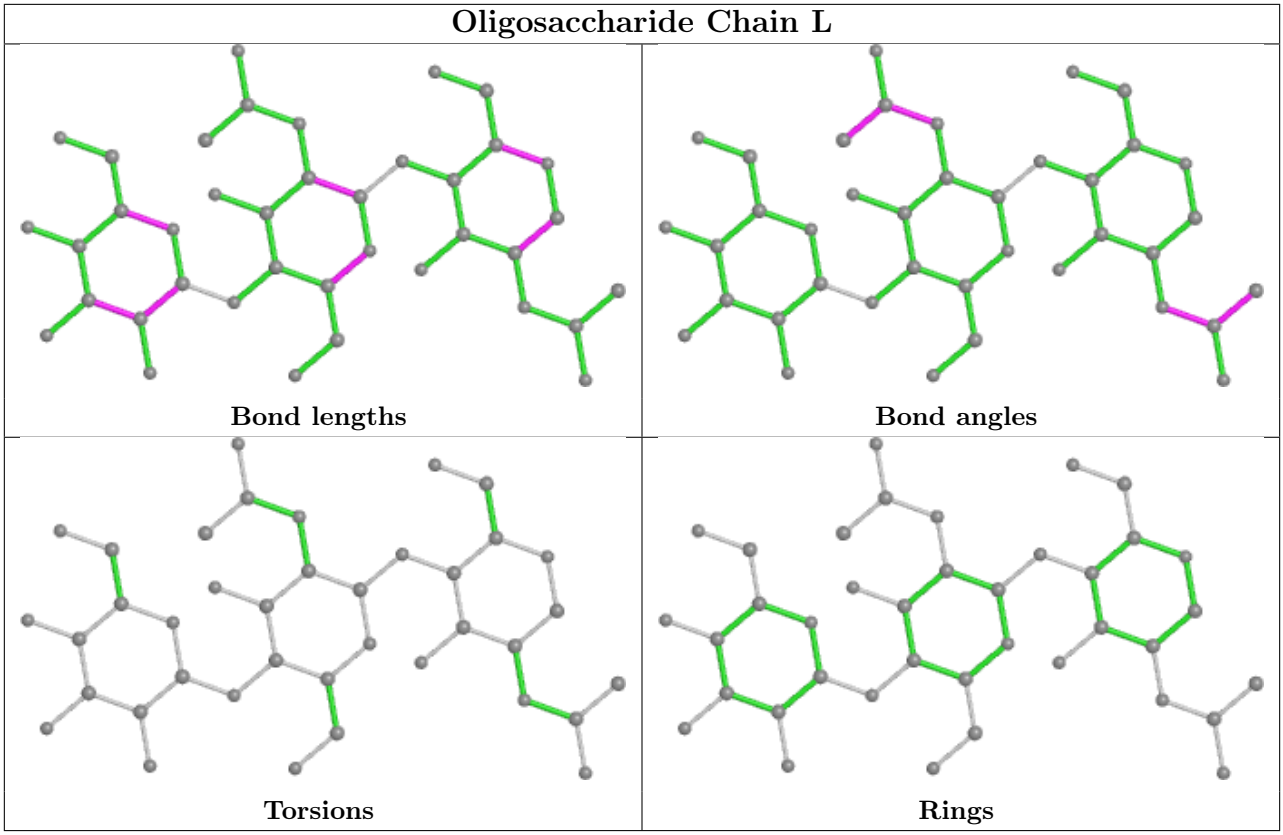
Bond angles



Torsions



Rings



5.6 Ligand geometry (i)

6 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	$\#\|Z\| > 2$
7	NAG	C	701	1	14,14,15	1.53	2 (14%)	17,19,21	0.89	1 (5%)
7	NAG	D	703	1	14,14,15	1.57	2 (14%)	17,19,21	0.94	1 (5%)
7	NAG	C	702	1	14,14,15	1.43	2 (14%)	17,19,21	0.93	1 (5%)
7	NAG	C	703	1	14,14,15	1.84	2 (14%)	17,19,21	1.14	2 (11%)
7	NAG	D	702	1	14,14,15	1.56	2 (14%)	17,19,21	1.04	1 (5%)
7	NAG	D	701	1	14,14,15	1.62	2 (14%)	17,19,21	1.02	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	701	1	-	2/6/23/26	0/1/1/1
7	NAG	D	703	1	-	0/6/23/26	0/1/1/1
7	NAG	C	702	1	-	0/6/23/26	0/1/1/1
7	NAG	C	703	1	-	2/6/23/26	0/1/1/1
7	NAG	D	702	1	-	0/6/23/26	0/1/1/1
7	NAG	D	701	1	-	0/6/23/26	0/1/1/1

The worst 5 of 12 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	C	703	NAG	C1-C2	5.98	1.61	1.52
7	D	701	NAG	C1-C2	4.32	1.58	1.52
7	D	703	NAG	C1-C2	4.21	1.58	1.52
7	C	701	NAG	C1-C2	3.90	1.58	1.52
7	D	702	NAG	C1-C2	3.76	1.58	1.52

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	C	703	NAG	C8-C7-N2	2.70	120.67	116.10
7	D	701	NAG	C8-C7-N2	2.38	120.12	116.10
7	D	702	NAG	C8-C7-N2	2.32	120.03	116.10
7	D	703	NAG	C8-C7-N2	2.27	119.94	116.10
7	C	702	NAG	C8-C7-N2	2.19	119.81	116.10

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	C	703	NAG	O5-C5-C6-O6
7	C	703	NAG	C4-C5-C6-O6
7	C	701	NAG	O5-C5-C6-O6
7	C	701	NAG	C4-C5-C6-O6

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.

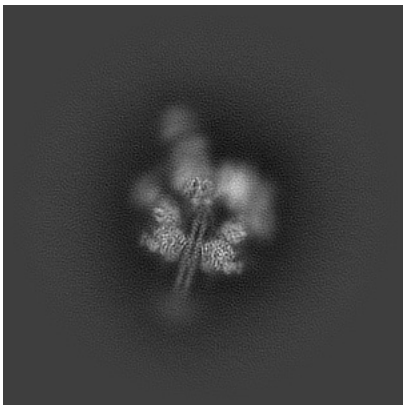
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-26163. These allow visual inspection of the internal detail of the map and identification of artifacts.

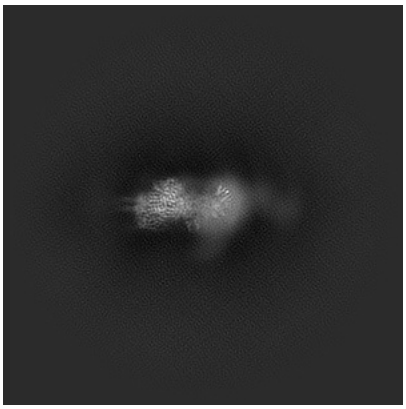
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

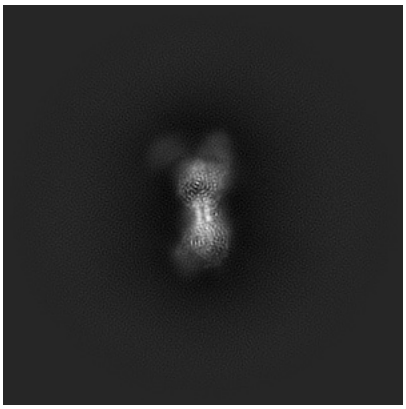
6.1.1 Primary map



X

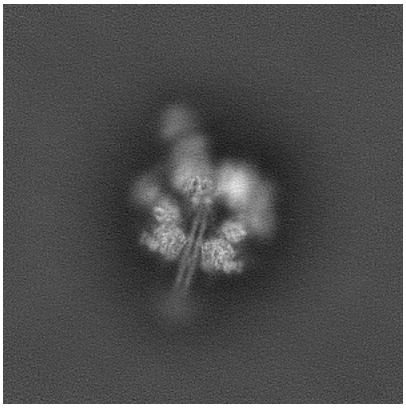


Y

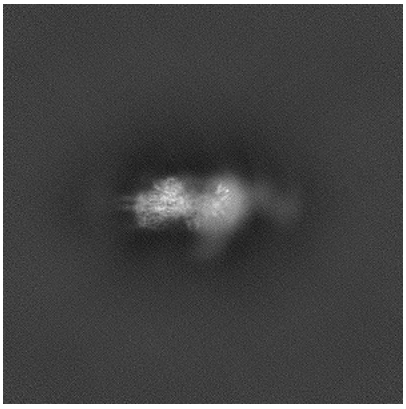


Z

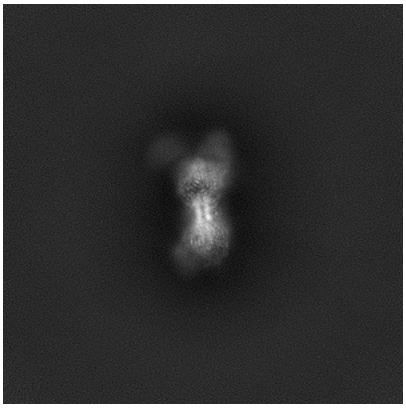
6.1.2 Raw map



X



Y

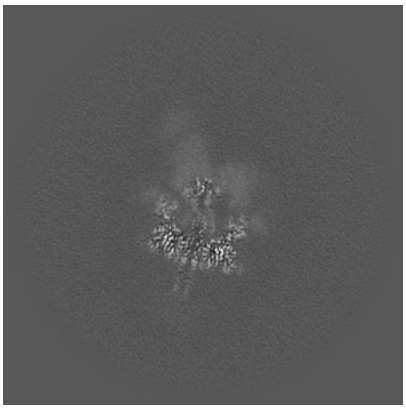


Z

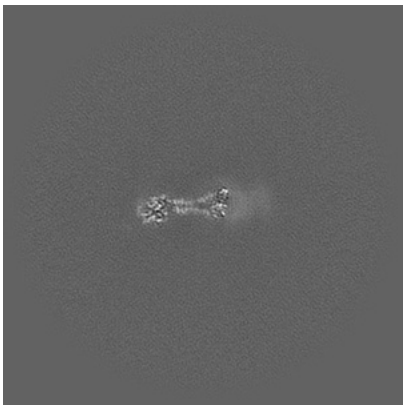
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

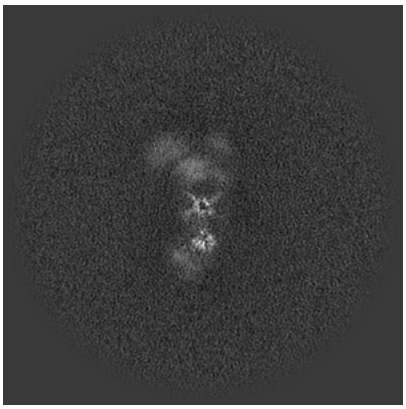
6.2.1 Primary map



X Index: 230

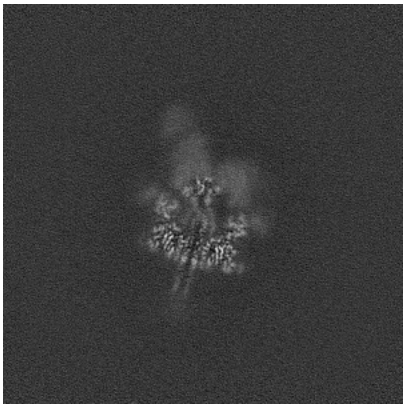


Y Index: 230

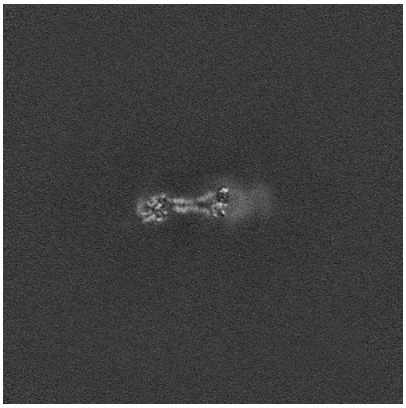


Z Index: 230

6.2.2 Raw map



X Index: 230



Y Index: 230

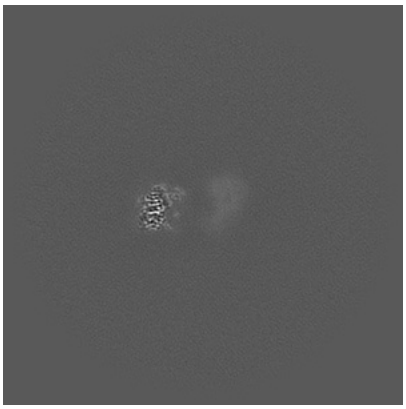
Z Index: 230

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

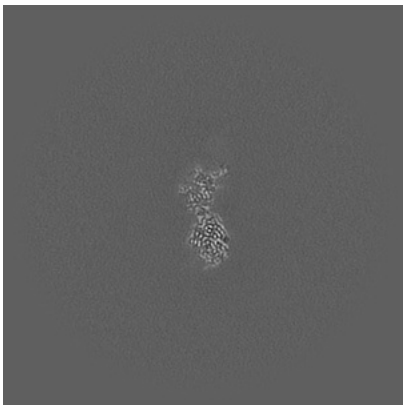
6.3 Largest variance slices (i)

6.3.1 Primary map

X Index: 235



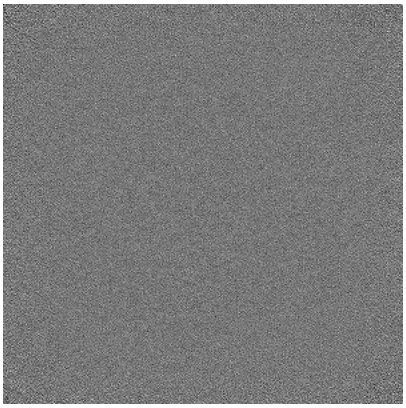
Y Index: 251



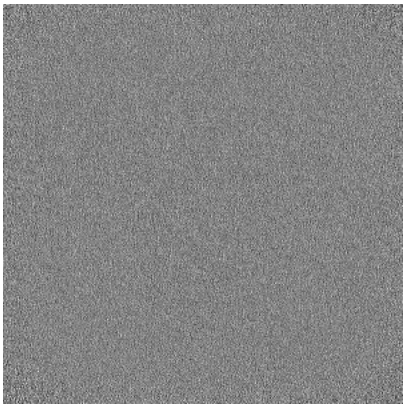
Z Index: 187

6.3.2 Raw map

X Index: 235



Y Index: 0



Z Index: 0

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

6.4.2 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.

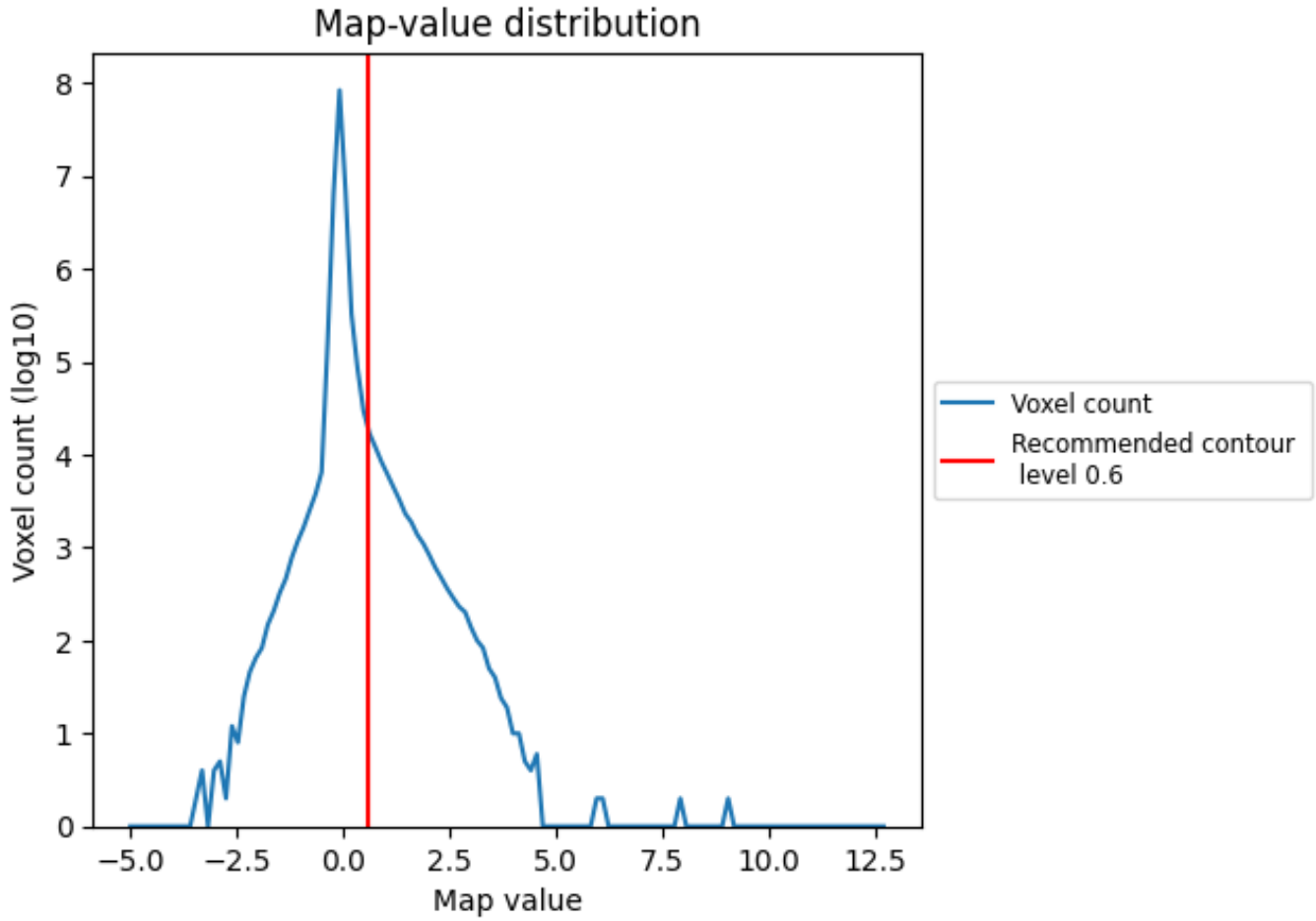
6.5 Mask visualisation (i)

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

7 Map analysis

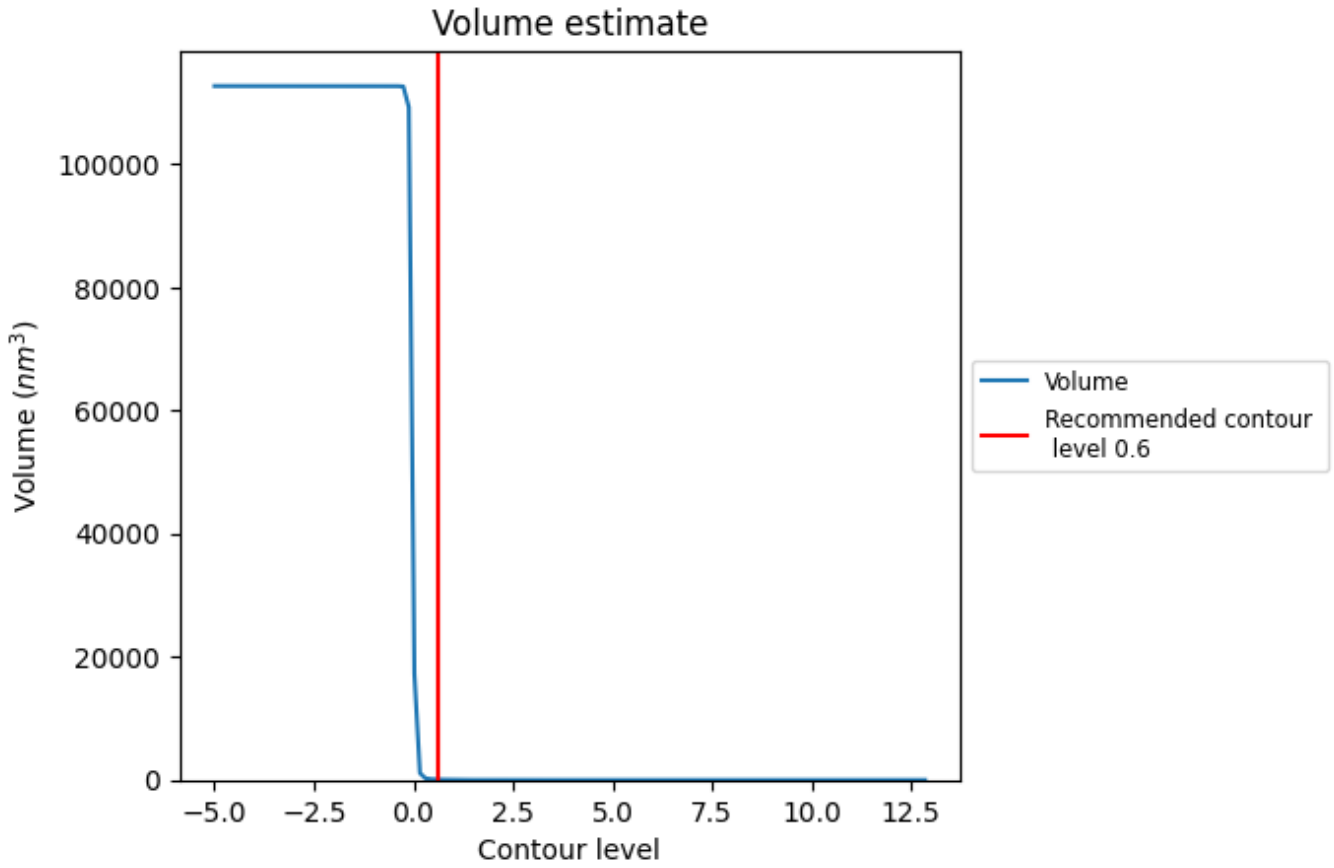
This section contains the results of statistical analysis of the map.

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.

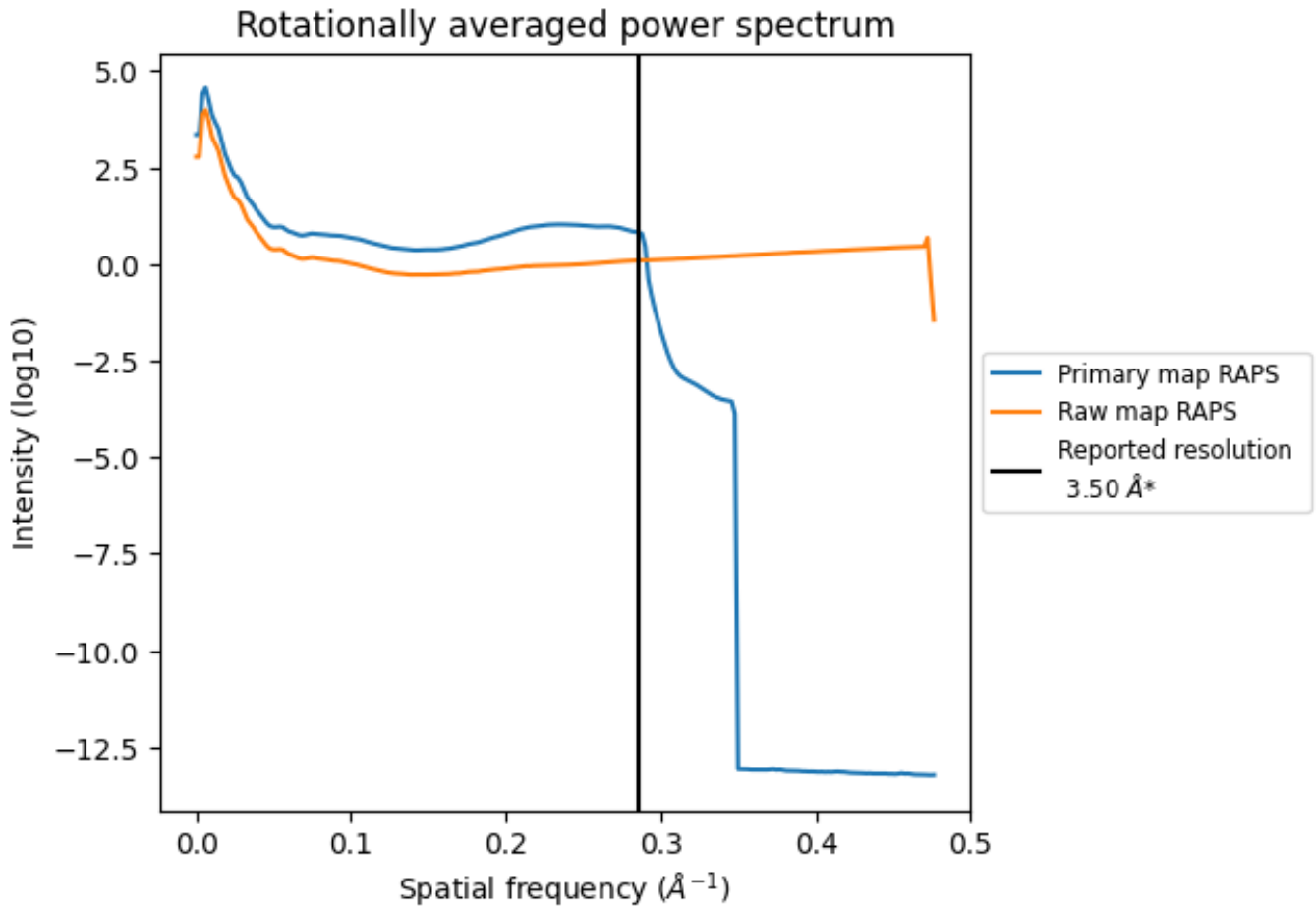
7.2 Volume estimate



The volume at the recommended contour level is 76 nm^3; this corresponds to an approximate mass of 69 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)

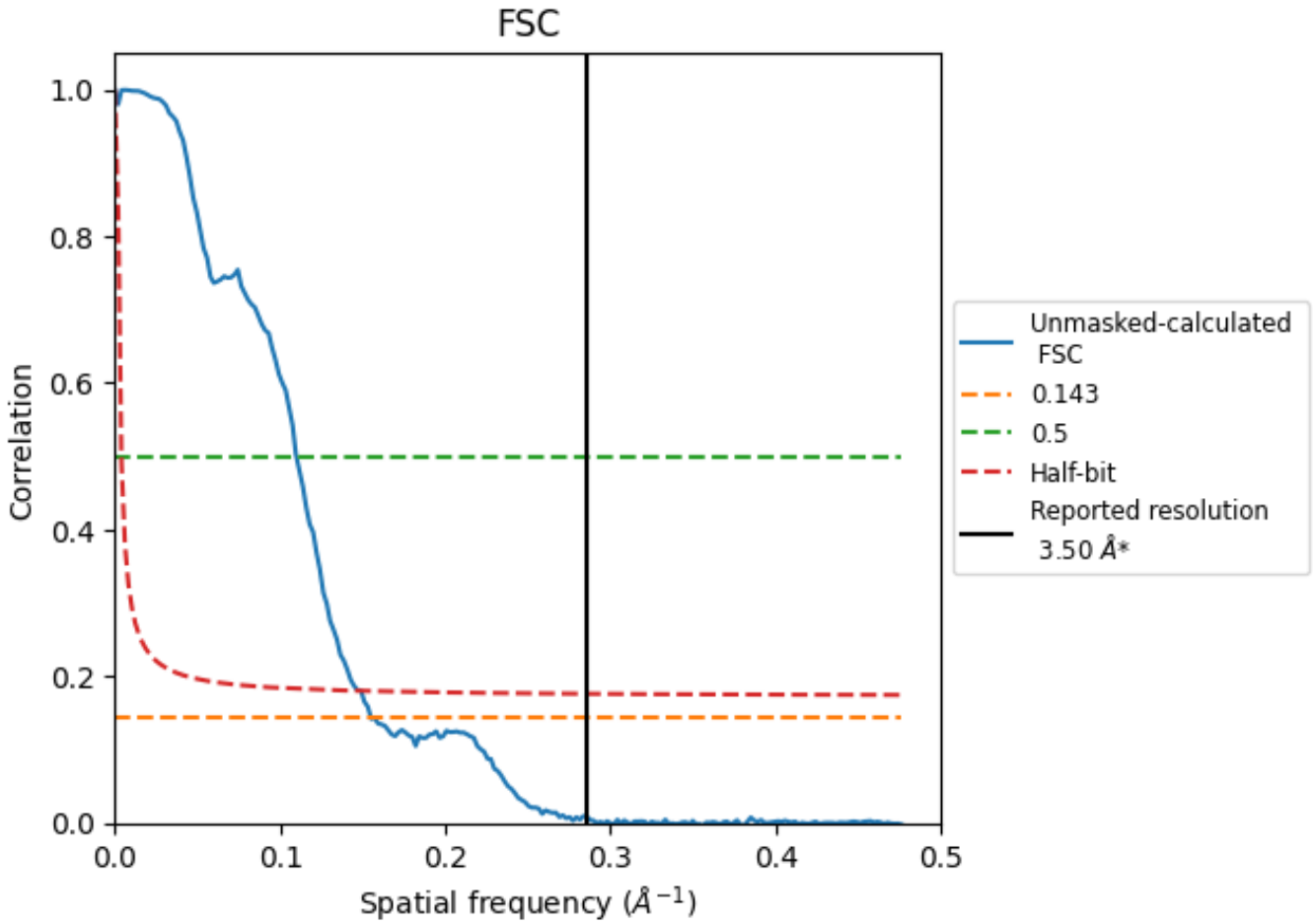


*Reported resolution corresponds to spatial frequency of 0.286 $Å^{-1}$

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 0.286 Å^{-1}

8.2 Resolution estimates (i)

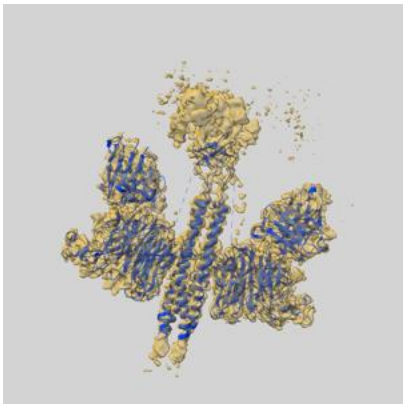
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.50	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	6.45	9.10	6.71

*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 6.45 differs from the reported value 3.5 by more than 10 %

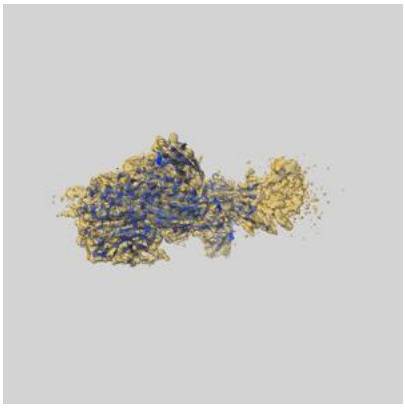
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-26163 and PDB model 7TY0. Per-residue inclusion information can be found in section 3 on page 11.

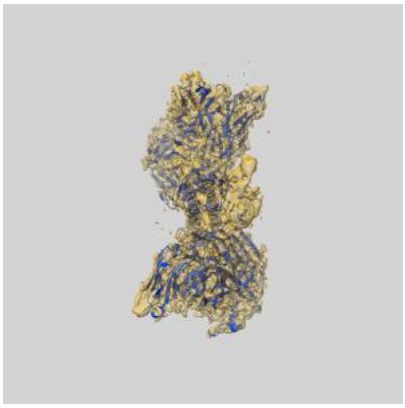
9.1 Map-model overlay



X



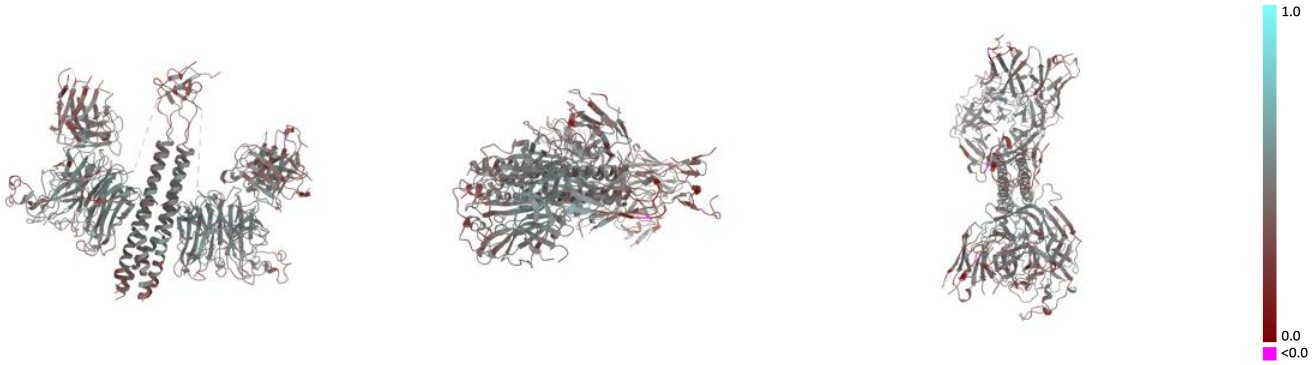
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.6 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.

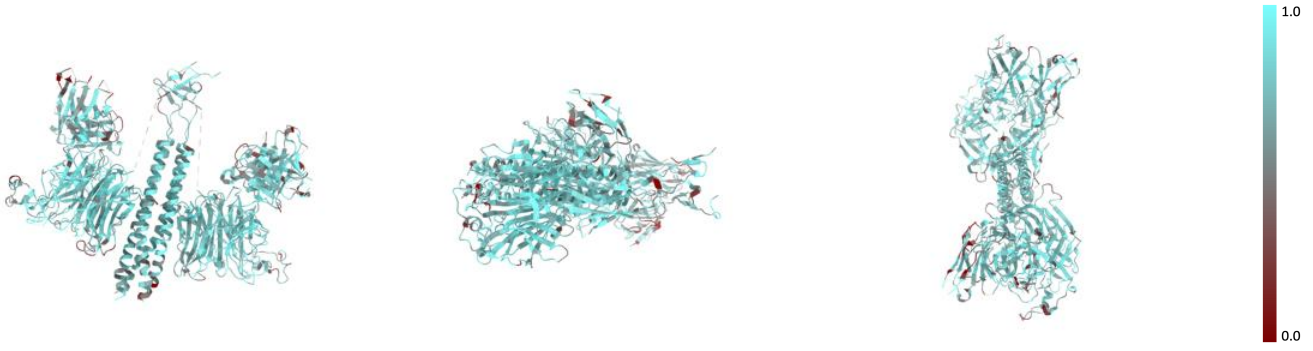
9.2 Q-score mapped to coordinate model



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.

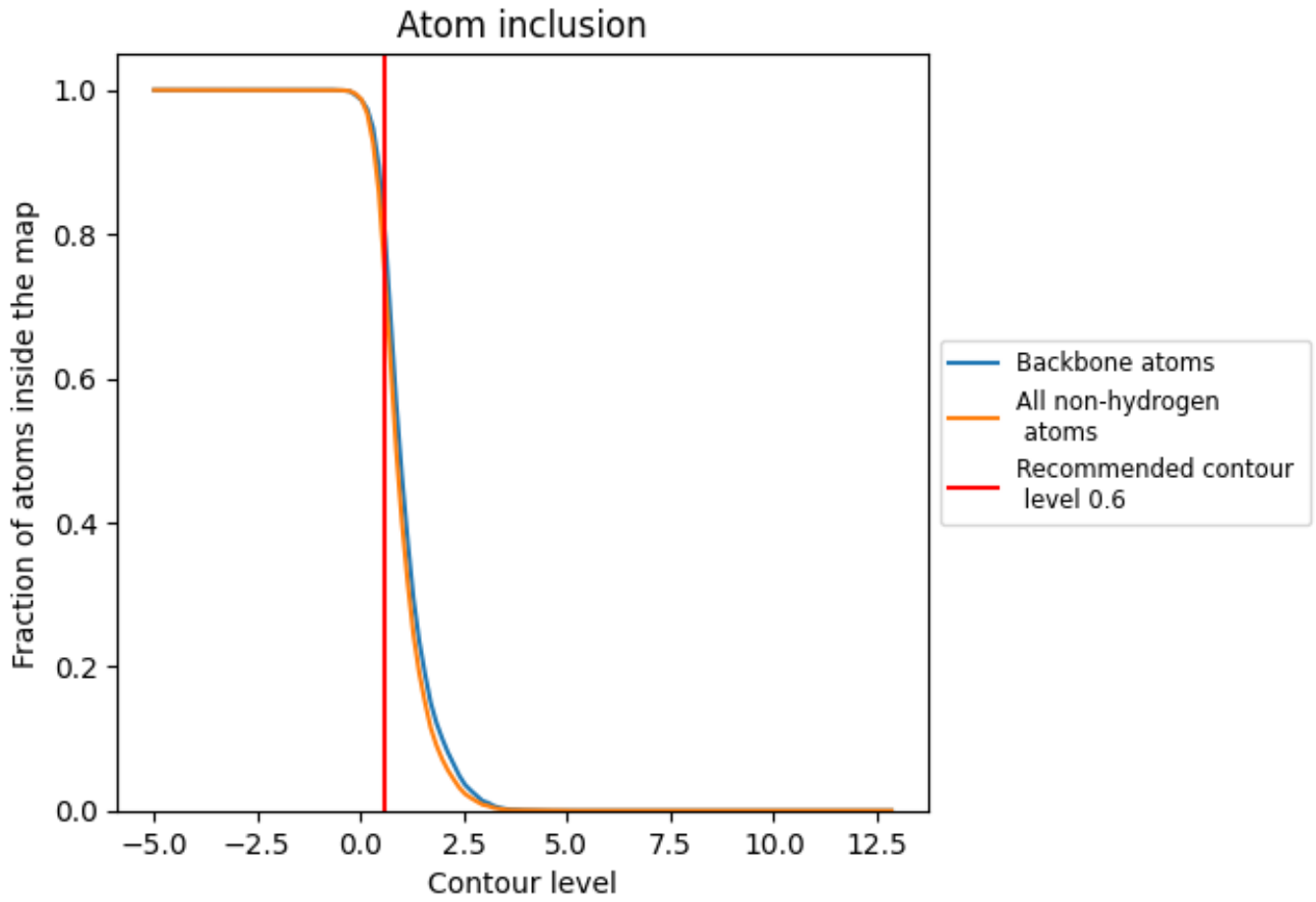
9.3 Atom inclusion mapped to coordinate model



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 (0.6).

9.4 Atom inclusion (i)



At the recommended contour level, 79% of all backbone atoms, 73% 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 (0.6) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7334	0.4390
A	0.7227	0.3930
B	0.7343	0.4130
C	0.7641	0.4630
D	0.7744	0.4570
E	0.3214	0.4090
F	0.1071	0.1670
G	0.0714	0.2030
H	0.2857	0.2170
I	0.3158	0.3760
J	0.7610	0.4250
K	0.6823	0.4030
L	0.0769	0.2310
M	0.3571	0.2800
N	0.6937	0.4300
O	0.6185	0.3870
P	0.2500	0.3130