Full wwPDB EM Validation Report

Nov 16, 2022 – 11:48 PM EST

PDB ID	:	7L8E
EMDB ID	:	EMD-23231
Title	:	BG505 SOSIP.v5.2(7S) in complex with the polyclonal Fab pAbC-1 from animal Rh.33172 (Wk38 time point)
Authors	:	Antanasijevic, A.; Sewall, L.M.; Ward, A.B.
Deposited on	:	2020-12-31
Resolution	:	4.20 Å(reported)
Based on initial models	:	4KTE, 6VL5

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 (i)) were used in the production of this report:

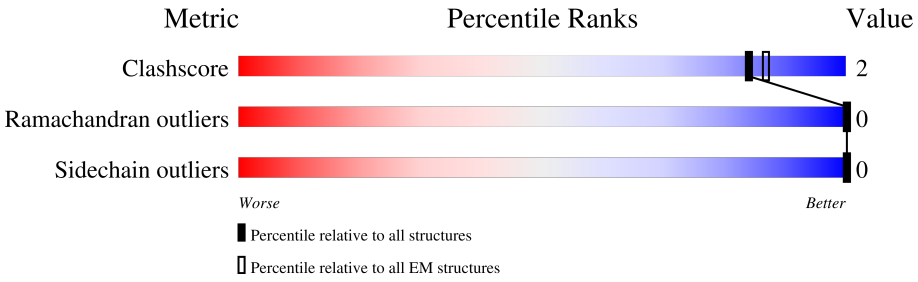
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al.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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 4.20 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	664	61% 6% 33%
1	B	664	17% 82%
1	C	664	64% 33%
1	D	664	18% 81%
1	E	664	61% 5% 34%
1	F	664	18% 81%
2	H	111	9% 93% 7%
3	L	99	25% 98%

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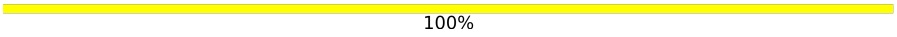
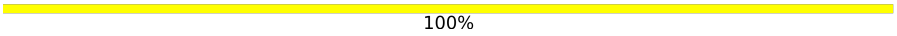
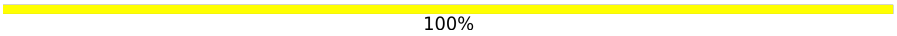
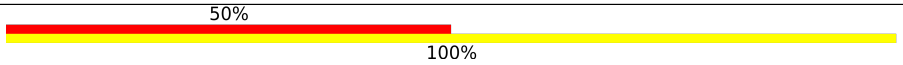
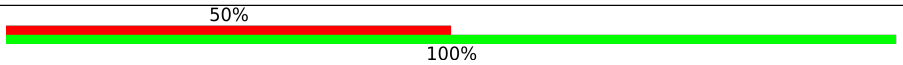
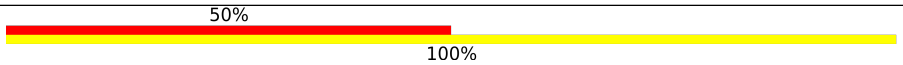
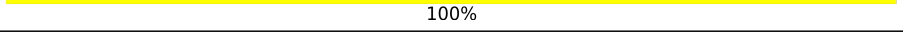
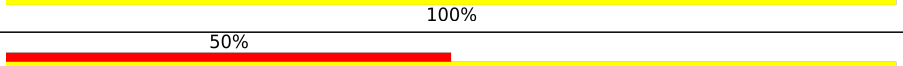
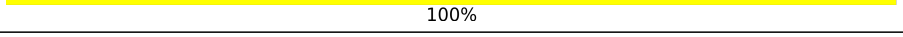
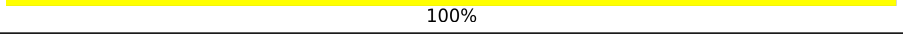
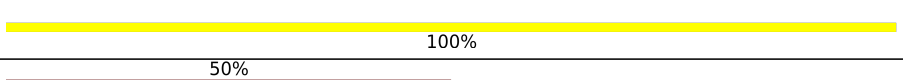
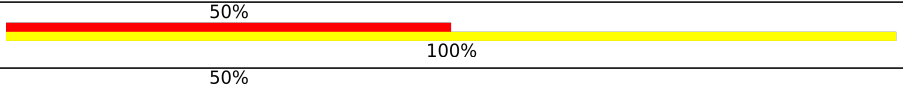
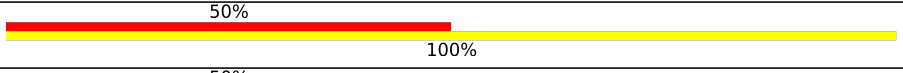
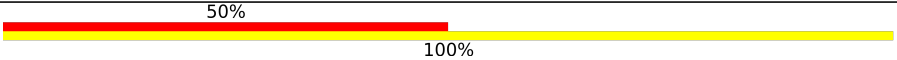
Mol	Chain	Length	Quality of chain
4	G	5	
4	Q	5	
4	X	5	
5	I	2	
5	J	2	
5	K	2	
5	M	2	
5	N	2	
5	O	2	
5	P	2	
5	R	2	
5	S	2	
5	T	2	
5	U	2	
5	V	2	
5	W	2	
5	Y	2	
5	Z	2	
5	a	2	
5	b	2	
5	c	2	

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 15827 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 Envelope glycoprotein gp160.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	C	444	Total	C	N	O	S	0	0
			3506	2204	618	656	28		
1	D	125	Total	C	N	O	S	0	0
			997	626	172	193	6		
1	E	441	Total	C	N	O	S	0	0
			3486	2192	615	651	28		
1	F	126	Total	C	N	O	S	0	0
			1003	629	173	195	6		
1	A	445	Total	C	N	O	S	0	0
			3514	2208	620	658	28		
1	B	121	Total	C	N	O	S	0	0
			968	609	168	185	6		

There are 330 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-1	MET	-	initiating methionine	UNP Q2N0S5
C	0	LYS	-	expression tag	UNP Q2N0S5
C	1	ARG	-	expression tag	UNP Q2N0S5
C	2	GLY	-	expression tag	UNP Q2N0S5
C	3	LEU	-	expression tag	UNP Q2N0S5
C	4	CYS	-	expression tag	UNP Q2N0S5
C	5	CYS	-	expression tag	UNP Q2N0S5
C	6	VAL	-	expression tag	UNP Q2N0S5
C	7	LEU	-	expression tag	UNP Q2N0S5
C	8	LEU	-	expression tag	UNP Q2N0S5
C	9	LEU	-	expression tag	UNP Q2N0S5
C	10	CYS	-	expression tag	UNP Q2N0S5
C	11	GLY	-	expression tag	UNP Q2N0S5
C	12	ALA	-	expression tag	UNP Q2N0S5
C	13	VAL	-	expression tag	UNP Q2N0S5
C	14	PHE	-	expression tag	UNP Q2N0S5
C	15	VAL	-	expression tag	UNP Q2N0S5
C	16	SER	-	expression tag	UNP Q2N0S5

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Chain	Residue	Modelled	Actual	Comment	Reference
C	17	PRO	-	expression tag	UNP Q2N0S5
C	18	SER	-	expression tag	UNP Q2N0S5
C	19	GLN	-	expression tag	UNP Q2N0S5
C	20	GLU	-	expression tag	UNP Q2N0S5
C	21	ILE	-	expression tag	UNP Q2N0S5
C	22	HIS	-	expression tag	UNP Q2N0S5
C	23	ALA	-	expression tag	UNP Q2N0S5
C	24	ARG	-	expression tag	UNP Q2N0S5
C	25	PHE	-	expression tag	UNP Q2N0S5
C	26	ARG	-	expression tag	UNP Q2N0S5
C	27	ARG	-	expression tag	UNP Q2N0S5
C	28	GLY	-	expression tag	UNP Q2N0S5
C	29	ALA	-	expression tag	UNP Q2N0S5
C	30	ARG	-	expression tag	UNP Q2N0S5
C	64	LYS	GLU	conflict	UNP Q2N0S5
C	73	CYS	ALA	conflict	UNP Q2N0S5
C	240	THR	PRO	conflict	UNP Q2N0S5
C	241	ASN	SER	conflict	UNP Q2N0S5
C	271	ILE	MET	conflict	UNP Q2N0S5
C	288	LEU	PHE	conflict	UNP Q2N0S5
C	290	GLU	THR	conflict	UNP Q2N0S5
C	291	SER	PRO	conflict	UNP Q2N0S5
C	304	VAL	ARG	conflict	UNP Q2N0S5
C	316	TRP	ALA	conflict	UNP Q2N0S5
C	319	TYR	ALA	conflict	UNP Q2N0S5
C	332	ASN	THR	conflict	UNP Q2N0S5
C	501	CYS	ALA	conflict	UNP Q2N0S5
C	510	ARG	GLU	conflict	UNP Q2N0S5
C	511	ARG	LYS	conflict	UNP Q2N0S5
C	520	SER	PHE	conflict	UNP Q2N0S5
C	560	PRO	ILE	conflict	UNP Q2N0S5
C	562	CYS	ALA	conflict	UNP Q2N0S5
C	569	ASP	LEU	conflict	UNP Q2N0S5
C	571	HIS	VAL	conflict	UNP Q2N0S5
C	586	HIS	ARG	conflict	UNP Q2N0S5
C	606	CYS	THR	conflict	UNP Q2N0S5
C	663	GLU	ALA	conflict	UNP Q2N0S5
D	1	MET	-	initiating methionine	UNP Q2N0S5
D	2	LYS	-	expression tag	UNP Q2N0S5
D	3	ARG	-	expression tag	UNP Q2N0S5
D	4	GLY	-	expression tag	UNP Q2N0S5
D	5	LEU	-	expression tag	UNP Q2N0S5

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Chain	Residue	Modelled	Actual	Comment	Reference
D	6	CYS	-	expression tag	UNP Q2N0S5
D	7	CYS	-	expression tag	UNP Q2N0S5
D	8	VAL	-	expression tag	UNP Q2N0S5
D	9	LEU	-	expression tag	UNP Q2N0S5
D	10	LEU	-	expression tag	UNP Q2N0S5
D	11	LEU	-	expression tag	UNP Q2N0S5
D	12	CYS	-	expression tag	UNP Q2N0S5
D	13	GLY	-	expression tag	UNP Q2N0S5
D	14	ALA	-	expression tag	UNP Q2N0S5
D	15	VAL	-	expression tag	UNP Q2N0S5
D	16	PHE	-	expression tag	UNP Q2N0S5
D	17	VAL	-	expression tag	UNP Q2N0S5
D	18	SER	-	expression tag	UNP Q2N0S5
D	19	PRO	-	expression tag	UNP Q2N0S5
D	20	SER	-	expression tag	UNP Q2N0S5
D	21	GLN	-	expression tag	UNP Q2N0S5
D	22	GLU	-	expression tag	UNP Q2N0S5
D	23	ILE	-	expression tag	UNP Q2N0S5
D	24	HIS	-	expression tag	UNP Q2N0S5
D	25	ALA	-	expression tag	UNP Q2N0S5
D	26	ARG	-	expression tag	UNP Q2N0S5
D	27	PHE	-	expression tag	UNP Q2N0S5
D	28	ARG	-	expression tag	UNP Q2N0S5
D	29	ARG	-	expression tag	UNP Q2N0S5
D	30	GLY	-	expression tag	UNP Q2N0S5
D	31	ALA	-	expression tag	UNP Q2N0S5
D	32	ARG	-	expression tag	UNP Q2N0S5
D	66	LYS	GLU	conflict	UNP Q2N0S5
D	75	CYS	ALA	conflict	UNP Q2N0S5
D	242	THR	PRO	conflict	UNP Q2N0S5
D	243	ASN	SER	conflict	UNP Q2N0S5
D	273	ILE	MET	conflict	UNP Q2N0S5
D	290	LEU	PHE	conflict	UNP Q2N0S5
D	292	GLU	THR	conflict	UNP Q2N0S5
D	293	SER	PRO	conflict	UNP Q2N0S5
D	306	VAL	ARG	conflict	UNP Q2N0S5
D	316	TRP	ALA	conflict	UNP Q2N0S5
D	319	TYR	ALA	conflict	UNP Q2N0S5
D	333	ASN	THR	conflict	UNP Q2N0S5
D	501	CYS	ALA	conflict	UNP Q2N0S5
D	509	ARG	GLU	conflict	UNP Q2N0S5
D	510	ARG	LYS	conflict	UNP Q2N0S5

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Chain	Residue	Modelled	Actual	Comment	Reference
D	519	SER	PHE	conflict	UNP Q2N0S5
D	559	PRO	ILE	conflict	UNP Q2N0S5
D	561	CYS	ALA	conflict	UNP Q2N0S5
D	568	ASP	LEU	conflict	UNP Q2N0S5
D	570	HIS	VAL	conflict	UNP Q2N0S5
D	585	HIS	ARG	conflict	UNP Q2N0S5
D	605	CYS	THR	conflict	UNP Q2N0S5
D	662	GLU	ALA	conflict	UNP Q2N0S5
E	-1	MET	-	initiating methionine	UNP Q2N0S5
E	0	LYS	-	expression tag	UNP Q2N0S5
E	1	ARG	-	expression tag	UNP Q2N0S5
E	2	GLY	-	expression tag	UNP Q2N0S5
E	3	LEU	-	expression tag	UNP Q2N0S5
E	4	CYS	-	expression tag	UNP Q2N0S5
E	5	CYS	-	expression tag	UNP Q2N0S5
E	6	VAL	-	expression tag	UNP Q2N0S5
E	7	LEU	-	expression tag	UNP Q2N0S5
E	8	LEU	-	expression tag	UNP Q2N0S5
E	9	LEU	-	expression tag	UNP Q2N0S5
E	10	CYS	-	expression tag	UNP Q2N0S5
E	11	GLY	-	expression tag	UNP Q2N0S5
E	12	ALA	-	expression tag	UNP Q2N0S5
E	13	VAL	-	expression tag	UNP Q2N0S5
E	14	PHE	-	expression tag	UNP Q2N0S5
E	15	VAL	-	expression tag	UNP Q2N0S5
E	16	SER	-	expression tag	UNP Q2N0S5
E	17	PRO	-	expression tag	UNP Q2N0S5
E	18	SER	-	expression tag	UNP Q2N0S5
E	19	GLN	-	expression tag	UNP Q2N0S5
E	20	GLU	-	expression tag	UNP Q2N0S5
E	21	ILE	-	expression tag	UNP Q2N0S5
E	22	HIS	-	expression tag	UNP Q2N0S5
E	23	ALA	-	expression tag	UNP Q2N0S5
E	24	ARG	-	expression tag	UNP Q2N0S5
E	25	PHE	-	expression tag	UNP Q2N0S5
E	26	ARG	-	expression tag	UNP Q2N0S5
E	27	ARG	-	expression tag	UNP Q2N0S5
E	28	GLY	-	expression tag	UNP Q2N0S5
E	29	ALA	-	expression tag	UNP Q2N0S5
E	30	ARG	-	expression tag	UNP Q2N0S5
E	64	LYS	GLU	conflict	UNP Q2N0S5
E	73	CYS	ALA	conflict	UNP Q2N0S5

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Chain	Residue	Modelled	Actual	Comment	Reference
E	240	THR	PRO	conflict	UNP Q2N0S5
E	241	ASN	SER	conflict	UNP Q2N0S5
E	271	ILE	MET	conflict	UNP Q2N0S5
E	288	LEU	PHE	conflict	UNP Q2N0S5
E	290	GLU	THR	conflict	UNP Q2N0S5
E	291	SER	PRO	conflict	UNP Q2N0S5
E	304	VAL	ARG	conflict	UNP Q2N0S5
E	316	TRP	ALA	conflict	UNP Q2N0S5
E	319	TYR	ALA	conflict	UNP Q2N0S5
E	332	ASN	THR	conflict	UNP Q2N0S5
E	501	CYS	ALA	conflict	UNP Q2N0S5
E	509	ARG	GLU	conflict	UNP Q2N0S5
E	510	ARG	LYS	conflict	UNP Q2N0S5
E	519	SER	PHE	conflict	UNP Q2N0S5
E	559	PRO	ILE	conflict	UNP Q2N0S5
E	561	CYS	ALA	conflict	UNP Q2N0S5
E	568	ASP	LEU	conflict	UNP Q2N0S5
E	570	HIS	VAL	conflict	UNP Q2N0S5
E	585	HIS	ARG	conflict	UNP Q2N0S5
E	605	CYS	THR	conflict	UNP Q2N0S5
E	662	GLU	ALA	conflict	UNP Q2N0S5
F	1	MET	-	initiating methionine	UNP Q2N0S5
F	2	LYS	-	expression tag	UNP Q2N0S5
F	3	ARG	-	expression tag	UNP Q2N0S5
F	4	GLY	-	expression tag	UNP Q2N0S5
F	5	LEU	-	expression tag	UNP Q2N0S5
F	6	CYS	-	expression tag	UNP Q2N0S5
F	7	CYS	-	expression tag	UNP Q2N0S5
F	8	VAL	-	expression tag	UNP Q2N0S5
F	9	LEU	-	expression tag	UNP Q2N0S5
F	10	LEU	-	expression tag	UNP Q2N0S5
F	11	LEU	-	expression tag	UNP Q2N0S5
F	12	CYS	-	expression tag	UNP Q2N0S5
F	13	GLY	-	expression tag	UNP Q2N0S5
F	14	ALA	-	expression tag	UNP Q2N0S5
F	15	VAL	-	expression tag	UNP Q2N0S5
F	16	PHE	-	expression tag	UNP Q2N0S5
F	17	VAL	-	expression tag	UNP Q2N0S5
F	18	SER	-	expression tag	UNP Q2N0S5
F	19	PRO	-	expression tag	UNP Q2N0S5
F	20	SER	-	expression tag	UNP Q2N0S5
F	21	GLN	-	expression tag	UNP Q2N0S5

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Chain	Residue	Modelled	Actual	Comment	Reference
F	22	GLU	-	expression tag	UNP Q2N0S5
F	23	ILE	-	expression tag	UNP Q2N0S5
F	24	HIS	-	expression tag	UNP Q2N0S5
F	25	ALA	-	expression tag	UNP Q2N0S5
F	26	ARG	-	expression tag	UNP Q2N0S5
F	27	PHE	-	expression tag	UNP Q2N0S5
F	28	ARG	-	expression tag	UNP Q2N0S5
F	29	ARG	-	expression tag	UNP Q2N0S5
F	30	GLY	-	expression tag	UNP Q2N0S5
F	31	ALA	-	expression tag	UNP Q2N0S5
F	32	ARG	-	expression tag	UNP Q2N0S5
F	66	LYS	GLU	conflict	UNP Q2N0S5
F	75	CYS	ALA	conflict	UNP Q2N0S5
F	242	THR	PRO	conflict	UNP Q2N0S5
F	243	ASN	SER	conflict	UNP Q2N0S5
F	273	ILE	MET	conflict	UNP Q2N0S5
F	290	LEU	PHE	conflict	UNP Q2N0S5
F	292	GLU	THR	conflict	UNP Q2N0S5
F	293	SER	PRO	conflict	UNP Q2N0S5
F	306	VAL	ARG	conflict	UNP Q2N0S5
F	316	TRP	ALA	conflict	UNP Q2N0S5
F	319	TYR	ALA	conflict	UNP Q2N0S5
F	333	ASN	THR	conflict	UNP Q2N0S5
F	501	CYS	ALA	conflict	UNP Q2N0S5
F	509	ARG	GLU	conflict	UNP Q2N0S5
F	510	ARG	LYS	conflict	UNP Q2N0S5
F	519	SER	PHE	conflict	UNP Q2N0S5
F	559	PRO	ILE	conflict	UNP Q2N0S5
F	561	CYS	ALA	conflict	UNP Q2N0S5
F	568	ASP	LEU	conflict	UNP Q2N0S5
F	570	HIS	VAL	conflict	UNP Q2N0S5
F	585	HIS	ARG	conflict	UNP Q2N0S5
F	605	CYS	THR	conflict	UNP Q2N0S5
F	662	GLU	ALA	conflict	UNP Q2N0S5
A	-1	MET	-	initiating methionine	UNP Q2N0S5
A	0	LYS	-	expression tag	UNP Q2N0S5
A	1	ARG	-	expression tag	UNP Q2N0S5
A	2	GLY	-	expression tag	UNP Q2N0S5
A	3	LEU	-	expression tag	UNP Q2N0S5
A	4	CYS	-	expression tag	UNP Q2N0S5
A	5	CYS	-	expression tag	UNP Q2N0S5
A	6	VAL	-	expression tag	UNP Q2N0S5

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Chain	Residue	Modelled	Actual	Comment	Reference
A	7	LEU	-	expression tag	UNP Q2N0S5
A	8	LEU	-	expression tag	UNP Q2N0S5
A	9	LEU	-	expression tag	UNP Q2N0S5
A	10	CYS	-	expression tag	UNP Q2N0S5
A	11	GLY	-	expression tag	UNP Q2N0S5
A	12	ALA	-	expression tag	UNP Q2N0S5
A	13	VAL	-	expression tag	UNP Q2N0S5
A	14	PHE	-	expression tag	UNP Q2N0S5
A	15	VAL	-	expression tag	UNP Q2N0S5
A	16	SER	-	expression tag	UNP Q2N0S5
A	17	PRO	-	expression tag	UNP Q2N0S5
A	18	SER	-	expression tag	UNP Q2N0S5
A	19	GLN	-	expression tag	UNP Q2N0S5
A	20	GLU	-	expression tag	UNP Q2N0S5
A	21	ILE	-	expression tag	UNP Q2N0S5
A	22	HIS	-	expression tag	UNP Q2N0S5
A	23	ALA	-	expression tag	UNP Q2N0S5
A	24	ARG	-	expression tag	UNP Q2N0S5
A	25	PHE	-	expression tag	UNP Q2N0S5
A	26	ARG	-	expression tag	UNP Q2N0S5
A	27	ARG	-	expression tag	UNP Q2N0S5
A	28	GLY	-	expression tag	UNP Q2N0S5
A	29	ALA	-	expression tag	UNP Q2N0S5
A	30	ARG	-	expression tag	UNP Q2N0S5
A	64	LYS	GLU	conflict	UNP Q2N0S5
A	73	CYS	ALA	conflict	UNP Q2N0S5
A	240	THR	PRO	conflict	UNP Q2N0S5
A	241	ASN	SER	conflict	UNP Q2N0S5
A	271	ILE	MET	conflict	UNP Q2N0S5
A	288	LEU	PHE	conflict	UNP Q2N0S5
A	290	GLU	THR	conflict	UNP Q2N0S5
A	291	SER	PRO	conflict	UNP Q2N0S5
A	304	VAL	ARG	conflict	UNP Q2N0S5
A	316	TRP	ALA	conflict	UNP Q2N0S5
A	319	TYR	ALA	conflict	UNP Q2N0S5
A	332	ASN	THR	conflict	UNP Q2N0S5
A	501	CYS	ALA	conflict	UNP Q2N0S5
A	509	ARG	GLU	conflict	UNP Q2N0S5
A	510	ARG	LYS	conflict	UNP Q2N0S5
A	519	SER	PHE	conflict	UNP Q2N0S5
A	559	PRO	ILE	conflict	UNP Q2N0S5
A	561	CYS	ALA	conflict	UNP Q2N0S5

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Chain	Residue	Modelled	Actual	Comment	Reference
A	568	ASP	LEU	conflict	UNP Q2N0S5
A	570	HIS	VAL	conflict	UNP Q2N0S5
A	585	HIS	ARG	conflict	UNP Q2N0S5
A	605	CYS	THR	conflict	UNP Q2N0S5
A	662	GLU	ALA	conflict	UNP Q2N0S5
B	1	MET	-	initiating methionine	UNP Q2N0S5
B	2	LYS	-	expression tag	UNP Q2N0S5
B	3	ARG	-	expression tag	UNP Q2N0S5
B	4	GLY	-	expression tag	UNP Q2N0S5
B	5	LEU	-	expression tag	UNP Q2N0S5
B	6	CYS	-	expression tag	UNP Q2N0S5
B	7	CYS	-	expression tag	UNP Q2N0S5
B	8	VAL	-	expression tag	UNP Q2N0S5
B	9	LEU	-	expression tag	UNP Q2N0S5
B	10	LEU	-	expression tag	UNP Q2N0S5
B	11	LEU	-	expression tag	UNP Q2N0S5
B	12	CYS	-	expression tag	UNP Q2N0S5
B	13	GLY	-	expression tag	UNP Q2N0S5
B	14	ALA	-	expression tag	UNP Q2N0S5
B	15	VAL	-	expression tag	UNP Q2N0S5
B	16	PHE	-	expression tag	UNP Q2N0S5
B	17	VAL	-	expression tag	UNP Q2N0S5
B	18	SER	-	expression tag	UNP Q2N0S5
B	19	PRO	-	expression tag	UNP Q2N0S5
B	20	SER	-	expression tag	UNP Q2N0S5
B	21	GLN	-	expression tag	UNP Q2N0S5
B	22	GLU	-	expression tag	UNP Q2N0S5
B	23	ILE	-	expression tag	UNP Q2N0S5
B	24	HIS	-	expression tag	UNP Q2N0S5
B	25	ALA	-	expression tag	UNP Q2N0S5
B	26	ARG	-	expression tag	UNP Q2N0S5
B	27	PHE	-	expression tag	UNP Q2N0S5
B	28	ARG	-	expression tag	UNP Q2N0S5
B	29	ARG	-	expression tag	UNP Q2N0S5
B	30	GLY	-	expression tag	UNP Q2N0S5
B	31	ALA	-	expression tag	UNP Q2N0S5
B	32	ARG	-	expression tag	UNP Q2N0S5
B	66	LYS	GLU	conflict	UNP Q2N0S5
B	75	CYS	ALA	conflict	UNP Q2N0S5
B	242	THR	PRO	conflict	UNP Q2N0S5
B	243	ASN	SER	conflict	UNP Q2N0S5
B	273	ILE	MET	conflict	UNP Q2N0S5

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Chain	Residue	Modelled	Actual	Comment	Reference
B	290	LEU	PHE	conflict	UNP Q2N0S5
B	292	GLU	THR	conflict	UNP Q2N0S5
B	293	SER	PRO	conflict	UNP Q2N0S5
B	306	VAL	ARG	conflict	UNP Q2N0S5
B	316	TRP	ALA	conflict	UNP Q2N0S5
B	319	TYR	ALA	conflict	UNP Q2N0S5
B	333	ASN	THR	conflict	UNP Q2N0S5
B	501	CYS	ALA	conflict	UNP Q2N0S5
B	509	ARG	GLU	conflict	UNP Q2N0S5
B	510	ARG	LYS	conflict	UNP Q2N0S5
B	519	SER	PHE	conflict	UNP Q2N0S5
B	559	PRO	ILE	conflict	UNP Q2N0S5
B	561	CYS	ALA	conflict	UNP Q2N0S5
B	568	ASP	LEU	conflict	UNP Q2N0S5
B	570	HIS	VAL	conflict	UNP Q2N0S5
B	585	HIS	ARG	conflict	UNP Q2N0S5
B	605	CYS	THR	conflict	UNP Q2N0S5
B	662	GLU	ALA	conflict	UNP Q2N0S5

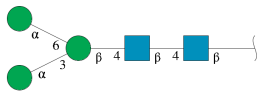
- Molecule 2 is a protein called Rh.33172 pAbC-1 Heavy Chain.

Mol	Chain	Residues	Atoms				AltConf	Trace
2	H	111	Total	C	N	O	0	0
			555	333	111	111		

- Molecule 3 is a protein called Rh.33172 pAbC-1 Light Chain.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	L	99	Total	C	N	O	0	0
			495	297	99	99		

- Molecule 4 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
4	G	5	Total	C	N	O	0	0
			61	34	2	25		

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Mol	Chain	Residues	Atoms	AltConf	Trace
4	Q	5	Total C N O 61 34 2 25	0	0
4	X	5	Total C N O 61 34 2 25	0	0

- Molecule 5 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
5	I	2	Total C N O 28 16 2 10	0	0
5	J	2	Total C N O 28 16 2 10	0	0
5	K	2	Total C N O 28 16 2 10	0	0
5	M	2	Total C N O 28 16 2 10	0	0
5	N	2	Total C N O 28 16 2 10	0	0
5	O	2	Total C N O 28 16 2 10	0	0
5	P	2	Total C N O 28 16 2 10	0	0
5	R	2	Total C N O 28 16 2 10	0	0
5	S	2	Total C N O 28 16 2 10	0	0
5	T	2	Total C N O 28 16 2 10	0	0
5	U	2	Total C N O 28 16 2 10	0	0
5	V	2	Total C N O 28 16 2 10	0	0
5	W	2	Total C N O 28 16 2 10	0	0
5	Y	2	Total C N O 28 16 2 10	0	0
5	Z	2	Total C N O 28 16 2 10	0	0

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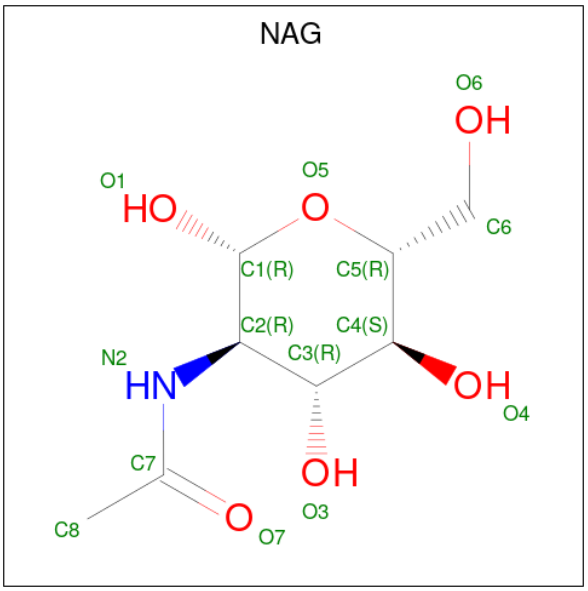
Mol	Chain	Residues	Atoms	AltConf	Trace
5	a	2	Total C N O 28 16 2 10	0	0
5	b	2	Total C N O 28 16 2 10	0	0
5	c	2	Total C N O 28 16 2 10	0	0

- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms	AltConf
6	C	1	Total C N O 154 88 11 55	0
6	C	1	Total C N O 154 88 11 55	0
6	C	1	Total C N O 154 88 11 55	0
6	C	1	Total C N O 154 88 11 55	0
6	C	1	Total C N O 154 88 11 55	0
6	C	1	Total C N O 154 88 11 55	0
6	C	1	Total C N O 154 88 11 55	0
6	C	1	Total C N O 154 88 11 55	0

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Mol	Chain	Residues	Atoms	AltConf
6	C	1	Total C N O 154 88 11 55	0
6	C	1	Total C N O 154 88 11 55	0
6	C	1	Total C N O 154 88 11 55	0
6	D	1	Total C N O 28 16 2 10	0
6	D	1	Total C N O 28 16 2 10	0
6	E	1	Total C N O 182 104 13 65	0
6	E	1	Total C N O 182 104 13 65	0
6	E	1	Total C N O 182 104 13 65	0
6	E	1	Total C N O 182 104 13 65	0
6	E	1	Total C N O 182 104 13 65	0
6	E	1	Total C N O 182 104 13 65	0
6	E	1	Total C N O 182 104 13 65	0
6	E	1	Total C N O 182 104 13 65	0
6	E	1	Total C N O 182 104 13 65	0
6	E	1	Total C N O 182 104 13 65	0
6	E	1	Total C N O 182 104 13 65	0
6	E	1	Total C N O 182 104 13 65	0
6	E	1	Total C N O 182 104 13 65	0
6	F	1	Total C N O 42 24 3 15	0
6	F	1	Total C N O 42 24 3 15	0
6	F	1	Total C N O 42 24 3 15	0

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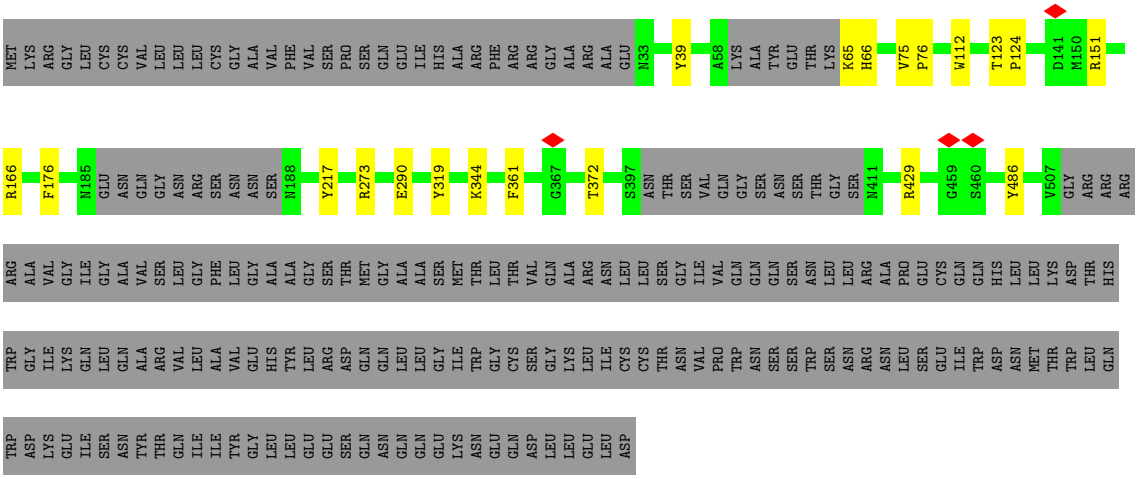
Mol	Chain	Residues	Atoms				AltConf
6	A	1	Total 168	C 96	N 12	O 60	0
6	A	1	Total 168	C 96	N 12	O 60	0
6	A	1	Total 168	C 96	N 12	O 60	0
6	A	1	Total 168	C 96	N 12	O 60	0
6	A	1	Total 168	C 96	N 12	O 60	0
6	A	1	Total 168	C 96	N 12	O 60	0
6	A	1	Total 168	C 96	N 12	O 60	0
6	A	1	Total 168	C 96	N 12	O 60	0
6	A	1	Total 168	C 96	N 12	O 60	0
6	A	1	Total 168	C 96	N 12	O 60	0
6	A	1	Total 168	C 96	N 12	O 60	0
6	A	1	Total 168	C 96	N 12	O 60	0
6	B	1	Total 42	C 24	N 3	O 15	0
6	B	1	Total 42	C 24	N 3	O 15	0
6	B	1	Total 42	C 24	N 3	O 15	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.

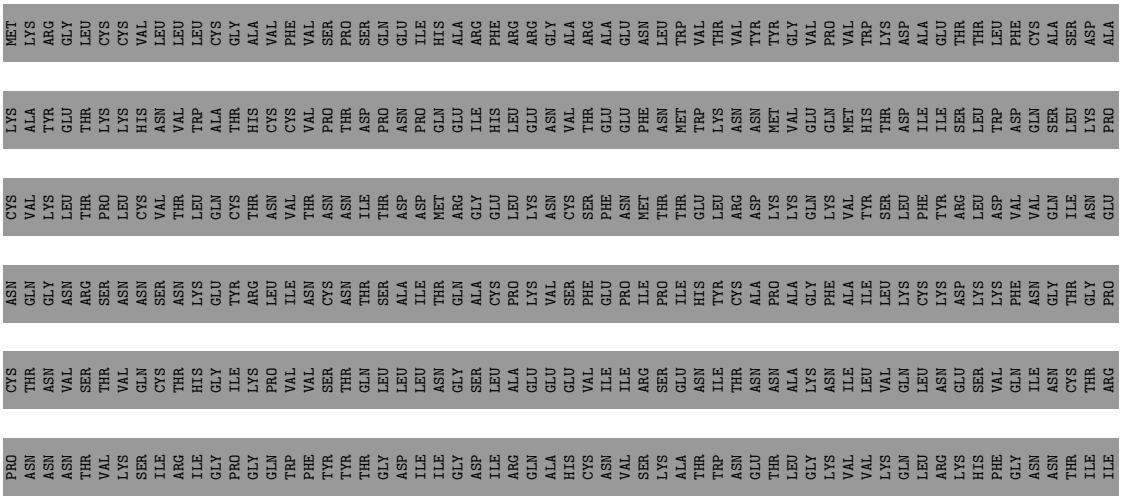
• Molecule 1: Envelope glycoprotein gp160

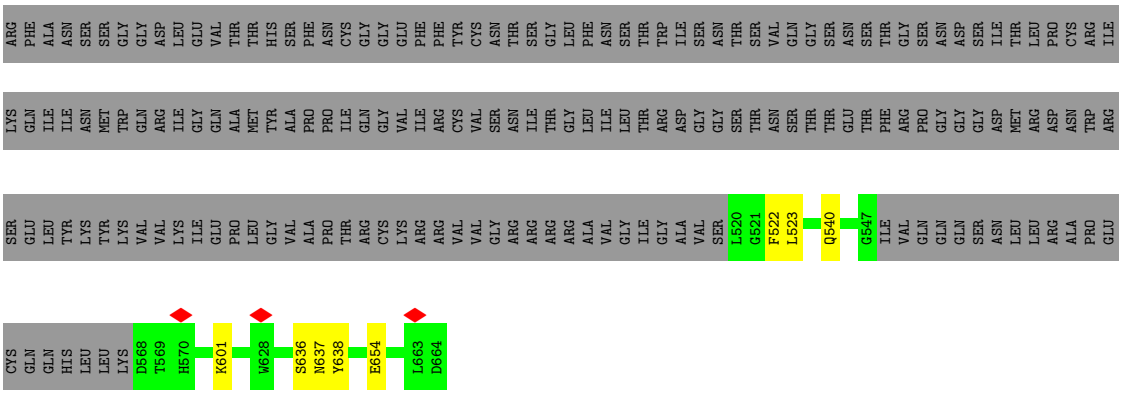
Chain C:



• Molecule 1: Envelope glycoprotein gp160

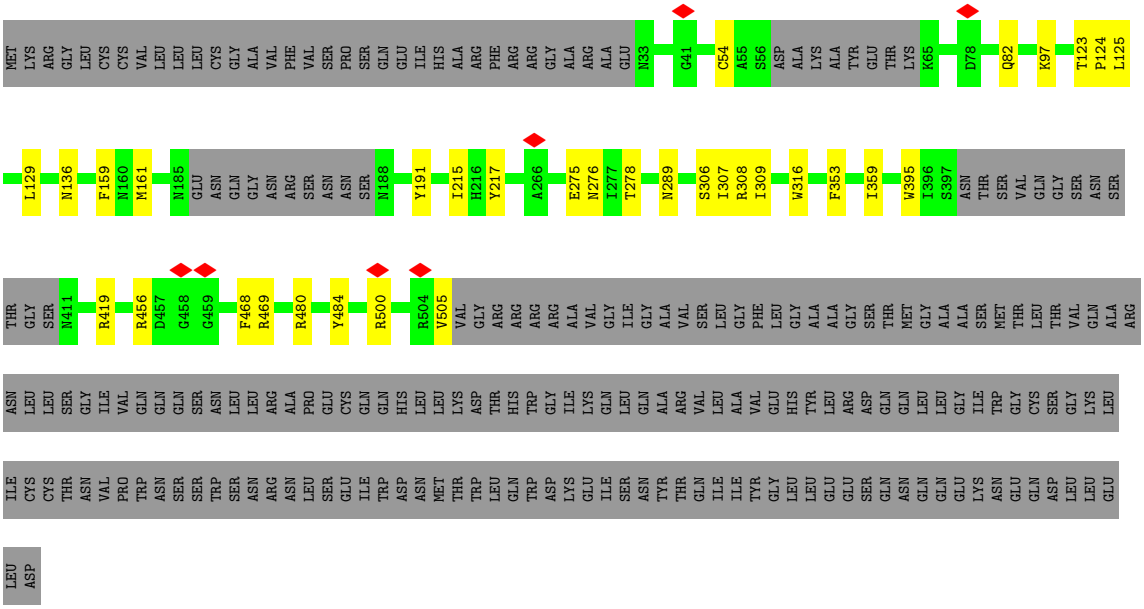
Chain D:





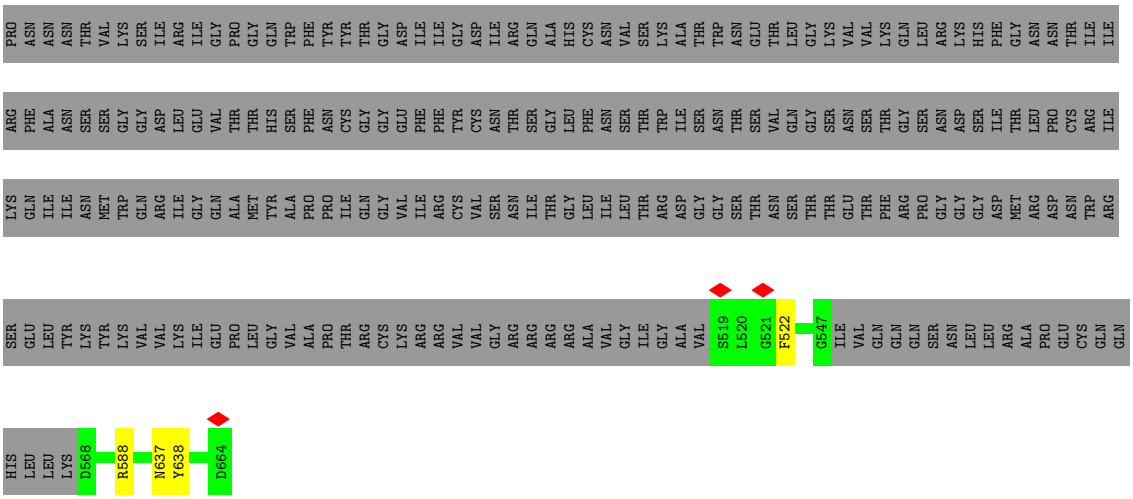
• Molecule 1: Envelope glycoprotein gp160

Chain E:



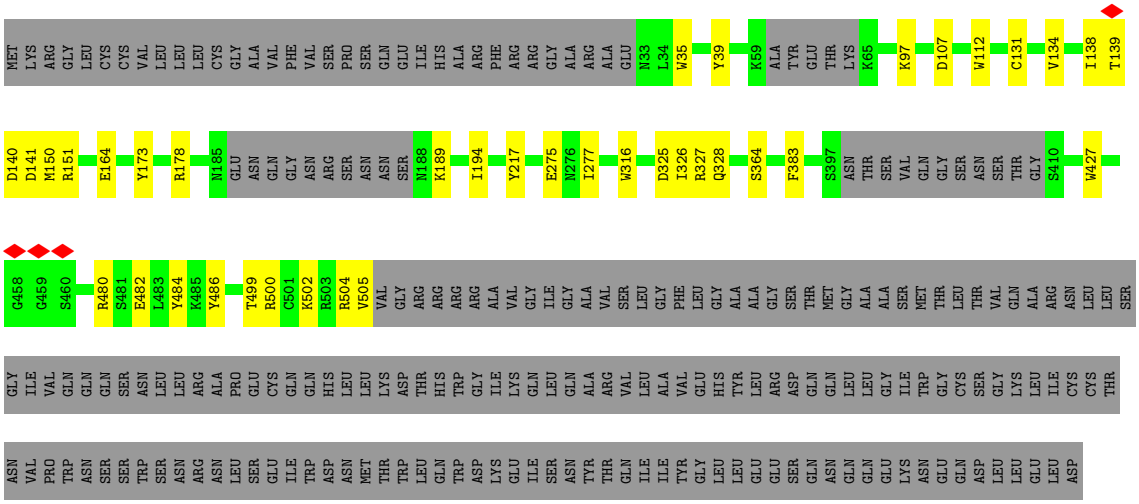
• Molecule 1: Envelope glycoprotein gp160

Chain F:



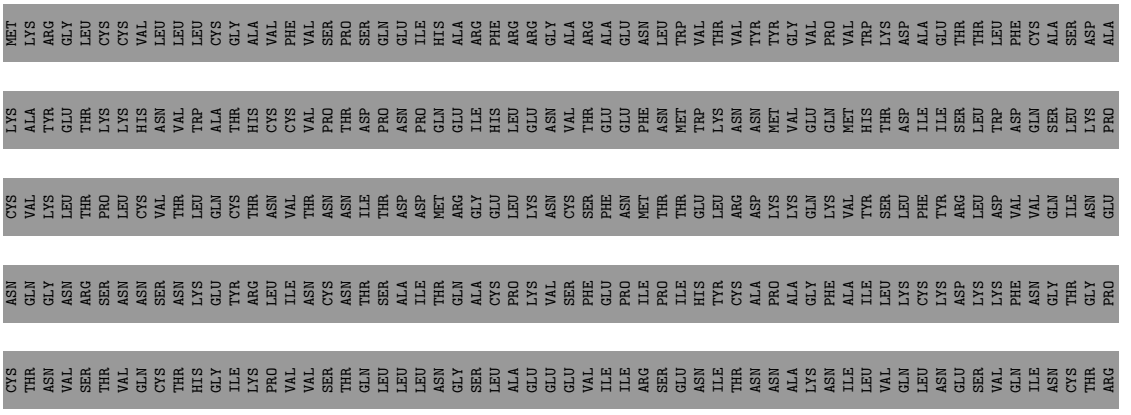
• Molecule 1: Envelope glycoprotein gp160

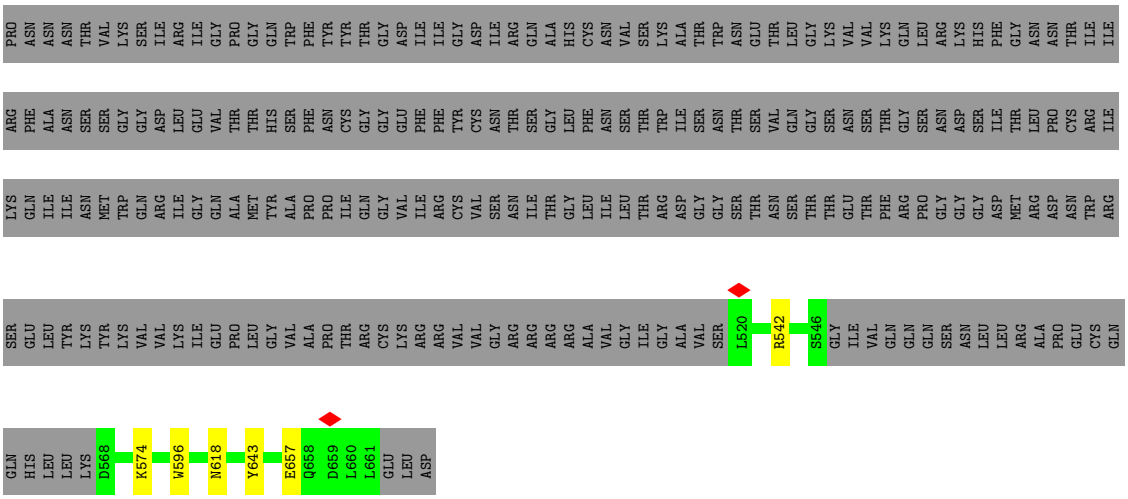
Chain A:



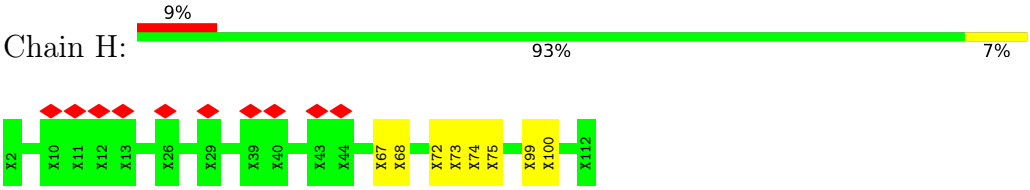
• Molecule 1: Envelope glycoprotein gp160

Chain B:

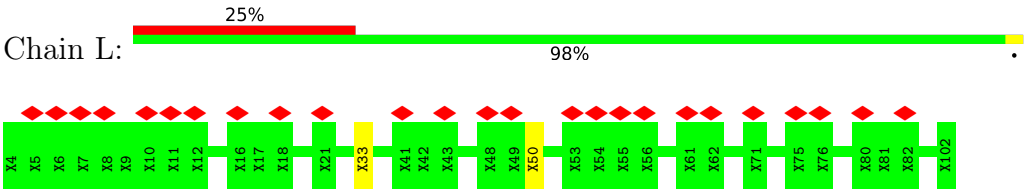




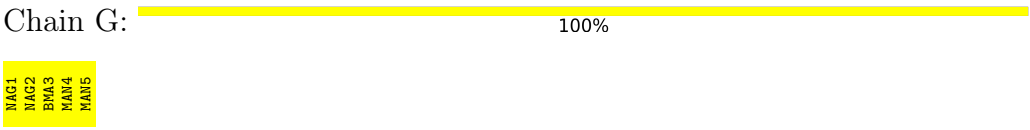
• Molecule 2: Rh.33172 pAbC-1 Heavy Chain



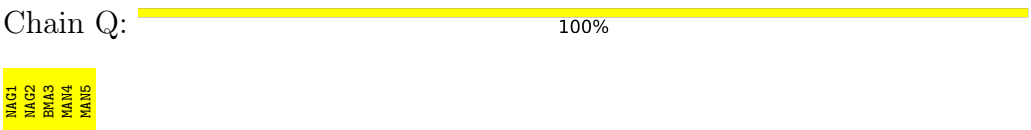
• Molecule 3: Rh.33172 pAbC-1 Light Chain



• Molecule 4: 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



• Molecule 4: 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

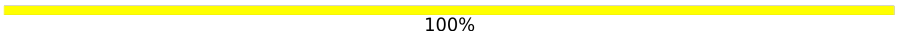


• Molecule 4: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain X:

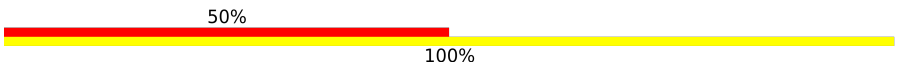
• Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain I:



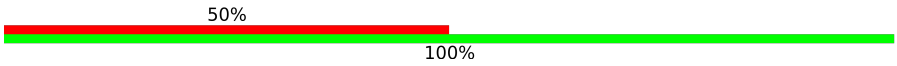
• Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain J:



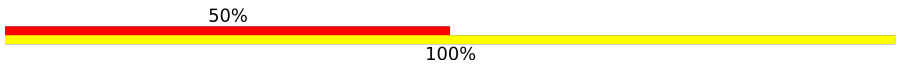
• Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain K:



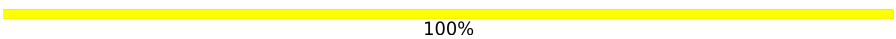
• Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain M:



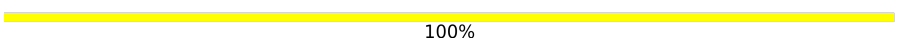
• Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain N:



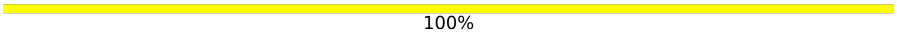
• Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain O:



• Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain P:

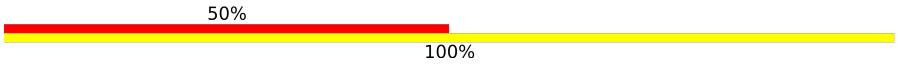


• Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain R:

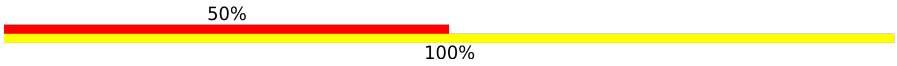
• Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain S:



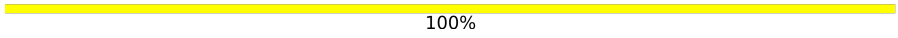
• Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain T:



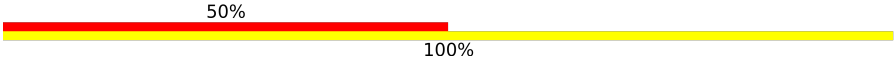
• Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain U:



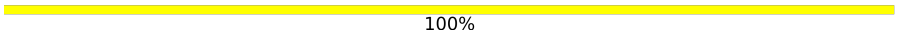
• Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain V:



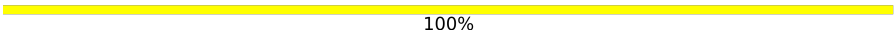
• Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain W:



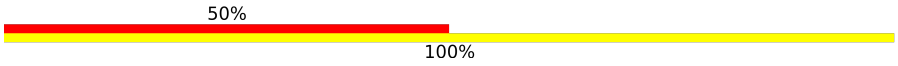
• Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Y:



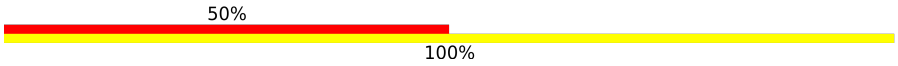
• Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Z:



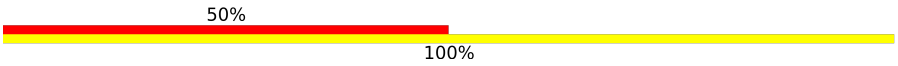
• Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain a:



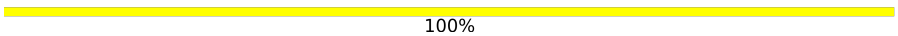
• Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain b:



• Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain c:




NAG1
NAG2

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	31914	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50.7	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	1600	Depositor
Magnification	29000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.069	Depositor
Minimum map value	-0.038	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.015	Depositor
Map size (Å)	329.59998, 329.59998, 329.59998	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.03, 1.03, 1.03	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: BMA, NAG, MAN

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	1.08	10/3586 (0.3%)	0.90	8/4868 (0.2%)
1	B	1.08	1/987 (0.1%)	0.83	1/1339 (0.1%)
1	C	1.09	7/3578 (0.2%)	0.94	7/4859 (0.1%)
1	D	1.10	1/1016 (0.1%)	0.93	2/1378 (0.1%)
1	E	1.10	7/3558 (0.2%)	0.91	6/4831 (0.1%)
1	F	1.05	1/1022 (0.1%)	0.80	2/1386 (0.1%)
All	All	1.09	27/13747 (0.2%)	0.90	26/18661 (0.1%)

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	319	TYR	CB-CG	-10.96	1.35	1.51
1	E	484	TYR	CB-CG	-9.40	1.37	1.51
1	E	484	TYR	CG-CD1	-7.46	1.29	1.39
1	C	217	TYR	CB-CG	-6.93	1.41	1.51
1	A	173	TYR	CB-CG	-6.73	1.41	1.51
1	A	112	TRP	CB-CG	-6.48	1.38	1.50
1	E	191	TYR	CB-CG	-6.25	1.42	1.51
1	A	316	TRP	CB-CG	-6.22	1.39	1.50
1	C	39	TYR	CB-CG	-6.18	1.42	1.51
1	A	39	TYR	CB-CG	-6.09	1.42	1.51
1	A	217	TYR	CB-CG	-5.93	1.42	1.51
1	A	427	TRP	CB-CG	-5.89	1.39	1.50
1	C	361	PHE	CB-CG	-5.72	1.41	1.51
1	C	112	TRP	CB-CG	-5.62	1.40	1.50
1	E	316	TRP	CB-CG	-5.50	1.40	1.50
1	E	484	TYR	CD1-CE1	-5.47	1.31	1.39
1	B	596	TRP	CB-CG	-5.34	1.40	1.50
1	C	176	PHE	CB-CG	-5.31	1.42	1.51
1	A	505	VAL	CB-CG2	5.29	1.64	1.52
1	D	654	GLU	CD-OE1	-5.28	1.19	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	191	TYR	CG-CD1	-5.19	1.32	1.39
1	E	505	VAL	CB-CG2	5.13	1.63	1.52
1	C	319	TYR	CD1-CE1	-5.13	1.31	1.39
1	A	482	GLU	CD-OE2	-5.11	1.20	1.25
1	A	164	GLU	CD-OE2	-5.11	1.20	1.25
1	A	486	TYR	CB-CG	-5.08	1.44	1.51
1	F	522	PHE	CB-CG	-5.02	1.42	1.51

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	178	ARG	NE-CZ-NH2	-8.76	115.92	120.30
1	C	429	ARG	NE-CZ-NH1	8.51	124.56	120.30
1	E	500	ARG	NE-CZ-NH2	-7.71	116.44	120.30
1	D	637	ASN	CB-CA-C	-7.65	95.10	110.40
1	E	480	ARG	NE-CZ-NH2	-7.38	116.61	120.30
1	A	173	TYR	CB-CG-CD2	-7.14	116.72	121.00
1	E	217	TYR	CB-CG-CD2	-6.63	117.02	121.00
1	E	419	ARG	NE-CZ-NH2	-6.36	117.12	120.30
1	C	166	ARG	NE-CZ-NH2	-6.28	117.16	120.30
1	D	638	TYR	N-CA-CB	6.01	121.42	110.60
1	A	504	ARG	NE-CZ-NH2	-5.78	117.41	120.30
1	C	151	ARG	NE-CZ-NH2	-5.74	117.43	120.30
1	A	480	ARG	NE-CZ-NH1	5.68	123.14	120.30
1	C	217	TYR	CB-CG-CD2	-5.57	117.66	121.00
1	A	39	TYR	CB-CG-CD2	-5.54	117.67	121.00
1	A	484	TYR	CB-CG-CD1	-5.54	117.68	121.00
1	B	643	TYR	CB-CG-CD2	-5.50	117.70	121.00
1	C	273	ARG	NE-CZ-NH2	-5.49	117.56	120.30
1	C	486	TYR	CB-CG-CD1	-5.40	117.76	121.00
1	C	39	TYR	CB-CG-CD1	-5.27	117.84	121.00
1	F	588	ARG	NE-CZ-NH2	5.24	122.92	120.30
1	A	383	PHE	CB-CG-CD1	5.22	124.46	120.80
1	E	469	ARG	NE-CZ-NH1	5.14	122.87	120.30
1	E	469	ARG	NE-CZ-NH2	-5.12	117.74	120.30
1	A	486	TYR	CB-CG-CD1	-5.03	117.98	121.00
1	F	638	TYR	CB-CG-CD1	-5.02	117.99	121.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3514	0	3451	23	0
1	B	968	0	930	4	0
1	C	3506	0	3441	5	0
1	D	997	0	955	4	0
1	E	3486	0	3422	22	0
1	F	1003	0	959	1	0
2	H	555	0	127	4	0
3	L	495	0	120	1	0
4	G	61	0	52	0	0
4	Q	61	0	52	0	0
4	X	61	0	52	1	0
5	I	28	0	25	0	0
5	J	28	0	25	0	0
5	K	28	0	25	0	0
5	M	28	0	25	0	0
5	N	28	0	25	0	0
5	O	28	0	25	0	0
5	P	28	0	25	0	0
5	R	28	0	25	0	0
5	S	28	0	25	0	0
5	T	28	0	25	0	0
5	U	28	0	25	0	0
5	V	28	0	25	0	0
5	W	28	0	25	0	0
5	Y	28	0	25	0	0
5	Z	28	0	25	4	0
5	a	28	0	25	0	0
5	b	28	0	25	0	0
5	c	28	0	25	0	0
6	A	168	0	156	2	0
6	B	42	0	39	1	0
6	C	154	0	143	4	0
6	D	28	0	26	1	0
6	E	182	0	169	4	0
6	F	42	0	39	0	0
All	All	15827	0	14583	69	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 (69) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:131:CYS:O	1:A:189:LYS:HD3	1.93	0.69
1:A:139:THR:O	1:A:151:ARG:HB2	1.98	0.63
1:C:65:LYS:HG3	1:C:66:HIS:CD2	2.34	0.63
5:Z:1:NAG:H3	5:Z:1:NAG:H83	1.80	0.63
5:Z:1:NAG:H3	5:Z:1:NAG:C8	2.30	0.61
1:E:82:GLN:HG2	1:E:82:GLN:O	2.01	0.61
1:A:364:SER:O	6:A:705:NAG:H82	2.01	0.59
1:A:35:TRP:CZ2	1:A:502:LYS:HD2	2.40	0.57
1:A:194:ILE:HD11	5:Z:2:NAG:H83	1.86	0.57
1:A:138:ILE:HG22	1:A:139:THR:O	2.06	0.56
1:E:125:LEU:HG	1:E:125:LEU:O	2.05	0.56
1:B:618:ASN:HB3	6:B:702:NAG:H83	1.86	0.55
1:A:150:MET:O	1:A:150:MET:HG3	2.06	0.55
1:E:306:SER:O	1:E:307:ILE:HD13	2.06	0.55
1:A:277:ILE:HG13	6:A:706:NAG:H81	1.89	0.55
5:Z:1:NAG:C1	5:Z:1:NAG:H82	2.36	0.55
1:E:289:ASN:O	6:E:709:NAG:H82	2.07	0.54
1:E:136:ASN:HB3	6:E:713:NAG:H82	1.90	0.54
1:E:353:PHE:CE1	1:E:456:ARG:HD3	2.45	0.52
1:E:307:ILE:HG22	1:E:308:ARG:N	2.24	0.52
1:E:359:ILE:HD12	1:E:468:PHE:HE1	1.74	0.52
1:D:522:PHE:CD2	1:D:523:LEU:HG	2.46	0.51
1:E:395:TRP:CE3	6:E:710:NAG:H61	2.46	0.51
1:A:134:VAL:HG12	1:A:138:ILE:CD1	2.40	0.51
1:E:161:MET:HE1	1:E:309:ILE:HG21	1.92	0.51
1:E:123:THR:N	1:E:124:PRO:CD	2.74	0.51
4:X:1:NAG:O7	4:X:1:NAG:O3	2.25	0.51
1:A:325:ASP:OD2	1:A:327:ARG:NH1	2.44	0.51
1:A:134:VAL:HG12	1:A:138:ILE:HD12	1.93	0.50
1:D:522:PHE:CE1	1:D:540:GLN:HA	2.46	0.50
1:E:276:ASN:OD1	1:E:276:ASN:C	2.50	0.50
1:A:131:CYS:O	1:A:189:LYS:CD	2.60	0.49
1:A:138:ILE:HG21	1:A:151:ARG:HA	1.93	0.49
1:E:129:LEU:HD22	1:E:159:PHE:CD2	2.48	0.49
1:D:601:LYS:NZ	1:B:657:GLU:OE1	2.46	0.48
1:E:359:ILE:HD12	1:E:468:PHE:CE1	2.48	0.48
1:A:139:THR:HG22	1:A:140:ASP:N	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:636:SER:HB2	6:D:701:NAG:HN2	1.80	0.47
3:L:33:UNK:O	3:L:50:UNK:N	2.47	0.47
1:E:97:LYS:NZ	1:E:275:GLU:OE2	2.48	0.46
1:E:307:ILE:CG2	1:E:308:ARG:N	2.78	0.46
1:A:134:VAL:O	1:A:138:ILE:HD12	2.15	0.46
6:C:702:NAG:HO3	6:C:702:NAG:C7	2.29	0.45
1:A:150:MET:HG2	1:A:326:ILE:HG22	1.99	0.45
1:A:141:ASP:O	1:A:150:MET:HB3	2.17	0.45
1:A:107:ASP:OD1	1:B:574:LYS:NZ	2.50	0.45
6:C:704:NAG:O3	6:C:704:NAG:C7	2.64	0.45
1:A:97:LYS:NZ	1:A:275:GLU:OE2	2.49	0.44
1:E:353:PHE:CZ	1:E:456:ARG:HD3	2.52	0.44
2:H:67:UNK:O	2:H:68:UNK:C	2.63	0.44
1:A:325:ASP:O	1:A:325:ASP:OD1	2.36	0.44
1:C:75:VAL:HA	1:C:76:PRO:HD3	1.91	0.43
1:C:123:THR:N	1:C:124:PRO:CD	2.81	0.43
1:E:125:LEU:O	1:E:125:LEU:CG	2.67	0.43
1:E:161:MET:CE	1:E:309:ILE:HG21	2.48	0.42
6:C:702:NAG:C7	6:C:702:NAG:O3	2.66	0.42
1:A:134:VAL:CG1	1:A:138:ILE:CD1	2.97	0.42
2:H:99:UNK:O	2:H:100:UNK:C	2.66	0.42
1:C:290:GLU:OE1	1:C:344:LYS:NZ	2.52	0.41
1:A:141:ASP:HB3	1:A:328:GLN:HE21	1.85	0.41
2:H:72:UNK:O	2:H:73:UNK:C	2.68	0.41
2:H:74:UNK:O	2:H:75:UNK:C	2.66	0.41
1:E:125:LEU:HD13	1:E:161:MET:SD	2.60	0.41
1:B:542:ARG:HG2	1:B:542:ARG:O	2.20	0.41
1:C:372:THR:HB	6:C:704:NAG:H83	2.02	0.41
1:E:278:THR:HG21	6:E:702:NAG:H3	2.03	0.40
1:E:54:CYS:SG	1:E:215:ILE:HG23	2.61	0.40
1:F:637:ASN:HD22	1:F:637:ASN:HA	1.66	0.40
1:A:499:THR:OG1	1:A:500:ARG:N	2.54	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	A	437/664 (66%)	431 (99%)	6 (1%)	0	100	100
1	B	117/664 (18%)	117 (100%)	0	0	100	100
1	C	436/664 (66%)	429 (98%)	7 (2%)	0	100	100
1	D	121/664 (18%)	118 (98%)	3 (2%)	0	100	100
1	E	433/664 (65%)	427 (99%)	6 (1%)	0	100	100
1	F	122/664 (18%)	122 (100%)	0	0	100	100
All	All	1666/3984 (42%)	1644 (99%)	22 (1%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	401/586 (68%)	401 (100%)	0	100	100
1	B	105/586 (18%)	105 (100%)	0	100	100
1	C	400/586 (68%)	400 (100%)	0	100	100
1	D	108/586 (18%)	108 (100%)	0	100	100
1	E	398/586 (68%)	398 (100%)	0	100	100
1	F	109/586 (19%)	109 (100%)	0	100	100
All	All	1521/3516 (43%)	1521 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	66	HIS

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Mol	Chain	Res	Type
1	A	328	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates

51 monosaccharides are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	NAG	G	1	4,1	14,14,15	1.95	6 (42%)	17,19,21	1.05	1 (5%)
4	NAG	G	2	4	14,14,15	1.90	4 (28%)	17,19,21	0.99	2 (11%)
4	BMA	G	3	4	11,11,12	1.41	3 (27%)	15,15,17	0.61	0
4	MAN	G	4	4	11,11,12	1.92	5 (45%)	15,15,17	0.69	0
4	MAN	G	5	4	11,11,12	1.88	4 (36%)	15,15,17	0.68	0
5	NAG	I	1	5,1	14,14,15	2.03	5 (35%)	17,19,21	1.04	1 (5%)
5	NAG	I	2	5	14,14,15	1.81	5 (35%)	17,19,21	0.95	1 (5%)
5	NAG	J	1	5,1	14,14,15	2.10	6 (42%)	17,19,21	1.01	0
5	NAG	J	2	5	14,14,15	1.98	6 (42%)	17,19,21	0.82	1 (5%)
5	NAG	K	1	5,1	14,14,15	0.38	0	17,19,21	0.48	0
5	NAG	K	2	5	14,14,15	0.38	0	17,19,21	0.39	0
5	NAG	M	1	5,1	14,14,15	2.13	6 (42%)	17,19,21	0.95	1 (5%)
5	NAG	M	2	5	14,14,15	1.93	5 (35%)	17,19,21	0.87	1 (5%)
5	NAG	N	1	5,1	14,14,15	2.08	6 (42%)	17,19,21	1.19	1 (5%)
5	NAG	N	2	5	14,14,15	1.94	5 (35%)	17,19,21	0.85	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
5	NAG	O	1	5,1	14,14,15	2.07	6 (42%)	17,19,21	1.00	1 (5%)
5	NAG	O	2	5	14,14,15	1.97	6 (42%)	17,19,21	0.87	1 (5%)
5	NAG	P	1	5,1	14,14,15	2.18	6 (42%)	17,19,21	1.24	1 (5%)
5	NAG	P	2	5	14,14,15	2.02	5 (35%)	17,19,21	0.81	0
4	NAG	Q	1	4,1	14,14,15	1.94	5 (35%)	17,19,21	0.95	0
4	NAG	Q	2	4	14,14,15	1.85	5 (35%)	17,19,21	0.93	1 (5%)
4	BMA	Q	3	4	11,11,12	1.42	3 (27%)	15,15,17	0.65	0
4	MAN	Q	4	4	11,11,12	1.93	6 (54%)	15,15,17	0.70	0
4	MAN	Q	5	4	11,11,12	1.87	5 (45%)	15,15,17	0.75	0
5	NAG	R	1	5,1	14,14,15	2.04	4 (28%)	17,19,21	1.05	2 (11%)
5	NAG	R	2	5	14,14,15	1.92	6 (42%)	17,19,21	0.89	1 (5%)
5	NAG	S	1	5,1	14,14,15	2.15	7 (50%)	17,19,21	1.02	1 (5%)
5	NAG	S	2	5	14,14,15	2.00	6 (42%)	17,19,21	0.91	1 (5%)
5	NAG	T	1	5,1	14,14,15	1.98	6 (42%)	17,19,21	1.07	1 (5%)
5	NAG	T	2	5	14,14,15	1.91	4 (28%)	17,19,21	0.84	1 (5%)
5	NAG	U	1	5,1	14,14,15	2.01	7 (50%)	17,19,21	1.19	2 (11%)
5	NAG	U	2	5	14,14,15	1.90	5 (35%)	17,19,21	1.01	2 (11%)
5	NAG	V	1	5,1	14,14,15	1.98	7 (50%)	17,19,21	1.21	2 (11%)
5	NAG	V	2	5	14,14,15	2.00	5 (35%)	17,19,21	0.80	0
5	NAG	W	1	5,1	14,14,15	2.17	7 (50%)	17,19,21	1.11	1 (5%)
5	NAG	W	2	5	14,14,15	1.94	5 (35%)	17,19,21	0.89	1 (5%)
4	NAG	X	1	4,1	14,14,15	0.40	0	17,19,21	0.53	0
4	NAG	X	2	4	14,14,15	0.40	0	17,19,21	0.52	0
4	BMA	X	3	4	11,11,12	0.29	0	15,15,17	0.48	0
4	MAN	X	4	4	11,11,12	0.26	0	15,15,17	0.52	0
4	MAN	X	5	4	11,11,12	0.26	0	15,15,17	0.51	0
5	NAG	Y	1	5,1	14,14,15	2.09	6 (42%)	17,19,21	1.09	1 (5%)
5	NAG	Y	2	5	14,14,15	1.87	4 (28%)	17,19,21	0.83	0
5	NAG	Z	1	5,1	14,14,15	0.37	0	17,19,21	0.42	0
5	NAG	Z	2	5	14,14,15	0.37	0	17,19,21	0.42	0
5	NAG	a	1	5,1	14,14,15	2.14	6 (42%)	17,19,21	1.02	1 (5%)
5	NAG	a	2	5	14,14,15	2.01	5 (35%)	17,19,21	0.85	0
5	NAG	b	1	5,1	14,14,15	2.17	7 (50%)	17,19,21	1.35	2 (11%)
5	NAG	b	2	5	14,14,15	2.13	7 (50%)	17,19,21	0.99	2 (11%)
5	NAG	c	1	5,1	14,14,15	2.03	7 (50%)	17,19,21	1.16	2 (11%)
5	NAG	c	2	5	14,14,15	1.87	5 (35%)	17,19,21	0.83	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	G	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	G	2	4	-	0/6/23/26	0/1/1/1
4	BMA	G	3	4	-	0/2/19/22	0/1/1/1
4	MAN	G	4	4	-	0/2/19/22	0/1/1/1
4	MAN	G	5	4	-	0/2/19/22	0/1/1/1
5	NAG	I	1	5,1	-	0/6/23/26	0/1/1/1
5	NAG	I	2	5	-	0/6/23/26	0/1/1/1
5	NAG	J	1	5,1	-	0/6/23/26	0/1/1/1
5	NAG	J	2	5	-	0/6/23/26	0/1/1/1
5	NAG	K	1	5,1	-	2/6/23/26	0/1/1/1
5	NAG	K	2	5	-	5/6/23/26	0/1/1/1
5	NAG	M	1	5,1	-	0/6/23/26	0/1/1/1
5	NAG	M	2	5	-	0/6/23/26	0/1/1/1
5	NAG	N	1	5,1	-	0/6/23/26	0/1/1/1
5	NAG	N	2	5	-	0/6/23/26	0/1/1/1
5	NAG	O	1	5,1	-	0/6/23/26	0/1/1/1
5	NAG	O	2	5	-	0/6/23/26	0/1/1/1
5	NAG	P	1	5,1	-	0/6/23/26	0/1/1/1
5	NAG	P	2	5	-	1/6/23/26	0/1/1/1
4	NAG	Q	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	Q	2	4	-	0/6/23/26	0/1/1/1
4	BMA	Q	3	4	-	0/2/19/22	0/1/1/1
4	MAN	Q	4	4	-	2/2/19/22	0/1/1/1
4	MAN	Q	5	4	-	1/2/19/22	0/1/1/1
5	NAG	R	1	5,1	-	0/6/23/26	0/1/1/1
5	NAG	R	2	5	-	0/6/23/26	0/1/1/1
5	NAG	S	1	5,1	-	0/6/23/26	0/1/1/1
5	NAG	S	2	5	-	0/6/23/26	0/1/1/1
5	NAG	T	1	5,1	-	0/6/23/26	0/1/1/1
5	NAG	T	2	5	-	0/6/23/26	0/1/1/1
5	NAG	U	1	5,1	-	0/6/23/26	0/1/1/1
5	NAG	U	2	5	-	0/6/23/26	0/1/1/1
5	NAG	V	1	5,1	-	0/6/23/26	0/1/1/1
5	NAG	V	2	5	-	0/6/23/26	0/1/1/1
5	NAG	W	1	5,1	-	0/6/23/26	0/1/1/1
5	NAG	W	2	5	-	0/6/23/26	0/1/1/1
4	NAG	X	1	4,1	-	5/6/23/26	0/1/1/1
4	NAG	X	2	4	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	BMA	X	3	4	-	2/2/19/22	0/1/1/1
4	MAN	X	4	4	-	1/2/19/22	0/1/1/1
4	MAN	X	5	4	-	1/2/19/22	0/1/1/1
5	NAG	Y	1	5,1	-	0/6/23/26	0/1/1/1
5	NAG	Y	2	5	-	0/6/23/26	0/1/1/1
5	NAG	Z	1	5,1	-	3/6/23/26	0/1/1/1
5	NAG	Z	2	5	-	3/6/23/26	0/1/1/1
5	NAG	a	1	5,1	-	0/6/23/26	0/1/1/1
5	NAG	a	2	5	-	0/6/23/26	0/1/1/1
5	NAG	b	1	5,1	-	0/6/23/26	0/1/1/1
5	NAG	b	2	5	-	0/6/23/26	0/1/1/1
5	NAG	c	1	5,1	-	0/6/23/26	0/1/1/1
5	NAG	c	2	5	-	0/6/23/26	0/1/1/1

All (229) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	W	1	NAG	C1-C2	5.62	1.60	1.52
5	J	1	NAG	C1-C2	5.29	1.60	1.52
5	M	1	NAG	C1-C2	5.23	1.60	1.52
5	R	1	NAG	C1-C2	5.17	1.60	1.52
5	S	1	NAG	C1-C2	5.13	1.60	1.52
5	a	1	NAG	C1-C2	5.12	1.60	1.52
5	P	1	NAG	C1-C2	5.11	1.60	1.52
5	b	2	NAG	C1-C2	5.00	1.59	1.52
5	Y	1	NAG	C1-C2	4.98	1.59	1.52
5	I	1	NAG	C1-C2	4.91	1.59	1.52
5	O	1	NAG	C1-C2	4.85	1.59	1.52
5	b	1	NAG	C1-C2	4.85	1.59	1.52
5	S	2	NAG	C1-C2	4.83	1.59	1.52
4	Q	1	NAG	C1-C2	4.80	1.59	1.52
5	N	1	NAG	C1-C2	4.76	1.59	1.52
5	c	1	NAG	C1-C2	4.74	1.59	1.52
5	P	2	NAG	C1-C2	4.74	1.59	1.52
4	G	1	NAG	C1-C2	4.71	1.59	1.52
5	V	2	NAG	C1-C2	4.65	1.59	1.52
5	a	2	NAG	C1-C2	4.63	1.59	1.52
5	U	1	NAG	C1-C2	4.57	1.59	1.52
5	N	2	NAG	C1-C2	4.43	1.59	1.52
5	O	2	NAG	C1-C2	4.43	1.59	1.52
5	T	1	NAG	C1-C2	4.42	1.58	1.52
5	T	2	NAG	C1-C2	4.42	1.58	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	J	2	NAG	C1-C2	4.42	1.58	1.52
5	M	2	NAG	C1-C2	4.34	1.58	1.52
5	W	2	NAG	C1-C2	4.33	1.58	1.52
5	R	2	NAG	C1-C2	4.26	1.58	1.52
5	Y	2	NAG	C1-C2	4.21	1.58	1.52
4	G	2	NAG	C1-C2	4.15	1.58	1.52
5	U	2	NAG	C1-C2	4.02	1.58	1.52
5	c	2	NAG	C1-C2	4.02	1.58	1.52
5	I	2	NAG	C1-C2	3.91	1.58	1.52
4	Q	2	NAG	C1-C2	3.85	1.58	1.52
5	V	1	NAG	C1-C2	3.76	1.58	1.52
5	P	2	NAG	O5-C5	3.40	1.50	1.43
5	b	2	NAG	O5-C5	3.21	1.49	1.43
5	V	2	NAG	O5-C5	3.19	1.49	1.43
4	G	4	MAN	C2-C3	3.19	1.57	1.52
5	a	2	NAG	O5-C5	3.17	1.49	1.43
5	N	2	NAG	O5-C5	3.17	1.49	1.43
5	J	2	NAG	O5-C5	3.16	1.49	1.43
5	U	2	NAG	O5-C5	3.14	1.49	1.43
4	Q	4	MAN	C2-C3	3.14	1.57	1.52
5	W	2	NAG	O5-C5	3.11	1.49	1.43
5	M	1	NAG	O5-C5	3.11	1.49	1.43
5	V	1	NAG	O5-C5	3.10	1.49	1.43
5	M	2	NAG	O5-C5	3.10	1.49	1.43
5	O	2	NAG	O5-C5	3.09	1.49	1.43
4	Q	4	MAN	O5-C5	3.09	1.49	1.43
4	G	5	MAN	O5-C5	3.09	1.49	1.43
5	Y	1	NAG	O5-C5	3.07	1.49	1.43
5	c	2	NAG	O5-C5	3.07	1.49	1.43
5	T	1	NAG	O5-C5	3.06	1.49	1.43
4	Q	5	MAN	C2-C3	3.05	1.57	1.52
4	G	2	NAG	O5-C5	3.05	1.49	1.43
5	P	1	NAG	O5-C5	3.03	1.49	1.43
5	Y	2	NAG	O5-C5	3.01	1.49	1.43
5	S	2	NAG	O5-C5	3.00	1.49	1.43
5	O	1	NAG	O5-C5	2.97	1.49	1.43
5	a	1	NAG	O5-C5	2.96	1.49	1.43
5	b	1	NAG	O5-C5	2.95	1.49	1.43
4	Q	5	MAN	O5-C5	2.95	1.49	1.43
4	G	4	MAN	O5-C5	2.95	1.49	1.43
5	N	1	NAG	O5-C5	2.94	1.49	1.43
5	J	1	NAG	O5-C5	2.94	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	G	5	MAN	C2-C3	2.93	1.56	1.52
4	Q	2	NAG	O5-C5	2.93	1.49	1.43
5	I	1	NAG	O5-C5	2.92	1.49	1.43
4	Q	1	NAG	O5-C5	2.91	1.49	1.43
5	T	2	NAG	O5-C5	2.90	1.49	1.43
5	R	2	NAG	O5-C5	2.88	1.49	1.43
5	c	1	NAG	O5-C5	2.87	1.49	1.43
5	P	1	NAG	C4-C5	2.86	1.59	1.53
5	S	1	NAG	O5-C5	2.83	1.49	1.43
4	G	4	MAN	C1-C2	2.81	1.58	1.52
5	b	2	NAG	C3-C2	2.81	1.58	1.52
5	I	2	NAG	O5-C5	2.77	1.49	1.43
5	U	1	NAG	O5-C5	2.74	1.49	1.43
4	G	1	NAG	O5-C5	2.71	1.48	1.43
5	R	1	NAG	O5-C5	2.70	1.48	1.43
4	G	5	MAN	C1-C2	2.69	1.58	1.52
5	W	1	NAG	O5-C5	2.69	1.48	1.43
5	R	2	NAG	C3-C2	2.68	1.58	1.52
5	N	1	NAG	C4-C5	2.67	1.58	1.53
5	S	2	NAG	C3-C2	2.65	1.58	1.52
5	V	1	NAG	C4-C5	2.63	1.58	1.53
5	a	2	NAG	C3-C2	2.58	1.58	1.52
5	c	2	NAG	C3-C2	2.56	1.58	1.52
5	T	1	NAG	O5-C1	2.56	1.47	1.43
5	J	2	NAG	C3-C2	2.56	1.57	1.52
4	Q	4	MAN	C1-C2	2.56	1.58	1.52
5	O	1	NAG	O5-C1	2.54	1.47	1.43
5	M	1	NAG	O5-C1	2.53	1.47	1.43
5	W	2	NAG	C3-C2	2.52	1.57	1.52
4	Q	5	MAN	C4-C5	2.50	1.58	1.53
5	a	1	NAG	O5-C1	2.50	1.47	1.43
5	V	1	NAG	C4-C3	2.50	1.58	1.52
5	T	2	NAG	C3-C2	2.49	1.57	1.52
5	b	1	NAG	O5-C1	2.49	1.47	1.43
5	b	1	NAG	C2-N2	2.48	1.50	1.46
5	V	1	NAG	C3-C2	2.47	1.57	1.52
5	M	2	NAG	C4-C5	2.46	1.58	1.53
4	G	4	MAN	C4-C5	2.45	1.58	1.53
5	M	2	NAG	C3-C2	2.45	1.57	1.52
5	I	2	NAG	C3-C2	2.45	1.57	1.52
5	J	1	NAG	O5-C1	2.45	1.47	1.43
4	Q	2	NAG	C3-C2	2.45	1.57	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	Q	4	MAN	C4-C5	2.44	1.58	1.53
5	U	1	NAG	C4-C5	2.44	1.58	1.53
5	V	2	NAG	C3-C2	2.43	1.57	1.52
4	Q	5	MAN	C1-C2	2.42	1.57	1.52
5	W	2	NAG	C4-C5	2.42	1.58	1.53
5	Y	1	NAG	C4-C5	2.42	1.58	1.53
5	J	2	NAG	C4-C5	2.40	1.58	1.53
5	O	1	NAG	C4-C5	2.40	1.58	1.53
5	S	1	NAG	C4-C5	2.40	1.58	1.53
5	V	2	NAG	C4-C5	2.40	1.58	1.53
5	b	1	NAG	C4-C3	2.40	1.58	1.52
5	N	1	NAG	O5-C1	2.40	1.47	1.43
5	O	2	NAG	C3-C2	2.39	1.57	1.52
5	O	2	NAG	C4-C5	2.38	1.58	1.53
5	U	2	NAG	C3-C2	2.38	1.57	1.52
5	J	1	NAG	C4-C5	2.37	1.58	1.53
5	a	1	NAG	C4-C5	2.37	1.58	1.53
4	Q	3	BMA	C2-C3	2.37	1.56	1.52
5	b	1	NAG	C4-C5	2.37	1.58	1.53
5	Y	2	NAG	C3-C2	2.36	1.57	1.52
4	G	2	NAG	C3-C2	2.36	1.57	1.52
5	U	2	NAG	C4-C5	2.35	1.58	1.53
5	a	1	NAG	C3-C2	2.35	1.57	1.52
5	P	2	NAG	C4-C5	2.35	1.58	1.53
5	W	1	NAG	O5-C1	2.34	1.47	1.43
4	G	5	MAN	C4-C5	2.34	1.58	1.53
4	G	3	BMA	O5-C5	2.33	1.48	1.43
5	N	2	NAG	C3-C2	2.33	1.57	1.52
4	G	1	NAG	C3-C2	2.33	1.57	1.52
4	G	2	NAG	C4-C5	2.33	1.57	1.53
4	Q	1	NAG	O5-C1	2.32	1.47	1.43
5	S	1	NAG	C4-C3	2.32	1.58	1.52
5	P	2	NAG	C3-C2	2.32	1.57	1.52
5	P	1	NAG	C4-C3	2.32	1.58	1.52
5	U	1	NAG	O5-C1	2.32	1.47	1.43
5	I	1	NAG	C4-C3	2.31	1.58	1.52
5	b	1	NAG	C3-C2	2.31	1.57	1.52
5	c	1	NAG	O5-C1	2.31	1.47	1.43
5	S	1	NAG	O5-C1	2.30	1.47	1.43
5	I	2	NAG	C4-C5	2.30	1.57	1.53
5	b	2	NAG	C4-C5	2.29	1.57	1.53
5	N	2	NAG	C4-C5	2.29	1.57	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	R	1	NAG	C4-C5	2.28	1.57	1.53
5	W	1	NAG	C2-N2	2.28	1.50	1.46
5	c	1	NAG	C4-C5	2.27	1.57	1.53
5	M	1	NAG	C4-C5	2.26	1.57	1.53
5	U	1	NAG	C3-C2	2.26	1.57	1.52
4	G	3	BMA	C2-C3	2.26	1.55	1.52
5	a	2	NAG	C4-C5	2.26	1.57	1.53
5	V	1	NAG	O5-C1	2.25	1.47	1.43
5	T	2	NAG	C4-C5	2.25	1.57	1.53
5	P	1	NAG	O5-C1	2.25	1.47	1.43
4	Q	3	BMA	O5-C5	2.24	1.48	1.43
5	N	1	NAG	C3-C2	2.23	1.57	1.52
5	Y	1	NAG	O5-C1	2.23	1.47	1.43
5	M	1	NAG	C3-C2	2.22	1.57	1.52
5	P	1	NAG	C3-C2	2.22	1.57	1.52
4	Q	2	NAG	C4-C3	2.22	1.58	1.52
5	c	1	NAG	C2-N2	2.21	1.50	1.46
5	S	1	NAG	C2-N2	2.21	1.50	1.46
5	Y	1	NAG	C4-C3	2.21	1.57	1.52
5	Y	2	NAG	C4-C5	2.21	1.57	1.53
5	U	1	NAG	C4-C3	2.20	1.57	1.52
4	Q	3	BMA	C1-C2	2.20	1.57	1.52
5	I	1	NAG	C4-C5	2.20	1.57	1.53
5	c	1	NAG	C4-C3	2.19	1.57	1.52
5	T	1	NAG	C4-C5	2.19	1.57	1.53
5	W	1	NAG	C3-C2	2.19	1.57	1.52
5	R	2	NAG	C4-C5	2.18	1.57	1.53
5	S	2	NAG	C4-C5	2.18	1.57	1.53
5	S	1	NAG	C3-C2	2.18	1.57	1.52
4	G	3	BMA	C1-C2	2.18	1.57	1.52
5	R	1	NAG	C4-C3	2.18	1.57	1.52
4	Q	2	NAG	C4-C5	2.18	1.57	1.53
5	N	1	NAG	C4-C3	2.15	1.57	1.52
5	T	1	NAG	C3-C2	2.15	1.57	1.52
5	Y	1	NAG	C3-C2	2.15	1.57	1.52
5	O	1	NAG	C4-C3	2.15	1.57	1.52
5	O	1	NAG	C3-C2	2.14	1.57	1.52
4	G	1	NAG	O5-C1	2.14	1.47	1.43
5	c	2	NAG	C4-C5	2.14	1.57	1.53
5	a	1	NAG	C4-C3	2.14	1.57	1.52
5	I	2	NAG	C4-C3	2.13	1.57	1.52
5	W	2	NAG	C4-C3	2.12	1.57	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	G	1	NAG	C4-C5	2.12	1.57	1.53
5	a	2	NAG	O5-C1	2.11	1.47	1.43
5	b	2	NAG	O5-C1	2.11	1.47	1.43
5	c	1	NAG	C3-C2	2.11	1.57	1.52
5	I	1	NAG	O5-C1	2.10	1.47	1.43
5	b	2	NAG	C4-C3	2.09	1.57	1.52
5	b	2	NAG	C2-N2	2.09	1.49	1.46
5	N	2	NAG	C4-C3	2.09	1.57	1.52
4	Q	4	MAN	O5-C1	2.08	1.47	1.43
4	Q	1	NAG	C3-C2	2.08	1.56	1.52
5	R	2	NAG	C4-C3	2.08	1.57	1.52
4	Q	5	MAN	C4-C3	2.08	1.57	1.52
5	W	1	NAG	C4-C5	2.08	1.57	1.53
5	T	1	NAG	C4-C3	2.07	1.57	1.52
5	J	2	NAG	O5-C1	2.07	1.47	1.43
5	O	2	NAG	C2-N2	2.07	1.49	1.46
5	U	2	NAG	C4-C3	2.07	1.57	1.52
5	J	2	NAG	C4-C3	2.07	1.57	1.52
4	G	1	NAG	C4-C3	2.05	1.57	1.52
5	O	2	NAG	C4-C3	2.05	1.57	1.52
4	Q	1	NAG	C4-C5	2.05	1.57	1.53
5	P	2	NAG	O5-C1	2.05	1.47	1.43
5	U	1	NAG	C2-N2	2.04	1.49	1.46
5	W	1	NAG	C4-C3	2.04	1.57	1.52
4	Q	4	MAN	C4-C3	2.04	1.57	1.52
5	R	2	NAG	C2-N2	2.04	1.49	1.46
5	J	1	NAG	C3-C2	2.03	1.56	1.52
5	M	1	NAG	C4-C3	2.02	1.57	1.52
5	M	2	NAG	C4-C3	2.01	1.57	1.52
5	V	2	NAG	C4-C3	2.01	1.57	1.52
5	S	2	NAG	C4-C3	2.01	1.57	1.52
5	V	1	NAG	C2-N2	2.01	1.49	1.46
4	G	4	MAN	C4-C3	2.01	1.57	1.52
5	J	1	NAG	C4-C3	2.00	1.57	1.52
5	S	2	NAG	O5-C1	2.00	1.46	1.43
5	c	2	NAG	C4-C3	2.00	1.57	1.52

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	b	1	NAG	C8-C7-N2	3.50	122.02	116.10
5	V	1	NAG	C1-C2-N2	-3.00	105.36	110.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	c	1	NAG	C8-C7-N2	2.91	121.03	116.10
5	W	1	NAG	C8-C7-N2	2.82	120.88	116.10
5	U	2	NAG	C8-C7-N2	2.77	120.79	116.10
5	b	2	NAG	C8-C7-N2	2.71	120.69	116.10
5	U	1	NAG	C8-C7-N2	2.70	120.66	116.10
4	G	2	NAG	C8-C7-N2	2.59	120.49	116.10
5	b	1	NAG	O7-C7-C8	-2.56	117.31	122.06
5	P	1	NAG	C8-C7-N2	2.46	120.27	116.10
5	N	1	NAG	C8-C7-N2	2.39	120.14	116.10
5	I	1	NAG	C8-C7-N2	2.36	120.09	116.10
5	S	1	NAG	C8-C7-N2	2.34	120.06	116.10
5	V	1	NAG	C8-C7-N2	2.34	120.06	116.10
5	Y	1	NAG	C8-C7-N2	2.32	120.03	116.10
5	U	2	NAG	O7-C7-C8	-2.30	117.79	122.06
4	G	1	NAG	C1-C2-N2	-2.29	106.58	110.49
4	Q	2	NAG	C8-C7-N2	2.21	119.85	116.10
5	R	2	NAG	C8-C7-N2	2.21	119.83	116.10
5	b	2	NAG	O7-C7-C8	-2.19	117.98	122.06
5	T	1	NAG	C8-C7-N2	2.17	119.78	116.10
5	a	1	NAG	C8-C7-N2	2.17	119.78	116.10
4	G	2	NAG	O7-C7-C8	-2.17	118.03	122.06
5	U	1	NAG	O7-C7-C8	-2.16	118.04	122.06
5	R	1	NAG	C1-O5-C5	2.14	115.10	112.19
5	S	2	NAG	C8-C7-N2	2.14	119.73	116.10
5	O	2	NAG	C8-C7-N2	2.12	119.69	116.10
5	O	1	NAG	C8-C7-N2	2.11	119.68	116.10
5	R	1	NAG	C8-C7-N2	2.11	119.67	116.10
5	W	2	NAG	C8-C7-N2	2.08	119.62	116.10
5	I	2	NAG	C8-C7-N2	2.07	119.60	116.10
5	M	1	NAG	C8-C7-N2	2.05	119.58	116.10
5	c	1	NAG	C1-C2-N2	-2.05	106.98	110.49
5	M	2	NAG	C8-C7-N2	2.04	119.56	116.10
5	T	2	NAG	C8-C7-N2	2.04	119.55	116.10
5	J	2	NAG	C8-C7-N2	2.00	119.49	116.10

There are no chirality outliers.

All (28) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	X	2	NAG	C8-C7-N2-C2
4	X	2	NAG	O7-C7-N2-C2
5	K	2	NAG	C1-C2-N2-C7

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Mol	Chain	Res	Type	Atoms
5	Z	1	NAG	C8-C7-N2-C2
5	Z	1	NAG	O7-C7-N2-C2
5	Z	2	NAG	C8-C7-N2-C2
5	Z	2	NAG	O7-C7-N2-C2
5	K	2	NAG	C8-C7-N2-C2
4	X	1	NAG	C8-C7-N2-C2
5	K	2	NAG	O7-C7-N2-C2
5	K	1	NAG	O5-C5-C6-O6
4	X	1	NAG	O5-C5-C6-O6
4	X	1	NAG	C4-C5-C6-O6
4	X	1	NAG	O7-C7-N2-C2
4	Q	4	MAN	O5-C5-C6-O6
4	X	3	BMA	C4-C5-C6-O6
5	Z	1	NAG	C1-C2-N2-C7
5	K	1	NAG	C4-C5-C6-O6
4	Q	5	MAN	O5-C5-C6-O6
4	X	4	MAN	O5-C5-C6-O6
4	X	3	BMA	O5-C5-C6-O6
4	X	5	MAN	O5-C5-C6-O6
5	P	2	NAG	O5-C5-C6-O6
5	Z	2	NAG	O5-C5-C6-O6
5	K	2	NAG	O5-C5-C6-O6
4	Q	4	MAN	C4-C5-C6-O6
5	K	2	NAG	C3-C2-N2-C7
4	X	1	NAG	C1-C2-N2-C7

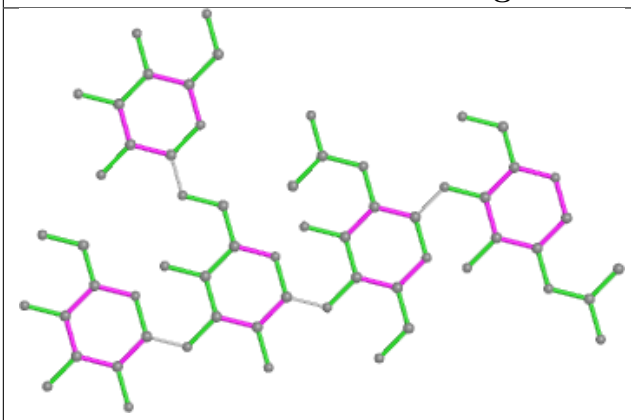
There are no ring outliers.

3 monomers are involved in 5 short contacts:

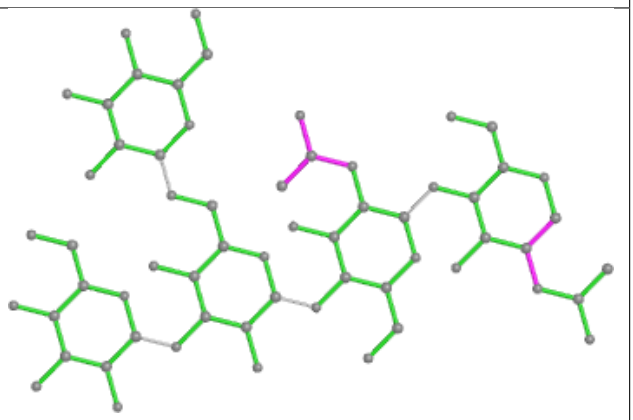
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	X	1	NAG	1	0
5	Z	1	NAG	3	0
5	Z	2	NAG	1	0

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

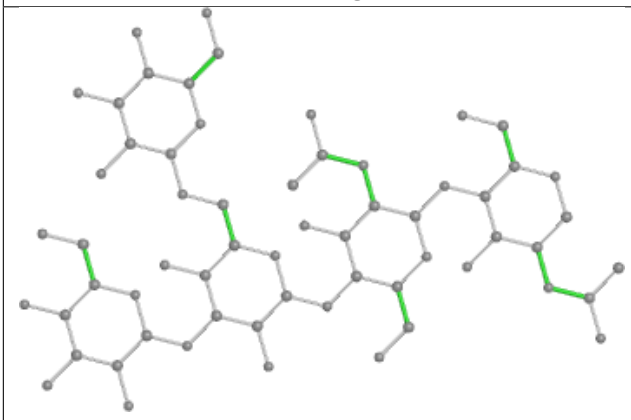
Oligosaccharide Chain G



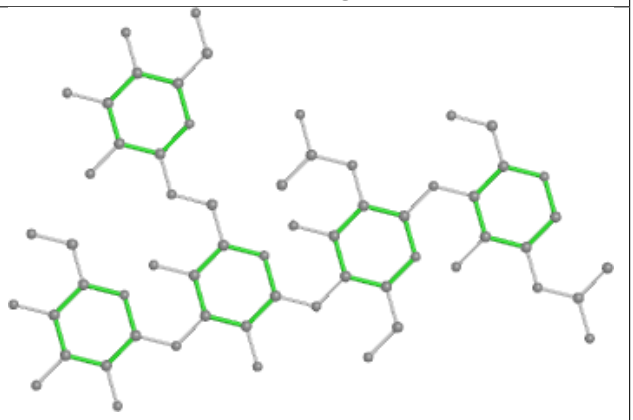
Bond lengths



Bond angles

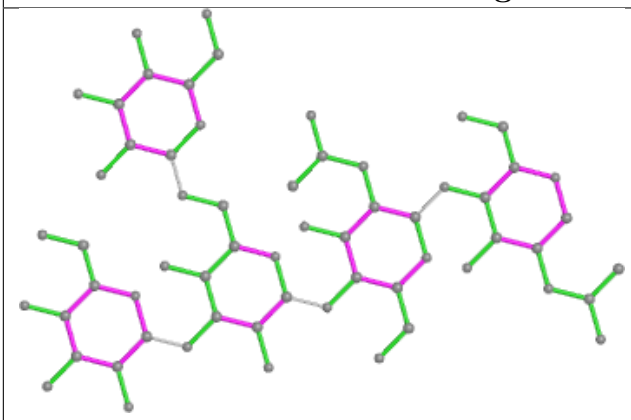


Torsions

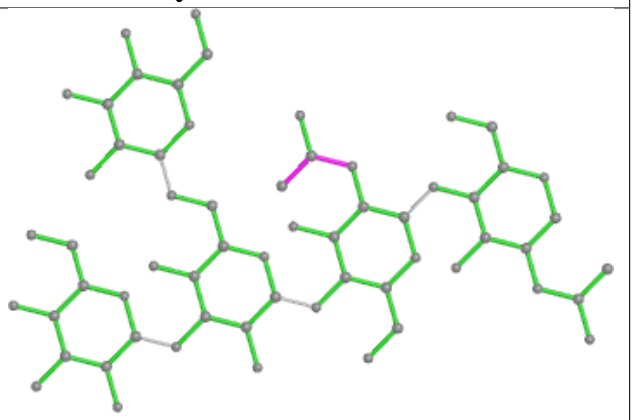


Rings

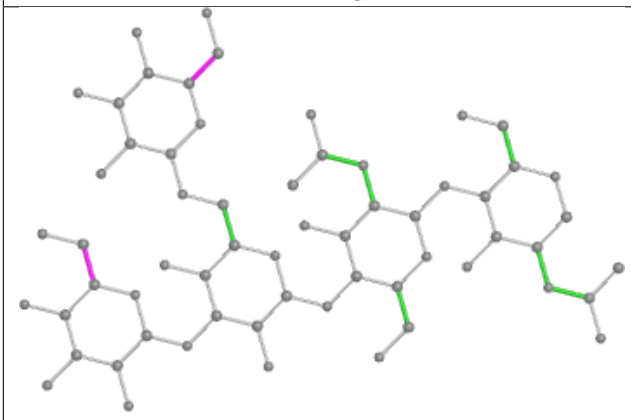
Oligosaccharide Chain Q



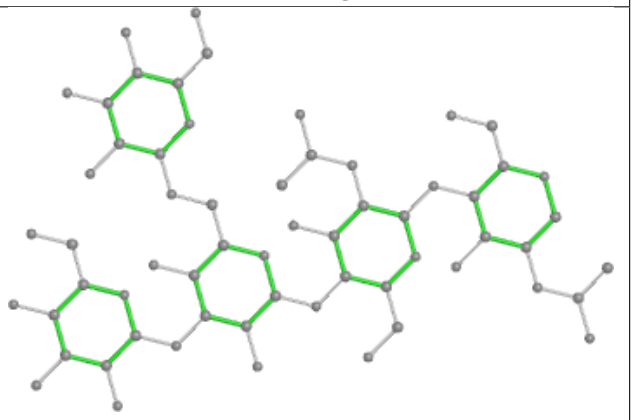
Bond lengths



Bond angles

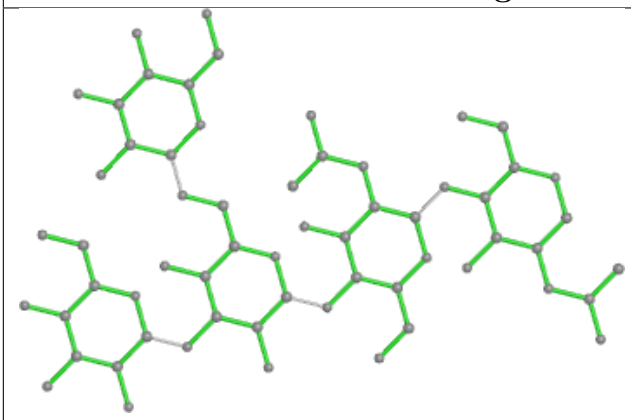


Torsions

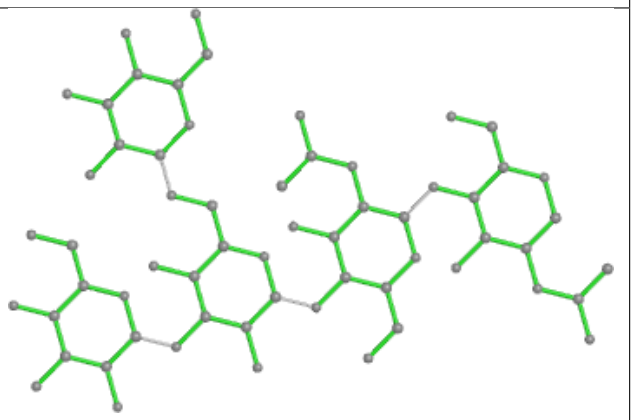


Rings

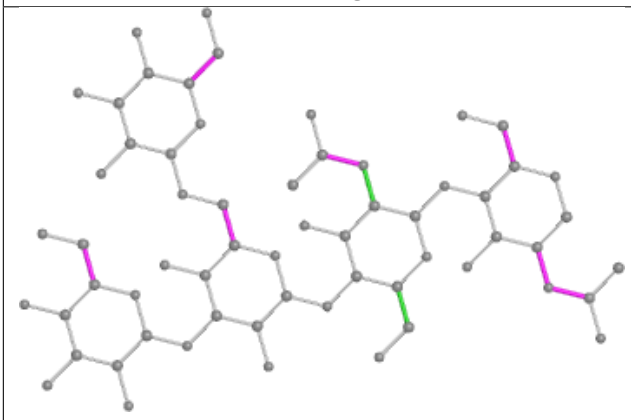
Oligosaccharide Chain X



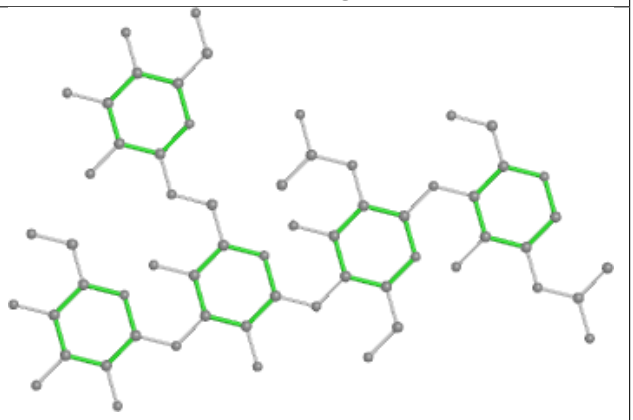
Bond lengths



Bond angles

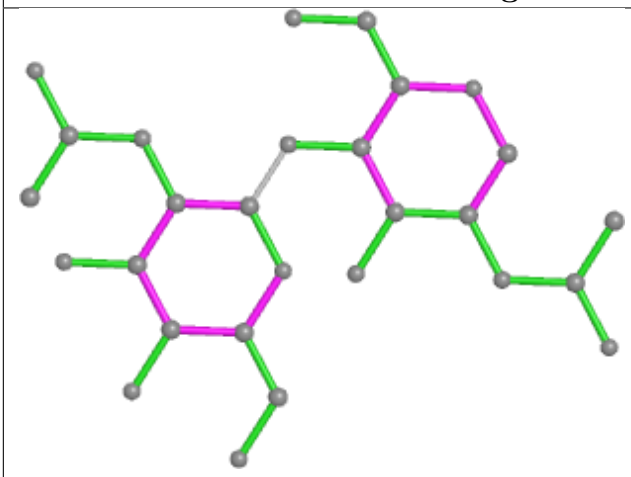


Torsions

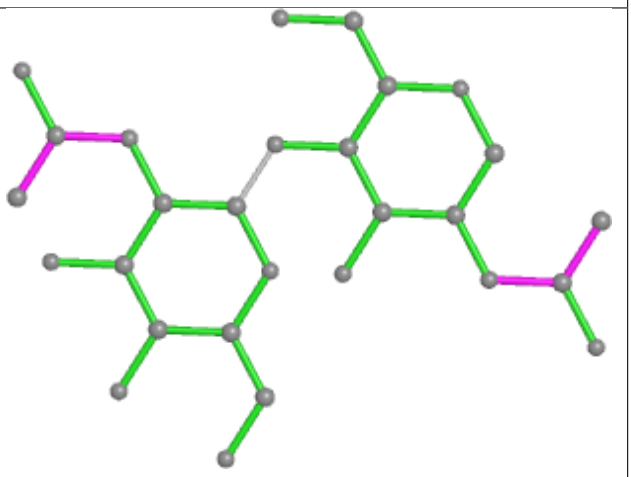


Rings

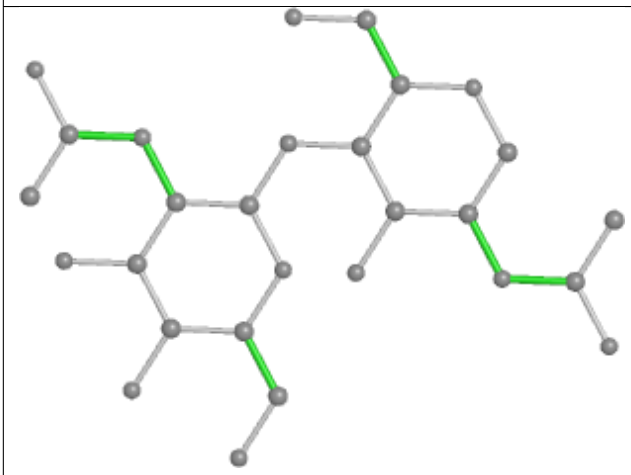
Oligosaccharide Chain I



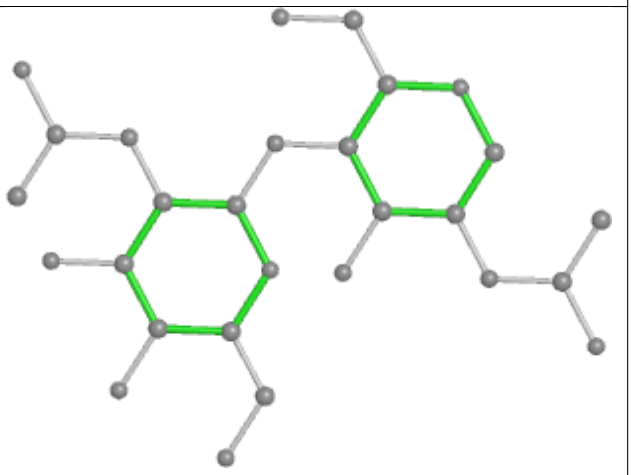
Bond lengths



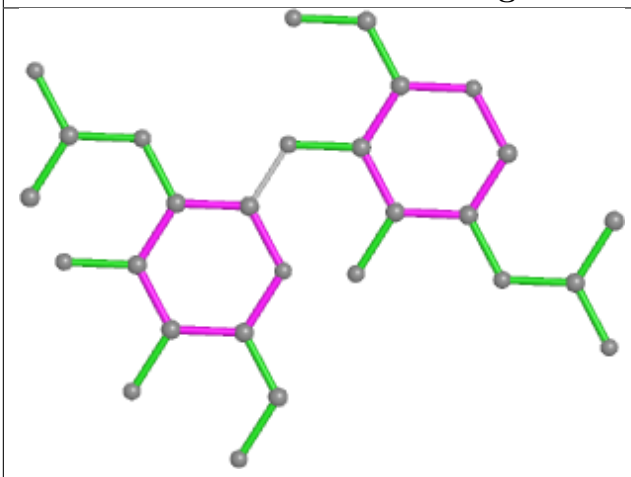
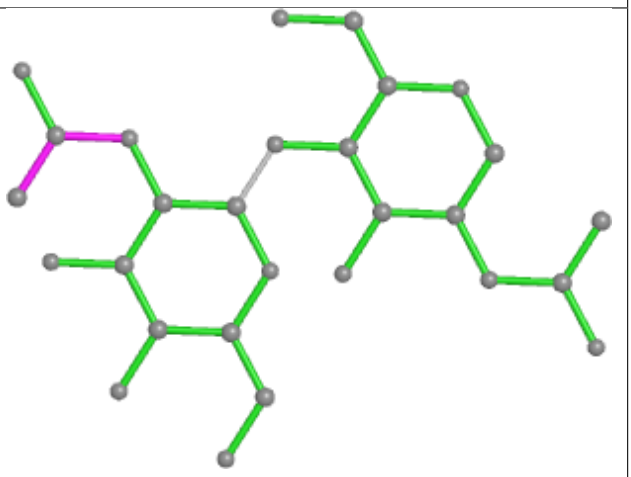
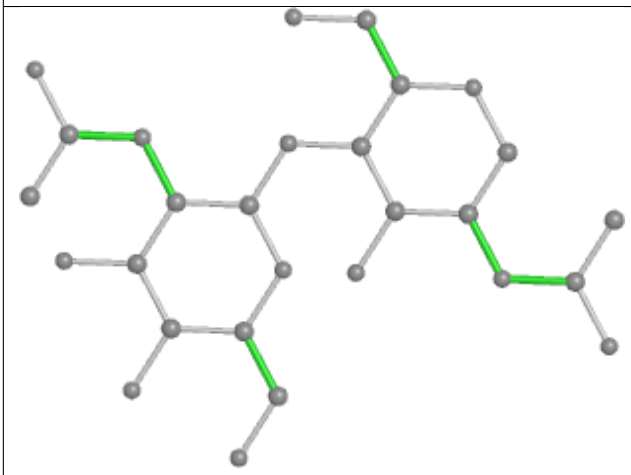
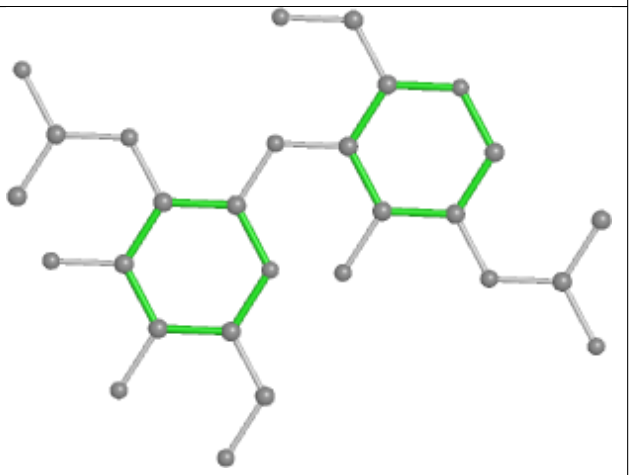
Bond angles



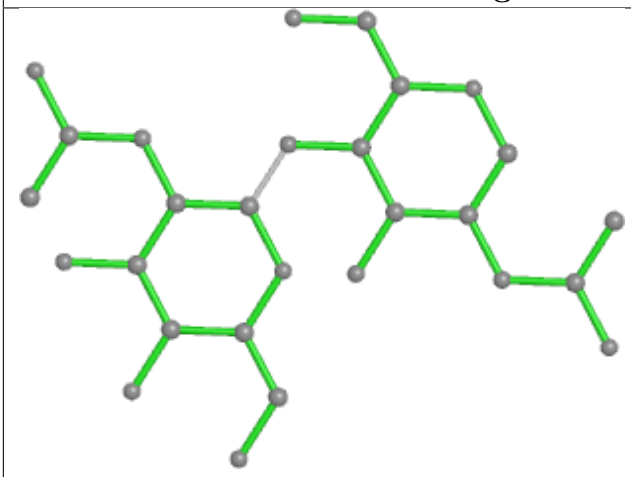
Torsions



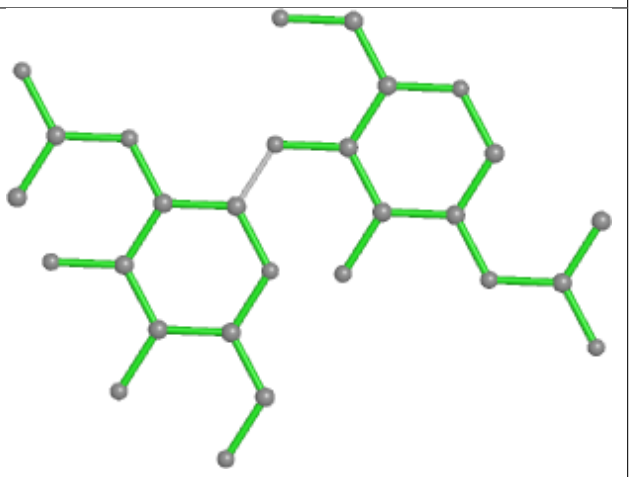
Rings

Oligosaccharide Chain J	
 Bond lengths	 Bond angles
 Torsions	 Rings

Oligosaccharide Chain K



Bond lengths



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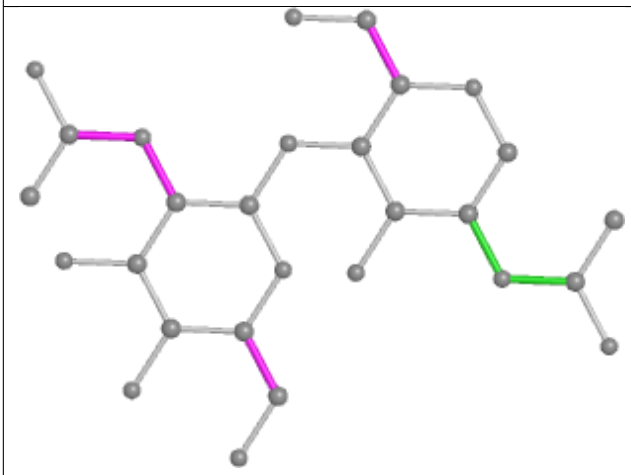

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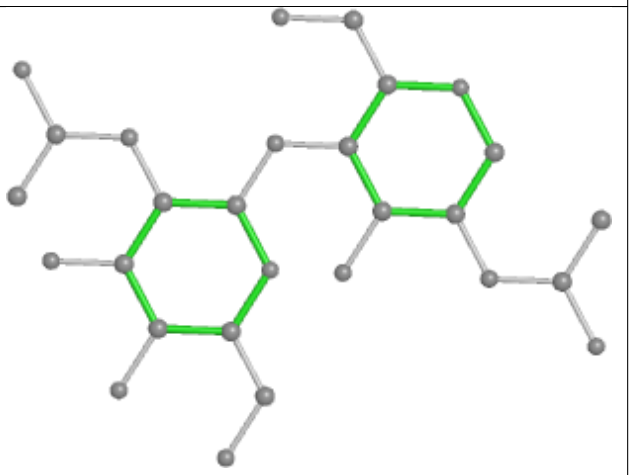
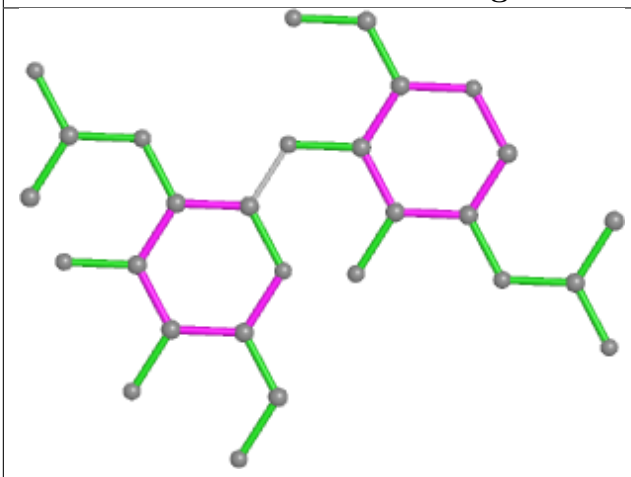


Rings

Oligosaccharide Chain M



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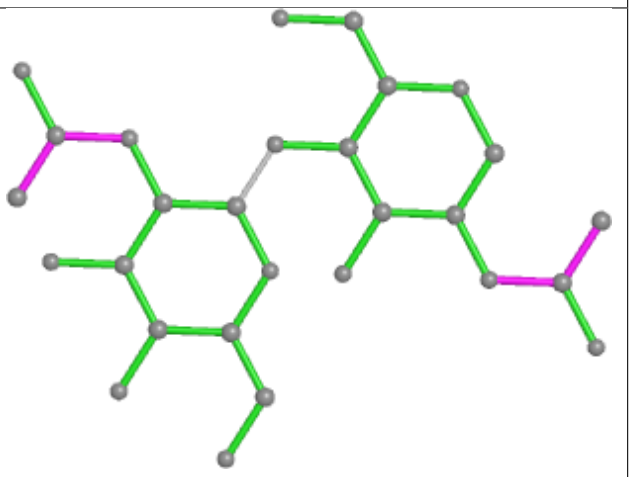
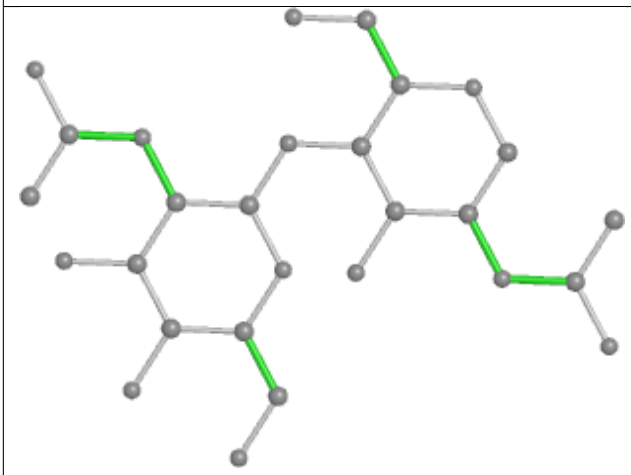


Bond angles



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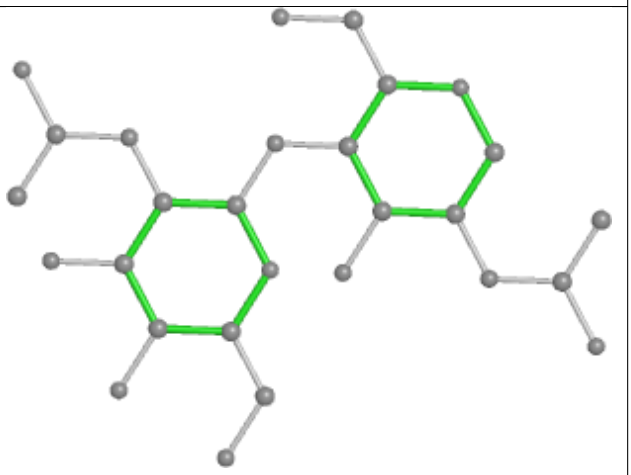
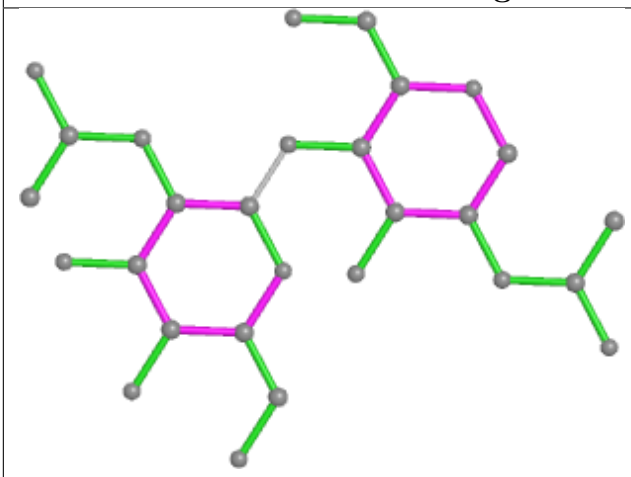
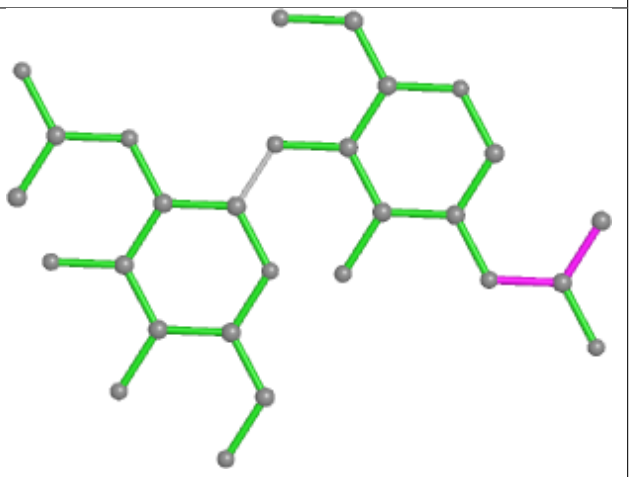
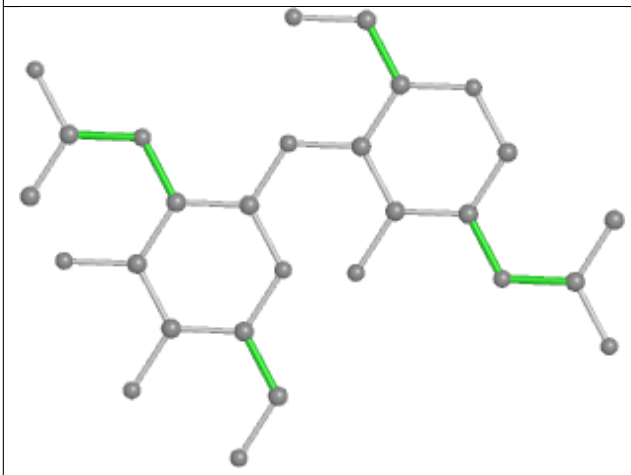
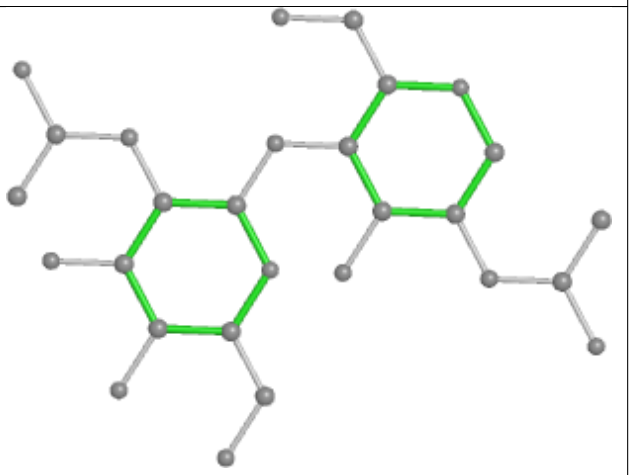
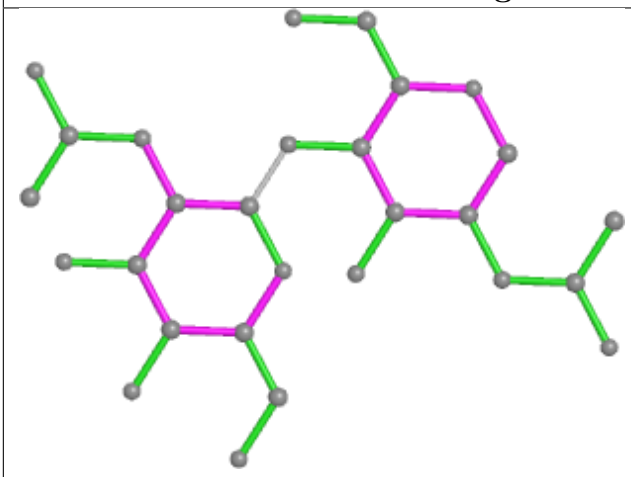
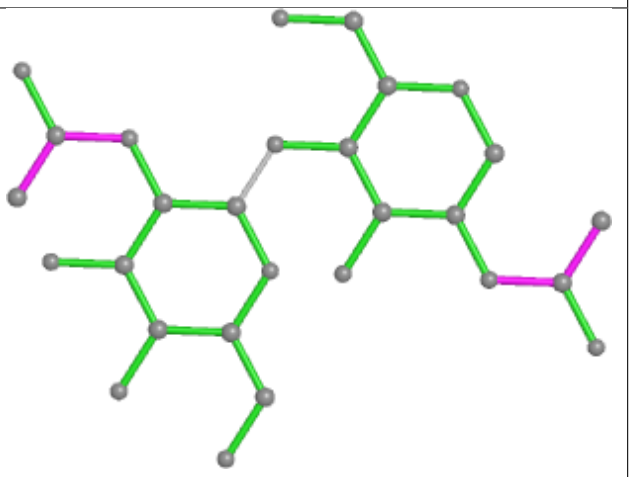
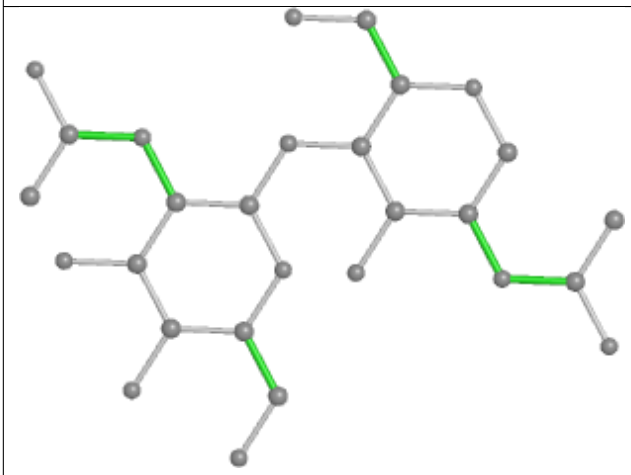
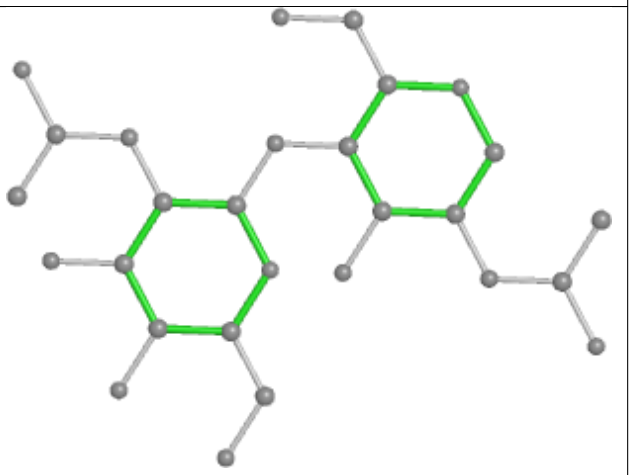
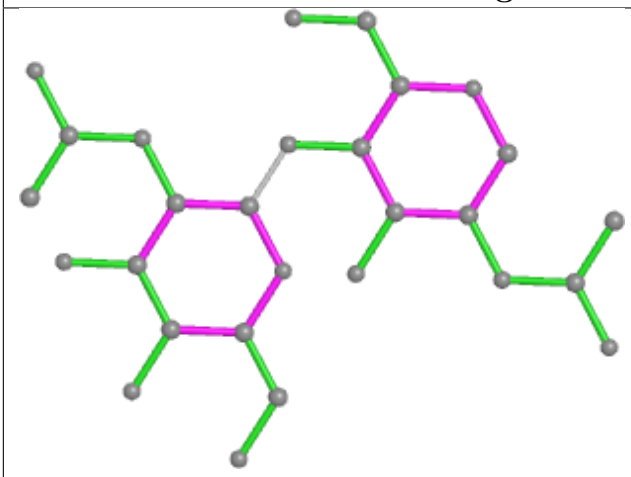
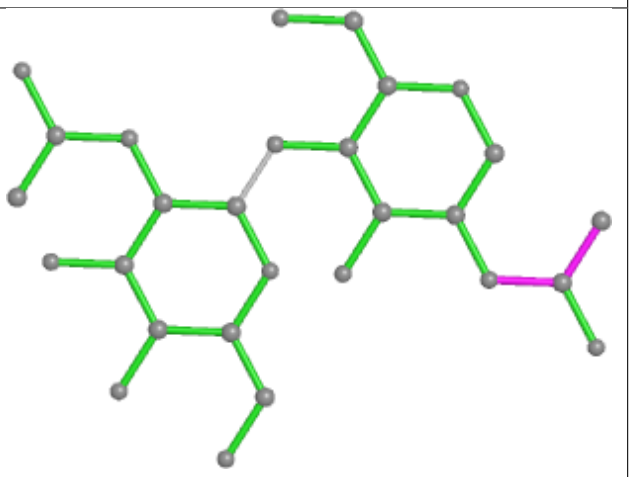
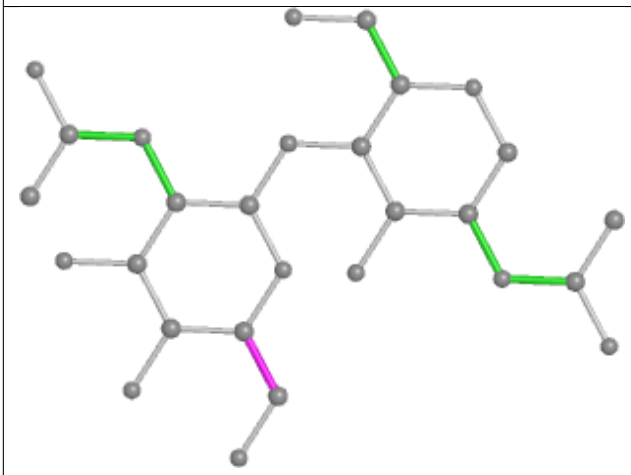
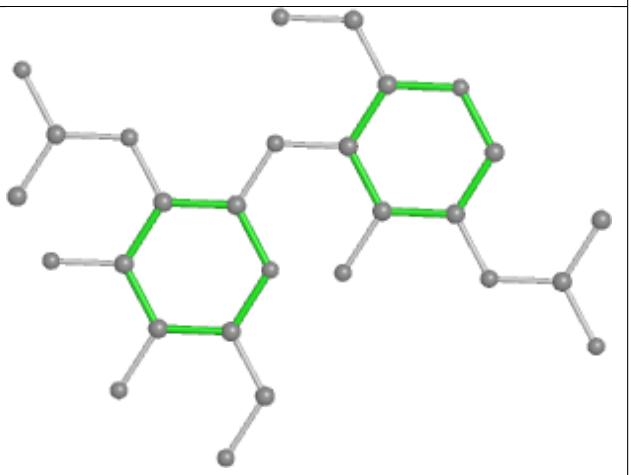
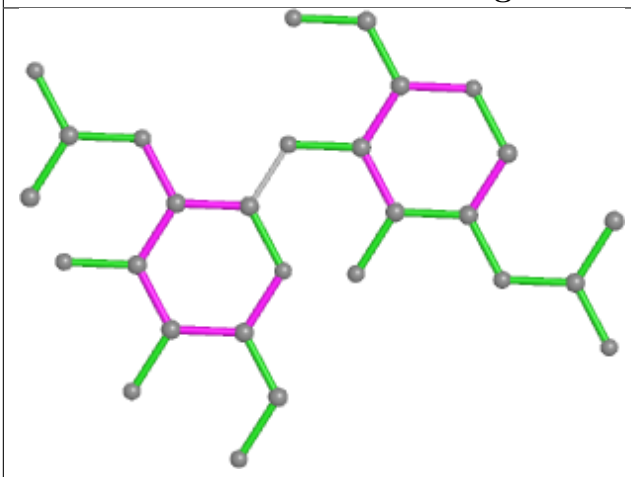
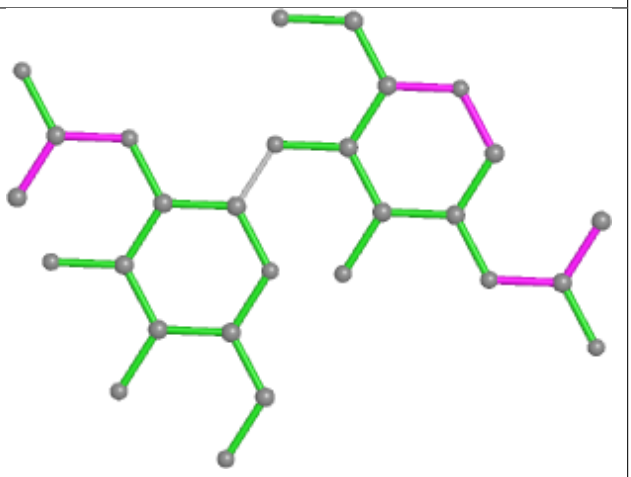
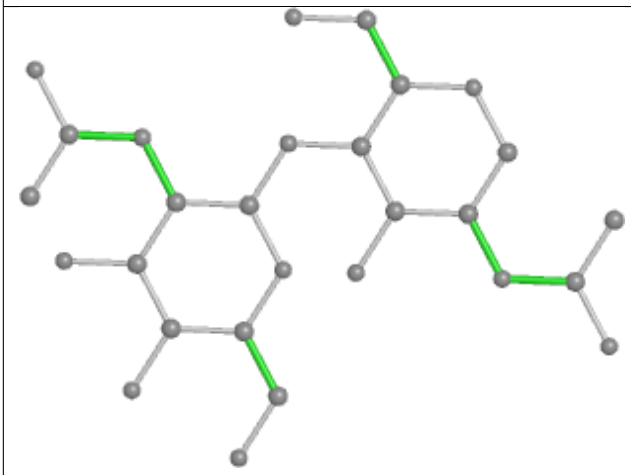
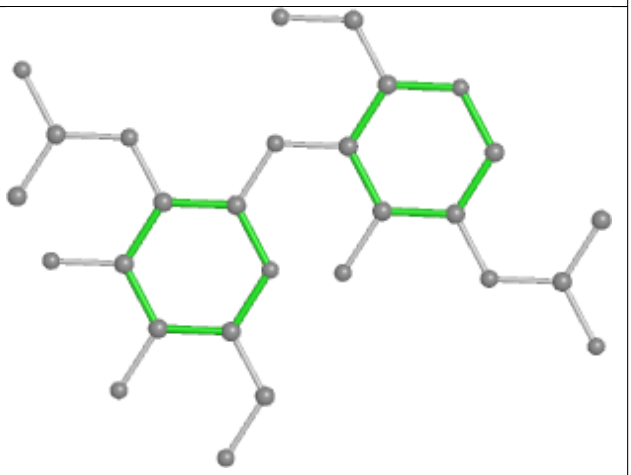


Rings

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

Oligosaccharide Chain O	
 Bond lengths	 Bond angles
 Torsions	 Rings

Oligosaccharide Chain P	
 Bond lengths	 Bond angles
 Torsions	 Rings

Oligosaccharide Chain R	
 Bond lengths	 Bond angles
 Torsions	 Rings

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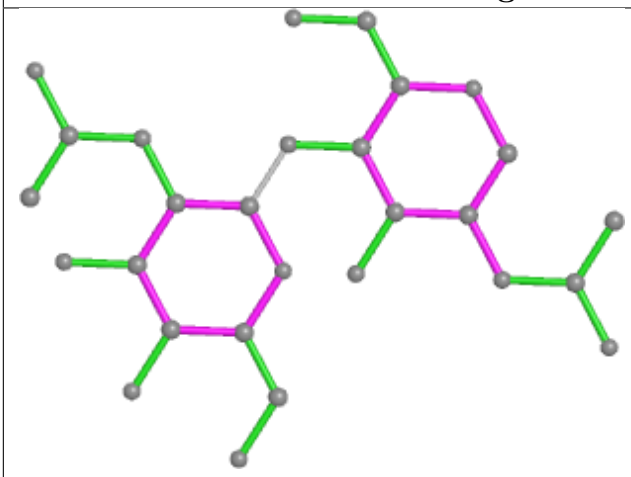
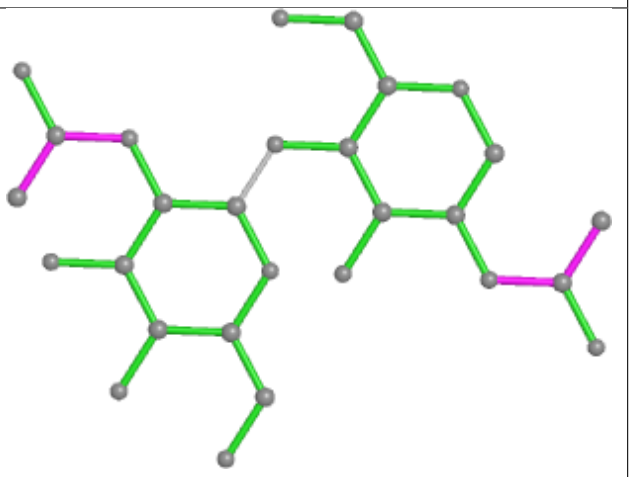
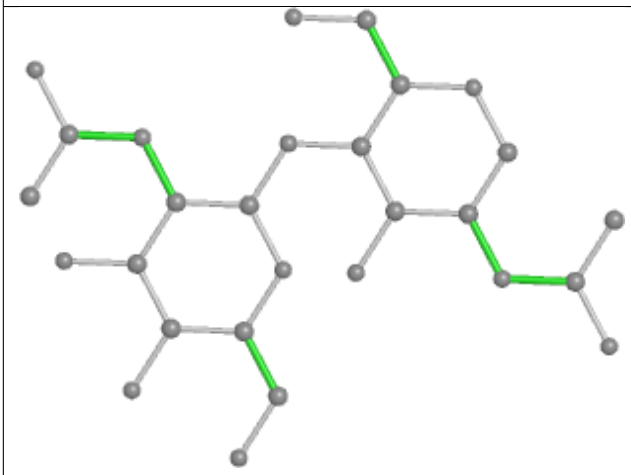
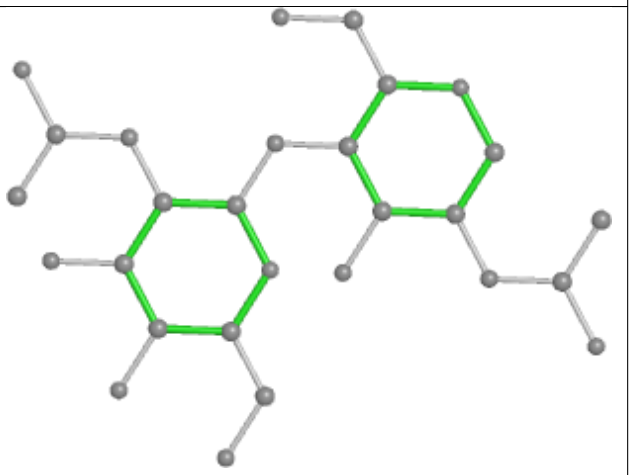
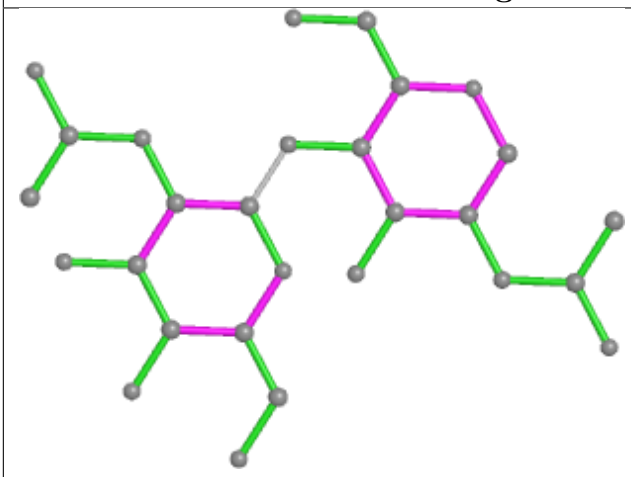
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

Oligosaccharide Chain T



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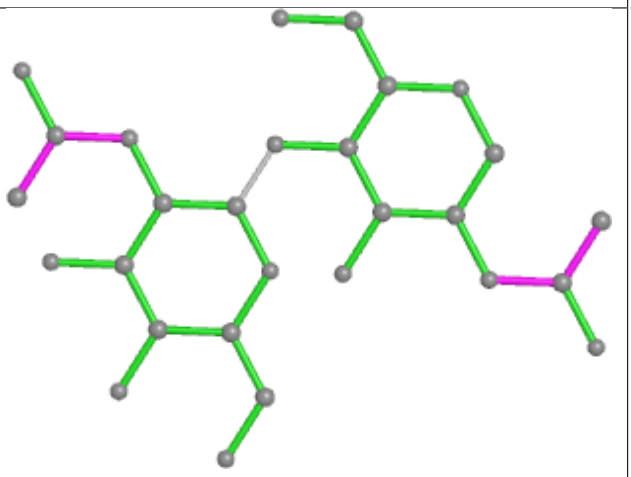
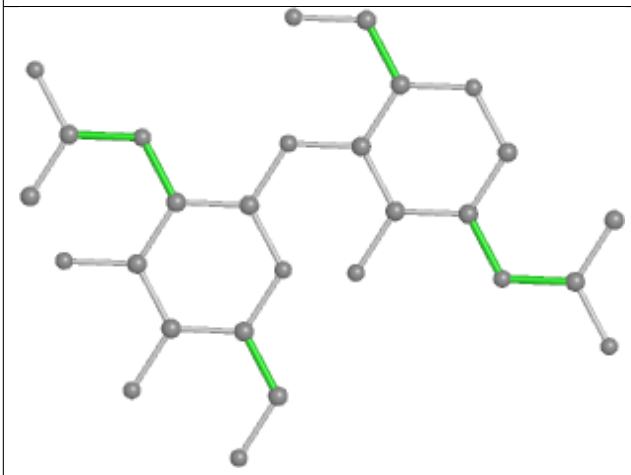
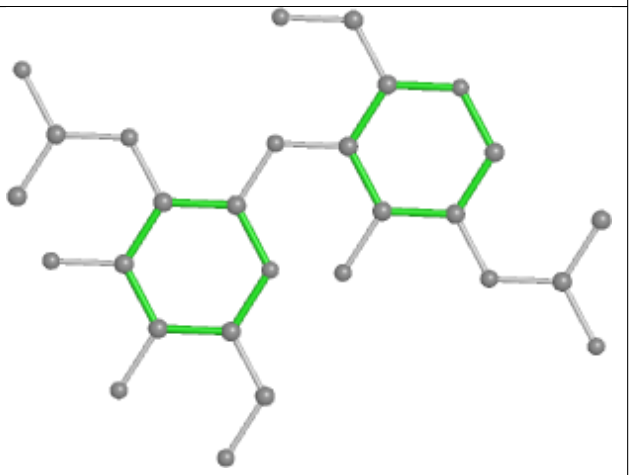


Bond angles

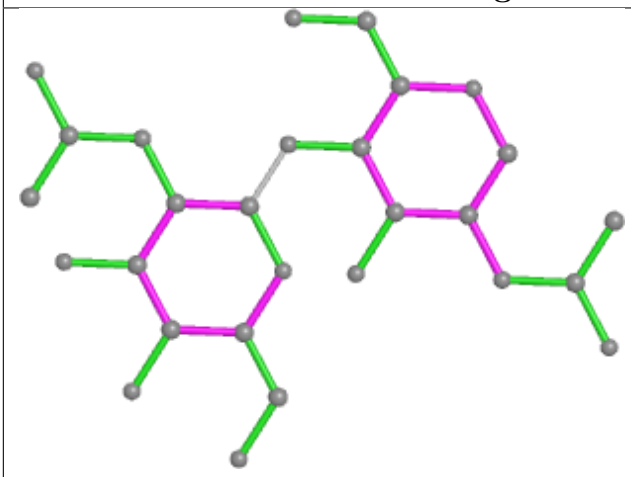


Torsions



Rings

Oligosaccharide Chain U



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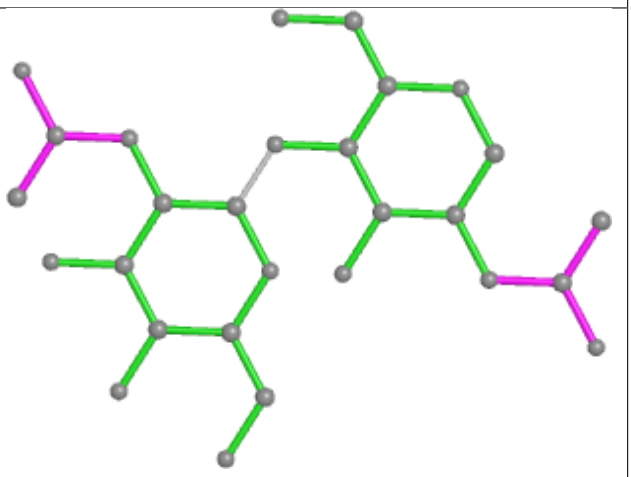

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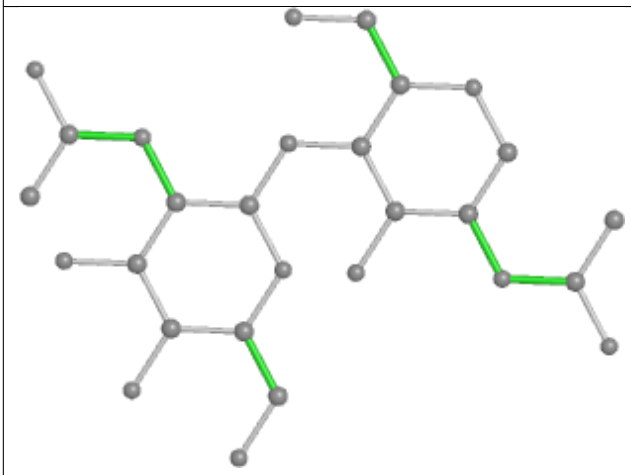

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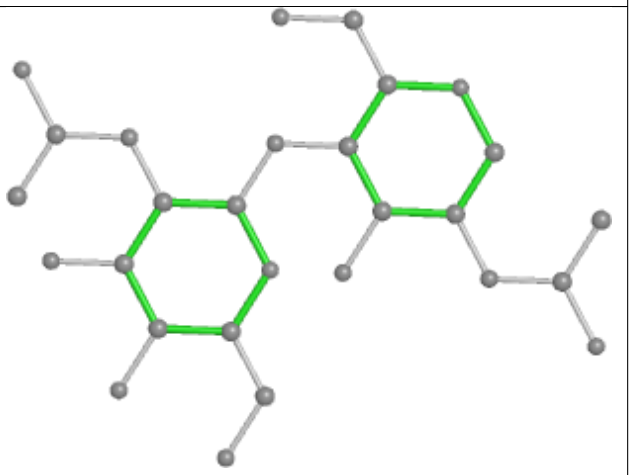
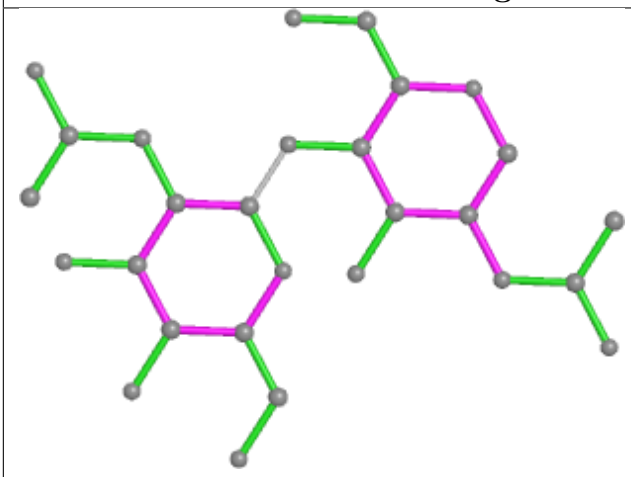
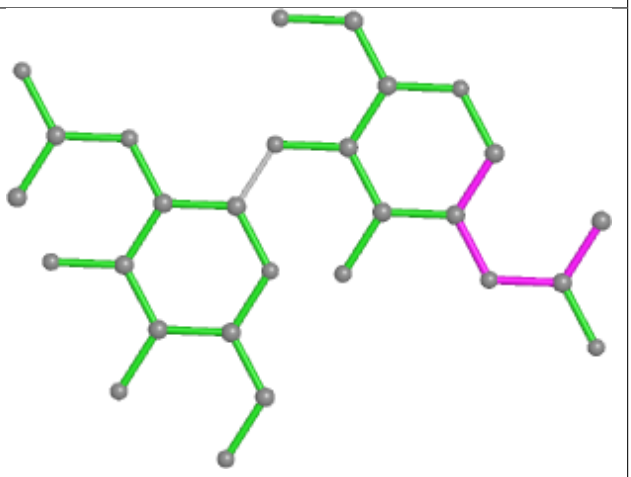


Rings

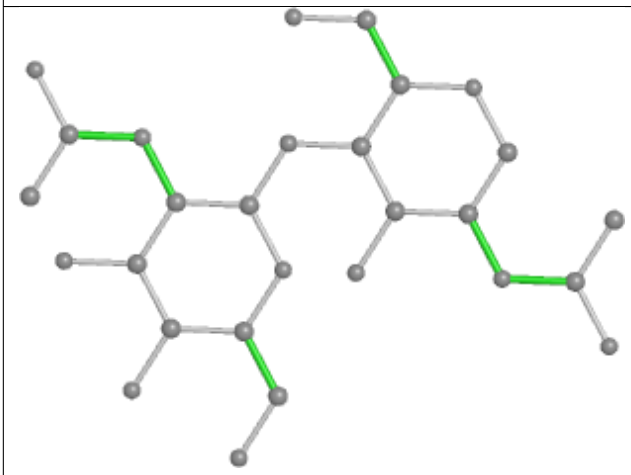
Oligosaccharide Chain V



Bond lengths



Bond angles



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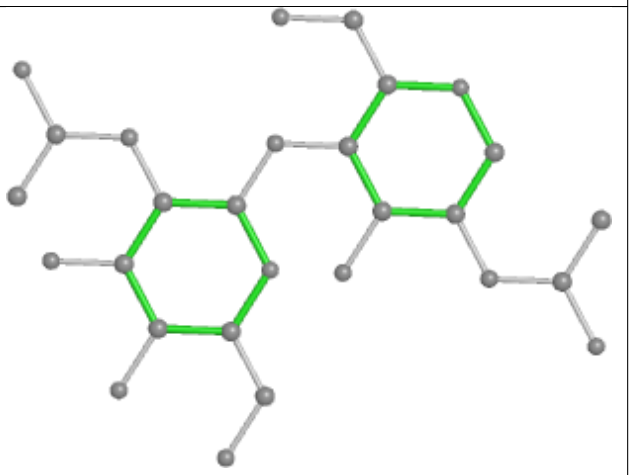
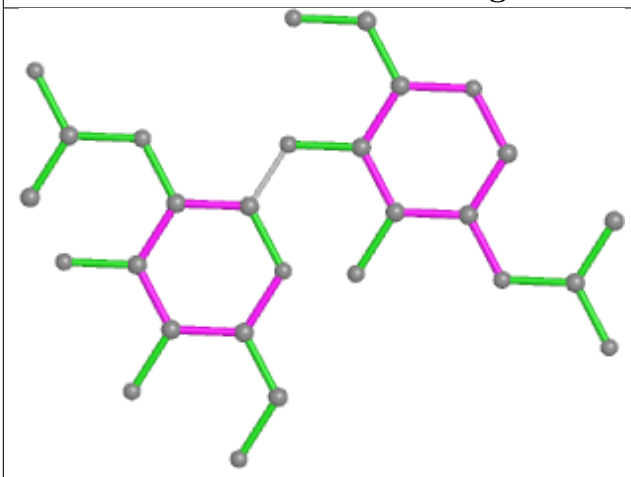
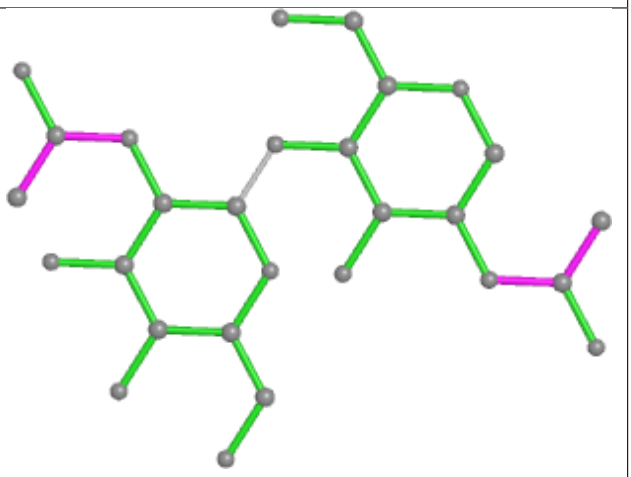


Rings

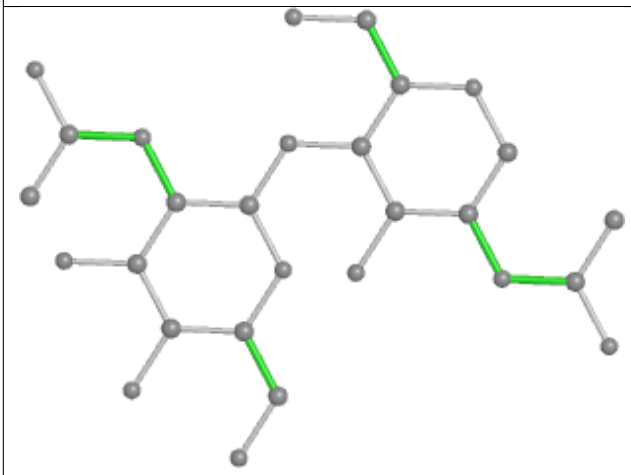
Oligosaccharide Chain W



Bond lengths



Bond angles



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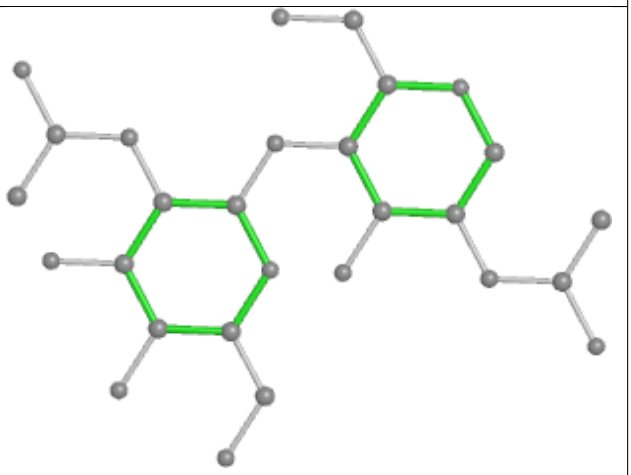
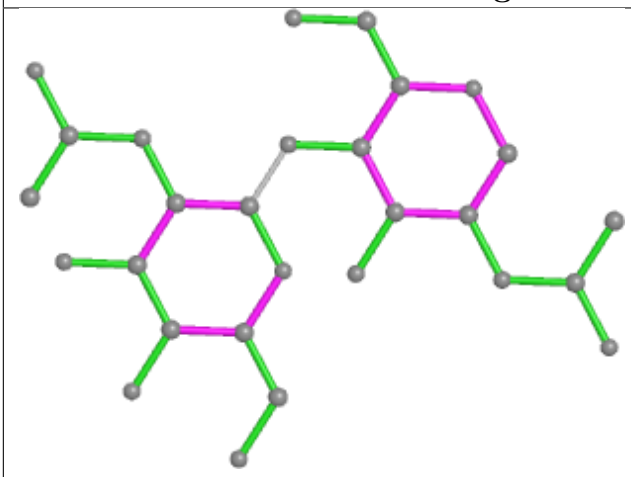
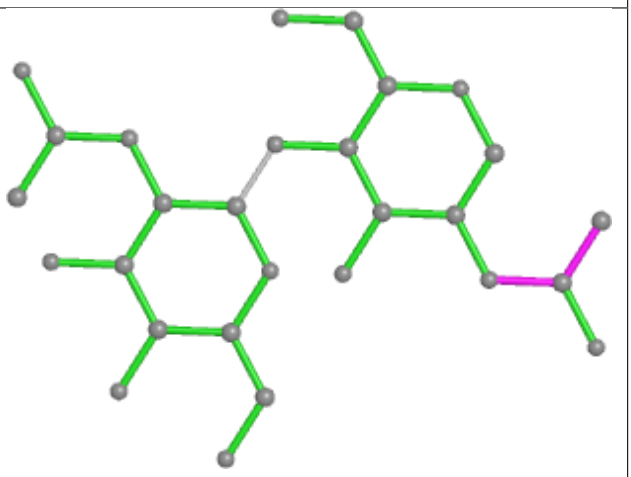
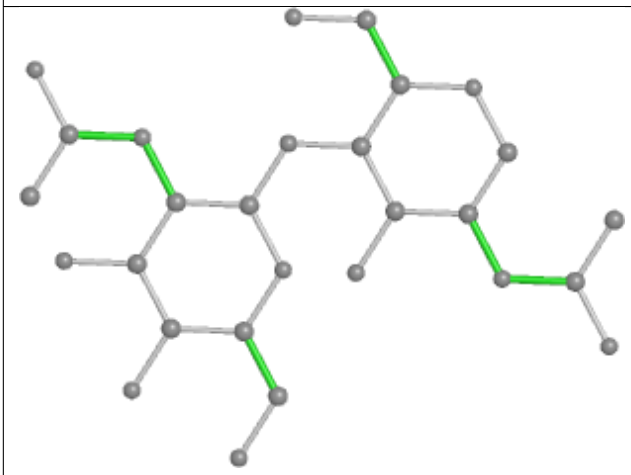
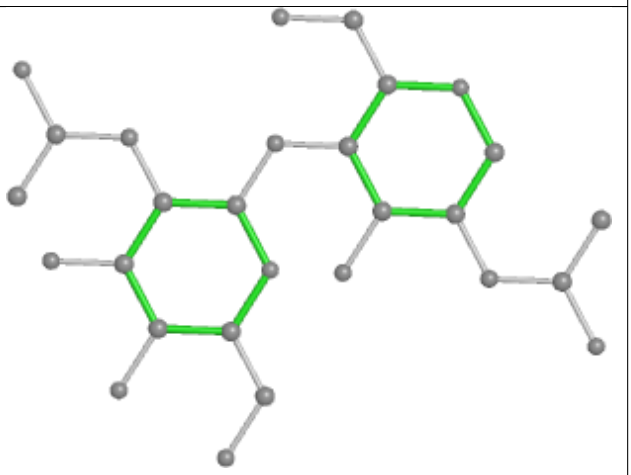
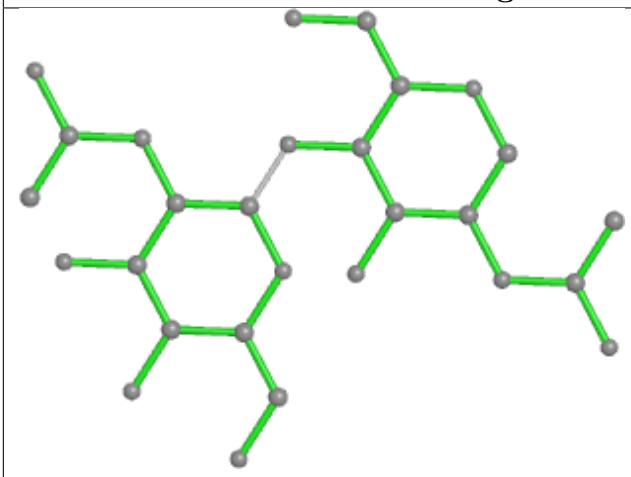


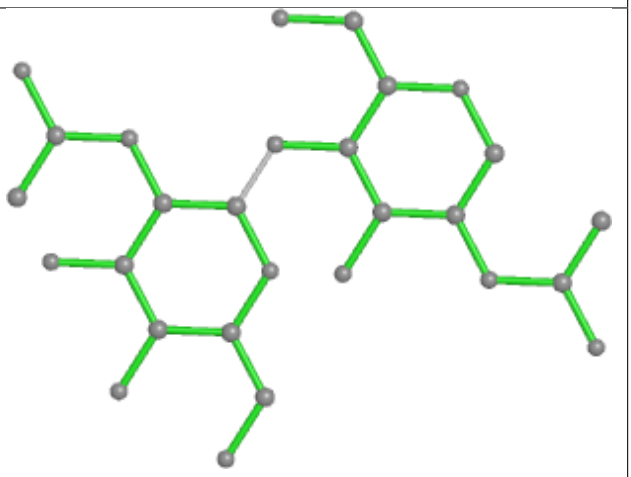
Rings

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

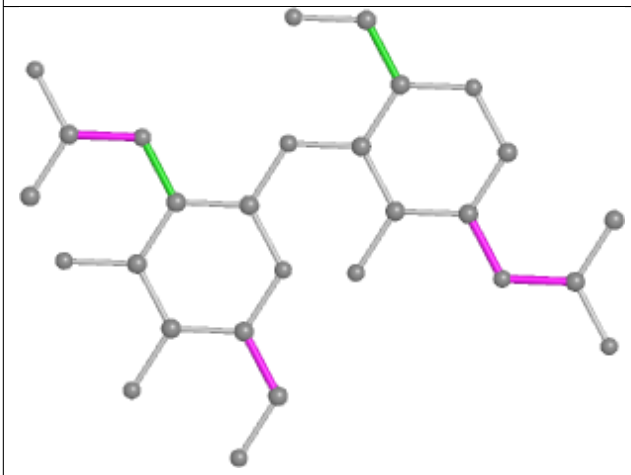
Oligosaccharide Chain Z



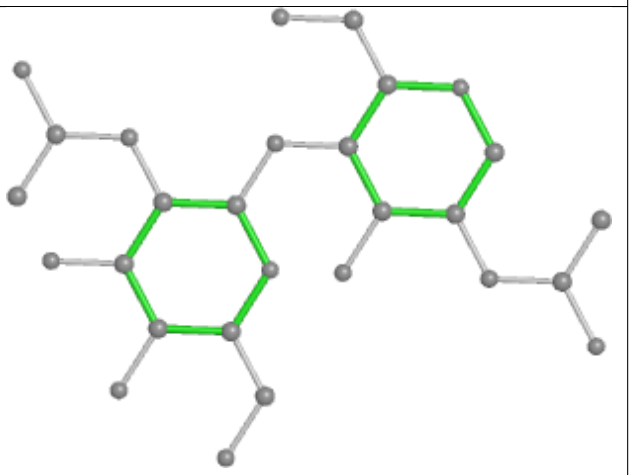
Bond lengths



Bond angles

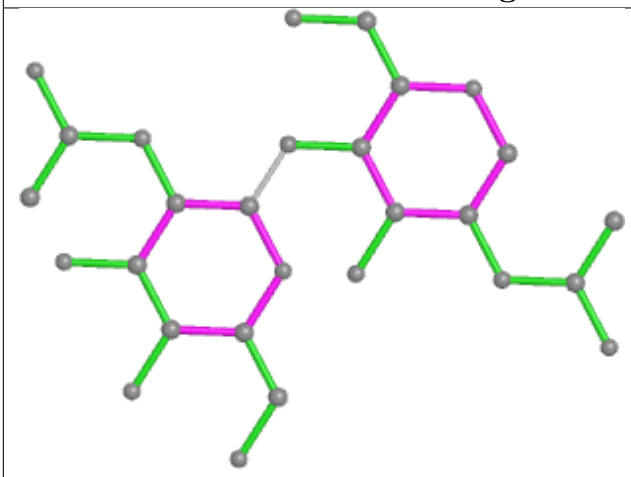


Torsions

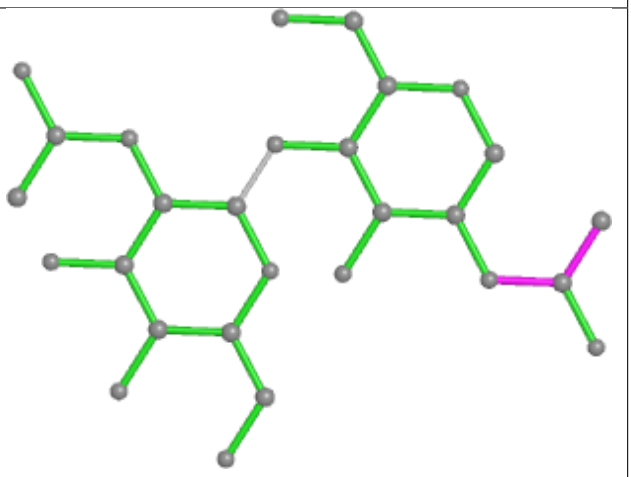


Rings

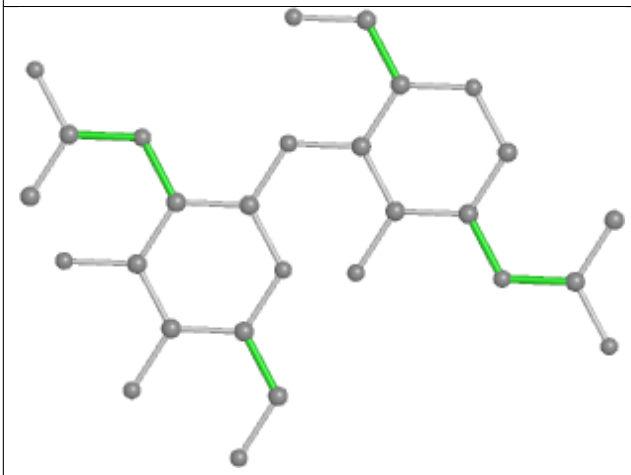
Oligosaccharide Chain a



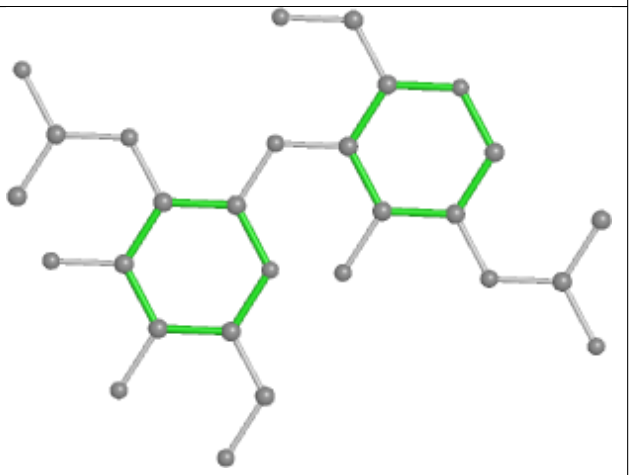
Bond lengths



Bond angles

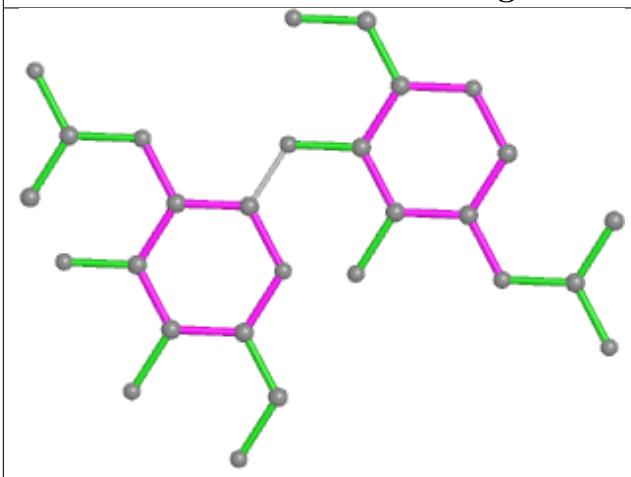


Torsions

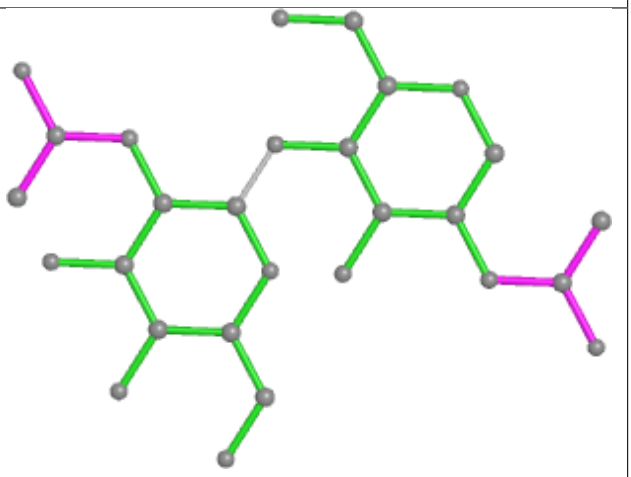


Rings

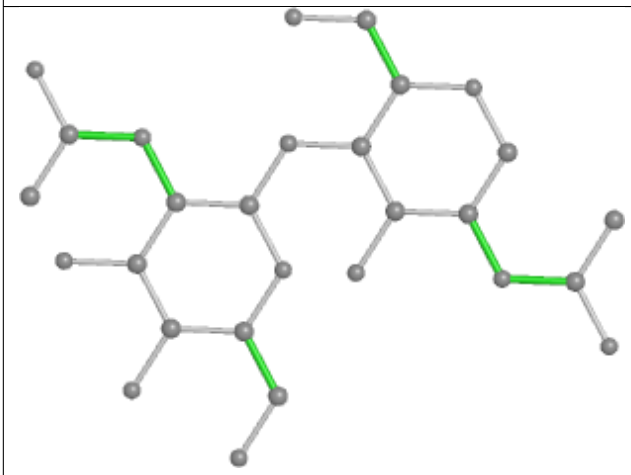
Oligosaccharide Chain b



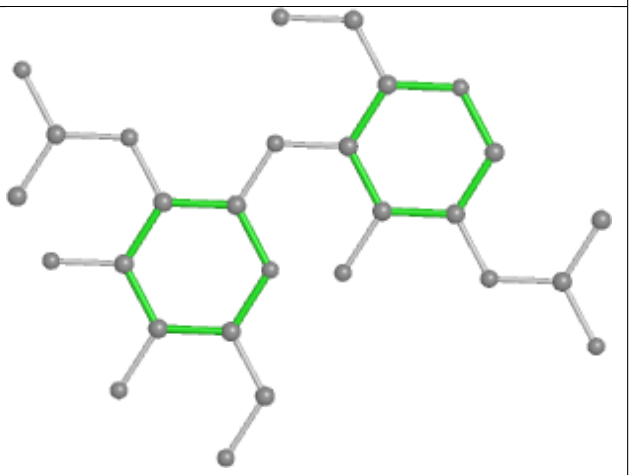
Bond lengths



Bond angles

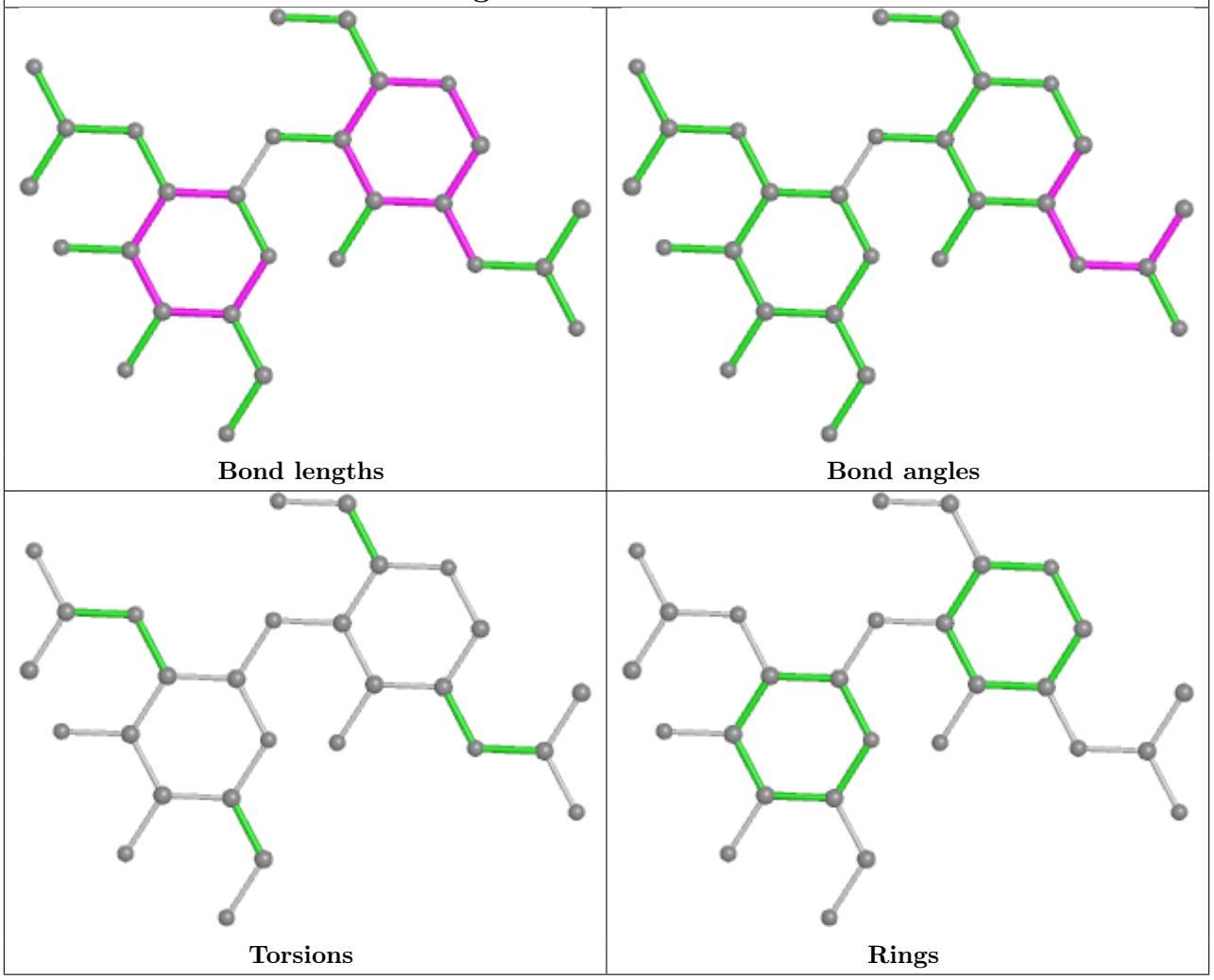


Torsions



Rings

Oligosaccharide Chain c



5.6 Ligand geometry (i)

44 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	$\#\|Z\| > 2$
6	NAG	F	701	1	14,14,15	0.40	0	17,19,21	0.50	0
6	NAG	E	708	1	14,14,15	0.38	0	17,19,21	0.44	0
6	NAG	C	707	1	14,14,15	2.15	6 (42%)	17,19,21	1.07	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
6	NAG	C	705	1	14,14,15	2.14	6 (42%)	17,19,21	0.98	1 (5%)
6	NAG	A	710	1	14,14,15	2.09	5 (35%)	17,19,21	1.00	1 (5%)
6	NAG	E	701	1	14,14,15	2.06	5 (35%)	17,19,21	1.00	1 (5%)
6	NAG	B	702	1	14,14,15	0.37	0	17,19,21	0.37	0
6	NAG	A	708	1	14,14,15	2.17	5 (35%)	17,19,21	0.95	1 (5%)
6	NAG	F	703	1	14,14,15	2.11	6 (42%)	17,19,21	0.94	1 (5%)
6	NAG	E	705	1	14,14,15	2.16	6 (42%)	17,19,21	1.03	1 (5%)
6	NAG	D	701	1	14,14,15	0.39	0	17,19,21	0.46	0
6	NAG	A	705	1	14,14,15	2.10	4 (28%)	17,19,21	1.05	1 (5%)
6	NAG	F	702	1	14,14,15	2.16	6 (42%)	17,19,21	0.92	0
6	NAG	E	703	1	14,14,15	1.97	5 (35%)	17,19,21	1.01	0
6	NAG	A	702	1	14,14,15	2.12	5 (35%)	17,19,21	1.05	2 (11%)
6	NAG	C	706	1	14,14,15	2.15	6 (42%)	17,19,21	1.02	1 (5%)
6	NAG	A	711	1	14,14,15	2.18	6 (42%)	17,19,21	0.95	2 (11%)
6	NAG	E	702	1	14,14,15	0.37	0	17,19,21	0.46	0
6	NAG	A	707	1	14,14,15	0.39	0	17,19,21	0.41	0
6	NAG	A	712	1	14,14,15	2.18	6 (42%)	17,19,21	1.01	1 (5%)
6	NAG	C	711	1	14,14,15	2.22	6 (42%)	17,19,21	1.04	1 (5%)
6	NAG	A	709	1	14,14,15	2.04	6 (42%)	17,19,21	1.09	1 (5%)
6	NAG	B	703	1	14,14,15	2.13	6 (42%)	17,19,21	0.98	1 (5%)
6	NAG	A	701	1	14,14,15	2.17	5 (35%)	17,19,21	0.97	1 (5%)
6	NAG	A	706	1	14,14,15	0.39	0	17,19,21	0.38	0
6	NAG	C	702	1	14,14,15	0.39	0	17,19,21	0.44	0
6	NAG	C	708	1	14,14,15	2.07	5 (35%)	17,19,21	1.03	1 (5%)
6	NAG	C	709	1	14,14,15	2.14	7 (50%)	17,19,21	1.07	1 (5%)
6	NAG	D	702	1	14,14,15	2.07	7 (50%)	17,19,21	1.00	1 (5%)
6	NAG	E	706	1	14,14,15	0.38	0	17,19,21	0.47	0
6	NAG	C	701	1	14,14,15	2.13	5 (35%)	17,19,21	0.97	1 (5%)
6	NAG	A	704	1	14,14,15	2.02	5 (35%)	17,19,21	1.06	1 (5%)
6	NAG	E	707	1	14,14,15	2.15	5 (35%)	17,19,21	0.93	0
6	NAG	E	711	1	14,14,15	2.16	5 (35%)	17,19,21	0.91	1 (5%)
6	NAG	E	704	1	14,14,15	2.20	5 (35%)	17,19,21	0.99	1 (5%)
6	NAG	E	712	1	14,14,15	2.18	6 (42%)	17,19,21	1.01	1 (5%)
6	NAG	C	710	1	14,14,15	2.19	6 (42%)	17,19,21	0.99	0
6	NAG	E	709	1	14,14,15	2.09	5 (35%)	17,19,21	1.08	3 (17%)
6	NAG	A	703	1	14,14,15	2.09	6 (42%)	17,19,21	1.06	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
6	NAG	E	713	1	14,14,15	2.15	5 (35%)	17,19,21	1.14	2 (11%)
6	NAG	C	703	1	14,14,15	2.04	6 (42%)	17,19,21	1.06	1 (5%)
6	NAG	E	710	1	14,14,15	2.12	5 (35%)	17,19,21	0.93	1 (5%)
6	NAG	B	701	1	14,14,15	2.21	5 (35%)	17,19,21	1.07	2 (11%)
6	NAG	C	704	1	14,14,15	0.38	0	17,19,21	0.42	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
6	NAG	F	701	1	-	4/6/23/26	0/1/1/1
6	NAG	E	708	1	-	2/6/23/26	0/1/1/1
6	NAG	C	707	1	-	1/6/23/26	0/1/1/1
6	NAG	C	705	1	-	0/6/23/26	0/1/1/1
6	NAG	A	710	1	-	0/6/23/26	0/1/1/1
6	NAG	E	701	1	-	1/6/23/26	0/1/1/1
6	NAG	B	702	1	-	3/6/23/26	0/1/1/1
6	NAG	A	708	1	-	2/6/23/26	0/1/1/1
6	NAG	F	703	1	-	0/6/23/26	0/1/1/1
6	NAG	E	705	1	-	0/6/23/26	0/1/1/1
6	NAG	D	701	1	-	3/6/23/26	0/1/1/1
6	NAG	A	705	1	-	0/6/23/26	0/1/1/1
6	NAG	F	702	1	-	0/6/23/26	0/1/1/1
6	NAG	E	703	1	-	2/6/23/26	0/1/1/1
6	NAG	A	702	1	-	0/6/23/26	0/1/1/1
6	NAG	C	706	1	-	0/6/23/26	0/1/1/1
6	NAG	A	711	1	-	0/6/23/26	0/1/1/1
6	NAG	E	702	1	-	2/6/23/26	0/1/1/1
6	NAG	A	707	1	-	4/6/23/26	0/1/1/1
6	NAG	A	712	1	-	0/6/23/26	0/1/1/1
6	NAG	C	711	1	-	0/6/23/26	0/1/1/1
6	NAG	A	709	1	-	1/6/23/26	0/1/1/1
6	NAG	B	703	1	-	0/6/23/26	0/1/1/1
6	NAG	A	701	1	-	0/6/23/26	0/1/1/1
6	NAG	A	706	1	-	2/6/23/26	0/1/1/1
6	NAG	C	702	1	-	4/6/23/26	0/1/1/1
6	NAG	C	708	1	-	1/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	NAG	C	709	1	-	0/6/23/26	0/1/1/1
6	NAG	D	702	1	-	0/6/23/26	0/1/1/1
6	NAG	E	706	1	-	4/6/23/26	0/1/1/1
6	NAG	C	701	1	-	0/6/23/26	0/1/1/1
6	NAG	A	704	1	-	1/6/23/26	0/1/1/1
6	NAG	E	707	1	-	1/6/23/26	0/1/1/1
6	NAG	E	711	1	-	0/6/23/26	0/1/1/1
6	NAG	E	704	1	-	0/6/23/26	0/1/1/1
6	NAG	E	712	1	-	0/6/23/26	0/1/1/1
6	NAG	C	710	1	-	2/6/23/26	0/1/1/1
6	NAG	E	709	1	-	2/6/23/26	0/1/1/1
6	NAG	A	703	1	-	0/6/23/26	0/1/1/1
6	NAG	E	713	1	-	0/6/23/26	0/1/1/1
6	NAG	C	703	1	-	1/6/23/26	0/1/1/1
6	NAG	E	710	1	-	0/6/23/26	0/1/1/1
6	NAG	B	701	1	-	1/6/23/26	0/1/1/1
6	NAG	C	704	1	-	5/6/23/26	0/1/1/1

All (188) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	701	NAG	C1-C2	5.75	1.60	1.52
6	C	701	NAG	C1-C2	5.55	1.60	1.52
6	E	704	NAG	C1-C2	5.51	1.60	1.52
6	A	711	NAG	C1-C2	5.47	1.60	1.52
6	B	701	NAG	C1-C2	5.41	1.60	1.52
6	C	711	NAG	C1-C2	5.40	1.60	1.52
6	E	713	NAG	C1-C2	5.40	1.60	1.52
6	A	708	NAG	C1-C2	5.39	1.60	1.52
6	E	707	NAG	C1-C2	5.38	1.60	1.52
6	E	712	NAG	C1-C2	5.34	1.60	1.52
6	A	702	NAG	C1-C2	5.31	1.60	1.52
6	F	702	NAG	C1-C2	5.28	1.60	1.52
6	C	705	NAG	C1-C2	5.27	1.60	1.52
6	C	706	NAG	C1-C2	5.26	1.60	1.52
6	C	707	NAG	C1-C2	5.26	1.60	1.52
6	B	703	NAG	C1-C2	5.24	1.60	1.52
6	E	711	NAG	C1-C2	5.22	1.60	1.52
6	A	712	NAG	C1-C2	5.21	1.60	1.52
6	E	705	NAG	C1-C2	5.21	1.60	1.52
6	E	701	NAG	C1-C2	5.19	1.60	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	710	NAG	C1-C2	5.19	1.60	1.52
6	C	710	NAG	C1-C2	5.10	1.60	1.52
6	A	704	NAG	C1-C2	5.01	1.59	1.52
6	A	705	NAG	C1-C2	5.01	1.59	1.52
6	C	703	NAG	C1-C2	4.95	1.59	1.52
6	F	703	NAG	C1-C2	4.95	1.59	1.52
6	A	703	NAG	C1-C2	4.92	1.59	1.52
6	C	708	NAG	C1-C2	4.89	1.59	1.52
6	E	710	NAG	C1-C2	4.88	1.59	1.52
6	E	703	NAG	C1-C2	4.77	1.59	1.52
6	C	709	NAG	C1-C2	4.76	1.59	1.52
6	D	702	NAG	C1-C2	4.73	1.59	1.52
6	E	709	NAG	C1-C2	4.71	1.59	1.52
6	A	709	NAG	C1-C2	4.60	1.59	1.52
6	C	710	NAG	O5-C5	3.46	1.50	1.43
6	A	712	NAG	O5-C5	3.37	1.50	1.43
6	C	711	NAG	O5-C5	3.37	1.50	1.43
6	E	711	NAG	O5-C5	3.35	1.50	1.43
6	A	708	NAG	O5-C5	3.34	1.50	1.43
6	E	704	NAG	O5-C5	3.34	1.50	1.43
6	E	709	NAG	O5-C5	3.33	1.50	1.43
6	E	710	NAG	O5-C5	3.29	1.50	1.43
6	A	705	NAG	O5-C5	3.27	1.50	1.43
6	E	712	NAG	O5-C5	3.26	1.50	1.43
6	A	709	NAG	O5-C5	3.24	1.50	1.43
6	C	709	NAG	O5-C5	3.20	1.49	1.43
6	D	702	NAG	O5-C5	3.19	1.49	1.43
6	B	701	NAG	O5-C5	3.18	1.49	1.43
6	F	702	NAG	O5-C5	3.16	1.49	1.43
6	C	706	NAG	O5-C5	3.14	1.49	1.43
6	A	710	NAG	O5-C5	3.14	1.49	1.43
6	A	711	NAG	O5-C5	3.13	1.49	1.43
6	A	703	NAG	O5-C5	3.12	1.49	1.43
6	C	707	NAG	O5-C5	3.11	1.49	1.43
6	E	701	NAG	O5-C5	3.11	1.49	1.43
6	C	705	NAG	O5-C5	3.09	1.49	1.43
6	C	708	NAG	O5-C5	3.08	1.49	1.43
6	B	703	NAG	O5-C5	3.08	1.49	1.43
6	E	709	NAG	O5-C1	3.06	1.48	1.43
6	E	707	NAG	O5-C5	3.05	1.49	1.43
6	A	705	NAG	O5-C1	3.04	1.48	1.43
6	E	705	NAG	O5-C5	3.03	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	F	703	NAG	O5-C5	3.02	1.49	1.43
6	A	702	NAG	O5-C5	3.02	1.49	1.43
6	E	704	NAG	O5-C1	3.02	1.48	1.43
6	A	704	NAG	O5-C5	3.01	1.49	1.43
6	C	703	NAG	O5-C5	3.00	1.49	1.43
6	E	713	NAG	O5-C5	3.00	1.49	1.43
6	C	711	NAG	O5-C1	2.98	1.48	1.43
6	E	712	NAG	O5-C1	2.98	1.48	1.43
6	A	708	NAG	O5-C1	2.97	1.48	1.43
6	A	712	NAG	O5-C1	2.96	1.48	1.43
6	C	701	NAG	O5-C5	2.94	1.49	1.43
6	C	710	NAG	O5-C1	2.94	1.48	1.43
6	E	703	NAG	O5-C5	2.94	1.49	1.43
6	B	701	NAG	O5-C1	2.89	1.48	1.43
6	A	701	NAG	O5-C5	2.89	1.49	1.43
6	C	708	NAG	O5-C1	2.87	1.48	1.43
6	F	703	NAG	O5-C1	2.85	1.48	1.43
6	E	701	NAG	O5-C1	2.84	1.48	1.43
6	E	710	NAG	O5-C1	2.83	1.48	1.43
6	A	702	NAG	C3-C2	2.81	1.58	1.52
6	E	707	NAG	O5-C1	2.80	1.48	1.43
6	B	703	NAG	O5-C1	2.80	1.48	1.43
6	E	711	NAG	O5-C1	2.78	1.48	1.43
6	F	702	NAG	O5-C1	2.77	1.48	1.43
6	E	713	NAG	O5-C1	2.76	1.48	1.43
6	A	710	NAG	O5-C1	2.76	1.48	1.43
6	A	709	NAG	O5-C1	2.75	1.48	1.43
6	C	707	NAG	C3-C2	2.75	1.58	1.52
6	C	703	NAG	O5-C1	2.74	1.48	1.43
6	A	711	NAG	O5-C1	2.73	1.48	1.43
6	C	709	NAG	O5-C1	2.73	1.48	1.43
6	C	701	NAG	O5-C1	2.70	1.48	1.43
6	E	705	NAG	O5-C1	2.70	1.48	1.43
6	C	705	NAG	O5-C1	2.70	1.48	1.43
6	A	704	NAG	O5-C1	2.68	1.48	1.43
6	E	703	NAG	O5-C1	2.67	1.48	1.43
6	E	705	NAG	C3-C2	2.67	1.58	1.52
6	C	706	NAG	O5-C1	2.64	1.47	1.43
6	C	707	NAG	O5-C1	2.64	1.47	1.43
6	A	701	NAG	O5-C1	2.63	1.47	1.43
6	D	702	NAG	O5-C1	2.62	1.47	1.43
6	C	709	NAG	C2-N2	2.56	1.50	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	702	NAG	O5-C1	2.55	1.47	1.43
6	B	701	NAG	C3-C2	2.54	1.57	1.52
6	C	708	NAG	C4-C5	2.51	1.58	1.53
6	E	707	NAG	C3-C2	2.48	1.57	1.52
6	A	703	NAG	O5-C1	2.48	1.47	1.43
6	E	710	NAG	C3-C2	2.46	1.57	1.52
6	C	706	NAG	C3-C2	2.44	1.57	1.52
6	A	701	NAG	C3-C2	2.43	1.57	1.52
6	C	710	NAG	C4-C5	2.42	1.58	1.53
6	A	709	NAG	C4-C5	2.40	1.58	1.53
6	E	704	NAG	C3-C2	2.40	1.57	1.52
6	C	705	NAG	C3-C2	2.38	1.57	1.52
6	F	703	NAG	C3-C2	2.37	1.57	1.52
6	E	713	NAG	C3-C2	2.36	1.57	1.52
6	A	705	NAG	C3-C2	2.36	1.57	1.52
6	C	711	NAG	C3-C2	2.36	1.57	1.52
6	C	701	NAG	C3-C2	2.35	1.57	1.52
6	A	711	NAG	C4-C5	2.35	1.58	1.53
6	C	709	NAG	C4-C5	2.34	1.58	1.53
6	D	702	NAG	C4-C5	2.34	1.58	1.53
6	F	703	NAG	C4-C5	2.33	1.57	1.53
6	E	710	NAG	C4-C5	2.32	1.57	1.53
6	E	711	NAG	C4-C5	2.32	1.57	1.53
6	E	701	NAG	C3-C2	2.30	1.57	1.52
6	A	703	NAG	C4-C5	2.30	1.57	1.53
6	C	710	NAG	C3-C2	2.29	1.57	1.52
6	F	702	NAG	C3-C2	2.29	1.57	1.52
6	B	703	NAG	C3-C2	2.29	1.57	1.52
6	F	702	NAG	C4-C5	2.28	1.57	1.53
6	B	701	NAG	C4-C5	2.28	1.57	1.53
6	D	702	NAG	C3-C2	2.27	1.57	1.52
6	E	711	NAG	C3-C2	2.27	1.57	1.52
6	E	709	NAG	C3-C2	2.26	1.57	1.52
6	A	712	NAG	C3-C2	2.26	1.57	1.52
6	C	706	NAG	C4-C5	2.25	1.57	1.53
6	A	710	NAG	C3-C2	2.25	1.57	1.52
6	C	709	NAG	C4-C3	2.25	1.58	1.52
6	A	711	NAG	C3-C2	2.24	1.57	1.52
6	C	709	NAG	C3-C2	2.23	1.57	1.52
6	E	705	NAG	C2-N2	2.23	1.50	1.46
6	E	712	NAG	C3-C2	2.23	1.57	1.52
6	C	710	NAG	C2-N2	2.22	1.50	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	703	NAG	C4-C5	2.22	1.57	1.53
6	A	709	NAG	C3-C2	2.21	1.57	1.52
6	A	712	NAG	C4-C5	2.21	1.57	1.53
6	C	707	NAG	C2-N2	2.19	1.50	1.46
6	A	703	NAG	C3-C2	2.19	1.57	1.52
6	A	708	NAG	C3-C2	2.18	1.57	1.52
6	C	703	NAG	C2-N2	2.16	1.50	1.46
6	E	709	NAG	C4-C5	2.15	1.57	1.53
6	E	707	NAG	C4-C5	2.15	1.57	1.53
6	E	703	NAG	C4-C5	2.15	1.57	1.53
6	A	704	NAG	C4-C5	2.15	1.57	1.53
6	A	708	NAG	C4-C5	2.14	1.57	1.53
6	E	712	NAG	C4-C5	2.13	1.57	1.53
6	C	705	NAG	C4-C5	2.12	1.57	1.53
6	C	708	NAG	C3-C2	2.10	1.57	1.52
6	C	703	NAG	C4-C5	2.10	1.57	1.53
6	D	702	NAG	C4-C3	2.10	1.57	1.52
6	A	710	NAG	C4-C5	2.10	1.57	1.53
6	E	713	NAG	C4-C5	2.08	1.57	1.53
6	D	702	NAG	C2-N2	2.08	1.49	1.46
6	C	705	NAG	C2-N2	2.07	1.49	1.46
6	A	704	NAG	C3-C2	2.07	1.56	1.52
6	E	705	NAG	C4-C5	2.07	1.57	1.53
6	C	711	NAG	C2-N2	2.07	1.49	1.46
6	E	703	NAG	C3-C2	2.06	1.56	1.52
6	A	709	NAG	C4-C3	2.06	1.57	1.52
6	B	703	NAG	C4-C3	2.05	1.57	1.52
6	C	707	NAG	C4-C5	2.04	1.57	1.53
6	C	711	NAG	C4-C5	2.04	1.57	1.53
6	E	704	NAG	C4-C5	2.04	1.57	1.53
6	A	701	NAG	C4-C5	2.03	1.57	1.53
6	F	702	NAG	C4-C3	2.03	1.57	1.52
6	A	703	NAG	C2-N2	2.03	1.49	1.46
6	A	702	NAG	C4-C5	2.03	1.57	1.53
6	C	706	NAG	C2-N2	2.03	1.49	1.46
6	A	711	NAG	C4-C3	2.02	1.57	1.52
6	F	703	NAG	C4-C3	2.02	1.57	1.52
6	C	701	NAG	C4-C5	2.01	1.57	1.53
6	A	712	NAG	C4-C3	2.01	1.57	1.52
6	E	701	NAG	C4-C5	2.00	1.57	1.53
6	E	712	NAG	C4-C3	2.00	1.57	1.52
6	C	703	NAG	C3-C2	2.00	1.56	1.52

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	C	709	NAG	C8-C7-N2	2.89	120.99	116.10
6	E	705	NAG	C8-C7-N2	2.73	120.72	116.10
6	C	711	NAG	C8-C7-N2	2.64	120.56	116.10
6	C	706	NAG	C8-C7-N2	2.63	120.55	116.10
6	E	713	NAG	C8-C7-N2	2.59	120.49	116.10
6	A	702	NAG	C8-C7-N2	2.56	120.43	116.10
6	D	702	NAG	C8-C7-N2	2.50	120.33	116.10
6	A	703	NAG	C8-C7-N2	2.48	120.30	116.10
6	C	703	NAG	C8-C7-N2	2.45	120.25	116.10
6	E	712	NAG	C8-C7-N2	2.44	120.22	116.10
6	C	705	NAG	C8-C7-N2	2.42	120.20	116.10
6	E	709	NAG	C8-C7-N2	2.41	120.18	116.10
6	A	712	NAG	C8-C7-N2	2.41	120.18	116.10
6	C	708	NAG	C1-C2-N2	-2.41	106.38	110.49
6	A	704	NAG	C8-C7-N2	2.36	120.09	116.10
6	A	705	NAG	C8-C7-N2	2.27	119.95	116.10
6	E	713	NAG	O7-C7-C8	-2.26	117.86	122.06
6	F	703	NAG	C8-C7-N2	2.22	119.87	116.10
6	A	710	NAG	C8-C7-N2	2.20	119.83	116.10
6	A	711	NAG	O7-C7-C8	-2.18	118.00	122.06
6	B	703	NAG	C8-C7-N2	2.18	119.80	116.10
6	E	704	NAG	O5-C1-C2	-2.18	107.85	111.29
6	A	701	NAG	C1-O5-C5	2.17	115.13	112.19
6	A	708	NAG	C8-C7-N2	2.16	119.75	116.10
6	B	701	NAG	C2-N2-C7	2.14	125.95	122.90
6	E	709	NAG	C1-C2-N2	-2.14	106.84	110.49
6	E	701	NAG	C1-O5-C5	2.12	115.06	112.19
6	A	711	NAG	C8-C7-N2	2.12	119.68	116.10
6	B	701	NAG	C8-C7-N2	2.10	119.65	116.10
6	E	711	NAG	C8-C7-N2	2.08	119.62	116.10
6	A	709	NAG	C1-C2-N2	-2.08	106.94	110.49
6	C	707	NAG	C8-C7-N2	2.03	119.54	116.10
6	A	702	NAG	O7-C7-C8	-2.03	118.29	122.06
6	C	701	NAG	C1-O5-C5	2.02	114.92	112.19
6	E	709	NAG	O7-C7-C8	-2.01	118.32	122.06
6	E	710	NAG	C8-C7-N2	2.01	119.50	116.10

There are no chirality outliers.

All (49) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	C	704	NAG	C3-C2-N2-C7
6	C	704	NAG	C8-C7-N2-C2
6	C	704	NAG	O7-C7-N2-C2
6	E	708	NAG	C8-C7-N2-C2
6	E	708	NAG	O7-C7-N2-C2
6	F	701	NAG	C8-C7-N2-C2
6	F	701	NAG	O7-C7-N2-C2
6	A	706	NAG	C8-C7-N2-C2
6	A	706	NAG	O7-C7-N2-C2
6	B	702	NAG	C3-C2-N2-C7
6	B	702	NAG	C8-C7-N2-C2
6	B	702	NAG	O7-C7-N2-C2
6	C	704	NAG	C4-C5-C6-O6
6	E	706	NAG	C8-C7-N2-C2
6	F	701	NAG	O5-C5-C6-O6
6	E	706	NAG	O5-C5-C6-O6
6	A	707	NAG	O5-C5-C6-O6
6	D	701	NAG	C8-C7-N2-C2
6	D	701	NAG	O7-C7-N2-C2
6	C	704	NAG	O5-C5-C6-O6
6	A	707	NAG	C4-C5-C6-O6
6	C	702	NAG	C8-C7-N2-C2
6	E	706	NAG	O7-C7-N2-C2
6	E	706	NAG	C4-C5-C6-O6
6	F	701	NAG	C4-C5-C6-O6
6	C	702	NAG	O7-C7-N2-C2
6	E	703	NAG	O5-C5-C6-O6
6	C	702	NAG	C1-C2-N2-C7
6	E	702	NAG	C8-C7-N2-C2
6	A	708	NAG	O5-C5-C6-O6
6	E	707	NAG	O5-C5-C6-O6
6	C	710	NAG	O5-C5-C6-O6
6	E	701	NAG	O5-C5-C6-O6
6	C	708	NAG	O5-C5-C6-O6
6	C	703	NAG	O5-C5-C6-O6
6	E	709	NAG	C4-C5-C6-O6
6	E	702	NAG	O7-C7-N2-C2
6	D	701	NAG	O5-C5-C6-O6
6	A	709	NAG	O5-C5-C6-O6
6	A	704	NAG	O5-C5-C6-O6
6	A	707	NAG	C8-C7-N2-C2
6	C	702	NAG	C3-C2-N2-C7
6	C	707	NAG	C3-C2-N2-C7

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Mol	Chain	Res	Type	Atoms
6	A	707	NAG	O7-C7-N2-C2
6	E	709	NAG	O5-C5-C6-O6
6	E	703	NAG	C4-C5-C6-O6
6	C	710	NAG	C3-C2-N2-C7
6	B	701	NAG	C3-C2-N2-C7
6	A	708	NAG	C4-C5-C6-O6

There are no ring outliers.

10 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	702	NAG	1	0
6	D	701	NAG	1	0
6	A	705	NAG	1	0
6	E	702	NAG	1	0
6	A	706	NAG	1	0
6	C	702	NAG	2	0
6	E	709	NAG	1	0
6	E	713	NAG	1	0
6	E	710	NAG	1	0
6	C	704	NAG	2	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

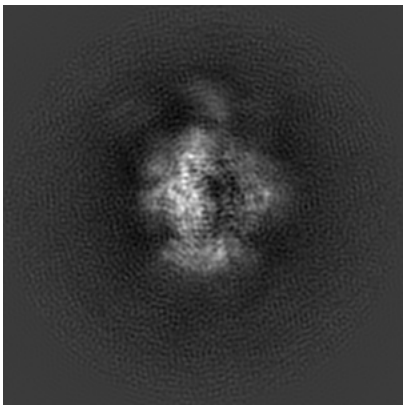
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-23231. These allow visual inspection of the internal detail of the map and identification of artifacts.

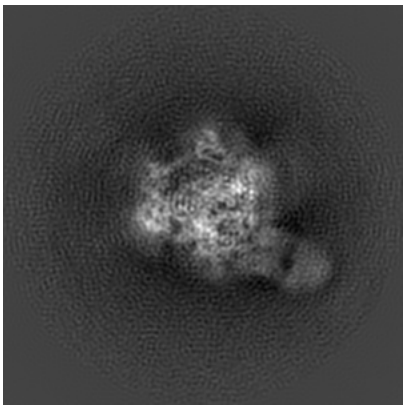
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

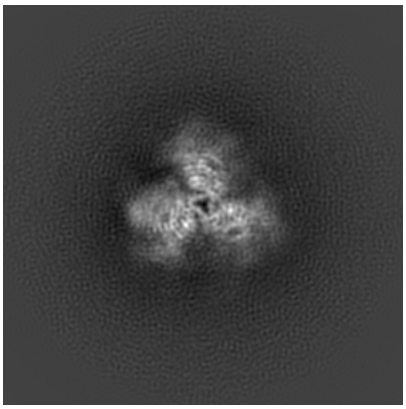
6.1.1 Primary map



X

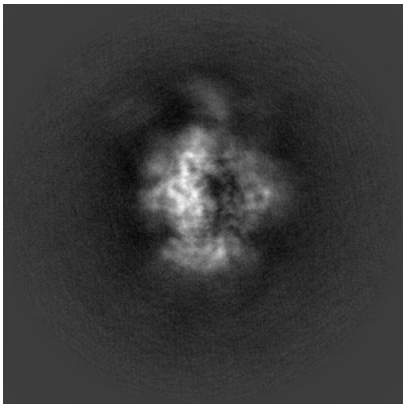


Y

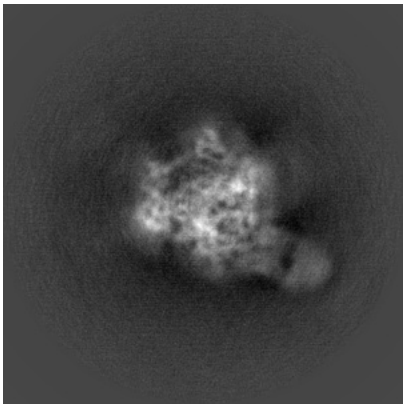


Z

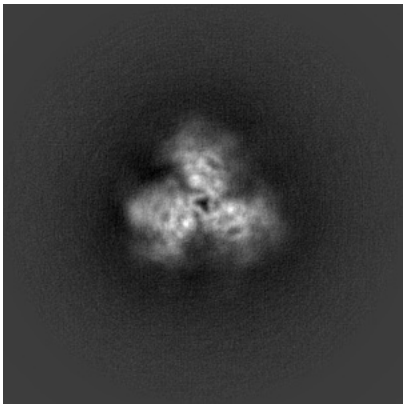
6.1.2 Raw map



X



Y

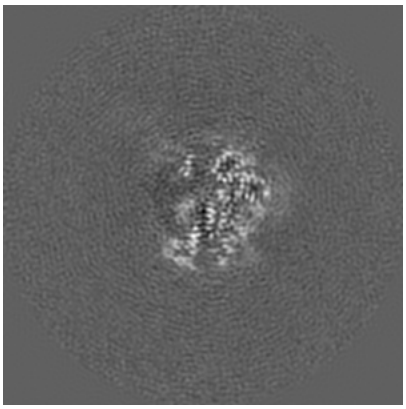


Z

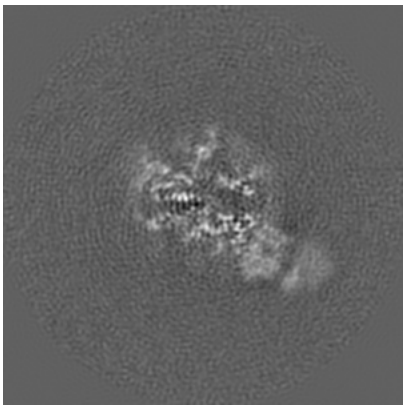
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

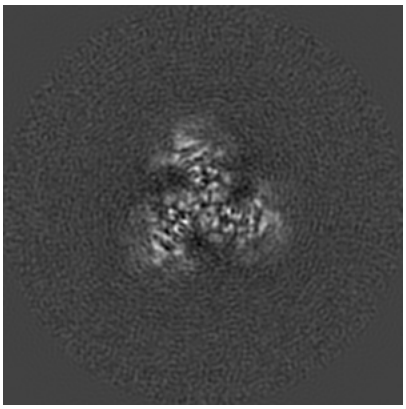
6.2.1 Primary map



X Index: 160

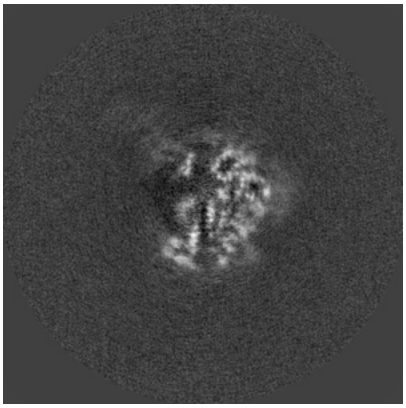


Y Index: 160

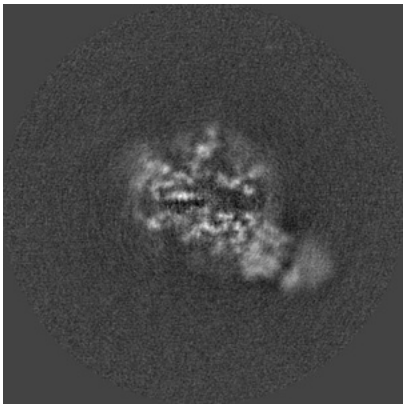


Z Index: 160

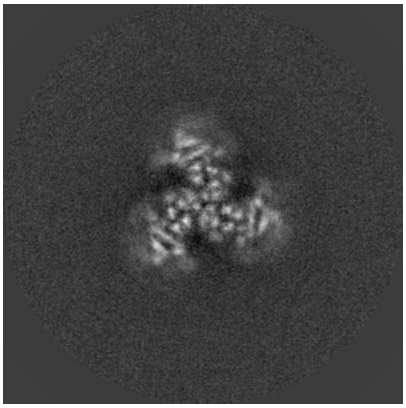
6.2.2 Raw map



X Index: 160



Y Index: 160

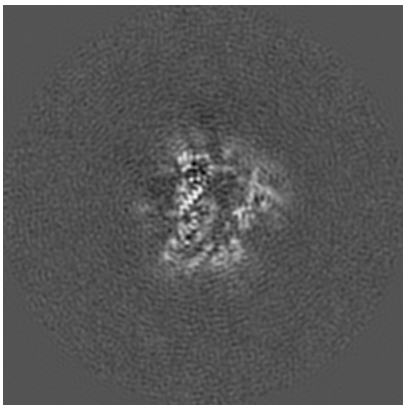


Z Index: 160

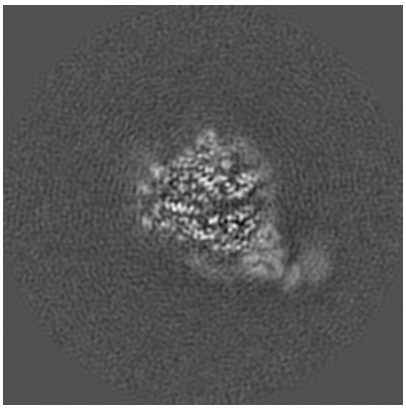
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

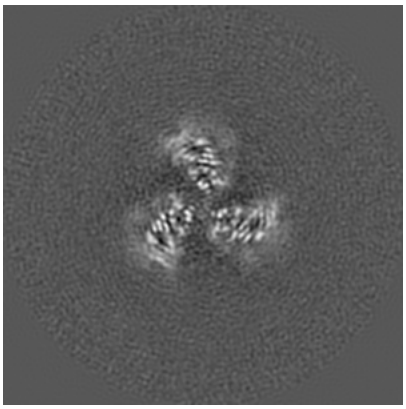
6.3.1 Primary map



X Index: 147

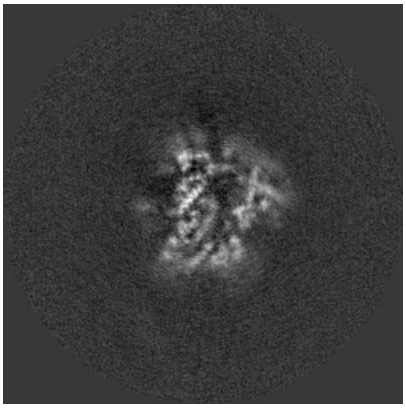


Y Index: 154

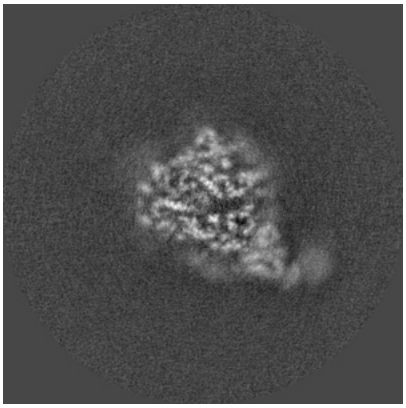


Z Index: 167

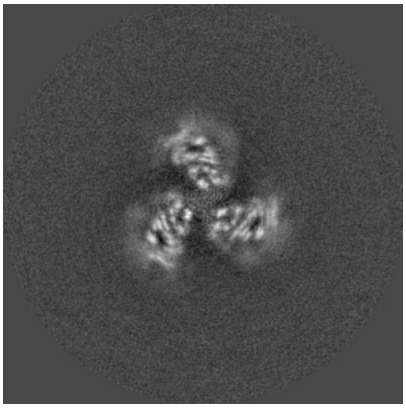
6.3.2 Raw map



X Index: 147



Y Index: 153



Z Index: 166

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

6.4 Orthogonal surface views (i)

6.4.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.015. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 Raw map

X Y Z

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

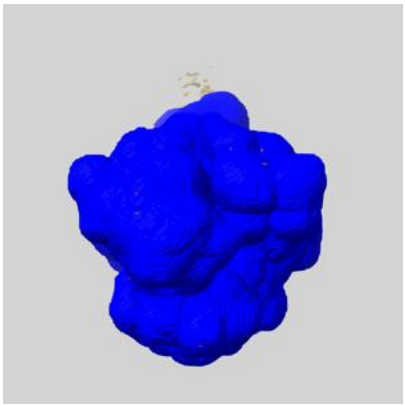
6.5 Mask visualisation (i)

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

A mask typically either:

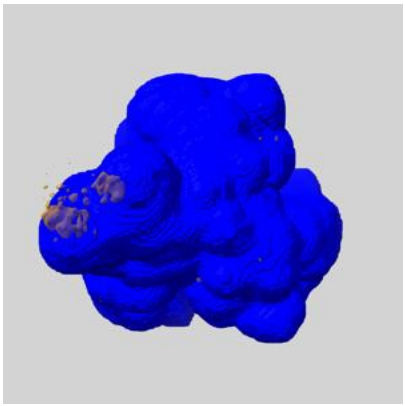
- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

6.5.1 emd_23231_msk_1.map (i)



X

Y

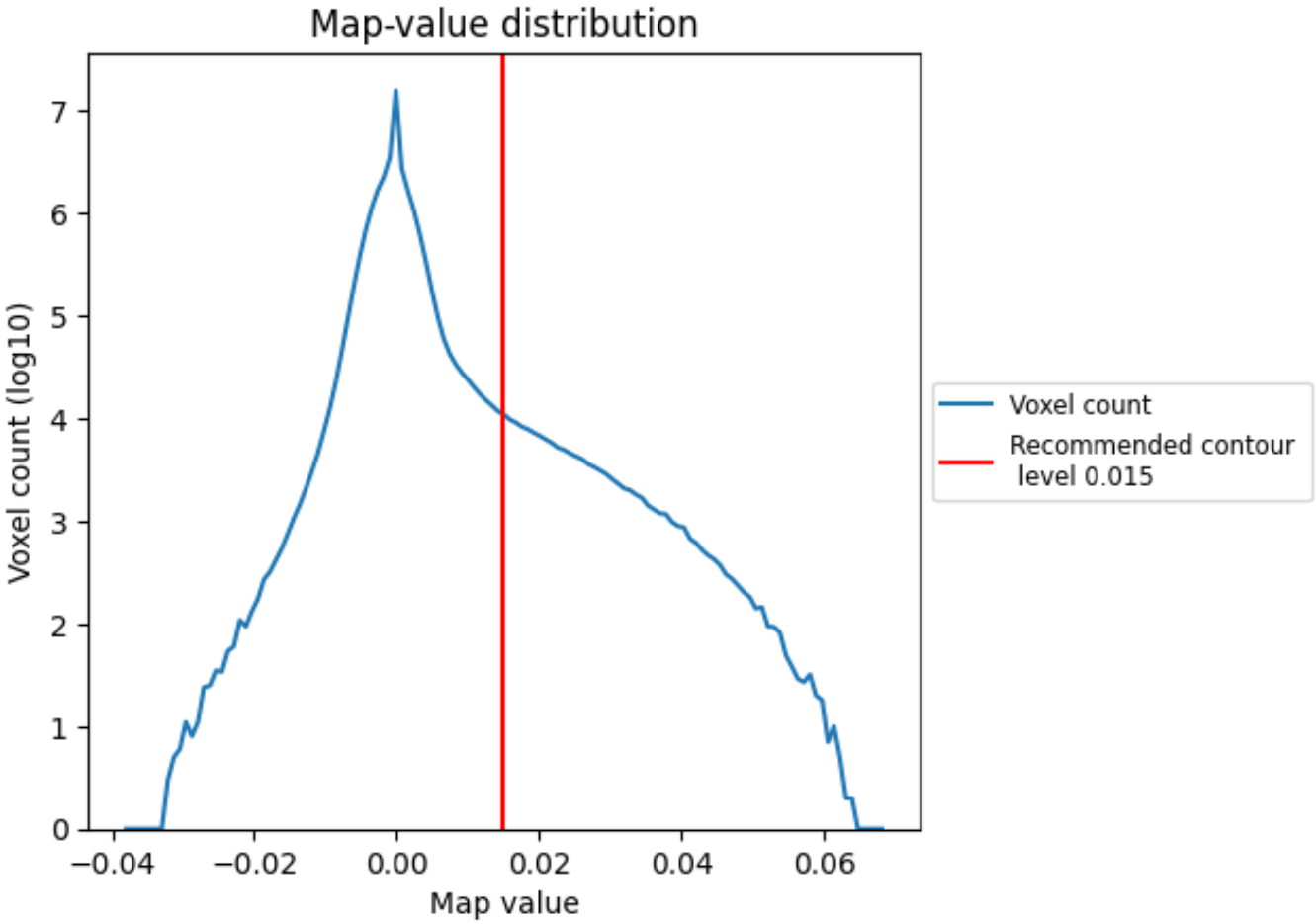


Z

7 Map analysis

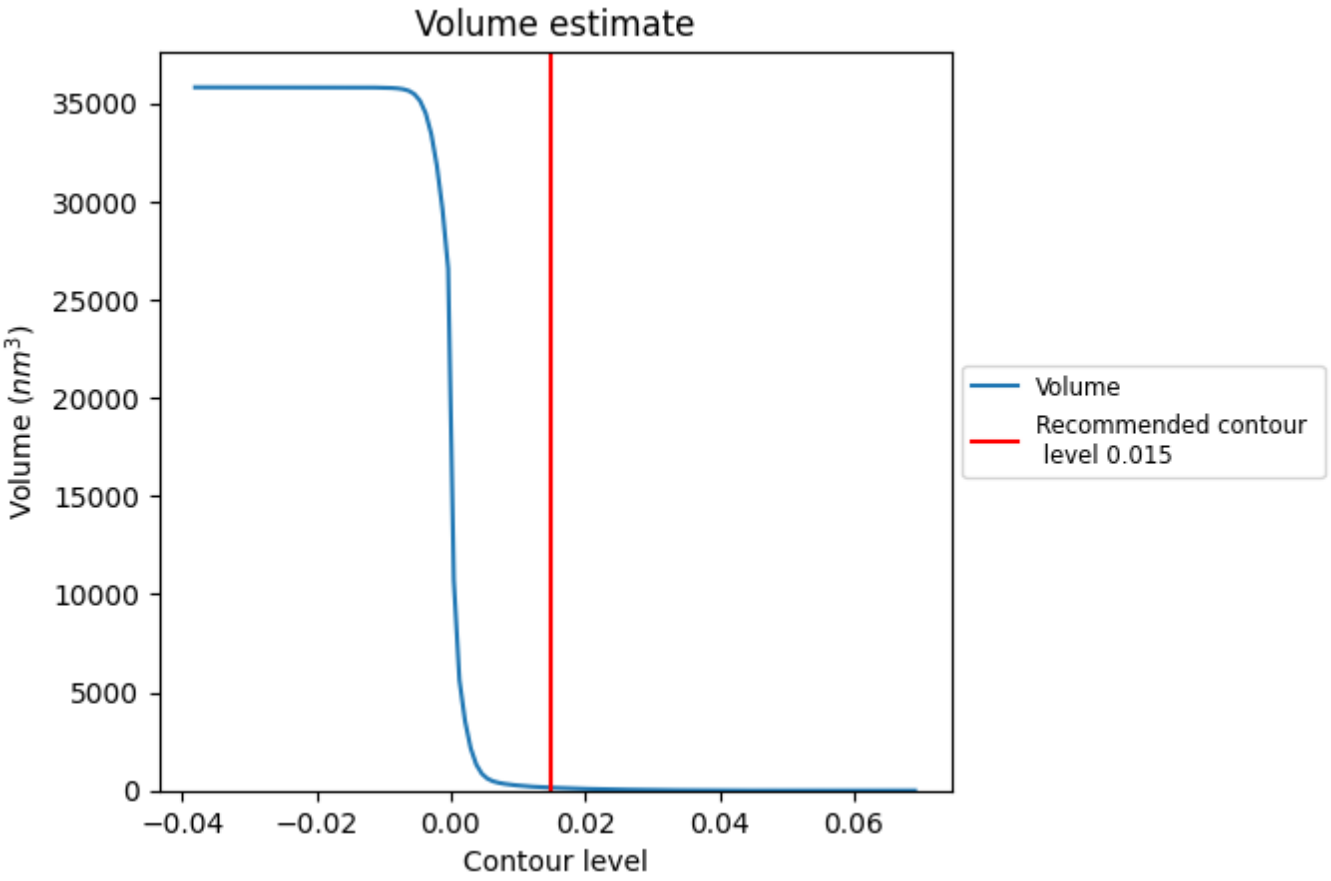
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

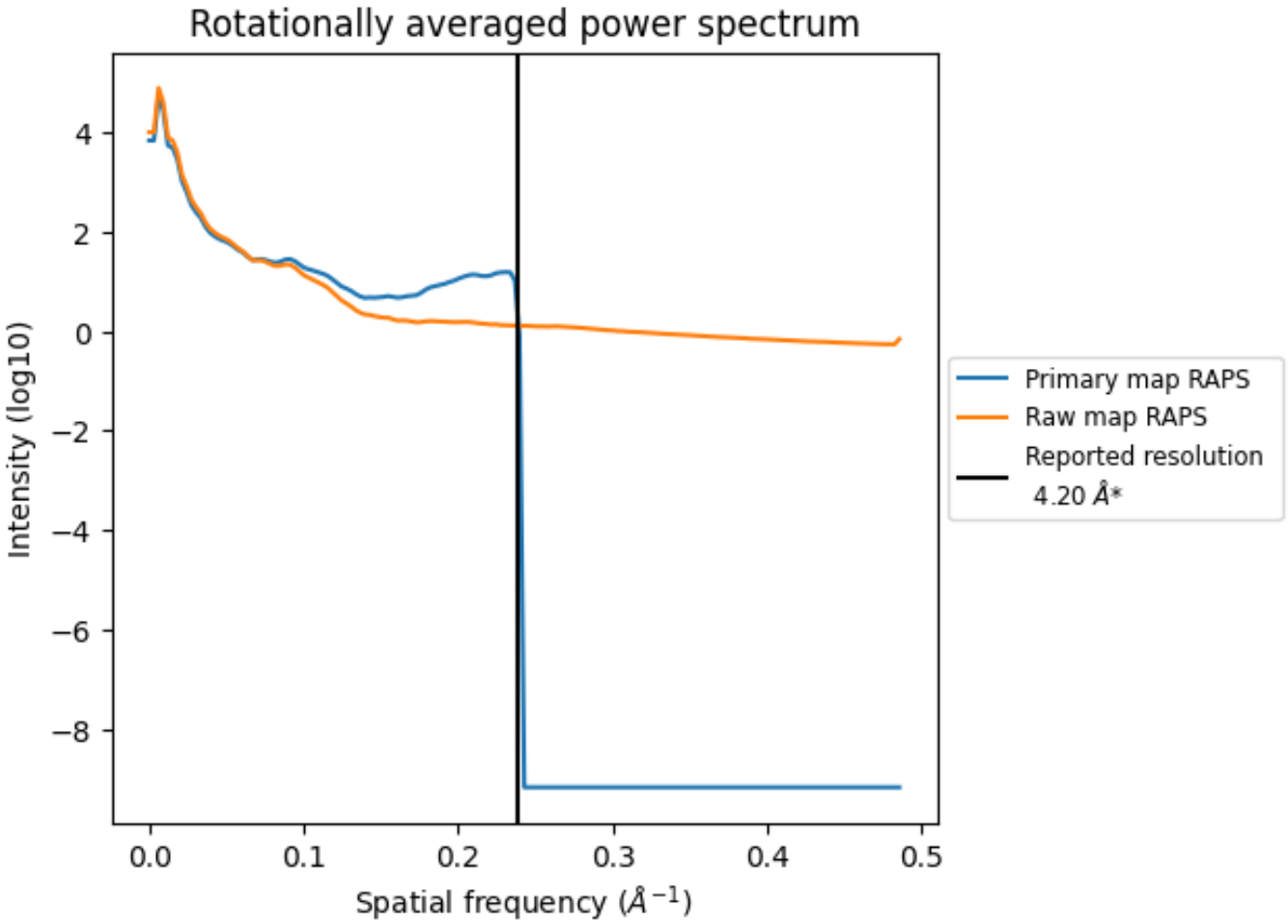
7.2 Volume estimate



The volume at the recommended contour level is 147 nm^3; this corresponds to an approximate mass of 133 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)

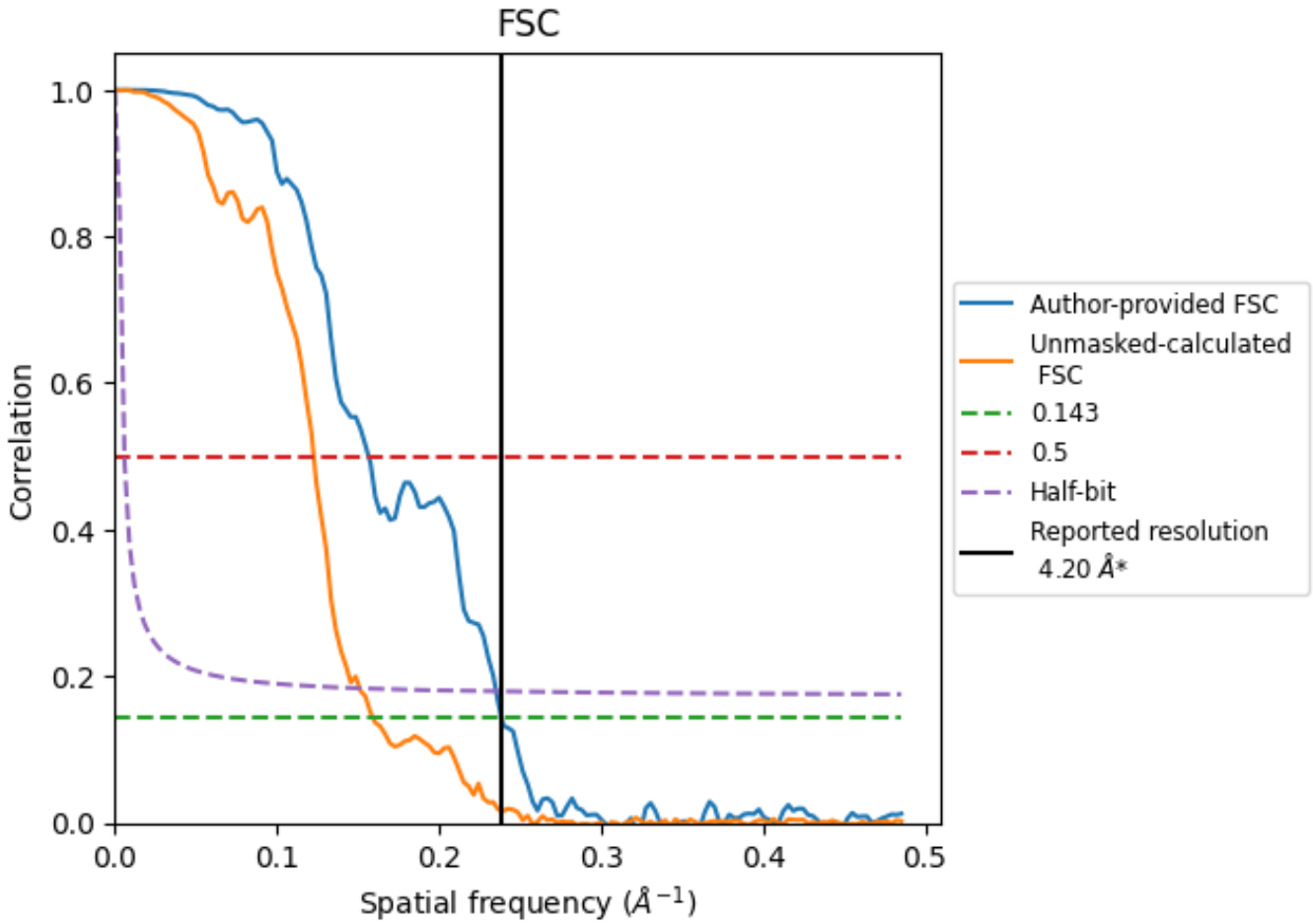


*Reported resolution corresponds to spatial frequency of 0.238 Å^{-1}

8 Fourier-Shell correlation

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.238 Å^{-1}

8.2 Resolution estimates (i)

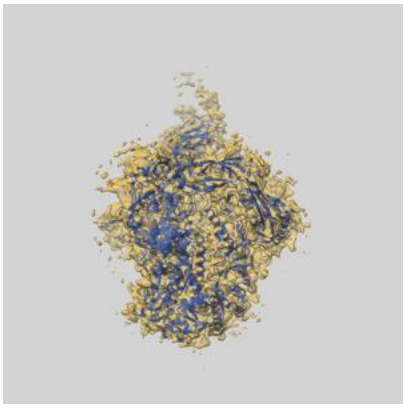
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.20	-	-
Author-provided FSC curve	4.19	6.39	4.25
Unmasked-calculated*	6.27	8.14	6.62

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 6.27 differs from the reported value 4.2 by more than 10 %

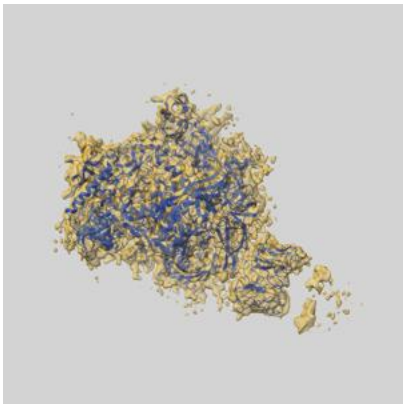
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-23231 and PDB model 7L8E. Per-residue inclusion information can be found in section 3 on page 17.

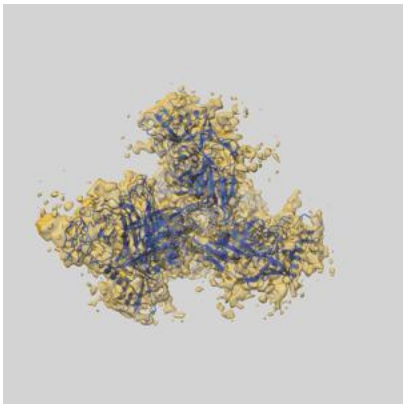
9.1 Map-model overlay



X



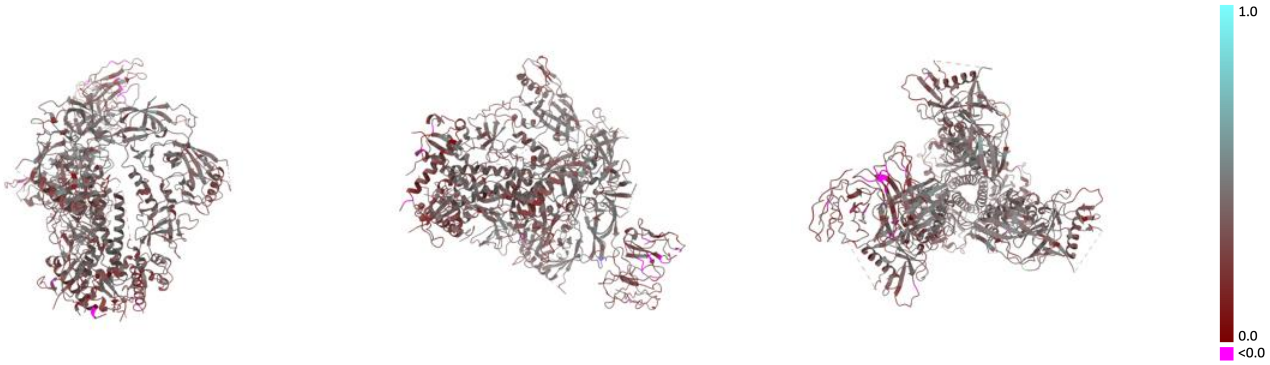
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.015 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.

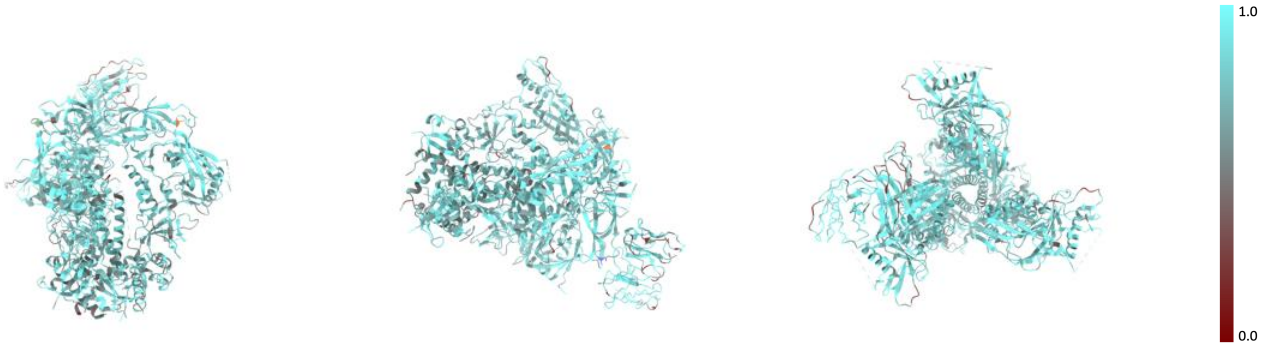
9.2 Q-score mapped to coordinate model (i)



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.

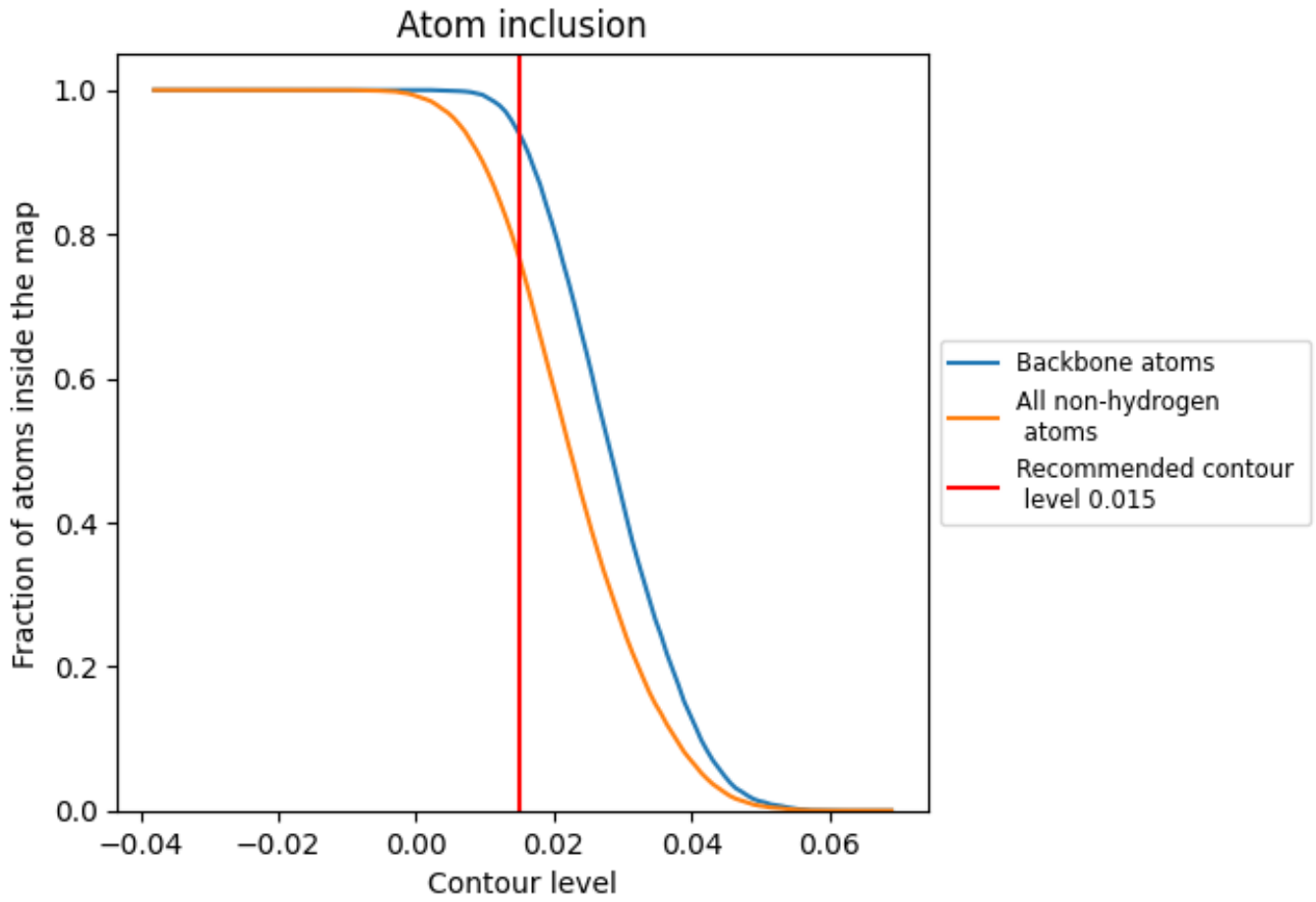
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.015).

9.4 Atom inclusion (i)



At the recommended contour level, 94% of all backbone atoms, 77% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.015) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7665	0.3620
A	0.7970	0.3850
B	0.7389	0.3320
C	0.7838	0.3770
D	0.7219	0.3150
E	0.7793	0.3800
F	0.7167	0.3270
G	0.7377	0.3990
H	0.8432	0.2800
I	0.5714	0.3980
J	0.5357	0.3860
K	0.3929	0.3580
L	0.7091	0.2660
M	0.4286	0.2850
N	0.7500	0.4080
O	0.6786	0.3820
P	0.7143	0.3530
Q	0.7049	0.3820
R	0.5000	0.3080
S	0.5714	0.3680
T	0.4643	0.3110
U	0.7143	0.4020
V	0.4286	0.2900
W	0.7500	0.3560
X	0.7541	0.4140
Y	0.5357	0.3340
Z	0.4643	0.2900
a	0.6071	0.3720
b	0.2143	0.2360
c	0.8214	0.3890