



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 08:27 AM UTC

PDB ID : 7L8F / pdb_00007l8f
EMDB ID : EMD-23232
Title : BG505 SOSIP.v5.2(7S) in complex with the polyclonal Fab pAbC-2 from animal Rh.33172 (Wk38 time point)
Authors : Antanasijevic, A.; Sewall, L.M.; Ward, A.B.
Deposited on : 2020-12-31
Resolution : 3.66 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 ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

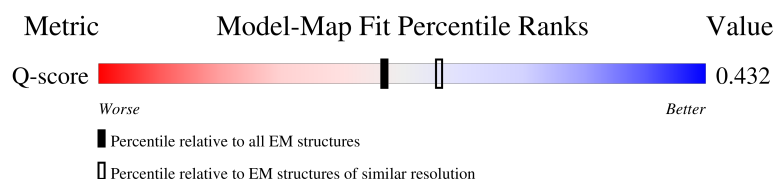
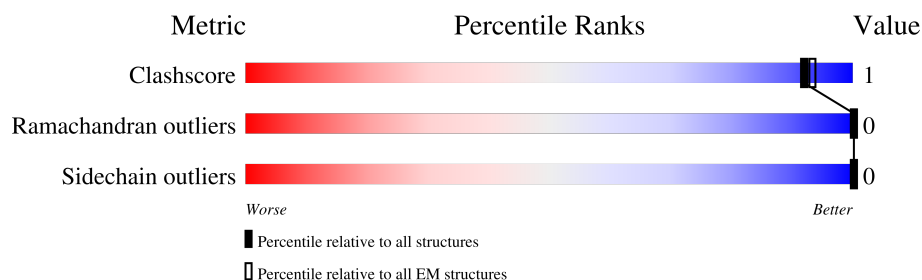
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance

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

The reported resolution of this entry is 3.66 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	11491 (3.16 - 4.16)

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 $\leq 5\%$. 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	 63% 33%
1	B	664	 18% 81%
1	C	664	 5% 62% 5% 33%
1	D	664	 18% 81%

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Mol	Chain	Length	Quality of chain
1	E	664	
1	F	664	
2	H	127	
3	L	107	
4	G	5	
4	K	5	
4	Q	5	
5	I	2	
5	J	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	

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 15840 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	446	Total	C	N	O	S	0	0
			3523	2214	622	659	28		
1	D	123	Total	C	N	O	S	0	0
			979	616	170	187	6		
1	E	444	Total	C	N	O	S	0	0
			3508	2205	619	656	28		
1	F	123	Total	C	N	O	S	0	0
			980	617	170	187	6		
1	A	445	Total	C	N	O	S	0	0
			3515	2210	620	657	28		
1	B	124	Total	C	N	O	S	0	0
			988	621	172	189	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	509	ARG	GLU	conflict	UNP Q2N0S5
C	510	ARG	LYS	conflict	UNP Q2N0S5
C	519	SER	PHE	conflict	UNP Q2N0S5
C	559	PRO	ILE	conflict	UNP Q2N0S5
C	561	CYS	ALA	conflict	UNP Q2N0S5
C	568	ASP	LEU	conflict	UNP Q2N0S5
C	570	HIS	VAL	conflict	UNP Q2N0S5
C	585	HIS	ARG	conflict	UNP Q2N0S5
C	605	CYS	THR	conflict	UNP Q2N0S5
C	662	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

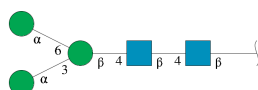
- Molecule 2 is a protein called Rh.33172 pAbC-2 Heavy Chain.

Mol	Chain	Residues	Atoms				AltConf	Trace
2	H	127	Total	C	N	O	0	0
			635	381	127	127		

- Molecule 3 is a protein called Rh.33172 pAbC-2 Light Chain.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	L	107	Total	C	N	O	0	0
			535	321	107	107		

- 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.



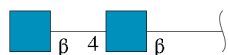
Mol	Chain	Residues	Atoms				AltConf	Trace
4	G	5	Total	C	N	O	0	0
			61	34	2	25		

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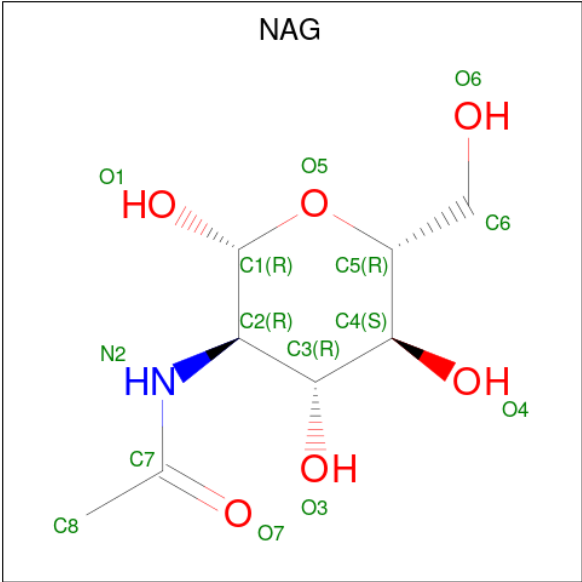
Mol	Chain	Residues	Atoms				AltConf	Trace
4	K	5	Total	C	N	O	0	0
			61	34	2	25		
4	Q	5	Total	C	N	O	0	0
			61	34	2	25		

- 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	0	0
			28	16	2	10		
5	J	2	Total	C	N	O	0	0
			28	16	2	10		
5	M	2	Total	C	N	O	0	0
			28	16	2	10		
5	N	2	Total	C	N	O	0	0
			28	16	2	10		
5	O	2	Total	C	N	O	0	0
			28	16	2	10		
5	P	2	Total	C	N	O	0	0
			28	16	2	10		
5	R	2	Total	C	N	O	0	0
			28	16	2	10		
5	S	2	Total	C	N	O	0	0
			28	16	2	10		
5	T	2	Total	C	N	O	0	0
			28	16	2	10		
5	U	2	Total	C	N	O	0	0
			28	16	2	10		
5	V	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



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

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Mol	Chain	Residues	Atoms				AltConf
6	C	1	Total	C	N	O	0
			14	8	1	5	
6	D	1	Total	C	N	O	0
			14	8	1	5	
6	D	1	Total	C	N	O	0
			14	8	1	5	
6	D	1	Total	C	N	O	0
			14	8	1	5	
6	E	1	Total	C	N	O	0
			14	8	1	5	
6	E	1	Total	C	N	O	0
			14	8	1	5	
6	E	1	Total	C	N	O	0
			14	8	1	5	
6	E	1	Total	C	N	O	0
			14	8	1	5	
6	E	1	Total	C	N	O	0
			14	8	1	5	
6	E	1	Total	C	N	O	0
			14	8	1	5	
6	E	1	Total	C	N	O	0
			14	8	1	5	
6	E	1	Total	C	N	O	0
			14	8	1	5	
6	E	1	Total	C	N	O	0
			14	8	1	5	
6	E	1	Total	C	N	O	0
			14	8	1	5	
6	F	1	Total	C	N	O	0
			14	8	1	5	
6	F	1	Total	C	N	O	0
			14	8	1	5	
6	A	1	Total	C	N	O	0
			14	8	1	5	
6	A	1	Total	C	N	O	0
			14	8	1	5	

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





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



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



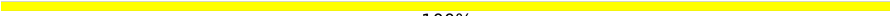
- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



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



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

Chain O:  100%

NAG1
NAG2

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

Chain P:  100%

NAG1
NAG2

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

Chain R:  50% 100%

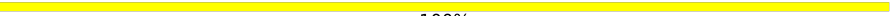
♦
NAG1
NAG2

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

Chain S:  50% 100%

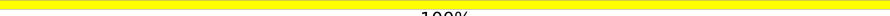
♦
NAG1
NAG2

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

Chain T:  100%

NAG1
NAG2

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

Chain U:  100%

NAG1
NAG2

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

Chain V:  100%

MAG1
MAG2

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	66171	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 ($e^-/\text{\AA}^2$)	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	0.149	Depositor
Minimum map value	-0.080	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.025	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	1.13	0/3587	1.26	29/4870 (0.6%)
1	B	1.07	1/1007 (0.1%)	1.07	4/1366 (0.3%)
1	C	1.09	1/3595 (0.0%)	1.25	20/4879 (0.4%)
1	D	1.07	0/998	1.08	3/1354 (0.2%)
1	E	1.08	1/3580 (0.0%)	1.26	34/4860 (0.7%)
1	F	1.07	0/999	1.12	4/1355 (0.3%)
All	All	1.09	3/13766 (0.0%)	1.22	94/18684 (0.5%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	661	LEU	CB-CG	6.91	1.67	1.53
1	C	374	HIS	CB-CG	-6.47	1.41	1.50
1	E	348	GLN	CG-CD	-5.26	1.39	1.52

All (94) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	492	GLU	CA-C-N	8.42	128.15	119.56
1	C	492	GLU	C-N-CA	8.42	128.15	119.56
1	C	298	ARG	CA-C-N	8.21	127.85	119.56
1	C	298	ARG	C-N-CA	8.21	127.85	119.56
1	A	492	GLU	CA-C-N	7.99	127.71	119.56
1	A	492	GLU	C-N-CA	7.99	127.71	119.56
1	A	298	ARG	CA-C-N	7.84	127.48	119.56
1	A	298	ARG	C-N-CA	7.84	127.48	119.56
1	C	437	PRO	N-CA-C	-7.64	103.13	110.47
1	E	298	ARG	CA-C-N	7.12	126.75	119.56
1	E	298	ARG	C-N-CA	7.12	126.75	119.56
1	F	605	CYS	N-CA-C	-7.11	99.95	110.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	205	CYS	CA-C-N	7.08	126.79	119.56
1	C	205	CYS	C-N-CA	7.08	126.79	119.56
1	E	205	CYS	CA-C-N	6.98	126.68	119.56
1	E	205	CYS	C-N-CA	6.98	126.68	119.56
1	E	276	ASN	CA-CB-CG	6.87	119.47	112.60
1	A	500	ARG	N-CA-C	6.84	121.48	113.20
1	E	492	GLU	CA-C-N	6.79	126.93	119.87
1	E	492	GLU	C-N-CA	6.79	126.93	119.87
1	E	425	ASN	N-CA-C	-6.79	99.53	110.32
1	A	342	LEU	N-CA-C	-6.78	104.64	113.12
1	C	237	GLY	CA-C-N	6.67	126.63	119.76
1	C	237	GLY	C-N-CA	6.67	126.63	119.76
1	E	237	GLY	CA-C-N	6.59	126.54	119.76
1	E	237	GLY	C-N-CA	6.59	126.54	119.76
1	C	110	SER	N-CA-C	-6.58	105.88	114.04
1	E	219	ALA	CA-C-N	6.58	126.75	120.31
1	E	219	ALA	C-N-CA	6.58	126.75	120.31
1	A	276	ASN	CA-CB-CG	6.50	119.10	112.60
1	A	437	PRO	N-CA-C	-6.49	104.24	110.47
1	E	437	PRO	N-CA-C	-6.46	103.67	110.58
1	C	106	THR	N-CA-C	-6.46	105.70	113.97
1	B	608	VAL	CA-C-N	6.44	126.42	119.78
1	B	608	VAL	C-N-CA	6.44	126.42	119.78
1	A	205	CYS	CA-C-N	6.44	126.13	119.56
1	A	205	CYS	C-N-CA	6.44	126.13	119.56
1	A	497	ALA	CA-C-N	6.44	126.20	119.76
1	A	497	ALA	C-N-CA	6.44	126.20	119.76
1	F	608	VAL	CA-C-N	6.33	126.24	119.85
1	F	608	VAL	C-N-CA	6.33	126.24	119.85
1	E	236	THR	N-CA-C	6.27	117.97	110.44
1	A	237	GLY	CA-C-N	6.23	126.20	119.78
1	A	237	GLY	C-N-CA	6.23	126.20	119.78
1	C	219	ALA	CA-C-N	6.15	126.12	120.03
1	C	219	ALA	C-N-CA	6.15	126.12	120.03
1	E	320	THR	N-CA-C	6.12	120.36	113.01
1	F	636	SER	N-CA-C	6.09	118.71	111.71
1	E	80	ASN	CA-C-N	6.04	125.72	119.56
1	E	80	ASN	C-N-CA	6.04	125.72	119.56
1	E	141	ASP	N-CA-C	-6.04	101.34	110.28
1	A	299	PRO	N-CA-C	6.04	121.41	113.86
1	B	614	TRP	N-CA-C	-5.98	104.72	112.68
1	E	437	PRO	CA-C-N	5.89	125.80	119.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	437	PRO	C-N-CA	5.89	125.80	119.85
1	B	548	ILE	N-CA-C	-5.86	106.10	111.67
1	E	75	VAL	CA-C-N	5.81	125.78	120.03
1	E	75	VAL	C-N-CA	5.81	125.78	120.03
1	A	437	PRO	CA-C-N	5.79	125.69	119.85
1	A	437	PRO	C-N-CA	5.79	125.69	119.85
1	A	219	ALA	CA-C-N	5.77	125.96	120.31
1	A	219	ALA	C-N-CA	5.77	125.96	120.31
1	A	297	THR	N-CA-C	5.75	118.02	108.99
1	E	496	VAL	N-CA-C	5.67	116.28	108.12
1	D	608	VAL	CA-C-N	5.66	125.64	120.03
1	D	608	VAL	C-N-CA	5.66	125.64	120.03
1	A	436	ALA	CA-C-N	5.66	123.79	119.66
1	A	436	ALA	C-N-CA	5.66	123.79	119.66
1	A	184	ILE	N-CA-C	5.51	116.17	110.82
1	C	425	ASN	N-CA-C	-5.49	100.75	109.76
1	E	78	ASP	CA-C-N	5.34	125.01	119.56
1	E	78	ASP	C-N-CA	5.34	125.01	119.56
1	C	424	ILE	N-CA-C	5.24	115.50	108.17
1	C	315	GLN	N-CA-C	5.19	116.86	108.41
1	C	213	ILE	N-CA-C	-5.16	102.26	108.45
1	A	194	ILE	N-CA-C	5.15	117.49	111.05
1	A	123	THR	CA-C-N	5.14	124.81	119.56
1	A	123	THR	C-N-CA	5.14	124.81	119.56
1	E	379	GLY	N-CA-C	-5.13	108.54	115.36
1	C	194	ILE	N-CA-C	5.08	117.40	111.05
1	E	120	VAL	N-CA-C	5.08	115.65	109.30
1	A	199	SER	N-CA-C	5.08	116.97	108.99
1	D	614	TRP	N-CA-C	-5.08	103.69	110.55
1	A	277	ILE	N-CA-C	5.06	115.78	110.62
1	A	393	SER	N-CA-C	5.06	117.38	110.55
1	E	312	GLY	CA-C-N	5.05	126.15	119.84
1	E	312	GLY	C-N-CA	5.05	126.15	119.84
1	E	109	ILE	CB-CA-C	-5.04	105.33	112.14
1	E	497	ALA	CA-C-N	5.02	124.78	119.76
1	E	497	ALA	C-N-CA	5.02	124.78	119.76
1	C	261	LEU	CA-C-N	5.01	129.24	122.07
1	C	261	LEU	C-N-CA	5.01	129.24	122.07
1	E	261	LEU	CA-C-N	5.00	129.22	122.07
1	E	261	LEU	C-N-CA	5.00	129.22	122.07

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	3515	0	3454	7	0
1	B	988	0	950	0	0
1	C	3523	0	3464	14	0
1	D	979	0	942	2	0
1	E	3508	0	3446	10	0
1	F	980	0	945	5	0
2	H	635	0	153	4	0
3	L	535	0	136	1	0
4	G	61	0	52	0	0
4	K	61	0	52	0	0
4	Q	61	0	52	0	0
5	I	28	0	25	0	0
5	J	28	0	25	1	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
6	A	182	0	169	0	0
6	B	42	0	39	1	0
6	C	210	0	195	1	0
6	D	42	0	39	1	0
6	E	182	0	169	0	0
6	F	28	0	26	0	0
All	All	15840	0	14558	44	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 1.

All (44) 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:F:624:ASP:O	1:F:624:ASP:OD1	2.12	0.68
1:E:183:GLN:HG2	1:E:191:TYR:CE2	2.28	0.68
1:C:294:ILE:CG2	1:C:447:SER:OG	2.43	0.66
1:C:164:GLU:HG3	1:C:165:LEU:HG	1.78	0.64
1:E:242:VAL:HG12	1:E:243:SER:N	2.15	0.59
1:E:242:VAL:CG1	1:E:243:SER:N	2.68	0.56
1:E:65:LYS:O	1:E:65:LYS:HG3	2.06	0.56
1:C:65:LYS:O	1:C:65:LYS:HG3	2.04	0.56
1:C:294:ILE:HG23	1:C:294:ILE:O	2.06	0.56
1:E:123:THR:N	1:E:124:PRO:CD	2.70	0.55
1:A:99:ASN:OD1	1:A:102:GLU:HB3	2.07	0.54
1:A:305:LYS:HE3	2:H:101:UNK:HA	1.89	0.54
6:B:703:NAG:O7	6:B:703:NAG:O3	2.24	0.54
1:E:232:LYS:NZ	1:E:269:GLU:OE2	2.42	0.53
1:A:114:GLN:HA	1:A:117:LYS:HG2	1.90	0.53
1:A:167:ASP:OD2	1:A:168:LYS:NZ	2.41	0.53
1:E:183:GLN:CG	1:E:191:TYR:CE2	2.92	0.52
5:J:1:NAG:H61	5:J:2:NAG:HN2	1.74	0.52
1:E:328:GLN:HE22	1:E:417:PRO:HB3	1.75	0.52
1:F:650:GLN:HA	1:F:650:GLN:OE1	2.10	0.51
1:D:636:SER:HB3	6:D:701:NAG:C7	2.41	0.50
1:F:631:TRP:CZ2	1:F:635:ILE:HD13	2.47	0.49
1:A:117:LYS:N	1:A:118:PRO:CD	2.76	0.49
1:C:297:THR:HB	1:C:330:HIS:CD2	2.48	0.48
1:C:105:HIS:O	1:C:105:HIS:CG	2.68	0.47
1:A:113:ASP:O	1:A:117:LYS:HG2	2.14	0.46
1:C:123:THR:N	1:C:124:PRO:CD	2.78	0.46
1:C:297:THR:HB	1:C:330:HIS:NE2	2.30	0.46
1:C:97:LYS:NZ	1:C:275:GLU:OE2	2.49	0.46
1:C:80:ASN:HB3	1:C:82:GLN:HE21	1.80	0.45
2:H:40:UNK:O	2:H:41:UNK:C	2.61	0.45
1:E:474:ASP:OD1	1:E:475:MET:N	2.49	0.45
1:F:629:LEU:O	1:F:633:LYS:HG2	2.17	0.44
1:E:141:ASP:O	1:E:150:MET:HB2	2.18	0.43
1:C:234:ASN:O	6:C:707:NAG:H82	2.19	0.43
1:A:114:GLN:HA	1:A:117:LYS:CG	2.49	0.42
2:H:76:UNK:O	2:H:77:UNK:C	2.65	0.42
1:F:611:ASN:HB2	1:F:614:TRP:CE2	2.54	0.42
1:D:614:TRP:O	1:D:615:SER:C	2.61	0.41
1:C:294:ILE:HG22	1:C:447:SER:OG	2.20	0.41
1:C:54:CYS:SG	1:C:215:ILE:HG23	2.60	0.41
3:L:99:UNK:O	3:L:100:UNK:C	2.69	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:65:LYS:O	1:C:65:LYS:CG	2.68	0.40
2:H:55:UNK:O	2:H:56:UNK:C	2.69	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%)	428 (98%)	9 (2%)	0	100	100
1	B	120/664 (18%)	118 (98%)	2 (2%)	0	100	100
1	C	438/664 (66%)	429 (98%)	9 (2%)	0	100	100
1	D	119/664 (18%)	119 (100%)	0	0	100	100
1	E	436/664 (66%)	431 (99%)	5 (1%)	0	100	100
1	F	119/664 (18%)	116 (98%)	3 (2%)	0	100	100
All	All	1669/3984 (42%)	1641 (98%)	28 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	401/586 (68%)	401 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	107/586 (18%)	107 (100%)	0	100	100
1	C	402/586 (69%)	402 (100%)	0	100	100
1	D	106/586 (18%)	106 (100%)	0	100	100
1	E	400/586 (68%)	400 (100%)	0	100	100
1	F	106/586 (18%)	106 (100%)	0	100	100
All	All	1522/3516 (43%)	1522 (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 (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	82	GLN
1	D	591	GLN
1	E	246	GLN
1	E	328	GLN
1	F	575	GLN
1	F	591	GLN
1	A	170	GLN
1	A	374	HIS
1	A	432	GLN
1	B	591	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 ⓘ

37 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	1,4	14,14,15	2.06	5 (35%)	17,19,21	1.15	3 (17%)
4	NAG	G	2	4	14,14,15	1.85	4 (28%)	17,19,21	0.93	1 (5%)
4	BMA	G	3	4	11,11,12	1.35	2 (18%)	15,15,17	0.62	0
4	MAN	G	4	4	11,11,12	1.91	4 (36%)	15,15,17	0.64	0
4	MAN	G	5	4	11,11,12	1.86	5 (45%)	15,15,17	0.65	0
5	NAG	I	1	1,5	14,14,15	2.14	7 (50%)	17,19,21	1.19	2 (11%)
5	NAG	I	2	5	14,14,15	2.03	5 (35%)	17,19,21	0.93	0
5	NAG	J	1	1,5	14,14,15	0.40	0	17,19,21	0.48	0
5	NAG	J	2	5	14,14,15	0.38	0	17,19,21	0.42	0
4	NAG	K	1	1,4	14,14,15	1.99	5 (35%)	17,19,21	1.18	2 (11%)
4	NAG	K	2	4	14,14,15	2.00	5 (35%)	17,19,21	1.27	2 (11%)
4	BMA	K	3	4	11,11,12	1.42	3 (27%)	15,15,17	0.60	0
4	MAN	K	4	4	11,11,12	1.94	4 (36%)	15,15,17	0.79	0
4	MAN	K	5	4	11,11,12	1.90	4 (36%)	15,15,17	0.63	0
5	NAG	M	1	1,5	14,14,15	2.09	4 (28%)	17,19,21	1.17	1 (5%)
5	NAG	M	2	5	14,14,15	2.03	6 (42%)	17,19,21	0.87	1 (5%)
5	NAG	N	1	1,5	14,14,15	2.08	4 (28%)	17,19,21	1.11	2 (11%)
5	NAG	N	2	5	14,14,15	1.97	6 (42%)	17,19,21	0.90	1 (5%)
5	NAG	O	1	1,5	14,14,15	2.16	6 (42%)	17,19,21	1.41	3 (17%)
5	NAG	O	2	5	14,14,15	2.08	4 (28%)	17,19,21	0.85	0
5	NAG	P	1	1,5	14,14,15	2.08	5 (35%)	17,19,21	1.09	2 (11%)
5	NAG	P	2	5	14,14,15	1.97	4 (28%)	17,19,21	0.90	1 (5%)
4	NAG	Q	1	1,4	14,14,15	1.96	3 (21%)	17,19,21	1.10	1 (5%)
4	NAG	Q	2	4	14,14,15	1.82	4 (28%)	17,19,21	0.92	1 (5%)
4	BMA	Q	3	4	11,11,12	1.44	3 (27%)	15,15,17	0.60	0
4	MAN	Q	4	4	11,11,12	1.88	4 (36%)	15,15,17	0.81	0
4	MAN	Q	5	4	11,11,12	1.87	5 (45%)	15,15,17	0.72	0
5	NAG	R	1	1,5	14,14,15	2.00	3 (21%)	17,19,21	1.03	0
5	NAG	R	2	5	14,14,15	2.00	5 (35%)	17,19,21	0.84	0
5	NAG	S	1	1,5	14,14,15	1.94	3 (21%)	17,19,21	1.18	2 (11%)
5	NAG	S	2	5	14,14,15	2.02	6 (42%)	17,19,21	0.86	1 (5%)
5	NAG	T	1	1,5	14,14,15	2.04	5 (35%)	17,19,21	1.19	3 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	NAG	T	2	5	14,14,15	1.81	4 (28%)	17,19,21	1.37	2 (11%)
5	NAG	U	1	1,5	14,14,15	2.04	5 (35%)	17,19,21	1.13	1 (5%)
5	NAG	U	2	5	14,14,15	2.01	5 (35%)	17,19,21	1.08	1 (5%)
5	NAG	V	1	1,5	14,14,15	1.95	3 (21%)	17,19,21	1.18	2 (11%)
5	NAG	V	2	5	14,14,15	1.94	4 (28%)	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	1,4	-	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	1,5	-	0/6/23/26	0/1/1/1
5	NAG	I	2	5	-	1/6/23/26	0/1/1/1
5	NAG	J	1	1,5	-	3/6/23/26	0/1/1/1
5	NAG	J	2	5	-	4/6/23/26	0/1/1/1
4	NAG	K	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	K	2	4	-	0/6/23/26	0/1/1/1
4	BMA	K	3	4	-	0/2/19/22	0/1/1/1
4	MAN	K	4	4	-	1/2/19/22	0/1/1/1
4	MAN	K	5	4	-	0/2/19/22	0/1/1/1
5	NAG	M	1	1,5	-	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	1,5	-	1/6/23/26	0/1/1/1
5	NAG	N	2	5	-	0/6/23/26	0/1/1/1
5	NAG	O	1	1,5	-	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	1,5	-	0/6/23/26	0/1/1/1
5	NAG	P	2	5	-	0/6/23/26	0/1/1/1
4	NAG	Q	1	1,4	-	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	-	1/2/19/22	0/1/1/1
4	MAN	Q	5	4	-	1/2/19/22	0/1/1/1
5	NAG	R	1	1,5	-	0/6/23/26	0/1/1/1
5	NAG	R	2	5	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	S	1	1,5	-	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	1,5	-	0/6/23/26	0/1/1/1
5	NAG	T	2	5	-	2/6/23/26	0/1/1/1
5	NAG	U	1	1,5	-	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	1,5	-	0/6/23/26	0/1/1/1
5	NAG	V	2	5	-	0/6/23/26	0/1/1/1

All (154) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	I	1	NAG	C1-C2	5.57	1.59	1.52
5	M	1	NAG	C1-C2	5.50	1.59	1.52
4	G	1	NAG	C1-C2	5.49	1.59	1.52
5	N	1	NAG	C1-C2	5.39	1.59	1.52
4	Q	1	NAG	C1-C2	5.27	1.59	1.52
5	T	1	NAG	C1-C2	5.27	1.59	1.52
5	P	1	NAG	C1-C2	5.20	1.59	1.52
5	R	1	NAG	C1-C2	5.17	1.59	1.52
5	U	1	NAG	C1-C2	5.13	1.59	1.52
5	S	1	NAG	C1-C2	5.10	1.59	1.52
4	K	1	NAG	C1-C2	5.09	1.59	1.52
5	O	2	NAG	C1-C2	5.05	1.59	1.52
5	O	1	NAG	C1-C2	5.04	1.59	1.52
4	K	2	NAG	C1-C2	5.03	1.59	1.52
5	V	1	NAG	C1-C2	4.96	1.59	1.52
5	R	2	NAG	C1-C2	4.83	1.58	1.52
5	S	2	NAG	C1-C2	4.80	1.58	1.52
5	I	2	NAG	C1-C2	4.78	1.58	1.52
5	M	2	NAG	C1-C2	4.76	1.58	1.52
5	P	2	NAG	C1-C2	4.72	1.58	1.52
5	U	2	NAG	C1-C2	4.66	1.58	1.52
5	N	2	NAG	C1-C2	4.61	1.58	1.52
5	V	2	NAG	C1-C2	4.59	1.58	1.52
4	G	2	NAG	C1-C2	4.48	1.58	1.52
4	Q	2	NAG	C1-C2	4.18	1.58	1.52
5	T	2	NAG	C1-C2	4.01	1.57	1.52
5	O	2	NAG	O5-C5	3.37	1.50	1.43
5	M	2	NAG	O5-C5	3.29	1.49	1.43
4	G	4	MAN	O5-C5	3.28	1.49	1.43
4	K	5	MAN	O5-C5	3.27	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	U	2	NAG	O5-C5	3.13	1.49	1.43
4	Q	4	MAN	C2-C3	3.13	1.57	1.52
4	G	5	MAN	O5-C5	3.11	1.49	1.43
4	K	4	MAN	O5-C5	3.11	1.49	1.43
5	S	2	NAG	O5-C5	3.10	1.49	1.43
5	R	2	NAG	O5-C5	3.10	1.49	1.43
5	N	2	NAG	O5-C5	3.09	1.49	1.43
4	Q	5	MAN	O5-C5	3.09	1.49	1.43
5	V	2	NAG	O5-C5	3.09	1.49	1.43
5	P	2	NAG	O5-C5	3.07	1.49	1.43
4	Q	5	MAN	C2-C3	3.04	1.57	1.52
4	G	4	MAN	C2-C3	3.03	1.57	1.52
5	I	2	NAG	O5-C5	3.03	1.49	1.43
4	Q	4	MAN	O5-C5	3.01	1.49	1.43
4	Q	2	NAG	O5-C5	2.99	1.49	1.43
4	K	5	MAN	C2-C3	2.98	1.57	1.52
5	P	1	NAG	O5-C5	2.97	1.49	1.43
4	K	4	MAN	C2-C3	2.96	1.57	1.52
4	K	4	MAN	C1-C2	2.95	1.59	1.52
4	G	5	MAN	C2-C3	2.92	1.57	1.52
4	K	1	NAG	O5-C5	2.88	1.49	1.43
5	N	1	NAG	O5-C5	2.88	1.49	1.43
5	O	1	NAG	C4-C5	2.86	1.59	1.53
5	M	1	NAG	O5-C5	2.83	1.48	1.43
5	U	1	NAG	O5-C5	2.83	1.48	1.43
5	O	1	NAG	O5-C5	2.81	1.48	1.43
5	T	2	NAG	C3-C2	2.80	1.58	1.52
5	U	2	NAG	C3-C2	2.77	1.58	1.52
4	G	4	MAN	C1-C2	2.75	1.58	1.52
5	R	1	NAG	O5-C5	2.74	1.48	1.43
4	G	2	NAG	O5-C5	2.72	1.48	1.43
5	S	1	NAG	O5-C5	2.69	1.48	1.43
4	K	2	NAG	O5-C5	2.68	1.48	1.43
5	T	2	NAG	O5-C5	2.63	1.48	1.43
5	T	1	NAG	O5-C1	2.58	1.48	1.43
4	Q	4	MAN	C1-C2	2.58	1.58	1.52
5	V	1	NAG	O5-C5	2.57	1.48	1.43
4	K	5	MAN	C1-C2	2.54	1.58	1.52
4	G	1	NAG	O5-C5	2.54	1.48	1.43
4	Q	3	BMA	O5-C5	2.53	1.48	1.43
5	I	2	NAG	C3-C2	2.53	1.57	1.52
5	I	2	NAG	C4-C5	2.51	1.58	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	K	4	MAN	C4-C5	2.51	1.58	1.53
4	G	5	MAN	C1-C2	2.50	1.58	1.52
5	T	1	NAG	O5-C5	2.50	1.48	1.43
4	Q	1	NAG	O5-C5	2.49	1.48	1.43
5	O	2	NAG	C3-C2	2.47	1.57	1.52
4	Q	4	MAN	C4-C5	2.47	1.58	1.53
5	P	2	NAG	C3-C2	2.47	1.57	1.52
5	I	1	NAG	O5-C5	2.47	1.48	1.43
4	Q	5	MAN	C4-C5	2.47	1.58	1.53
5	N	2	NAG	C3-C2	2.45	1.57	1.52
5	M	2	NAG	C3-C2	2.44	1.57	1.52
4	K	2	NAG	C3-C2	2.44	1.57	1.52
4	G	4	MAN	C4-C5	2.42	1.58	1.53
5	R	1	NAG	C4-C5	2.41	1.58	1.53
5	I	1	NAG	C3-C2	2.41	1.57	1.52
4	G	5	MAN	C4-C5	2.40	1.58	1.53
5	R	2	NAG	C3-C2	2.40	1.57	1.52
5	V	2	NAG	C3-C2	2.40	1.57	1.52
5	N	1	NAG	O5-C1	2.39	1.47	1.43
4	K	3	BMA	O5-C5	2.38	1.48	1.43
5	M	1	NAG	C4-C5	2.37	1.58	1.53
5	O	1	NAG	C4-C3	2.36	1.58	1.52
5	S	2	NAG	C3-C2	2.36	1.57	1.52
4	Q	5	MAN	C1-C2	2.35	1.57	1.52
4	K	5	MAN	C4-C5	2.33	1.58	1.53
5	S	2	NAG	C4-C5	2.33	1.58	1.53
4	G	1	NAG	C3-C2	2.32	1.57	1.52
5	U	1	NAG	C4-C5	2.31	1.58	1.53
5	P	1	NAG	C4-C5	2.30	1.57	1.53
4	G	3	BMA	O5-C5	2.30	1.47	1.43
5	U	2	NAG	C2-N2	2.29	1.50	1.46
5	O	2	NAG	C4-C5	2.28	1.57	1.53
4	G	2	NAG	C3-C2	2.25	1.57	1.52
4	K	2	NAG	C2-N2	2.24	1.50	1.46
5	P	2	NAG	C4-C5	2.24	1.57	1.53
5	S	1	NAG	C4-C5	2.24	1.57	1.53
4	Q	2	NAG	C3-C2	2.23	1.57	1.52
5	O	1	NAG	C3-C2	2.22	1.57	1.52
5	T	1	NAG	C2-N2	2.21	1.49	1.46
5	O	1	NAG	C2-N2	2.21	1.49	1.46
4	Q	1	NAG	C3-C2	2.21	1.57	1.52
5	M	2	NAG	C4-C5	2.21	1.57	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	V	2	NAG	C4-C5	2.21	1.57	1.53
5	I	1	NAG	O5-C1	2.20	1.47	1.43
5	N	1	NAG	C3-C2	2.20	1.57	1.52
5	I	1	NAG	C4-C3	2.20	1.58	1.52
5	I	2	NAG	C2-N2	2.20	1.49	1.46
4	G	3	BMA	C2-C3	2.18	1.55	1.52
5	N	2	NAG	C4-C5	2.17	1.57	1.53
4	G	1	NAG	O5-C1	2.17	1.47	1.43
5	T	2	NAG	C4-C5	2.17	1.57	1.53
4	K	1	NAG	C4-C5	2.16	1.57	1.53
4	K	1	NAG	C3-C2	2.16	1.57	1.52
5	R	2	NAG	C4-C5	2.15	1.57	1.53
5	U	2	NAG	C4-C5	2.15	1.57	1.53
4	Q	3	BMA	C1-C2	2.15	1.57	1.52
5	P	1	NAG	C3-C2	2.14	1.57	1.52
5	S	2	NAG	C4-C3	2.14	1.57	1.52
5	V	1	NAG	C4-C5	2.13	1.57	1.53
5	U	1	NAG	C4-C3	2.13	1.57	1.52
4	K	3	BMA	C1-C2	2.12	1.57	1.52
4	K	3	BMA	C2-C3	2.12	1.55	1.52
5	P	1	NAG	O5-C1	2.12	1.47	1.43
5	T	1	NAG	C3-C2	2.11	1.56	1.52
4	Q	3	BMA	C2-C3	2.11	1.55	1.52
5	M	1	NAG	O5-C1	2.10	1.47	1.43
5	S	2	NAG	C2-N2	2.08	1.49	1.46
4	K	1	NAG	O5-C1	2.07	1.47	1.43
5	U	1	NAG	O5-C1	2.07	1.47	1.43
5	N	2	NAG	C2-N2	2.07	1.49	1.46
5	N	2	NAG	C4-C3	2.06	1.57	1.52
5	I	1	NAG	C2-N2	2.06	1.49	1.46
4	G	5	MAN	C4-C3	2.05	1.57	1.52
5	R	2	NAG	C2-N2	2.04	1.49	1.46
5	M	2	NAG	C4-C3	2.04	1.57	1.52
4	K	2	NAG	C4-C3	2.03	1.57	1.52
4	G	1	NAG	C2-N2	2.03	1.49	1.46
5	M	2	NAG	C2-N2	2.01	1.49	1.46
5	I	1	NAG	C4-C5	2.01	1.57	1.53
4	Q	2	NAG	C4-C5	2.01	1.57	1.53
4	Q	5	MAN	C4-C3	2.00	1.57	1.52
4	G	2	NAG	C2-N2	2.00	1.49	1.46

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	K	2	NAG	C8-C7-N2	3.63	122.13	116.12
5	T	2	NAG	C2-N2-C7	3.13	127.10	122.90
5	N	1	NAG	C8-C7-N2	2.80	120.77	116.12
5	O	1	NAG	C8-C7-N2	2.80	120.76	116.12
4	G	1	NAG	C8-C7-N2	2.74	120.66	116.12
5	V	1	NAG	C8-C7-N2	2.72	120.63	116.12
5	I	1	NAG	C8-C7-N2	2.69	120.58	116.12
5	T	1	NAG	C8-C7-N2	2.69	120.57	116.12
5	U	2	NAG	C8-C7-N2	2.60	120.43	116.12
5	M	1	NAG	C8-C7-N2	2.55	120.35	116.12
5	S	1	NAG	C8-C7-N2	2.52	120.30	116.12
5	U	1	NAG	C8-C7-N2	2.52	120.30	116.12
5	N	1	NAG	O7-C7-C8	-2.39	117.79	122.05
4	G	2	NAG	C8-C7-N2	2.38	120.07	116.12
4	Q	1	NAG	C8-C7-N2	2.34	120.01	116.12
4	K	2	NAG	O7-C7-C8	-2.32	117.93	122.05
5	P	1	NAG	C1-C2-N2	-2.32	106.78	110.43
4	K	1	NAG	C1-O5-C5	2.25	115.20	112.19
4	K	1	NAG	C8-C7-N2	2.21	119.79	116.12
5	P	1	NAG	C8-C7-N2	2.21	119.79	116.12
5	O	1	NAG	O5-C5-C6	-2.21	103.36	107.66
5	N	2	NAG	C8-C7-N2	2.20	119.77	116.12
4	G	1	NAG	O7-C7-C8	-2.20	118.14	122.05
5	S	1	NAG	C1-C2-N2	-2.18	106.99	110.43
5	S	2	NAG	C8-C7-N2	2.14	119.67	116.12
5	P	2	NAG	C8-C7-N2	2.14	119.67	116.12
5	I	1	NAG	O7-C7-C8	-2.11	118.30	122.05
4	G	1	NAG	C1-O5-C5	2.10	115.01	112.19
5	T	1	NAG	C1-O5-C5	2.10	115.00	112.19
4	Q	2	NAG	C8-C7-N2	2.10	119.60	116.12
5	O	1	NAG	O4-C4-C3	-2.08	105.48	110.38
5	V	1	NAG	O7-C7-C8	-2.04	118.42	122.05
5	M	2	NAG	C8-C7-N2	2.03	119.48	116.12
5	T	1	NAG	O7-C7-C8	-2.02	118.46	122.05
5	T	2	NAG	C1-C2-N2	2.00	113.59	110.43

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	J	1	NAG	C8-C7-N2-C2
5	J	2	NAG	C8-C7-N2-C2
5	J	2	NAG	O7-C7-N2-C2

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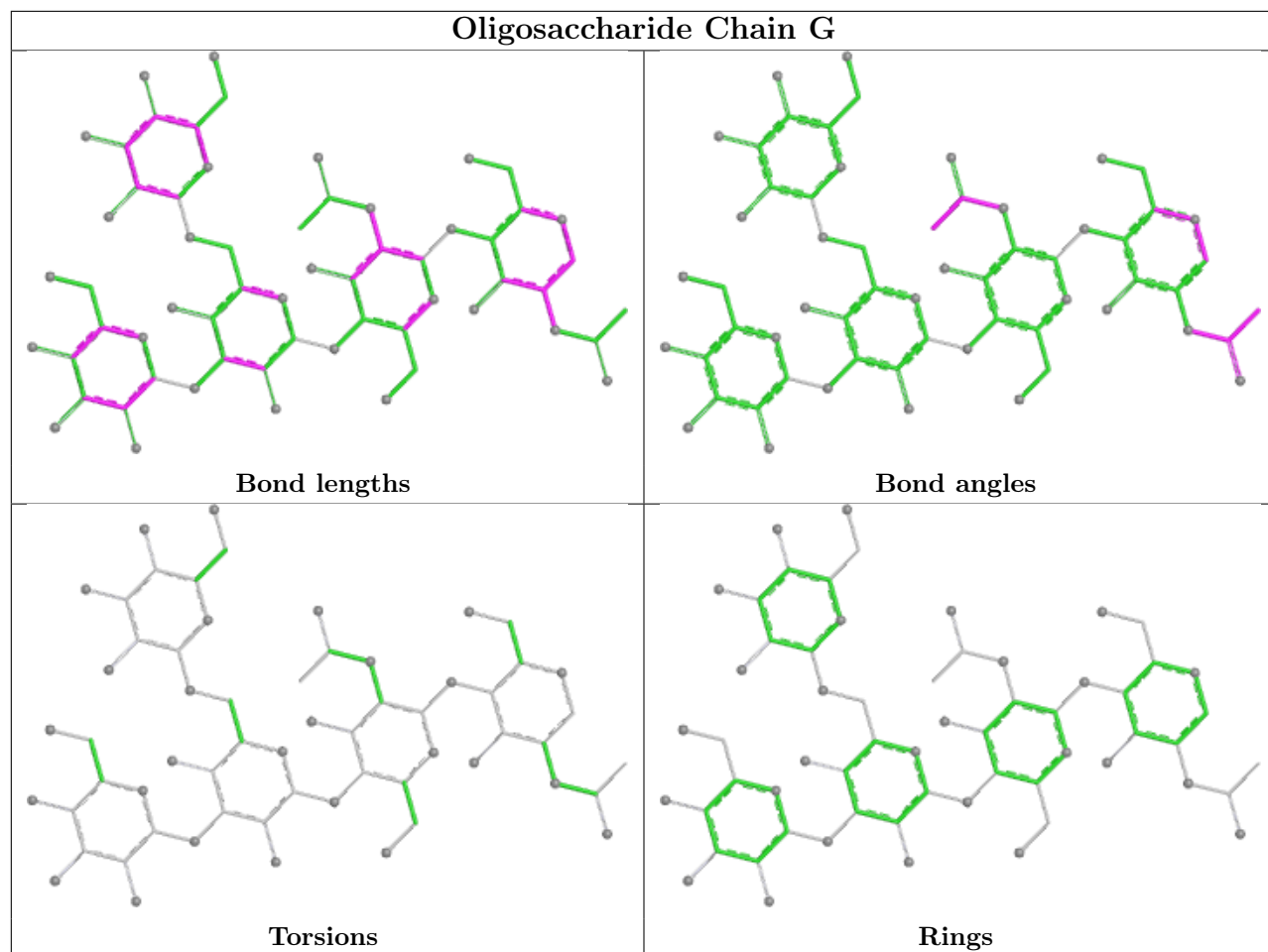
Mol	Chain	Res	Type	Atoms
5	J	1	NAG	O7-C7-N2-C2
5	J	2	NAG	C4-C5-C6-O6
5	J	2	NAG	O5-C5-C6-O6
4	Q	5	MAN	O5-C5-C6-O6
5	I	2	NAG	O5-C5-C6-O6
4	Q	4	MAN	O5-C5-C6-O6
4	K	4	MAN	O5-C5-C6-O6
5	T	2	NAG	C1-C2-N2-C7
5	J	1	NAG	C1-C2-N2-C7
5	N	1	NAG	C1-C2-N2-C7
5	T	2	NAG	C3-C2-N2-C7

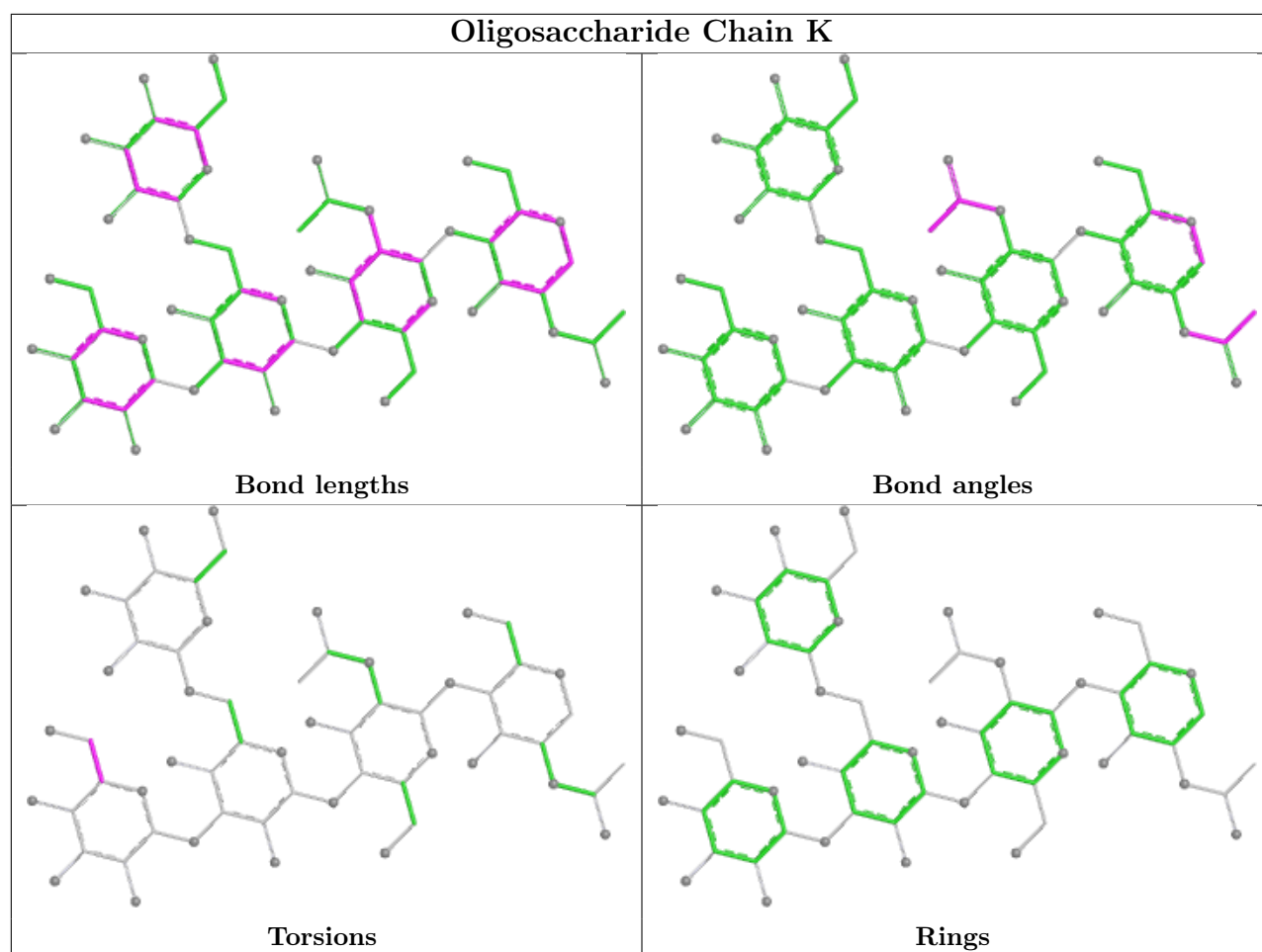
There are no ring outliers.

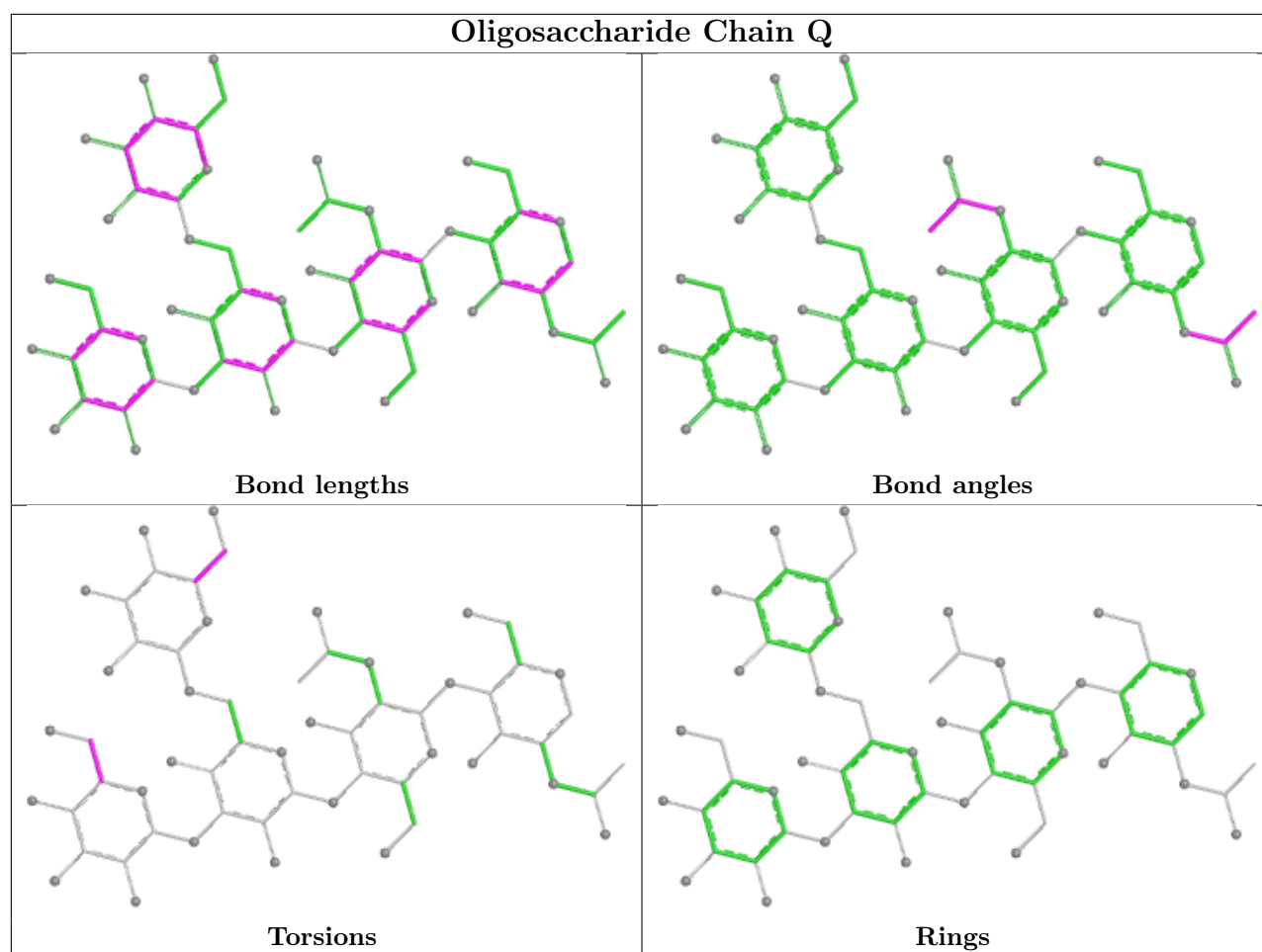
2 monomers are involved in 1 short contact:

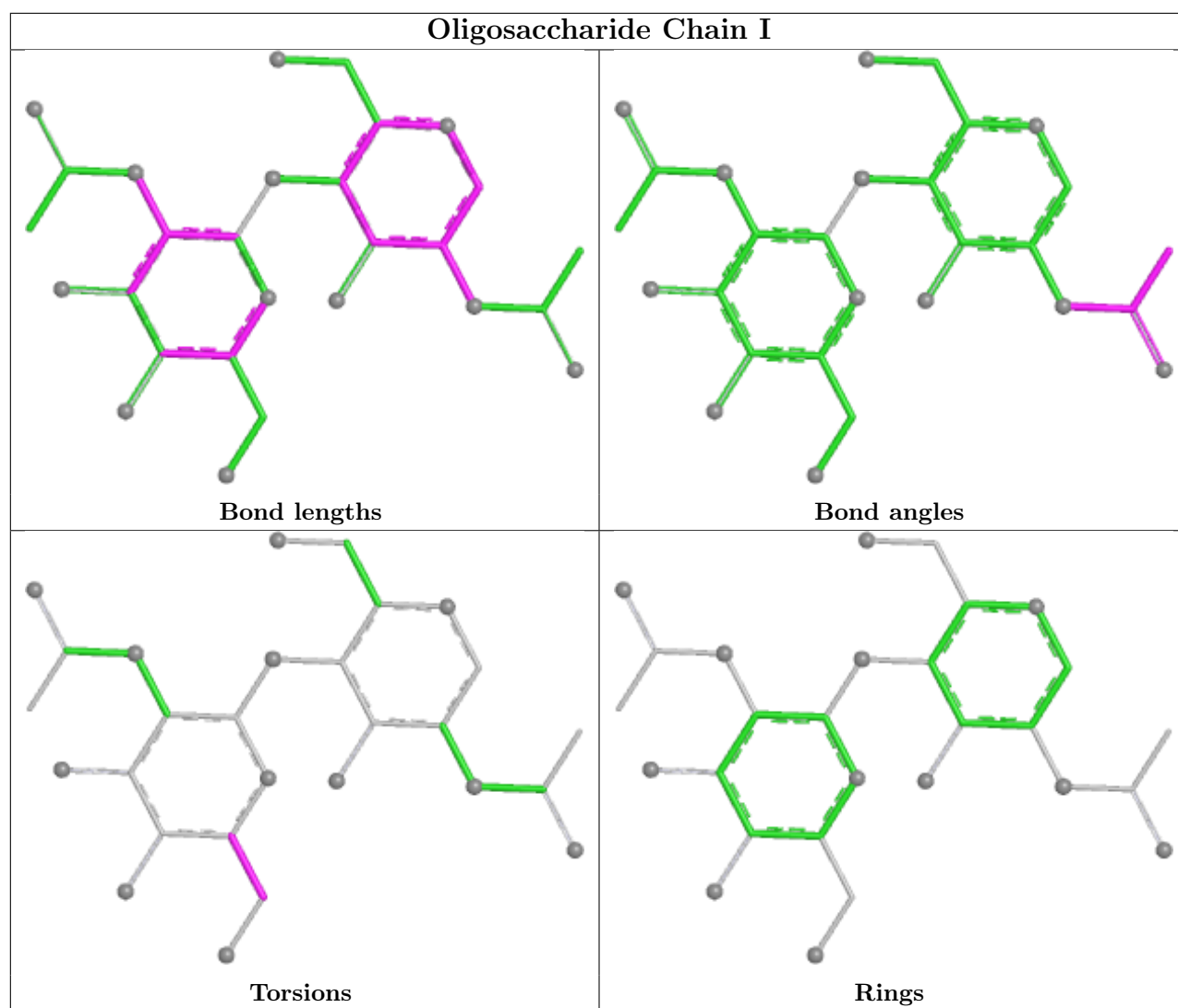
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	J	2	NAG	1	0
5	J	1	NAG	1	0

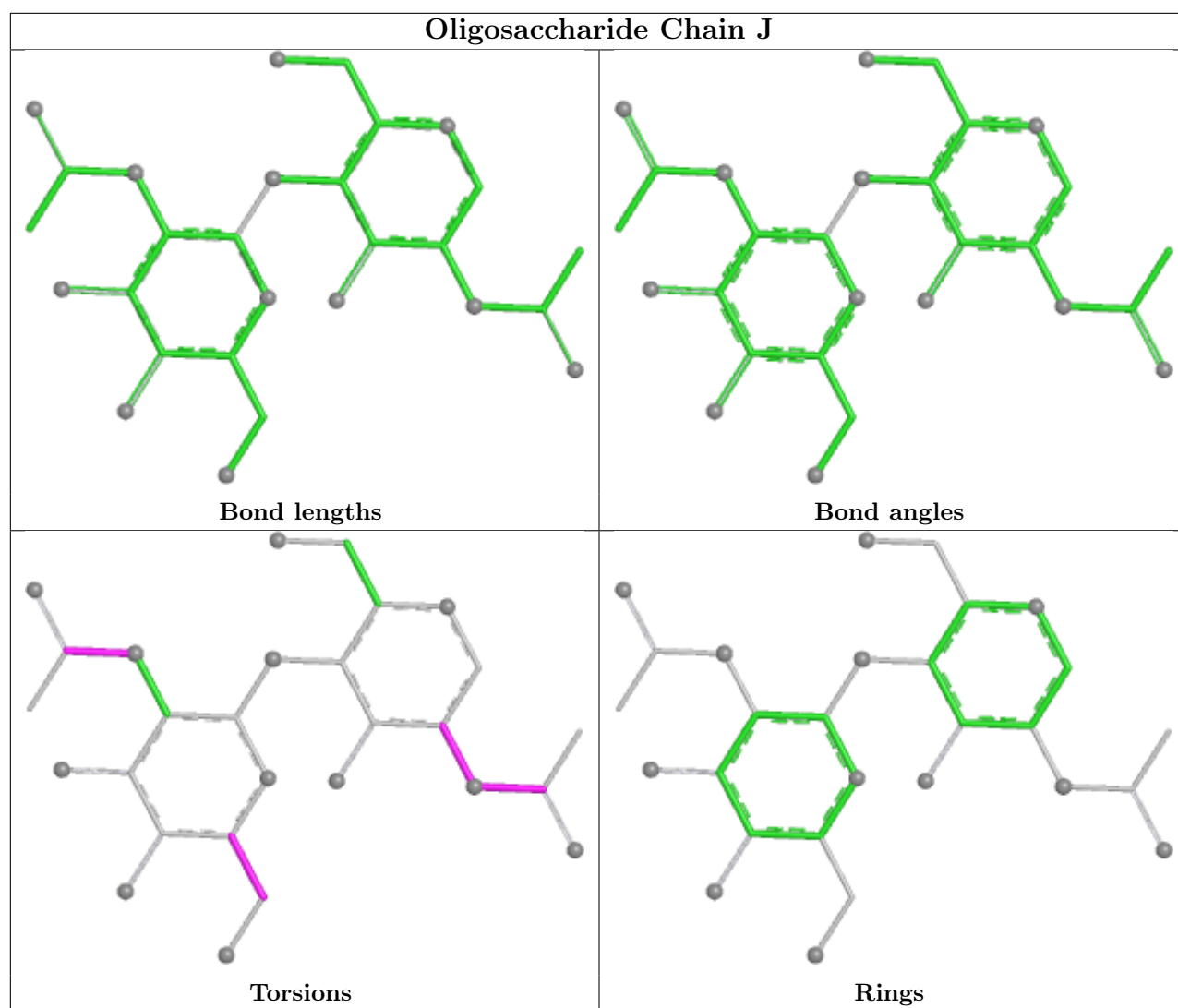
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

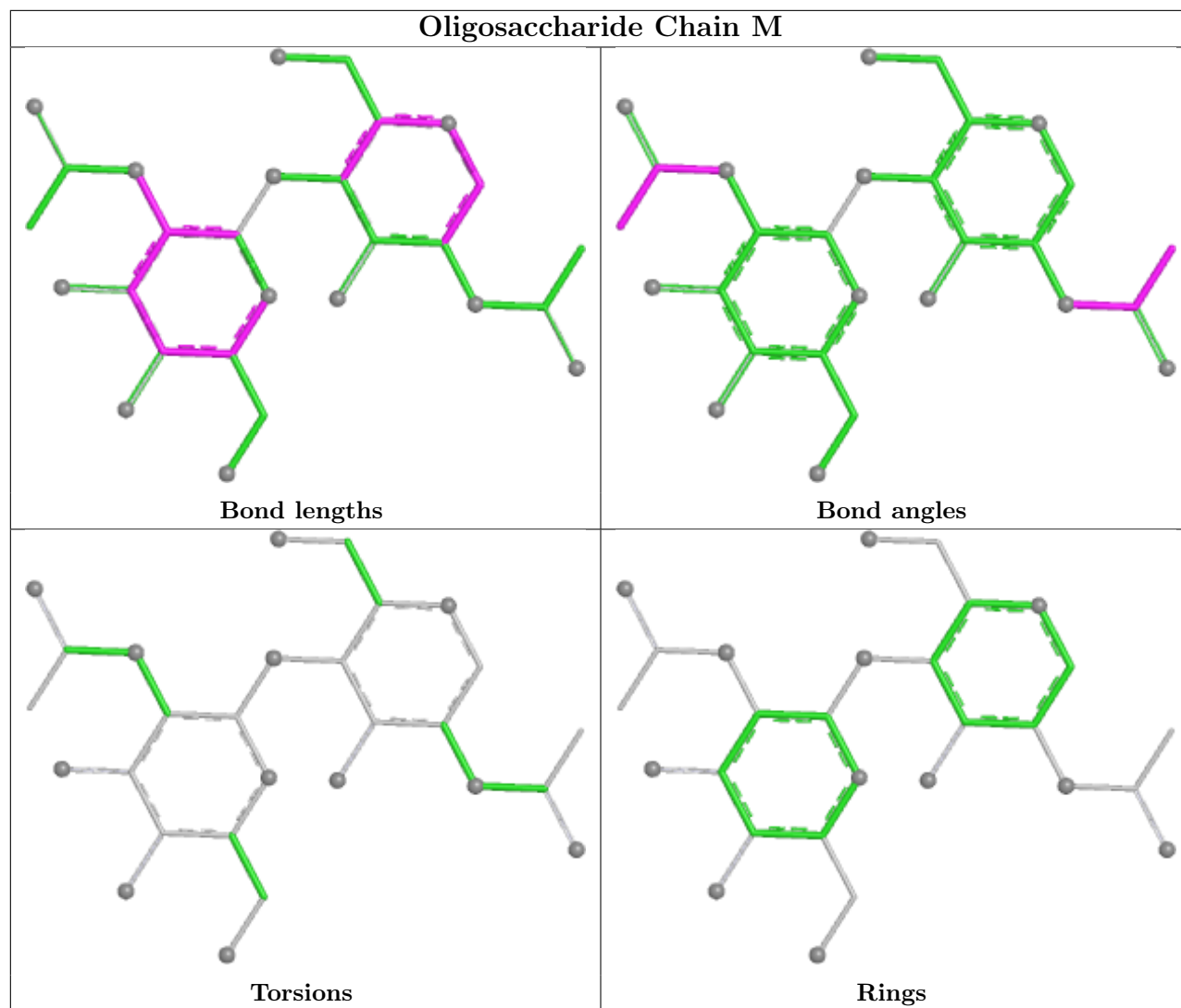


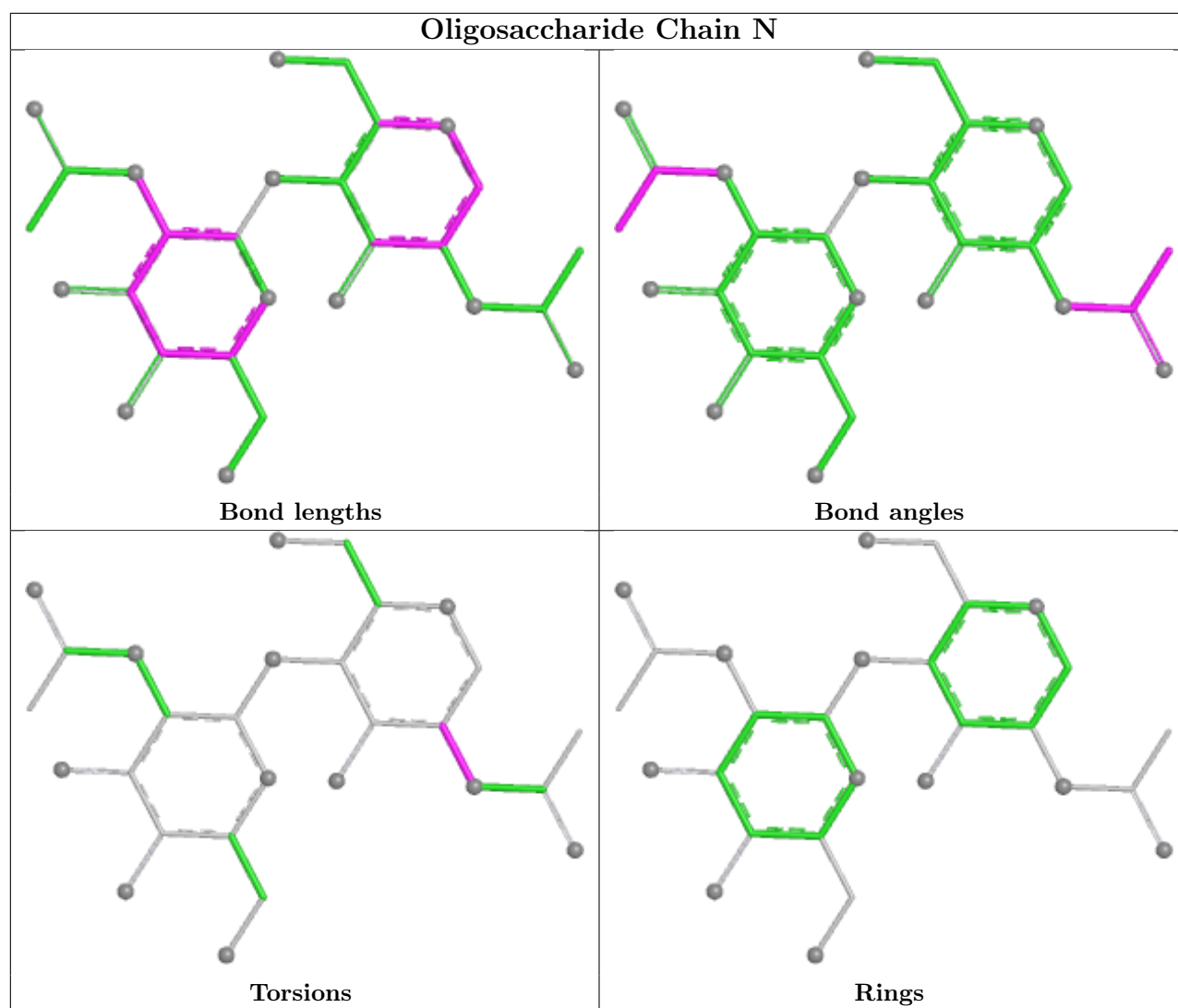


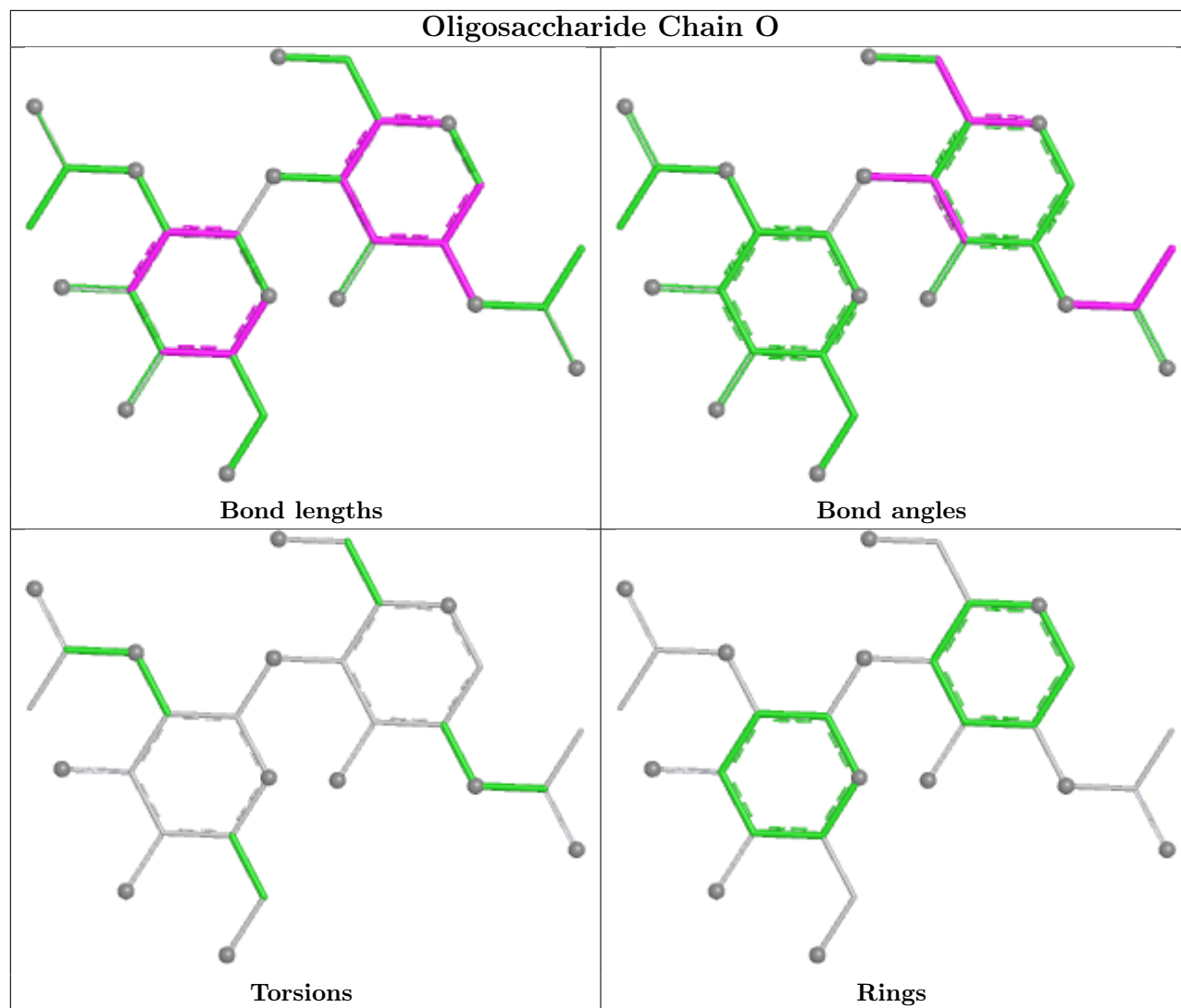


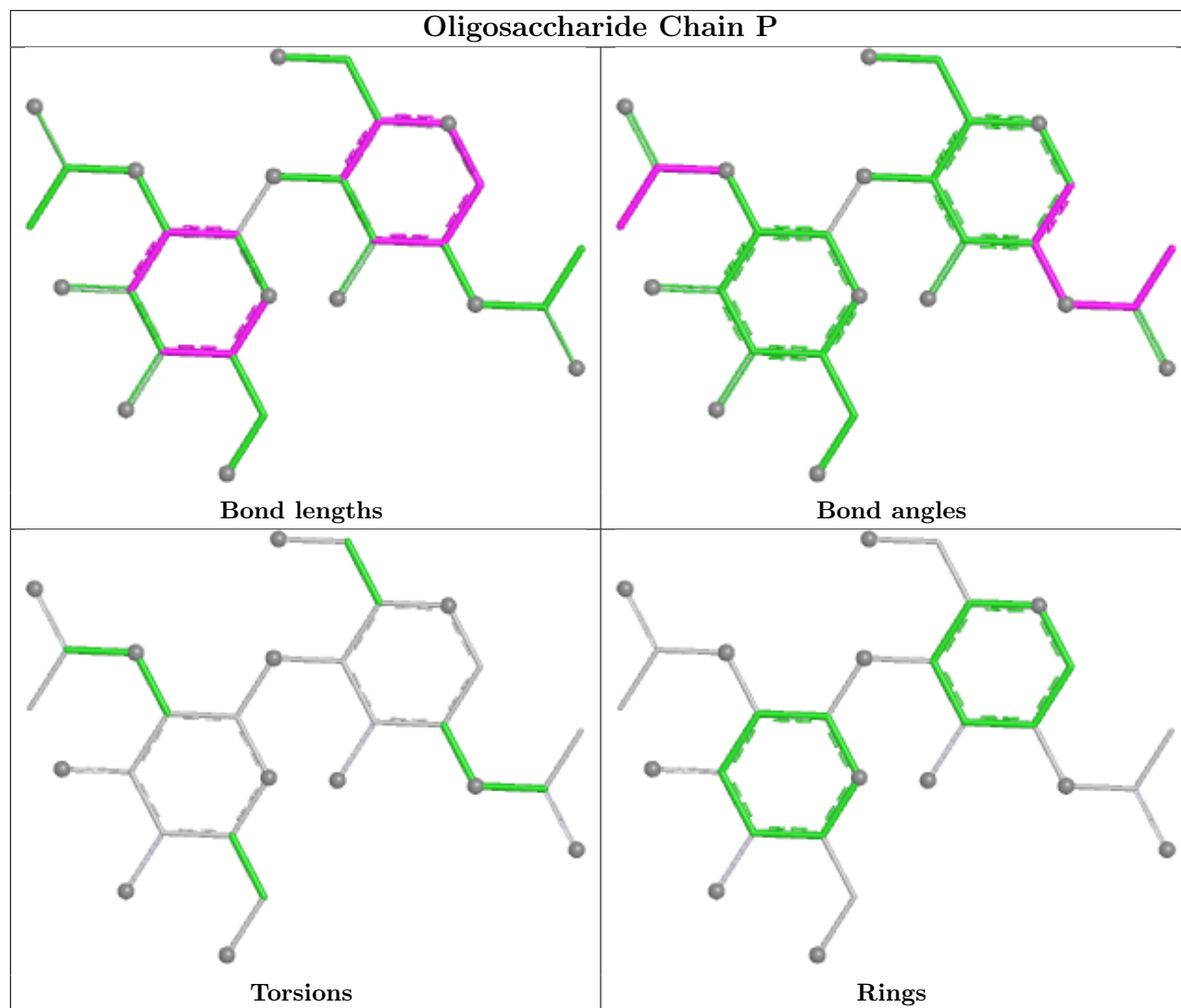


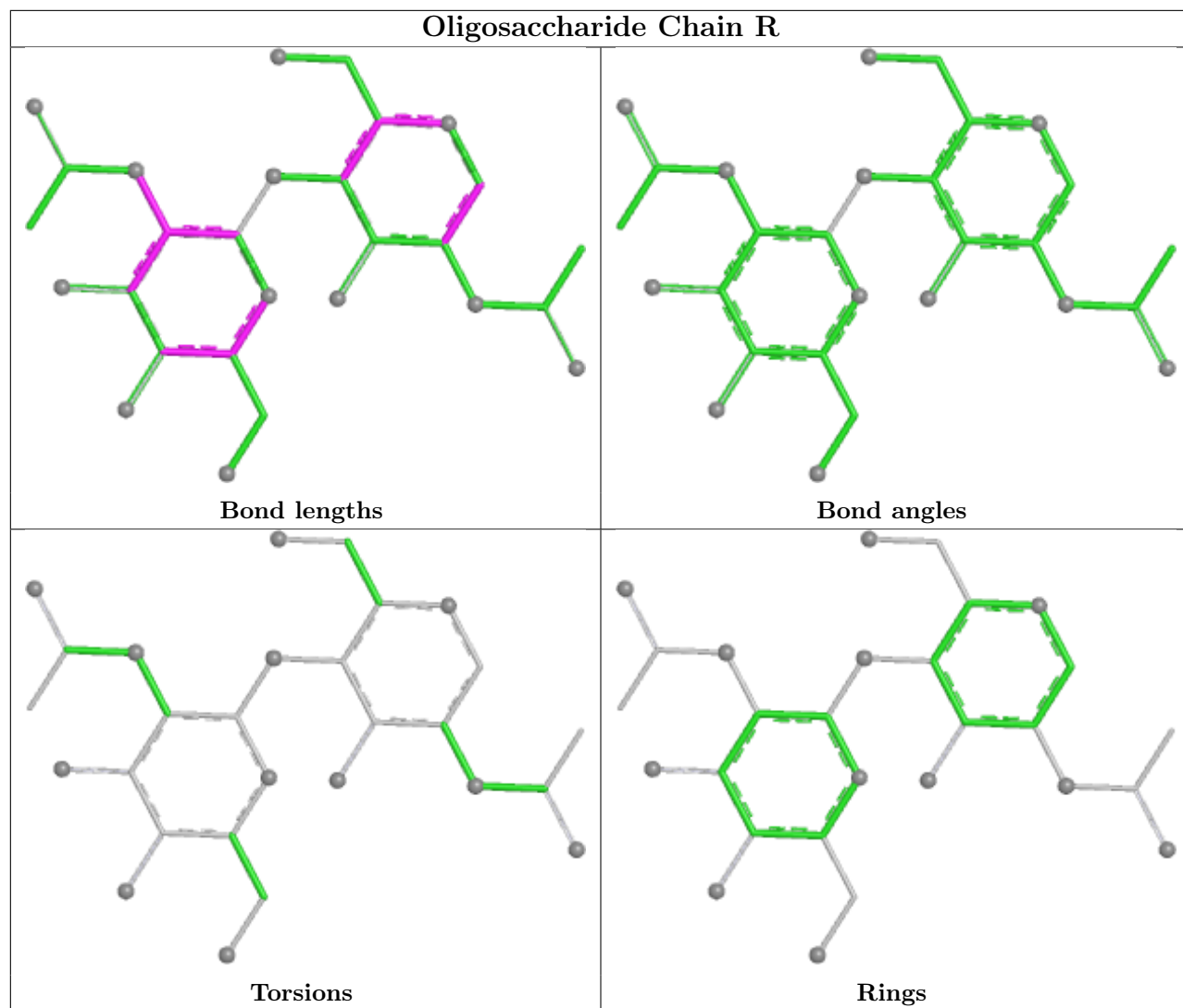


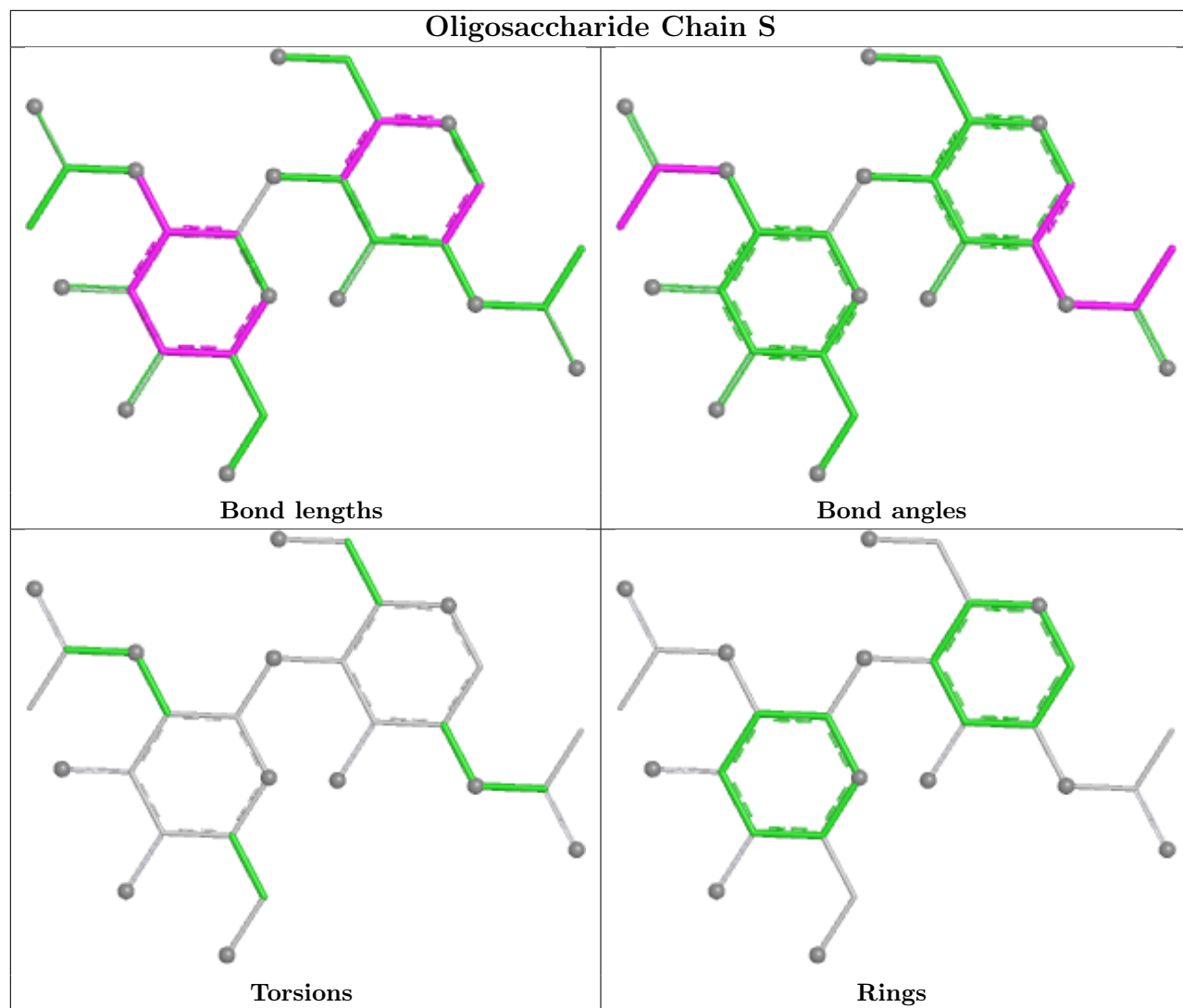


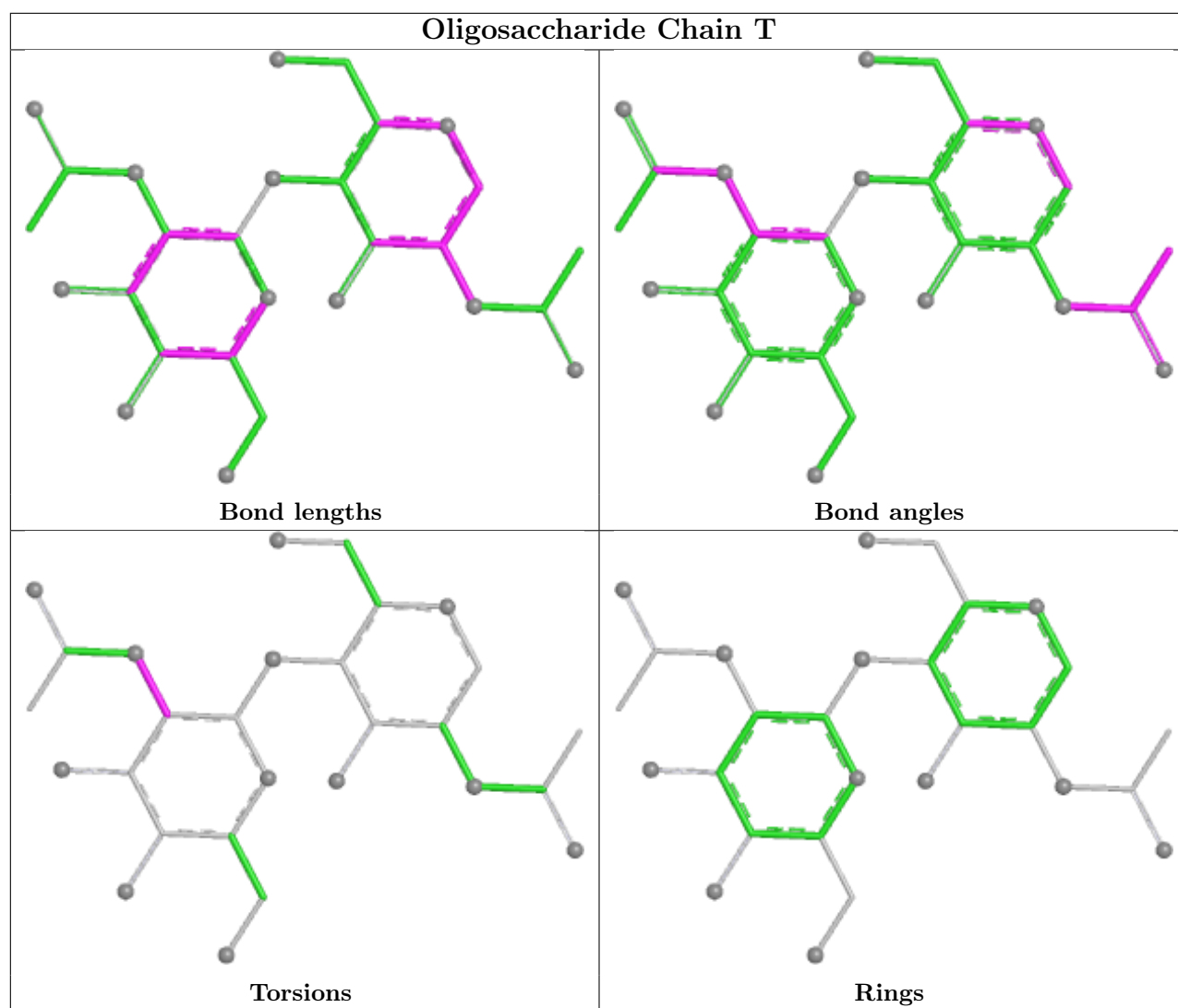


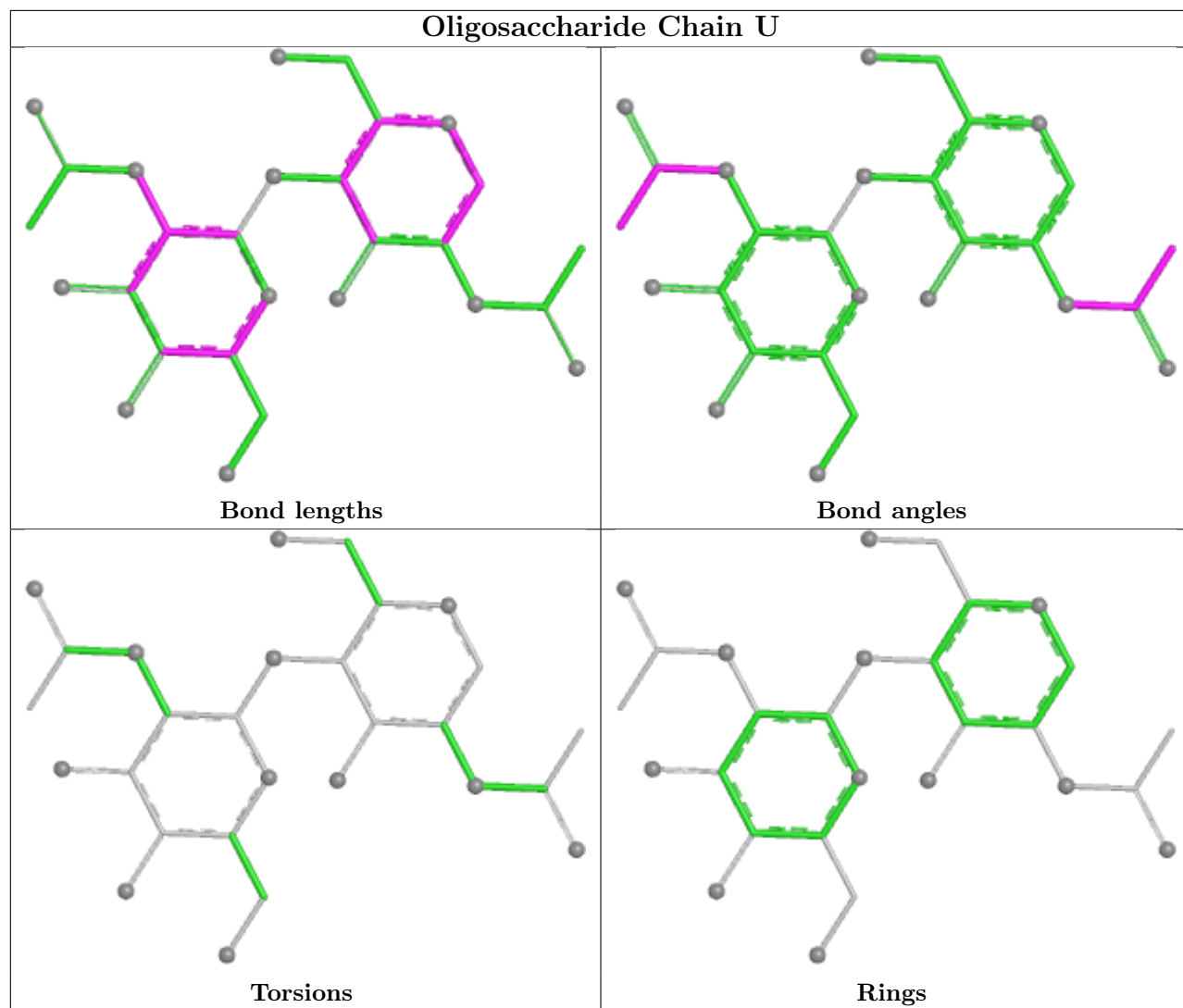


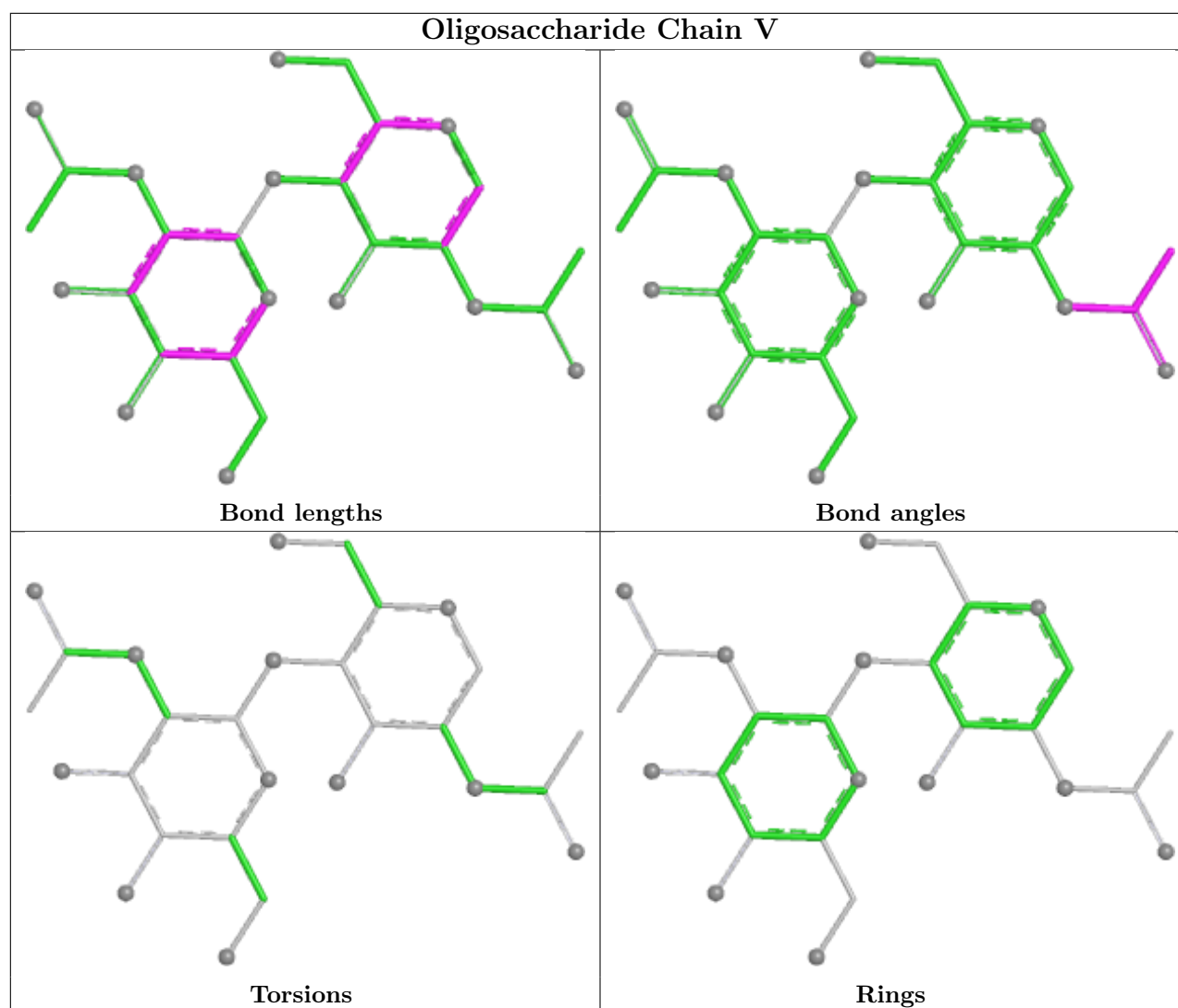












5.6 Ligand geometry [i](#)

49 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	E	703	1	14,14,15	2.27	6 (42%)	17,19,21	1.10	0
6	NAG	E	713	1	14,14,15	2.15	7 (50%)	17,19,21	1.06	1 (5%)
6	NAG	F	702	1	14,14,15	0.37	0	17,19,21	0.39	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	NAG	D	703	1	14,14,15	2.24	4 (28%)	17,19,21	1.15	2 (11%)
6	NAG	E	701	1	14,14,15	2.13	5 (35%)	17,19,21	1.07	1 (5%)
6	NAG	C	710	1	14,14,15	2.23	5 (35%)	17,19,21	0.94	0
6	NAG	C	714	1	14,14,15	2.21	7 (50%)	17,19,21	1.11	1 (5%)
6	NAG	A	709	1	14,14,15	2.19	5 (35%)	17,19,21	0.99	1 (5%)
6	NAG	A	711	1	14,14,15	2.63	5 (35%)	17,19,21	1.37	2 (11%)
6	NAG	E	709	1	14,14,15	2.26	6 (42%)	17,19,21	1.18	2 (11%)
6	NAG	A	713	1	14,14,15	2.08	5 (35%)	17,19,21	1.02	1 (5%)
6	NAG	B	703	1	14,14,15	0.37	0	17,19,21	0.48	0
6	NAG	C	705	1	14,14,15	1.96	5 (35%)	17,19,21	1.13	1 (5%)
6	NAG	A	701	1	14,14,15	2.14	4 (28%)	17,19,21	0.99	1 (5%)
6	NAG	D	702	1	14,14,15	0.39	0	17,19,21	0.49	0
6	NAG	E	706	1	14,14,15	0.39	0	17,19,21	0.45	0
6	NAG	E	705	1	14,14,15	2.16	5 (35%)	17,19,21	1.17	3 (17%)
6	NAG	C	712	1	14,14,15	2.29	7 (50%)	17,19,21	1.03	2 (11%)
6	NAG	A	705	1	14,14,15	2.26	6 (42%)	17,19,21	1.39	3 (17%)
6	NAG	C	704	1	14,14,15	2.12	5 (35%)	17,19,21	1.07	1 (5%)
6	NAG	C	706	1	14,14,15	2.12	5 (35%)	17,19,21	1.11	2 (11%)
6	NAG	B	701	1	14,14,15	0.37	0	17,19,21	0.49	0
6	NAG	A	707	1	14,14,15	2.10	6 (42%)	17,19,21	1.06	1 (5%)
6	NAG	A	704	1	14,14,15	0.39	0	17,19,21	0.51	0
6	NAG	A	710	1	14,14,15	2.18	6 (42%)	17,19,21	1.21	2 (11%)
6	NAG	C	715	1	14,14,15	2.21	6 (42%)	17,19,21	1.01	1 (5%)
6	NAG	E	708	1	14,14,15	2.24	6 (42%)	17,19,21	1.02	1 (5%)
6	NAG	E	712	1	14,14,15	2.32	6 (42%)	17,19,21	1.01	0
6	NAG	A	703	1	14,14,15	2.07	4 (28%)	17,19,21	1.02	0
6	NAG	B	702	1	14,14,15	2.27	7 (50%)	17,19,21	1.01	2 (11%)
6	NAG	E	702	1	14,14,15	2.16	4 (28%)	17,19,21	0.96	0
6	NAG	A	712	1	14,14,15	2.18	6 (42%)	17,19,21	0.97	1 (5%)
6	NAG	C	708	1	14,14,15	2.07	4 (28%)	17,19,21	1.10	2 (11%)
6	NAG	C	702	1	14,14,15	2.15	5 (35%)	17,19,21	1.00	0
6	NAG	F	701	1	14,14,15	2.22	6 (42%)	17,19,21	0.95	0
6	NAG	A	706	1	14,14,15	2.11	4 (28%)	17,19,21	1.10	1 (5%)
6	NAG	C	709	1	14,14,15	2.22	5 (35%)	17,19,21	1.00	1 (5%)
6	NAG	C	707	1	14,14,15	0.39	0	17,19,21	0.50	0
6	NAG	A	708	1	14,14,15	2.15	7 (50%)	17,19,21	1.04	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	NAG	E	704	1	14,14,15	2.15	5 (35%)	17,19,21	1.01	1 (5%)
6	NAG	E	710	1	14,14,15	0.38	0	17,19,21	0.46	0
6	NAG	A	702	1	14,14,15	2.21	5 (35%)	17,19,21	1.14	3 (17%)
6	NAG	C	703	1	14,14,15	2.16	4 (28%)	17,19,21	0.99	1 (5%)
6	NAG	E	707	1	14,14,15	0.37	0	17,19,21	0.47	0
6	NAG	C	711	1	14,14,15	2.10	6 (42%)	17,19,21	1.03	2 (11%)
6	NAG	E	711	1	14,14,15	2.12	7 (50%)	17,19,21	1.28	3 (17%)
6	NAG	C	713	1	14,14,15	2.29	6 (42%)	17,19,21	1.02	1 (5%)
6	NAG	D	701	1	14,14,15	0.39	0	17,19,21	0.42	0
6	NAG	C	701	1	14,14,15	2.15	5 (35%)	17,19,21	0.99	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	E	703	1	-	1/6/23/26	0/1/1/1
6	NAG	E	713	1	-	0/6/23/26	0/1/1/1
6	NAG	F	702	1	-	4/6/23/26	0/1/1/1
6	NAG	D	703	1	-	0/6/23/26	0/1/1/1
6	NAG	E	701	1	-	1/6/23/26	0/1/1/1
6	NAG	C	710	1	-	0/6/23/26	0/1/1/1
6	NAG	C	714	1	-	1/6/23/26	0/1/1/1
6	NAG	A	709	1	-	2/6/23/26	0/1/1/1
6	NAG	A	711	1	-	1/6/23/26	0/1/1/1
6	NAG	E	709	1	-	0/6/23/26	0/1/1/1
6	NAG	A	713	1	-	0/6/23/26	0/1/1/1
6	NAG	B	703	1	-	1/6/23/26	0/1/1/1
6	NAG	C	705	1	-	1/6/23/26	0/1/1/1
6	NAG	A	701	1	-	0/6/23/26	0/1/1/1
6	NAG	D	702	1	-	3/6/23/26	0/1/1/1
6	NAG	E	706	1	-	2/6/23/26	0/1/1/1
6	NAG	E	705	1	-	1/6/23/26	0/1/1/1
6	NAG	C	712	1	-	1/6/23/26	0/1/1/1
6	NAG	A	705	1	-	2/6/23/26	0/1/1/1
6	NAG	C	704	1	-	0/6/23/26	0/1/1/1
6	NAG	C	706	1	-	0/6/23/26	0/1/1/1
6	NAG	B	701	1	-	4/6/23/26	0/1/1/1
6	NAG	A	707	1	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	NAG	A	704	1	-	3/6/23/26	0/1/1/1
6	NAG	A	710	1	-	0/6/23/26	0/1/1/1
6	NAG	C	715	1	-	0/6/23/26	0/1/1/1
6	NAG	E	708	1	-	0/6/23/26	0/1/1/1
6	NAG	E	712	1	-	0/6/23/26	0/1/1/1
6	NAG	A	703	1	-	0/6/23/26	0/1/1/1
6	NAG	B	702	1	-	0/6/23/26	0/1/1/1
6	NAG	E	702	1	-	0/6/23/26	0/1/1/1
6	NAG	A	712	1	-	0/6/23/26	0/1/1/1
6	NAG	C	708	1	-	0/6/23/26	0/1/1/1
6	NAG	C	702	1	-	1/6/23/26	0/1/1/1
6	NAG	F	701	1	-	0/6/23/26	0/1/1/1
6	NAG	A	706	1	-	0/6/23/26	0/1/1/1
6	NAG	C	709	1	-	0/6/23/26	0/1/1/1
6	NAG	C	707	1	-	1/6/23/26	0/1/1/1
6	NAG	A	708	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	710	1	-	4/6/23/26	0/1/1/1
6	NAG	A	702	1	-	1/6/23/26	0/1/1/1
6	NAG	C	703	1	-	0/6/23/26	0/1/1/1
6	NAG	E	707	1	-	2/6/23/26	0/1/1/1
6	NAG	C	711	1	-	0/6/23/26	0/1/1/1
6	NAG	E	711	1	-	0/6/23/26	0/1/1/1
6	NAG	C	713	1	-	0/6/23/26	0/1/1/1
6	NAG	D	701	1	-	3/6/23/26	0/1/1/1
6	NAG	C	701	1	-	0/6/23/26	0/1/1/1

All (212) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	711	NAG	C1-C2	7.67	1.62	1.52
6	E	712	NAG	C1-C2	6.15	1.60	1.52
6	E	703	NAG	C1-C2	6.09	1.60	1.52
6	A	705	NAG	C1-C2	6.02	1.60	1.52
6	A	702	NAG	C1-C2	5.99	1.60	1.52
6	C	713	NAG	C1-C2	5.97	1.60	1.52
6	C	710	NAG	C1-C2	5.95	1.60	1.52
6	E	702	NAG	C1-C2	5.90	1.60	1.52
6	C	702	NAG	C1-C2	5.85	1.60	1.52
6	E	708	NAG	C1-C2	5.84	1.60	1.52
6	C	709	NAG	C1-C2	5.80	1.60	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	703	NAG	C1-C2	5.77	1.60	1.52
6	A	701	NAG	C1-C2	5.76	1.60	1.52
6	C	703	NAG	C1-C2	5.74	1.60	1.52
6	C	715	NAG	C1-C2	5.71	1.60	1.52
6	C	712	NAG	C1-C2	5.71	1.60	1.52
6	E	709	NAG	C1-C2	5.69	1.60	1.52
6	C	701	NAG	C1-C2	5.66	1.60	1.52
6	B	702	NAG	C1-C2	5.63	1.60	1.52
6	D	703	NAG	C1-C2	5.63	1.60	1.52
6	A	712	NAG	C1-C2	5.60	1.60	1.52
6	E	704	NAG	C1-C2	5.60	1.60	1.52
6	E	705	NAG	C1-C2	5.55	1.59	1.52
6	A	710	NAG	C1-C2	5.55	1.59	1.52
6	A	706	NAG	C1-C2	5.55	1.59	1.52
6	C	704	NAG	C1-C2	5.54	1.59	1.52
6	E	701	NAG	C1-C2	5.50	1.59	1.52
6	F	701	NAG	C1-C2	5.47	1.59	1.52
6	A	709	NAG	C1-C2	5.46	1.59	1.52
6	A	707	NAG	C1-C2	5.37	1.59	1.52
6	E	713	NAG	C1-C2	5.28	1.59	1.52
6	C	714	NAG	C1-C2	5.28	1.59	1.52
6	A	713	NAG	C1-C2	5.27	1.59	1.52
6	C	706	NAG	C1-C2	5.20	1.59	1.52
6	C	705	NAG	C1-C2	5.08	1.59	1.52
6	A	708	NAG	C1-C2	5.01	1.59	1.52
6	C	708	NAG	C1-C2	4.98	1.59	1.52
6	C	711	NAG	C1-C2	4.79	1.58	1.52
6	E	711	NAG	C1-C2	4.58	1.58	1.52
6	F	701	NAG	O5-C5	3.60	1.50	1.43
6	E	711	NAG	O5-C5	3.60	1.50	1.43
6	C	711	NAG	O5-C5	3.55	1.50	1.43
6	C	712	NAG	O5-C5	3.52	1.50	1.43
6	A	711	NAG	C3-C2	3.46	1.59	1.52
6	A	709	NAG	O5-C5	3.44	1.50	1.43
6	B	702	NAG	O5-C5	3.40	1.50	1.43
6	C	708	NAG	O5-C5	3.37	1.50	1.43
6	C	714	NAG	O5-C5	3.37	1.50	1.43
6	C	706	NAG	O5-C5	3.36	1.50	1.43
6	A	708	NAG	O5-C5	3.36	1.50	1.43
6	E	709	NAG	O5-C5	3.28	1.49	1.43
6	E	712	NAG	O5-C5	3.28	1.49	1.43
6	E	708	NAG	O5-C5	3.26	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	C	715	NAG	O5-C5	3.25	1.49	1.43
6	C	701	NAG	O5-C5	3.24	1.49	1.43
6	E	703	NAG	O5-C5	3.23	1.49	1.43
6	C	713	NAG	O5-C5	3.23	1.49	1.43
6	A	706	NAG	O5-C5	3.20	1.49	1.43
6	E	701	NAG	O5-C5	3.20	1.49	1.43
6	D	703	NAG	O5-C5	3.19	1.49	1.43
6	C	703	NAG	O5-C5	3.17	1.49	1.43
6	A	710	NAG	O5-C5	3.17	1.49	1.43
6	C	709	NAG	O5-C5	3.16	1.49	1.43
6	E	713	NAG	O5-C5	3.15	1.49	1.43
6	A	705	NAG	O5-C5	3.14	1.49	1.43
6	A	712	NAG	O5-C5	3.12	1.49	1.43
6	C	704	NAG	O5-C5	3.10	1.49	1.43
6	C	702	NAG	O5-C5	3.10	1.49	1.43
6	C	710	NAG	O5-C5	3.07	1.49	1.43
6	E	704	NAG	O5-C5	3.03	1.49	1.43
6	E	705	NAG	O5-C5	3.01	1.49	1.43
6	A	711	NAG	O5-C5	3.01	1.49	1.43
6	A	713	NAG	O5-C5	2.96	1.49	1.43
6	E	702	NAG	O5-C5	2.95	1.49	1.43
6	A	701	NAG	O5-C5	2.91	1.49	1.43
6	A	707	NAG	O5-C5	2.90	1.49	1.43
6	D	703	NAG	C3-C2	2.90	1.58	1.52
6	C	705	NAG	O5-C5	2.87	1.49	1.43
6	E	711	NAG	O5-C1	2.85	1.48	1.43
6	A	710	NAG	O5-C1	2.84	1.48	1.43
6	A	702	NAG	O5-C5	2.81	1.48	1.43
6	E	708	NAG	O5-C1	2.80	1.48	1.43
6	C	713	NAG	O5-C1	2.80	1.48	1.43
6	C	712	NAG	O5-C1	2.76	1.48	1.43
6	A	709	NAG	O5-C1	2.76	1.48	1.43
6	C	711	NAG	O5-C1	2.75	1.48	1.43
6	A	703	NAG	O5-C5	2.73	1.48	1.43
6	E	712	NAG	O5-C1	2.67	1.48	1.43
6	B	702	NAG	O5-C1	2.66	1.48	1.43
6	E	703	NAG	O5-C1	2.66	1.48	1.43
6	E	709	NAG	O5-C1	2.65	1.48	1.43
6	C	715	NAG	O5-C1	2.64	1.48	1.43
6	A	702	NAG	O5-C1	2.64	1.48	1.43
6	E	713	NAG	O5-C1	2.64	1.48	1.43
6	C	714	NAG	O5-C1	2.62	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	C	706	NAG	O5-C1	2.61	1.48	1.43
6	C	710	NAG	O5-C1	2.61	1.48	1.43
6	E	701	NAG	O5-C1	2.60	1.48	1.43
6	A	708	NAG	O5-C1	2.59	1.48	1.43
6	E	704	NAG	O5-C1	2.57	1.48	1.43
6	C	708	NAG	O5-C1	2.56	1.48	1.43
6	C	702	NAG	O5-C1	2.55	1.48	1.43
6	A	713	NAG	O5-C1	2.54	1.48	1.43
6	D	703	NAG	O5-C1	2.54	1.48	1.43
6	C	701	NAG	O5-C1	2.53	1.48	1.43
6	A	705	NAG	C3-C2	2.50	1.57	1.52
6	A	705	NAG	O5-C1	2.49	1.47	1.43
6	F	701	NAG	O5-C1	2.47	1.47	1.43
6	E	705	NAG	C3-C2	2.47	1.57	1.52
6	C	714	NAG	C3-C2	2.45	1.57	1.52
6	A	708	NAG	C3-C2	2.45	1.57	1.52
6	C	709	NAG	O5-C1	2.44	1.47	1.43
6	C	709	NAG	C3-C2	2.44	1.57	1.52
6	A	706	NAG	O5-C1	2.42	1.47	1.43
6	A	712	NAG	C3-C2	2.42	1.57	1.52
6	E	712	NAG	C3-C2	2.42	1.57	1.52
6	C	704	NAG	O5-C1	2.42	1.47	1.43
6	A	701	NAG	O5-C1	2.41	1.47	1.43
6	B	702	NAG	C4-C5	2.39	1.58	1.53
6	B	702	NAG	C3-C2	2.38	1.57	1.52
6	A	712	NAG	O5-C1	2.37	1.47	1.43
6	C	706	NAG	C3-C2	2.37	1.57	1.52
6	F	701	NAG	C4-C5	2.37	1.58	1.53
6	C	711	NAG	C4-C5	2.37	1.58	1.53
6	E	705	NAG	O5-C1	2.36	1.47	1.43
6	A	711	NAG	O5-C1	2.36	1.47	1.43
6	A	708	NAG	C4-C5	2.36	1.58	1.53
6	A	707	NAG	C3-C2	2.36	1.57	1.52
6	C	714	NAG	C4-C5	2.34	1.58	1.53
6	E	702	NAG	O5-C1	2.33	1.47	1.43
6	C	705	NAG	O5-C1	2.33	1.47	1.43
6	E	709	NAG	C3-C2	2.33	1.57	1.52
6	C	712	NAG	C3-C2	2.32	1.57	1.52
6	C	710	NAG	C3-C2	2.32	1.57	1.52
6	E	713	NAG	C4-C5	2.31	1.58	1.53
6	F	701	NAG	C3-C2	2.31	1.57	1.52
6	C	703	NAG	C3-C2	2.30	1.57	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	C	713	NAG	C3-C2	2.30	1.57	1.52
6	C	703	NAG	O5-C1	2.30	1.47	1.43
6	E	711	NAG	C4-C5	2.29	1.57	1.53
6	E	709	NAG	C2-N2	2.29	1.50	1.46
6	C	706	NAG	C4-C5	2.28	1.57	1.53
6	E	711	NAG	C3-C2	2.28	1.57	1.52
6	A	701	NAG	C3-C2	2.27	1.57	1.52
6	A	703	NAG	O5-C1	2.26	1.47	1.43
6	E	702	NAG	C3-C2	2.26	1.57	1.52
6	E	705	NAG	C4-C5	2.26	1.57	1.53
6	C	712	NAG	C4-C5	2.24	1.57	1.53
6	A	712	NAG	C4-C5	2.24	1.57	1.53
6	A	707	NAG	O5-C1	2.24	1.47	1.43
6	E	701	NAG	C4-C5	2.24	1.57	1.53
6	A	709	NAG	C3-C2	2.24	1.57	1.52
6	C	711	NAG	C3-C2	2.24	1.57	1.52
6	C	714	NAG	C2-N2	2.22	1.49	1.46
6	E	708	NAG	C3-C2	2.21	1.57	1.52
6	E	709	NAG	C4-C5	2.21	1.57	1.53
6	C	712	NAG	C2-N2	2.21	1.49	1.46
6	E	703	NAG	C3-C2	2.20	1.57	1.52
6	E	703	NAG	C4-C5	2.19	1.57	1.53
6	A	702	NAG	C3-C2	2.18	1.57	1.52
6	A	710	NAG	C3-C2	2.18	1.57	1.52
6	A	706	NAG	C3-C2	2.18	1.57	1.52
6	A	707	NAG	C4-C5	2.17	1.57	1.53
6	C	708	NAG	C3-C2	2.17	1.57	1.52
6	E	712	NAG	C4-C5	2.17	1.57	1.53
6	A	713	NAG	C3-C2	2.17	1.57	1.52
6	E	711	NAG	C4-C3	2.17	1.58	1.52
6	C	715	NAG	C3-C2	2.17	1.57	1.52
6	C	702	NAG	C3-C2	2.16	1.57	1.52
6	A	710	NAG	C2-N2	2.16	1.49	1.46
6	E	713	NAG	C3-C2	2.16	1.57	1.52
6	E	704	NAG	C3-C2	2.15	1.57	1.52
6	C	705	NAG	C3-C2	2.15	1.57	1.52
6	E	704	NAG	C4-C5	2.15	1.57	1.53
6	C	709	NAG	C2-N2	2.14	1.49	1.46
6	C	704	NAG	C3-C2	2.14	1.57	1.52
6	C	701	NAG	C4-C5	2.13	1.57	1.53
6	E	711	NAG	C2-N2	2.13	1.49	1.46
6	E	713	NAG	C2-N2	2.13	1.49	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	C	713	NAG	C4-C5	2.13	1.57	1.53
6	C	701	NAG	C3-C2	2.12	1.56	1.52
6	E	701	NAG	C3-C2	2.12	1.56	1.52
6	A	713	NAG	C4-C5	2.11	1.57	1.53
6	E	712	NAG	C2-N2	2.11	1.49	1.46
6	C	714	NAG	C4-C3	2.11	1.57	1.52
6	C	715	NAG	C2-N2	2.11	1.49	1.46
6	A	709	NAG	C4-C5	2.11	1.57	1.53
6	B	702	NAG	C2-N2	2.10	1.49	1.46
6	A	708	NAG	C4-C3	2.10	1.57	1.52
6	A	708	NAG	C2-N2	2.09	1.49	1.46
6	C	713	NAG	C2-N2	2.08	1.49	1.46
6	B	702	NAG	C4-C3	2.08	1.57	1.52
6	C	704	NAG	C4-C5	2.08	1.57	1.53
6	E	708	NAG	C2-N2	2.07	1.49	1.46
6	A	705	NAG	C2-N2	2.06	1.49	1.46
6	C	715	NAG	C4-C5	2.05	1.57	1.53
6	C	705	NAG	C4-C5	2.05	1.57	1.53
6	C	702	NAG	C4-C5	2.05	1.57	1.53
6	A	705	NAG	C4-C5	2.04	1.57	1.53
6	C	711	NAG	C4-C3	2.04	1.57	1.52
6	E	708	NAG	C4-C5	2.04	1.57	1.53
6	A	703	NAG	C3-C2	2.03	1.56	1.52
6	A	707	NAG	C2-N2	2.03	1.49	1.46
6	A	711	NAG	C2-N2	2.03	1.49	1.46
6	A	710	NAG	C4-C5	2.02	1.57	1.53
6	E	703	NAG	C4-C3	2.02	1.57	1.52
6	A	712	NAG	C4-C3	2.02	1.57	1.52
6	C	710	NAG	C4-C5	2.02	1.57	1.53
6	E	713	NAG	C4-C3	2.01	1.57	1.52
6	A	702	NAG	C4-C5	2.00	1.57	1.53
6	F	701	NAG	C4-C3	2.00	1.57	1.52
6	C	712	NAG	C4-C3	2.00	1.57	1.52

All (49) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	705	NAG	C2-N2-C7	3.30	127.32	122.90
6	E	709	NAG	C8-C7-N2	3.07	121.21	116.12
6	E	711	NAG	C8-C7-N2	3.04	121.16	116.12
6	A	711	NAG	C2-N2-C7	2.93	126.83	122.90
6	A	710	NAG	O7-C7-C8	-2.73	117.19	122.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	710	NAG	C8-C7-N2	2.73	120.64	116.12
6	C	705	NAG	C1-C2-N2	-2.71	106.16	110.43
6	C	706	NAG	O7-C7-C8	-2.64	117.36	122.05
6	A	711	NAG	C1-C2-N2	-2.62	106.31	110.43
6	C	704	NAG	C8-C7-N2	2.56	120.36	116.12
6	C	712	NAG	C8-C7-N2	2.55	120.36	116.12
6	E	705	NAG	C8-C7-N2	2.55	120.35	116.12
6	C	708	NAG	C8-C7-N2	2.50	120.26	116.12
6	A	705	NAG	C1-C2-N2	2.48	114.35	110.43
6	E	711	NAG	O7-C7-C8	-2.45	117.69	122.05
6	E	709	NAG	O7-C7-C8	-2.44	117.71	122.05
6	E	713	NAG	C8-C7-N2	2.42	120.12	116.12
6	C	714	NAG	C8-C7-N2	2.41	120.12	116.12
6	A	706	NAG	C8-C7-N2	2.38	120.07	116.12
6	C	709	NAG	C8-C7-N2	2.37	120.05	116.12
6	C	715	NAG	C8-C7-N2	2.34	120.00	116.12
6	A	702	NAG	C8-C7-N2	2.33	119.98	116.12
6	E	711	NAG	C1-C2-N2	-2.33	106.77	110.43
6	D	703	NAG	C8-C7-N2	2.28	119.90	116.12
6	A	705	NAG	O5-C1-C2	-2.27	107.78	111.29
6	C	706	NAG	C8-C7-N2	2.27	119.88	116.12
6	A	707	NAG	C8-C7-N2	2.25	119.84	116.12
6	E	704	NAG	C8-C7-N2	2.24	119.84	116.12
6	A	709	NAG	C8-C7-N2	2.24	119.83	116.12
6	D	703	NAG	C1-O5-C5	2.23	115.18	112.19
6	C	711	NAG	C1-C2-N2	-2.23	106.92	110.43
6	C	713	NAG	C8-C7-N2	2.23	119.81	116.12
6	A	702	NAG	C1-O5-C5	2.22	115.16	112.19
6	A	708	NAG	C1-C2-N2	-2.19	106.99	110.43
6	A	713	NAG	C8-C7-N2	2.19	119.74	116.12
6	C	708	NAG	O7-C7-C8	-2.18	118.17	122.05
6	E	708	NAG	C8-C7-N2	2.17	119.72	116.12
6	A	708	NAG	C8-C7-N2	2.16	119.71	116.12
6	E	705	NAG	C1-O5-C5	2.16	115.08	112.19
6	B	702	NAG	O7-C7-C8	-2.14	118.24	122.05
6	E	705	NAG	O7-C7-C8	-2.11	118.29	122.05
6	B	702	NAG	C8-C7-N2	2.09	119.58	116.12
6	C	711	NAG	C8-C7-N2	2.09	119.58	116.12
6	E	701	NAG	C8-C7-N2	2.08	119.58	116.12
6	A	712	NAG	C8-C7-N2	2.06	119.53	116.12
6	C	712	NAG	O7-C7-C8	-2.06	118.39	122.05
6	C	703	NAG	C8-C7-N2	2.04	119.51	116.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	701	NAG	C1-O5-C5	2.04	114.92	112.19
6	A	702	NAG	O7-C7-C8	-2.00	118.49	122.05

There are no chirality outliers.

All (40) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	D	701	NAG	C3-C2-N2-C7
6	D	701	NAG	C8-C7-N2-C2
6	D	701	NAG	O7-C7-N2-C2
6	D	702	NAG	C1-C2-N2-C7
6	D	702	NAG	C8-C7-N2-C2
6	D	702	NAG	O7-C7-N2-C2
6	E	706	NAG	C8-C7-N2-C2
6	E	706	NAG	O7-C7-N2-C2
6	E	707	NAG	C8-C7-N2-C2
6	E	707	NAG	O7-C7-N2-C2
6	E	710	NAG	C8-C7-N2-C2
6	E	710	NAG	O7-C7-N2-C2
6	A	705	NAG	C1-C2-N2-C7
6	B	701	NAG	C8-C7-N2-C2
6	B	701	NAG	O7-C7-N2-C2
6	B	701	NAG	O5-C5-C6-O6
6	B	701	NAG	C4-C5-C6-O6
6	F	702	NAG	C8-C7-N2-C2
6	A	704	NAG	C8-C7-N2-C2
6	E	710	NAG	O5-C5-C6-O6
6	F	702	NAG	C4-C5-C6-O6
6	E	710	NAG	C4-C5-C6-O6
6	F	702	NAG	O7-C7-N2-C2
6	A	704	NAG	O7-C7-N2-C2
6	A	709	NAG	O5-C5-C6-O6
6	F	702	NAG	O5-C5-C6-O6
6	E	701	NAG	O5-C5-C6-O6
6	C	707	NAG	O5-C5-C6-O6
6	C	712	NAG	O5-C5-C6-O6
6	A	702	NAG	O5-C5-C6-O6
6	C	702	NAG	O5-C5-C6-O6
6	E	703	NAG	O5-C5-C6-O6
6	C	714	NAG	O5-C5-C6-O6
6	E	705	NAG	O5-C5-C6-O6
6	C	705	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
6	A	704	NAG	O5-C5-C6-O6
6	A	709	NAG	C4-C5-C6-O6
6	A	705	NAG	C3-C2-N2-C7
6	A	711	NAG	C3-C2-N2-C7
6	B	703	NAG	C3-C2-N2-C7

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	703	NAG	1	0
6	C	707	NAG	1	0
6	D	701	NAG	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

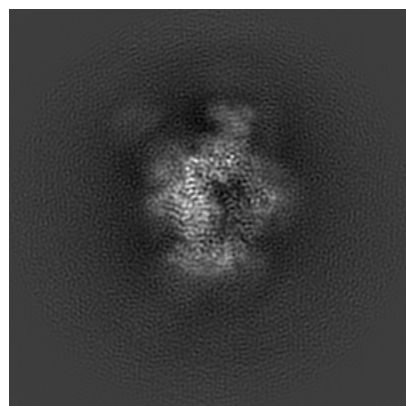
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-23232. These allow visual inspection of the internal detail of the map and identification of artifacts.

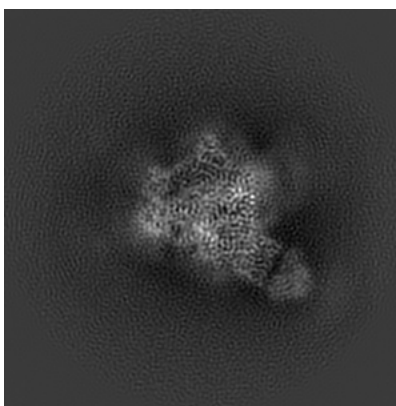
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

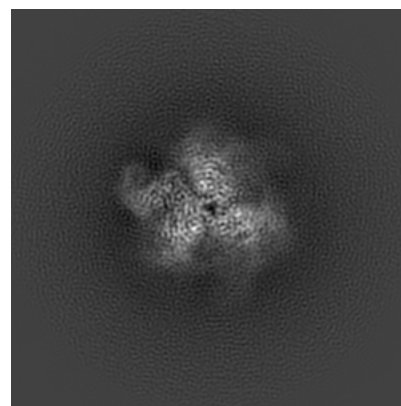
6.1.1 Primary map



X

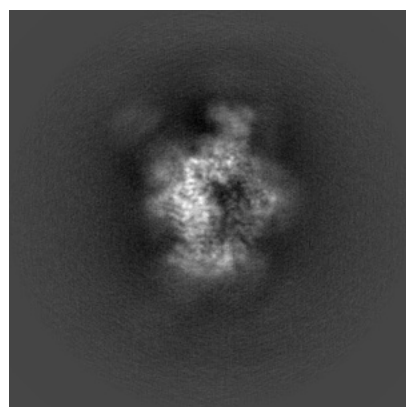


Y

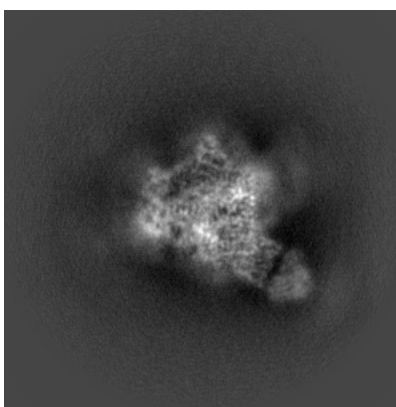


Z

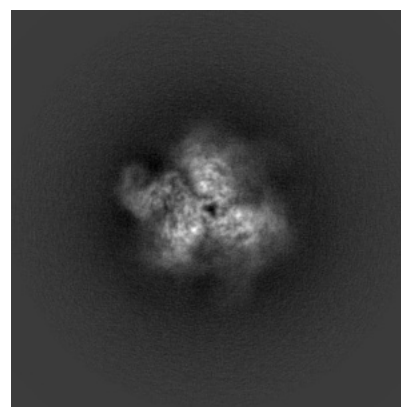
6.1.2 Raw map



X



Y

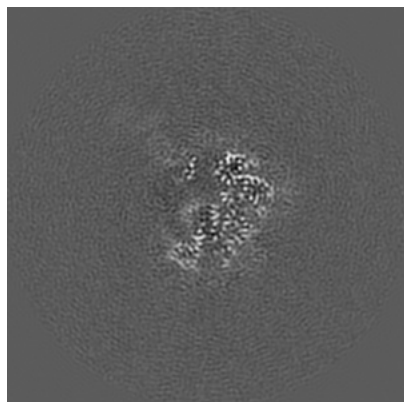


Z

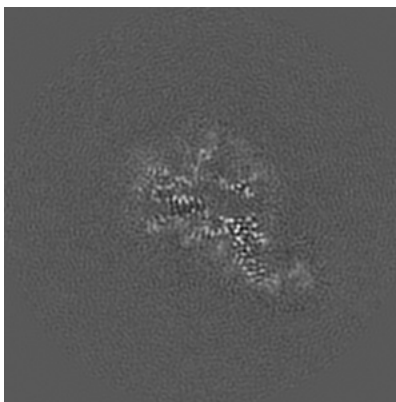
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

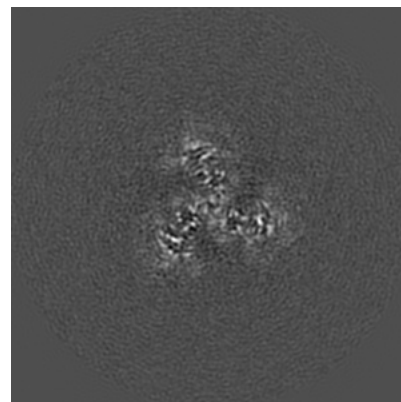
6.2.1 Primary map



X Index: 160

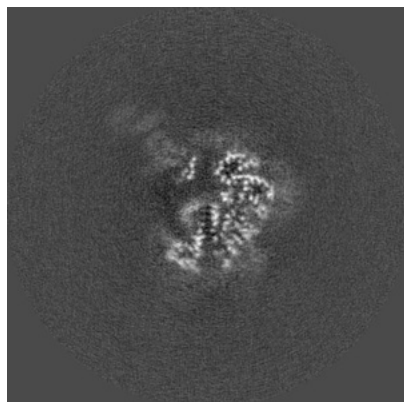


Y Index: 160

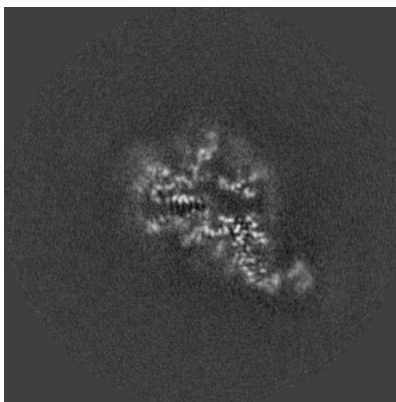


Z Index: 160

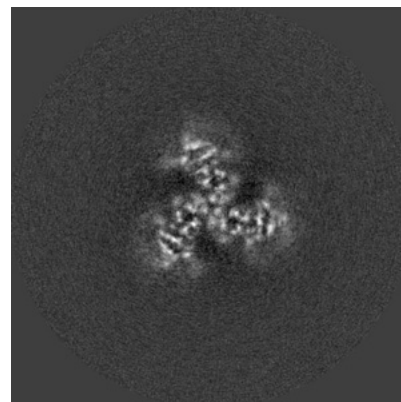
6.2.2 Raw map



X Index: 160



Y Index: 160

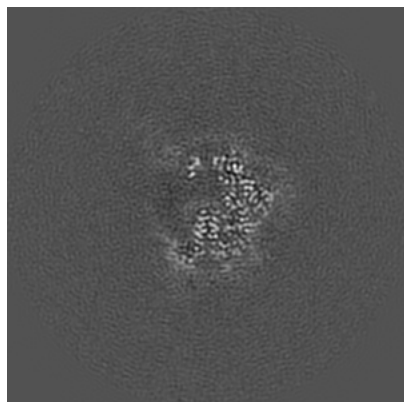


Z Index: 160

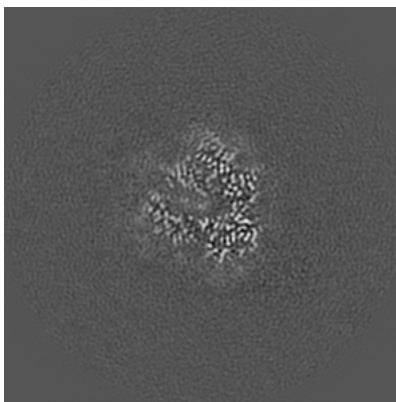
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

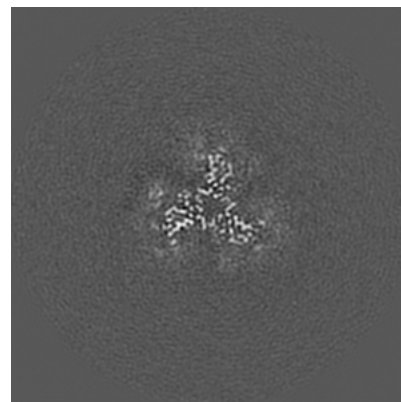
6.3.1 Primary map



X Index: 157

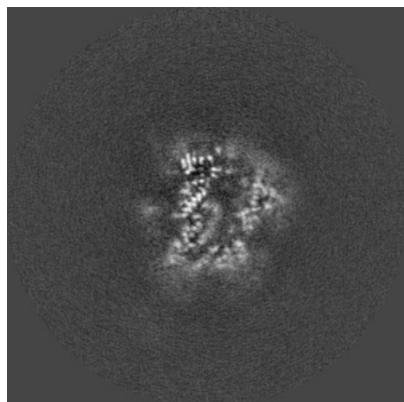


Y Index: 146

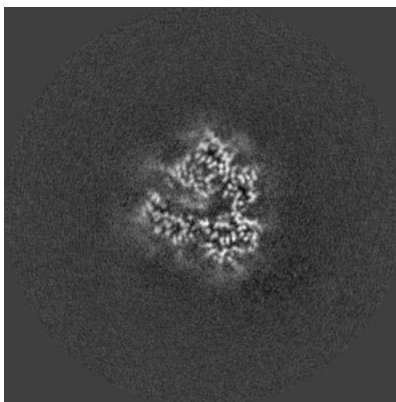


Z Index: 183

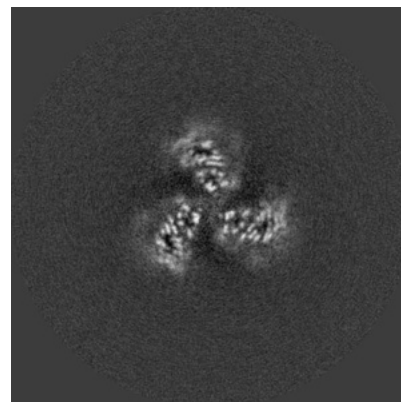
6.3.2 Raw map



X Index: 147



Y Index: 145

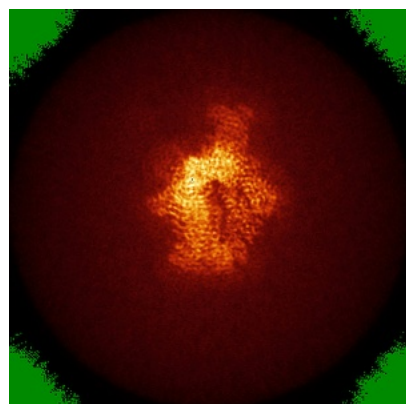


Z Index: 166

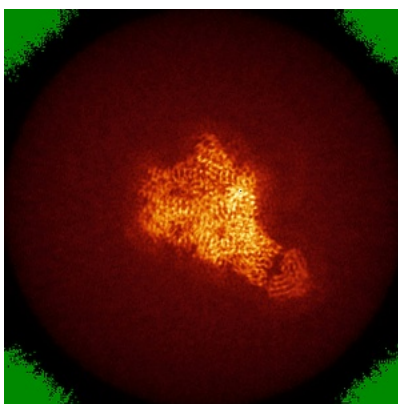
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

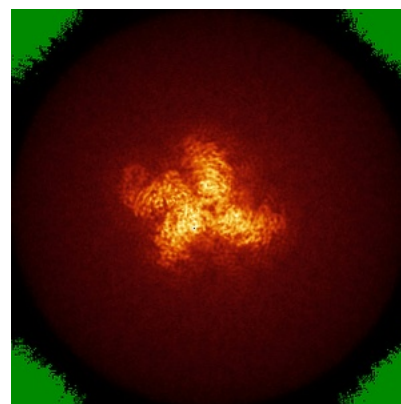
6.4.1 Primary map



X

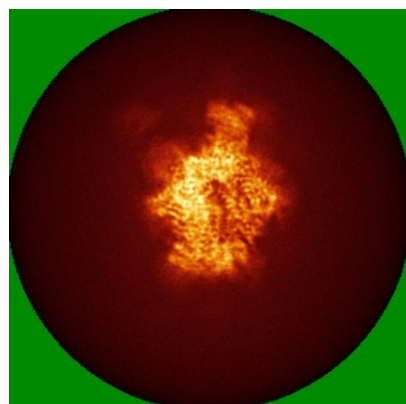


Y

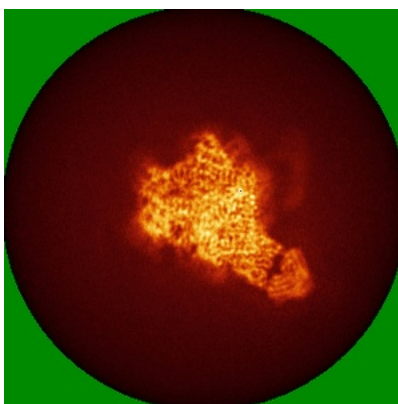


Z

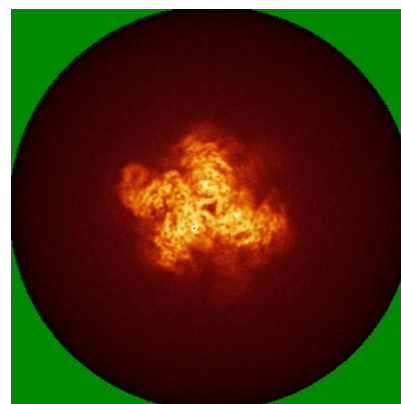
6.4.2 Raw map



X



Y



Z

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

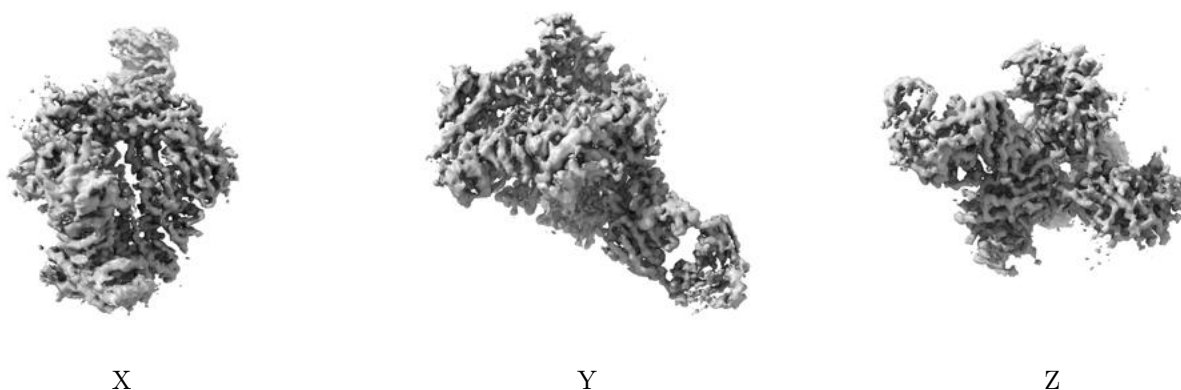
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.025. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

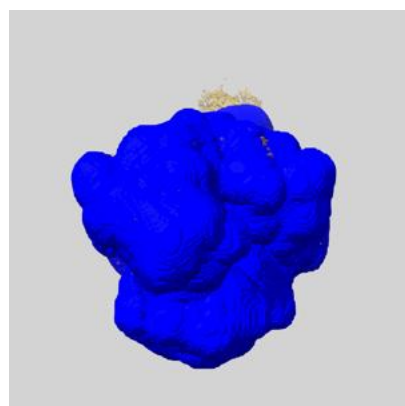
6.6 Mask visualisation [i](#)

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

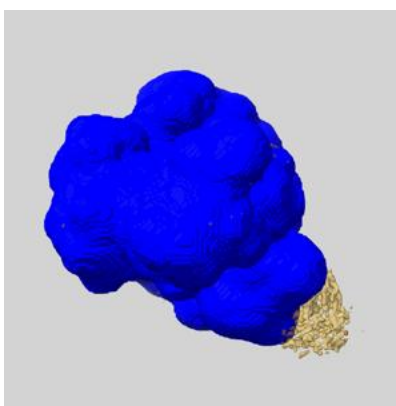
A mask typically either:

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

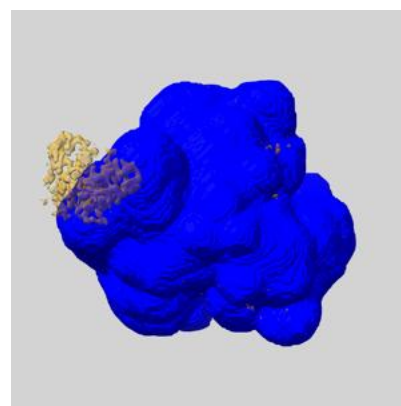
6.6.1 emd_23232_msk_1.map [i](#)



X



Y

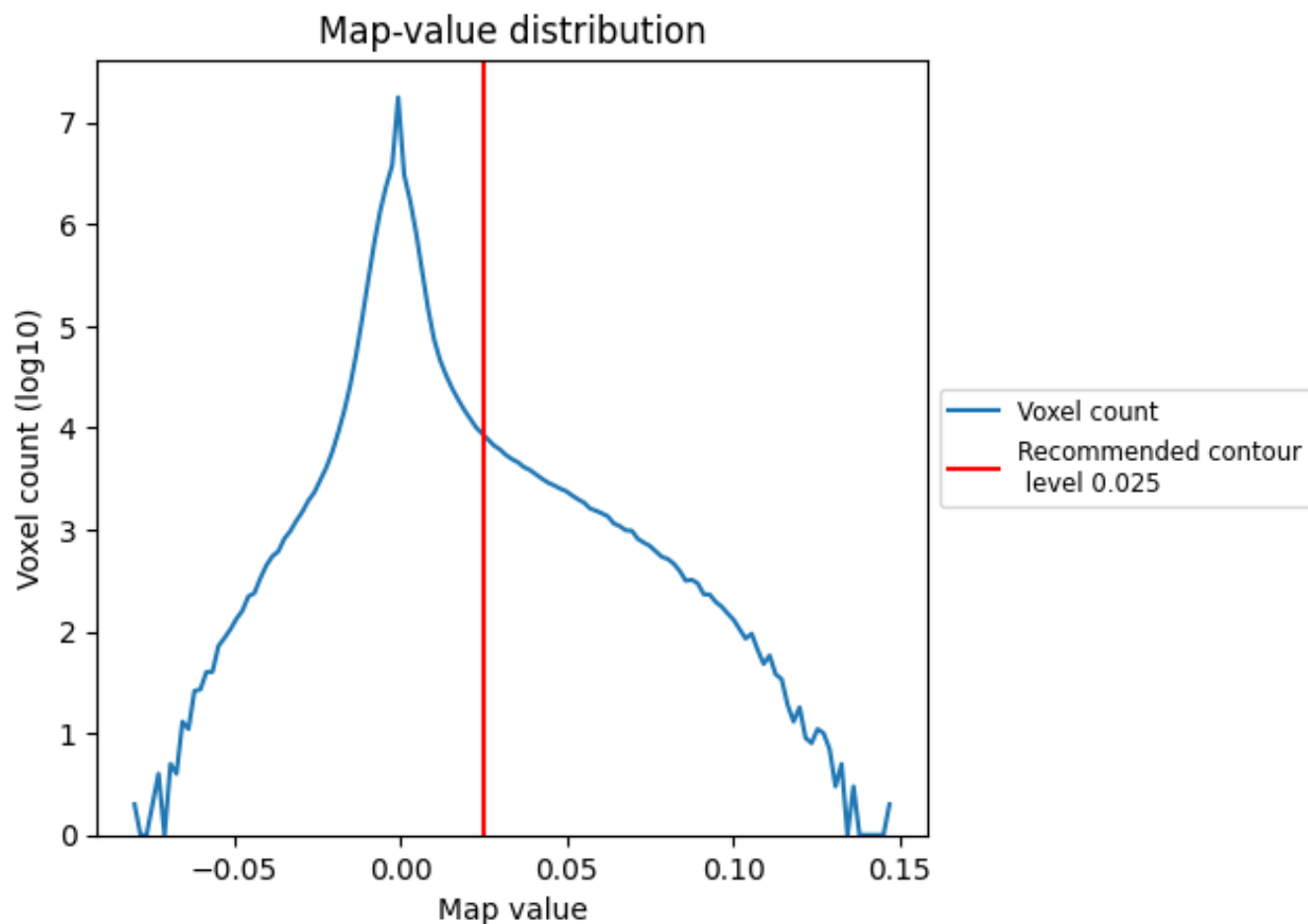


Z

7 Map analysis [i](#)

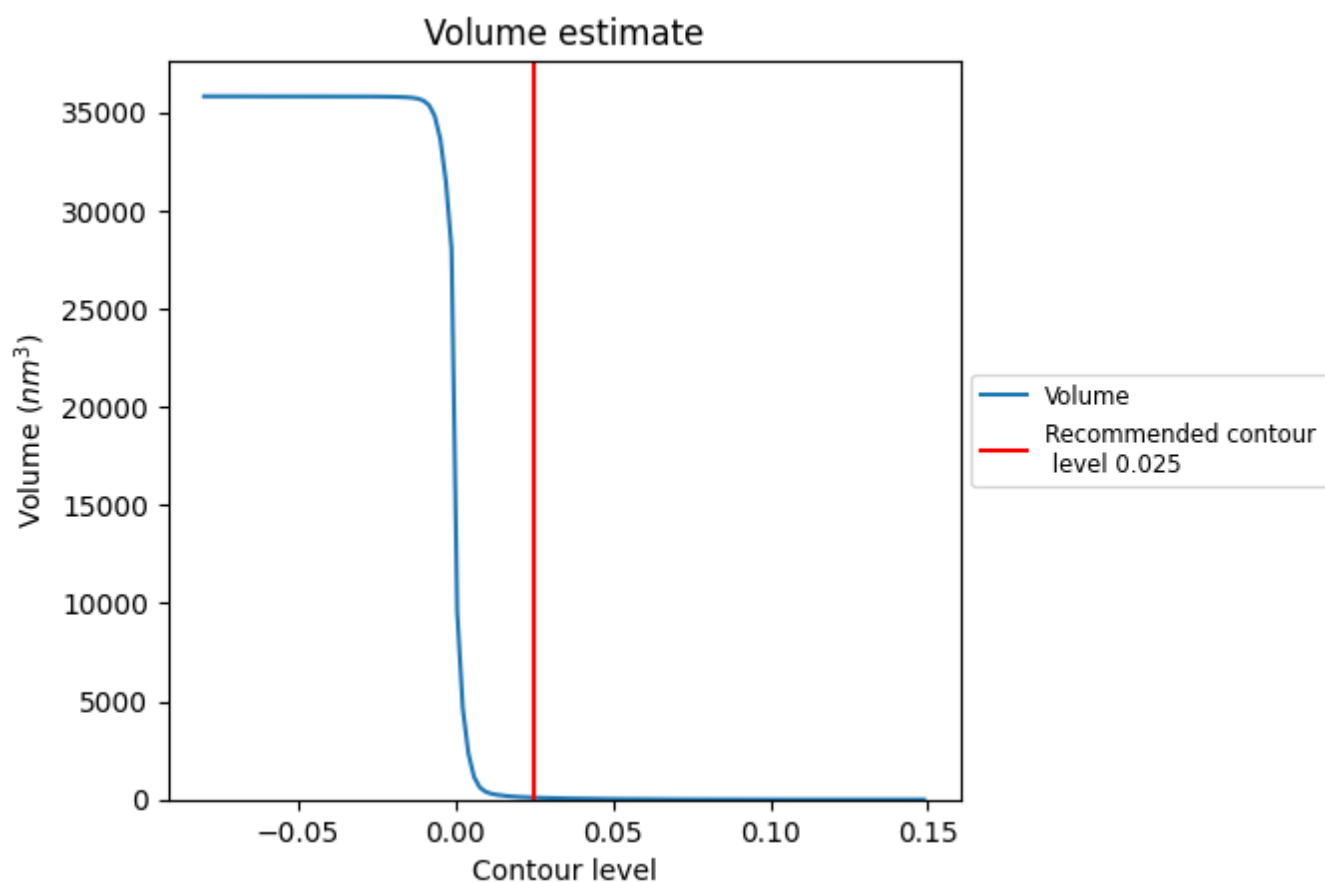
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

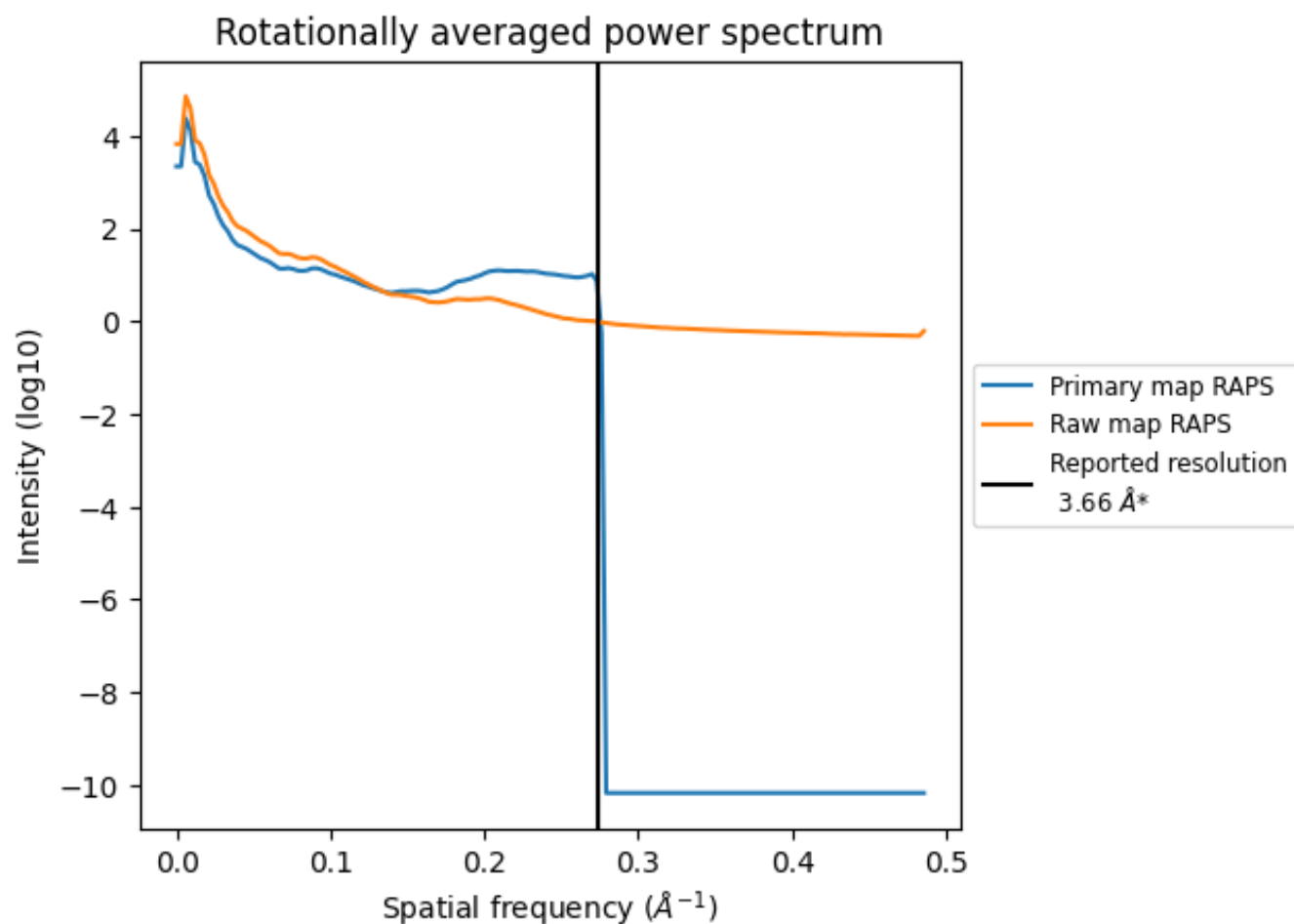
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 100 nm³; this corresponds to an approximate mass of 90 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 ⓘ

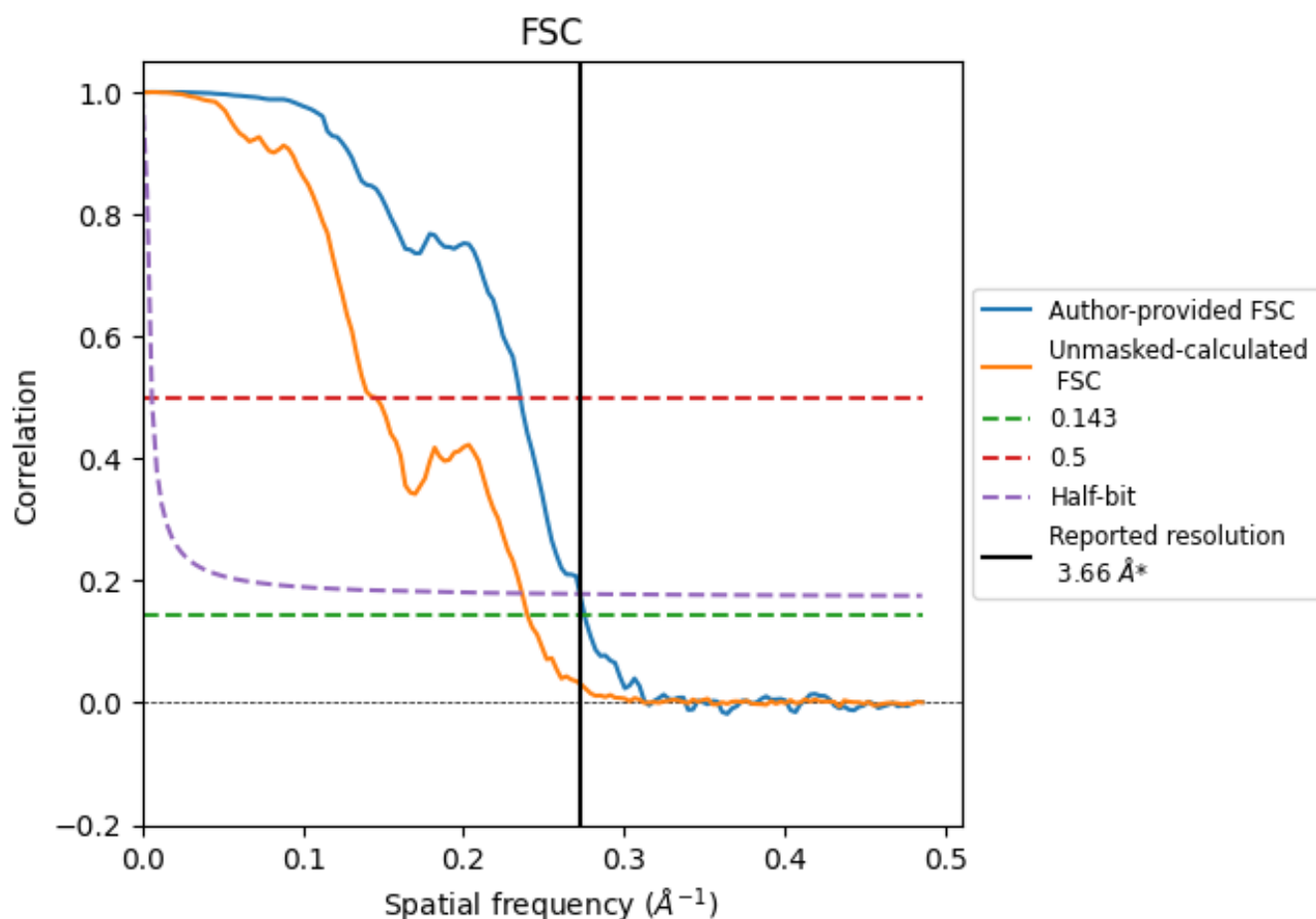


*Reported resolution corresponds to spatial frequency of 0.273 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.273 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

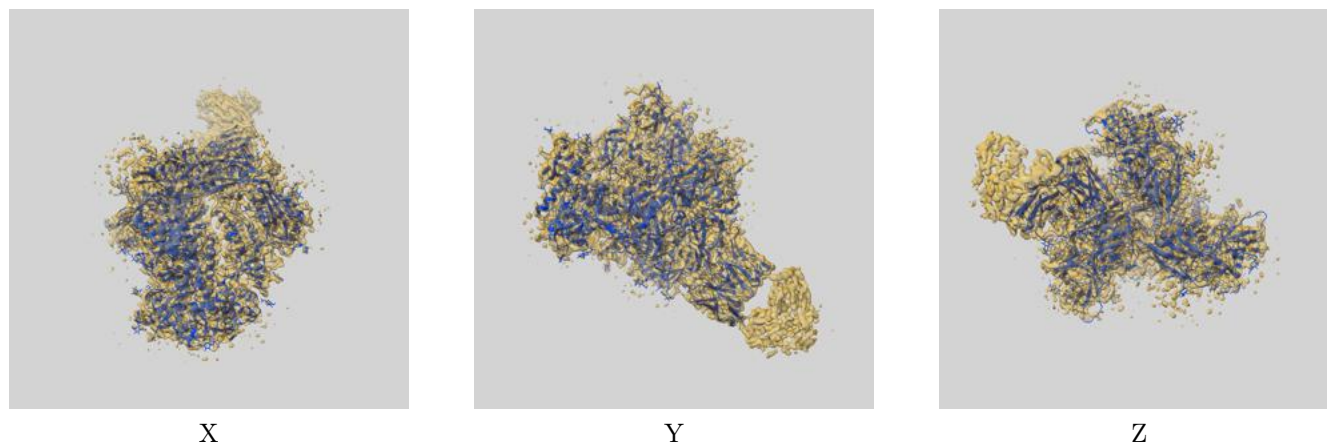
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.66	-	-
Author-provided FSC curve	3.63	4.25	3.67
Unmasked-calculated*	4.17	6.91	4.23

*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 4.17 differs from the reported value 3.66 by more than 10 %

9 Map-model fit [i](#)

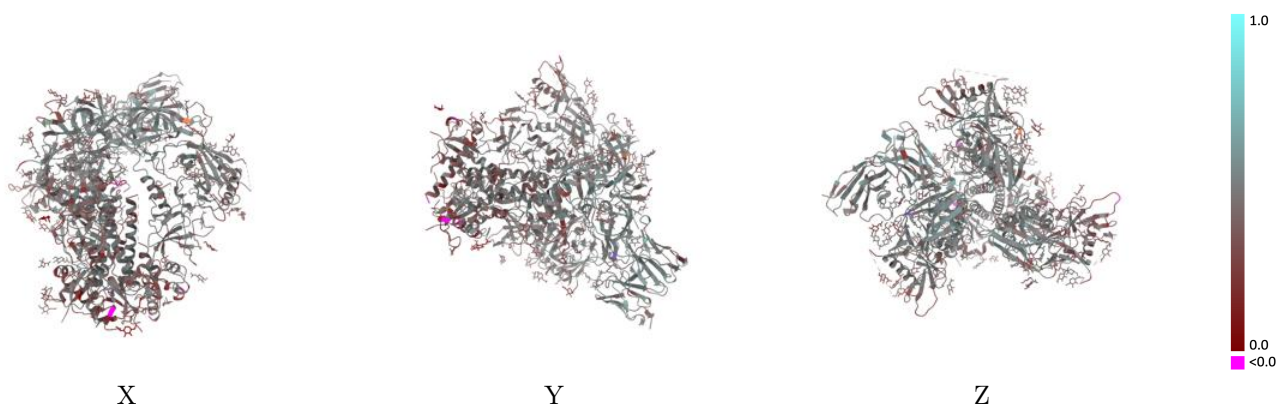
This section contains information regarding the fit between EMDB map EMD-23232 and PDB model 7L8F. Per-residue inclusion information can be found in section [3](#) on page [17](#).

9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 0.025 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](#)

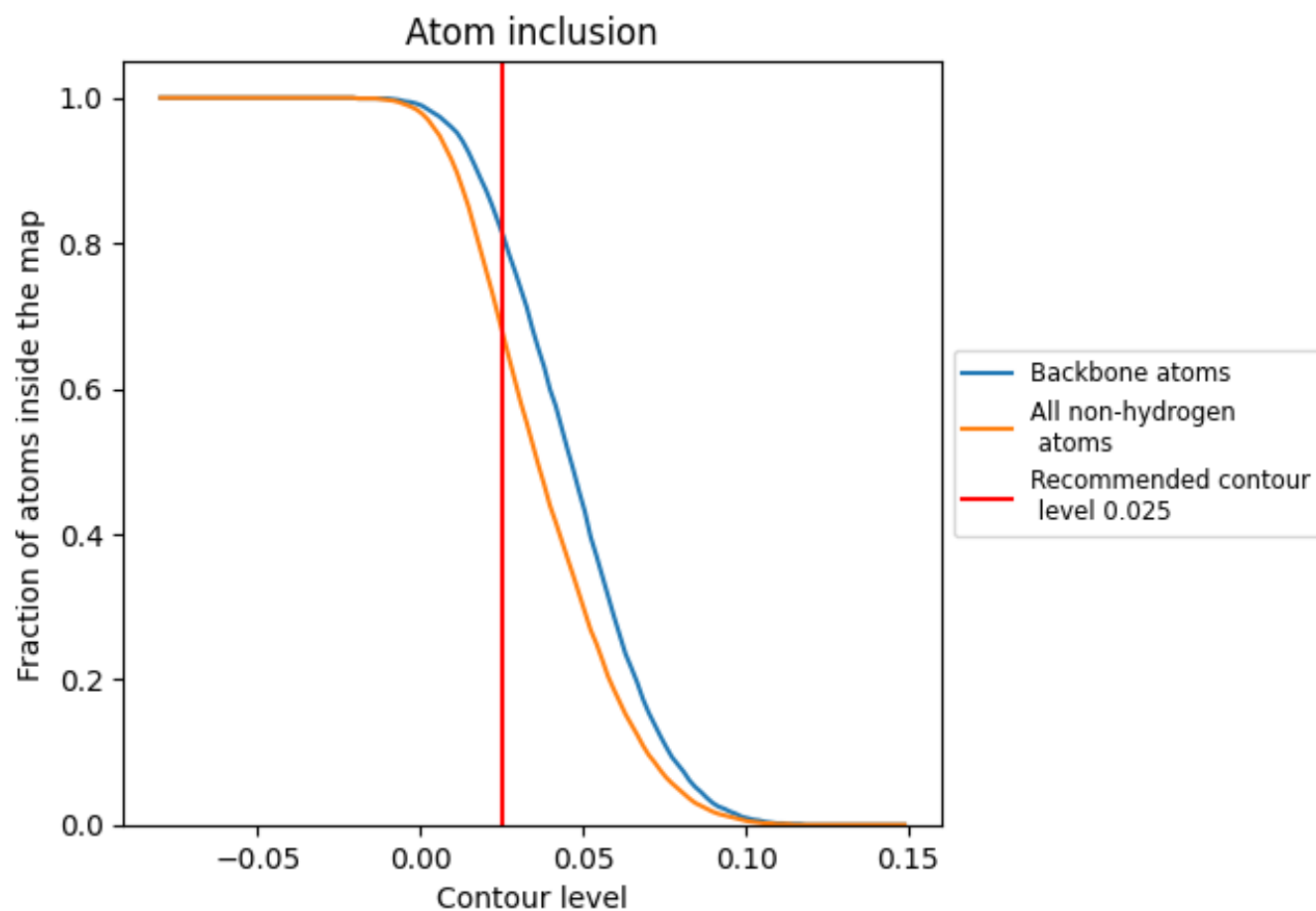


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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](#)

This section was not generated.

9.4 Atom inclusion [i](#)



At the recommended contour level, 82% of all backbone atoms, 68% 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 (0.025) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6820	 0.4320
A	 0.7160	 0.4570
B	 0.6120	 0.3860
C	 0.6850	 0.4290
D	 0.6080	 0.3800
E	 0.6820	 0.4430
F	 0.5940	 0.3760
G	 0.4920	 0.4280
H	 0.8440	 0.4820
I	 0.4640	 0.2910
J	 0.5360	 0.4240
K	 0.5250	 0.3900
L	 0.8430	 0.4690
M	 0.3930	 0.4180
N	 0.3570	 0.4260
O	 0.6790	 0.4110
P	 0.6070	 0.3600
Q	 0.5080	 0.4010
R	 0.3570	 0.3540
S	 0.3930	 0.2710
T	 0.5000	 0.3960
U	 0.6070	 0.4670
V	 0.6790	 0.4560

