Full wwPDB EM Validation Report (i)

Aug 17, 2026 – 08:47 PM EDT

PDB ID	:	9OGL / pdb_00009ogl
EMDB ID	:	EMD-70469
Title	:	BG505 MD39.3 SOSIP.664 in complex with 3BC315, BG18 and VRC01 Fabs
Authors	:	Ozorowski, G.; Phulera, S.; Ward, A.B.
Deposited on	:	2025-04-30
Resolution	:	3.10 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the (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 (1)) were used in the production of this report:

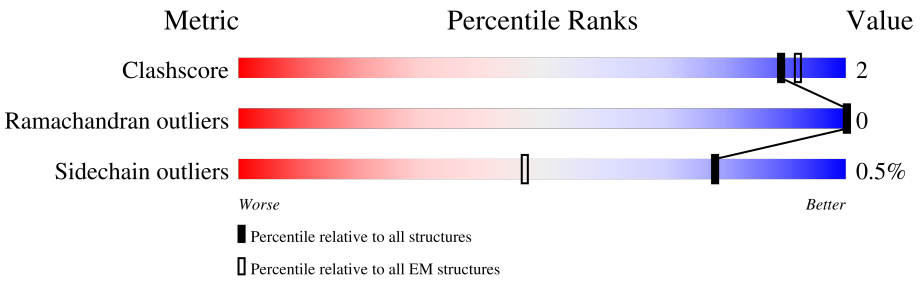
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4-5-2 with Phenix2.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

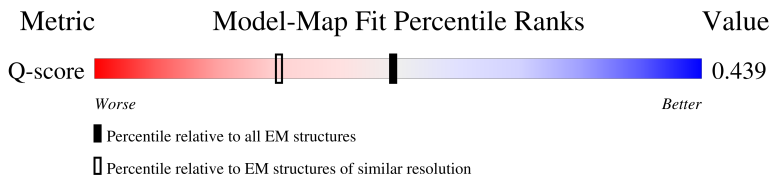
1 Overall quality at a glance (i)

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

The reported resolution of this entry is 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	14724 (2.60 - 3.60)

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	233	17% 49% 5% 45%
1	F	233	18% 54% • 45%
1	I	233	21% 54% • 45%
2	E	214	15% 44% • • 50%

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Mol	Chain	Length	Quality of chain
2	G	214	15% 48% 50%
2	J	214	18% 46% 50%
3	K	224	51% 47%
3	N	224	50% 47%
3	P	224	50% 47%
4	M	210	43% 54%
4	O	210	7% 47% 53%
4	Q	210	11% 44% 54%
5	H	232	8% 53% 46%
6	L	216	16% 48% 50%
7	A	642	82% 6% 12%
7	B	642	5% 86% 13%
7	C	642	80% 6% 14%
8	R	3	100%
8	e	3	33% 67%
9	S	4	25% 75%
10	T	10	10% 10% 70% 20%
10	a	10	90% 10%
11	U	6	33% 33% 67%
11	c	6	17% 83% 17%
12	V	2	100% 50% 50%
13	W	2	50% 100%
13	X	2	100%
13	b	2	50% 50%
13	d	2	50% 50%

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Mol	Chain	Length	Quality of chain
13	h	2	100%
14	Y	5	20% 20% 80%
14	f	5	20% 100%
15	Z	7	29% 14% 86%
16	g	10	10% 80% 10%
17	i	6	17% 33% 67%

2 Entry composition (i)

There are 18 unique types of molecules in this entry. The entry contains 27177 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 BG18 Fab heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	D	127	995	626	176	187	6	0	0
1	F	129	1007	632	178	191	6	0	0
1	I	127	995	626	176	187	6	0	0

- Molecule 2 is a protein called BG18 Fab light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	E	106	806	501	140	162	3	0	0
2	G	106	806	501	140	162	3	0	0
2	J	106	806	501	140	162	3	0	0

- Molecule 3 is a protein called VRC01 Fab heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	K	119	955	603	173	171	8	0	0
3	N	119	955	603	173	171	8	0	0
3	P	119	955	603	173	171	8	0	0

- Molecule 4 is a protein called VRC01 Fab light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	M	97	751	474	129	146	2	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	O	98	758	479	130	147	2	0	0
4	Q	97	751	474	129	146	2	0	0

- Molecule 5 is a protein called 3BC315 Fab heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	H	126	995	637	173	178	7	0	0

- Molecule 6 is a protein called 3BC315 Fab light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	L	108	804	505	134	162	3	0	0

- Molecule 7 is a protein called Envelope glycoprotein gp160.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	A	566	4464	2806	783	843	32	0	0
7	B	557	4393	2758	771	831	33	0	0
7	C	554	4374	2753	764	825	32	0	0

There are 93 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	106	GLU	THR	conflict	UNP A0A6H1VFU0
A	240	GLN	PRO	conflict	UNP A0A6H1VFU0
A	271	ILE	MET	conflict	UNP A0A6H1VFU0
A	288	LEU	PHE	conflict	UNP A0A6H1VFU0
A	291	SER	PRO	conflict	UNP A0A6H1VFU0
A	304	VAL	ARG	conflict	UNP A0A6H1VFU0
A	319	TYR	ALA	conflict	UNP A0A6H1VFU0
A	363	GLN	ASN	conflict	UNP A0A6H1VFU0
A	375	SER	TYR	conflict	UNP A0A6H1VFU0
A	501	CYS	ALA	conflict	UNP A0A6H1VFU0
A	503E	SER	-	linker	UNP A0A6H1VFU0
A	503F	HIS	-	linker	UNP A0A6H1VFU0

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Chain	Residue	Modelled	Actual	Comment	Reference
A	503G	SER	-	linker	UNP A0A6H1VFU0
A	503H	GLY	-	linker	UNP A0A6H1VFU0
A	503I	SER	-	linker	UNP A0A6H1VFU0
A	503J	GLY	-	linker	UNP A0A6H1VFU0
A	503K	GLY	-	linker	UNP A0A6H1VFU0
A	503L	SER	-	linker	UNP A0A6H1VFU0
A	503M	GLY	-	linker	UNP A0A6H1VFU0
A	503N	SER	-	linker	UNP A0A6H1VFU0
A	503O	GLY	-	linker	UNP A0A6H1VFU0
A	503P	GLY	-	linker	UNP A0A6H1VFU0
A	503Q	HIS	-	linker	UNP A0A6H1VFU0
A	503R	ALA	-	linker	UNP A0A6H1VFU0
A	519	SER	PHE	conflict	UNP A0A6H1VCU6
A	559	PRO	ILE	conflict	UNP A0A6H1VCU6
A	561	PRO	ALA	conflict	UNP A0A6H1VCU6
A	568	ASP	LEU	conflict	UNP A0A6H1VCU6
A	570	HIS	VAL	conflict	UNP A0A6H1VCU6
A	585	HIS	ARG	conflict	UNP A0A6H1VCU6
A	605	CYS	THR	conflict	UNP A0A6H1VCU6
B	106	GLU	THR	conflict	UNP A0A6H1VFU0
B	240	GLN	PRO	conflict	UNP A0A6H1VFU0
B	271	ILE	MET	conflict	UNP A0A6H1VFU0
B	288	LEU	PHE	conflict	UNP A0A6H1VFU0
B	291	SER	PRO	conflict	UNP A0A6H1VFU0
B	304	VAL	ARG	conflict	UNP A0A6H1VFU0
B	319	TYR	ALA	conflict	UNP A0A6H1VFU0
B	363	GLN	ASN	conflict	UNP A0A6H1VFU0
B	375	SER	TYR	conflict	UNP A0A6H1VFU0
B	501	CYS	ALA	conflict	UNP A0A6H1VFU0
B	503E	SER	-	linker	UNP A0A6H1VFU0
B	503F	HIS	-	linker	UNP A0A6H1VFU0
B	503G	SER	-	linker	UNP A0A6H1VFU0
B	503H	GLY	-	linker	UNP A0A6H1VFU0
B	503I	SER	-	linker	UNP A0A6H1VFU0
B	503J	GLY	-	linker	UNP A0A6H1VFU0
B	503K	GLY	-	linker	UNP A0A6H1VFU0
B	503L	SER	-	linker	UNP A0A6H1VFU0
B	503M	GLY	-	linker	UNP A0A6H1VFU0
B	503N	SER	-	linker	UNP A0A6H1VFU0
B	503O	GLY	-	linker	UNP A0A6H1VFU0
B	503P	GLY	-	linker	UNP A0A6H1VFU0
B	503Q	HIS	-	linker	UNP A0A6H1VFU0

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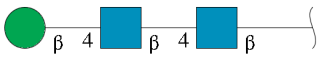
Chain	Residue	Modelled	Actual	Comment	Reference
B	503R	ALA	-	linker	UNP A0A6H1VFU0
B	503Z	SER	PHE	conflict	UNP A0A6H1VCU6
B	559	PRO	ILE	conflict	UNP A0A6H1VCU6
B	561	PRO	ALA	conflict	UNP A0A6H1VCU6
B	568	ASP	LEU	conflict	UNP A0A6H1VCU6
B	570	HIS	VAL	conflict	UNP A0A6H1VCU6
B	585	HIS	ARG	conflict	UNP A0A6H1VCU6
B	605	CYS	THR	conflict	UNP A0A6H1VCU6
C	106	GLU	THR	conflict	UNP A0A6H1VFU0
C	240	GLN	PRO	conflict	UNP A0A6H1VFU0
C	271	ILE	MET	conflict	UNP A0A6H1VFU0
C	288	LEU	PHE	conflict	UNP A0A6H1VFU0
C	291	SER	PRO	conflict	UNP A0A6H1VFU0
C	304	VAL	ARG	conflict	UNP A0A6H1VFU0
C	319	TYR	ALA	conflict	UNP A0A6H1VFU0
C	363	GLN	ASN	conflict	UNP A0A6H1VFU0
C	375	SER	TYR	conflict	UNP A0A6H1VFU0
C	501	CYS	ALA	conflict	UNP A0A6H1VFU0
C	502F	SER	-	linker	UNP A0A6H1VFU0
C	502G	HIS	-	linker	UNP A0A6H1VFU0
C	502H	SER	-	linker	UNP A0A6H1VFU0
C	502I	GLY	-	linker	UNP A0A6H1VFU0
C	502J	SER	-	linker	UNP A0A6H1VFU0
C	502K	GLY	-	linker	UNP A0A6H1VFU0
C	502L	GLY	-	linker	UNP A0A6H1VFU0
C	502M	SER	-	linker	UNP A0A6H1VFU0
C	502N	GLY	-	linker	UNP A0A6H1VFU0
C	502O	SER	-	linker	UNP A0A6H1VFU0
C	502P	GLY	-	linker	UNP A0A6H1VFU0
C	502Q	GLY	-	linker	UNP A0A6H1VFU0
C	502R	HIS	-	linker	UNP A0A6H1VFU0
C	502S	ALA	-	linker	UNP A0A6H1VFU0
C	503A	SER	PHE	conflict	UNP A0A6H1VCU6
C	559	PRO	ILE	conflict	UNP A0A6H1VCU6
C	561	PRO	ALA	conflict	UNP A0A6H1VCU6
C	568	ASP	LEU	conflict	UNP A0A6H1VCU6
C	570	HIS	VAL	conflict	UNP A0A6H1VCU6
C	585	HIS	ARG	conflict	UNP A0A6H1VCU6
C	605	CYS	THR	conflict	UNP A0A6H1VCU6

- Molecule 8 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.

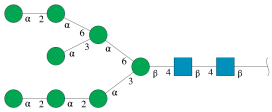


Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
8	R	3	39	22	2	15	0	0
8	e	3	39	22	2	15	0	0

- Molecule 9 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		
9	S	4	50	28	2	20	0	0

- Molecule 10 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-[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		
10	T	10	116	64	2	50	0	0
10	a	10	116	64	2	50	0	0

- Molecule 11 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-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		
11	U	6	72	40	2	30	0	0
11	c	6	72	40	2	30	0	0

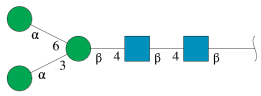
- Molecule 12 is an oligosaccharide called alpha-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
12	V	2	24	14	1	9	0	0

- Molecule 13 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

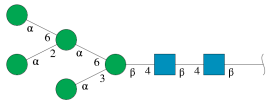
Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
13	W	2	28	16	2	10	0	0
13	X	2	28	16	2	10	0	0
13	b	2	28	16	2	10	0	0
13	d	2	28	16	2	10	0	0
13	h	2	28	16	2	10	0	0

- Molecule 14 is an oligosaccharide called 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.



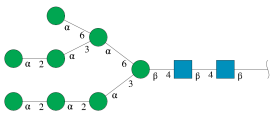
Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
14	Y	5	61	34	2	25	0	0
14	f	5	61	34	2	25	0	0

- Molecule 15 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)-[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.



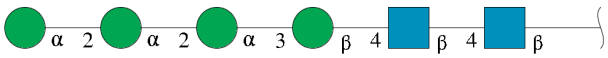
Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
15	Z	7	83	46	2	35	0	0

- Molecule 16 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]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.



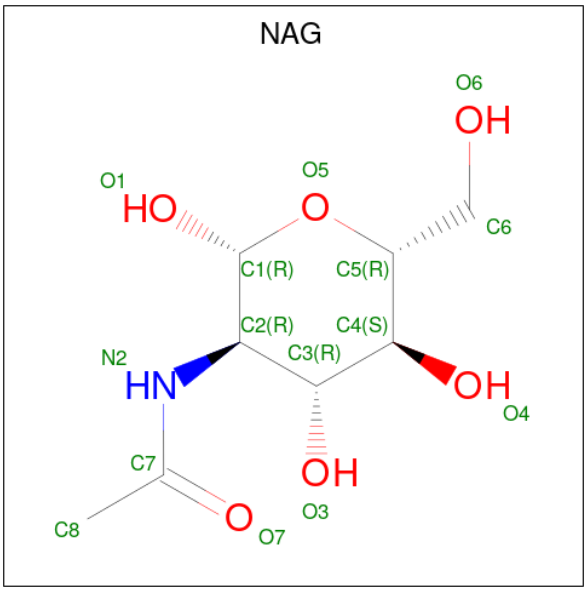
Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
16	g	10	116	64	2	50	0	0

- Molecule 17 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-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		
17	i	6	72	40	2	30	0	0

- Molecule 18 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



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

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

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Continued from previous page...

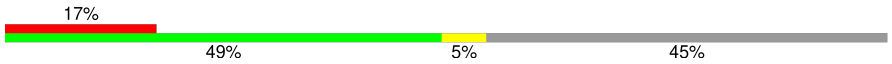
Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
18	C	1	14	8	1	5	0
			Total	C	N	O	
18	C	1	14	8	1	5	0
			Total	C	N	O	
18	C	1	14	8	1	5	0
			Total	C	N	O	
18	C	1	14	8	1	5	0
			Total	C	N	O	
18	C	1	14	8	1	5	0
			Total	C	N	O	
18	C	1	14	8	1	5	0
			Total	C	N	O	
18	C	1	14	8	1	5	0
			Total	C	N	O	
18	C	1	14	8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

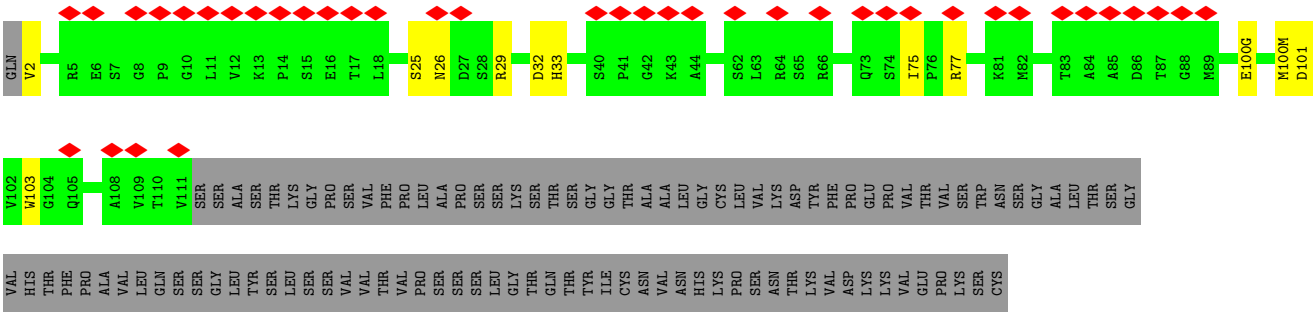
3 Residue-property plots (i)

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: BG18 Fab heavy chain

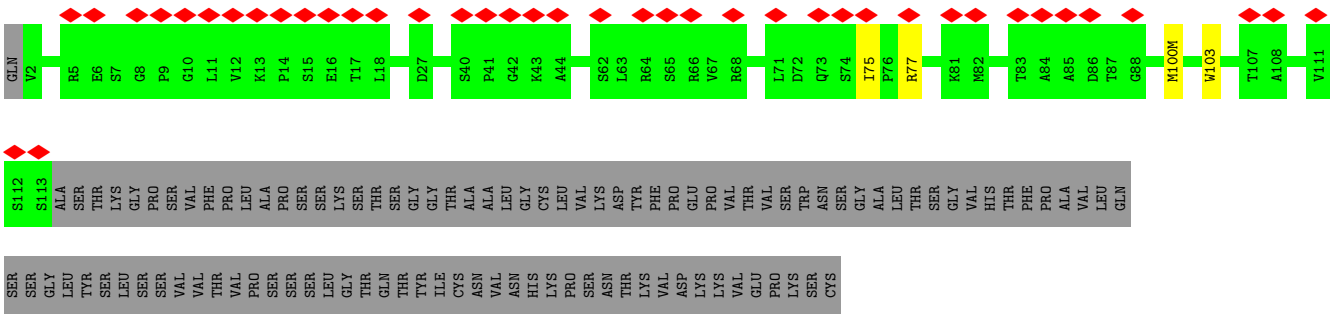
Chain D:





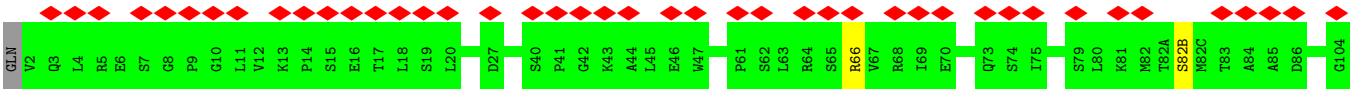
- Molecule 1: BG18 Fab heavy chain

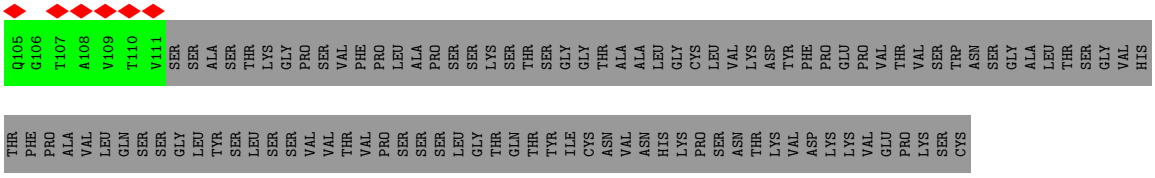
Chain F:



- Molecule 1: BG18 Fab heavy chain

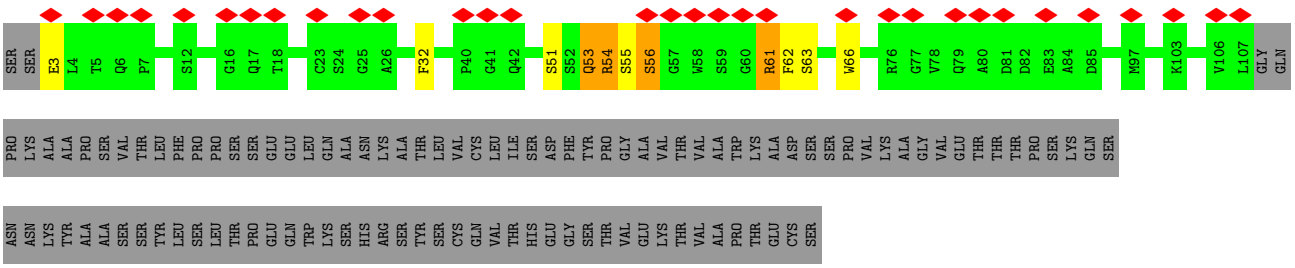
Chain I:





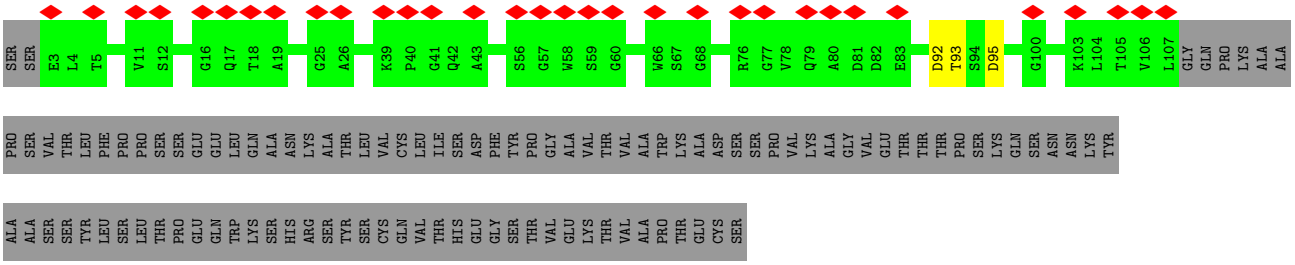
• Molecule 2: BG18 Fab light chain

Chain E:



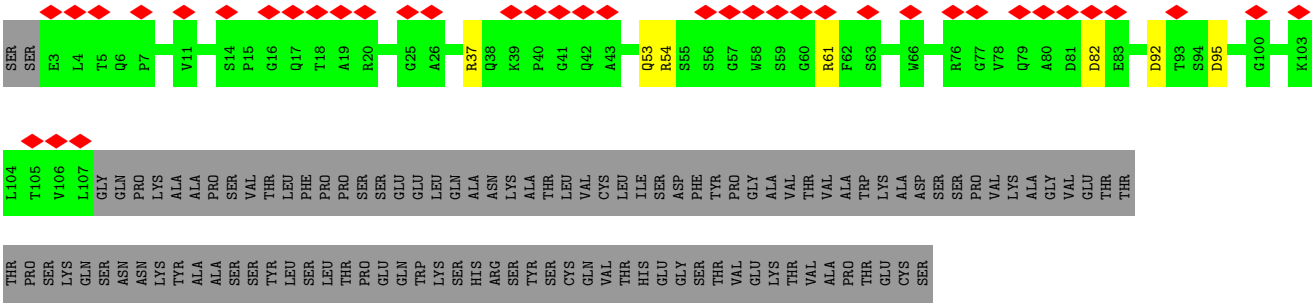
• Molecule 2: BG18 Fab light chain

Chain G:



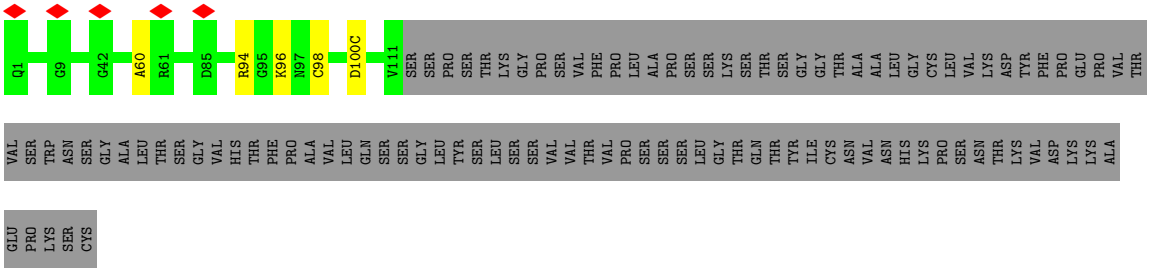
• Molecule 2: BG18 Fab light chain

Chain J:



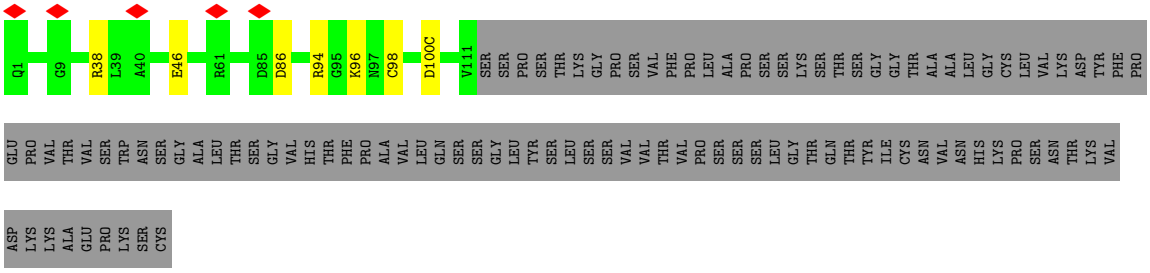
• Molecule 3: VRC01 Fab heavy chain

Chain K:



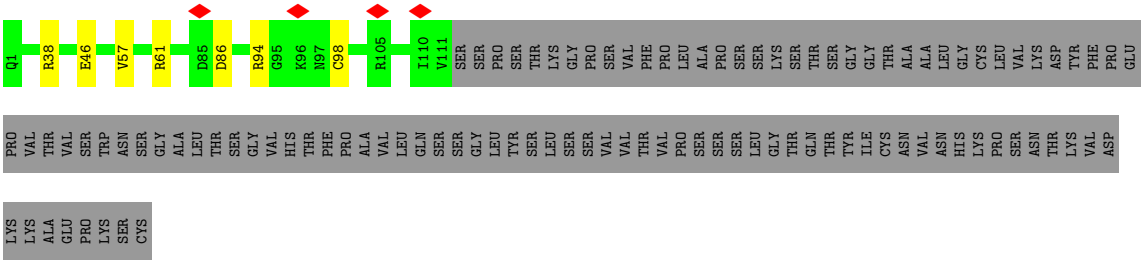
• Molecule 3: VRC01 Fab heavy chain

Chain N:



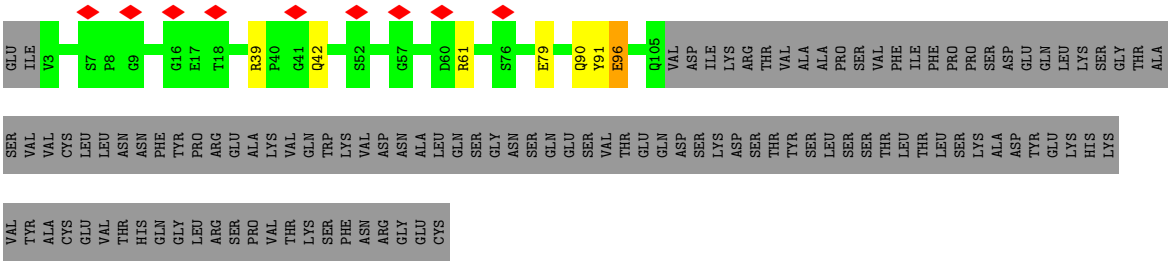
• Molecule 3: VRC01 Fab heavy chain

Chain P:



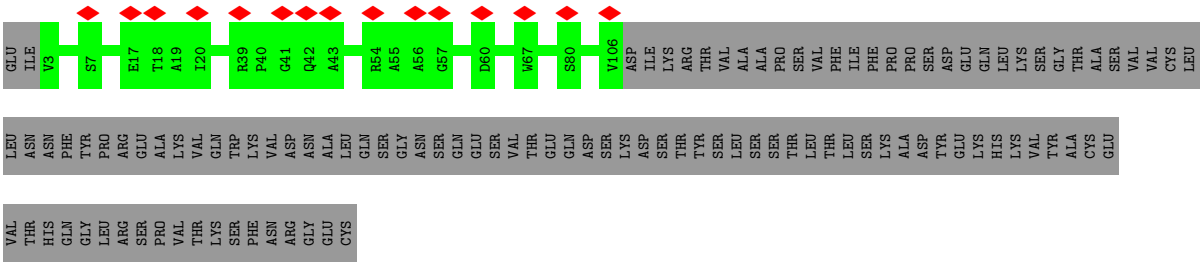
• Molecule 4: VRC01 Fab light chain

Chain M:



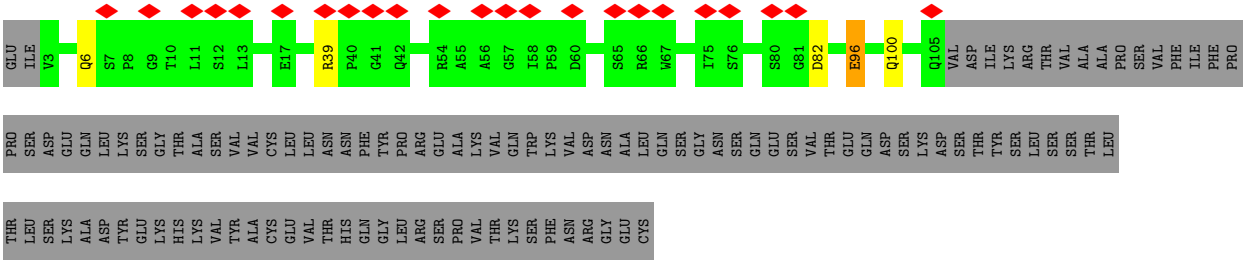
• Molecule 4: VRC01 Fab light chain

Chain O:



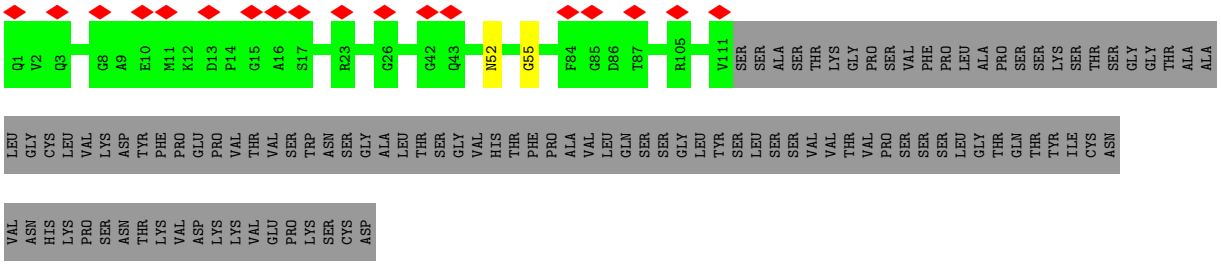
- Molecule 4: VRC01 Fab light chain

Chain Q:



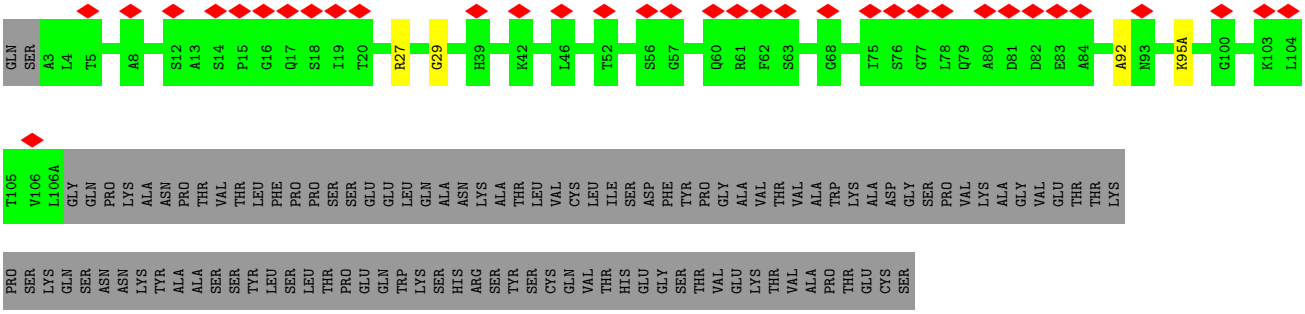
- Molecule 5: 3BC315 Fab heavy chain

Chain H:



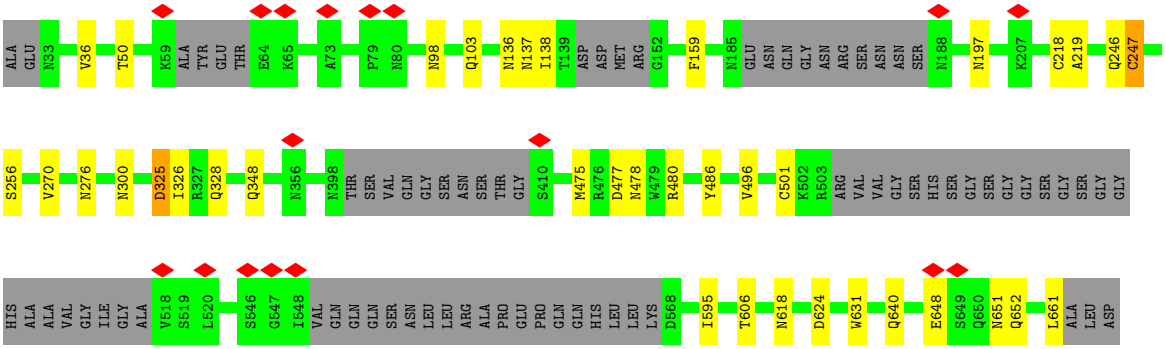
- Molecule 6: 3BC315 Fab light chain

Chain L:



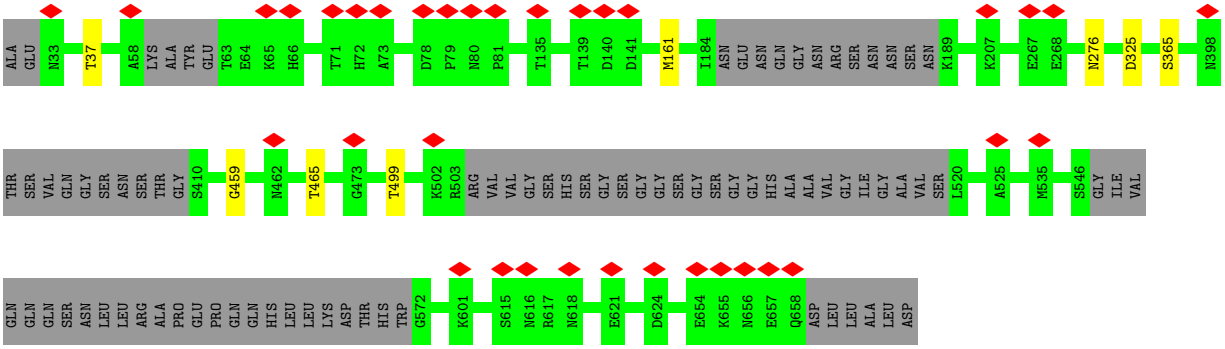
- Molecule 7: Envelope glycoprotein gp160

Chain A:



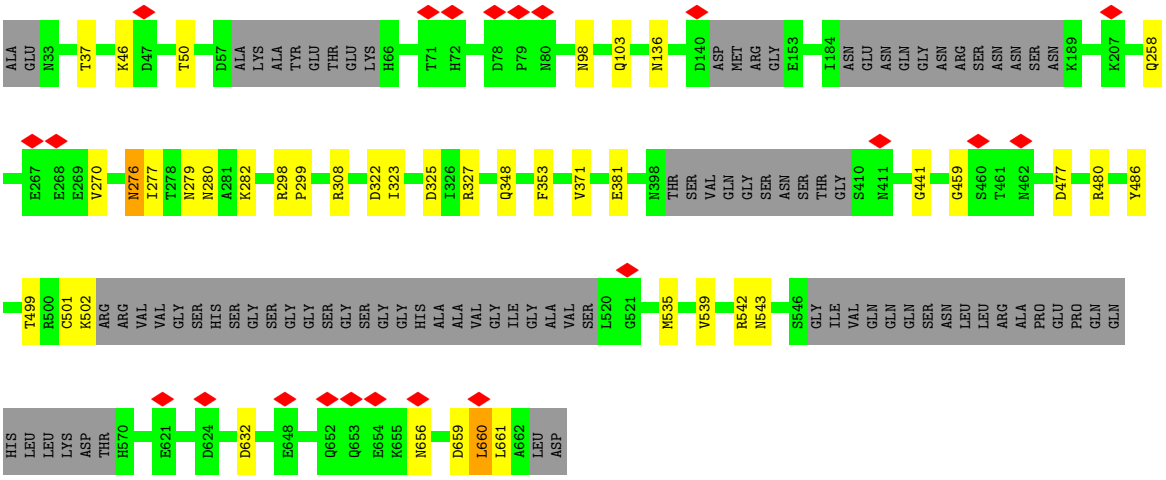
• Molecule 7: Envelope glycoprotein gp160

Chain B:



• Molecule 7: Envelope glycoprotein gp160

Chain C:



• Molecule 8: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain R: 100%

• Molecule 8: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain e: 33% 67%

• Molecule 9: 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 S: 25% 75%

• Molecule 10: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-[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

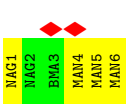
Chain T: 10% 10% 70% 20%

• Molecule 10: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-[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 a: 90% 10%

• Molecule 11: alpha-D-mannopyranose-(1-2)-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 U: 33% 33% 67%



• Molecule 11: alpha-D-mannopyranose-(1-2)-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

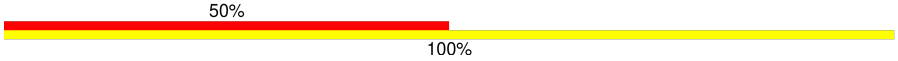
Chain c:

• Molecule 12: alpha-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain V:

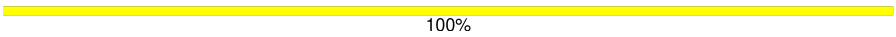
• Molecule 13: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain W:



• Molecule 13: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain X:



• Molecule 13: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain b:

• Molecule 13: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

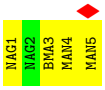
Chain d:

• Molecule 13: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain h: 100%

• Molecule 14: 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 Y: 20% 20% 80%



• Molecule 14: 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 f: 20% 100%

• Molecule 15: alpha-D-mannopyranose-(1-2)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)-[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

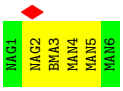
Chain Z: 29% 14% 86%

• Molecule 16: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]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: 10% 80% 10%

• Molecule 17: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-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 i:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	243503	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS GLACIOS	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/Å^2$)	45	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	190000	Depositor
Image detector	TFS FALCON 4i (4k x 4k)	Depositor
Maximum map value	1.533	Depositor
Minimum map value	-0.917	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.028	Depositor
Recommended contour level	0.17	Depositor
Map size (Å)	413.56, 413.56, 413.56	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.0339, 1.0339, 1.0339	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: MAN, FUC, NAG, BMA

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	0.25	0/1021	0.62	0/1390
1	F	0.22	0/1033	0.54	0/1406
1	I	0.24	0/1021	0.58	0/1390
2	E	0.31	0/825	0.76	3/1122 (0.3%)
2	G	0.20	0/825	0.50	0/1122
2	J	0.20	0/825	0.51	0/1122
3	K	0.25	0/980	0.58	0/1327
3	N	0.25	0/980	0.56	0/1327
3	P	0.25	0/980	0.59	0/1327
4	M	0.22	0/771	0.54	0/1048
4	O	0.21	0/778	0.49	0/1058
4	Q	0.23	0/771	0.48	0/1048
5	H	0.22	0/1023	0.53	0/1385
6	L	0.24	0/821	0.53	0/1115
7	A	0.28	0/4552	0.60	2/6177 (0.0%)
7	B	0.25	0/4479	0.54	1/6077 (0.0%)
7	C	0.29	0/4462	0.61	3/6058 (0.0%)
All	All	0.26	0/26147	0.58	9/35499 (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
2	E	0	2
2	J	0	1
All	All	0	3

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	56	SER	N-CA-C	-13.05	96.02	112.72
7	C	659	ASP	N-CA-C	-8.67	103.22	113.88
7	C	276	ASN	N-CA-C	-7.17	102.06	111.02
7	A	247	CYS	CA-CB-SG	6.85	130.15	114.40
2	E	55	SER	CA-C-N	-6.28	111.15	122.46
2	E	55	SER	C-N-CA	-6.28	111.15	122.46
7	C	661	LEU	N-CA-C	-5.36	99.39	110.80
7	A	501	CYS	CA-CB-SG	5.15	126.24	114.40
7	B	276	ASN	N-CA-C	-5.02	100.16	108.75

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	E	54	ARG	Sidechain
2	E	61	ARG	Sidechain
2	J	61	ARG	Sidechain

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	995	0	962	7	0
1	F	1007	0	972	2	0
1	I	995	0	962	1	0
2	E	806	0	776	11	0
2	G	806	0	776	2	0
2	J	806	0	776	4	0
3	K	955	0	929	3	0
3	N	955	0	929	4	0
3	P	955	0	929	5	0
4	M	751	0	711	4	0
4	O	758	0	720	0	0
4	Q	751	0	711	3	0
5	H	995	0	960	2	0
6	L	804	0	786	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	A	4464	0	4367	32	0
7	B	4393	0	4300	5	0
7	C	4374	0	4273	29	0
8	R	39	0	34	0	0
8	e	39	0	34	0	0
9	S	50	0	43	0	0
10	T	116	0	97	2	0
10	a	116	0	97	1	0
11	U	72	0	61	0	0
11	c	72	0	61	1	0
12	V	24	0	22	0	0
13	W	28	0	25	0	0
13	X	28	0	25	0	0
13	b	28	0	25	0	0
13	d	28	0	25	0	0
13	h	28	0	25	0	0
14	Y	61	0	52	0	0
14	f	61	0	52	0	0
15	Z	83	0	70	0	0
16	g	116	0	97	1	0
17	i	72	0	61	0	0
18	A	210	0	195	0	0
18	B	154	0	143	0	0
18	C	182	0	169	0	0
All	All	27177	0	26252	94	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 2.

All (94) 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)
2:E:66:TRP:CE2	7:A:138:ILE:HG23	1.97	0.97
2:E:66:TRP:NE1	7:A:138:ILE:HG23	1.97	0.79
1:D:2:VAL:N	1:D:26:ASN:OD1	2.15	0.79
7:C:46:LYS:NZ	7:C:632:ASP:OD2	2.18	0.77
2:E:56:SER:HB2	7:A:138:ILE:HD11	1.66	0.76
4:Q:6:GLN:O	4:Q:100:GLN:NE2	2.22	0.73
7:A:475:MET:SD	7:A:478:ASN:ND2	2.63	0.72
7:A:218:CYS:HA	7:A:247:CYS:HB3	1.71	0.72
2:G:95:ASP:O	11:c:5:MAN:O3	2.06	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:53:GLN:NE2	7:C:136:ASN:OD1	2.24	0.70
7:A:138:ILE:O	7:A:138:ILE:HG22	1.91	0.70
2:E:56:SER:HB2	7:A:138:ILE:CD1	2.22	0.69
3:K:94:ARG:NH2	3:K:98:CYS:SG	2.66	0.68
7:A:652:GLN:NE2	7:C:535:MET:O	2.25	0.68
4:Q:39:ARG:NH1	4:Q:82:ASP:O	2.29	0.66
7:A:197:ASN:O	7:C:308:ARG:NH1	2.29	0.66
7:C:325:ASP:OD2	16:g:5:MAN:O4	2.09	0.66
4:M:96:GLU:OE1	7:C:459:GLY:N	2.27	0.65
2:E:56:SER:CB	7:A:138:ILE:HD11	2.28	0.64
7:B:325:ASP:OD2	10:a:5:MAN:O4	2.07	0.64
7:A:661:LEU:HD12	7:C:502:LYS:H	1.63	0.63
7:A:648:GLU:O	7:A:652:GLN:NE2	2.32	0.63
2:E:32:PHE:CD1	7:A:138:ILE:HG21	2.33	0.63
3:K:96:LYS:N	3:K:100(C):ASP:O	2.30	0.63
7:A:595:ILE:O	7:A:651:ASN:ND2	2.33	0.61
7:C:477:ASP:OD1	7:C:480:ARG:NH1	2.34	0.61
3:N:38:ARG:NH1	3:N:86:ASP:OD1	2.34	0.60
7:C:298:ARG:NH1	7:C:381:GLU:OE2	2.35	0.59
1:I:66:ARG:NH1	1:I:82(B):SER:O	2.35	0.59
2:E:51:SER:OG	10:T:6:MAN:O4	2.21	0.59
7:A:640:GLN:OE1	7:C:542:ARG:NH2	2.36	0.59
1:D:33:HIS:NE2	10:T:9:MAN:O2	2.36	0.58
7:A:661:LEU:CD1	7:C:502:LYS:H	2.17	0.58
7:A:300:ASN:ND2	7:A:326:ILE:O	2.37	0.58
4:M:61:ARG:NH1	4:M:79:GLU:OE2	2.37	0.57
7:A:256:SER:O	7:A:478:ASN:ND2	2.34	0.57
3:N:94:ARG:NH2	3:N:98:CYS:SG	2.77	0.57
7:A:138:ILE:O	7:A:138:ILE:CG2	2.53	0.57
7:A:98:ASN:ND2	7:A:486:TYR:O	2.38	0.56
7:C:98:ASN:ND2	7:C:486:TYR:O	2.38	0.56
1:D:100(M):MET:O	1:D:103:TRP:NE1	2.39	0.55
7:A:477:ASP:OD1	7:A:480:ARG:NH1	2.40	0.55
2:E:32:PHE:HD1	7:A:138:ILE:HG21	1.72	0.54
7:A:270:VAL:O	7:A:348:GLN:NE2	2.42	0.53
1:F:100(M):MET:O	1:F:103:TRP:NE1	2.42	0.52
5:H:52:ASN:ND2	7:A:624:ASP:OD2	2.39	0.52
2:E:3:GLU:OE1	2:E:3:GLU:N	2.43	0.51
7:C:277:ILE:HG12	7:C:353:PHE:CZ	2.46	0.51
2:J:37:ARG:NH1	2:J:82:ASP:OD1	2.43	0.51
7:C:280:ASN:C	7:C:282:LYS:H	2.18	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:100(G):GLU:OE2	7:A:328:GLN:N	2.44	0.50
7:C:539:VAL:O	7:C:543:ASN:ND2	2.43	0.50
7:C:299:PRO:O	7:C:327:ARG:NE	2.45	0.49
1:D:29:ARG:NE	1:D:32:ASP:OD2	2.43	0.48
3:P:57:VAL:O	7:B:365:SER:OG	2.31	0.48
2:E:62:PHE:O	2:E:63:SER:OG	2.28	0.48
3:P:94:ARG:NH2	3:P:98:CYS:SG	2.87	0.48
7:C:37:THR:OG1	7:C:499:THR:OG1	2.28	0.47
7:C:270:VAL:O	7:C:348:GLN:NE2	2.44	0.47
1:F:75:ILE:O	1:F:77:ARG:N	2.47	0.47
4:M:39:ARG:NH2	4:M:42:GLN:OE1	2.45	0.47
2:J:92:ASP:OD1	2:J:95:ASP:N	2.47	0.47
1:D:2:VAL:N	1:D:25:SER:O	2.47	0.47
2:G:92:ASP:OD1	2:G:93:THR:N	2.43	0.47
7:C:280:ASN:C	7:C:282:LYS:N	2.72	0.46
7:C:298:ARG:NH2	7:C:441:GLY:O	2.43	0.46
2:J:54:ARG:NH1	7:C:323:ILE:O	2.48	0.46
3:N:38:ARG:NH2	3:N:46:GLU:OE1	2.44	0.45
3:N:96:LYS:N	3:N:100(C):ASP:O	2.47	0.45
5:H:52:ASN:O	5:H:55:GLY:N	2.48	0.44
7:A:50:THR:O	7:A:103:GLN:NE2	2.50	0.44
7:A:219:ALA:O	7:A:246:GLN:NE2	2.47	0.44
7:C:279:ASN:ND2	7:C:280:ASN:O	2.50	0.44
7:C:258:GLN:NE2	7:C:371:VAL:O	2.43	0.44
7:A:496:VAL:O	7:A:631:TRP:NE1	2.38	0.43
7:B:37:THR:OG1	7:B:499:THR:OG1	2.34	0.43
4:M:90:GLN:HG2	4:M:91:TYR:H	1.84	0.42
3:P:38:ARG:NH2	3:P:46:GLU:OE1	2.52	0.42
1:D:75:ILE:O	1:D:77:ARG:N	2.53	0.42
7:C:322:ASP:OD1	7:C:323:ILE:N	2.48	0.41
3:P:38:ARG:NH1	3:P:86:ASP:OD1	2.53	0.41
7:C:656:ASN:O	7:C:660:LEU:HB2	2.20	0.41
6:L:92:ALA:HB3	6:L:95(A):LYS:HB3	2.03	0.41
6:L:27:ARG:O	6:L:29:GLY:N	2.52	0.41
7:A:325:ASP:OD1	7:A:325:ASP:N	2.33	0.41
7:C:499:THR:OG1	7:C:501:CYS:SG	2.79	0.41
2:E:53:GLN:HB3	7:A:325:ASP:HB3	2.02	0.41
3:K:60:ALA:HA	7:C:459:GLY:HA3	2.02	0.41
7:C:280:ASN:O	7:C:282:LYS:N	2.53	0.41
3:P:61:ARG:NH1	7:B:465:THR:O	2.55	0.40
4:Q:96:GLU:OE2	7:B:459:GLY:N	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:C:50:THR:O	7:C:103:GLN:NE2	2.53	0.40
7:A:36:VAL:O	7:A:606:THR:OG1	2.32	0.40
7:A:136:ASN:O	7:A:137:ASN:HB2	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	125/233 (54%)	121 (97%)	4 (3%)	0	100	100
1	F	127/233 (54%)	126 (99%)	1 (1%)	0	100	100
1	I	125/233 (54%)	123 (98%)	2 (2%)	0	100	100
2	E	104/214 (49%)	101 (97%)	3 (3%)	0	100	100
2	G	104/214 (49%)	104 (100%)	0	0	100	100
2	J	104/214 (49%)	103 (99%)	1 (1%)	0	100	100
3	K	117/224 (52%)	116 (99%)	1 (1%)	0	100	100
3	N	117/224 (52%)	114 (97%)	3 (3%)	0	100	100
3	P	117/224 (52%)	115 (98%)	2 (2%)	0	100	100
4	M	95/210 (45%)	92 (97%)	3 (3%)	0	100	100
4	O	96/210 (46%)	92 (96%)	4 (4%)	0	100	100
4	Q	95/210 (45%)	91 (96%)	4 (4%)	0	100	100
5	H	124/232 (53%)	124 (100%)	0	0	100	100
6	L	106/216 (49%)	103 (97%)	3 (3%)	0	100	100
7	A	552/642 (86%)	532 (96%)	20 (4%)	0	100	100
7	B	545/642 (85%)	534 (98%)	11 (2%)	0	100	100
7	C	540/642 (84%)	522 (97%)	18 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	3193/5017 (64%)	3113 (98%)	80 (2%)	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	108/200 (54%)	107 (99%)	1 (1%)	70	80
1	F	110/200 (55%)	110 (100%)	0	100	100
1	I	108/200 (54%)	108 (100%)	0	100	100
2	E	90/183 (49%)	87 (97%)	3 (3%)	33	63
2	G	90/183 (49%)	90 (100%)	0	100	100
2	J	90/183 (49%)	90 (100%)	0	100	100
3	K	101/192 (53%)	101 (100%)	0	100	100
3	N	101/192 (53%)	101 (100%)	0	100	100
3	P	101/192 (53%)	101 (100%)	0	100	100
4	M	80/182 (44%)	79 (99%)	1 (1%)	61	77
4	O	81/182 (44%)	81 (100%)	0	100	100
4	Q	80/182 (44%)	79 (99%)	1 (1%)	61	77
5	H	104/196 (53%)	104 (100%)	0	100	100
6	L	89/182 (49%)	89 (100%)	0	100	100
7	A	503/560 (90%)	499 (99%)	4 (1%)	73	81
7	B	495/560 (88%)	494 (100%)	1 (0%)	87	89
7	C	493/560 (88%)	491 (100%)	2 (0%)	84	86
All	All	2824/4329 (65%)	2811 (100%)	13 (0%)	78	85

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	101	ASP
2	E	53	GLN
2	E	54	ARG
2	E	61	ARG
4	M	96	GLU
4	Q	96	GLU
7	A	159	PHE
7	A	276	ASN
7	A	325	ASP
7	A	618	ASN
7	B	161	MET
7	C	276	ASN
7	C	660	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	26	ASN
1	F	26	ASN
5	H	100(A)	HIS
7	A	130	GLN
7	A	137	ASN
7	A	293	GLN
7	A	575	GLN
7	B	82	GLN
7	B	183	GLN
7	B	246	GLN
7	B	315	GLN
7	B	575	GLN
7	C	279	ASN
7	C	315	GLN
7	C	653	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)

87 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	$\#\|Z\| > 2$
8	NAG	R	1	8,7	14,14,15	0.72	0	17,19,21	1.34	2 (11%)
8	NAG	R	2	8	14,14,15	0.77	1 (7%)	17,19,21	1.09	1 (5%)
8	BMA	R	3	8	11,11,12	0.77	0	15,15,17	1.26	1 (6%)
9	NAG	S	1	7,9	14,14,15	0.77	0	17,19,21	1.03	1 (5%)
9	NAG	S	2	9	14,14,15	0.70	0	17,19,21	1.01	1 (5%)
9	BMA	S	3	9	11,11,12	0.73	0	15,15,17	0.97	0
9	MAN	S	4	9	11,11,12	0.74	0	15,15,17	1.01	1 (6%)
10	NAG	T	1	10,7	14,14,15	0.85	0	17,19,21	1.05	2 (11%)
10	MAN	T	10	10	11,11,12	0.71	0	15,15,17	1.29	1 (6%)
10	NAG	T	2	10	14,14,15	0.75	0	17,19,21	1.08	0
10	BMA	T	3	10	11,11,12	0.73	0	15,15,17	1.30	1 (6%)
10	MAN	T	4	10	11,11,12	0.77	0	15,15,17	1.23	2 (13%)
10	MAN	T	5	10	11,11,12	0.73	0	15,15,17	1.11	1 (6%)
10	MAN	T	6	10	11,11,12	0.77	0	15,15,17	0.98	1 (6%)
10	MAN	T	7	10	11,11,12	0.74	0	15,15,17	1.13	1 (6%)
10	MAN	T	8	10	11,11,12	0.73	0	15,15,17	1.03	1 (6%)
10	MAN	T	9	10	11,11,12	0.74	0	15,15,17	1.03	1 (6%)
11	NAG	U	1	11,7	14,14,15	0.76	0	17,19,21	1.60	3 (17%)
11	NAG	U	2	11	14,14,15	0.60	0	17,19,21	0.96	0
11	BMA	U	3	11	11,11,12	0.74	0	15,15,17	0.89	0
11	MAN	U	4	11	11,11,12	0.77	0	15,15,17	1.24	2 (13%)
11	MAN	U	5	11	11,11,12	0.76	0	15,15,17	1.04	1 (6%)
11	MAN	U	6	11	11,11,12	0.74	0	15,15,17	1.15	1 (6%)
12	NAG	V	1	12,7	14,14,15	0.79	0	17,19,21	2.39	5 (29%)
12	FUC	V	2	12	10,10,11	0.80	0	14,14,16	0.74	0
13	NAG	W	1	13,7	14,14,15	0.74	0	17,19,21	1.18	2 (11%)
13	NAG	W	2	13	14,14,15	0.67	0	17,19,21	1.00	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
13	NAG	X	1	13,7	14,14,15	0.71	0	17,19,21	1.57	3 (17%)
13	NAG	X	2	13	14,14,15	0.90	1 (7%)	17,19,21	1.13	1 (5%)
14	NAG	Y	1	14,7	14,14,15	0.77	0	17,19,21	1.26	2 (11%)
14	NAG	Y	2	14	14,14,15	0.70	0	17,19,21	0.89	0
14	BMA	Y	3	14	11,11,12	0.77	0	15,15,17	1.18	1 (6%)
14	MAN	Y	4	14	11,11,12	0.80	1 (9%)	15,15,17	1.02	1 (6%)
14	MAN	Y	5	14	11,11,12	0.75	0	15,15,17	0.99	1 (6%)
15	NAG	Z	1	15,7	14,14,15	0.85	0	17,19,21	0.87	0
15	NAG	Z	2	15	14,14,15	0.78	1 (7%)	17,19,21	0.83	0
15	BMA	Z	3	15	11,11,12	0.76	0	15,15,17	1.20	1 (6%)
15	MAN	Z	4	15	11,11,12	0.77	0	15,15,17	1.04	1 (6%)
15	MAN	Z	5	15	11,11,12	0.76	0	15,15,17	1.05	1 (6%)
15	MAN	Z	6	15	11,11,12	0.72	0	15,15,17	1.00	1 (6%)
15	MAN	Z	7	15	11,11,12	0.71	0	15,15,17	1.09	1 (6%)
10	NAG	a	1	10,7	14,14,15	0.84	0	17,19,21	1.23	2 (11%)
10	MAN	a	10	10	11,11,12	0.74	0	15,15,17	1.08	1 (6%)
10	NAG	a	2	10	14,14,15	0.78	0	17,19,21	1.25	2 (11%)
10	BMA	a	3	10	11,11,12	0.89	0	15,15,17	1.33	1 (6%)
10	MAN	a	4	10	11,11,12	0.75	0	15,15,17	1.10	1 (6%)
10	MAN	a	5	10	11,11,12	0.75	0	15,15,17	1.13	1 (6%)
10	MAN	a	6	10	11,11,12	0.79	1 (9%)	15,15,17	0.97	1 (6%)
10	MAN	a	7	10	11,11,12	0.75	0	15,15,17	0.96	1 (6%)
10	MAN	a	8	10	11,11,12	0.74	0	15,15,17	1.10	1 (6%)
10	MAN	a	9	10	11,11,12	0.76	0	15,15,17	1.08	1 (6%)
13	NAG	b	1	13,7	14,14,15	0.80	0	17,19,21	0.83	0
13	NAG	b	2	13	14,14,15	0.67	0	17,19,21	1.02	1 (5%)
11	NAG	c	1	11,7	14,14,15	0.73	0	17,19,21	1.31	2 (11%)
11	NAG	c	2	11	14,14,15	0.68	0	17,19,21	1.01	2 (11%)
11	BMA	c	3	11	11,11,12	0.81	0	15,15,17	1.23	1 (6%)
11	MAN	c	4	11	11,11,12	0.75	0	15,15,17	1.09	1 (6%)
11	MAN	c	5	11	11,11,12	0.72	0	15,15,17	1.27	1 (6%)
11	MAN	c	6	11	11,11,12	0.75	0	15,15,17	1.04	1 (6%)
13	NAG	d	1	13,7	14,14,15	0.72	0	17,19,21	0.97	0
13	NAG	d	2	13	14,14,15	0.68	0	17,19,21	0.99	1 (5%)
8	NAG	e	1	8,7	14,14,15	0.77	0	17,19,21	1.32	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
8	NAG	e	2	8	14,14,15	0.70	0	17,19,21	1.13	3 (17%)
8	BMA	e	3	8	11,11,12	0.70	0	15,15,17	0.91	0
14	NAG	f	1	14,7	14,14,15	0.73	0	17,19,21	1.16	1 (5%)
14	NAG	f	2	14	14,14,15	0.72	0	17,19,21	1.11	1 (5%)
14	BMA	f	3	14	11,11,12	0.75	0	15,15,17	1.12	1 (6%)
14	MAN	f	4	14	11,11,12	0.76	0	15,15,17	0.97	1 (6%)
14	MAN	f	5	14	11,11,12	0.68	0	15,15,17	1.22	1 (6%)
16	NAG	g	1	16,7	14,14,15	0.74	0	17,19,21	1.06	0
16	MAN	g	10	16	11,11,12	0.73	0	15,15,17	1.08	1 (6%)
16	NAG	g	2	16	14,14,15	0.75	0	17,19,21	1.05	1 (5%)
16	BMA	g	3	16	11,11,12	0.75	0	15,15,17	1.14	2 (13%)
16	MAN	g	4	16	11,11,12	0.78	0	15,15,17	0.97	1 (6%)
16	MAN	g	5	16	11,11,12	0.78	0	15,15,17	1.05	1 (6%)
16	MAN	g	6	16	11,11,12	0.79	1 (9%)	15,15,17	0.93	1 (6%)
16	MAN	g	7	16	11,11,12	0.82	1 (9%)	15,15,17	1.21	2 (13%)
16	MAN	g	8	16	11,11,12	0.77	0	15,15,17	1.07	1 (6%)
16	MAN	g	9	16	11,11,12	0.76	0	15,15,17	1.01	1 (6%)
13	NAG	h	1	13,7	14,14,15	0.69	0	17,19,21	1.72	2 (11%)
13	NAG	h	2	13	14,14,15	0.71	0	17,19,21	1.06	1 (5%)
17	NAG	i	1	17,7	14,14,15	0.70	0	17,19,21	0.98	0
17	NAG	i	2	17	14,14,15	0.67	0	17,19,21	0.97	1 (5%)
17	BMA	i	3	17	11,11,12	0.78	0	15,15,17	1.08	1 (6%)
17	MAN	i	4	17	11,11,12	0.77	0	15,15,17	1.04	1 (6%)
17	MAN	i	5	17	11,11,12	0.79	1 (9%)	15,15,17	0.92	1 (6%)
17	MAN	i	6	17	11,11,12	0.72	0	15,15,17	0.92	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	NAG	R	1	8,7	-	0/6/23/26	0/1/1/1
8	NAG	R	2	8	-	0/6/23/26	0/1/1/1
8	BMA	R	3	8	-	0/2/19/22	0/1/1/1
9	NAG	S	1	7,9	-	0/6/23/26	0/1/1/1
9	NAG	S	2	9	-	0/6/23/26	0/1/1/1
9	BMA	S	3	9	-	1/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	MAN	S	4	9	-	2/2/19/22	0/1/1/1
10	NAG	T	1	10,7	-	0/6/23/26	0/1/1/1
10	MAN	T	10	10	-	0/2/19/22	1/1/1/1
10	NAG	T	2	10	-	0/6/23/26	0/1/1/1
10	BMA	T	3	10	-	0/2/19/22	0/1/1/1
10	MAN	T	4	10	-	2/2/19/22	0/1/1/1
10	MAN	T	5	10	-	0/2/19/22	0/1/1/1
10	MAN	T	6	10	-	0/2/19/22	0/1/1/1
10	MAN	T	7	10	-	2/2/19/22	0/1/1/1
10	MAN	T	8	10	-	2/2/19/22	0/1/1/1
10	MAN	T	9	10	-	2/2/19/22	0/1/1/1
11	NAG	U	1	11,7	-	0/6/23/26	0/1/1/1
11	NAG	U	2	11	-	2/6/23/26	0/1/1/1
11	BMA	U	3	11	-	0/2/19/22	0/1/1/1
11	MAN	U	4	11	-	2/2/19/22	0/1/1/1
11	MAN	U	5	11	-	1/2/19/22	0/1/1/1
11	MAN	U	6	11	-	2/2/19/22	0/1/1/1
12	NAG	V	1	12,7	-	3/6/23/26	0/1/1/1
12	FUC	V	2	12	-	-	0/1/1/1
13	NAG	W	1	13,7	-	2/6/23/26	0/1/1/1
13	NAG	W	2	13	-	1/6/23/26	0/1/1/1
13	NAG	X	1	13,7	-	0/6/23/26	0/1/1/1
13	NAG	X	2	13	-	1/6/23/26	0/1/1/1
14	NAG	Y	1	14,7	-	0/6/23/26	0/1/1/1
14	NAG	Y	2	14	-	0/6/23/26	0/1/1/1
14	BMA	Y	3	14	-	0/2/19/22	0/1/1/1
14	MAN	Y	4	14	-	0/2/19/22	0/1/1/1
14	MAN	Y	5	14	-	1/2/19/22	0/1/1/1
15	NAG	Z	1	15,7	-	3/6/23/26	0/1/1/1
15	NAG	Z	2	15	-	2/6/23/26	0/1/1/1
15	BMA	Z	3	15	-	2/2/19/22	0/1/1/1
15	MAN	Z	4	15	-	1/2/19/22	0/1/1/1
15	MAN	Z	5	15	-	2/2/19/22	0/1/1/1
15	MAN	Z	6	15	-	2/2/19/22	0/1/1/1
15	MAN	Z	7	15	-	2/2/19/22	0/1/1/1
10	NAG	a	1	10,7	-	0/6/23/26	0/1/1/1
10	MAN	a	10	10	-	2/2/19/22	0/1/1/1
10	NAG	a	2	10	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	BMA	a	3	10	-	2/2/19/22	0/1/1/1
10	MAN	a	4	10	-	0/2/19/22	0/1/1/1
10	MAN	a	5	10	-	0/2/19/22	0/1/1/1
10	MAN	a	6	10	-	1/2/19/22	0/1/1/1
10	MAN	a	7	10	-	2/2/19/22	0/1/1/1
10	MAN	a	8	10	-	1/2/19/22	0/1/1/1
10	MAN	a	9	10	-	0/2/19/22	0/1/1/1
13	NAG	b	1	13,7	-	0/6/23/26	0/1/1/1
13	NAG	b	2	13	-	1/6/23/26	0/1/1/1
11	NAG	c	1	11,7	-	1/6/23/26	0/1/1/1
11	NAG	c	2	11	-	0/6/23/26	0/1/1/1
11	BMA	c	3	11	-	2/2/19/22	0/1/1/1
11	MAN	c	4	11	-	1/2/19/22	0/1/1/1
11	MAN	c	5	11	-	1/2/19/22	0/1/1/1
11	MAN	c	6	11	-	0/2/19/22	0/1/1/1
13	NAG	d	1	13,7	-	2/6/23/26	0/1/1/1
13	NAG	d	2	13	-	1/6/23/26	0/1/1/1
8	NAG	e	1	8,7	-	0/6/23/26	0/1/1/1
8	NAG	e	2	8	-	2/6/23/26	0/1/1/1
8	BMA	e	3	8	-	1/2/19/22	0/1/1/1
14	NAG	f	1	14,7	-	0/6/23/26	0/1/1/1
14	NAG	f	2	14	-	0/6/23/26	0/1/1/1
14	BMA	f	3	14	-	1/2/19/22	0/1/1/1
14	MAN	f	4	14	-	2/2/19/22	0/1/1/1
14	MAN	f	5	14	-	2/2/19/22	0/1/1/1
16	NAG	g	1	16,7	-	1/6/23/26	0/1/1/1
16	MAN	g	10	16	-	2/2/19/22	0/1/1/1
16	NAG	g	2	16	-	0/6/23/26	0/1/1/1
16	BMA	g	3	16	-	2/2/19/22	0/1/1/1
16	MAN	g	4	16	-	2/2/19/22	0/1/1/1
16	MAN	g	5	16	-	0/2/19/22	0/1/1/1
16	MAN	g	6	16	-	0/2/19/22	0/1/1/1
16	MAN	g	7	16	-	2/2/19/22	0/1/1/1
16	MAN	g	8	16	-	2/2/19/22	0/1/1/1
16	MAN	g	9	16	-	2/2/19/22	0/1/1/1
13	NAG	h	1	13,7	-	2/6/23/26	0/1/1/1
13	NAG	h	2	13	-	0/6/23/26	0/1/1/1
17	NAG	i	1	17,7	-	0/6/23/26	0/1/1/1
17	NAG	i	2	17	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	BMA	i	3	17	-	1/2/19/22	0/1/1/1
17	MAN	i	4	17	-	2/2/19/22	0/1/1/1
17	MAN	i	5	17	-	2/2/19/22	0/1/1/1
17	MAN	i	6	17	-	2/2/19/22	0/1/1/1

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	X	2	NAG	C1-C2	2.73	1.56	1.52
17	i	5	MAN	O5-C1	-2.07	1.40	1.43
14	Y	4	MAN	O5-C1	-2.05	1.40	1.43
15	Z	2	NAG	O5-C1	-2.05	1.40	1.43
16	g	6	MAN	O5-C1	-2.04	1.40	1.43
8	R	2	NAG	O5-C1	-2.04	1.40	1.43
16	g	7	MAN	O5-C1	-2.03	1.40	1.43
10	a	6	MAN	O5-C1	-2.02	1.40	1.43

All (96) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	V	1	NAG	C2-N2-C7	6.49	131.60	122.90
13	h	1	NAG	C2-N2-C7	5.62	130.43	122.90
12	V	1	NAG	C1-O5-C5	4.97	118.85	112.19
10	T	10	MAN	C1-O5-C5	4.19	117.80	112.19
11	c	5	MAN	C1-O5-C5	3.86	117.36	112.19
8	R	3	BMA	C1-O5-C5	3.81	117.29	112.19
14	f	5	MAN	C1-O5-C5	3.55	116.95	112.19
10	a	3	BMA	C1-O5-C5	3.53	116.92	112.19
8	R	1	NAG	O4-C4-C5	3.53	118.02	109.32
11	U	1	NAG	O5-C1-C2	-3.50	105.88	111.29
8	e	1	NAG	C1-O5-C5	3.39	116.73	112.19
10	T	3	BMA	C1-O5-C5	3.39	116.72	112.19
14	Y	3	BMA	C1-O5-C5	3.37	116.70	112.19
11	U	1	NAG	C1-O5-C5	3.31	116.63	112.19
14	Y	1	NAG	C1-O5-C5	3.31	116.62	112.19
15	Z	3	BMA	C1-O5-C5	3.24	116.52	112.19
13	X	1	NAG	O4-C4-C3	-3.21	102.81	110.38
11	U	6	MAN	C1-O5-C5	3.20	116.48	112.19
10	T	7	MAN	C1-O5-C5	3.19	116.46	112.19
14	f	3	BMA	C1-O5-C5	3.12	116.36	112.19
10	a	5	MAN	C1-O5-C5	3.06	116.29	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	g	10	MAN	C1-O5-C5	3.03	116.25	112.19
10	a	10	MAN	C1-O5-C5	3.00	116.21	112.19
16	g	2	NAG	C1-O5-C5	2.97	116.16	112.19
13	W	1	NAG	C1-O5-C5	2.96	116.16	112.19
15	Z	7	MAN	C1-O5-C5	2.94	116.12	112.19
13	X	1	NAG	C1-O5-C5	2.92	116.11	112.19
10	a	9	MAN	C1-O5-C5	2.92	116.10	112.19
10	a	8	MAN	C1-O5-C5	2.89	116.06	112.19
10	T	4	MAN	C1-O5-C5	2.88	116.05	112.19
11	c	1	NAG	C1-O5-C5	2.85	116.01	112.19
13	X	2	NAG	C1-O5-C5	2.85	116.00	112.19
8	R	1	NAG	C1-O5-C5	2.84	116.00	112.19
10	T	8	MAN	C1-O5-C5	2.84	115.99	112.19
10	a	2	NAG	O3-C3-C2	-2.78	103.62	109.40
10	T	5	MAN	C1-O5-C5	2.78	115.92	112.19
11	U	5	MAN	C1-O5-C5	2.77	115.89	112.19
10	a	1	NAG	O3-C3-C2	-2.77	103.66	109.40
9	S	4	MAN	C1-O5-C5	2.71	115.82	112.19
10	a	4	MAN	C1-O5-C5	2.69	115.79	112.19
16	g	3	BMA	C1-O5-C5	2.69	115.79	112.19
16	g	5	MAN	C1-O5-C5	2.69	115.79	112.19
13	h	2	NAG	C1-O5-C5	2.66	115.76	112.19
10	a	1	NAG	O4-C4-C5	-2.66	102.76	109.32
17	i	4	MAN	C1-O5-C5	2.66	115.75	112.19
16	g	8	MAN	C1-O5-C5	2.63	115.71	112.19
16	g	9	MAN	C1-O5-C5	2.60	115.67	112.19
14	Y	4	MAN	C1-O5-C5	2.58	115.65	112.19
9	S	1	NAG	C1-O5-C5	2.58	115.64	112.19
15	Z	6	MAN	C1-O5-C5	2.57	115.63	112.19
11	c	6	MAN	C1-O5-C5	2.57	115.63	112.19
17	i	3	BMA	O3-C3-C2	-2.55	104.84	110.05
11	U	4	MAN	C1-O5-C5	2.52	115.56	112.19
17	i	2	NAG	C1-O5-C5	2.47	115.50	112.19
11	c	4	MAN	C1-O5-C5	2.47	115.49	112.19
8	e	2	NAG	C1-O5-C5	2.46	115.48	112.19
14	Y	5	MAN	C1-O5-C5	2.46	115.48	112.19
8	R	2	NAG	C1-O5-C5	2.45	115.47	112.19
10	T	6	MAN	C1-O5-C5	2.44	115.46	112.19
12	V	1	NAG	O5-C5-C6	-2.43	102.93	107.66
15	Z	5	MAN	C1-O5-C5	2.42	115.42	112.19
14	f	4	MAN	C1-O5-C5	2.42	115.42	112.19
15	Z	4	MAN	C1-O5-C5	2.41	115.42	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	X	1	NAG	O4-C4-C5	2.39	115.21	109.32
10	T	9	MAN	C1-O5-C5	2.38	115.37	112.19
13	b	2	NAG	C1-O5-C5	2.34	115.32	112.19
13	W	2	NAG	C1-O5-C5	2.33	115.31	112.19
11	c	3	BMA	C1-C2-C3	-2.33	106.25	109.64
11	c	2	NAG	O4-C4-C3	-2.33	104.89	110.38
16	g	3	BMA	O3-C3-C2	-2.33	105.30	110.05
8	e	2	NAG	O4-C4-C3	-2.32	104.91	110.38
10	a	6	MAN	C1-O5-C5	2.32	115.29	112.19
16	g	4	MAN	C1-O5-C5	2.31	115.29	112.19
10	a	2	NAG	O4-C4-C5	-2.29	103.69	109.32
10	T	1	NAG	O4-C4-C5	-2.27	103.74	109.32
10	T	4	MAN	C1-C2-C3	2.25	112.92	109.64
13	d	2	NAG	C1-O5-C5	2.24	115.18	112.19
14	f	1	NAG	O4-C4-C3	-2.24	105.11	110.38
12	V	1	NAG	O4-C4-C5	2.21	114.78	109.32
11	U	4	MAN	O3-C3-C2	-2.21	105.55	110.05
11	U	1	NAG	C2-N2-C7	2.20	125.84	122.90
16	g	7	MAN	C1-O5-C5	2.16	115.09	112.19
14	f	2	NAG	C4-C3-C2	-2.15	107.87	111.02
16	g	6	MAN	C1-O5-C5	2.13	115.04	112.19
17	i	5	MAN	C1-O5-C5	2.09	114.98	112.19
11	c	2	NAG	C1-O5-C5	2.09	114.98	112.19
13	h	1	NAG	C8-C7-N2	2.07	119.55	116.12
13	W	1	NAG	O5-C1-C2	-2.06	108.10	111.29
8	e	2	NAG	O5-C1-C2	-2.06	108.10	111.29
11	c	1	NAG	O4-C4-C3	-2.06	105.53	110.38
16	g	7	MAN	C3-C4-C5	2.04	113.93	110.23
12	V	1	NAG	C6-C5-C4	2.03	118.01	113.02
9	S	2	NAG	C1-O5-C5	2.03	114.91	112.19
10	T	1	NAG	O3-C3-C2	-2.03	105.19	109.40
14	Y	1	NAG	O4-C4-C3	-2.02	105.61	110.38
10	a	7	MAN	C1-O5-C5	2.01	114.88	112.19

There are no chirality outliers.

All (87) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
15	Z	1	NAG	O5-C5-C6-O6
11	c	3	BMA	O5-C5-C6-O6
10	T	8	MAN	C4-C5-C6-O6
14	f	4	MAN	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
15	Z	2	NAG	O5-C5-C6-O6
16	g	7	MAN	O5-C5-C6-O6
16	g	9	MAN	O5-C5-C6-O6
17	i	6	MAN	O5-C5-C6-O6
10	a	3	BMA	C4-C5-C6-O6
11	U	2	NAG	C4-C5-C6-O6
8	e	2	NAG	O5-C5-C6-O6
13	W	1	NAG	O5-C5-C6-O6
14	f	4	MAN	C4-C5-C6-O6
16	g	10	MAN	O5-C5-C6-O6
15	Z	2	NAG	C4-C5-C6-O6
9	S	4	MAN	O5-C5-C6-O6
17	i	4	MAN	O5-C5-C6-O6
10	T	9	MAN	O5-C5-C6-O6
15	Z	1	NAG	C4-C5-C6-O6
15	Z	6	MAN	O5-C5-C6-O6
10	T	9	MAN	C4-C5-C6-O6
11	c	3	BMA	C4-C5-C6-O6
16	g	9	MAN	C4-C5-C6-O6
16	g	8	MAN	O5-C5-C6-O6
10	T	8	MAN	O5-C5-C6-O6
10	T	4	MAN	O5-C5-C6-O6
10	a	3	BMA	O5-C5-C6-O6
10	T	4	MAN	C4-C5-C6-O6
11	U	6	MAN	O5-C5-C6-O6
13	W	1	NAG	C4-C5-C6-O6
15	Z	6	MAN	C4-C5-C6-O6
16	g	7	MAN	C4-C5-C6-O6
11	U	2	NAG	O5-C5-C6-O6
17	i	6	MAN	C4-C5-C6-O6
17	i	5	MAN	O5-C5-C6-O6
12	V	1	NAG	C8-C7-N2-C2
12	V	1	NAG	O7-C7-N2-C2
13	h	1	NAG	C8-C7-N2-C2
13	h	1	NAG	O7-C7-N2-C2
10	a	10	MAN	O5-C5-C6-O6
11	U	4	MAN	O5-C5-C6-O6
14	f	5	MAN	O5-C5-C6-O6
15	Z	5	MAN	O5-C5-C6-O6
15	Z	7	MAN	O5-C5-C6-O6
8	e	2	NAG	C4-C5-C6-O6
16	g	3	BMA	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
16	g	3	BMA	O5-C5-C6-O6
11	U	5	MAN	O5-C5-C6-O6
17	i	4	MAN	C4-C5-C6-O6
14	f	3	BMA	O5-C5-C6-O6
15	Z	3	BMA	O5-C5-C6-O6
16	g	10	MAN	C4-C5-C6-O6
9	S	4	MAN	C4-C5-C6-O6
10	a	7	MAN	C4-C5-C6-O6
15	Z	3	BMA	C4-C5-C6-O6
16	g	8	MAN	C4-C5-C6-O6
11	c	4	MAN	O5-C5-C6-O6
11	U	6	MAN	C4-C5-C6-O6
13	W	2	NAG	O5-C5-C6-O6
13	X	2	NAG	O5-C5-C6-O6
13	b	2	NAG	O5-C5-C6-O6
10	a	8	MAN	O5-C5-C6-O6
14	Y	5	MAN	O5-C5-C6-O6
8	e	3	BMA	O5-C5-C6-O6
9	S	3	BMA	O5-C5-C6-O6
11	c	5	MAN	O5-C5-C6-O6
13	d	2	NAG	O5-C5-C6-O6
13	d	1	NAG	O5-C5-C6-O6
10	a	6	MAN	O5-C5-C6-O6
10	a	7	MAN	O5-C5-C6-O6
17	i	3	BMA	O5-C5-C6-O6
10	T	7	MAN	C4-C5-C6-O6
10	T	7	MAN	O5-C5-C6-O6
11	U	4	MAN	C4-C5-C6-O6
16	g	4	MAN	C4-C5-C6-O6
14	f	5	MAN	C4-C5-C6-O6
12	V	1	NAG	O5-C5-C6-O6
15	Z	5	MAN	C4-C5-C6-O6
17	i	5	MAN	C4-C5-C6-O6
15	Z	7	MAN	C4-C5-C6-O6
10	a	10	MAN	C4-C5-C6-O6
15	Z	1	NAG	C1-C2-N2-C7
16	g	1	NAG	C1-C2-N2-C7
15	Z	4	MAN	O5-C5-C6-O6
16	g	4	MAN	O5-C5-C6-O6
13	d	1	NAG	C4-C5-C6-O6
11	c	1	NAG	O5-C5-C6-O6

All (1) ring outliers are listed below:

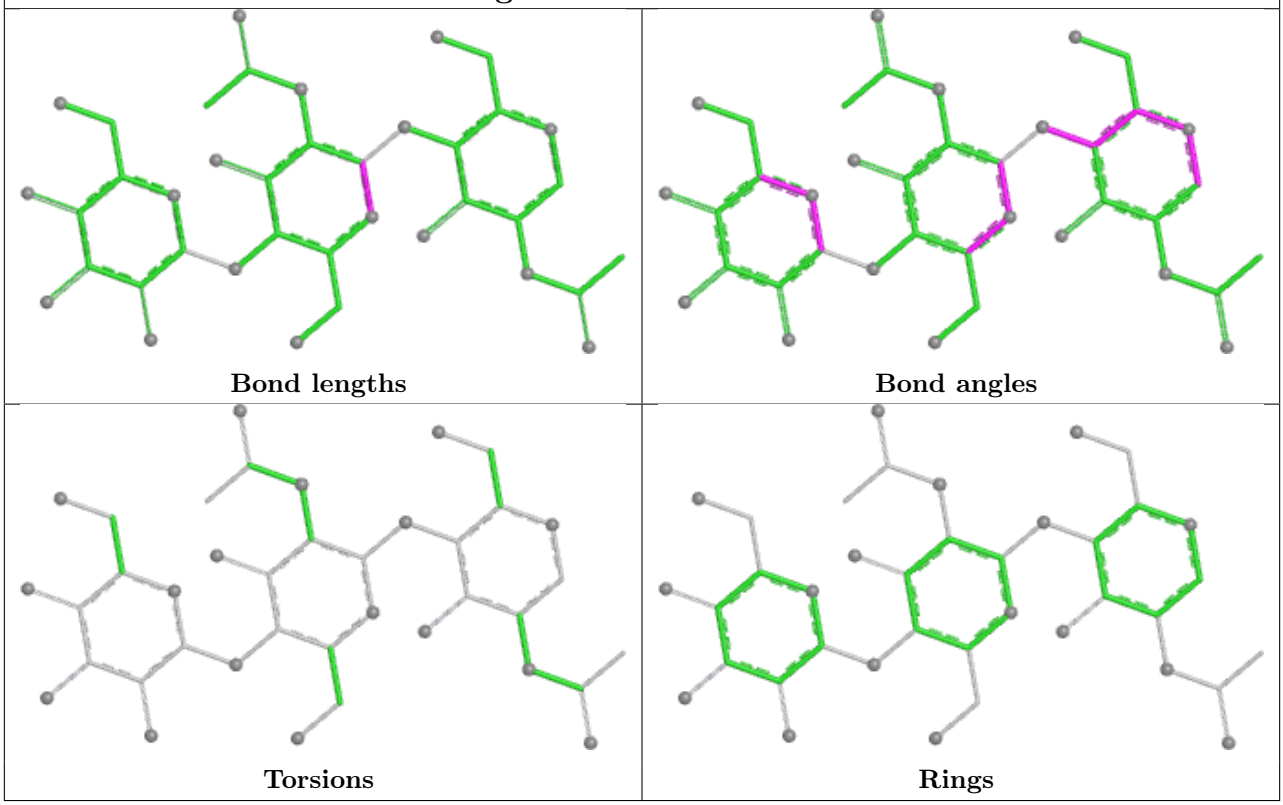
Mol	Chain	Res	Type	Atoms
10	T	10	MAN	C1-C2-C3-C4-C5-O5

5 monomers are involved in 5 short contacts:

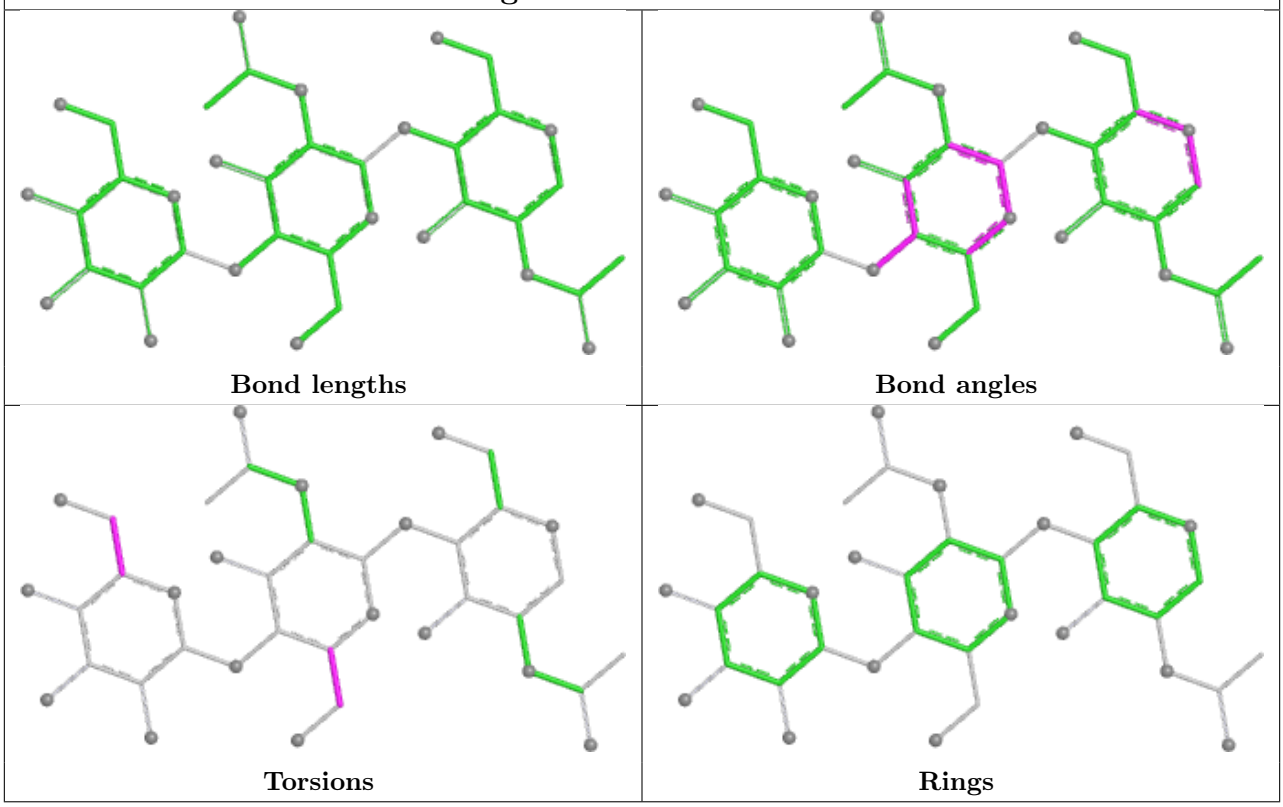
Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	c	5	MAN	1	0
16	g	5	MAN	1	0
10	a	5	MAN	1	0
10	T	9	MAN	1	0
10	T	6	MAN	1	0

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

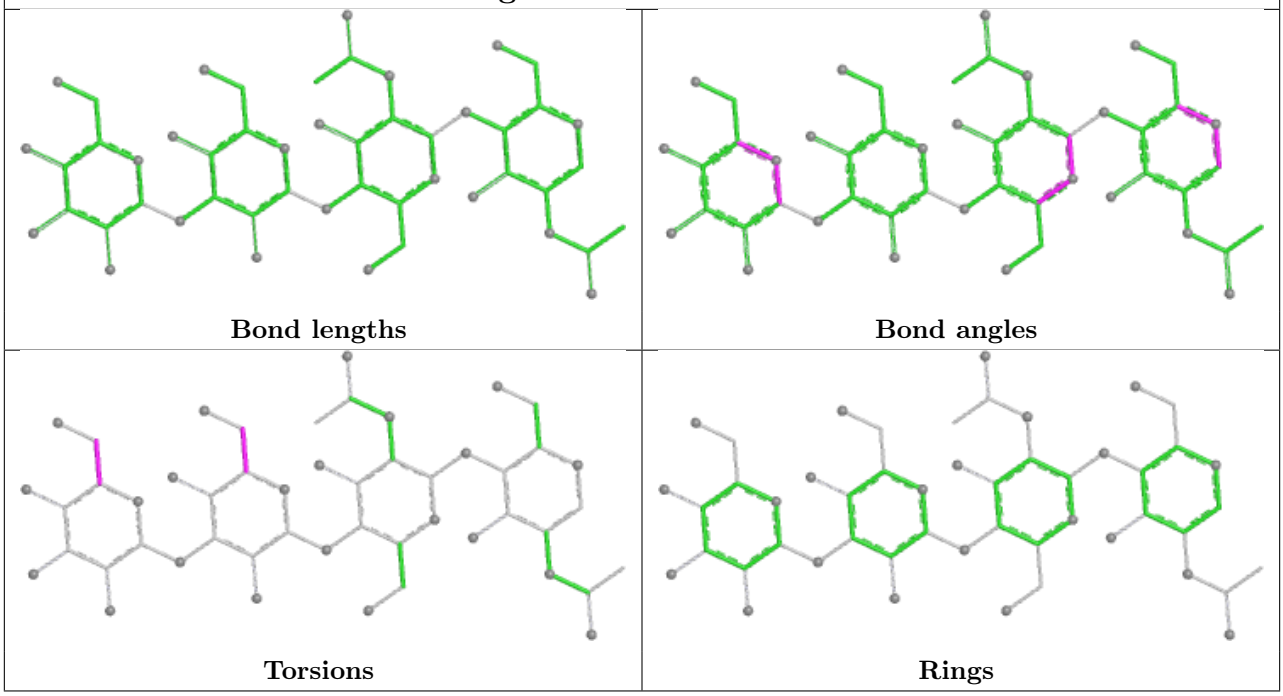
Oligosaccharide Chain R



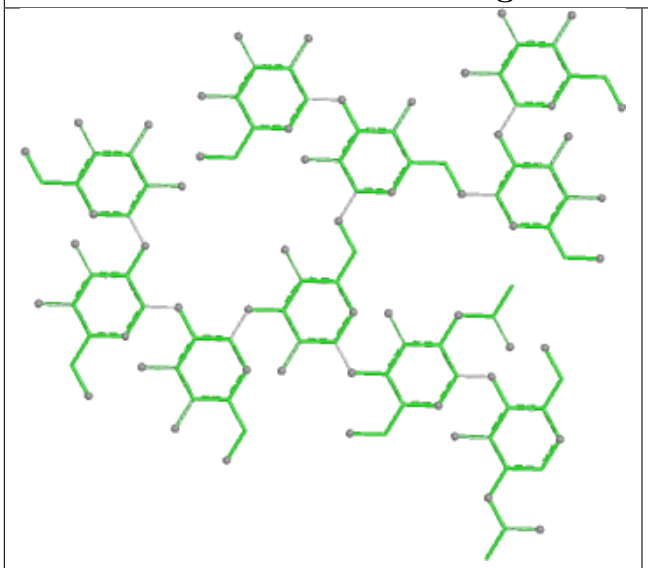
Oligosaccharide Chain e



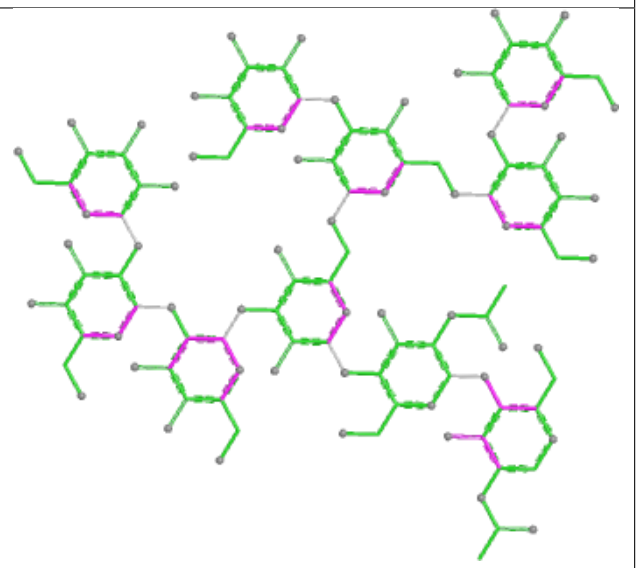
Oligosaccharide Chain S



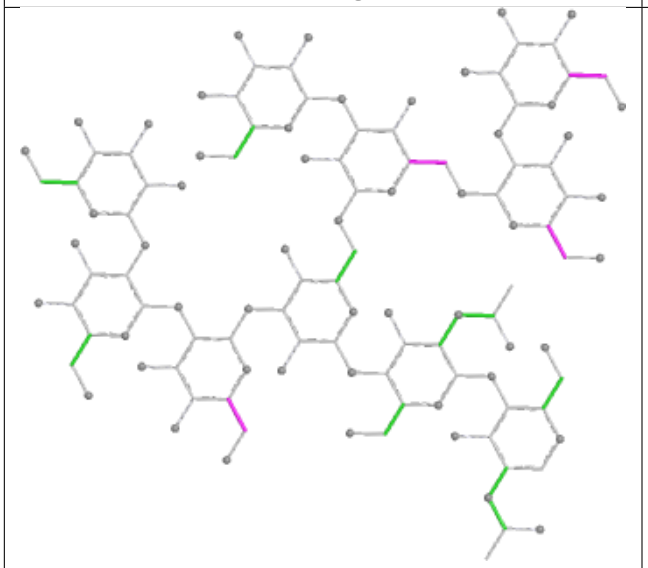
Oligosaccharide Chain T



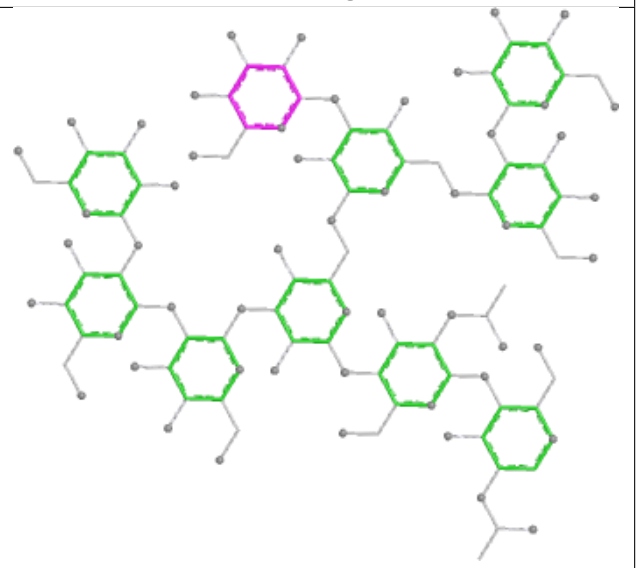
Bond lengths



Bond angles

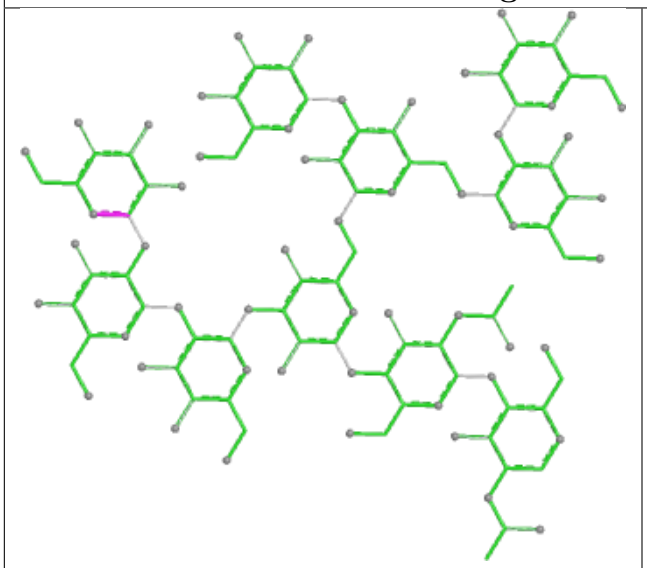


Torsions

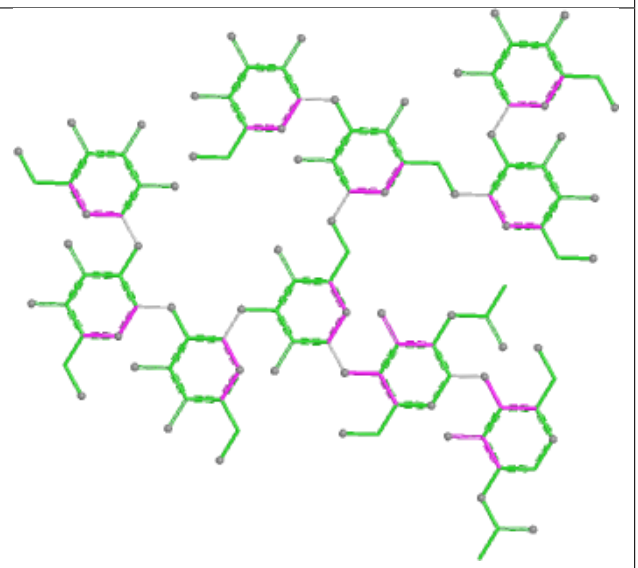


Rings

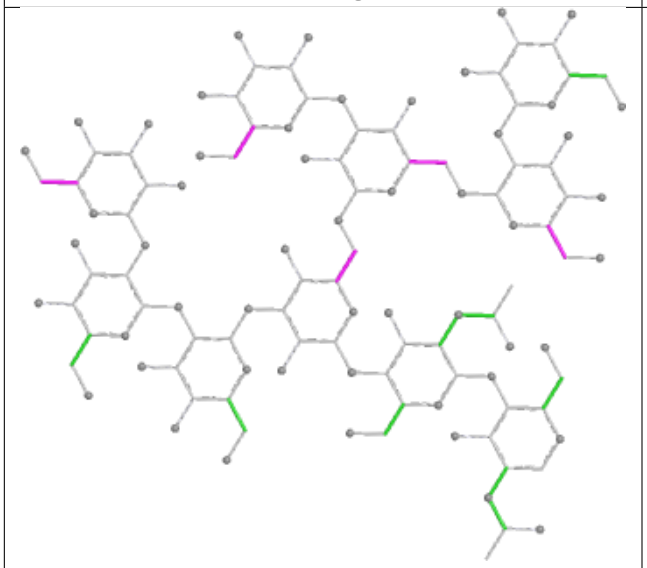
Oligosaccharide Chain a



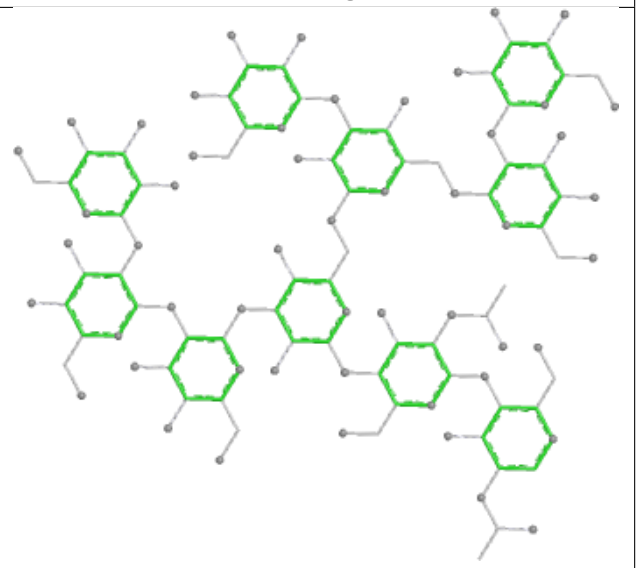
Bond lengths



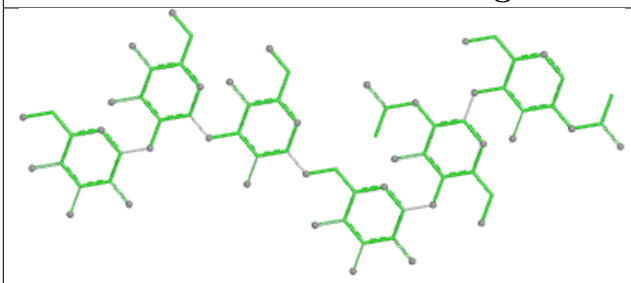
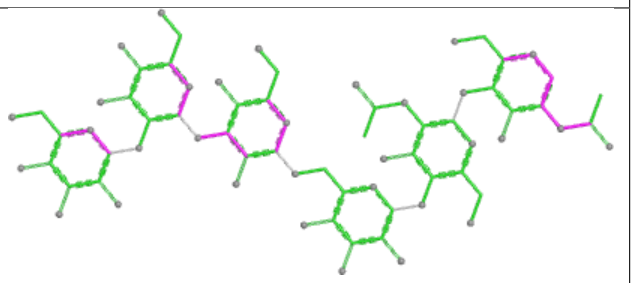
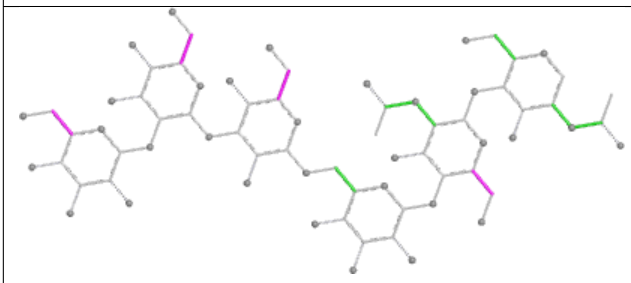
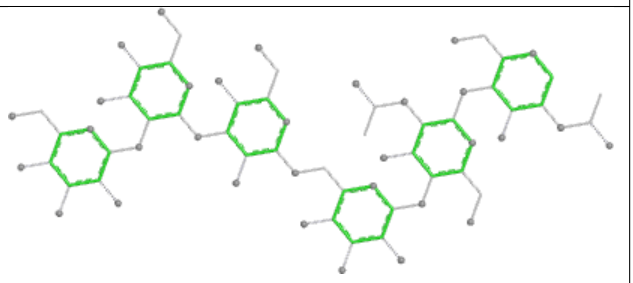
Bond angles

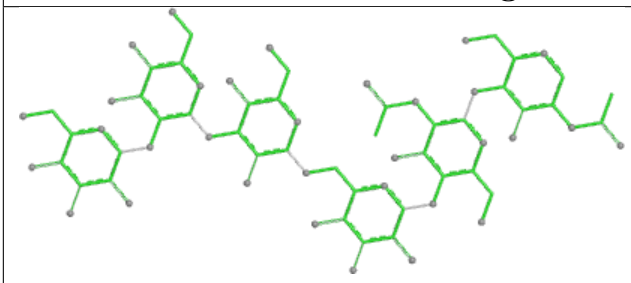
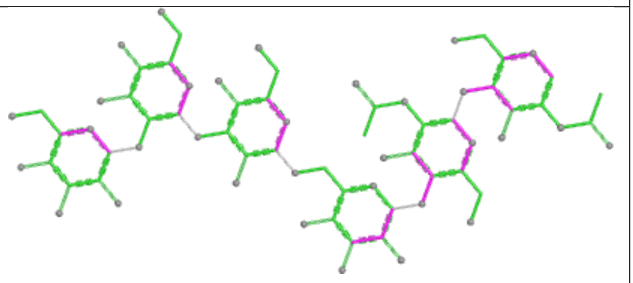
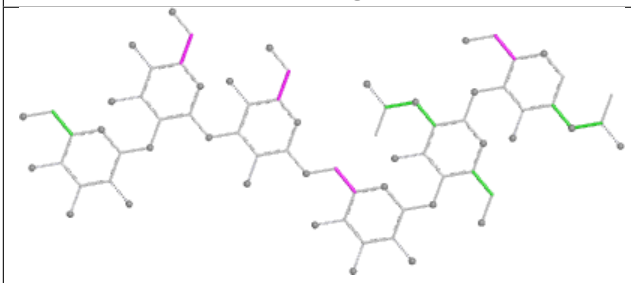
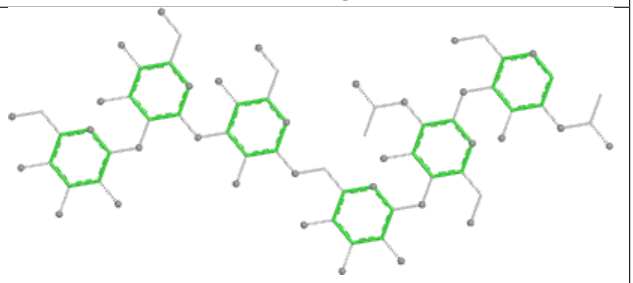


Torsions

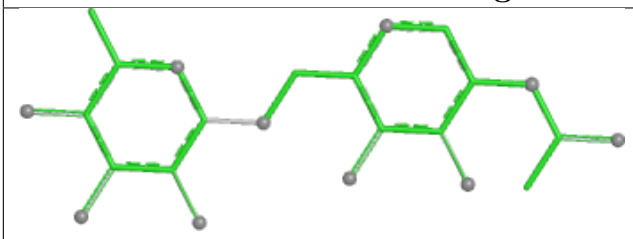


Rings

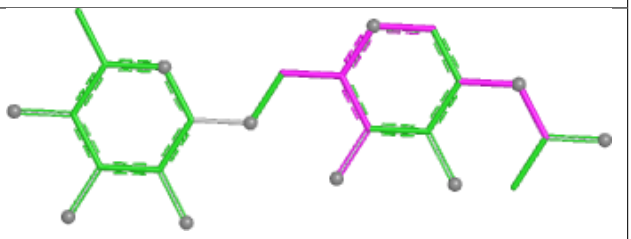
Oligosaccharide Chain U	
 Bond lengths	 Bond angles
 Torsions	 Rings

Oligosaccharide Chain c	
 Bond lengths	 Bond angles
 Torsions	 Rings

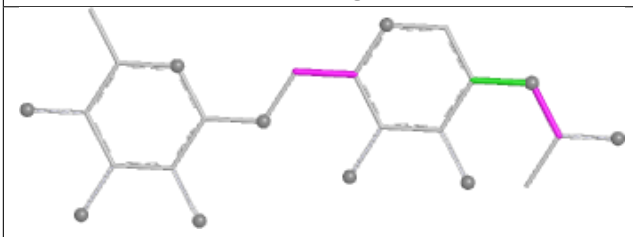
Oligosaccharide Chain V



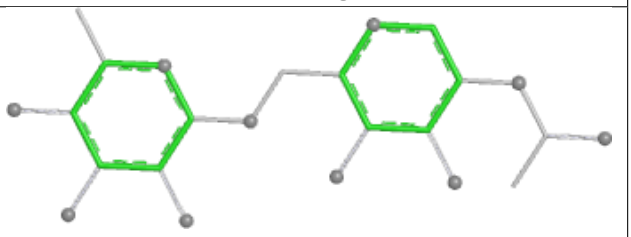
Bond lengths



Bond angles

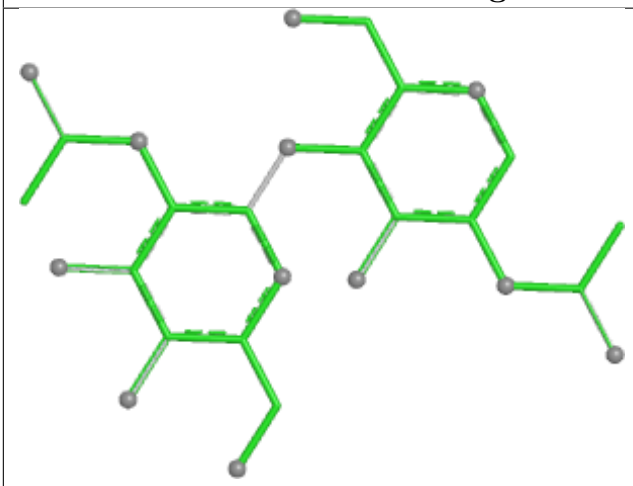


Torsions



Rings

Oligosaccharide Chain W



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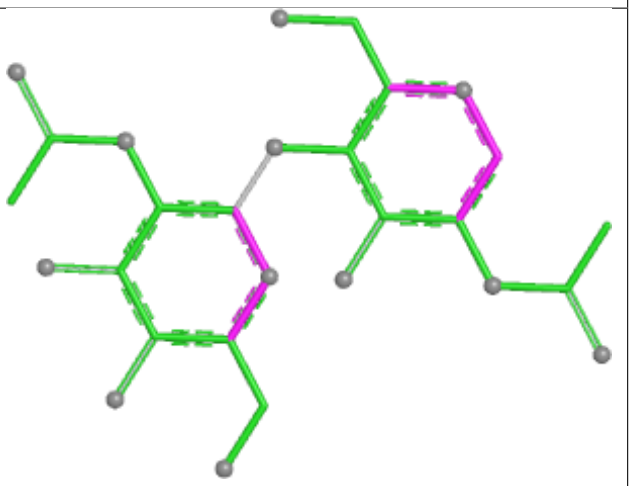

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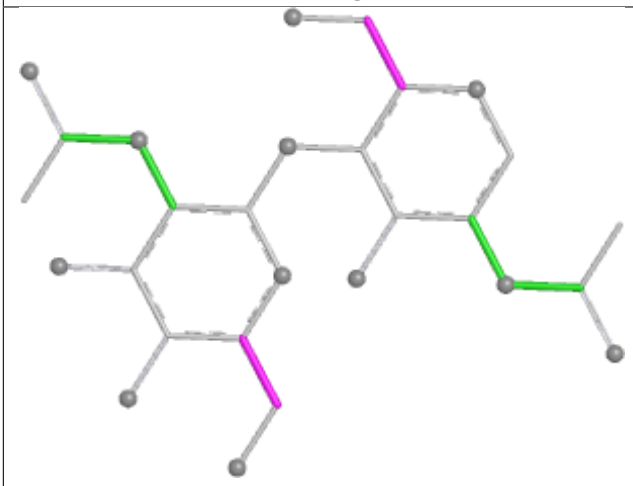

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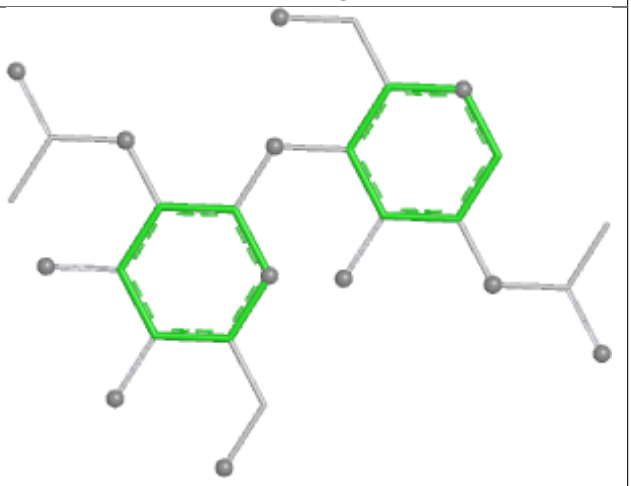
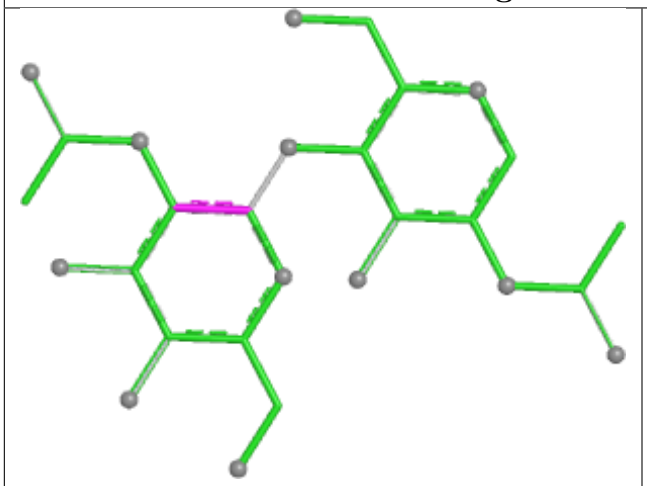
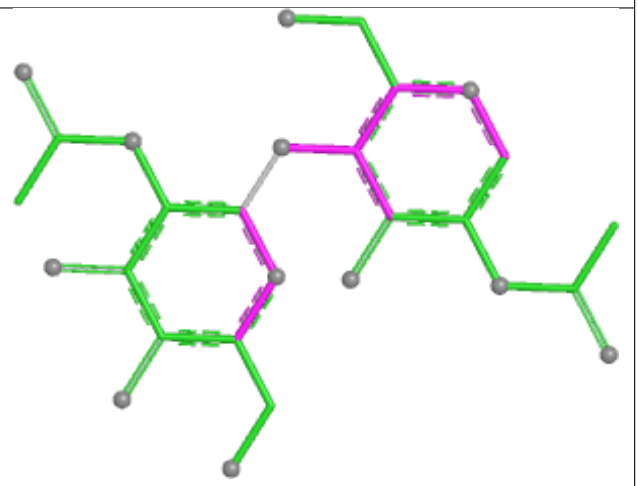


Rings

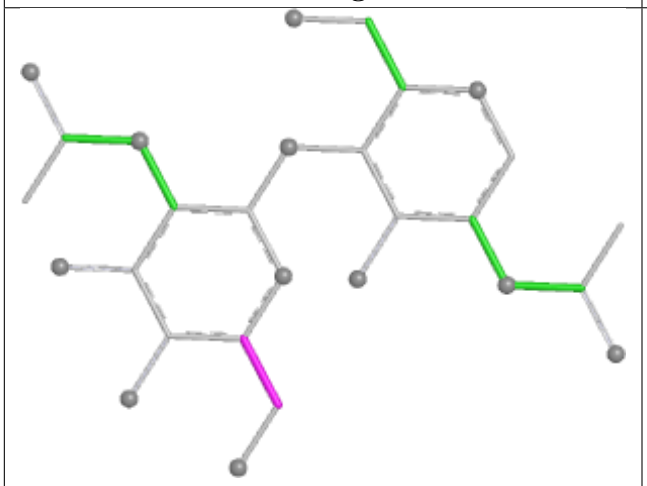
Oligosaccharide Chain X



Bond lengths



Bond angles



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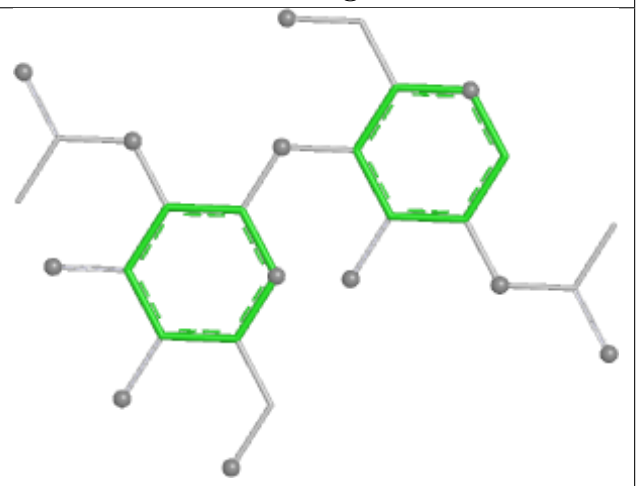
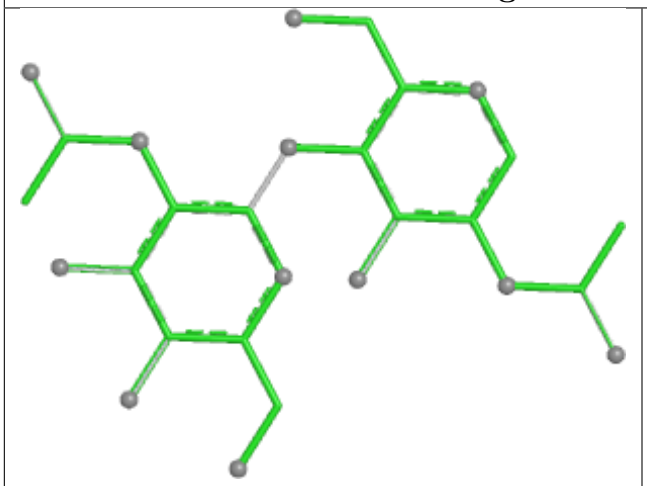


Rings

Oligosaccharide Chain b



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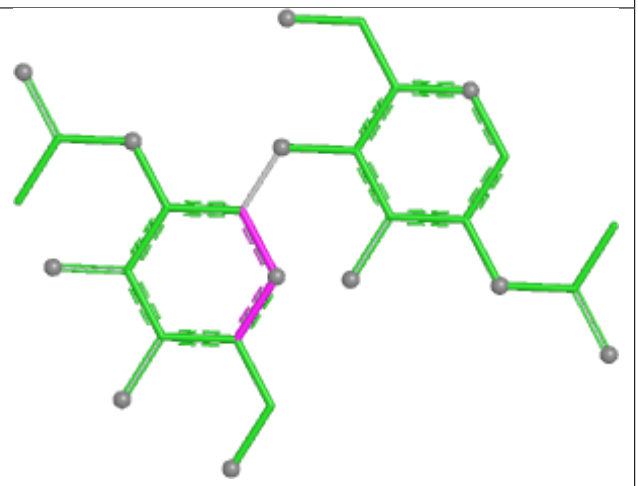

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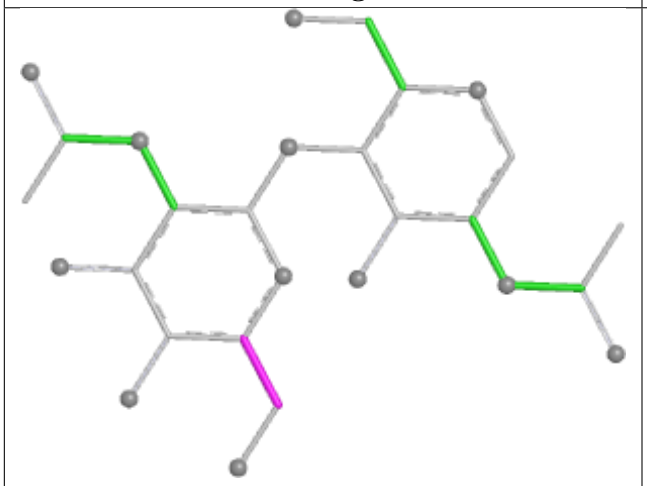

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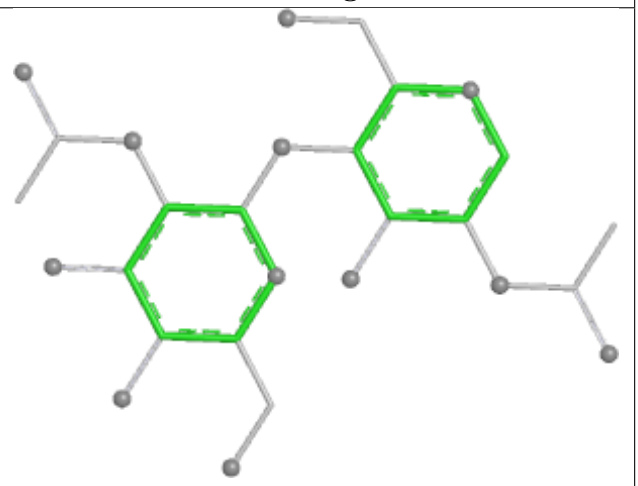
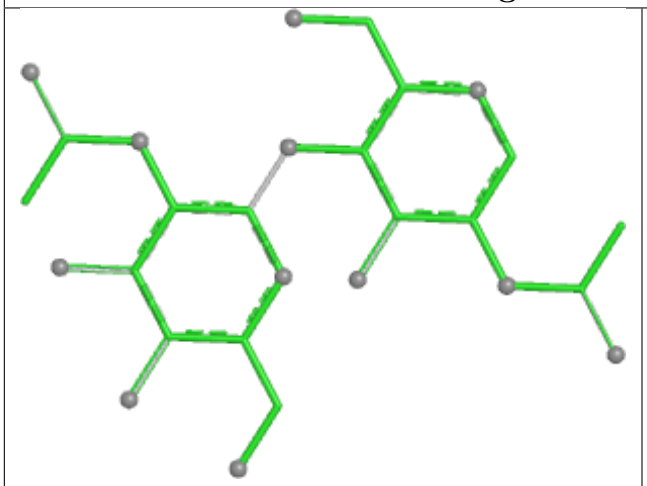
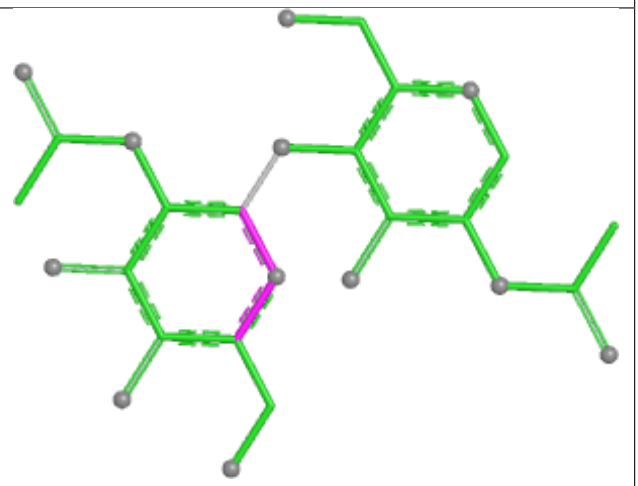


Rings

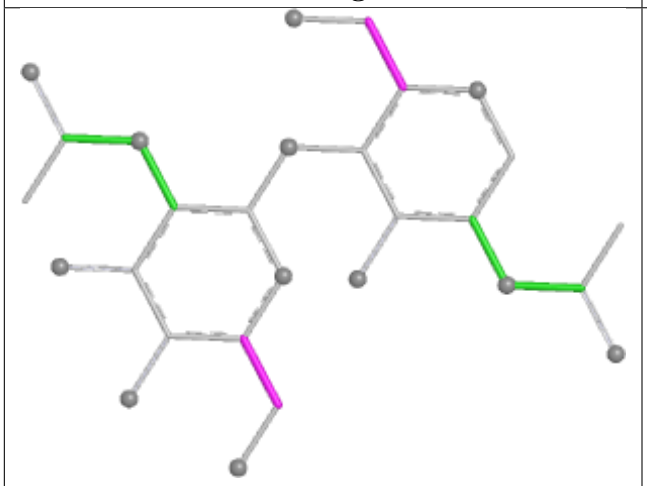
Oligosaccharide Chain d



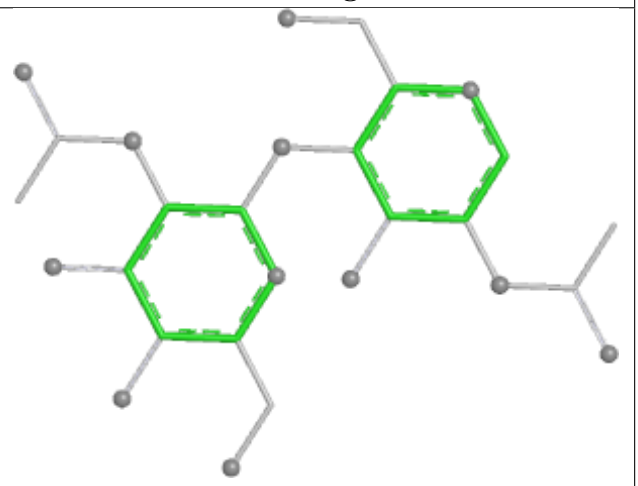
Bond lengths



Bond angles

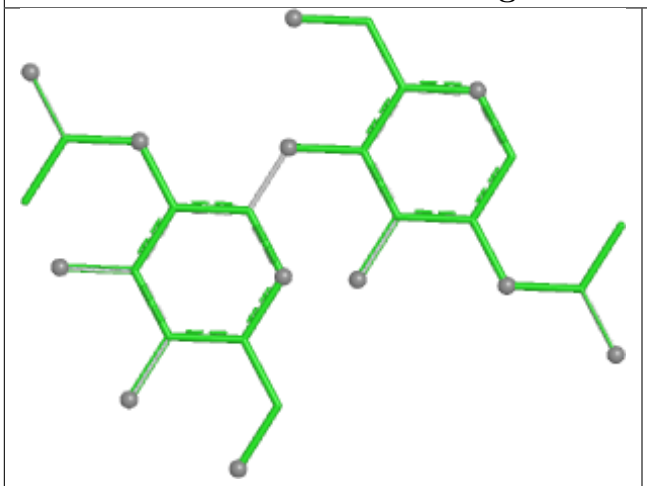


Torsions

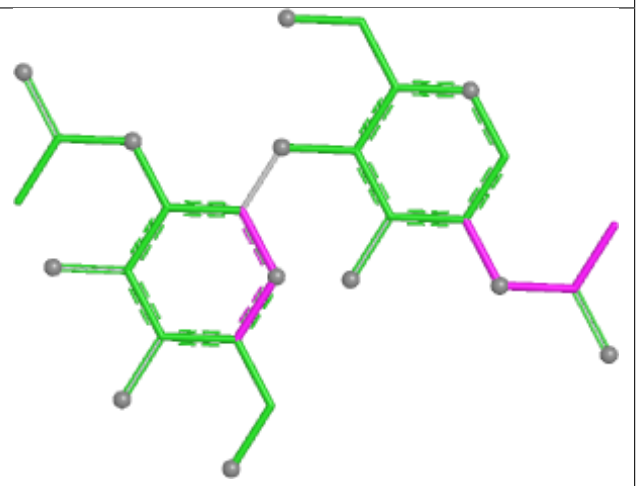


Rings

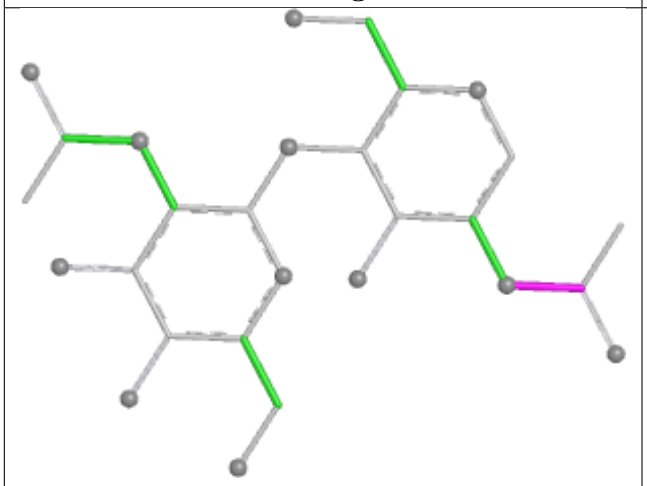
Oligosaccharide Chain h



Bond lengths



Bond angles



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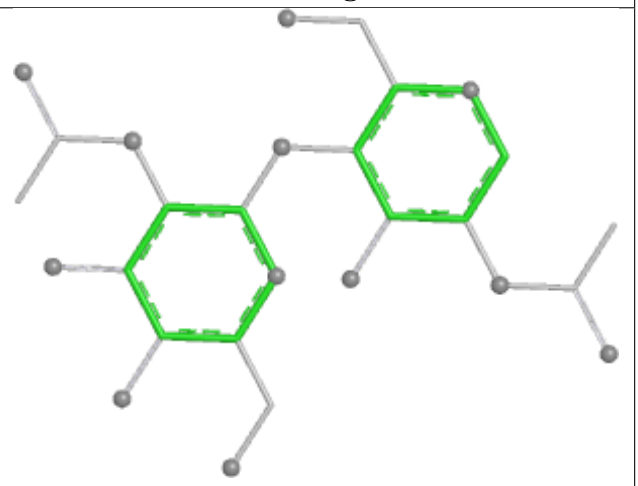
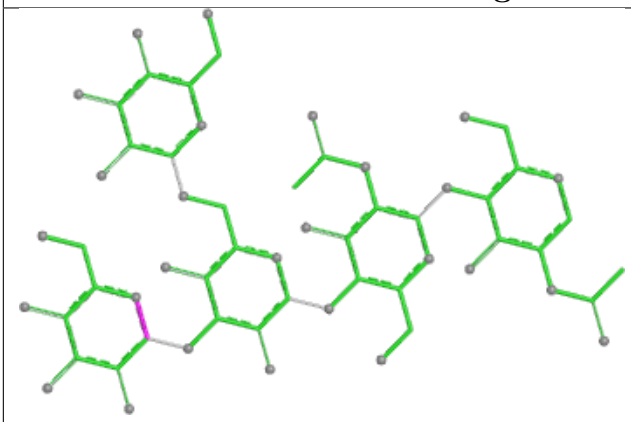
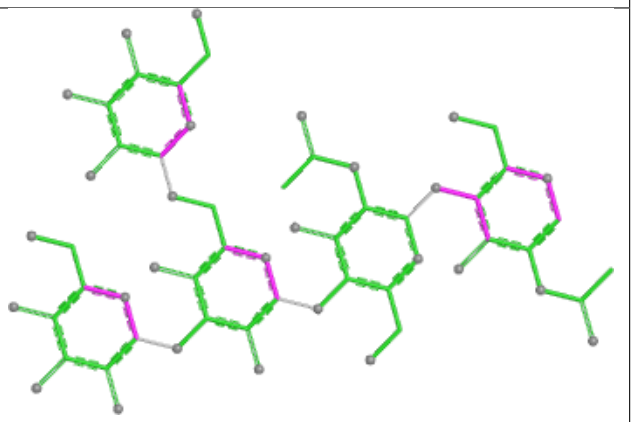
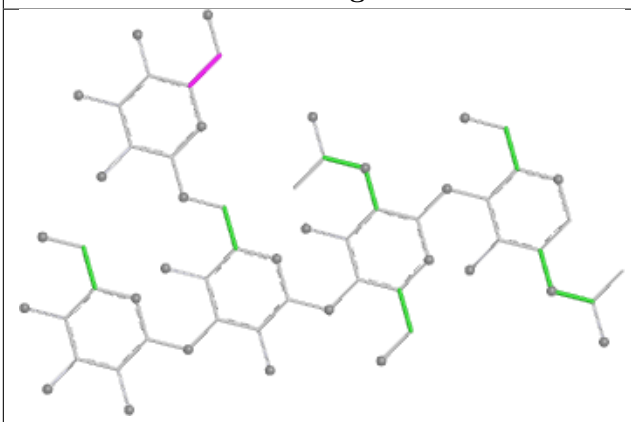
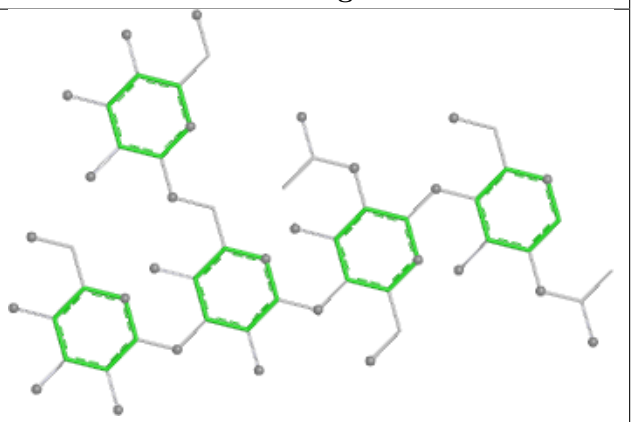
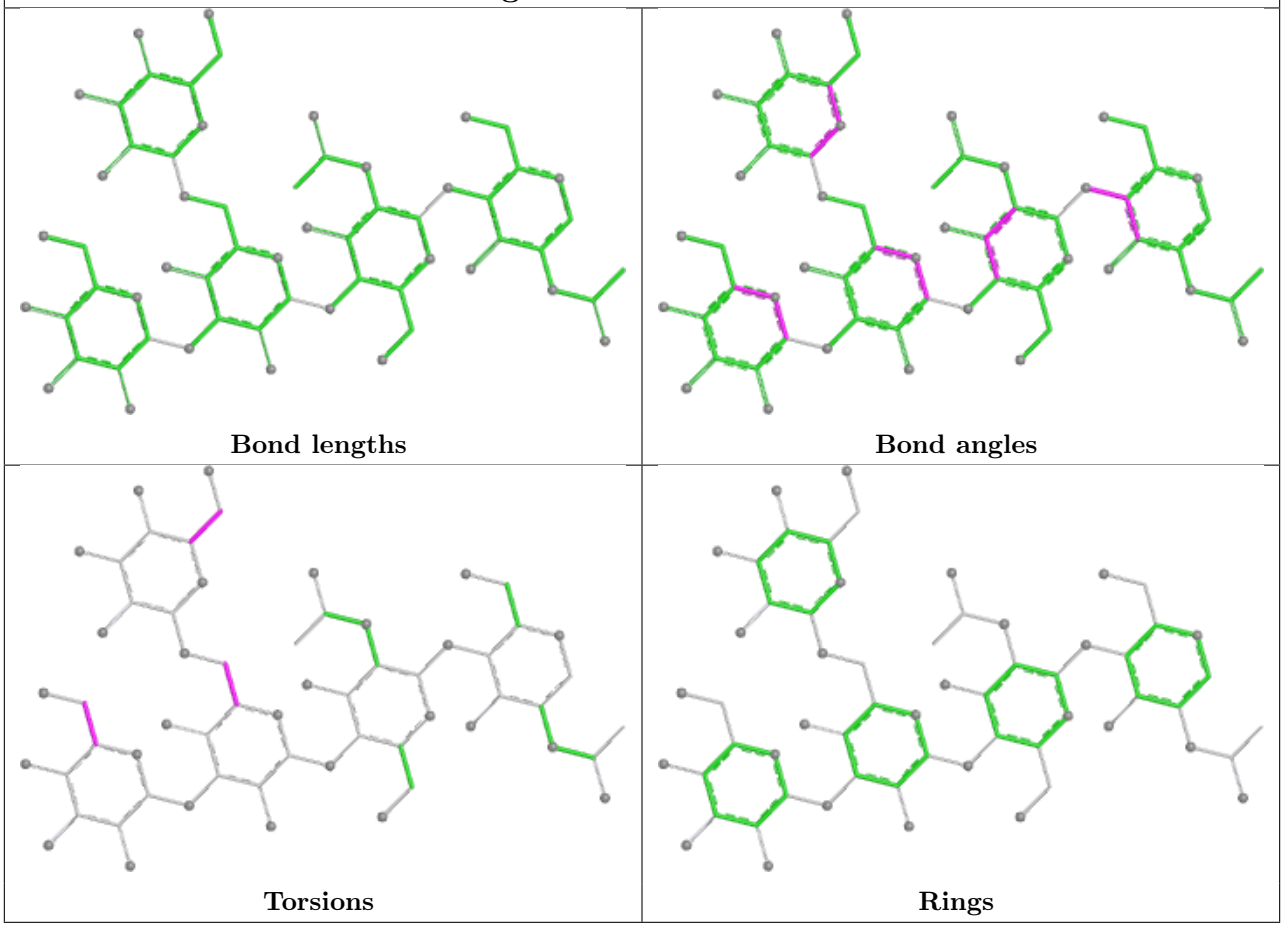
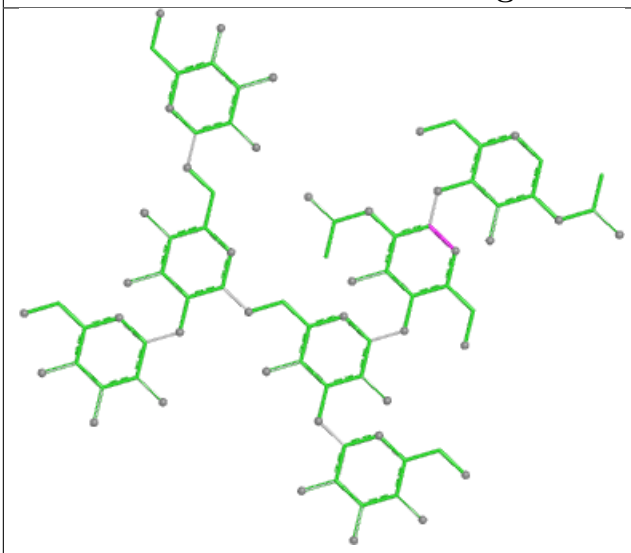
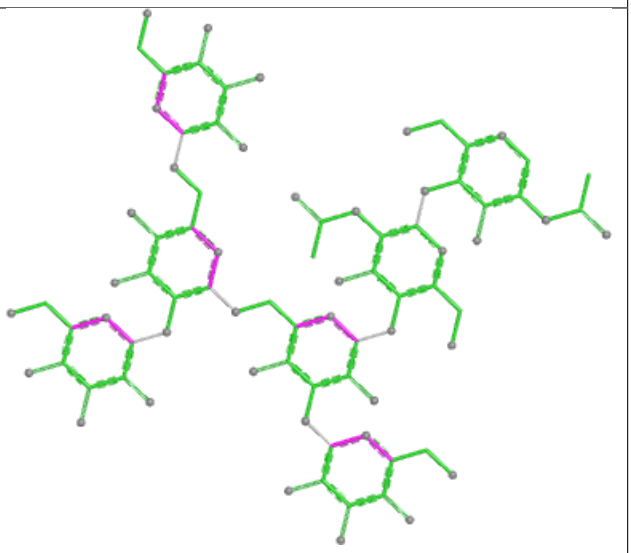
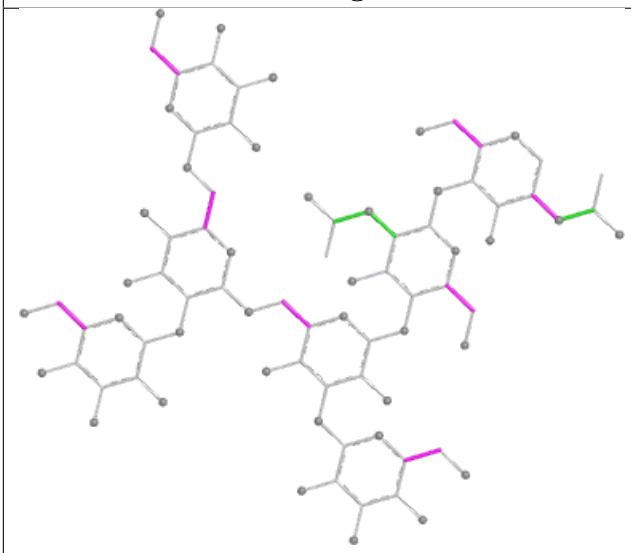
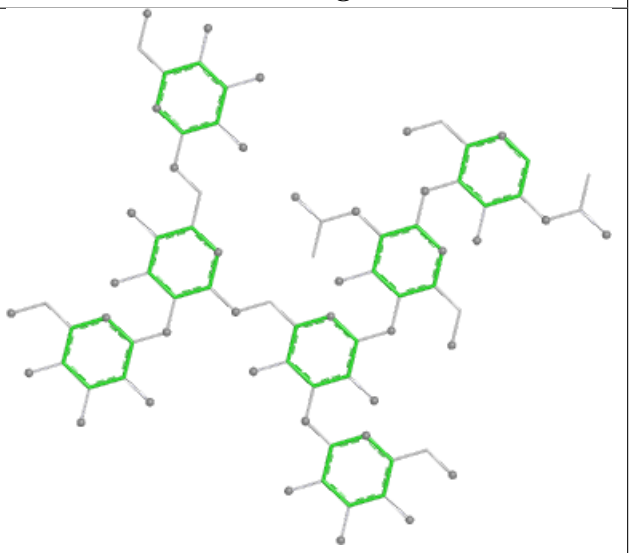


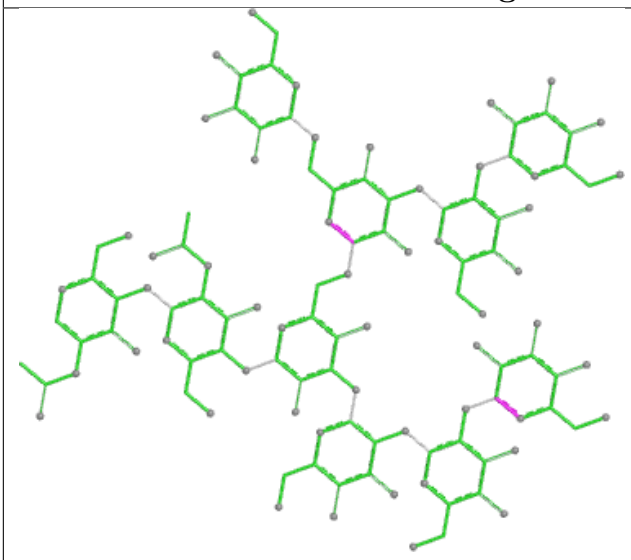
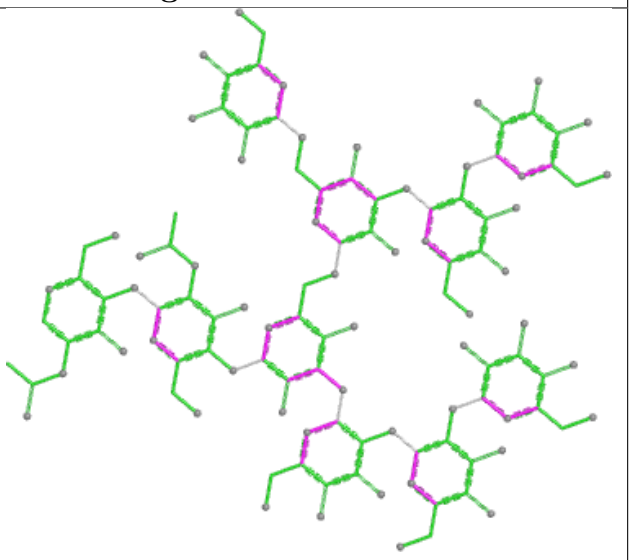
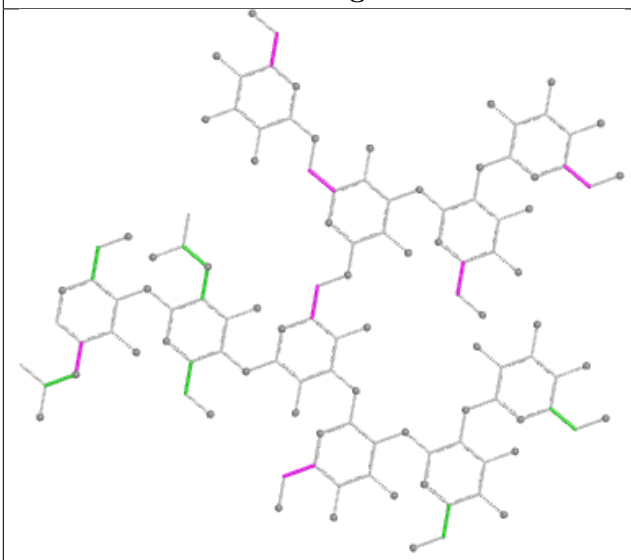
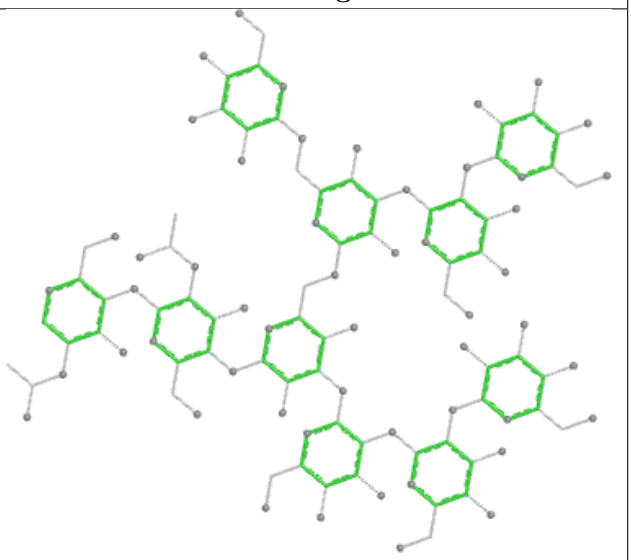
Rings

Oligosaccharide Chain Y	
 Bond lengths	 Bond angles
 Torsions	 Rings

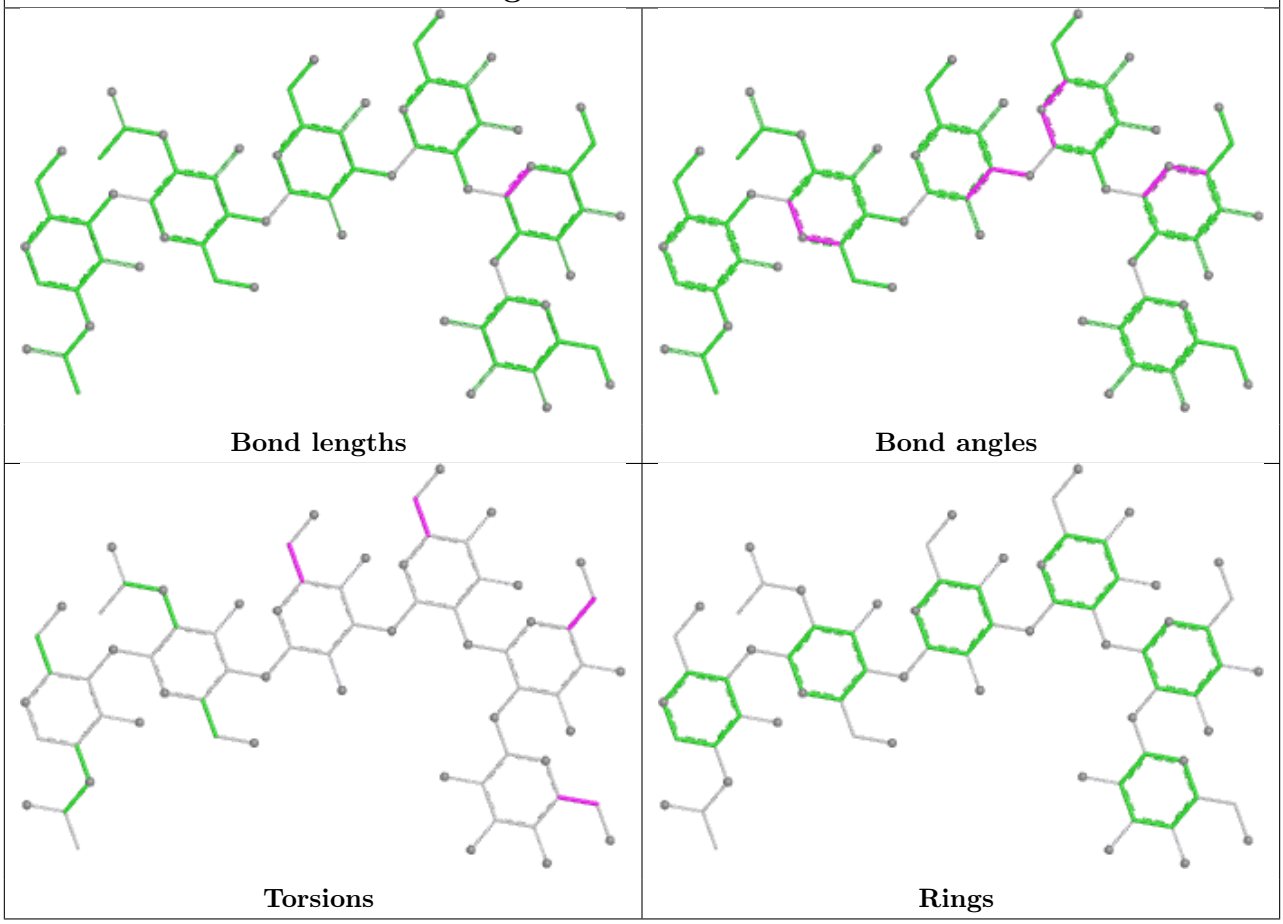
Oligosaccharide Chain f



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

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

Oligosaccharide Chain i



5.6 Ligand geometry (i)

39 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	$\#\|Z\| > 2$
18	NAG	C	711	7	14,14,15	0.69	0	17,19,21	0.92	0
18	NAG	B	708	7	14,14,15	0.67	0	17,19,21	0.88	0
18	NAG	A	705	7	14,14,15	0.66	0	17,19,21	1.02	0
18	NAG	C	706	7	14,14,15	0.70	0	17,19,21	0.93	0
18	NAG	C	705	7	14,14,15	0.74	0	17,19,21	0.81	0
18	NAG	B	703	7	14,14,15	0.65	0	17,19,21	0.91	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
18	NAG	C	701	7	14,14,15	0.69	0	17,19,21	1.03	1 (5%)
18	NAG	C	704	7	14,14,15	0.68	0	17,19,21	1.11	1 (5%)
18	NAG	C	708	7	14,14,15	0.66	0	17,19,21	0.96	1 (5%)
18	NAG	B	710	7	14,14,15	0.69	0	17,19,21	0.87	0
18	NAG	A	713	7	14,14,15	0.73	0	17,19,21	0.99	1 (5%)
18	NAG	C	703	7	14,14,15	0.69	0	17,19,21	0.99	1 (5%)
18	NAG	C	709	7	14,14,15	0.69	0	17,19,21	0.94	1 (5%)
18	NAG	B	702	7	14,14,15	0.74	0	17,19,21	1.10	1 (5%)
18	NAG	B	711	7	14,14,15	0.67	0	17,19,21	0.89	0
18	NAG	B	705	7	14,14,15	0.71	0	17,19,21	1.02	0
18	NAG	B	707	7	14,14,15	0.69	0	17,19,21	1.06	1 (5%)
18	NAG	A	706	7	14,14,15	0.72	0	17,19,21	1.32	2 (11%)
18	NAG	A	709	7	14,14,15	0.77	0	17,19,21	0.92	1 (5%)
18	NAG	C	702	7	14,14,15	0.68	0	17,19,21	1.12	2 (11%)
18	NAG	A	701	7	14,14,15	0.70	0	17,19,21	1.15	2 (11%)
18	NAG	A	711	7	14,14,15	0.70	0	17,19,21	1.07	1 (5%)
18	NAG	B	704	7	14,14,15	0.71	0	17,19,21	1.04	1 (5%)
18	NAG	A	708	7	14,14,15	0.74	0	17,19,21	0.92	0
18	NAG	C	707	7	14,14,15	0.67	0	17,19,21	0.99	0
18	NAG	B	706	7	14,14,15	0.63	0	17,19,21	1.84	3 (17%)
18	NAG	A	710	7	14,14,15	0.86	1 (7%)	17,19,21	1.31	1 (5%)
18	NAG	A	712	7	14,14,15	0.77	0	17,19,21	0.98	1 (5%)
18	NAG	A	702	7	14,14,15	0.68	0	17,19,21	1.12	1 (5%)
18	NAG	A	714	7	14,14,15	0.72	0	17,19,21	0.94	1 (5%)
18	NAG	C	713	7	14,14,15	0.70	0	17,19,21	1.00	0
18	NAG	C	712	7	14,14,15	0.71	0	17,19,21	0.91	0
18	NAG	B	709	7	14,14,15	0.66	0	17,19,21	0.96	1 (5%)
18	NAG	B	701	7	14,14,15	0.70	0	17,19,21	0.91	0
18	NAG	C	710	7	14,14,15	0.72	0	17,19,21	0.91	0
18	NAG	A	703	7	14,14,15	0.73	0	17,19,21	1.13	1 (5%)
18	NAG	A	707	7	14,14,15	0.74	0	17,19,21	0.88	0
18	NAG	A	715	7	14,14,15	0.69	0	17,19,21	0.99	1 (5%)
18	NAG	A	704	7	14,14,15	0.67	0	17,19,21	0.97	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
18	NAG	C	711	7	-	1/6/23/26	0/1/1/1
18	NAG	B	708	7	-	1/6/23/26	0/1/1/1
18	NAG	A	705	7	-	1/6/23/26	0/1/1/1
18	NAG	C	706	7	-	1/6/23/26	0/1/1/1
18	NAG	C	705	7	-	0/6/23/26	0/1/1/1
18	NAG	B	703	7	-	0/6/23/26	0/1/1/1
18	NAG	C	701	7	-	1/6/23/26	0/1/1/1
18	NAG	C	704	7	-	1/6/23/26	0/1/1/1
18	NAG	C	708	7	-	1/6/23/26	0/1/1/1
18	NAG	B	710	7	-	0/6/23/26	0/1/1/1
18	NAG	A	713	7	-	1/6/23/26	0/1/1/1
18	NAG	C	703	7	-	1/6/23/26	0/1/1/1
18	NAG	C	709	7	-	0/6/23/26	0/1/1/1
18	NAG	B	702	7	-	0/6/23/26	0/1/1/1
18	NAG	B	711	7	-	1/6/23/26	0/1/1/1
18	NAG	B	705	7	-	1/6/23/26	0/1/1/1
18	NAG	B	707	7	-	1/6/23/26	0/1/1/1
18	NAG	A	706	7	-	0/6/23/26	0/1/1/1
18	NAG	A	709	7	-	0/6/23/26	0/1/1/1
18	NAG	C	702	7	-	1/6/23/26	0/1/1/1
18	NAG	A	701	7	-	1/6/23/26	0/1/1/1
18	NAG	A	711	7	-	0/6/23/26	0/1/1/1
18	NAG	B	704	7	-	0/6/23/26	0/1/1/1
18	NAG	A	708	7	-	2/6/23/26	0/1/1/1
18	NAG	C	707	7	-	1/6/23/26	0/1/1/1
18	NAG	B	706	7	-	3/6/23/26	0/1/1/1
18	NAG	A	710	7	-	2/6/23/26	0/1/1/1
18	NAG	A	712	7	-	1/6/23/26	0/1/1/1
18	NAG	A	702	7	-	1/6/23/26	0/1/1/1
18	NAG	A	714	7	-	1/6/23/26	0/1/1/1
18	NAG	C	713	7	-	0/6/23/26	0/1/1/1
18	NAG	C	712	7	-	0/6/23/26	0/1/1/1
18	NAG	B	709	7	-	1/6/23/26	0/1/1/1
18	NAG	B	701	7	-	2/6/23/26	0/1/1/1
18	NAG	C	710	7	-	0/6/23/26	0/1/1/1
18	NAG	A	703	7	-	1/6/23/26	0/1/1/1
18	NAG	A	707	7	-	2/6/23/26	0/1/1/1
18	NAG	A	715	7	-	1/6/23/26	0/1/1/1
18	NAG	A	704	7	-	1/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	A	710	NAG	C1-C2	2.17	1.55	1.52

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	B	706	NAG	C2-N2-C7	5.58	130.38	122.90
18	A	710	NAG	C2-N2-C7	3.31	127.34	122.90
18	A	706	NAG	C2-N2-C7	3.30	127.33	122.90
18	C	704	NAG	C1-O5-C5	3.10	116.34	112.19
18	B	702	NAG	C1-O5-C5	2.99	116.19	112.19
18	A	702	NAG	C1-O5-C5	2.93	116.12	112.19
18	A	712	NAG	C1-O5-C5	2.86	116.02	112.19
18	A	711	NAG	C1-O5-C5	2.86	116.01	112.19
18	A	701	NAG	C1-O5-C5	2.85	116.00	112.19
18	A	713	NAG	C1-O5-C5	2.79	115.92	112.19
18	C	702	NAG	C1-O5-C5	2.74	115.86	112.19
18	B	706	NAG	C1-O5-C5	2.69	115.79	112.19
18	B	707	NAG	C1-O5-C5	2.64	115.72	112.19
18	A	706	NAG	C1-O5-C5	2.59	115.66	112.19
18	A	709	NAG	C1-O5-C5	2.54	115.59	112.19
18	A	703	NAG	C1-O5-C5	2.49	115.53	112.19
18	B	706	NAG	C8-C7-N2	2.46	120.19	116.12
18	C	701	NAG	C1-O5-C5	2.41	115.42	112.19
18	C	703	NAG	C1-O5-C5	2.35	115.34	112.19
18	A	714	NAG	C1-O5-C5	2.24	115.19	112.19
18	A	704	NAG	C1-O5-C5	2.18	115.11	112.19
18	B	704	NAG	C1-O5-C5	2.15	115.07	112.19
18	C	702	NAG	C2-N2-C7	2.11	125.72	122.90
18	C	709	NAG	C2-N2-C7	2.05	125.65	122.90
18	A	715	NAG	C1-O5-C5	2.04	114.92	112.19
18	B	709	NAG	C1-O5-C5	2.03	114.91	112.19
18	A	701	NAG	C2-N2-C7	2.02	125.61	122.90
18	C	708	NAG	C1-O5-C5	2.01	114.88	112.19
18	B	703	NAG	C2-N2-C7	2.01	125.60	122.90

There are no chirality outliers.

All (33) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
18	A	707	NAG	O5-C5-C6-O6
18	A	708	NAG	O5-C5-C6-O6
18	A	708	NAG	C4-C5-C6-O6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
18	B	706	NAG	C8-C7-N2-C2
18	B	706	NAG	O7-C7-N2-C2
18	A	707	NAG	C4-C5-C6-O6
18	A	703	NAG	O5-C5-C6-O6
18	A	714	NAG	O5-C5-C6-O6
18	B	707	NAG	O5-C5-C6-O6
18	B	708	NAG	O5-C5-C6-O6
18	C	704	NAG	O5-C5-C6-O6
18	A	702	NAG	O5-C5-C6-O6
18	A	705	NAG	O5-C5-C6-O6
18	C	707	NAG	O5-C5-C6-O6
18	A	715	NAG	O5-C5-C6-O6
18	B	705	NAG	O5-C5-C6-O6
18	C	702	NAG	O5-C5-C6-O6
18	C	706	NAG	O5-C5-C6-O6
18	C	708	NAG	O5-C5-C6-O6
18	A	701	NAG	O5-C5-C6-O6
18	A	704	NAG	O5-C5-C6-O6
18	B	709	NAG	O5-C5-C6-O6
18	B	711	NAG	O5-C5-C6-O6
18	C	703	NAG	O5-C5-C6-O6
18	C	711	NAG	O5-C5-C6-O6
18	B	701	NAG	O5-C5-C6-O6
18	A	712	NAG	O5-C5-C6-O6
18	C	701	NAG	O5-C5-C6-O6
18	B	706	NAG	O5-C5-C6-O6
18	A	710	NAG	O5-C5-C6-O6
18	A	710	NAG	C1-C2-N2-C7
18	B	701	NAG	C1-C2-N2-C7
18	A	713	NAG	O5-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.

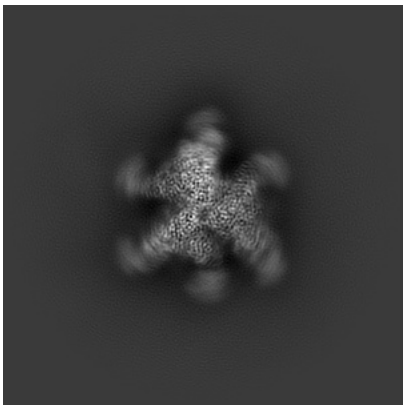
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-70469. These allow visual inspection of the internal detail of the map and identification of artifacts.

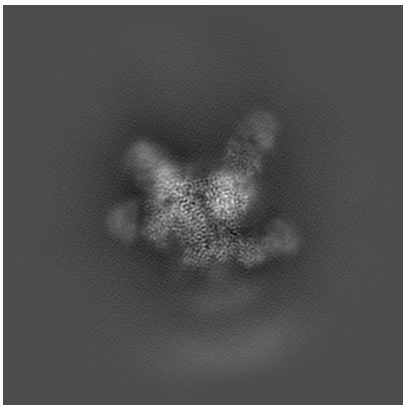
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections (i)

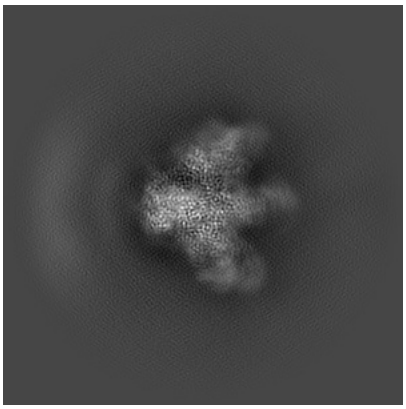
6.1.1 Primary map



X

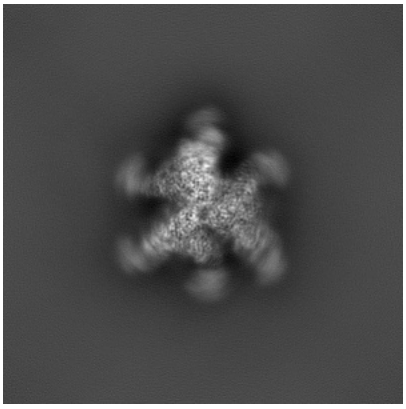


Y



Z

6.1.2 Raw map



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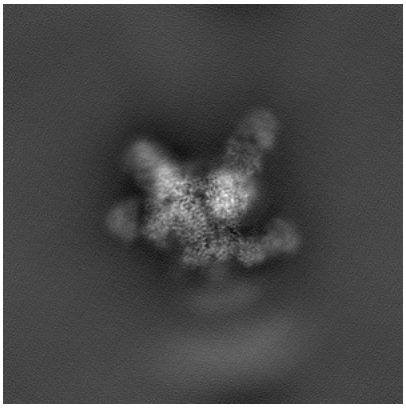
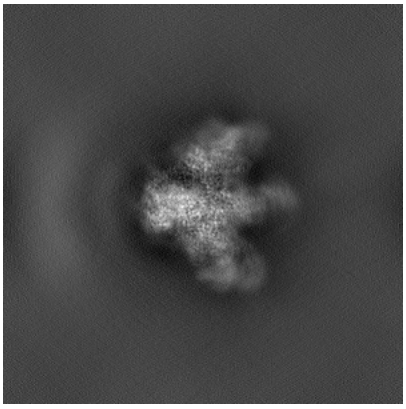


Y

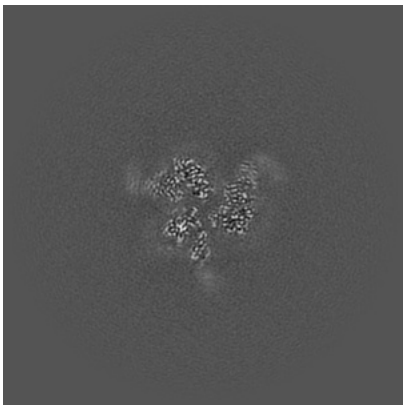


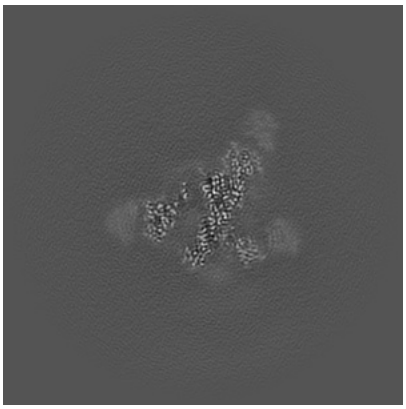
Z

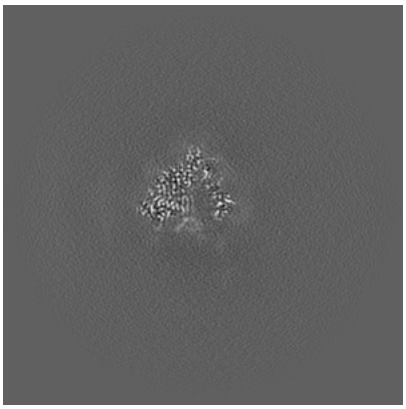
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

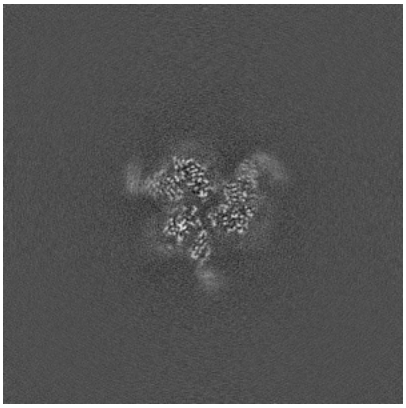
6.2.1 Primary map

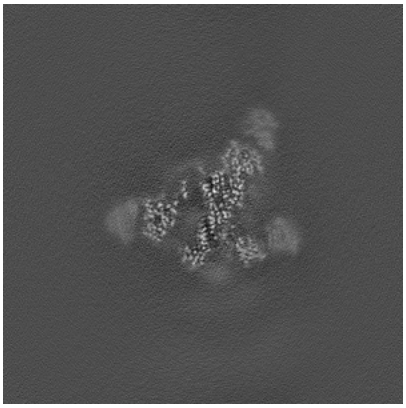

X Index: 200

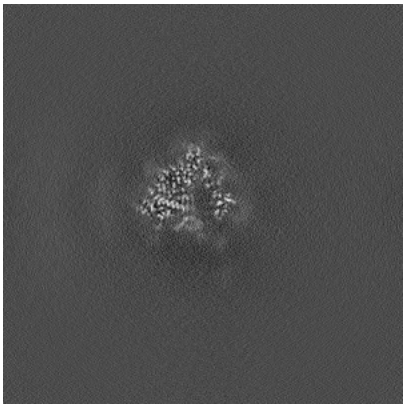

Y Index: 200


Z Index: 200

6.2.2 Raw map


X Index: 200

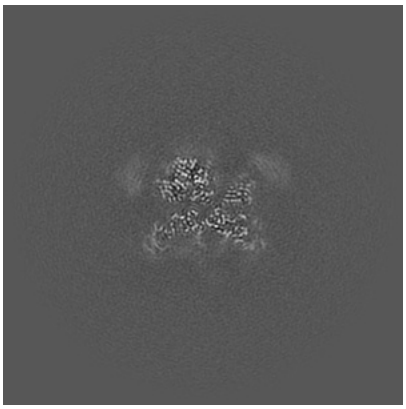

Y Index: 200

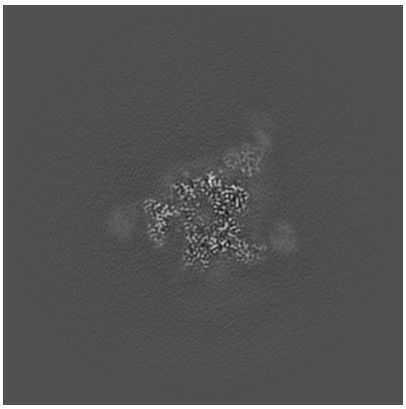

Z Index: 200

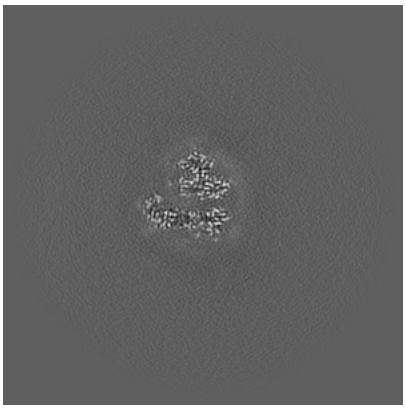
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

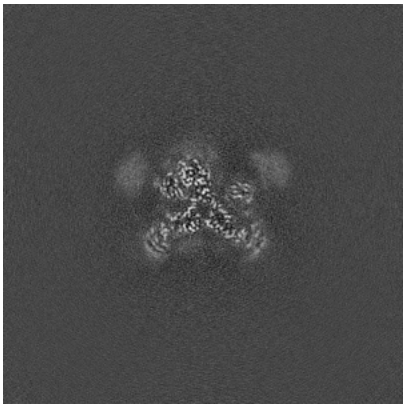
6.3.1 Primary map

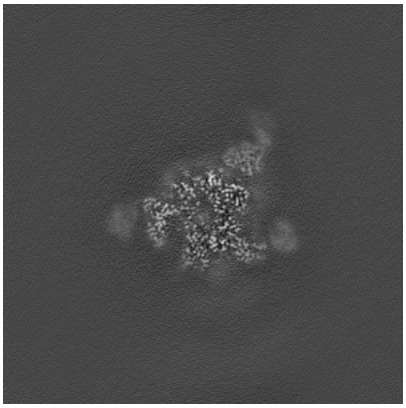

X Index: 208

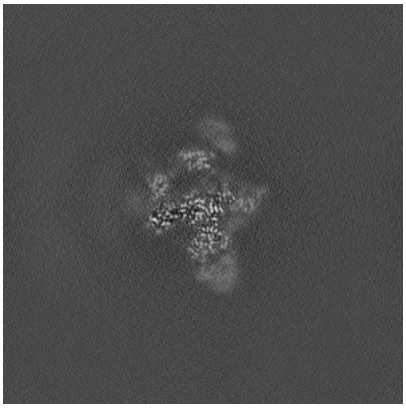

Y Index: 193


Z Index: 188

6.3.2 Raw map


X Index: 212

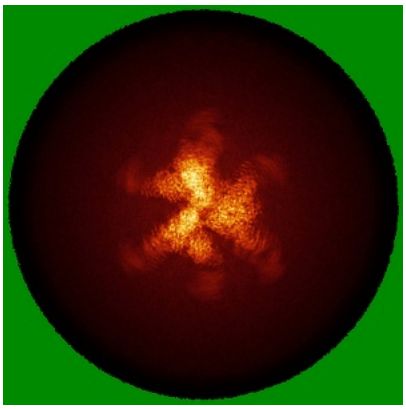

Y Index: 193

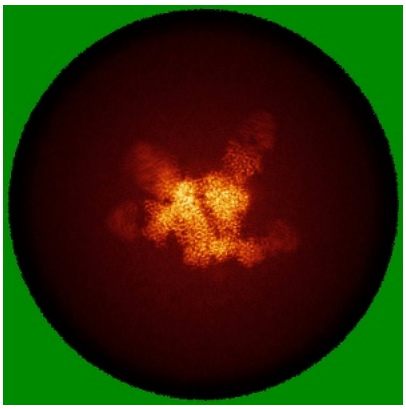

Z Index: 223

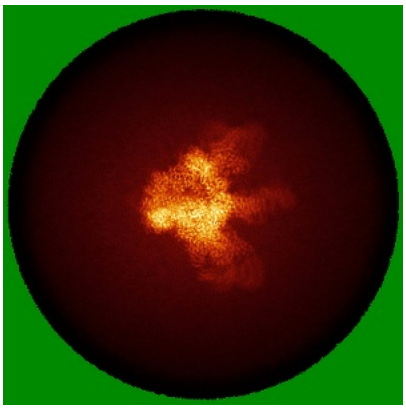
The images above show the largest variance slices of the map in three orthogonal directions.

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

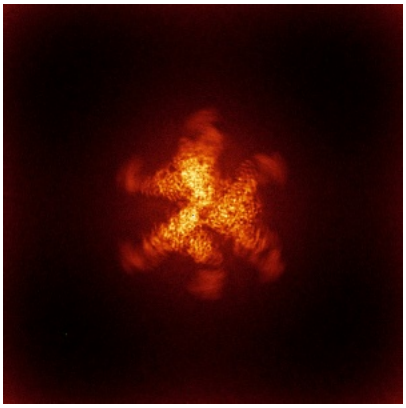
6.4.1 Primary map

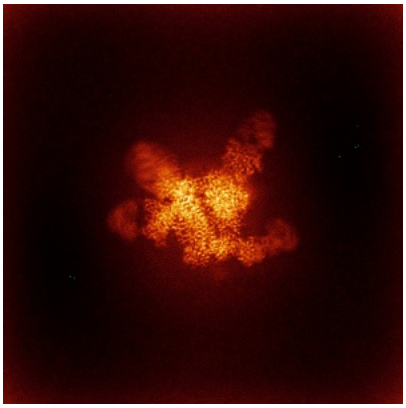

X

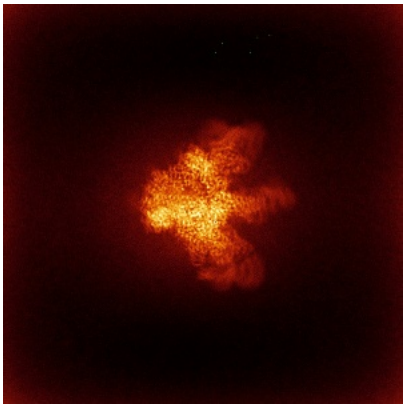

Y


Z

6.4.2 Raw map


X

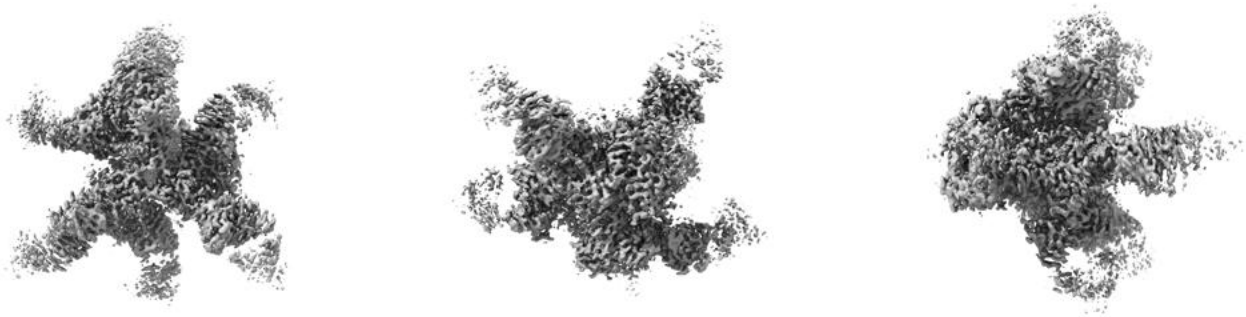

Y


Z

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

6.5 Orthogonal surface views (i)

6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.17. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map

X Y Z

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

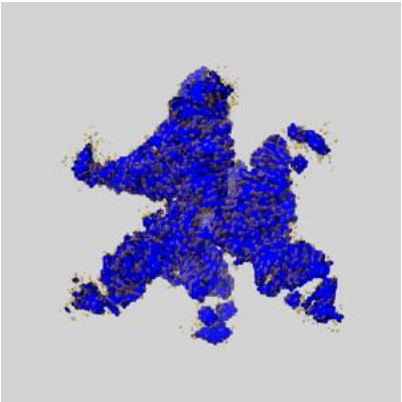
6.6 Mask visualisation (i)

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

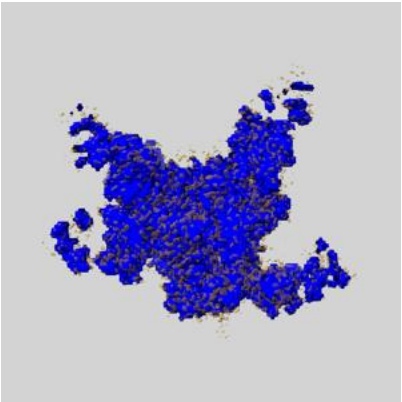
A mask typically either:

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

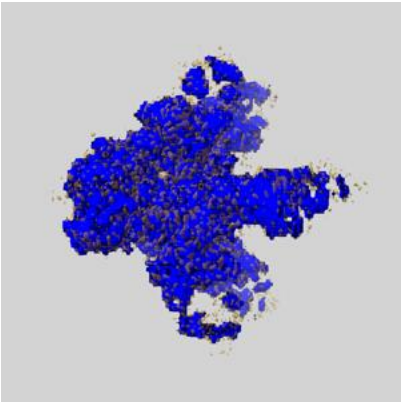
6.6.1 emd_70469_msk_1.map (i)



X



Y

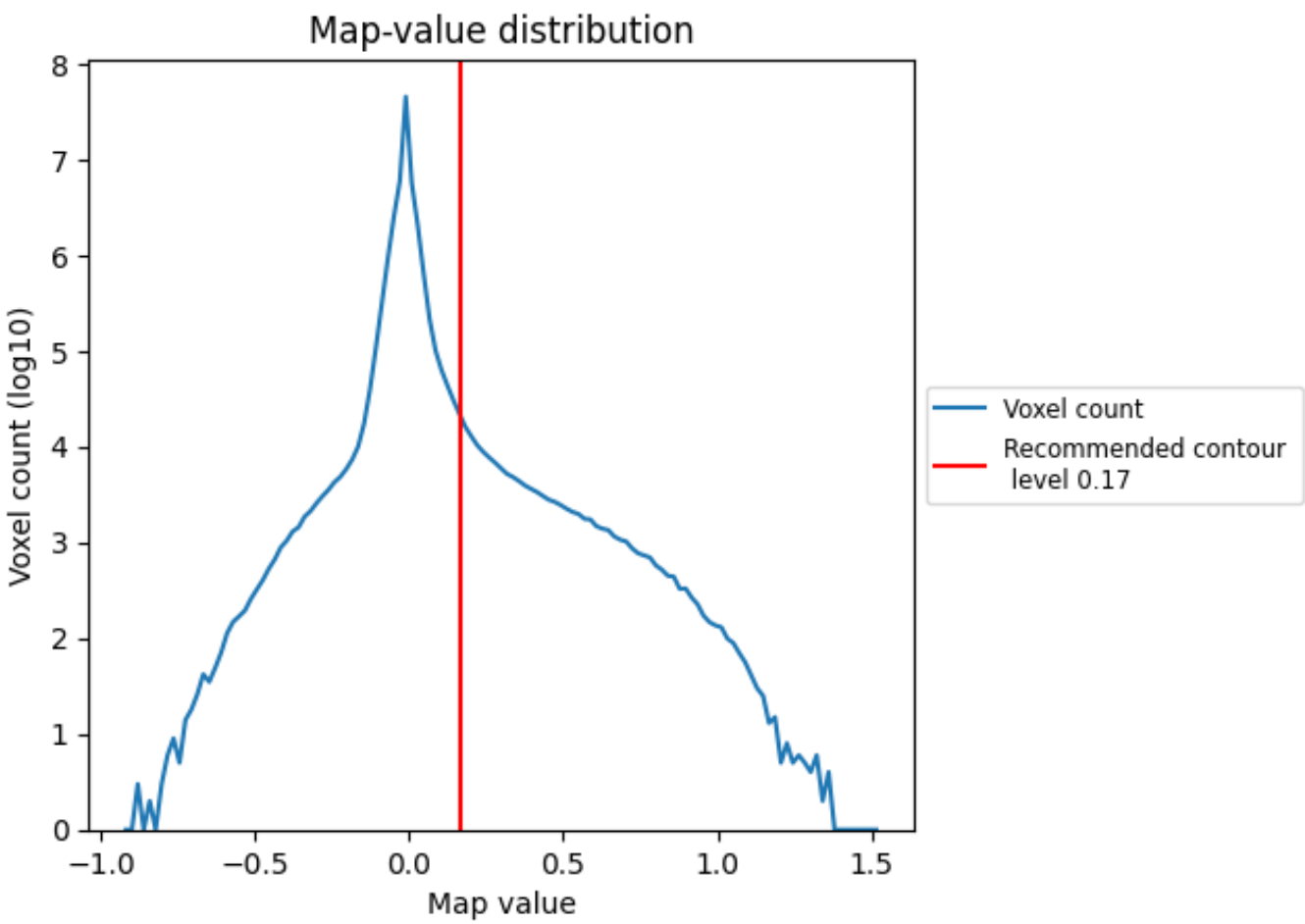


Z

7 Map analysis (i)

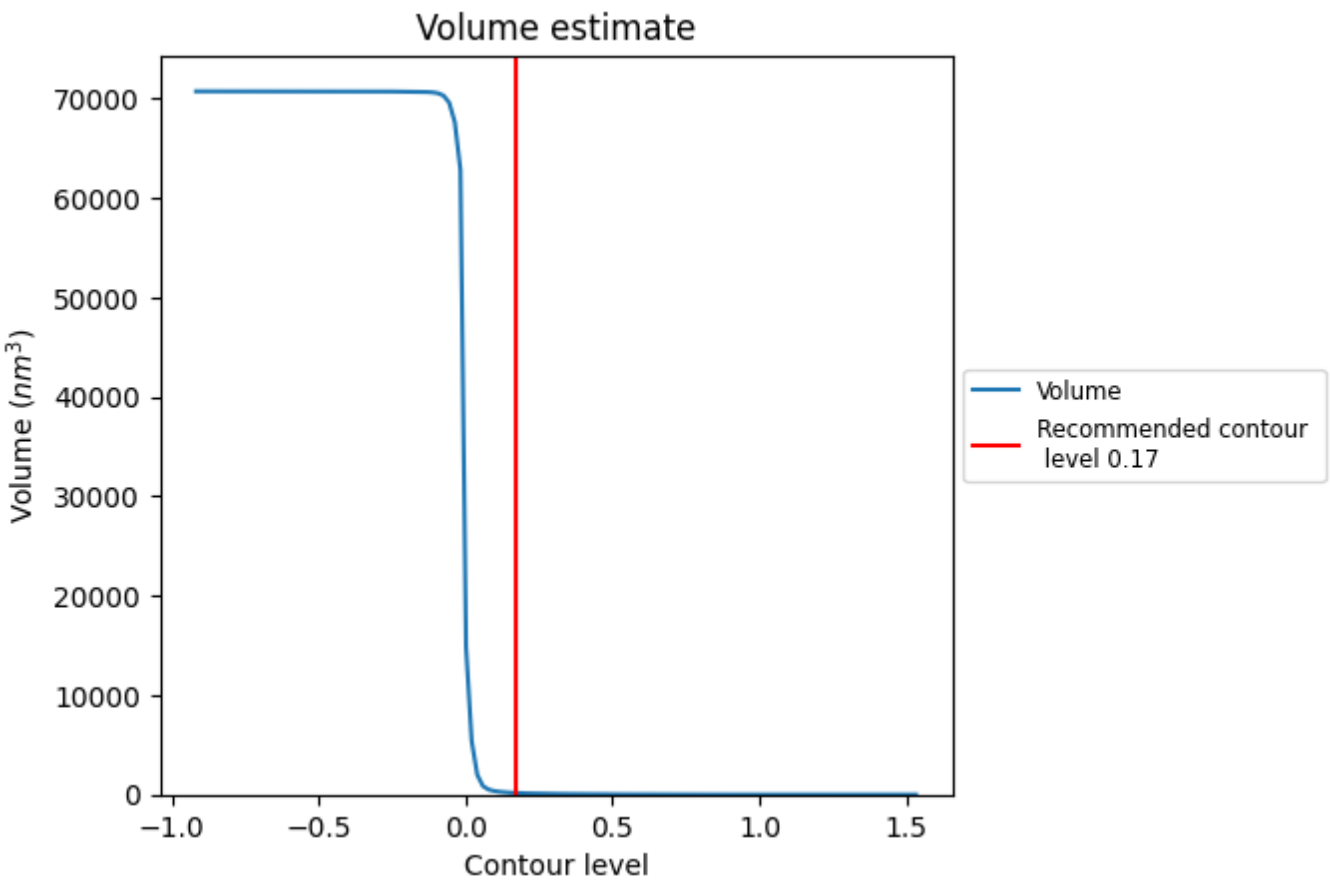
This section contains the results of statistical analysis of the map.

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.

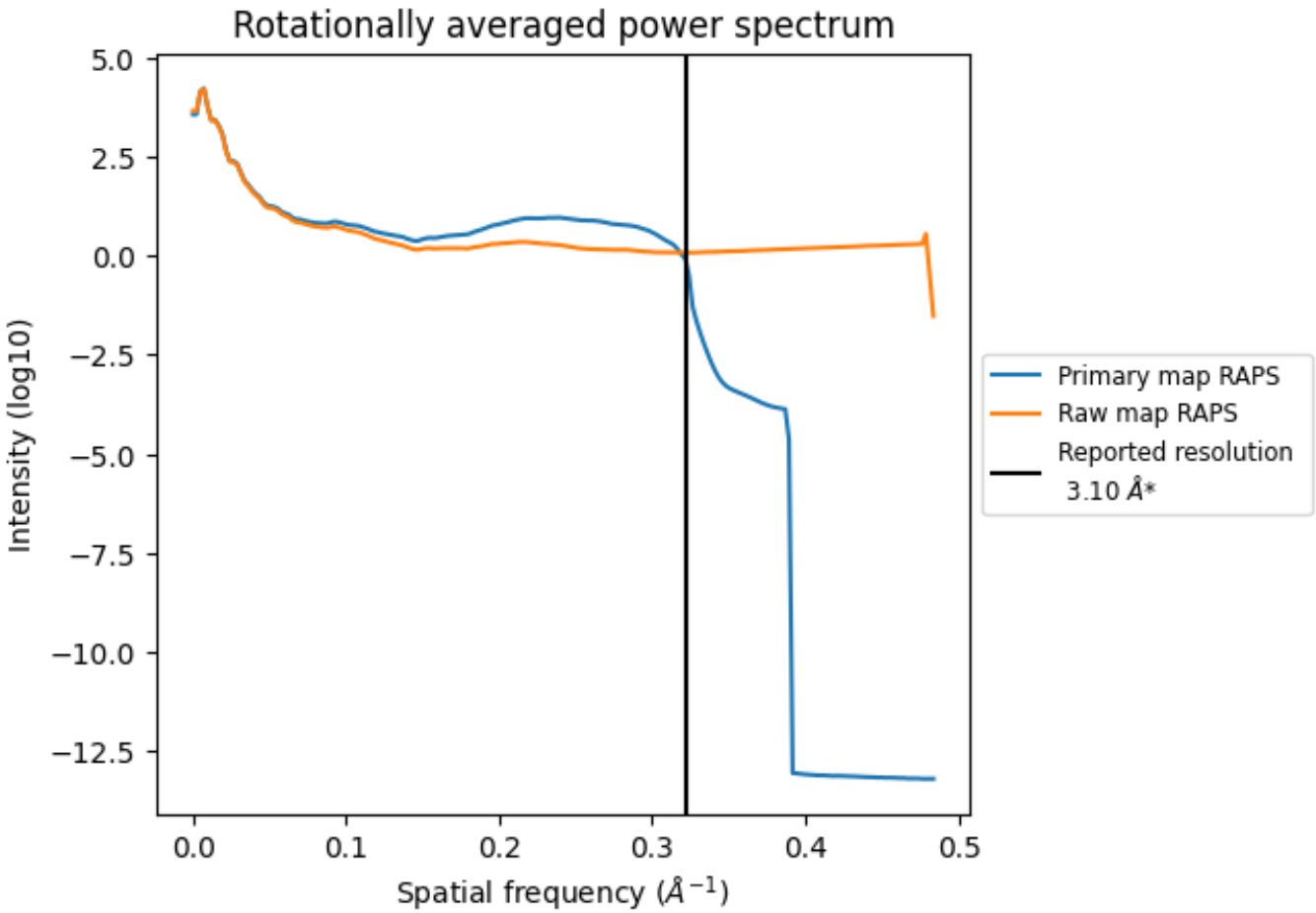
7.2 Volume estimate (i)



The volume at the recommended contour level is 159 nm^3; this corresponds to an approximate mass of 144 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)

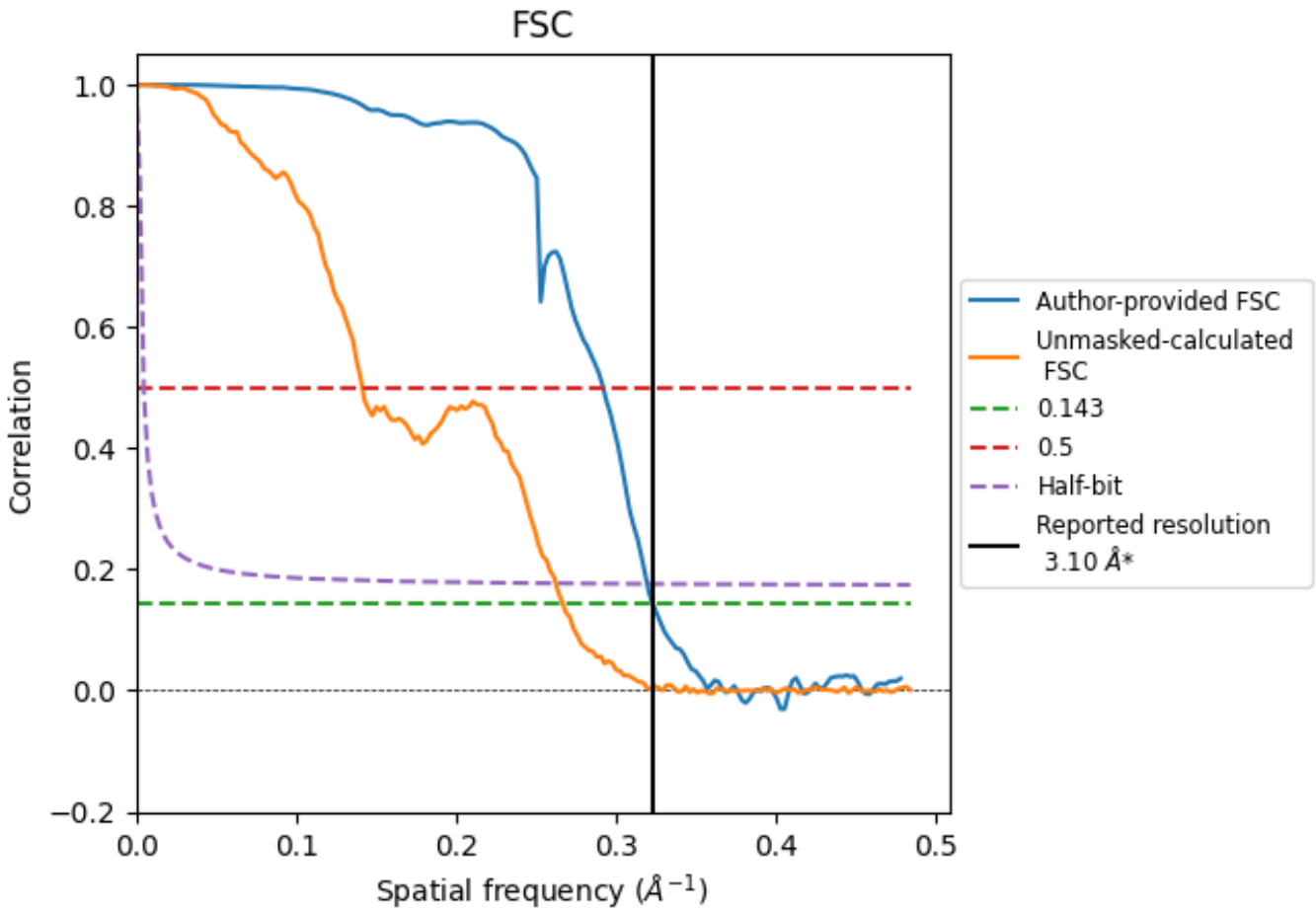


*Reported resolution corresponds to spatial frequency of 0.323 Å^{-1}

8 Fourier-Shell correlation (i)

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 (i)



*Reported resolution corresponds to spatial frequency of 0.323 Å^{-1}

8.2 Resolution estimates (i)

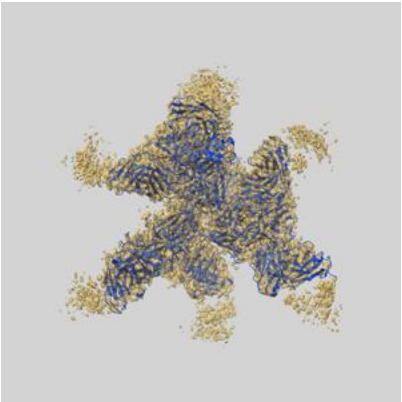
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.10	-	-
Author-provided FSC curve	3.10	3.43	3.13
Unmasked-calculated*	3.75	7.08	3.82

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.75 differs from the reported value 3.1 by more than 10 %

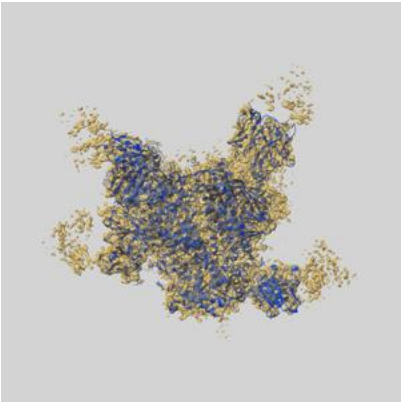
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-70469 and PDB model 9OGL. Per-residue inclusion information can be found in section 3 on page 15.

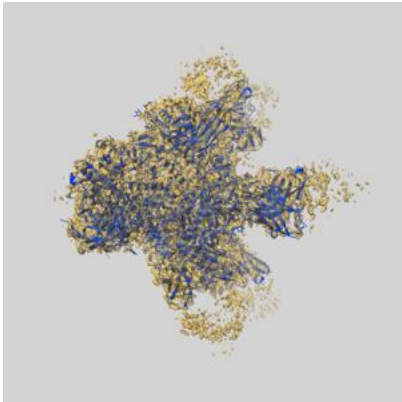
9.1 Map-model overlay (i)



X



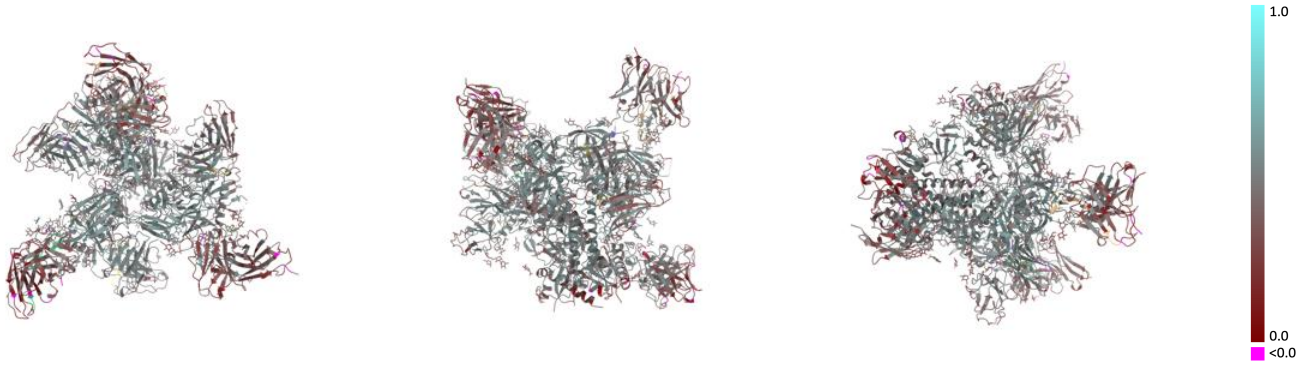
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.17 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

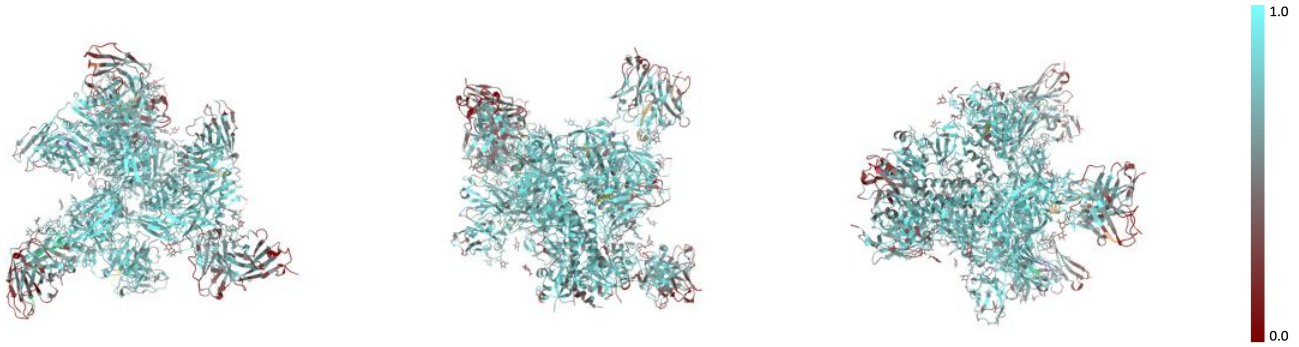
9.2 Q-score mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

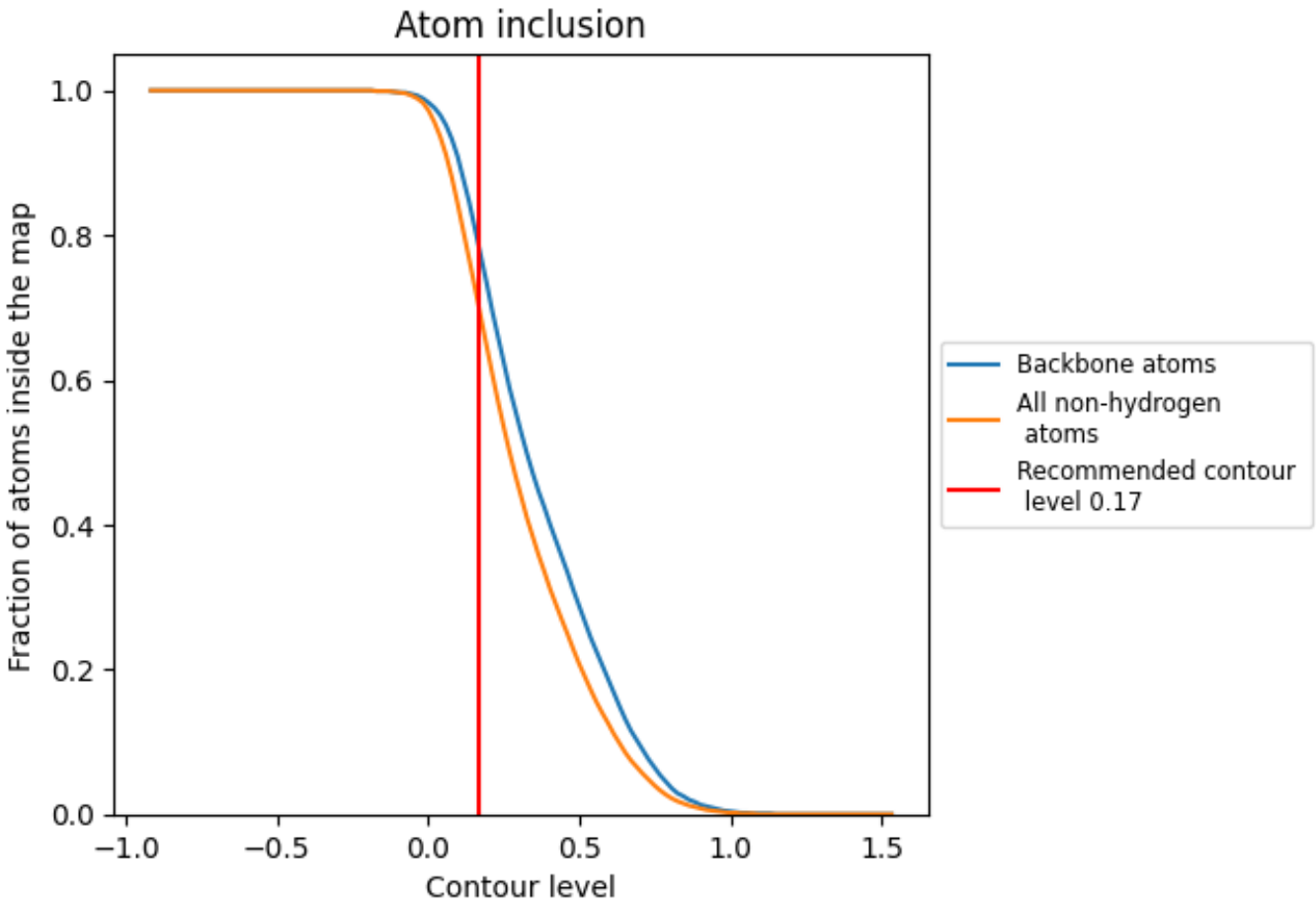
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.17).

9.4 Atom inclusion (i)



At the recommended contour level, 78% of all backbone atoms, 70% 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 (0.17) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6970	0.4390
A	0.7800	0.4950
B	0.7530	0.4730
C	0.7670	0.4780
D	0.5520	0.3530
E	0.5540	0.3650
F	0.5430	0.3520
G	0.5290	0.3480
H	0.6710	0.4030
I	0.5140	0.3080
J	0.5130	0.3310
K	0.7820	0.5000
L	0.5400	0.3490
M	0.6860	0.4300
N	0.7550	0.4840
O	0.6770	0.4230
P	0.7450	0.4710
Q	0.6290	0.4010
R	0.5900	0.3760
S	0.8000	0.4630
T	0.7500	0.4410
U	0.5690	0.3270
V	0.2500	0.3590
W	0.6070	0.4080
X	0.6070	0.4540
Y	0.6390	0.4730
Z	0.6510	0.4140
a	0.7240	0.4280
b	0.7140	0.4380
c	0.5420	0.3450
d	0.6430	0.4310
e	0.7440	0.4220
f	0.6560	0.3280
g	0.7070	0.4360
h	0.6430	0.3290
i	0.5280	0.3560