Full wwPDB EM Validation Report

Jan 27, 2025 – 01:11 PM EST

PDB ID	:	9AUG
EMDB ID	:	EMD-43879
Title	:	Cryo-EM structure of CH848.d949.10.17.GS-DH270.UCA3.G57R
Authors	:	Zhang, Q.E.; Acharya, P.
Deposited on	:	2024-02-29
Resolution	:	3.80 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ 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:

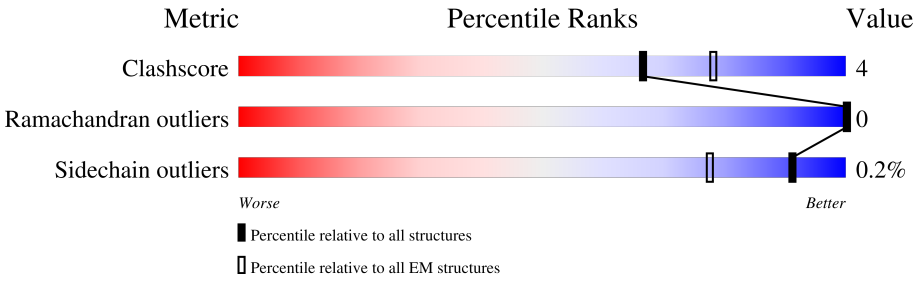
EMDB validation analysis	:	0.0.1.dev113
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.40

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.80 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	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	469	10% 89% 9%
1	B	469	12% 90% 8%
1	C	469	8% 86% 12%
2	D	153	73% 7% 20%
2	E	153	14% 71% 9% 20%
2	F	153	13% 71% 10% 20%
3	G	232	45% 9% 46%
3	H	232	6% 49% 5% 46%

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Mol	Chain	Length	Quality of chain
3	I	232	5% 45% 9% 46%
4	J	216	14% 46% 5% 49%
4	K	216	16% 46% 5% 49%
4	L	216	14% 45% 6% 49%
5	M	5	40% 60%
5	R	5	40% 40% 60%
5	W	5	40% 60%
6	N	8	25% 25% 75%
6	S	8	25% 25% 75%
6	X	8	25% 25% 75%
7	O	3	33% 100%
7	T	3	33% 67% 33%
7	Y	3	33% 67% 33%
8	P	2	100%
8	Q	2	50% 100%
8	U	2	100%
8	V	2	50% 100%
8	Z	2	100%
8	a	2	50% 100%

2 Entry composition (i)

There are 9 unique types of molecules in this entry. The entry contains 20211 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 HIV-1 BG505 DS-SOSIP glycoprotein gp120.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	460	Total	C	N	O	S	0	0
			3590	2245	622	694	29		
1	B	460	Total	C	N	O	S	0	0
			3590	2245	622	694	29		
1	C	460	Total	C	N	O	S	0	0
			3590	2245	622	694	29		

There are 432 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	47	GLU	ASP	conflict	UNP Q2N0S6
A	49	LYS	GLU	conflict	UNP Q2N0S6
A	59	ARG	LYS	conflict	UNP Q2N0S6
A	63	LYS	THR	conflict	UNP Q2N0S6
A	65	VAL	LYS	conflict	UNP Q2N0S6
A	80	SER	ASN	conflict	UNP Q2N0S6
A	84	LEU	ILE	conflict	UNP Q2N0S6
A	85	VAL	HIS	conflict	UNP Q2N0S6
A	87	GLY	GLU	conflict	UNP Q2N0S6
A	92	ASN	GLU	conflict	UNP Q2N0S6
A	99	ASP	ASN	conflict	UNP Q2N0S6
A	102	ASP	GLU	conflict	UNP Q2N0S6
A	106	GLU	THR	conflict	UNP Q2N0S6
A	130	ILE	GLN	conflict	UNP Q2N0S6
A	?	-	THR	deletion	UNP Q2N0S6
A	?	-	ASN	deletion	UNP Q2N0S6
A	?	-	VAL	deletion	UNP Q2N0S6
A	?	-	THR	deletion	UNP Q2N0S6
A	?	-	ASN	deletion	UNP Q2N0S6
A	?	-	ASN	deletion	UNP Q2N0S6
A	?	-	ILE	deletion	UNP Q2N0S6
A	132	SER	THR	conflict	UNP Q2N0S6
A	134	ALA	ASP	conflict	UNP Q2N0S6
A	135	GLY	MET	conflict	UNP Q2N0S6

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Chain	Residue	Modelled	Actual	Comment	Reference
A	136	SER	ARG	conflict	UNP Q2N0S6
A	138	GLY	-	insertion	UNP Q2N0S6
A	149	VAL	-	insertion	UNP Q2N0S6
A	150	GLU	-	insertion	UNP Q2N0S6
A	154	MET	LEU	conflict	UNP Q2N0S6
A	161	THR	MET	conflict	UNP Q2N0S6
A	165	ILE	LEU	conflict	UNP Q2N0S6
A	169	GLU	LYS	conflict	UNP Q2N0S6
A	170	LYS	GLN	conflict	UNP Q2N0S6
A	172	GLU	VAL	conflict	UNP Q2N0S6
A	174	ALA	SER	conflict	UNP Q2N0S6
A	178	LYS	ARG	conflict	UNP Q2N0S6
A	179	PRO	LEU	conflict	UNP Q2N0S6
A	181	ILE	VAL	conflict	UNP Q2N0S6
A	183	PRO	GLN	conflict	UNP Q2N0S6
A	184	LEU	ILE	conflict	UNP Q2N0S6
A	185	SER	ASN	conflict	UNP Q2N0S6
A	?	-	ASN	deletion	UNP Q2N0S6
A	?	-	GLN	deletion	UNP Q2N0S6
A	?	-	GLY	deletion	UNP Q2N0S6
A	?	-	ASN	deletion	UNP Q2N0S6
A	?	-	ARG	deletion	UNP Q2N0S6
A	?	-	SER	deletion	UNP Q2N0S6
A	185b	THR	ASN	conflict	UNP Q2N0S6
A	187	ASN	SER	conflict	UNP Q2N0S6
A	188	THR	ASN	conflict	UNP Q2N0S6
A	189	SER	LYS	conflict	UNP Q2N0S6
A	201	CYS	ILE	conflict	UNP Q2N0S6
A	209	THR	SER	conflict	UNP Q2N0S6
A	223	TYR	PHE	conflict	UNP Q2N0S6
A	229	ASN	LYS	conflict	UNP Q2N0S6
A	231	GLU	LYS	conflict	UNP Q2N0S6
A	232	THR	LYS	conflict	UNP Q2N0S6
A	240	SER	PRO	conflict	UNP Q2N0S6
A	241	ASN	SER	conflict	UNP Q2N0S6
A	252	ARG	LYS	conflict	UNP Q2N0S6
A	268	LYS	GLU	conflict	UNP Q2N0S6
A	270	ILE	VAL	conflict	UNP Q2N0S6
A	271	VAL	MET	conflict	UNP Q2N0S6
A	277	LEU	ILE	conflict	UNP Q2N0S6
A	283	ILE	ASN	conflict	UNP Q2N0S6
A	285	ILE	LEU	conflict	UNP Q2N0S6

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Chain	Residue	Modelled	Actual	Comment	Reference
A	287	HIS	GLN	conflict	UNP Q2N0S6
A	288	LEU	PHE	conflict	UNP Q2N0S6
A	289	HIS	ASN	conflict	UNP Q2N0S6
A	293	GLU	GLN	conflict	UNP Q2N0S6
A	295	VAL	ASN	conflict	UNP Q2N0S6
A	307	VAL	ILE	conflict	UNP Q2N0S6
A	316	THR	ALA	conflict	UNP Q2N0S6
A	327	LYS	ARG	conflict	UNP Q2N0S6
A	332	ASN	THR	conflict	UNP Q2N0S6
A	333	ILE	VAL	conflict	UNP Q2N0S6
A	335	GLU	LYS	conflict	UNP Q2N0S6
A	336	GLU	ALA	conflict	UNP Q2N0S6
A	337	LYS	THR	conflict	UNP Q2N0S6
A	340	ASP	GLU	conflict	UNP Q2N0S6
A	343	GLN	GLY	conflict	UNP Q2N0S6
A	346	GLY	VAL	conflict	UNP Q2N0S6
A	347	ILE	LYS	conflict	UNP Q2N0S6
A	348	GLU	GLN	conflict	UNP Q2N0S6
A	350	GLN	ARG	conflict	UNP Q2N0S6
A	354	PRO	GLY	conflict	UNP Q2N0S6
A	356	LYS	ASN	conflict	UNP Q2N0S6
A	?	-	ILE	deletion	UNP Q2N0S6
A	?	-	ARG	deletion	UNP Q2N0S6
A	360	LYS	PHE	conflict	UNP Q2N0S6
A	361	TYR	ALA	conflict	UNP Q2N0S6
A	363	GLN	-	insertion	UNP Q2N0S6
A	365	ALA	SER	conflict	UNP Q2N0S6
A	369	MET	LEU	conflict	UNP Q2N0S6
A	371	ILE	VAL	conflict	UNP Q2N0S6
A	389	ASN	GLY	conflict	UNP Q2N0S6
A	392	ASN	-	insertion	UNP Q2N0S6
A	393	GLY	-	insertion	UNP Q2N0S6
A	394	THR	-	insertion	UNP Q2N0S6
A	395	TYR	-	insertion	UNP Q2N0S6
A	397	GLY	SER	conflict	UNP Q2N0S6
A	400	TYR	TRP	conflict	UNP Q2N0S6
A	403	THR	ASN	conflict	UNP Q2N0S6
A	404	ASN	THR	conflict	UNP Q2N0S6
A	406	SER	VAL	conflict	UNP Q2N0S6
A	407	ALA	GLN	conflict	UNP Q2N0S6
A	408	ASN	GLY	conflict	UNP Q2N0S6
A	411	THR	ASN	conflict	UNP Q2N0S6

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Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	GLY	deletion	UNP Q2N0S6
A	?	-	SER	deletion	UNP Q2N0S6
A	?	-	ASN	deletion	UNP Q2N0S6
A	?	-	ASP	deletion	UNP Q2N0S6
A	?	-	SER	deletion	UNP Q2N0S6
A	417	GLN	PRO	conflict	UNP Q2N0S6
A	429	GLY	ARG	conflict	UNP Q2N0S6
A	430	VAL	ILE	conflict	UNP Q2N0S6
A	432	ARG	GLN	conflict	UNP Q2N0S6
A	433	CYS	ALA	conflict	UNP Q2N0S6
A	440	ALA	GLN	conflict	UNP Q2N0S6
A	442	ASN	VAL	conflict	UNP Q2N0S6
A	444	THR	ARG	conflict	UNP Q2N0S6
A	446	ARG	VAL	conflict	UNP Q2N0S6
A	453	LEU	ILE	conflict	UNP Q2N0S6
A	460	THR	SER	conflict	UNP Q2N0S6
A	461	ASN	THR	conflict	UNP Q2N0S6
A	462	SER	ASN	conflict	UNP Q2N0S6
A	463	ASN	SER	conflict	UNP Q2N0S6
A	464	GLU	THR	conflict	UNP Q2N0S6
A	471	ALA	GLY	conflict	UNP Q2N0S6
A	499	THR	-	expression tag	UNP Q2N0S6
A	500	ARG	-	expression tag	UNP Q2N0S6
A	501	CYS	-	expression tag	UNP Q2N0S6
A	502	LYS	-	expression tag	UNP Q2N0S6
A	503	ARG	-	expression tag	UNP Q2N0S6
A	504	ARG	-	expression tag	UNP Q2N0S6
A	505	VAL	-	expression tag	UNP Q2N0S6
A	506	VAL	-	expression tag	UNP Q2N0S6
A	507	GLY	-	expression tag	UNP Q2N0S6
A	508	ARG	-	expression tag	UNP Q2N0S6
A	509	ARG	-	expression tag	UNP Q2N0S6
A	510	ARG	-	expression tag	UNP Q2N0S6
A	511	ARG	-	expression tag	UNP Q2N0S6
A	512	ARG	-	expression tag	UNP Q2N0S6
A	513	ARG	-	expression tag	UNP Q2N0S6
B	47	GLU	ASP	conflict	UNP Q2N0S6
B	49	LYS	GLU	conflict	UNP Q2N0S6
B	59	ARG	LYS	conflict	UNP Q2N0S6
B	63	LYS	THR	conflict	UNP Q2N0S6
B	65	VAL	LYS	conflict	UNP Q2N0S6
B	80	SER	ASN	conflict	UNP Q2N0S6

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Chain	Residue	Modelled	Actual	Comment	Reference
B	84	LEU	ILE	conflict	UNP Q2N0S6
B	85	VAL	HIS	conflict	UNP Q2N0S6
B	87	GLY	GLU	conflict	UNP Q2N0S6
B	92	ASN	GLU	conflict	UNP Q2N0S6
B	99	ASP	ASN	conflict	UNP Q2N0S6
B	102	ASP	GLU	conflict	UNP Q2N0S6
B	106	GLU	THR	conflict	UNP Q2N0S6
B	130	ILE	GLN	conflict	UNP Q2N0S6
B	?	-	THR	deletion	UNP Q2N0S6
B	?	-	ASN	deletion	UNP Q2N0S6
B	?	-	VAL	deletion	UNP Q2N0S6
B	?	-	THR	deletion	UNP Q2N0S6
B	?	-	ASN	deletion	UNP Q2N0S6
B	?	-	ASN	deletion	UNP Q2N0S6
B	?	-	ILE	deletion	UNP Q2N0S6
B	132	SER	THR	conflict	UNP Q2N0S6
B	134	ALA	ASP	conflict	UNP Q2N0S6
B	135	GLY	MET	conflict	UNP Q2N0S6
B	136	SER	ARG	conflict	UNP Q2N0S6
B	138	GLY	-	insertion	UNP Q2N0S6
B	149	VAL	-	insertion	UNP Q2N0S6
B	150	GLU	-	insertion	UNP Q2N0S6
B	154	MET	LEU	conflict	UNP Q2N0S6
B	161	THR	MET	conflict	UNP Q2N0S6
B	165	ILE	LEU	conflict	UNP Q2N0S6
B	169	GLU	LYS	conflict	UNP Q2N0S6
B	170	LYS	GLN	conflict	UNP Q2N0S6
B	172	GLU	VAL	conflict	UNP Q2N0S6
B	174	ALA	SER	conflict	UNP Q2N0S6
B	178	LYS	ARG	conflict	UNP Q2N0S6
B	179	PRO	LEU	conflict	UNP Q2N0S6
B	181	ILE	VAL	conflict	UNP Q2N0S6
B	183	PRO	GLN	conflict	UNP Q2N0S6
B	184	LEU	ILE	conflict	UNP Q2N0S6
B	185	SER	ASN	conflict	UNP Q2N0S6
B	?	-	ASN	deletion	UNP Q2N0S6
B	?	-	GLN	deletion	UNP Q2N0S6
B	?	-	GLY	deletion	UNP Q2N0S6
B	?	-	ASN	deletion	UNP Q2N0S6
B	?	-	ARG	deletion	UNP Q2N0S6
B	?	-	SER	deletion	UNP Q2N0S6
B	185b	THR	ASN	conflict	UNP Q2N0S6

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Chain	Residue	Modelled	Actual	Comment	Reference
B	187	ASN	SER	conflict	UNP Q2N0S6
B	188	THR	ASN	conflict	UNP Q2N0S6
B	189	SER	LYS	conflict	UNP Q2N0S6
B	201	CYS	ILE	conflict	UNP Q2N0S6
B	209	THR	SER	conflict	UNP Q2N0S6
B	223	TYR	PHE	conflict	UNP Q2N0S6
B	229	ASN	LYS	conflict	UNP Q2N0S6
B	231	GLU	LYS	conflict	UNP Q2N0S6
B	232	THR	LYS	conflict	UNP Q2N0S6
B	240	SER	PRO	conflict	UNP Q2N0S6
B	241	ASN	SER	conflict	UNP Q2N0S6
B	252	ARG	LYS	conflict	UNP Q2N0S6
B	268	LYS	GLU	conflict	UNP Q2N0S6
B	270	ILE	VAL	conflict	UNP Q2N0S6
B	271	VAL	MET	conflict	UNP Q2N0S6
B	277	LEU	ILE	conflict	UNP Q2N0S6
B	283	ILE	ASN	conflict	UNP Q2N0S6
B	285	ILE	LEU	conflict	UNP Q2N0S6
B	287	HIS	GLN	conflict	UNP Q2N0S6
B	288	LEU	PHE	conflict	UNP Q2N0S6
B	289	HIS	ASN	conflict	UNP Q2N0S6
B	293	GLU	GLN	conflict	UNP Q2N0S6
B	295	VAL	ASN	conflict	UNP Q2N0S6
B	307	VAL	ILE	conflict	UNP Q2N0S6
B	316	THR	ALA	conflict	UNP Q2N0S6
B	327	LYS	ARG	conflict	UNP Q2N0S6
B	332	ASN	THR	conflict	UNP Q2N0S6
B	333	ILE	VAL	conflict	UNP Q2N0S6
B	335	GLU	LYS	conflict	UNP Q2N0S6
B	336	GLU	ALA	conflict	UNP Q2N0S6
B	337	LYS	THR	conflict	UNP Q2N0S6
B	340	ASP	GLU	conflict	UNP Q2N0S6
B	343	GLN	GLY	conflict	UNP Q2N0S6
B	346	GLY	VAL	conflict	UNP Q2N0S6
B	347	ILE	LYS	conflict	UNP Q2N0S6
B	348	GLU	GLN	conflict	UNP Q2N0S6
B	350	GLN	ARG	conflict	UNP Q2N0S6
B	354	PRO	GLY	conflict	UNP Q2N0S6
B	356	LYS	ASN	conflict	UNP Q2N0S6
B	?	-	ILE	deletion	UNP Q2N0S6
B	?	-	ARG	deletion	UNP Q2N0S6
B	360	LYS	PHE	conflict	UNP Q2N0S6

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Chain	Residue	Modelled	Actual	Comment	Reference
B	361	TYR	ALA	conflict	UNP Q2N0S6
B	363	GLN	-	insertion	UNP Q2N0S6
B	365	ALA	SER	conflict	UNP Q2N0S6
B	369	MET	LEU	conflict	UNP Q2N0S6
B	371	ILE	VAL	conflict	UNP Q2N0S6
B	389	ASN	GLY	conflict	UNP Q2N0S6
B	392	ASN	-	insertion	UNP Q2N0S6
B	393	GLY	-	insertion	UNP Q2N0S6
B	394	THR	-	insertion	UNP Q2N0S6
B	395	TYR	-	insertion	UNP Q2N0S6
B	397	GLY	SER	conflict	UNP Q2N0S6
B	400	TYR	TRP	conflict	UNP Q2N0S6
B	403	THR	ASN	conflict	UNP Q2N0S6
B	404	ASN	THR	conflict	UNP Q2N0S6
B	406	SER	VAL	conflict	UNP Q2N0S6
B	407	ALA	GLN	conflict	UNP Q2N0S6
B	408	ASN	GLY	conflict	UNP Q2N0S6
B	411	THR	ASN	conflict	UNP Q2N0S6
B	?	-	GLY	deletion	UNP Q2N0S6
B	?	-	SER	deletion	UNP Q2N0S6
B	?	-	ASN	deletion	UNP Q2N0S6
B	?	-	ASP	deletion	UNP Q2N0S6
B	?	-	SER	deletion	UNP Q2N0S6
B	417	GLN	PRO	conflict	UNP Q2N0S6
B	429	GLY	ARG	conflict	UNP Q2N0S6
B	430	VAL	ILE	conflict	UNP Q2N0S6
B	432	ARG	GLN	conflict	UNP Q2N0S6
B	433	CYS	ALA	conflict	UNP Q2N0S6
B	440	ALA	GLN	conflict	UNP Q2N0S6
B	442	ASN	VAL	conflict	UNP Q2N0S6
B	444	THR	ARG	conflict	UNP Q2N0S6
B	446	ARG	VAL	conflict	UNP Q2N0S6
B	453	LEU	ILE	conflict	UNP Q2N0S6
B	460	THR	SER	conflict	UNP Q2N0S6
B	461	ASN	THR	conflict	UNP Q2N0S6
B	462	SER	ASN	conflict	UNP Q2N0S6
B	463	ASN	SER	conflict	UNP Q2N0S6
B	464	GLU	THR	conflict	UNP Q2N0S6
B	471	ALA	GLY	conflict	UNP Q2N0S6
B	499	THR	-	expression tag	UNP Q2N0S6
B	500	ARG	-	expression tag	UNP Q2N0S6
B	501	CYS	-	expression tag	UNP Q2N0S6

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Chain	Residue	Modelled	Actual	Comment	Reference
B	502	LYS	-	expression tag	UNP Q2N0S6
B	503	ARG	-	expression tag	UNP Q2N0S6
B	504	ARG	-	expression tag	UNP Q2N0S6
B	505	VAL	-	expression tag	UNP Q2N0S6
B	506	VAL	-	expression tag	UNP Q2N0S6
B	507	GLY	-	expression tag	UNP Q2N0S6
B	508	ARG	-	expression tag	UNP Q2N0S6
B	509	ARG	-	expression tag	UNP Q2N0S6
B	510	ARG	-	expression tag	UNP Q2N0S6
B	511	ARG	-	expression tag	UNP Q2N0S6
B	512	ARG	-	expression tag	UNP Q2N0S6
B	513	ARG	-	expression tag	UNP Q2N0S6
C	47	GLU	ASP	conflict	UNP Q2N0S6
C	49	LYS	GLU	conflict	UNP Q2N0S6
C	59	ARG	LYS	conflict	UNP Q2N0S6
C	63	LYS	THR	conflict	UNP Q2N0S6
C	65	VAL	LYS	conflict	UNP Q2N0S6
C	80	SER	ASN	conflict	UNP Q2N0S6
C	84	LEU	ILE	conflict	UNP Q2N0S6
C	85	VAL	HIS	conflict	UNP Q2N0S6
C	87	GLY	GLU	conflict	UNP Q2N0S6
C	92	ASN	GLU	conflict	UNP Q2N0S6
C	99	ASP	ASN	conflict	UNP Q2N0S6
C	102	ASP	GLU	conflict	UNP Q2N0S6
C	106	GLU	THR	conflict	UNP Q2N0S6
C	130	ILE	GLN	conflict	UNP Q2N0S6
C	?	-	THR	deletion	UNP Q2N0S6
C	?	-	ASN	deletion	UNP Q2N0S6
C	?	-	VAL	deletion	UNP Q2N0S6
C	?	-	THR	deletion	UNP Q2N0S6
C	?	-	ASN	deletion	UNP Q2N0S6
C	?	-	ASN	deletion	UNP Q2N0S6
C	?	-	ILE	deletion	UNP Q2N0S6
C	132	SER	THR	conflict	UNP Q2N0S6
C	134	ALA	ASP	conflict	UNP Q2N0S6
C	135	GLY	MET	conflict	UNP Q2N0S6
C	136	SER	ARG	conflict	UNP Q2N0S6
C	138	GLY	-	insertion	UNP Q2N0S6
C	149	VAL	-	insertion	UNP Q2N0S6
C	150	GLU	-	insertion	UNP Q2N0S6
C	154	MET	LEU	conflict	UNP Q2N0S6
C	161	THR	MET	conflict	UNP Q2N0S6

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Chain	Residue	Modelled	Actual	Comment	Reference
C	165	ILE	LEU	conflict	UNP Q2N0S6
C	169	GLU	LYS	conflict	UNP Q2N0S6
C	170	LYS	GLN	conflict	UNP Q2N0S6
C	172	GLU	VAL	conflict	UNP Q2N0S6
C	174	ALA	SER	conflict	UNP Q2N0S6
C	178	LYS	ARG	conflict	UNP Q2N0S6
C	179	PRO	LEU	conflict	UNP Q2N0S6
C	181	ILE	VAL	conflict	UNP Q2N0S6
C	183	PRO	GLN	conflict	UNP Q2N0S6
C	184	LEU	ILE	conflict	UNP Q2N0S6
C	185	SER	ASN	conflict	UNP Q2N0S6
C	?	-	ASN	deletion	UNP Q2N0S6
C	?	-	GLN	deletion	UNP Q2N0S6
C	?	-	GLY	deletion	UNP Q2N0S6
C	?	-	ASN	deletion	UNP Q2N0S6
C	?	-	ARG	deletion	UNP Q2N0S6
C	?	-	SER	deletion	UNP Q2N0S6
C	185b	THR	ASN	conflict	UNP Q2N0S6
C	187	ASN	SER	conflict	UNP Q2N0S6
C	188	THR	ASN	conflict	UNP Q2N0S6
C	189	SER	LYS	conflict	UNP Q2N0S6
C	201	CYS	ILE	conflict	UNP Q2N0S6
C	209	THR	SER	conflict	UNP Q2N0S6
C	223	TYR	PHE	conflict	UNP Q2N0S6
C	229	ASN	LYS	conflict	UNP Q2N0S6
C	231	GLU	LYS	conflict	UNP Q2N0S6
C	232	THR	LYS	conflict	UNP Q2N0S6
C	240	SER	PRO	conflict	UNP Q2N0S6
C	241	ASN	SER	conflict	UNP Q2N0S6
C	252	ARG	LYS	conflict	UNP Q2N0S6
C	268	LYS	GLU	conflict	UNP Q2N0S6
C	270	ILE	VAL	conflict	UNP Q2N0S6
C	271	VAL	MET	conflict	UNP Q2N0S6
C	277	LEU	ILE	conflict	UNP Q2N0S6
C	283	ILE	ASN	conflict	UNP Q2N0S6
C	285	ILE	LEU	conflict	UNP Q2N0S6
C	287	HIS	GLN	conflict	UNP Q2N0S6
C	288	LEU	PHE	conflict	UNP Q2N0S6
C	289	HIS	ASN	conflict	UNP Q2N0S6
C	293	GLU	GLN	conflict	UNP Q2N0S6
C	295	VAL	ASN	conflict	UNP Q2N0S6
C	307	VAL	ILE	conflict	UNP Q2N0S6

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Chain	Residue	Modelled	Actual	Comment	Reference
C	316	THR	ALA	conflict	UNP Q2N0S6
C	327	LYS	ARG	conflict	UNP Q2N0S6
C	332	ASN	THR	conflict	UNP Q2N0S6
C	333	ILE	VAL	conflict	UNP Q2N0S6
C	335	GLU	LYS	conflict	UNP Q2N0S6
C	336	GLU	ALA	conflict	UNP Q2N0S6
C	337	LYS	THR	conflict	UNP Q2N0S6
C	340	ASP	GLU	conflict	UNP Q2N0S6
C	343	GLN	GLY	conflict	UNP Q2N0S6
C	346	GLY	VAL	conflict	UNP Q2N0S6
C	347	ILE	LYS	conflict	UNP Q2N0S6
C	348	GLU	GLN	conflict	UNP Q2N0S6
C	350	GLN	ARG	conflict	UNP Q2N0S6
C	354	PRO	GLY	conflict	UNP Q2N0S6
C	356	LYS	ASN	conflict	UNP Q2N0S6
C	?	-	ILE	deletion	UNP Q2N0S6
C	?	-	ARG	deletion	UNP Q2N0S6
C	360	LYS	PHE	conflict	UNP Q2N0S6
C	361	TYR	ALA	conflict	UNP Q2N0S6
C	363	GLN	-	insertion	UNP Q2N0S6
C	365	ALA	SER	conflict	UNP Q2N0S6
C	369	MET	LEU	conflict	UNP Q2N0S6
C	371	ILE	VAL	conflict	UNP Q2N0S6
C	389	ASN	GLY	conflict	UNP Q2N0S6
C	392	ASN	-	insertion	UNP Q2N0S6
C	393	GLY	-	insertion	UNP Q2N0S6
C	394	THR	-	insertion	UNP Q2N0S6
C	395	TYR	-	insertion	UNP Q2N0S6
C	397	GLY	SER	conflict	UNP Q2N0S6
C	400	TYR	TRP	conflict	UNP Q2N0S6
C	403	THR	ASN	conflict	UNP Q2N0S6
C	404	ASN	THR	conflict	UNP Q2N0S6
C	406	SER	VAL	conflict	UNP Q2N0S6
C	407	ALA	GLN	conflict	UNP Q2N0S6
C	408	ASN	GLY	conflict	UNP Q2N0S6
C	411	THR	ASN	conflict	UNP Q2N0S6
C	?	-	GLY	deletion	UNP Q2N0S6
C	?	-	SER	deletion	UNP Q2N0S6
C	?	-	ASN	deletion	UNP Q2N0S6
C	?	-	ASP	deletion	UNP Q2N0S6
C	?	-	SER	deletion	UNP Q2N0S6
C	417	GLN	PRO	conflict	UNP Q2N0S6

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Chain	Residue	Modelled	Actual	Comment	Reference
C	429	GLY	ARG	conflict	UNP Q2N0S6
C	430	VAL	ILE	conflict	UNP Q2N0S6
C	432	ARG	GLN	conflict	UNP Q2N0S6
C	433	CYS	ALA	conflict	UNP Q2N0S6
C	440	ALA	GLN	conflict	UNP Q2N0S6
C	442	ASN	VAL	conflict	UNP Q2N0S6
C	444	THR	ARG	conflict	UNP Q2N0S6
C	446	ARG	VAL	conflict	UNP Q2N0S6
C	453	LEU	ILE	conflict	UNP Q2N0S6
C	460	THR	SER	conflict	UNP Q2N0S6
C	461	ASN	THR	conflict	UNP Q2N0S6
C	462	SER	ASN	conflict	UNP Q2N0S6
C	463	ASN	SER	conflict	UNP Q2N0S6
C	464	GLU	THR	conflict	UNP Q2N0S6
C	471	ALA	GLY	conflict	UNP Q2N0S6
C	499	THR	-	expression tag	UNP Q2N0S6
C	500	ARG	-	expression tag	UNP Q2N0S6
C	501	CYS	-	expression tag	UNP Q2N0S6
C	502	LYS	-	expression tag	UNP Q2N0S6
C	503	ARG	-	expression tag	UNP Q2N0S6
C	504	ARG	-	expression tag	UNP Q2N0S6
C	505	VAL	-	expression tag	UNP Q2N0S6
C	506	VAL	-	expression tag	UNP Q2N0S6
C	507	GLY	-	expression tag	UNP Q2N0S6
C	508	ARG	-	expression tag	UNP Q2N0S6
C	509	ARG	-	expression tag	UNP Q2N0S6
C	510	ARG	-	expression tag	UNP Q2N0S6
C	511	ARG	-	expression tag	UNP Q2N0S6
C	512	ARG	-	expression tag	UNP Q2N0S6
C	513	ARG	-	expression tag	UNP Q2N0S6

- Molecule 2 is a protein called HIV-1 BG505 DS-SOSIP glycoprotein gp41.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	D	123	Total	C	N	O	S	0	0
			979	617	169	187	6		
2	E	123	Total	C	N	O	S	0	0
			979	617	169	187	6		
2	F	123	Total	C	N	O	S	0	0
			979	617	169	187	6		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	559	PRO	ILE	conflict	UNP Q2N0S6
D	605	CYS	THR	conflict	UNP Q2N0S6
E	559	PRO	ILE	conflict	UNP Q2N0S6
E	605	CYS	THR	conflict	UNP Q2N0S6
F	559	PRO	ILE	conflict	UNP Q2N0S6
F	605	CYS	THR	conflict	UNP Q2N0S6

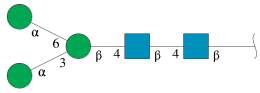
- Molecule 3 is a protein called UCA3.G57R heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	G	126	Total	C	N	O	S	0	0
			996	631	171	188	6		
3	H	126	Total	C	N	O	S	0	0
			996	631	171	188	6		
3	I	126	Total	C	N	O	S	0	0
			996	631	171	188	6		

- Molecule 4 is a protein called UCA3.G57R light chain.

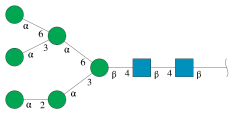
Mol	Chain	Residues	Atoms					AltConf	Trace
4	J	110	Total	C	N	O	S	0	0
			796	492	133	167	4		
4	K	110	Total	C	N	O	S	0	0
			796	492	133	167	4		
4	L	110	Total	C	N	O	S	0	0
			796	492	133	167	4		

- Molecule 5 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.



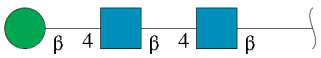
Mol	Chain	Residues	Atoms				AltConf	Trace
5	M	5	Total	C	N	O	0	0
			61	34	2	25		
5	R	5	Total	C	N	O	0	0
			61	34	2	25		
5	W	5	Total	C	N	O	0	0
			61	34	2	25		

- Molecule 6 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				AltConf	Trace
6	N	8	Total	C	N	O	0	0
			94	52	2	40		
6	S	8	Total	C	N	O	0	0
			94	52	2	40		
6	X	8	Total	C	N	O	0	0
			94	52	2	40		

- Molecule 7 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				AltConf	Trace
7	O	3	Total	C	N	O	0	0
			39	22	2	15		
7	T	3	Total	C	N	O	0	0
			39	22	2	15		
7	Y	3	Total	C	N	O	0	0
			39	22	2	15		

- Molecule 8 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
8	P	2	Total	C	N	O	0	0
			28	16	2	10		
8	Q	2	Total	C	N	O	0	0
			28	16	2	10		

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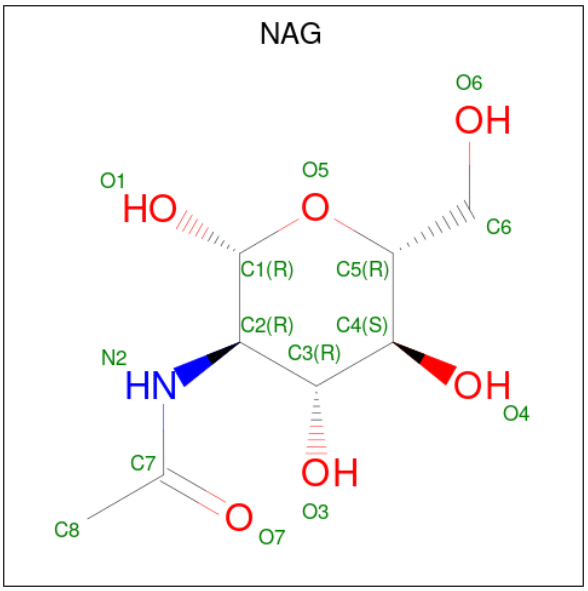
Mol	Chain	Residues	Atoms	AltConf	Trace
8	U	2	Total C N O 28 16 2 10	0	0
8	V	2	Total C N O 28 16 2 10	0	0
8	Z	2	Total C N O 28 16 2 10	0	0
8	a	2	Total C N O 28 16 2 10	0	0

- Molecule 9 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$) (labeled as "Ligand of Interest" by depositor).



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

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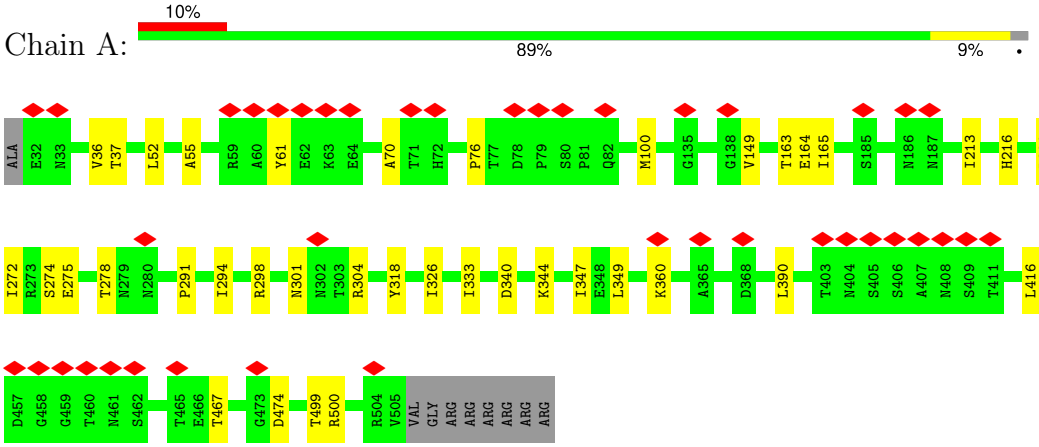
Mol	Chain	Residues	Atoms				AltConf
9	A	1	Total 14	C 8	N 1	O 5	0
9	A	1	Total 14	C 8	N 1	O 5	0
9	B	1	Total 14	C 8	N 1	O 5	0
9	B	1	Total 14	C 8	N 1	O 5	0
9	B	1	Total 14	C 8	N 1	O 5	0
9	B	1	Total 14	C 8	N 1	O 5	0
9	B	1	Total 14	C 8	N 1	O 5	0
9	B	1	Total 14	C 8	N 1	O 5	0
9	B	1	Total 14	C 8	N 1	O 5	0
9	B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

3 Residue-property plots

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.

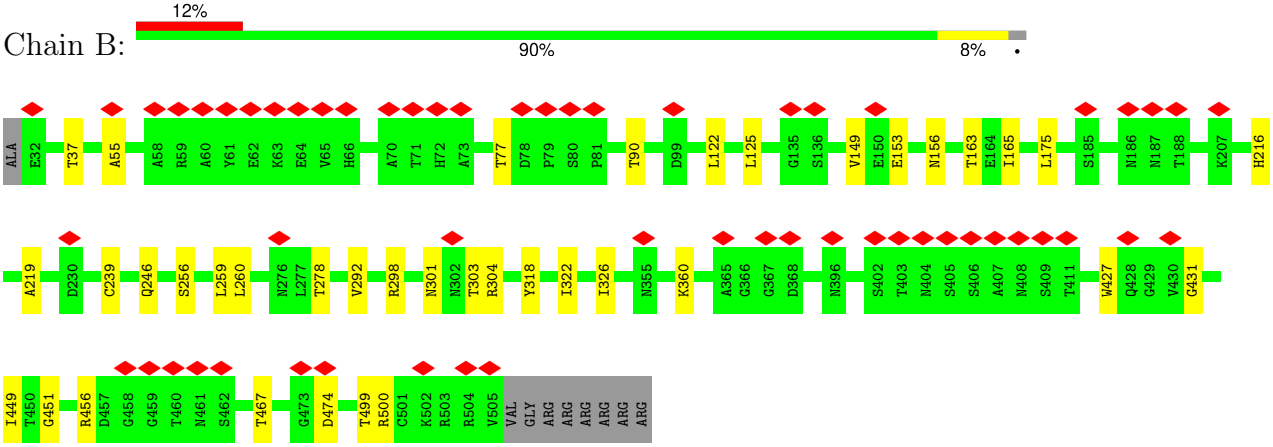
• Molecule 1: HIV-1 BG505 DS-SOSIP glycoprotein gp120

Chain A:



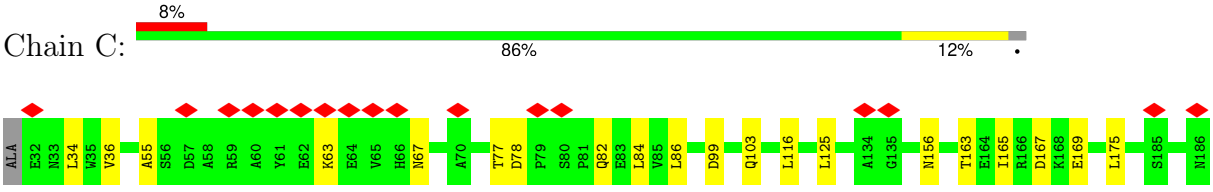
• Molecule 1: HIV-1 BG505 DS-SOSIP glycoprotein gp120

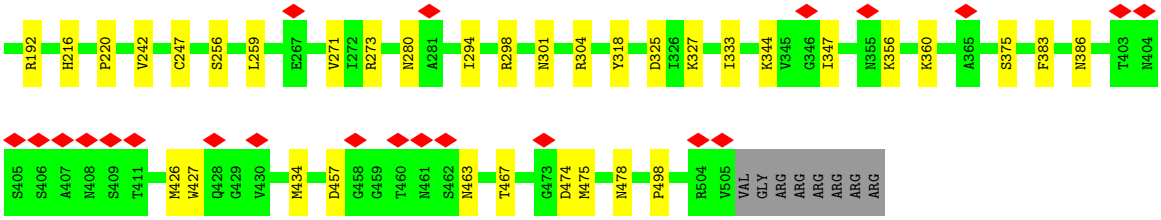
Chain B:



• Molecule 1: HIV-1 BG505 DS-SOSIP glycoprotein gp120

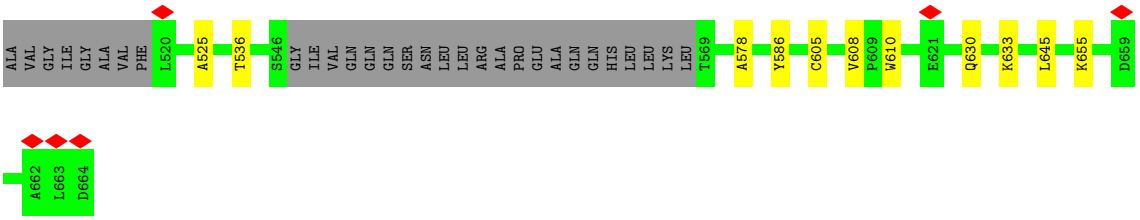
Chain C:





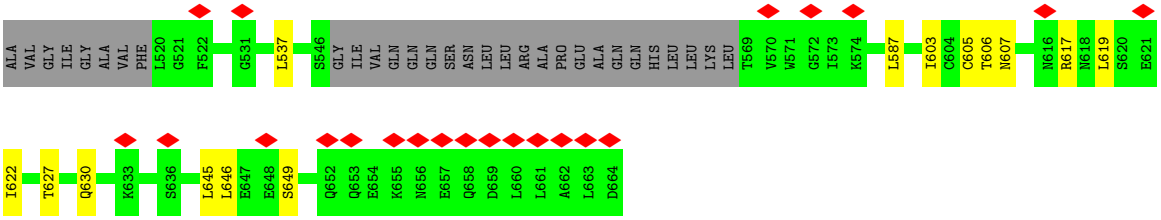
• Molecule 2: HIV-1 BG505 DS-SOSIP glycoprotein gp41

Chain D:



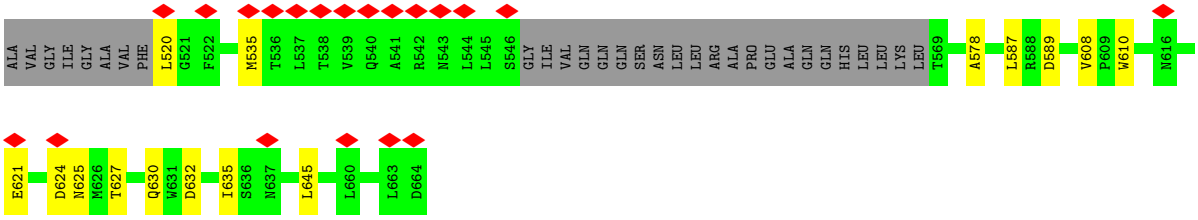
• Molecule 2: HIV-1 BG505 DS-SOSIP glycoprotein gp41

Chain E:



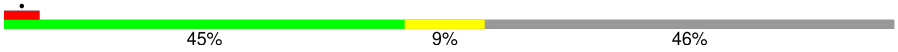
• Molecule 2: HIV-1 BG505 DS-SOSIP glycoprotein gp41

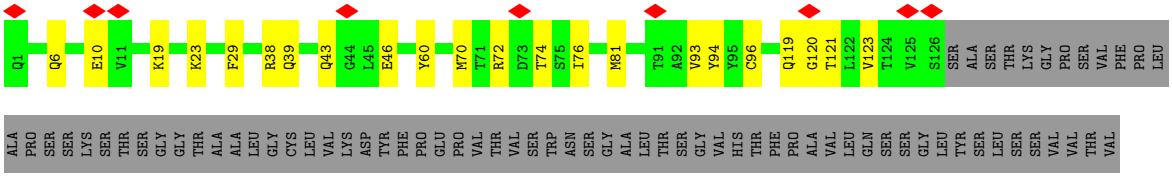
Chain F:



• Molecule 3: UCA3.G57R heavy chain

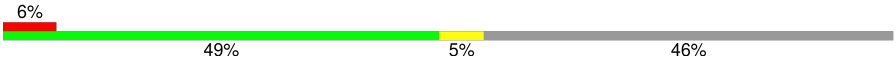
Chain G:

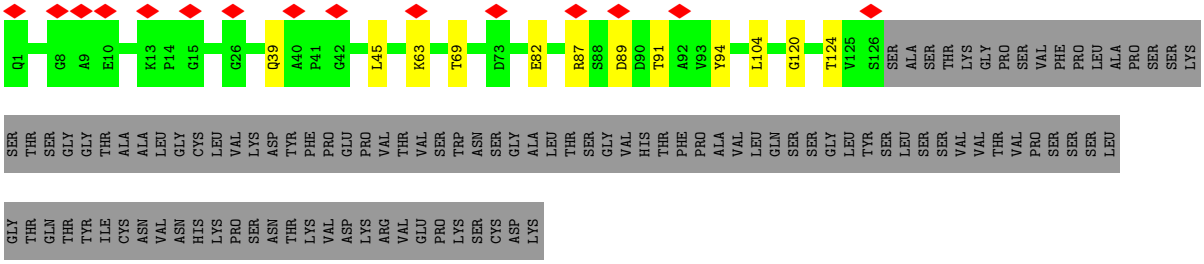




• Molecule 3: UCA3.G57R heavy chain

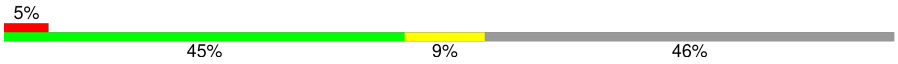
Chain H:

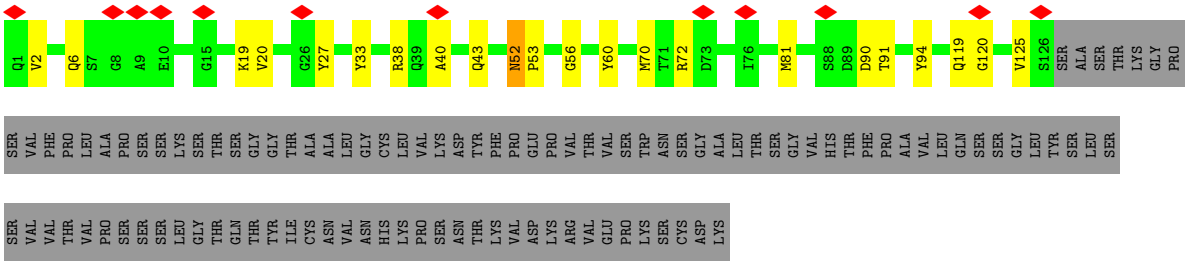




• Molecule 3: UCA3.G57R heavy chain

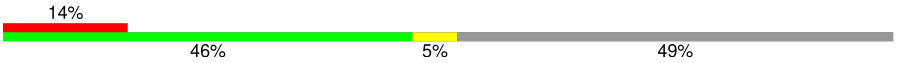
Chain I:

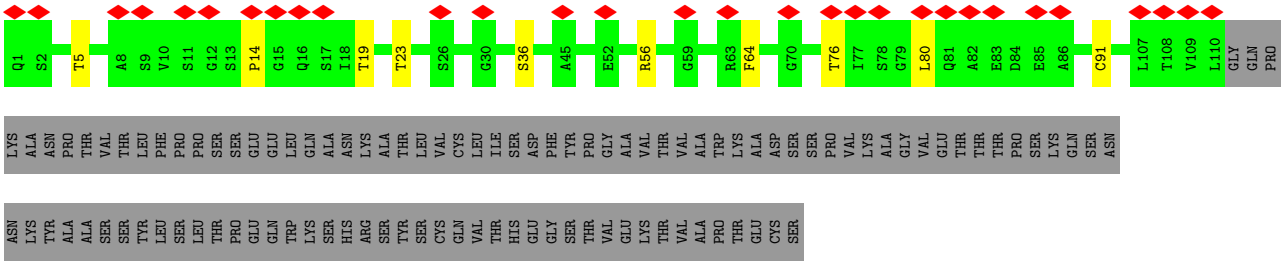




• Molecule 4: UCA3.G57R light chain

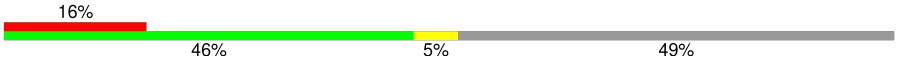
Chain J:

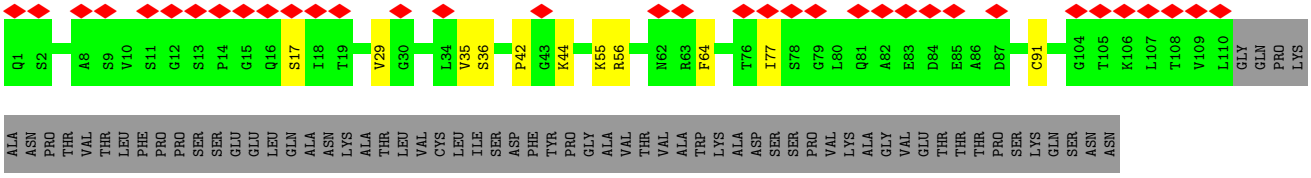




• Molecule 4: UCA3.G57R light chain

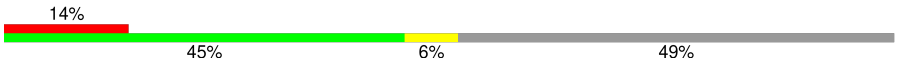
Chain K:

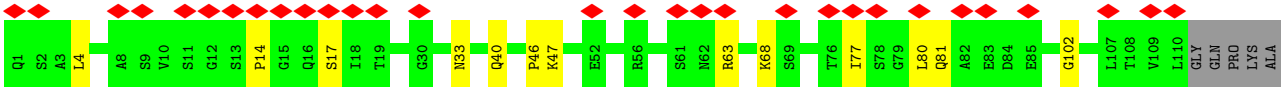


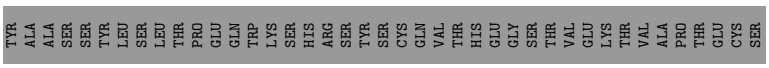


• Molecule 4: UCA3.G57R light chain

Chain L:





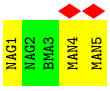


• Molecule 5: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain M:

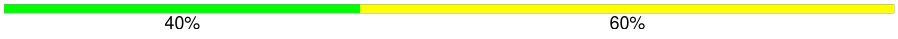
• Molecule 5: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain R:



• Molecule 5: 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 W:



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

Chain N:

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

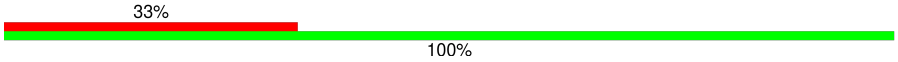
Chain S:

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

Chain X:

• Molecule 7: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain O:



• Molecule 7: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

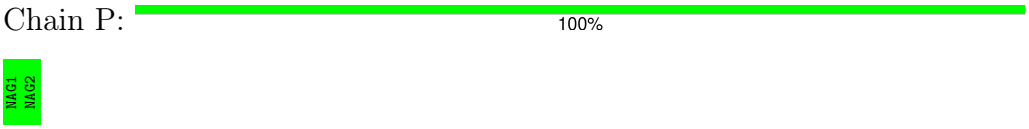
Chain T:

• Molecule 7: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Y:

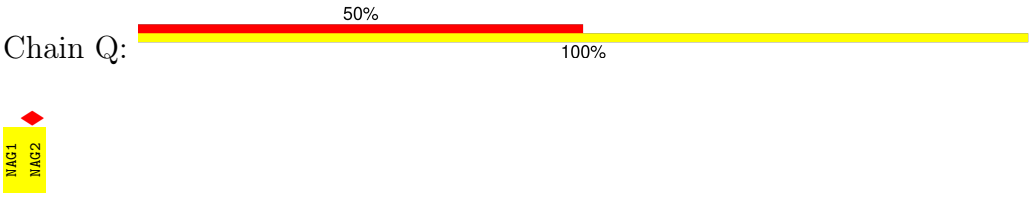
• Molecule 8: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain P:



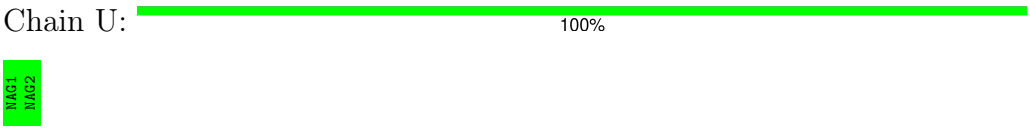
• Molecule 8: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Q:



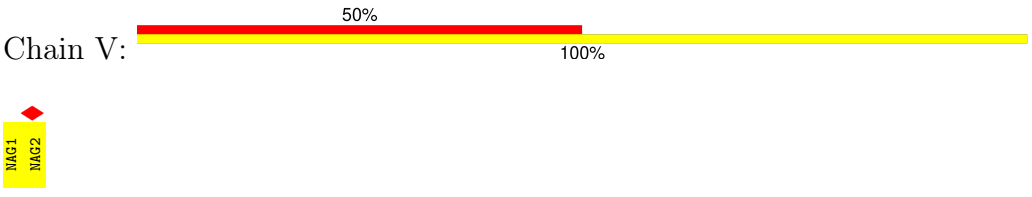
• Molecule 8: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain U:



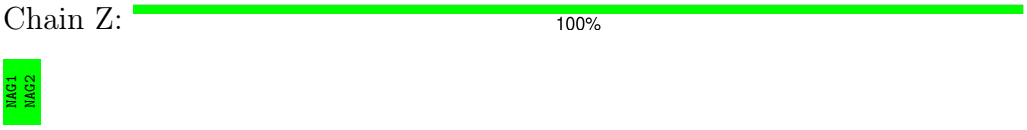
• Molecule 8: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain V:



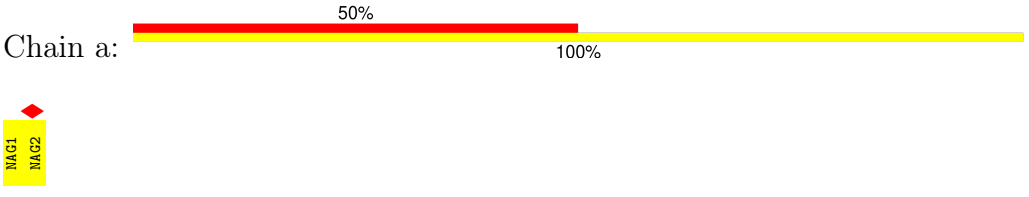
• Molecule 8: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Z:



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

Chain a:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	362409	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 ($e^-/Å^2$)	66.4	Depositor
Minimum defocus (nm)	350	Depositor
Maximum defocus (nm)	5000	Depositor
Magnification	81000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	1.232	Depositor
Minimum map value	-0.996	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.029	Depositor
Recommended contour level	0.2	Depositor
Map size (Å)	345.6, 345.6, 345.6	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.08, 1.08, 1.08	Depositor

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	0.29	0/3667	0.60	2/4988 (0.0%)
1	B	0.28	0/3667	0.60	0/4988
1	C	0.29	0/3667	0.60	1/4988 (0.0%)
2	D	0.30	0/996	0.60	0/1351
2	E	0.31	0/996	0.58	0/1351
2	F	0.30	0/996	0.66	2/1351 (0.1%)
3	G	0.28	0/1024	0.63	0/1390
3	H	0.29	0/1024	0.66	1/1390 (0.1%)
3	I	0.32	0/1024	0.68	0/1390
4	J	0.28	0/811	0.57	0/1100
4	K	0.30	0/811	0.62	0/1100
4	L	0.29	0/811	0.56	0/1100
All	All	0.29	0/19494	0.61	6/26487 (0.0%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	F	589	ASP	CB-CG-OD2	7.74	125.27	118.30
1	A	247	CYS	CA-CB-SG	6.60	125.88	114.00
1	C	247	CYS	CA-CB-SG	6.33	125.38	114.00
1	A	340	ASP	CB-CG-OD2	6.08	123.78	118.30
3	H	104	LEU	CA-CB-CG	5.37	127.65	115.30
2	F	624	ASP	CB-CG-OD1	5.33	123.10	118.30

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	3590	0	3491	23	0
1	B	3590	0	3491	23	0
1	C	3590	0	3491	35	0
2	D	979	0	957	8	0
2	E	979	0	957	9	0
2	F	979	0	957	10	0
3	G	996	0	945	12	0
3	H	996	0	945	6	0
3	I	996	0	945	14	0
4	J	796	0	772	5	0
4	K	796	0	772	5	0
4	L	796	0	772	6	0
5	M	61	0	52	0	0
5	R	61	0	52	0	0
5	W	61	0	52	0	0
6	N	94	0	79	0	0
6	S	94	0	79	0	0
6	X	94	0	79	0	0
7	O	39	0	34	0	0
7	T	39	0	34	0	0
7	Y	39	0	34	0	0
8	P	28	0	25	0	0
8	Q	28	0	25	0	0
8	U	28	0	25	0	0
8	V	28	0	25	0	0
8	Z	28	0	25	0	0
8	a	28	0	25	0	0
9	A	126	0	117	0	0
9	B	126	0	117	0	0
9	C	126	0	117	1	0
All	All	20211	0	19491	145	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (145) 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)
3:G:94:TYR:O	3:G:120:GLY:HA2	1.84	0.77
3:I:94:TYR:O	3:I:120:GLY:HA2	1.89	0.72
3:H:94:TYR:O	3:H:120:GLY:HA2	1.93	0.67
1:B:304:ARG:HB3	1:B:318:TYR:HB3	1.79	0.65
1:B:55:ALA:HB3	1:B:216:HIS:HB2	1.79	0.63
1:C:55:ALA:HB3	1:C:216:HIS:HB2	1.80	0.63
3:I:52:ASN:O	3:I:72:ARG:NH2	2.33	0.61
1:B:298:ARG:NH2	1:B:301:ASN:OD1	2.34	0.60
3:H:69:THR:HB	3:H:82:GLU:HB2	1.83	0.60
1:A:360:LYS:HB3	1:A:467:THR:HG22	1.83	0.59
4:J:36:SER:OG	4:J:91:CYS:SG	2.58	0.58
1:A:55:ALA:HB3	1:A:216:HIS:HB2	1.87	0.57
1:C:63:LYS:HD2	1:C:67:ASN:HD21	1.69	0.56
2:F:621:GLU:O	2:F:625:ASN:HB3	2.06	0.56
1:C:165:ILE:HG22	1:C:167:ASP:H	1.69	0.56
3:G:39:GLN:NE2	3:G:43:GLN:O	2.40	0.55
1:C:360:LYS:HB3	1:C:467:THR:HG22	1.89	0.54
1:C:304:ARG:HB3	1:C:318:TYR:HB3	1.89	0.54
4:K:36:SER:OG	4:K:91:CYS:SG	2.65	0.54
4:L:17:SER:HA	4:L:77:ILE:O	2.08	0.54
3:G:38:ARG:NH2	3:G:46:GLU:OE2	2.40	0.54
4:J:14:PRO:HA	4:J:80:LEU:HB3	1.89	0.54
1:C:280:ASN:ND2	1:C:457:ASP:O	2.41	0.54
3:I:53:PRO:HA	3:I:72:ARG:HE	1.71	0.54
1:A:304:ARG:HB3	1:A:318:TYR:HB3	1.90	0.54
3:I:56:GLY:HA2	3:I:72:ARG:HH22	1.72	0.53
3:I:20:VAL:HG21	3:I:94:TYR:HD2	1.73	0.53
1:A:298:ARG:NH2	1:A:301:ASN:OD1	2.42	0.53
1:C:220:PRO:HB3	2:F:578:ALA:HB1	1.90	0.52
2:D:630:GLN:HA	2:D:633:LYS:HD2	1.91	0.52
1:A:220:PRO:HB3	2:D:578:ALA:HB1	1.92	0.52
1:B:163:THR:HG23	1:B:165:ILE:H	1.75	0.52
2:E:627:THR:OG1	2:E:630:GLN:OE1	2.27	0.51
3:G:23:LYS:NZ	3:G:76:ILE:O	2.43	0.51
3:G:10:GLU:HB2	3:G:123:VAL:HG12	1.92	0.51
3:I:91:THR:HG22	3:I:125:VAL:H	1.76	0.51
4:K:56:ARG:NH1	4:K:64:PHE:O	2.43	0.51
2:E:606:THR:HG21	2:E:646:LEU:HG	1.93	0.50
3:G:6:GLN:NE2	3:G:96:CYS:SG	2.85	0.50
1:C:298:ARG:NH2	1:C:301:ASN:OD1	2.41	0.50
1:C:325:ASP:OD2	1:C:327:LYS:NZ	2.45	0.50
2:F:535:MET:SD	2:F:535:MET:N	2.85	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:122:LEU:HB3	1:B:125:LEU:HD12	1.94	0.49
1:B:278:THR:O	1:B:456:ARG:NH2	2.42	0.49
1:B:474:ASP:N	1:B:474:ASP:OD1	2.45	0.49
1:C:474:ASP:N	1:C:474:ASP:OD1	2.46	0.49
1:B:256:SER:OG	1:B:259:LEU:O	2.29	0.49
1:A:278:THR:O	1:A:456:ARG:NH2	2.45	0.49
1:B:260:LEU:HB2	1:B:451:GLY:H	1.78	0.49
1:B:427:TRP:HD1	1:B:431:GLY:HA2	1.77	0.49
1:A:36:VAL:HG22	2:D:610:TRP:HE3	1.77	0.49
4:L:40:GLN:HB3	4:L:46:PRO:HB3	1.95	0.49
1:C:99:ASP:OD2	1:C:103:GLN:NE2	2.46	0.48
3:I:2:VAL:HG11	3:I:27:TYR:HB3	1.95	0.48
3:G:19:LYS:HA	3:G:81:MET:O	2.13	0.48
1:A:272:ILE:HG12	1:A:349:LEU:HD13	1.94	0.48
4:L:33:ASN:OD1	4:L:68:LYS:NZ	2.41	0.48
1:A:70:ALA:HB3	1:A:213:ILE:HD11	1.96	0.48
3:I:38:ARG:NH1	3:I:90:ASP:OD1	2.46	0.48
1:A:37:THR:HG22	2:D:605:CYS:HA	1.96	0.47
3:H:87:ARG:NH2	3:H:89:ASP:OD1	2.47	0.47
3:G:93:VAL:HA	3:G:121:THR:O	2.15	0.47
1:C:116:LEU:HD21	1:C:434:MET:HE2	1.97	0.47
2:D:608:VAL:HG21	2:D:645:LEU:HB3	1.97	0.47
3:H:39:GLN:HB3	3:H:45:LEU:HG	1.97	0.47
2:F:608:VAL:HG21	2:F:645:LEU:HB3	1.96	0.47
2:F:632:ASP:HA	2:F:635:ILE:HG22	1.96	0.47
1:C:375:SER:HA	1:C:383:PHE:O	2.15	0.47
1:B:322:ILE:HD13	1:B:326:ILE:HD13	1.97	0.46
1:B:292:VAL:H	1:B:449:ILE:HG22	1.81	0.46
1:B:500:ARG:HE	2:E:619:LEU:HD13	1.80	0.46
1:B:149:VAL:HG23	1:B:153:GLU:H	1.79	0.46
4:K:17:SER:HA	4:K:77:ILE:O	2.15	0.46
1:C:36:VAL:HG22	2:F:610:TRP:HE3	1.80	0.46
1:B:37:THR:HG22	2:E:605:CYS:HA	1.98	0.45
1:C:163:THR:HG23	1:C:165:ILE:H	1.81	0.45
1:C:55:ALA:HB1	1:C:77:THR:HB	1.99	0.45
1:C:169:GLU:HB2	9:C:603:NAG:H61	1.98	0.45
4:J:19:THR:HG22	4:J:76:THR:HG22	1.99	0.45
1:A:149:VAL:HG12	1:A:326:ILE:HG13	1.97	0.45
1:C:256:SER:OG	1:C:259:LEU:O	2.34	0.45
3:H:91:THR:HG23	3:H:124:THR:HG22	1.98	0.45
3:H:94:TYR:O	3:H:120:GLY:CA	2.61	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:94:TYR:O	3:I:120:GLY:CA	2.63	0.45
1:A:61:TYR:HE2	1:A:76:PRO:HB3	1.81	0.45
1:C:156:ASN:HA	1:C:175:LEU:HD23	1.99	0.45
1:B:303:THR:OG1	1:B:304:ARG:N	2.49	0.45
1:C:386:ASN:N	1:C:386:ASN:OD1	2.48	0.45
3:G:60:TYR:HE1	3:G:70:MET:HG3	1.81	0.45
1:A:165:ILE:HD11	1:C:192:ARG:HH11	1.82	0.44
1:B:259:LEU:HD11	1:B:449:ILE:HD11	1.99	0.44
2:D:525:ALA:HB3	2:D:536:THR:HG21	1.99	0.44
1:C:325:ASP:OD2	3:I:33:TYR:OH	2.36	0.44
4:K:42:PRO:O	4:K:44:LYS:NZ	2.50	0.44
1:B:90:THR:HA	1:B:239:CYS:O	2.18	0.44
1:A:428:GLN:HE22	1:A:474:ASP:HA	1.82	0.44
4:K:29:VAL:HG13	4:K:35:VAL:HG21	2.00	0.43
1:B:55:ALA:HB1	1:B:77:THR:HB	2.00	0.43
1:B:499:THR:OG1	1:B:500:ARG:N	2.50	0.43
1:A:225:ILE:HD12	1:A:247:CYS:HA	2.00	0.43
3:G:43:GLN:N	3:G:43:GLN:OE1	2.52	0.43
3:I:6:GLN:H	3:I:119:GLN:HE22	1.66	0.43
1:A:265:LEU:HD21	1:A:291:PRO:HG3	2.00	0.43
1:B:156:ASN:HA	1:B:175:LEU:HD23	2.01	0.43
1:A:499:THR:OG1	1:A:500:ARG:N	2.49	0.43
2:E:617:ARG:HB3	2:E:622:ILE:HD11	2.01	0.43
2:E:607:ASN:OD1	2:E:649:SER:OG	2.36	0.43
1:C:86:LEU:HD12	1:C:242:VAL:HG13	2.00	0.43
1:C:356:LYS:NZ	1:C:463:ASN:O	2.46	0.43
1:A:163:THR:OG1	1:A:164:GLU:N	2.52	0.43
3:G:29:PHE:HZ	3:G:74:THR:HA	1.84	0.43
1:A:344:LYS:HA	1:A:347:ILE:HG22	2.01	0.42
4:L:4:LEU:HB2	4:L:102:GLY:HA2	2.01	0.42
4:L:63:ARG:NH1	4:L:81:GLN:OE1	2.52	0.42
3:I:60:TYR:HE1	3:I:70:MET:HG3	1.84	0.42
1:A:274:SER:OG	1:A:275:GLU:N	2.52	0.42
1:C:34:LEU:HD12	1:C:498:PRO:HB2	2.02	0.42
3:G:6:GLN:H	3:G:119:GLN:HE22	1.67	0.42
1:C:457:ASP:OD2	1:C:467:THR:OG1	2.33	0.42
1:C:125:LEU:HD23	1:C:125:LEU:HA	1.90	0.42
1:B:219:ALA:O	1:B:246:GLN:NE2	2.53	0.41
1:C:294:ILE:HD12	1:C:333:ILE:HD11	2.01	0.41
1:C:82:GLN:HE22	1:C:84:LEU:HB2	1.85	0.41
4:J:56:ARG:NH1	4:J:64:PHE:O	2.44	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:52:LEU:HD11	1:A:100:MET:HG2	2.03	0.41
1:B:360:LYS:HB2	1:B:467:THR:HG22	2.01	0.41
3:I:19:LYS:HA	3:I:81:MET:O	2.19	0.41
1:C:271:VAL:HG12	1:C:273:ARG:HE	1.85	0.41
2:E:587:LEU:HD23	2:E:587:LEU:HA	1.92	0.41
2:F:627:THR:OG1	2:F:630:GLN:OE1	2.30	0.41
1:A:390:LEU:HD11	1:A:416:LEU:HD21	2.03	0.41
1:C:78:ASP:N	1:C:78:ASP:OD1	2.54	0.41
1:C:344:LYS:HA	1:C:347:ILE:HG12	2.02	0.41
1:C:475:MET:SD	1:C:478:ASN:ND2	2.94	0.41
2:E:537:LEU:HD13	2:E:603:ILE:HD11	2.02	0.41
3:I:40:ALA:HB3	3:I:43:GLN:HB2	2.03	0.41
4:L:14:PRO:HA	4:L:80:LEU:HB2	2.03	0.41
1:C:426:MET:HG3	1:C:427:TRP:CD1	2.56	0.41
4:J:5:THR:OG1	4:J:23:THR:OG1	2.31	0.40
1:A:294:ILE:HD12	1:A:333:ILE:HD11	2.02	0.40
2:D:586:TYR:HE2	2:F:587:LEU:HD22	1.85	0.40
2:D:655:LYS:HD3	2:D:655:LYS:HA	1.80	0.40
2:E:645:LEU:HD23	2:E:645:LEU:HA	1.93	0.40
1:C:84:LEU:HD11	2:F:520:LEU:HD12	2.04	0.40
2:F:621:GLU:O	2:F:625:ASN:CB	2.70	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	458/469 (98%)	406 (89%)	52 (11%)	0	100	100
1	B	458/469 (98%)	412 (90%)	46 (10%)	0	100	100
1	C	458/469 (98%)	414 (90%)	44 (10%)	0	100	100
2	D	119/153 (78%)	113 (95%)	6 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	E	119/153 (78%)	116 (98%)	3 (2%)	0	100	100
2	F	119/153 (78%)	111 (93%)	8 (7%)	0	100	100
3	G	124/232 (53%)	118 (95%)	6 (5%)	0	100	100
3	H	124/232 (53%)	119 (96%)	5 (4%)	0	100	100
3	I	124/232 (53%)	119 (96%)	5 (4%)	0	100	100
4	J	108/216 (50%)	100 (93%)	8 (7%)	0	100	100
4	K	108/216 (50%)	100 (93%)	8 (7%)	0	100	100
4	L	108/216 (50%)	98 (91%)	10 (9%)	0	100	100
All	All	2427/3210 (76%)	2226 (92%)	201 (8%)	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	407/414 (98%)	407 (100%)	0	100	100
1	B	407/414 (98%)	407 (100%)	0	100	100
1	C	407/414 (98%)	407 (100%)	0	100	100
2	D	106/129 (82%)	106 (100%)	0	100	100
2	E	106/129 (82%)	106 (100%)	0	100	100
2	F	106/129 (82%)	106 (100%)	0	100	100
3	G	104/196 (53%)	103 (99%)	1 (1%)	73	80
3	H	104/196 (53%)	103 (99%)	1 (1%)	73	80
3	I	104/196 (53%)	103 (99%)	1 (1%)	73	80
4	J	90/182 (50%)	90 (100%)	0	100	100
4	K	90/182 (50%)	89 (99%)	1 (1%)	70	79
4	L	90/182 (50%)	89 (99%)	1 (1%)	70	79
All	All	2121/2763 (77%)	2116 (100%)	5 (0%)	91	94

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	G	72	ARG
3	H	63	LYS
3	I	52	ASN
4	K	55	LYS
4	L	47	LYS

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

Mol	Chain	Res	Type
3	I	52	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

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

5.5 Carbohydrates (i)

60 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	$\#\|Z\| > 2$
5	NAG	M	1	1,5	14,14,15	0.38	0	17,19,21	1.24	3 (17%)
5	NAG	M	2	5	14,14,15	0.24	0	17,19,21	0.58	0
5	BMA	M	3	5	11,11,12	0.74	0	15,15,17	0.72	0
5	MAN	M	4	5	11,11,12	0.81	0	15,15,17	1.12	2 (13%)
5	MAN	M	5	5	11,11,12	0.77	0	15,15,17	1.07	2 (13%)
6	NAG	N	1	1,6	14,14,15	0.24	0	17,19,21	0.64	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
6	NAG	N	2	6	14,14,15	0.26	0	17,19,21	0.46	0
6	BMA	N	3	6	11,11,12	0.64	0	15,15,17	1.05	1 (6%)
6	MAN	N	4	6	11,11,12	0.87	1 (9%)	15,15,17	1.32	2 (13%)
6	MAN	N	5	6	11,11,12	0.93	0	15,15,17	1.47	2 (13%)
6	MAN	N	6	6	11,11,12	0.74	0	15,15,17	1.01	2 (13%)
6	MAN	N	7	6	11,11,12	0.78	0	15,15,17	0.98	2 (13%)
6	MAN	N	8	6	11,11,12	0.79	0	15,15,17	1.14	2 (13%)
7	NAG	O	1	1,7	14,14,15	0.23	0	17,19,21	0.55	0
7	NAG	O	2	7	14,14,15	0.29	0	17,19,21	0.51	0
7	BMA	O	3	7	11,11,12	0.80	0	15,15,17	0.80	0
8	NAG	P	1	1,8	14,14,15	0.33	0	17,19,21	0.46	0
8	NAG	P	2	8	14,14,15	0.30	0	17,19,21	0.57	0
8	NAG	Q	1	1,8	14,14,15	0.53	0	17,19,21	0.71	1 (5%)
8	NAG	Q	2	8	14,14,15	0.71	0	17,19,21	1.05	1 (5%)
5	NAG	R	1	1,5	14,14,15	0.43	0	17,19,21	1.18	2 (11%)
5	NAG	R	2	5	14,14,15	0.28	0	17,19,21	0.59	0
5	BMA	R	3	5	11,11,12	0.75	0	15,15,17	0.83	0
5	MAN	R	4	5	11,11,12	0.81	0	15,15,17	1.11	2 (13%)
5	MAN	R	5	5	11,11,12	0.80	0	15,15,17	1.05	2 (13%)
6	NAG	S	1	1,6	14,14,15	0.24	0	17,19,21	0.62	0
6	NAG	S	2	6	14,14,15	0.26	0	17,19,21	0.53	0
6	BMA	S	3	6	11,11,12	0.83	0	15,15,17	0.94	1 (6%)
6	MAN	S	4	6	11,11,12	0.76	0	15,15,17	1.23	2 (13%)
6	MAN	S	5	6	11,11,12	0.95	0	15,15,17	1.40	2 (13%)
6	MAN	S	6	6	11,11,12	0.75	0	15,15,17	1.03	2 (13%)
6	MAN	S	7	6	11,11,12	0.75	0	15,15,17	1.04	2 (13%)
6	MAN	S	8	6	11,11,12	0.80	0	15,15,17	1.20	2 (13%)
7	NAG	T	1	1,7	14,14,15	0.27	0	17,19,21	0.61	1 (5%)
7	NAG	T	2	7	14,14,15	0.35	0	17,19,21	0.51	0
7	BMA	T	3	7	11,11,12	0.78	0	15,15,17	0.82	0
8	NAG	U	1	1,8	14,14,15	0.28	0	17,19,21	0.47	0
8	NAG	U	2	8	14,14,15	0.28	0	17,19,21	0.56	0
8	NAG	V	1	1,8	14,14,15	0.61	0	17,19,21	0.76	1 (5%)
8	NAG	V	2	8	14,14,15	0.63	0	17,19,21	1.05	1 (5%)
5	NAG	W	1	1,5	14,14,15	0.39	0	17,19,21	1.16	2 (11%)
5	NAG	W	2	5	14,14,15	0.29	0	17,19,21	0.54	0
5	BMA	W	3	5	11,11,12	0.74	0	15,15,17	0.77	0
5	MAN	W	4	5	11,11,12	0.77	0	15,15,17	1.10	2 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
5	MAN	W	5	5	11,11,12	0.79	0	15,15,17	1.03	2 (13%)
6	NAG	X	1	1,6	14,14,15	0.22	0	17,19,21	0.61	0
6	NAG	X	2	6	14,14,15	0.23	0	17,19,21	0.49	0
6	BMA	X	3	6	11,11,12	0.71	0	15,15,17	1.01	1 (6%)
6	MAN	X	4	6	11,11,12	0.90	1 (9%)	15,15,17	1.40	1 (6%)
6	MAN	X	5	6	11,11,12	1.02	0	15,15,17	1.72	4 (26%)
6	MAN	X	6	6	11,11,12	0.72	0	15,15,17	1.09	2 (13%)
6	MAN	X	7	6	11,11,12	0.81	0	15,15,17	0.97	2 (13%)
6	MAN	X	8	6	11,11,12	0.79	0	15,15,17	1.20	2 (13%)
7	NAG	Y	1	1,7	14,14,15	0.23	0	17,19,21	0.57	0
7	NAG	Y	2	7	14,14,15	0.31	0	17,19,21	0.56	0
7	BMA	Y	3	7	11,11,12	0.75	0	15,15,17	0.88	1 (6%)
8	NAG	Z	1	1,8	14,14,15	0.32	0	17,19,21	0.45	0
8	NAG	Z	2	8	14,14,15	0.28	0	17,19,21	0.56	0
8	NAG	a	1	1,8	14,14,15	0.60	0	17,19,21	0.66	1 (5%)
8	NAG	a	2	8	14,14,15	0.52	0	17,19,21	1.07	1 (5%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	M	1	1,5	-	4/6/23/26	0/1/1/1
5	NAG	M	2	5	-	0/6/23/26	0/1/1/1
5	BMA	M	3	5	-	0/2/19/22	0/1/1/1
5	MAN	M	4	5	-	0/2/19/22	0/1/1/1
5	MAN	M	5	5	-	0/2/19/22	0/1/1/1
6	NAG	N	1	1,6	-	4/6/23/26	0/1/1/1
6	NAG	N	2	6	-	1/6/23/26	0/1/1/1
6	BMA	N	3	6	-	1/2/19/22	0/1/1/1
6	MAN	N	4	6	-	0/2/19/22	0/1/1/1
6	MAN	N	5	6	-	1/2/19/22	0/1/1/1
6	MAN	N	6	6	-	0/2/19/22	0/1/1/1
6	MAN	N	7	6	-	1/2/19/22	0/1/1/1
6	MAN	N	8	6	-	1/2/19/22	0/1/1/1
7	NAG	O	1	1,7	-	1/6/23/26	0/1/1/1
7	NAG	O	2	7	-	1/6/23/26	0/1/1/1
7	BMA	O	3	7	-	1/2/19/22	0/1/1/1
8	NAG	P	1	1,8	-	1/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	NAG	P	2	8	-	4/6/23/26	0/1/1/1
8	NAG	Q	1	1,8	-	0/6/23/26	0/1/1/1
8	NAG	Q	2	8	-	4/6/23/26	0/1/1/1
5	NAG	R	1	1,5	-	4/6/23/26	0/1/1/1
5	NAG	R	2	5	-	2/6/23/26	0/1/1/1
5	BMA	R	3	5	-	2/2/19/22	0/1/1/1
5	MAN	R	4	5	-	2/2/19/22	0/1/1/1
5	MAN	R	5	5	-	0/2/19/22	0/1/1/1
6	NAG	S	1	1,6	-	3/6/23/26	0/1/1/1
6	NAG	S	2	6	-	1/6/23/26	0/1/1/1
6	BMA	S	3	6	-	1/2/19/22	0/1/1/1
6	MAN	S	4	6	-	0/2/19/22	0/1/1/1
6	MAN	S	5	6	-	1/2/19/22	0/1/1/1
6	MAN	S	6	6	-	2/2/19/22	0/1/1/1
6	MAN	S	7	6	-	1/2/19/22	0/1/1/1
6	MAN	S	8	6	-	1/2/19/22	0/1/1/1
7	NAG	T	1	1,7	-	2/6/23/26	0/1/1/1
7	NAG	T	2	7	-	1/6/23/26	0/1/1/1
7	BMA	T	3	7	-	1/2/19/22	0/1/1/1
8	NAG	U	1	1,8	-	2/6/23/26	0/1/1/1
8	NAG	U	2	8	-	4/6/23/26	0/1/1/1
8	NAG	V	1	1,8	-	0/6/23/26	0/1/1/1
8	NAG	V	2	8	-	3/6/23/26	0/1/1/1
5	NAG	W	1	1,5	-	3/6/23/26	0/1/1/1
5	NAG	W	2	5	-	0/6/23/26	0/1/1/1
5	BMA	W	3	5	-	0/2/19/22	0/1/1/1
5	MAN	W	4	5	-	0/2/19/22	0/1/1/1
5	MAN	W	5	5	-	0/2/19/22	0/1/1/1
6	NAG	X	1	1,6	-	3/6/23/26	0/1/1/1
6	NAG	X	2	6	-	2/6/23/26	0/1/1/1
6	BMA	X	3	6	-	1/2/19/22	0/1/1/1
6	MAN	X	4	6	-	1/2/19/22	0/1/1/1
6	MAN	X	5	6	-	1/2/19/22	0/1/1/1
6	MAN	X	6	6	-	0/2/19/22	0/1/1/1
6	MAN	X	7	6	-	2/2/19/22	0/1/1/1
6	MAN	X	8	6	-	1/2/19/22	0/1/1/1
7	NAG	Y	1	1,7	-	1/6/23/26	0/1/1/1
7	NAG	Y	2	7	-	1/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	BMA	Y	3	7	-	1/2/19/22	0/1/1/1
8	NAG	Z	1	1,8	-	0/6/23/26	0/1/1/1
8	NAG	Z	2	8	-	4/6/23/26	0/1/1/1
8	NAG	a	1	1,8	-	1/6/23/26	0/1/1/1
8	NAG	a	2	8	-	4/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	X	4	MAN	C1-C2	2.55	1.58	1.52
6	N	4	MAN	C1-C2	2.42	1.58	1.52

All (61) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	X	5	MAN	C1-O5-C5	4.42	118.11	112.19
6	N	5	MAN	C1-O5-C5	4.10	117.68	112.19
6	X	4	MAN	C1-O5-C5	3.89	117.40	112.19
6	S	5	MAN	C1-O5-C5	3.70	117.15	112.19
6	N	4	MAN	C1-O5-C5	3.67	117.11	112.19
6	S	8	MAN	C1-O5-C5	3.64	117.07	112.19
6	X	8	MAN	C1-O5-C5	3.63	117.06	112.19
6	S	4	MAN	C1-O5-C5	3.32	116.63	112.19
5	W	1	NAG	C2-N2-C7	3.31	127.34	122.90
5	M	1	NAG	C2-N2-C7	3.31	127.33	122.90
5	R	1	NAG	C2-N2-C7	3.30	127.33	122.90
6	N	8	MAN	C1-O5-C5	3.28	116.59	112.19
8	Q	2	NAG	C2-N2-C7	3.24	127.25	122.90
8	a	2	NAG	C2-N2-C7	3.21	127.20	122.90
8	V	2	NAG	C2-N2-C7	3.21	127.20	122.90
6	X	6	MAN	C1-O5-C5	3.20	116.47	112.19
5	M	5	MAN	C1-O5-C5	3.00	116.20	112.19
5	M	4	MAN	C1-O5-C5	2.97	116.17	112.19
5	R	4	MAN	C1-O5-C5	2.95	116.13	112.19
5	R	5	MAN	C1-O5-C5	2.94	116.13	112.19
5	W	4	MAN	C1-O5-C5	2.92	116.09	112.19
6	X	5	MAN	O2-C2-C3	-2.91	104.12	110.15
6	S	7	MAN	C1-O5-C5	2.83	115.98	112.19
5	W	5	MAN	C1-O5-C5	2.83	115.98	112.19
6	S	6	MAN	C1-O5-C5	2.83	115.98	112.19
6	N	6	MAN	C1-O5-C5	2.79	115.92	112.19
5	M	1	NAG	C1-O5-C5	2.70	115.80	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	N	3	BMA	C1-O5-C5	2.56	115.62	112.19
8	V	1	NAG	C1-O5-C5	2.53	115.57	112.19
5	R	1	NAG	C1-O5-C5	2.52	115.56	112.19
8	Q	1	NAG	C1-O5-C5	2.44	115.46	112.19
6	N	7	MAN	C1-O5-C5	2.43	115.44	112.19
6	S	5	MAN	O2-C2-C3	-2.43	105.12	110.15
5	W	1	NAG	C1-O5-C5	2.38	115.38	112.19
6	S	4	MAN	O2-C2-C3	-2.38	105.22	110.15
6	X	7	MAN	C1-O5-C5	2.33	115.31	112.19
6	X	3	BMA	C1-O5-C5	2.28	115.25	112.19
8	a	1	NAG	C1-O5-C5	2.25	115.20	112.19
6	X	5	MAN	C2-C3-C4	2.24	114.79	110.86
5	W	4	MAN	O2-C2-C3	-2.22	105.55	110.15
6	N	5	MAN	O2-C2-C3	-2.19	105.61	110.15
6	S	8	MAN	O2-C2-C3	-2.18	105.64	110.15
6	X	8	MAN	O2-C2-C3	-2.16	105.68	110.15
6	N	8	MAN	O2-C2-C3	-2.16	105.68	110.15
5	M	1	NAG	C1-C2-N2	2.16	113.83	110.43
5	R	4	MAN	O2-C2-C3	-2.15	105.69	110.15
6	X	6	MAN	O2-C2-C3	-2.15	105.69	110.15
5	M	5	MAN	O2-C2-C3	-2.15	105.70	110.15
6	N	6	MAN	O2-C2-C3	-2.14	105.71	110.15
6	S	3	BMA	C1-O5-C5	2.14	115.06	112.19
6	N	7	MAN	O2-C2-C3	-2.13	105.73	110.15
6	X	7	MAN	O2-C2-C3	-2.13	105.74	110.15
5	R	5	MAN	O2-C2-C3	-2.13	105.75	110.15
5	W	5	MAN	O2-C2-C3	-2.11	105.77	110.15
7	T	1	NAG	C1-O5-C5	2.10	115.00	112.19
7	Y	3	BMA	C1-O5-C5	2.10	115.00	112.19
6	S	6	MAN	O2-C2-C3	-2.10	105.81	110.15
5	M	4	MAN	O2-C2-C3	-2.09	105.82	110.15
6	S	7	MAN	O2-C2-C3	-2.09	105.82	110.15
6	X	5	MAN	C1-C2-C3	2.03	112.61	109.64
6	N	4	MAN	O2-C2-C3	-2.00	106.00	110.15

There are no chirality outliers.

All (84) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	N	1	NAG	O5-C5-C6-O6
5	R	2	NAG	O5-C5-C6-O6
6	N	1	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
6	X	7	MAN	O5-C5-C6-O6
8	Z	2	NAG	O5-C5-C6-O6
7	T	1	NAG	C4-C5-C6-O6
8	P	2	NAG	O5-C5-C6-O6
5	R	2	NAG	C4-C5-C6-O6
7	T	1	NAG	O5-C5-C6-O6
8	P	2	NAG	C4-C5-C6-O6
6	N	1	NAG	C8-C7-N2-C2
6	N	1	NAG	O7-C7-N2-C2
6	S	1	NAG	C8-C7-N2-C2
6	S	1	NAG	O7-C7-N2-C2
6	X	1	NAG	C8-C7-N2-C2
6	X	1	NAG	O7-C7-N2-C2
8	P	2	NAG	C8-C7-N2-C2
8	P	2	NAG	O7-C7-N2-C2
8	U	2	NAG	C8-C7-N2-C2
8	U	2	NAG	O7-C7-N2-C2
8	Z	2	NAG	C8-C7-N2-C2
8	Z	2	NAG	O7-C7-N2-C2
8	U	1	NAG	O5-C5-C6-O6
6	N	8	MAN	O5-C5-C6-O6
6	X	2	NAG	C4-C5-C6-O6
8	U	2	NAG	C4-C5-C6-O6
7	Y	3	BMA	O5-C5-C6-O6
8	U	1	NAG	C4-C5-C6-O6
8	Z	2	NAG	C4-C5-C6-O6
6	X	2	NAG	O5-C5-C6-O6
8	U	2	NAG	O5-C5-C6-O6
6	X	8	MAN	O5-C5-C6-O6
7	O	1	NAG	O5-C5-C6-O6
6	X	7	MAN	C4-C5-C6-O6
6	X	5	MAN	O5-C5-C6-O6
6	N	7	MAN	O5-C5-C6-O6
5	R	1	NAG	C4-C5-C6-O6
7	O	3	BMA	O5-C5-C6-O6
6	S	1	NAG	O5-C5-C6-O6
6	S	8	MAN	O5-C5-C6-O6
6	X	1	NAG	O5-C5-C6-O6
7	O	2	NAG	O5-C5-C6-O6
7	Y	1	NAG	O5-C5-C6-O6
7	T	2	NAG	O5-C5-C6-O6
6	N	5	MAN	O5-C5-C6-O6

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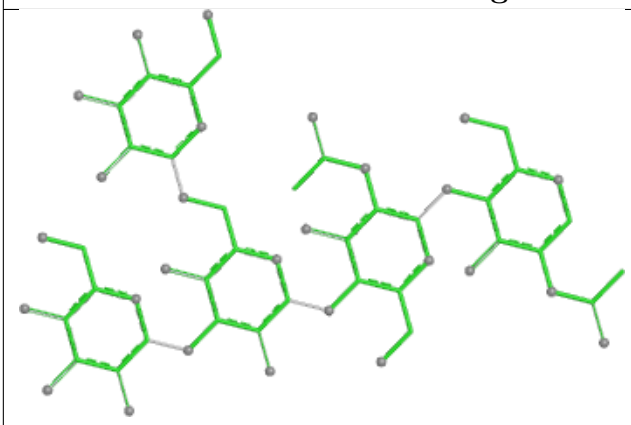
Mol	Chain	Res	Type	Atoms
7	Y	2	NAG	O5-C5-C6-O6
8	Q	2	NAG	C4-C5-C6-O6
5	R	1	NAG	O5-C5-C6-O6
6	S	5	MAN	O5-C5-C6-O6
6	S	7	MAN	O5-C5-C6-O6
7	T	3	BMA	O5-C5-C6-O6
8	a	2	NAG	C4-C5-C6-O6
5	R	4	MAN	O5-C5-C6-O6
5	R	3	BMA	O5-C5-C6-O6
5	R	4	MAN	C4-C5-C6-O6
5	R	3	BMA	C4-C5-C6-O6
6	N	3	BMA	C4-C5-C6-O6
8	P	1	NAG	O5-C5-C6-O6
6	S	6	MAN	C4-C5-C6-O6
8	Q	2	NAG	O5-C5-C6-O6
6	S	2	NAG	O5-C5-C6-O6
6	N	2	NAG	C4-C5-C6-O6
5	R	1	NAG	C3-C2-N2-C7
8	a	2	NAG	O5-C5-C6-O6
6	X	3	BMA	C4-C5-C6-O6
8	a	1	NAG	C4-C5-C6-O6
5	M	1	NAG	C4-C5-C6-O6
6	S	6	MAN	O5-C5-C6-O6
5	M	1	NAG	C1-C2-N2-C7
5	R	1	NAG	C1-C2-N2-C7
5	W	1	NAG	C1-C2-N2-C7
8	Q	2	NAG	C1-C2-N2-C7
8	V	2	NAG	C1-C2-N2-C7
8	a	2	NAG	C1-C2-N2-C7
6	S	3	BMA	C4-C5-C6-O6
5	M	1	NAG	C3-C2-N2-C7
5	W	1	NAG	C3-C2-N2-C7
8	Q	2	NAG	C3-C2-N2-C7
8	V	2	NAG	C3-C2-N2-C7
8	a	2	NAG	C3-C2-N2-C7
8	V	2	NAG	C4-C5-C6-O6
6	X	4	MAN	O5-C5-C6-O6
5	M	1	NAG	O5-C5-C6-O6
5	W	1	NAG	C4-C5-C6-O6

There are no ring outliers.

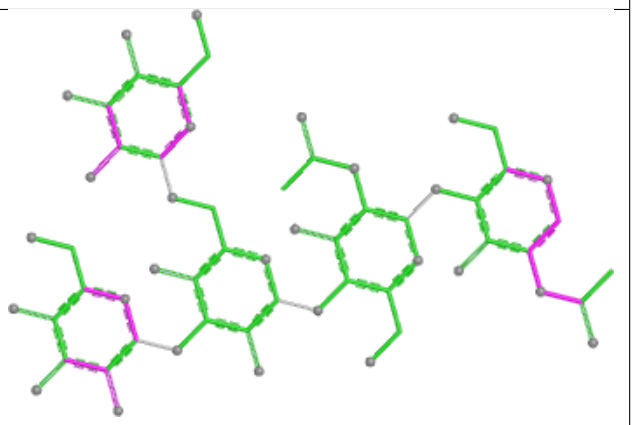
No monomer is involved in short contacts.

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

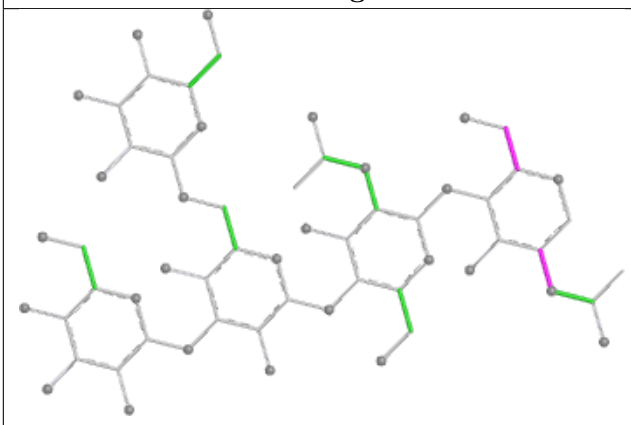
Oligosaccharide Chain M



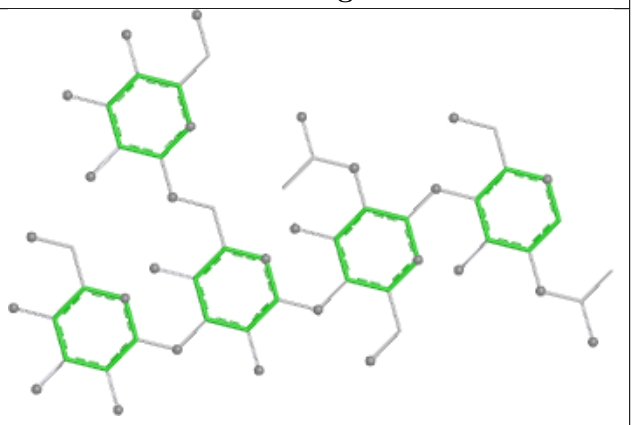
Bond lengths



Bond angles

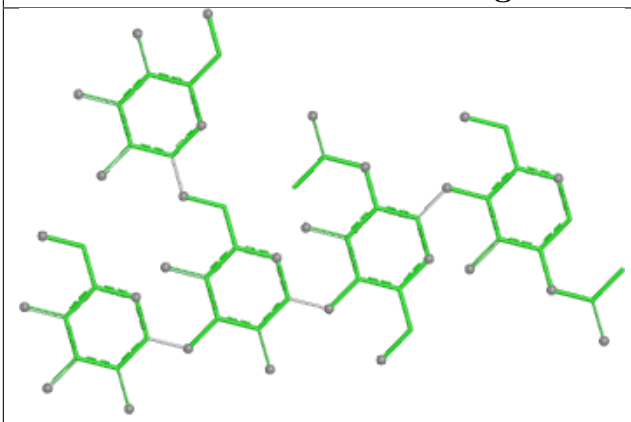


Torsions

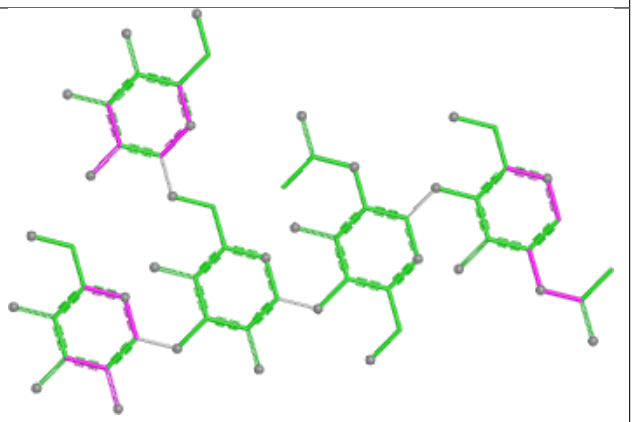


Rings

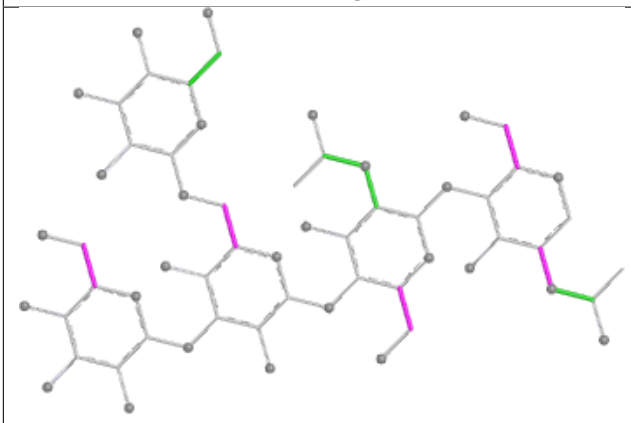
Oligosaccharide Chain R



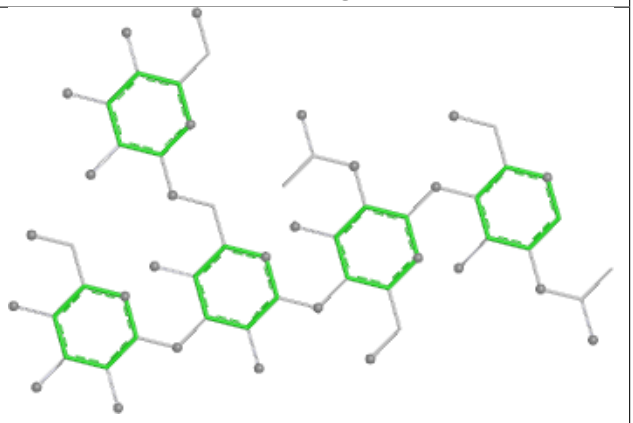
Bond lengths



Bond angles

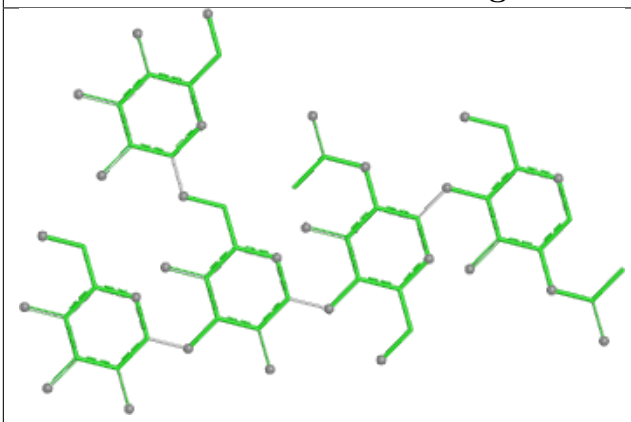


Torsions

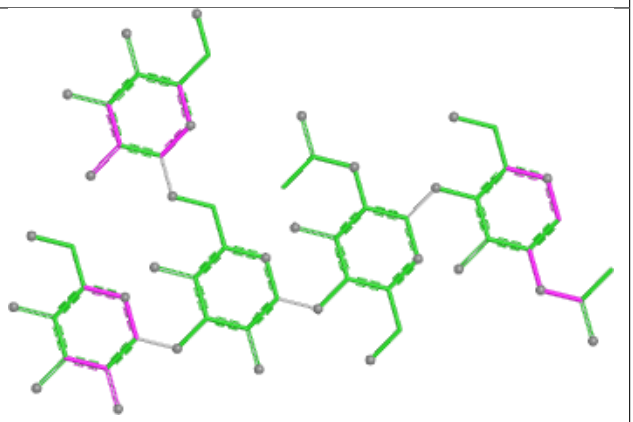


Rings

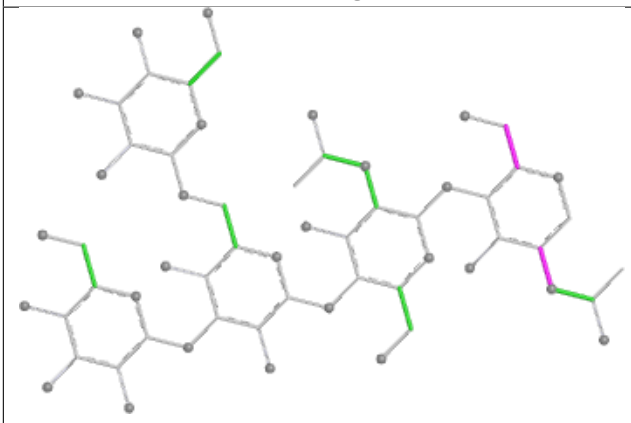
Oligosaccharide Chain W



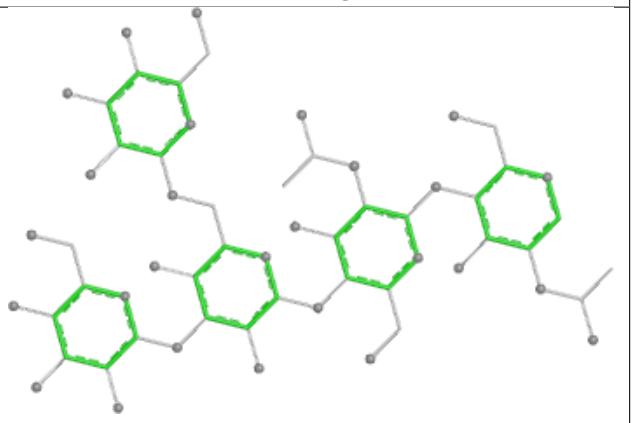
Bond lengths



Bond angles

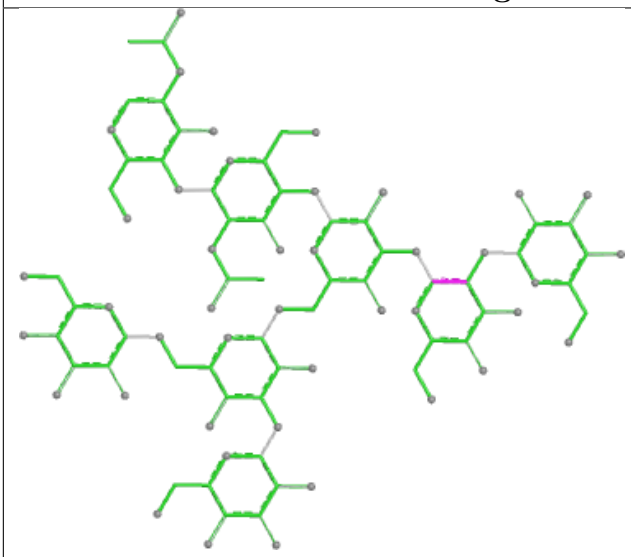


Torsions

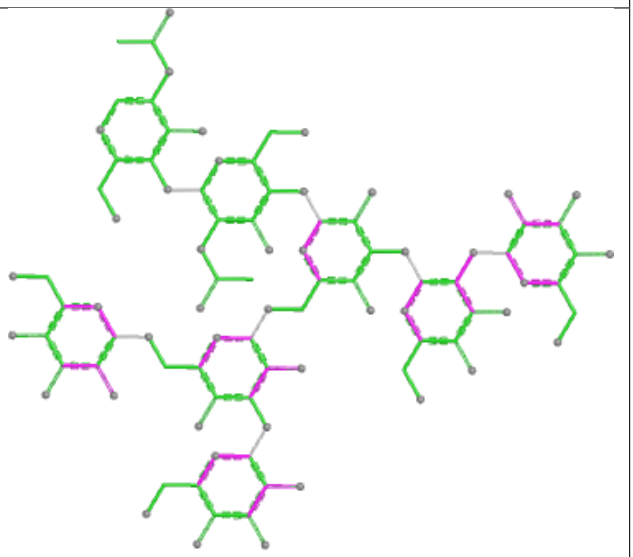


Rings

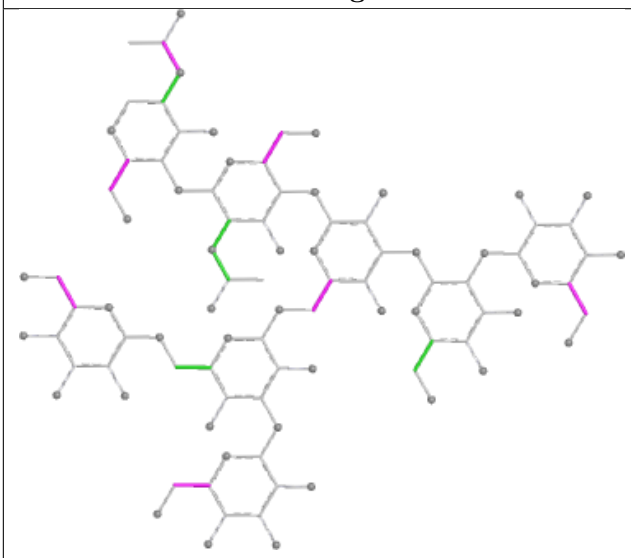
Oligosaccharide Chain N



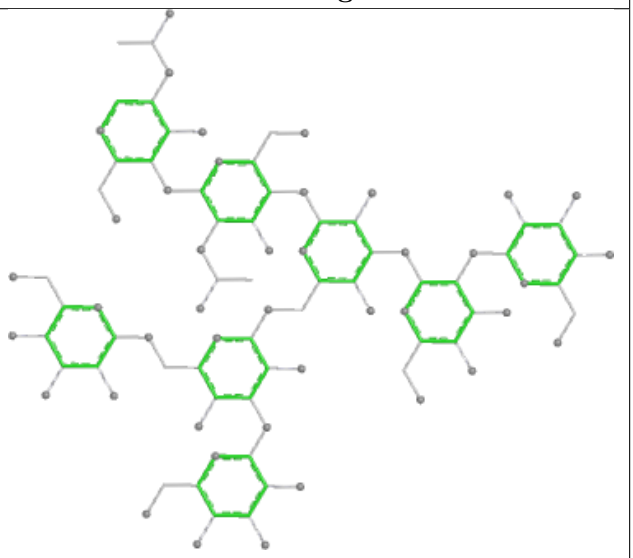
Bond lengths



Bond angles

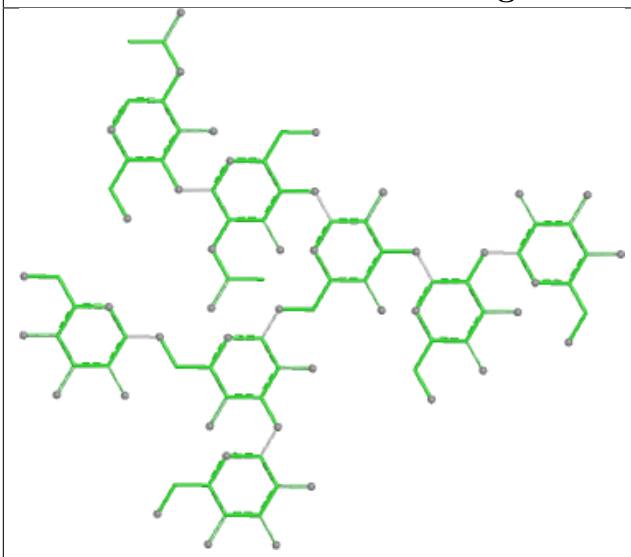


Torsions

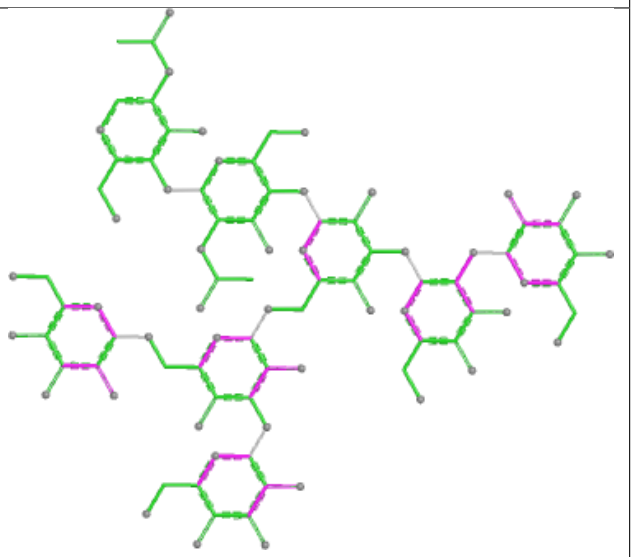


Rings

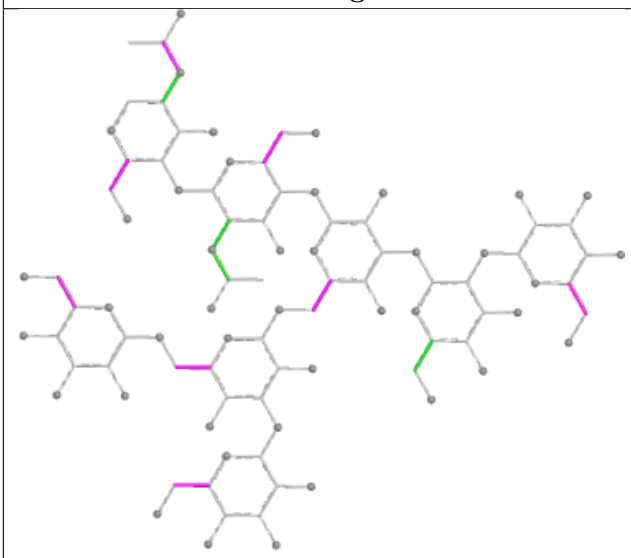
Oligosaccharide Chain S



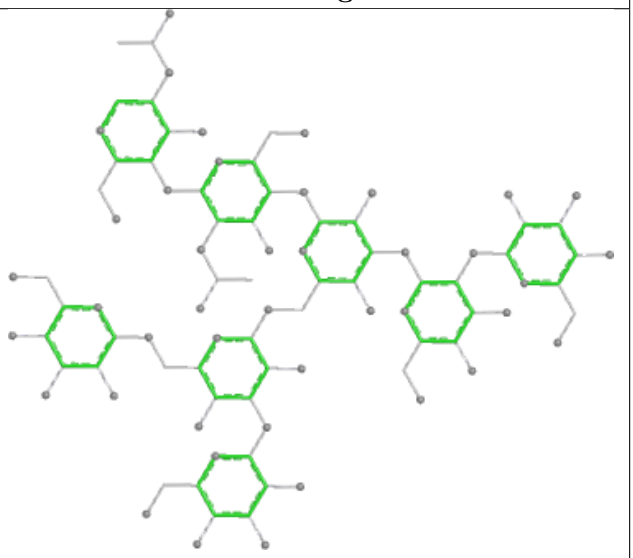
Bond lengths



Bond angles

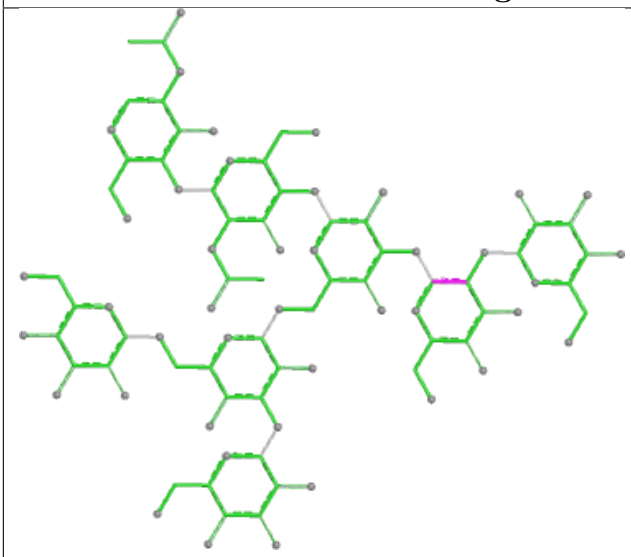


Torsions

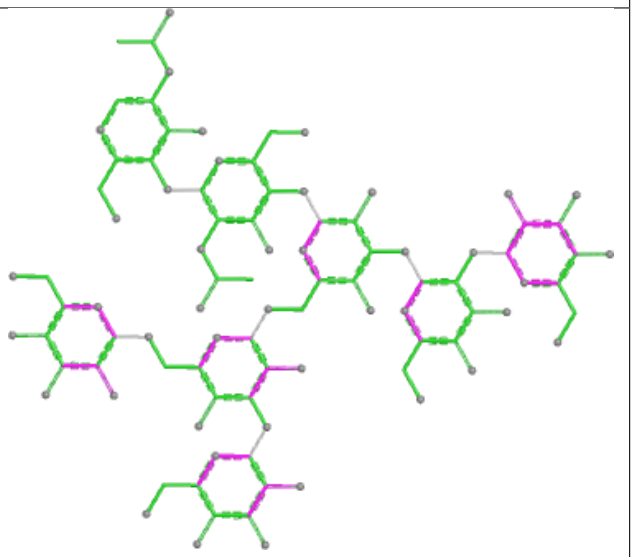


Rings

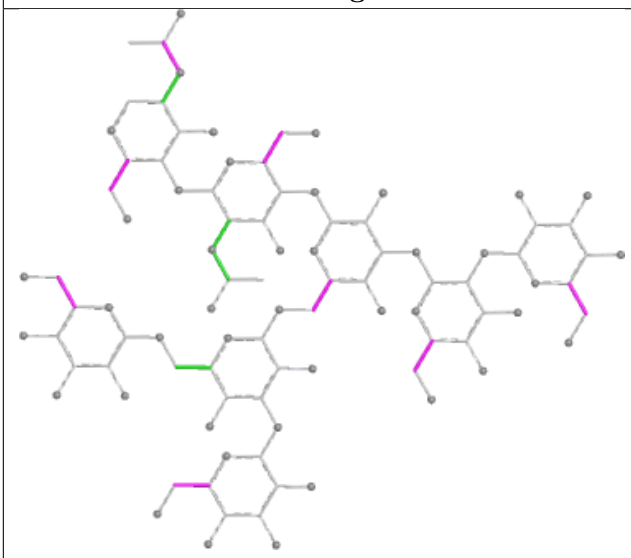
Oligosaccharide Chain X



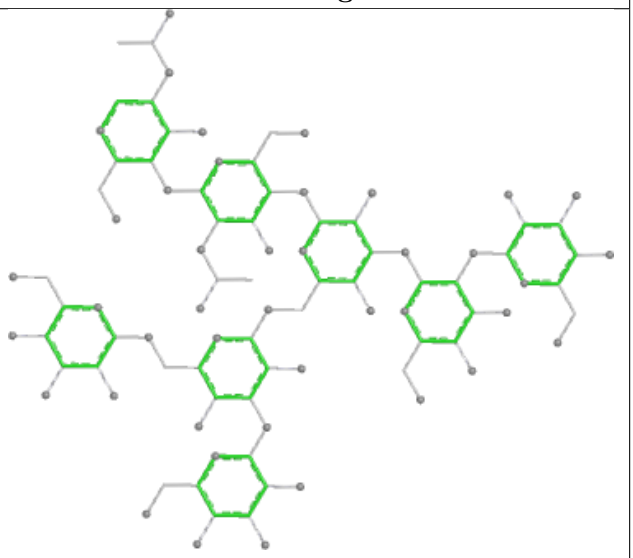
Bond lengths



Bond angles

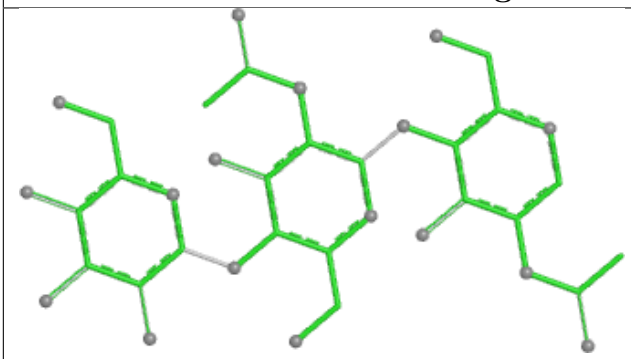


Torsions

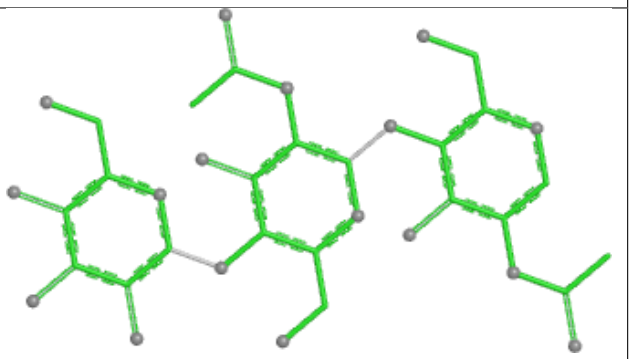


Rings

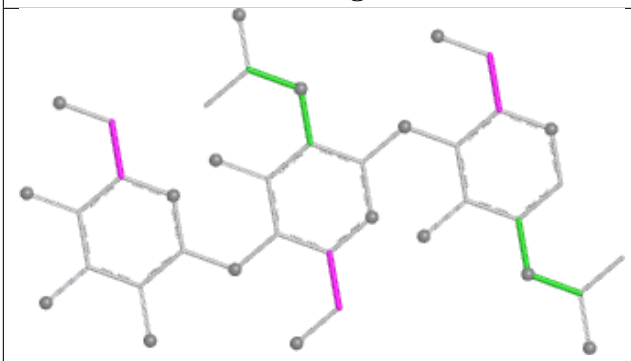
Oligosaccharide Chain O



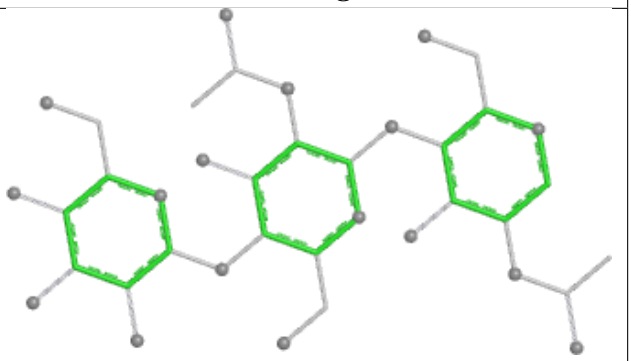
Bond lengths



Bond angles

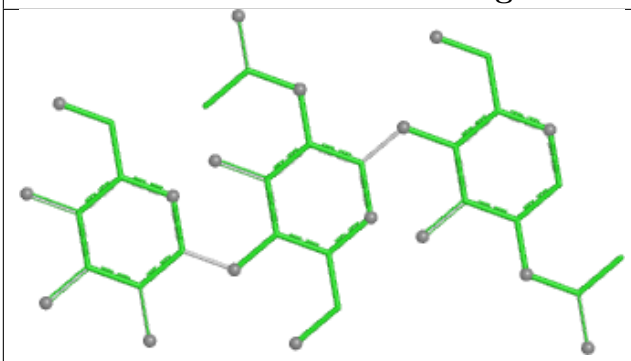


Torsions

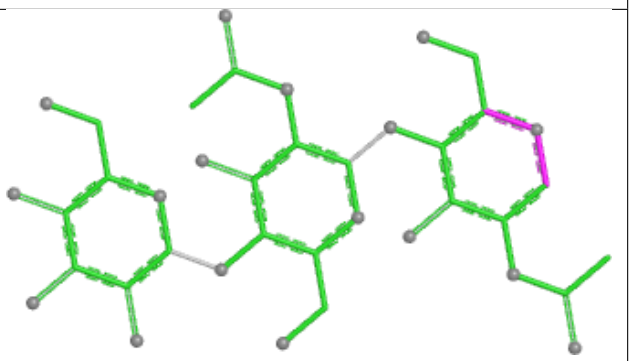


Rings

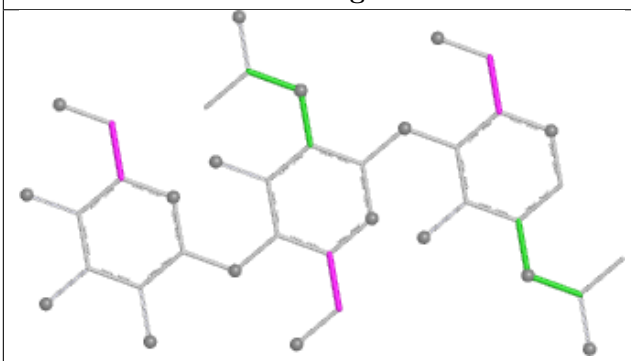
Oligosaccharide Chain T



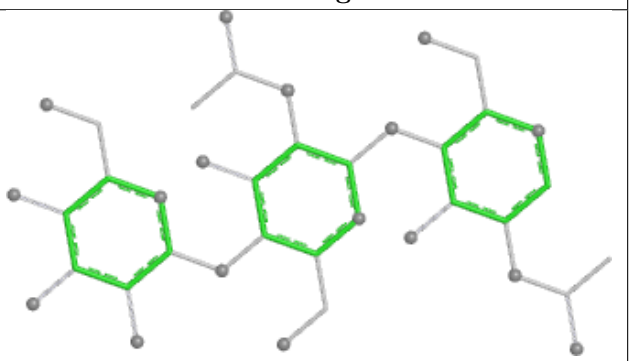
Bond lengths



Bond angles

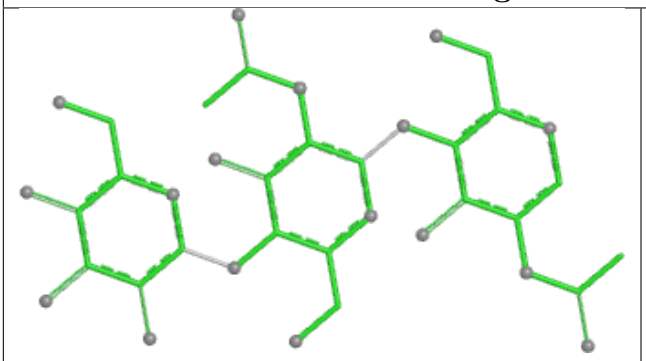


Torsions

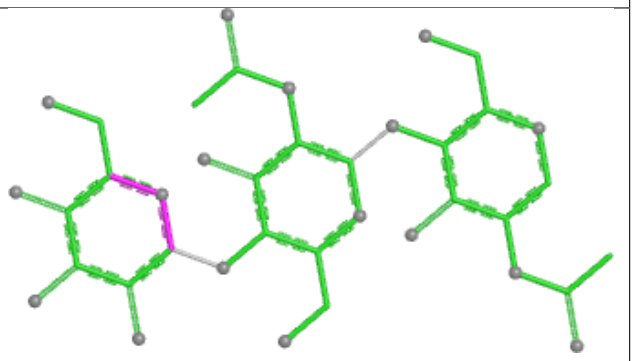


Rings

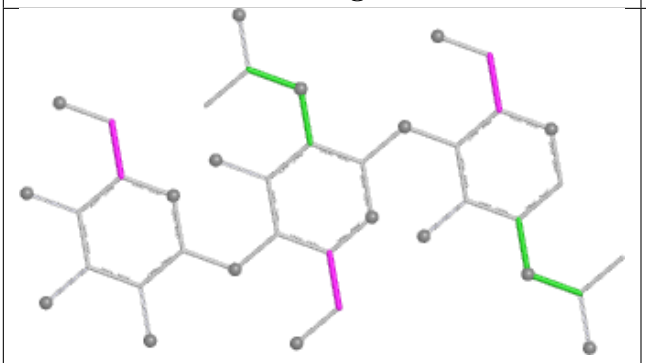
Oligosaccharide Chain Y



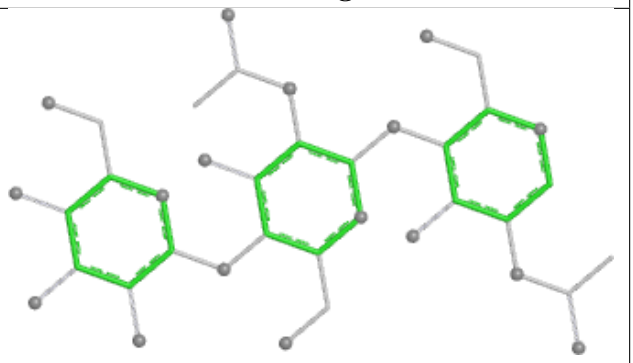
Bond lengths



Bond angles

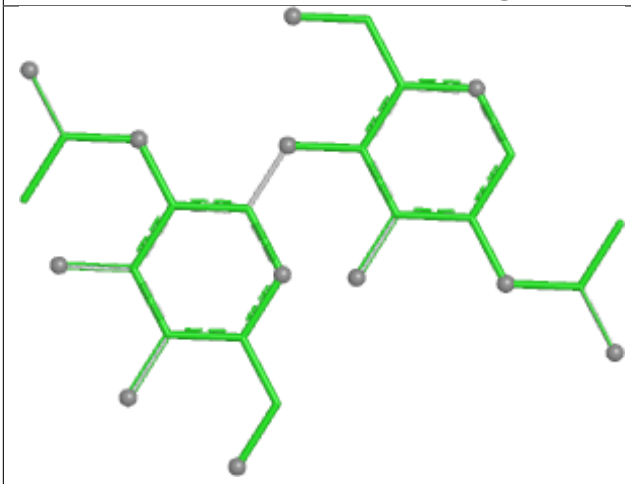


Torsions

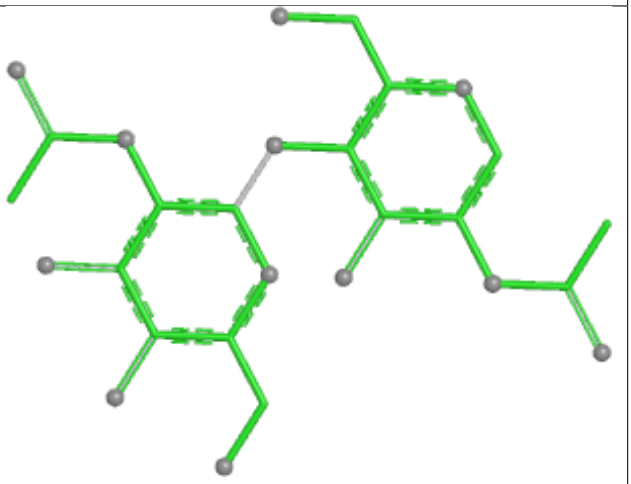


Rings

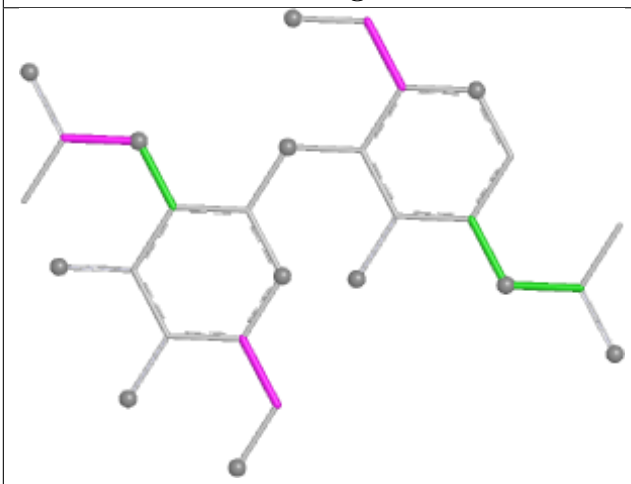
Oligosaccharide Chain P



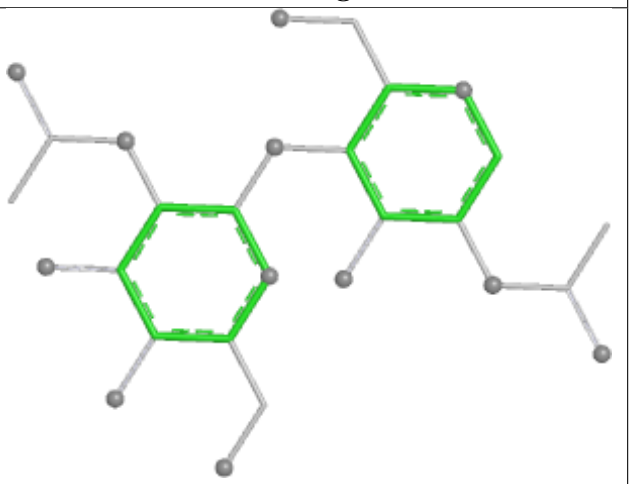
Bond lengths



Bond angles

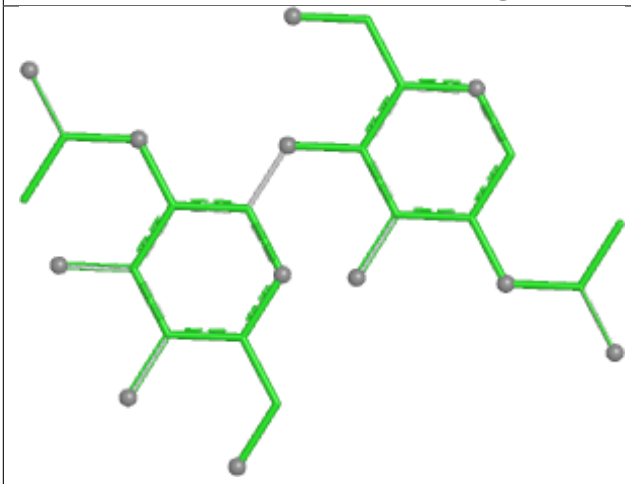


Torsions

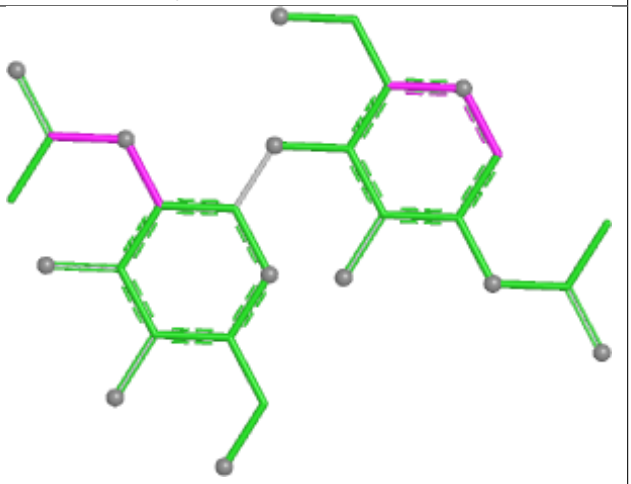


Rings

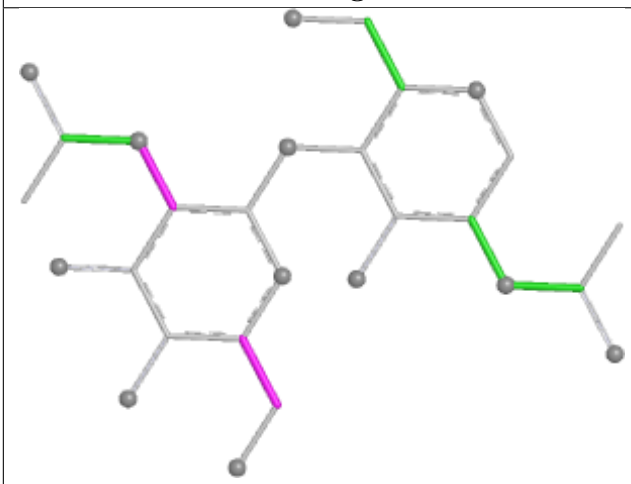
Oligosaccharide Chain Q



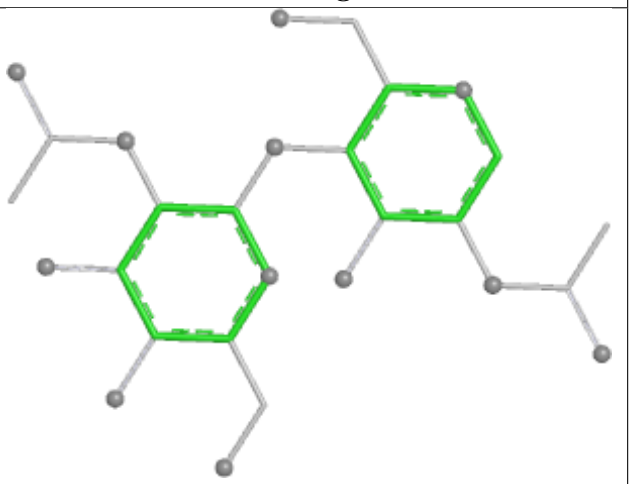
Bond lengths



Bond angles

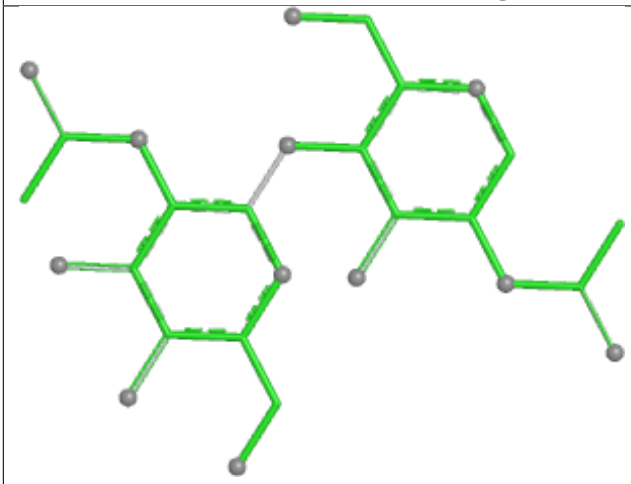


Torsions

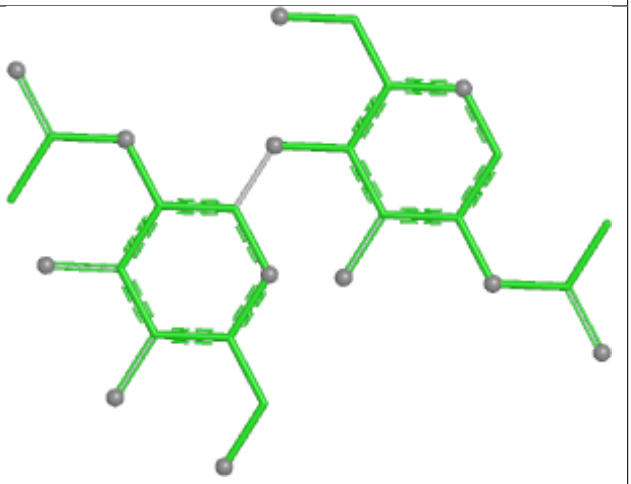


Rings

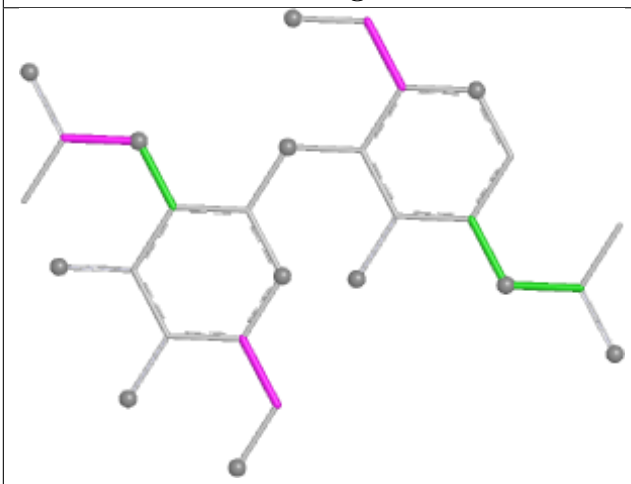
Oligosaccharide Chain U



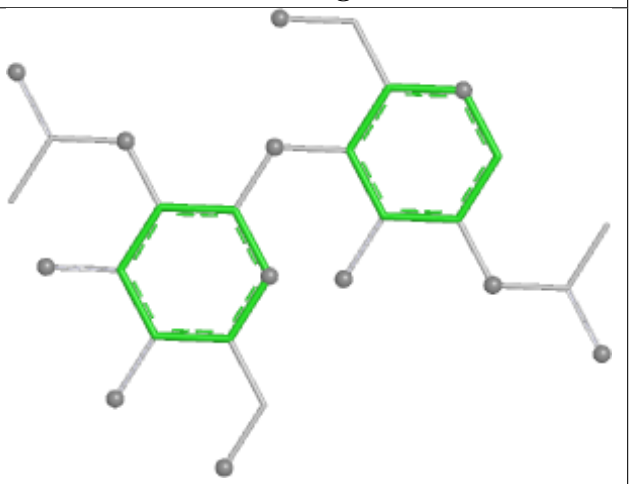
Bond lengths



Bond angles

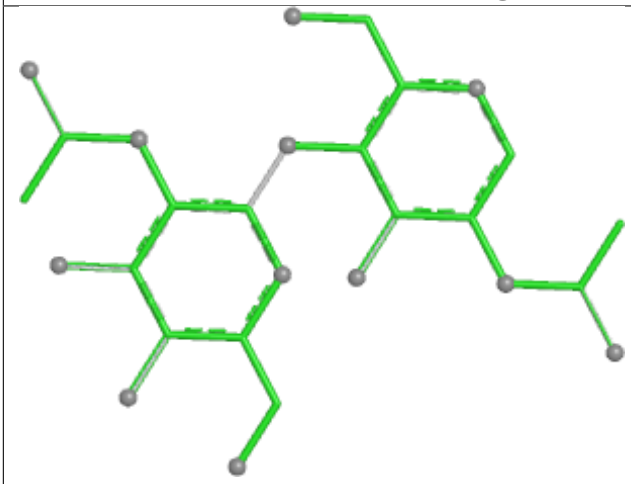


Torsions

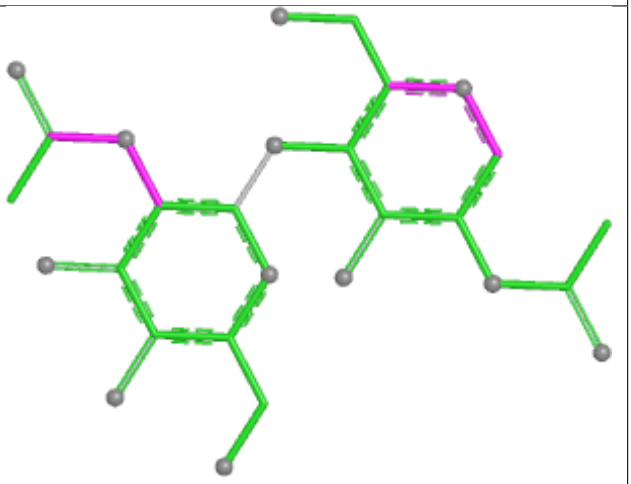


Rings

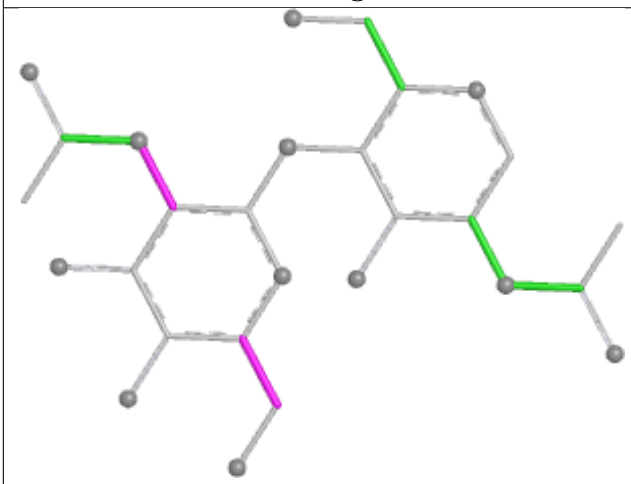
Oligosaccharide Chain V



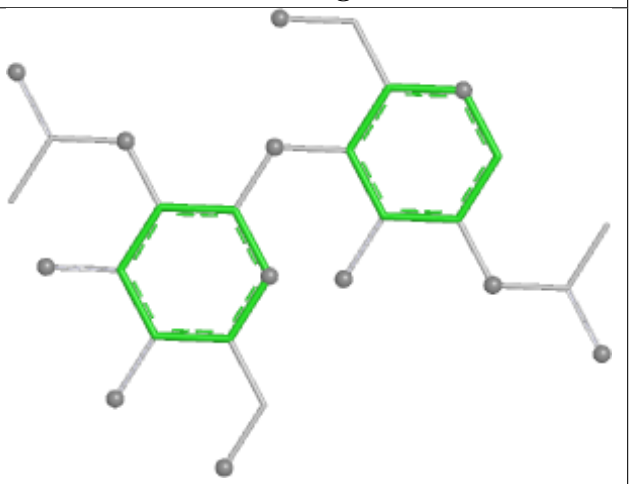
Bond lengths



Bond angles

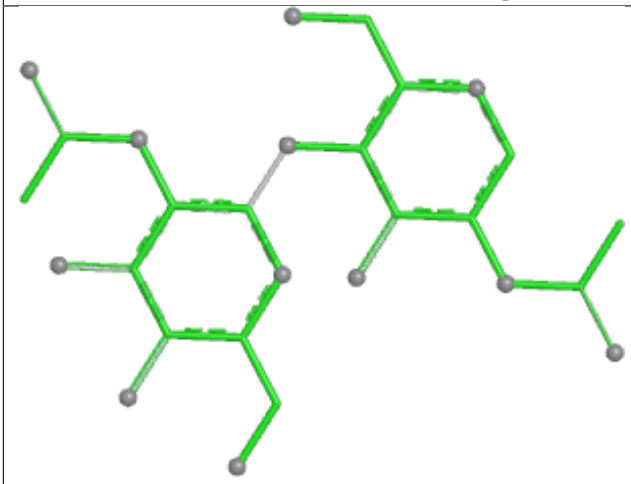


Torsions

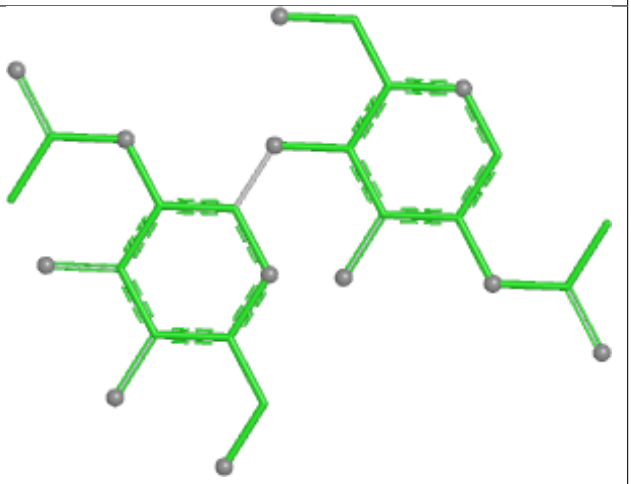


Rings

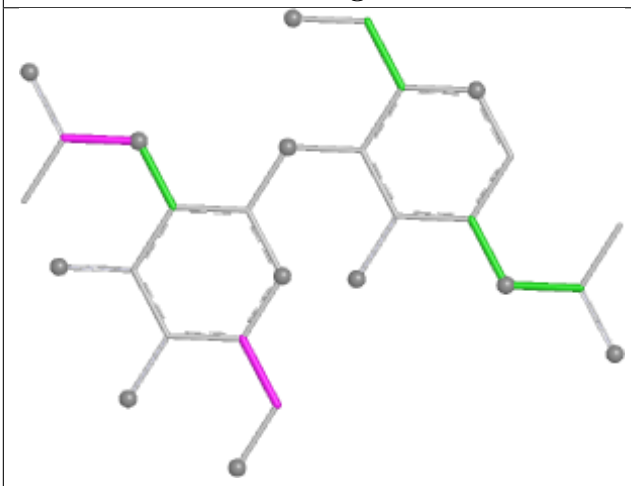
Oligosaccharide Chain Z



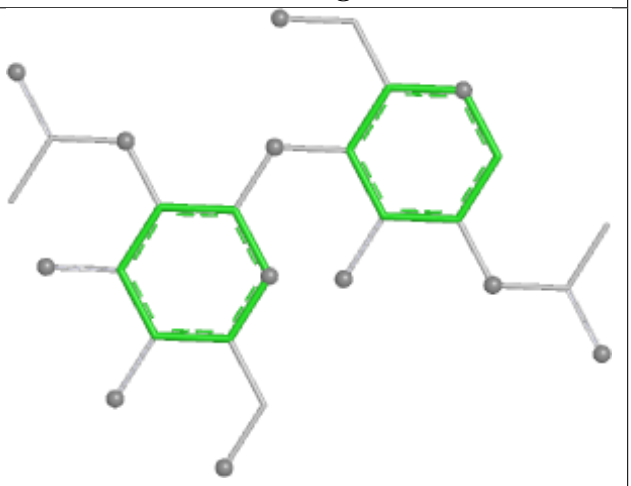
Bond lengths



Bond angles

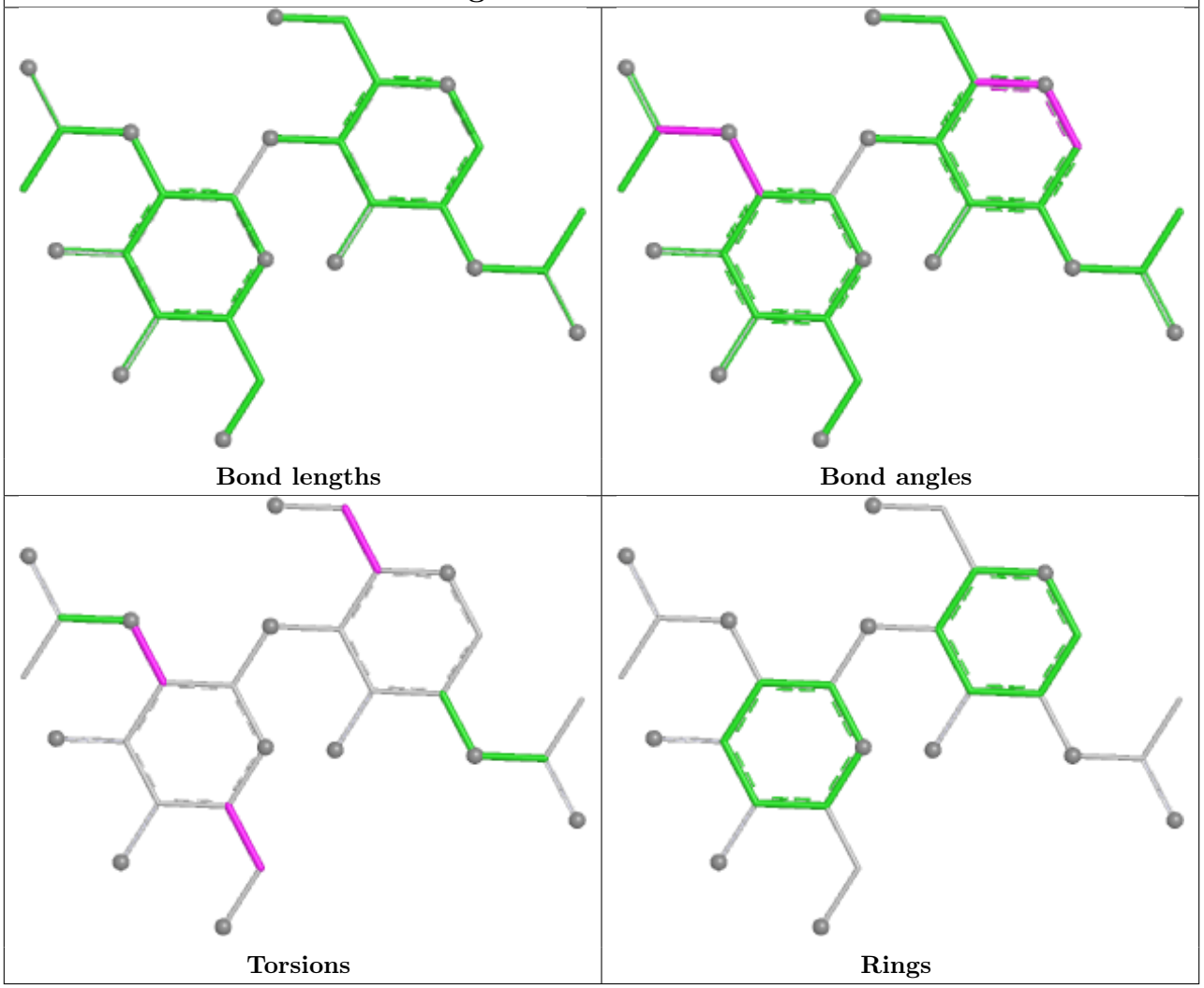


Torsions



Rings

Oligosaccharide Chain a



5.6 Ligand geometry (i)

27 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	$\#\|Z\| > 2$
9	NAG	B	608	1	14,14,15	0.43	0	17,19,21	0.65	1 (5%)
9	NAG	C	609	1	14,14,15	0.37	0	17,19,21	0.43	0
9	NAG	A	609	1	14,14,15	0.39	0	17,19,21	0.45	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
9	NAG	A	605	1	14,14,15	0.44	0	17,19,21	0.53	0
9	NAG	A	603	1	14,14,15	0.45	0	17,19,21	1.03	1 (5%)
9	NAG	B	609	1	14,14,15	0.35	0	17,19,21	0.47	0
9	NAG	C	604	1	14,14,15	0.81	1 (7%)	17,19,21	1.15	2 (11%)
9	NAG	A	608	1	14,14,15	0.38	0	17,19,21	0.71	1 (5%)
9	NAG	B	606	1	14,14,15	0.36	0	17,19,21	0.53	0
9	NAG	C	602	1	14,14,15	0.45	0	17,19,21	1.06	1 (5%)
9	NAG	C	606	1	14,14,15	0.62	0	17,19,21	0.46	0
9	NAG	A	607	1	14,14,15	0.39	0	17,19,21	0.55	0
9	NAG	C	601	1	14,14,15	0.59	0	17,19,21	1.15	2 (11%)
9	NAG	B	602	1	14,14,15	0.46	0	17,19,21	1.05	1 (5%)
9	NAG	A	602	1	14,14,15	0.45	0	17,19,21	1.04	1 (5%)
9	NAG	B	607	1	14,14,15	0.39	0	17,19,21	0.46	0
9	NAG	B	601	1	14,14,15	0.44	0	17,19,21	1.08	1 (5%)
9	NAG	C	603	1	14,14,15	0.48	0	17,19,21	1.02	1 (5%)
9	NAG	A	601	1	14,14,15	0.47	0	17,19,21	1.09	2 (11%)
9	NAG	C	605	1	14,14,15	0.43	0	17,19,21	0.50	0
9	NAG	B	604	1	14,14,15	0.65	1 (7%)	17,19,21	1.08	2 (11%)
9	NAG	A	604	1	14,14,15	0.73	1 (7%)	17,19,21	1.15	2 (11%)
9	NAG	B	605	1	14,14,15	0.52	0	17,19,21	0.54	0
9	NAG	A	606	1	14,14,15	0.33	0	17,19,21	0.55	0
9	NAG	C	608	1	14,14,15	0.46	0	17,19,21	0.73	1 (5%)
9	NAG	B	603	1	14,14,15	0.51	0	17,19,21	1.03	1 (5%)
9	NAG	C	607	1	14,14,15	0.43	0	17,19,21	0.50	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
9	NAG	B	608	1	-	2/6/23/26	0/1/1/1
9	NAG	C	609	1	-	2/6/23/26	0/1/1/1
9	NAG	A	609	1	-	1/6/23/26	0/1/1/1
9	NAG	A	605	1	-	2/6/23/26	0/1/1/1
9	NAG	A	603	1	-	3/6/23/26	0/1/1/1
9	NAG	B	609	1	-	0/6/23/26	0/1/1/1
9	NAG	C	604	1	-	4/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	NAG	A	608	1	-	2/6/23/26	0/1/1/1
9	NAG	B	606	1	-	2/6/23/26	0/1/1/1
9	NAG	C	602	1	-	4/6/23/26	0/1/1/1
9	NAG	C	606	1	-	2/6/23/26	0/1/1/1
9	NAG	A	607	1	-	2/6/23/26	0/1/1/1
9	NAG	C	601	1	-	2/6/23/26	0/1/1/1
9	NAG	B	602	1	-	2/6/23/26	0/1/1/1
9	NAG	A	602	1	-	4/6/23/26	0/1/1/1
9	NAG	B	607	1	-	1/6/23/26	0/1/1/1
9	NAG	B	601	1	-	4/6/23/26	0/1/1/1
9	NAG	C	603	1	-	4/6/23/26	0/1/1/1
9	NAG	A	601	1	-	4/6/23/26	0/1/1/1
9	NAG	C	605	1	-	2/6/23/26	0/1/1/1
9	NAG	B	604	1	-	3/6/23/26	0/1/1/1
9	NAG	A	604	1	-	4/6/23/26	0/1/1/1
9	NAG	B	605	1	-	2/6/23/26	0/1/1/1
9	NAG	A	606	1	-	1/6/23/26	0/1/1/1
9	NAG	C	608	1	-	0/6/23/26	0/1/1/1
9	NAG	B	603	1	-	4/6/23/26	0/1/1/1
9	NAG	C	607	1	-	1/6/23/26	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	C	604	NAG	C1-C2	2.66	1.56	1.52
9	A	604	NAG	C1-C2	2.27	1.55	1.52
9	B	604	NAG	C1-C2	2.02	1.55	1.52

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	C	603	NAG	C2-N2-C7	3.27	127.28	122.90
9	A	603	NAG	C2-N2-C7	3.25	127.26	122.90
9	C	602	NAG	C2-N2-C7	3.25	127.25	122.90
9	B	601	NAG	C2-N2-C7	3.25	127.25	122.90
9	A	602	NAG	C2-N2-C7	3.25	127.25	122.90
9	B	603	NAG	C2-N2-C7	3.25	127.25	122.90
9	B	602	NAG	C2-N2-C7	3.23	127.23	122.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	B	604	NAG	C2-N2-C7	3.21	127.20	122.90
9	A	601	NAG	C2-N2-C7	3.21	127.20	122.90
9	C	601	NAG	C2-N2-C7	3.20	127.18	122.90
9	A	604	NAG	C2-N2-C7	3.12	127.08	122.90
9	C	604	NAG	C2-N2-C7	3.09	127.04	122.90
9	C	604	NAG	C1-O5-C5	2.75	115.87	112.19
9	A	604	NAG	C1-O5-C5	2.70	115.81	112.19
9	C	608	NAG	C1-O5-C5	2.65	115.74	112.19
9	C	601	NAG	C1-O5-C5	2.60	115.67	112.19
9	A	608	NAG	C1-O5-C5	2.55	115.60	112.19
9	B	608	NAG	C1-O5-C5	2.30	115.27	112.19
9	A	601	NAG	C1-O5-C5	2.08	114.97	112.19
9	B	604	NAG	C1-O5-C5	2.07	114.97	112.19

There are no chirality outliers.

All (64) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	B	606	NAG	C4-C5-C6-O6
9	B	605	NAG	O5-C5-C6-O6
9	B	606	NAG	O5-C5-C6-O6
9	A	605	NAG	O5-C5-C6-O6
9	B	608	NAG	O5-C5-C6-O6
9	A	604	NAG	C4-C5-C6-O6
9	C	605	NAG	O5-C5-C6-O6
9	C	604	NAG	O5-C5-C6-O6
9	B	601	NAG	O5-C5-C6-O6
9	C	606	NAG	O5-C5-C6-O6
9	A	607	NAG	C4-C5-C6-O6
9	B	605	NAG	C4-C5-C6-O6
9	A	607	NAG	O5-C5-C6-O6
9	A	602	NAG	C4-C5-C6-O6
9	B	603	NAG	O5-C5-C6-O6
9	A	604	NAG	O5-C5-C6-O6
9	C	603	NAG	O5-C5-C6-O6
9	C	609	NAG	O5-C5-C6-O6
9	C	604	NAG	C4-C5-C6-O6
9	B	601	NAG	C4-C5-C6-O6
9	B	603	NAG	C4-C5-C6-O6
9	C	609	NAG	C4-C5-C6-O6
9	C	602	NAG	O5-C5-C6-O6
9	B	608	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
9	C	603	NAG	C4-C5-C6-O6
9	C	605	NAG	C4-C5-C6-O6
9	A	605	NAG	C4-C5-C6-O6
9	C	602	NAG	C4-C5-C6-O6
9	A	601	NAG	O5-C5-C6-O6
9	B	607	NAG	O5-C5-C6-O6
9	A	602	NAG	O5-C5-C6-O6
9	A	601	NAG	C4-C5-C6-O6
9	C	606	NAG	C4-C5-C6-O6
9	B	604	NAG	O5-C5-C6-O6
9	A	603	NAG	O5-C5-C6-O6
9	A	609	NAG	O5-C5-C6-O6
9	C	607	NAG	O5-C5-C6-O6
9	A	606	NAG	O5-C5-C6-O6
9	A	603	NAG	C1-C2-N2-C7
9	A	608	NAG	C4-C5-C6-O6
9	A	608	NAG	O5-C5-C6-O6
9	A	604	NAG	C3-C2-N2-C7
9	B	604	NAG	C3-C2-N2-C7
9	C	601	NAG	C3-C2-N2-C7
9	C	604	NAG	C3-C2-N2-C7
9	A	601	NAG	C1-C2-N2-C7
9	A	602	NAG	C1-C2-N2-C7
9	A	604	NAG	C1-C2-N2-C7
9	B	601	NAG	C1-C2-N2-C7
9	B	602	NAG	C1-C2-N2-C7
9	B	603	NAG	C1-C2-N2-C7
9	B	604	NAG	C1-C2-N2-C7
9	C	601	NAG	C1-C2-N2-C7
9	C	602	NAG	C1-C2-N2-C7
9	C	603	NAG	C1-C2-N2-C7
9	C	604	NAG	C1-C2-N2-C7
9	A	601	NAG	C3-C2-N2-C7
9	A	602	NAG	C3-C2-N2-C7
9	A	603	NAG	C3-C2-N2-C7
9	B	601	NAG	C3-C2-N2-C7
9	B	602	NAG	C3-C2-N2-C7
9	B	603	NAG	C3-C2-N2-C7
9	C	602	NAG	C3-C2-N2-C7
9	C	603	NAG	C3-C2-N2-C7

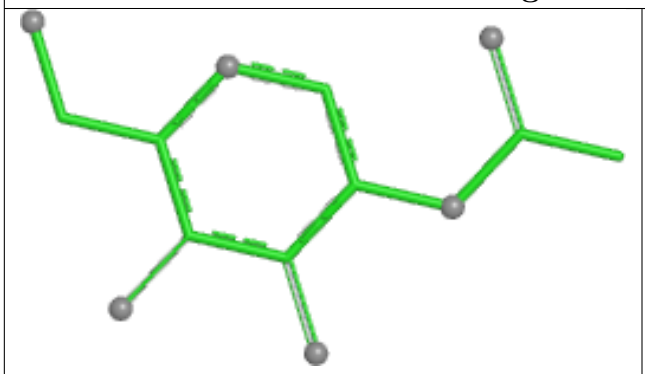
There are no ring outliers.

1 monomer is involved in 1 short contact:

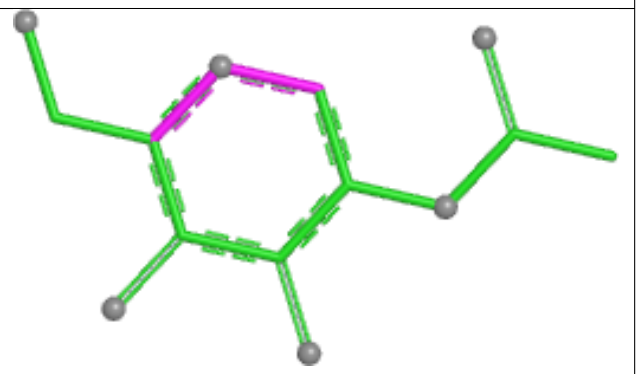
Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	C	603	NAG	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

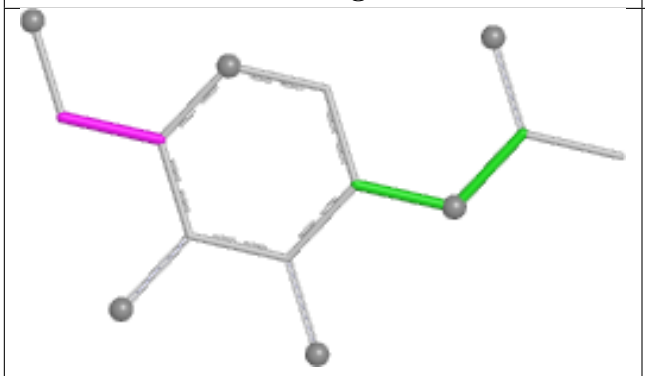
Ligand NAG B 608



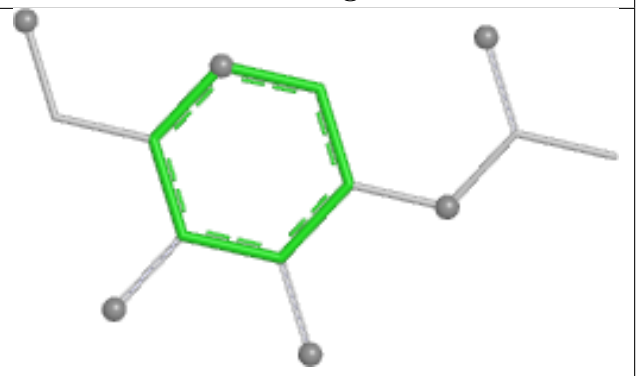
Bond lengths



Bond angles

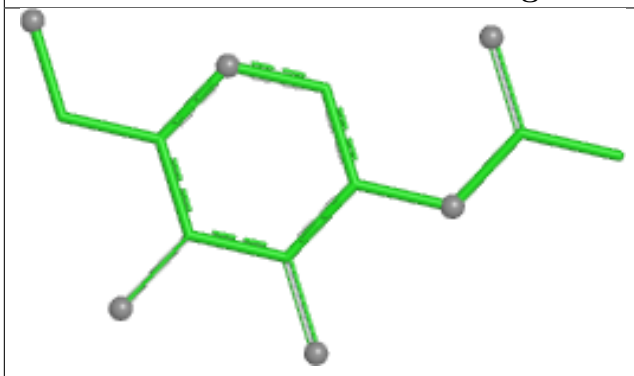


Torsions

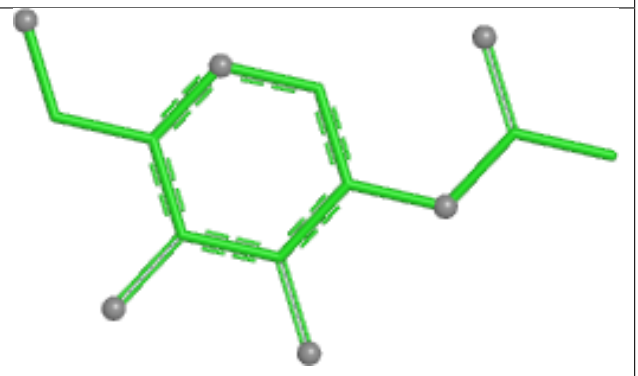


Rings

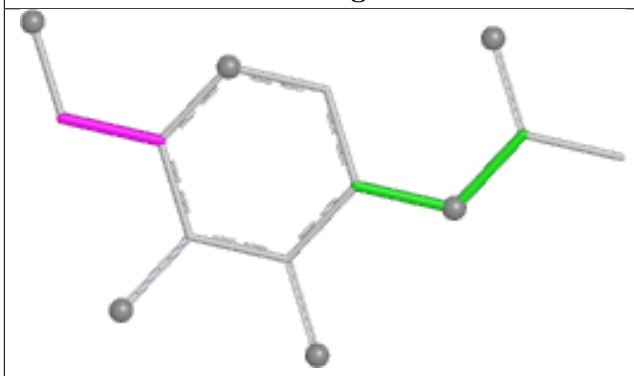
Ligand NAG C 609



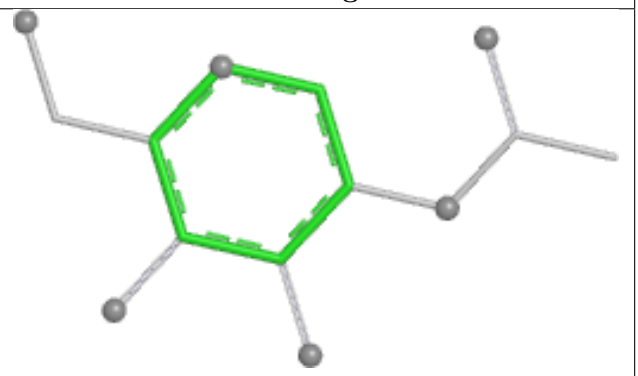
Bond lengths



Bond angles

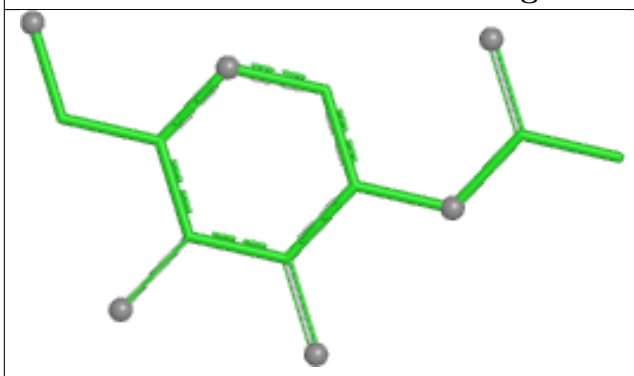


Torsions

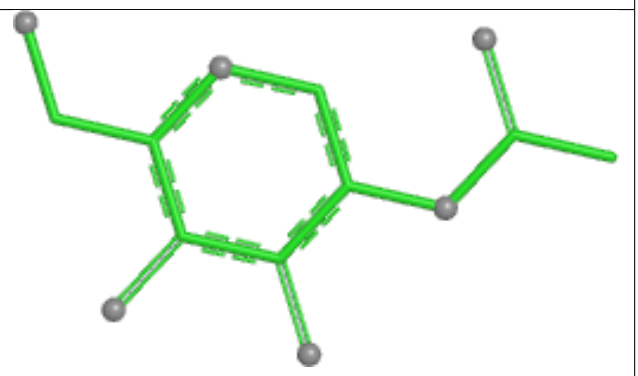


Rings

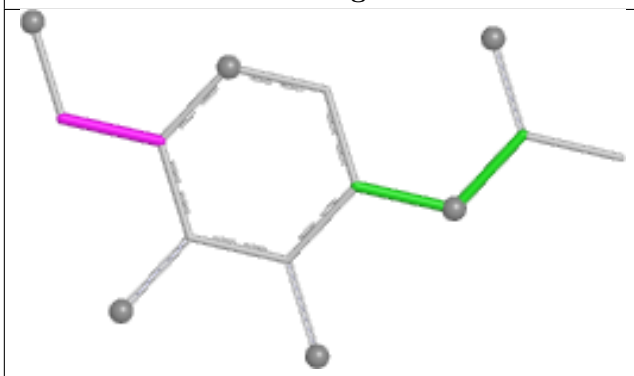
Ligand NAG A 609



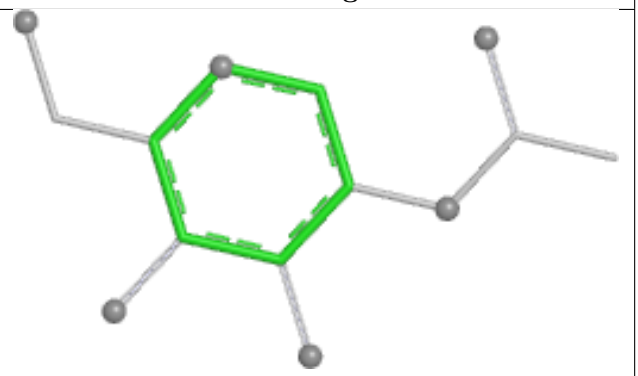
Bond lengths



Bond angles

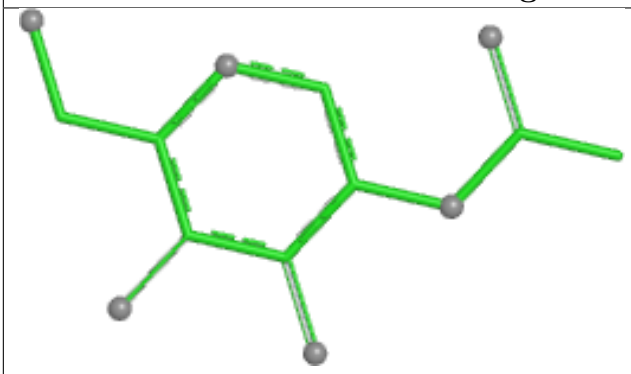


Torsions

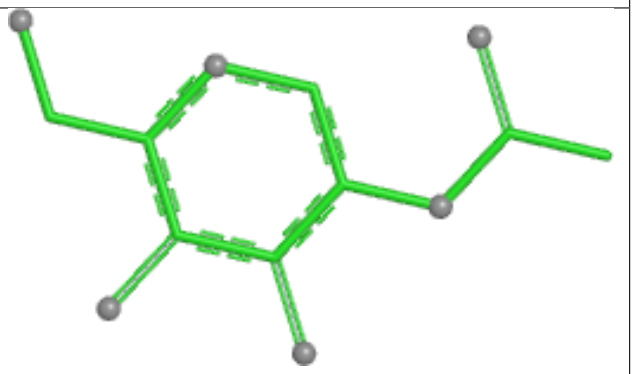


Rings

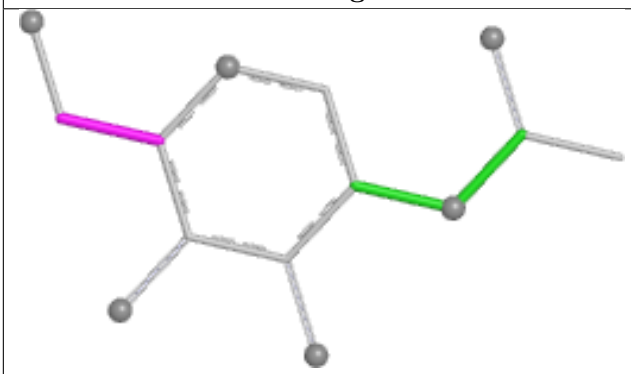
Ligand NAG A 605



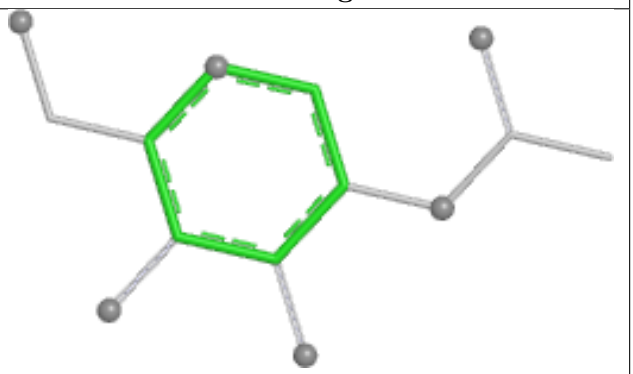
Bond lengths



Bond angles

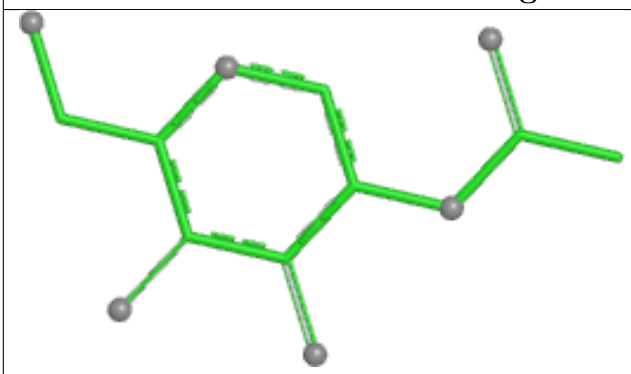


Torsions

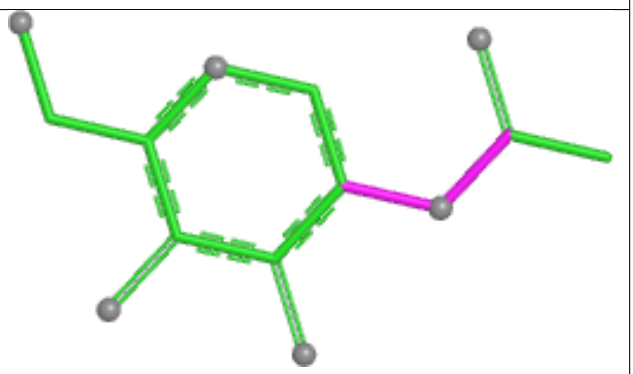


Rings

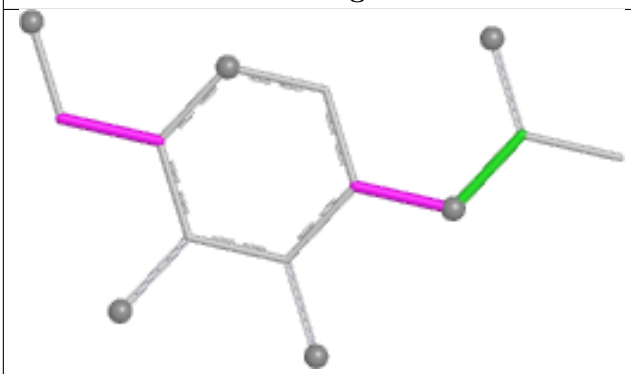
Ligand NAG A 603



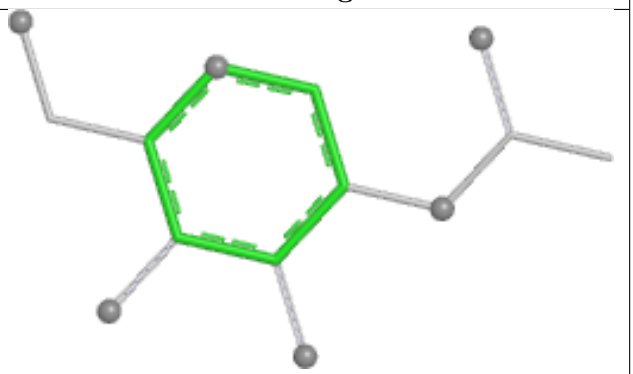
Bond lengths



Bond angles

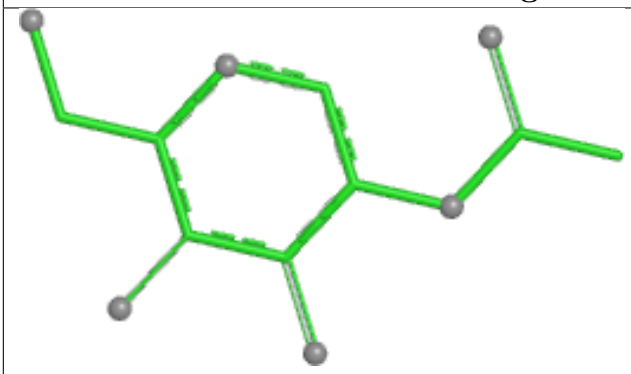


Torsions



Rings

Ligand NAG B 609



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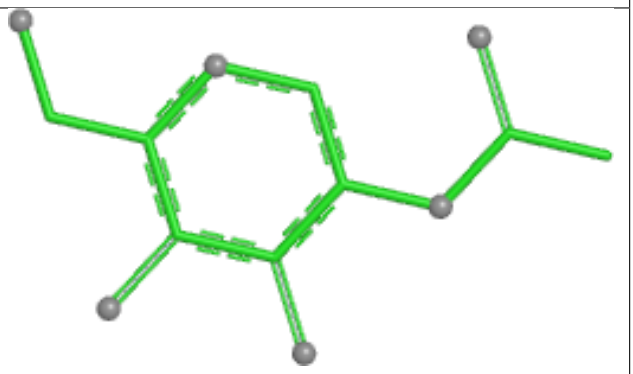
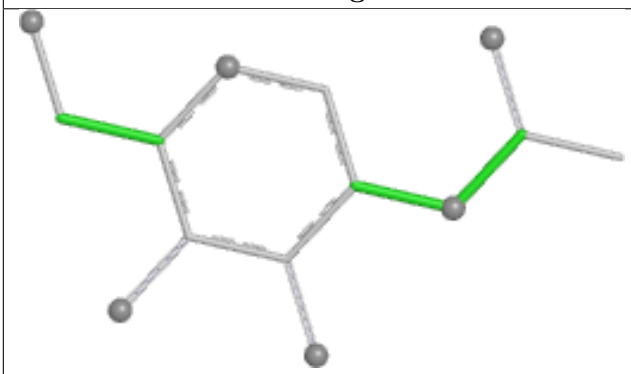
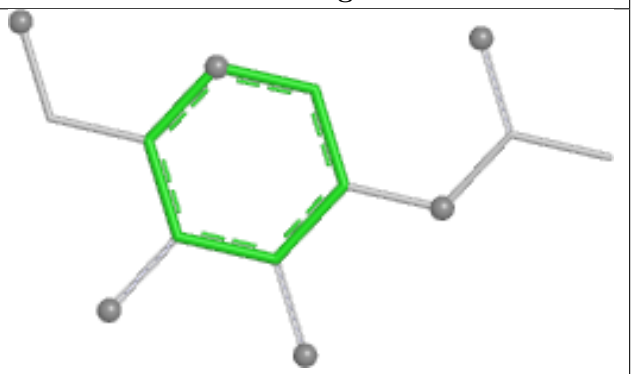


Bond angles

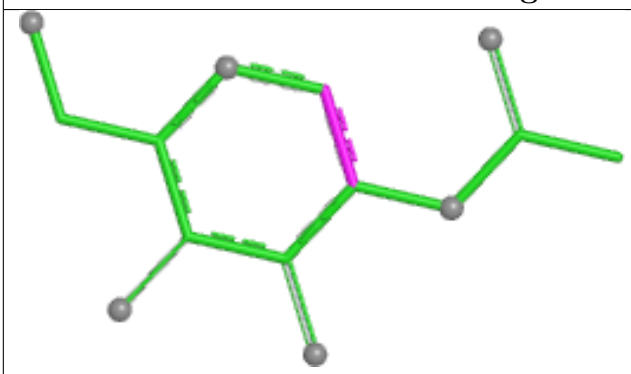


Torsions

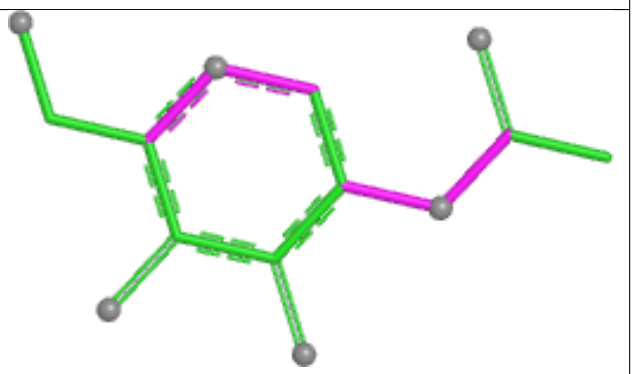


Rings

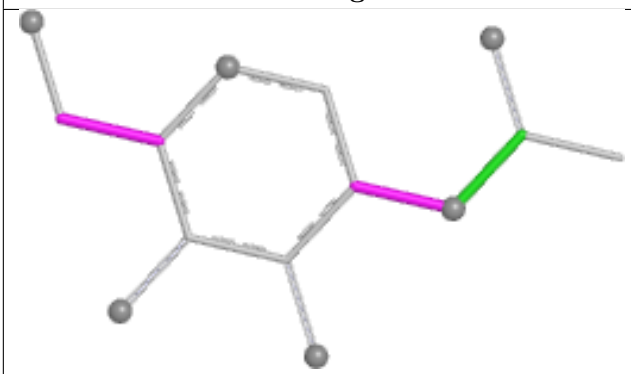
Ligand NAG C 604



Bond lengths



Bond angles



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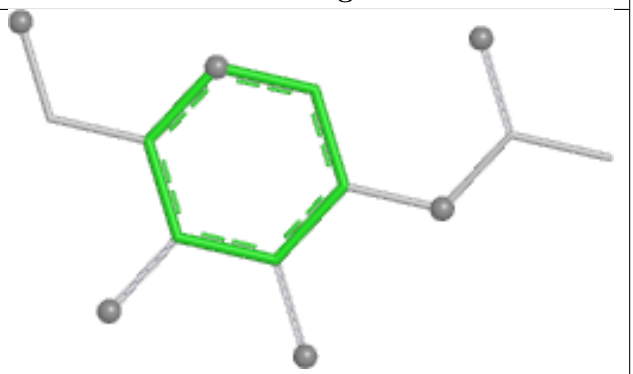
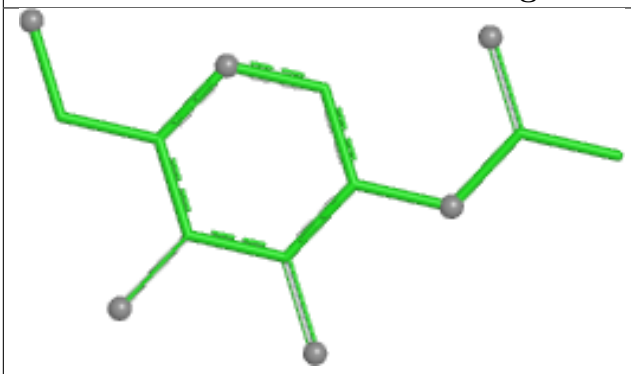


Rings

Ligand NAG A 608



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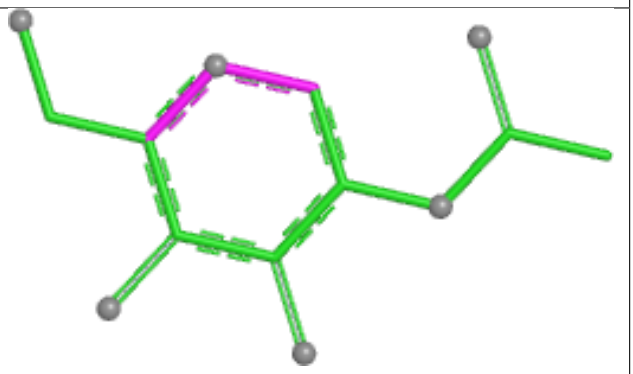
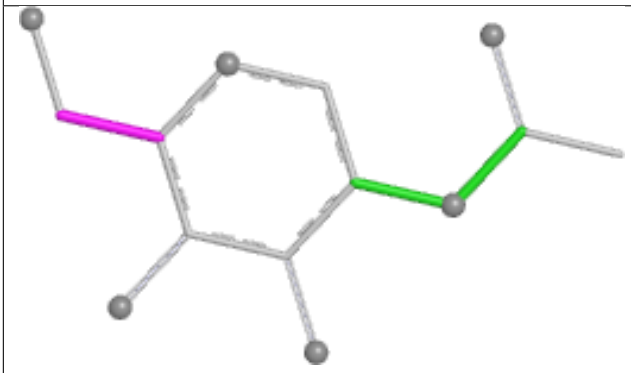
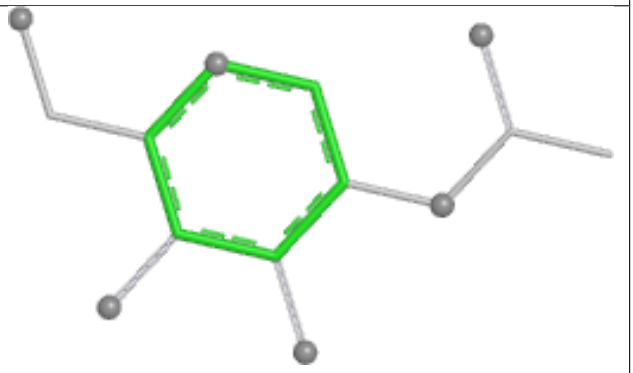


Bond angles

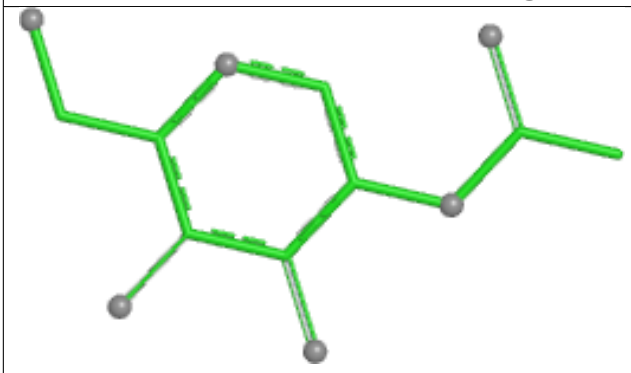


Torsions

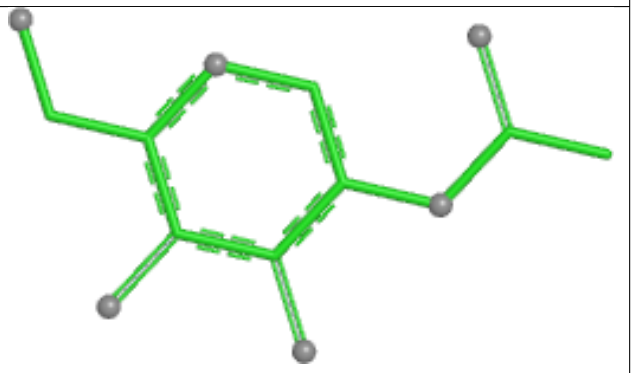


Rings

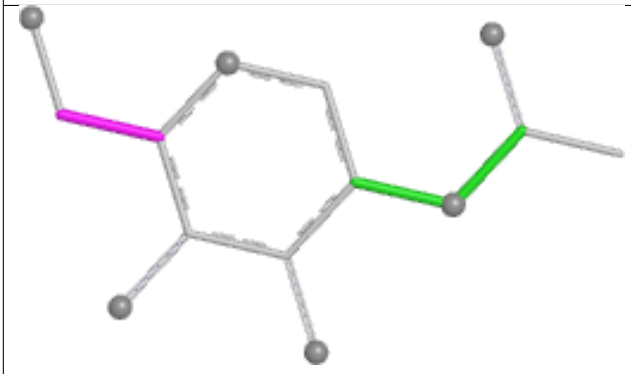
Ligand NAG B 606



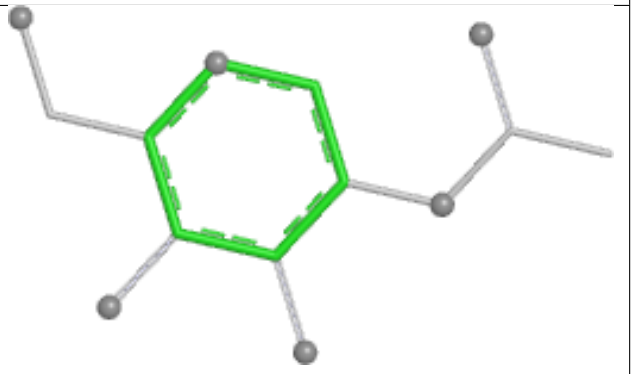
Bond lengths



Bond angles

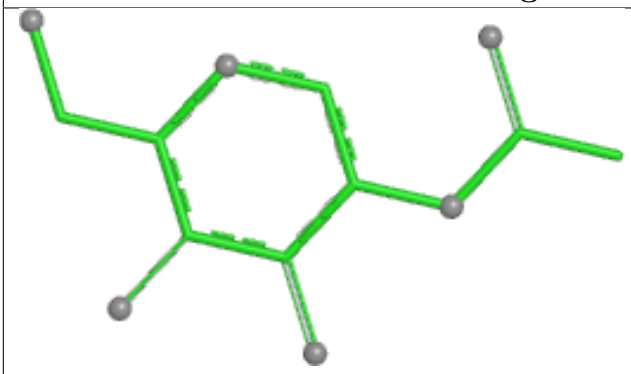


Torsions

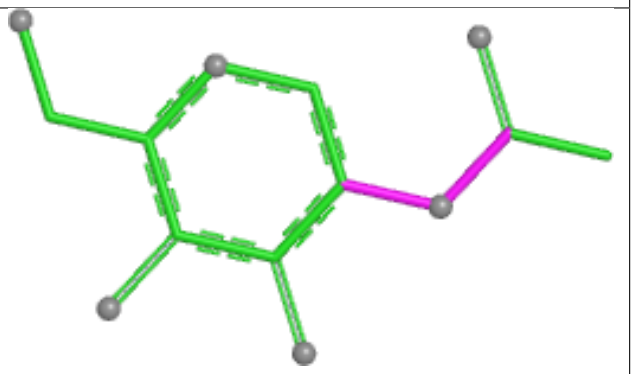


Rings

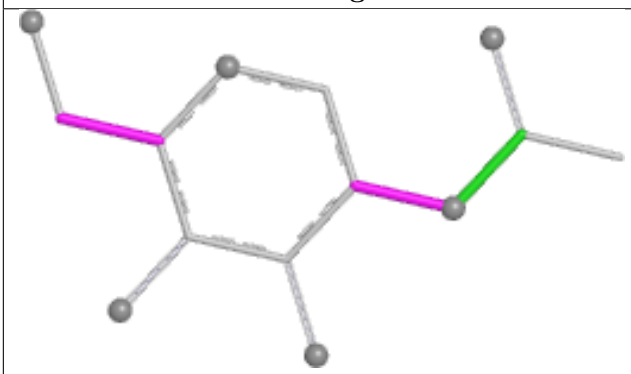
Ligand NAG C 602



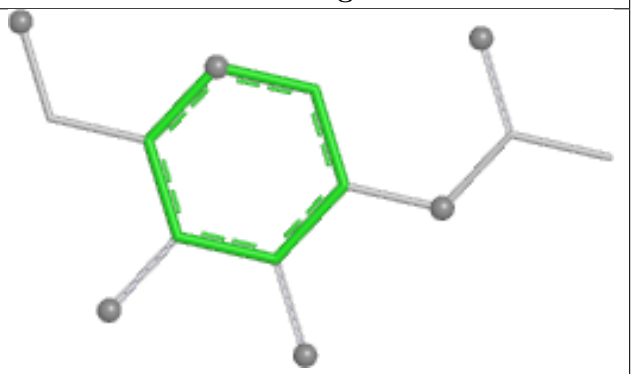
Bond lengths



Bond angles

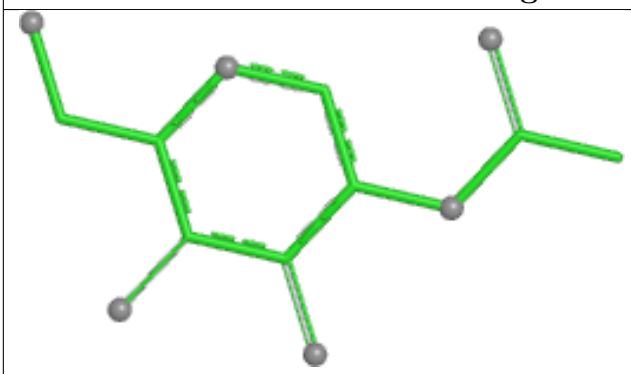


Torsions

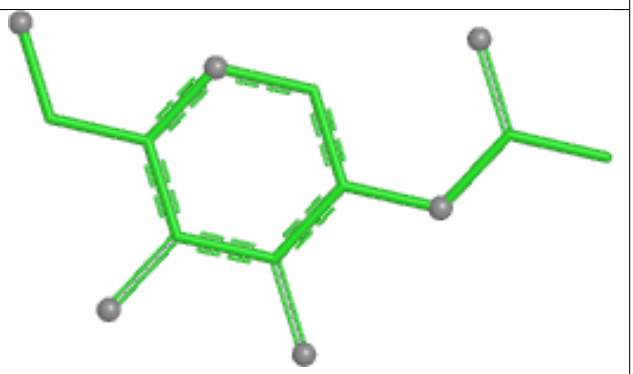


Rings

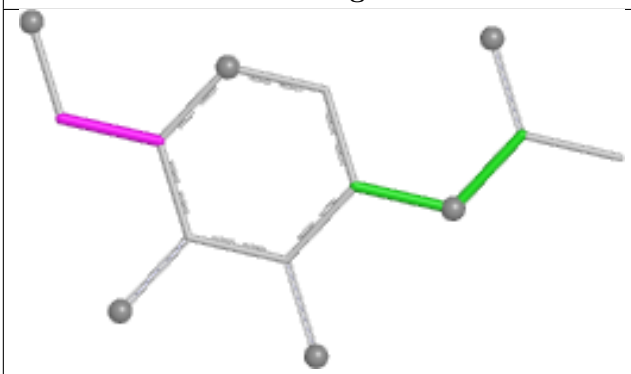
Ligand NAG C 606



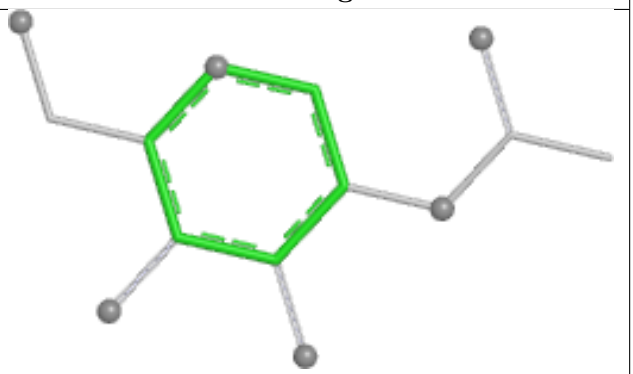
Bond lengths



Bond angles

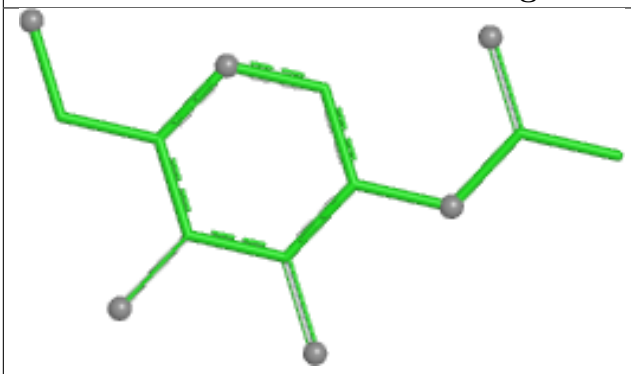


Torsions

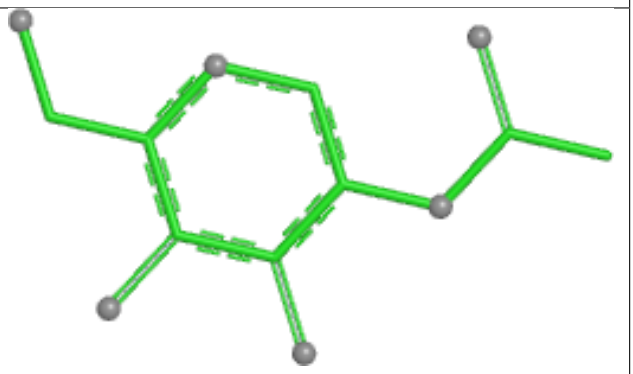


Rings

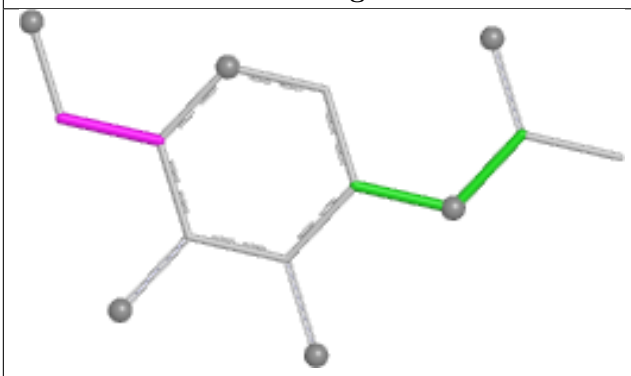
Ligand NAG A 607



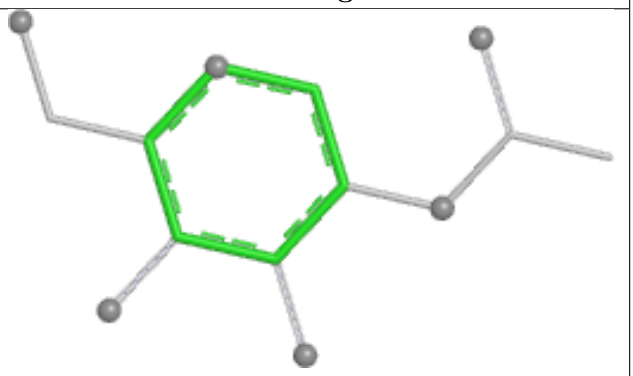
Bond lengths



Bond angles

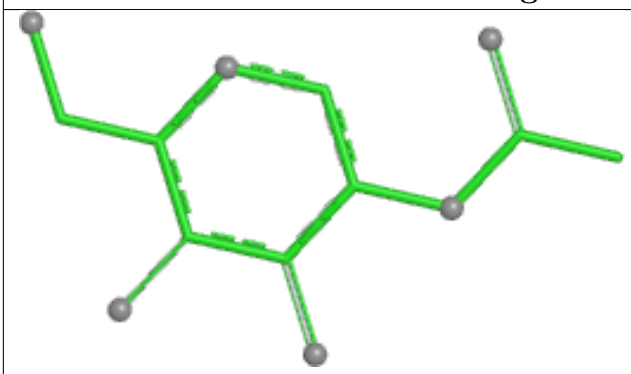


Torsions

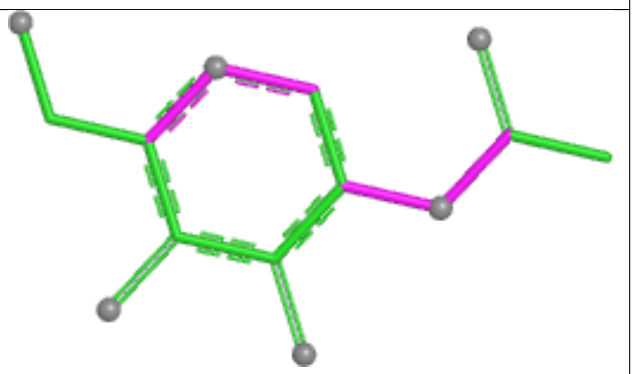


Rings

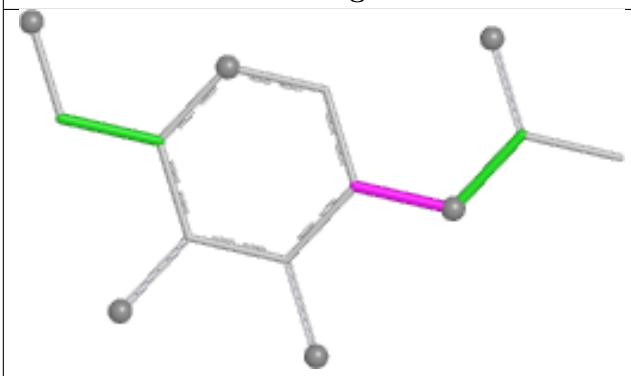
Ligand NAG C 601



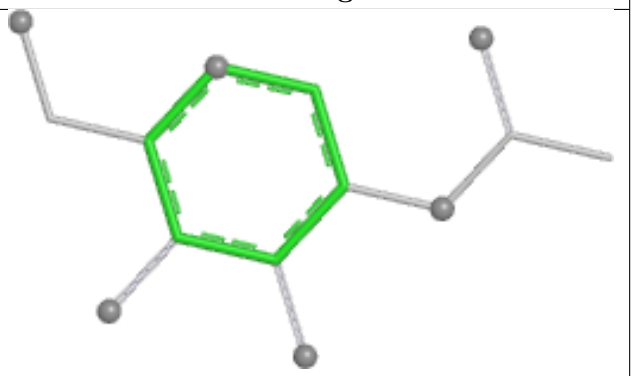
Bond lengths



Bond angles

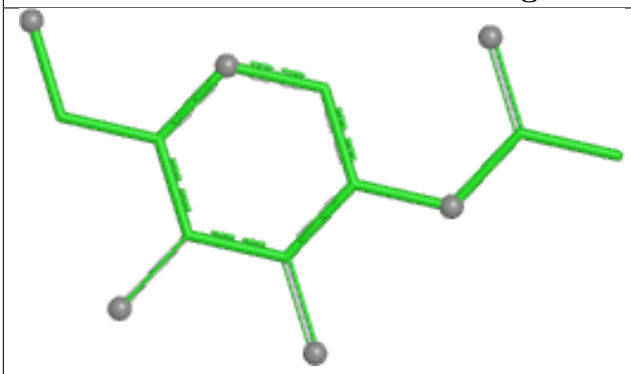


Torsions

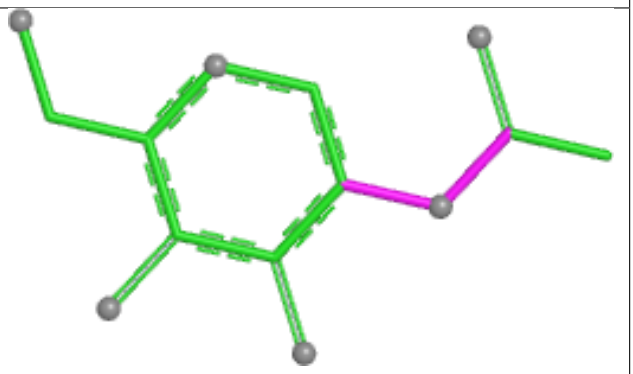


Rings

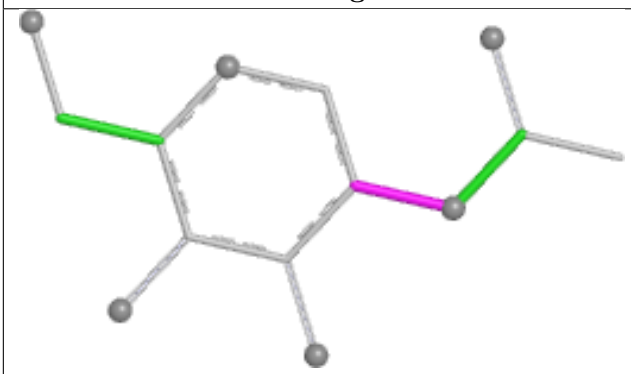
Ligand NAG B 602



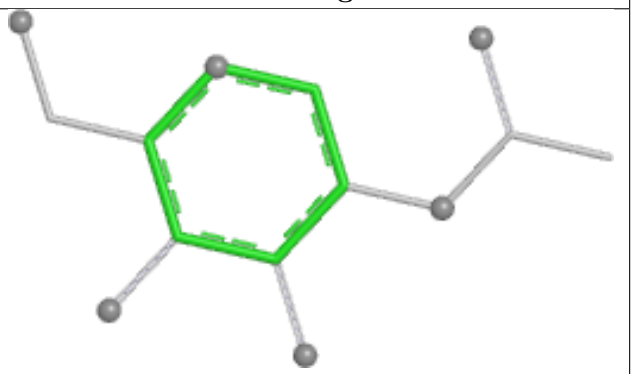
Bond lengths



Bond angles

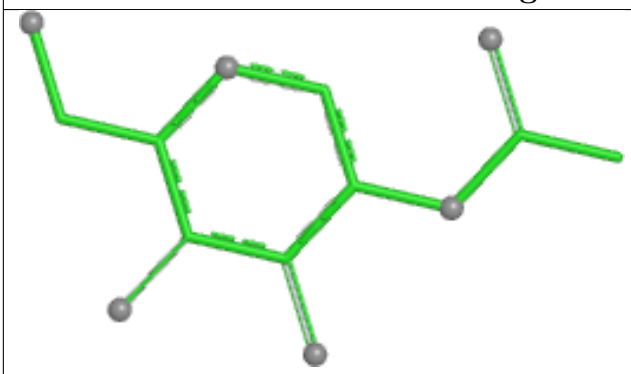


Torsions

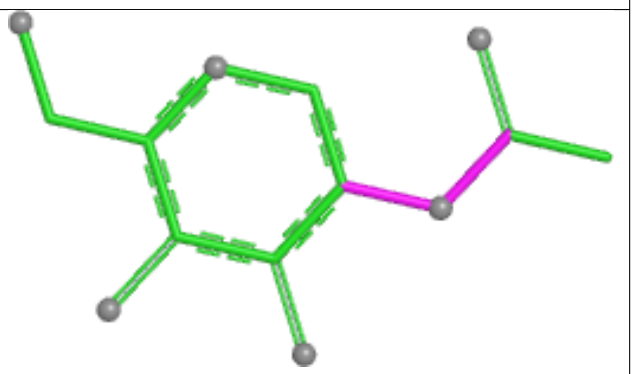


Rings

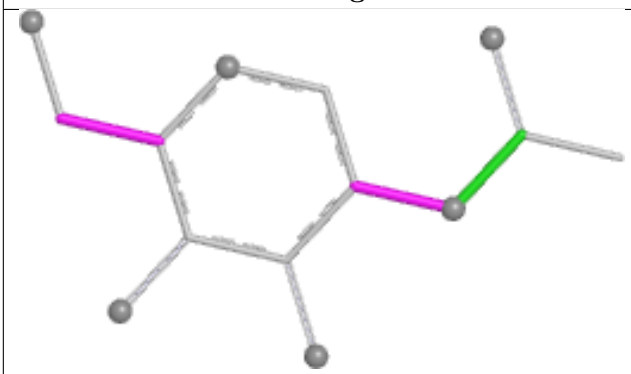
Ligand NAG A 602



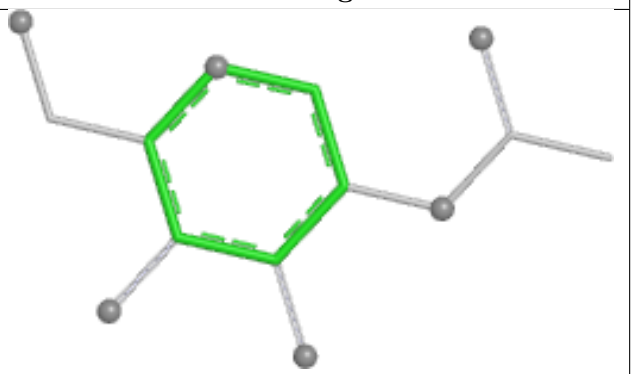
Bond lengths



Bond angles

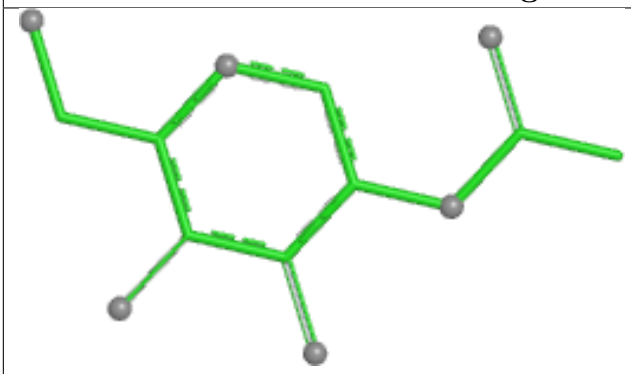


Torsions



Rings

Ligand NAG B 607



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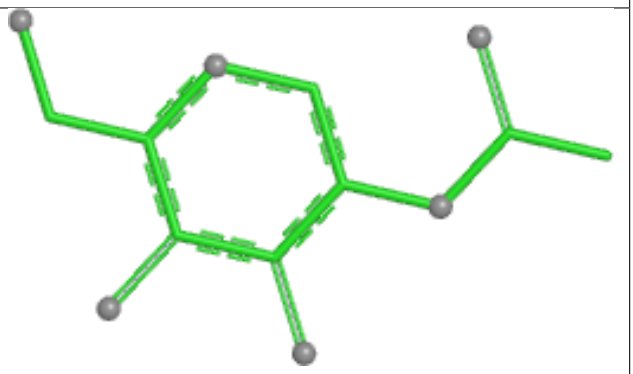
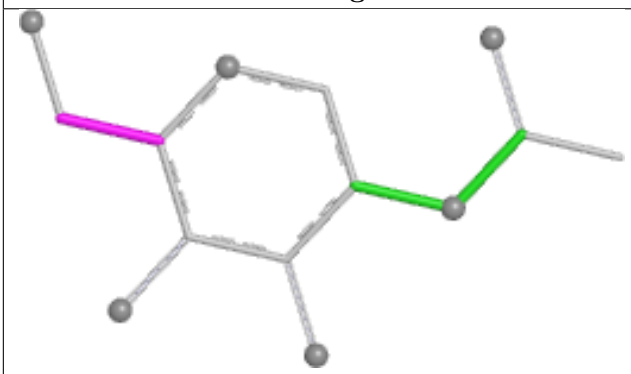
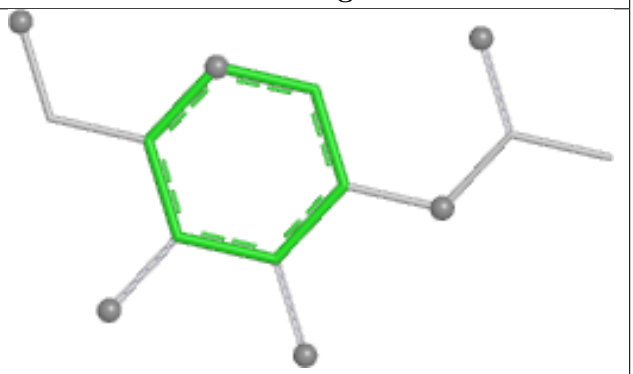


Bond angles

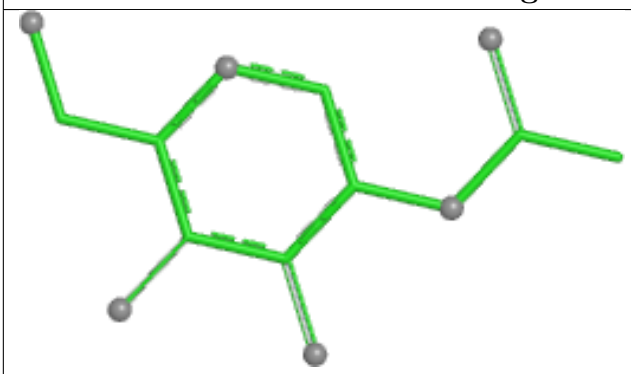


Torsions

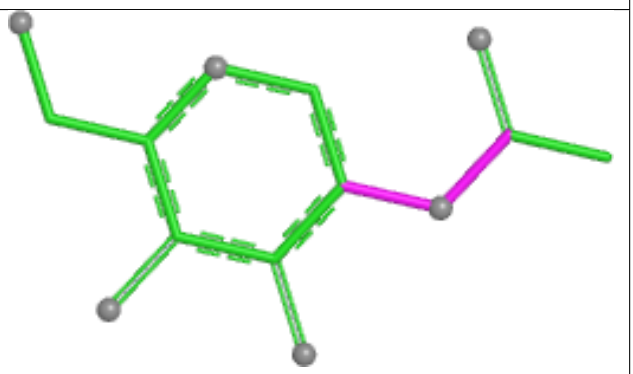


Rings

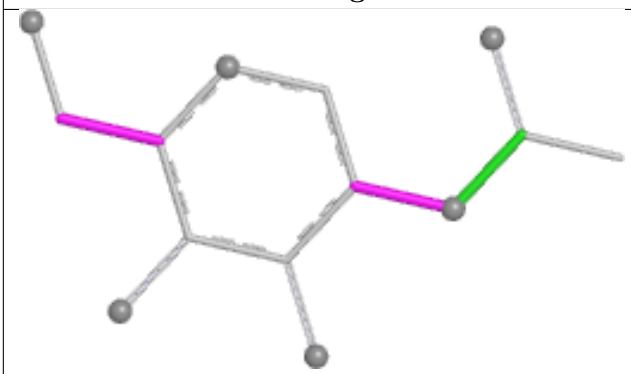
Ligand NAG B 601



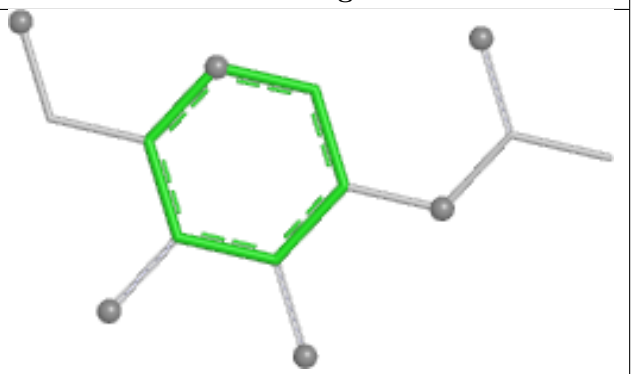
Bond lengths



Bond angles

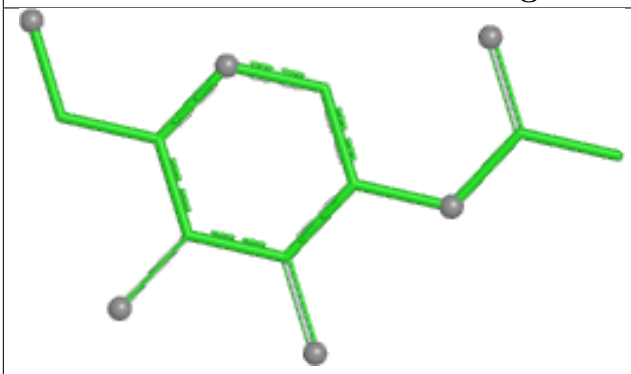


Torsions

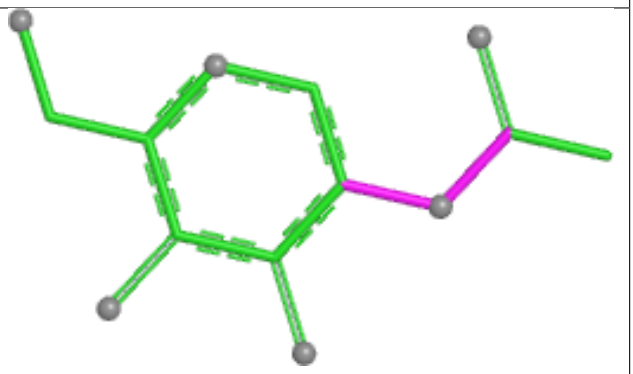


Rings

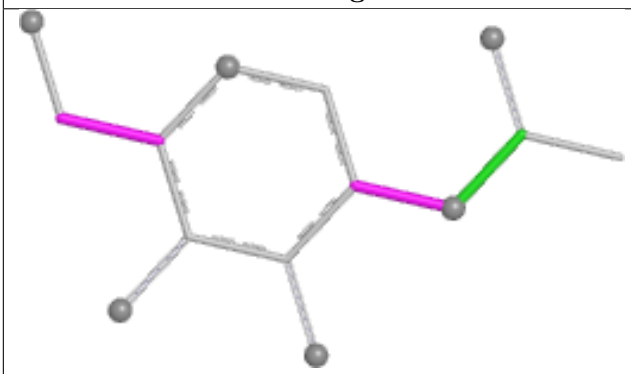
Ligand NAG C 603



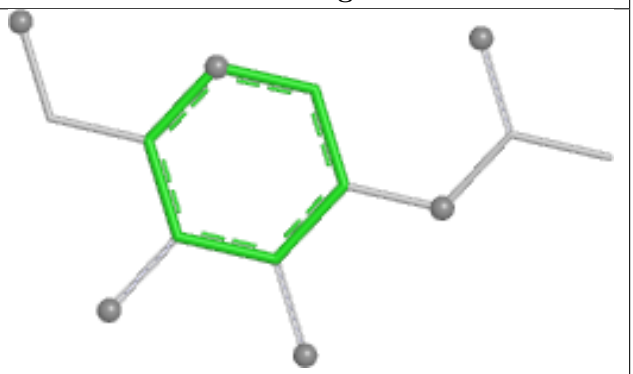
Bond lengths



Bond angles

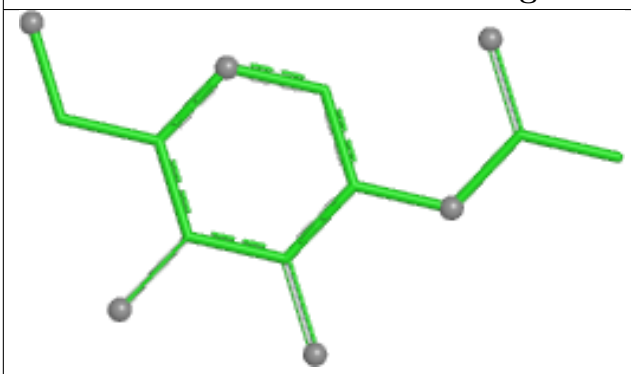


Torsions

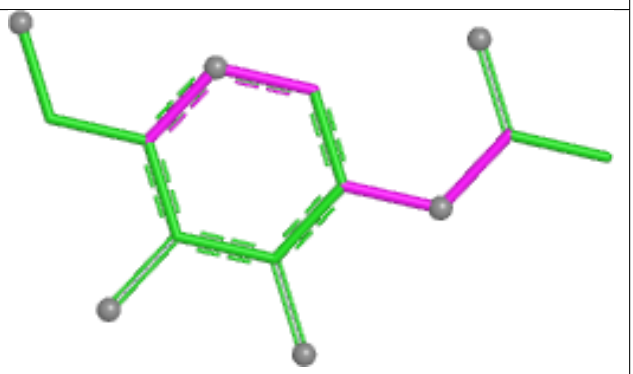


Rings

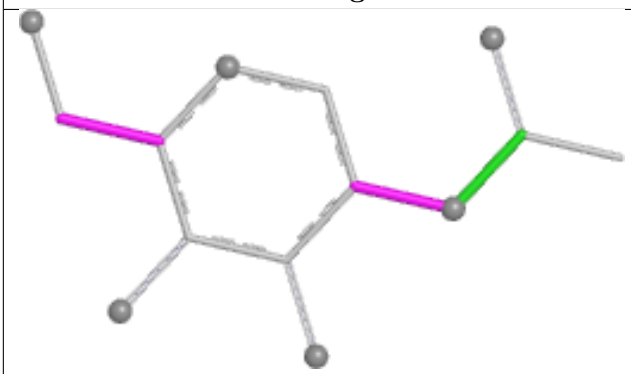
Ligand NAG A 601



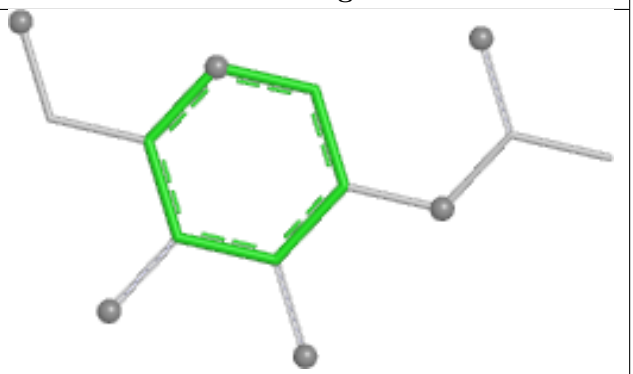
Bond lengths



Bond angles

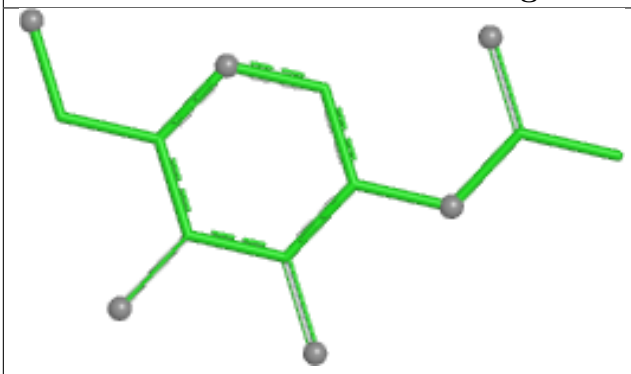


Torsions

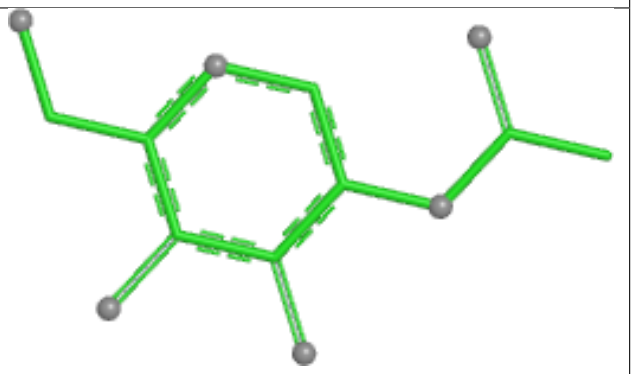


Rings

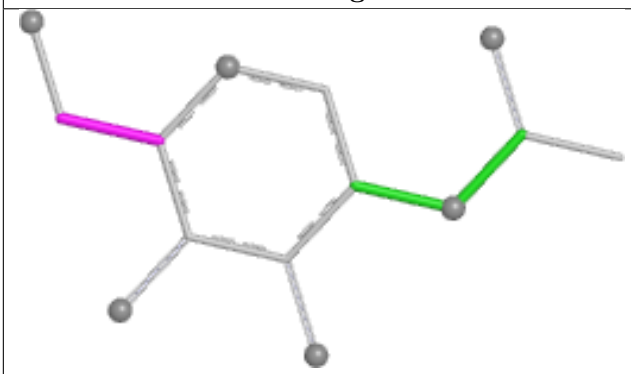
Ligand NAG C 605



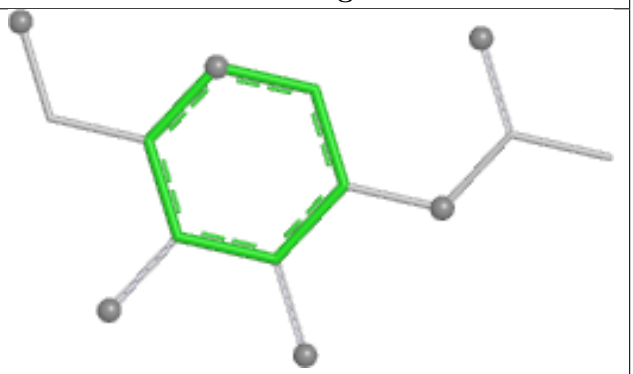
Bond lengths



Bond angles

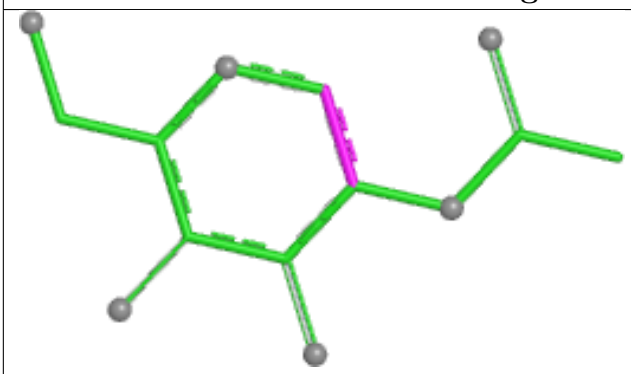


Torsions

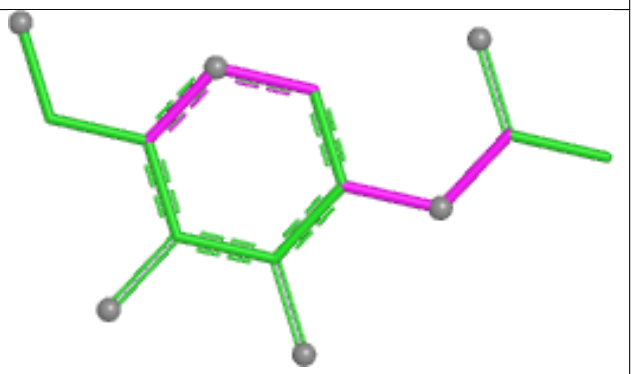


Rings

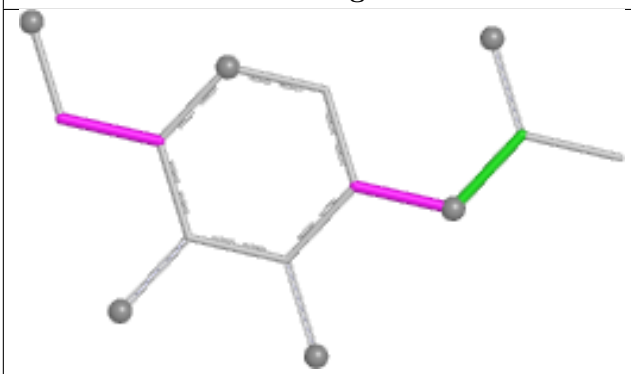
Ligand NAG B 604



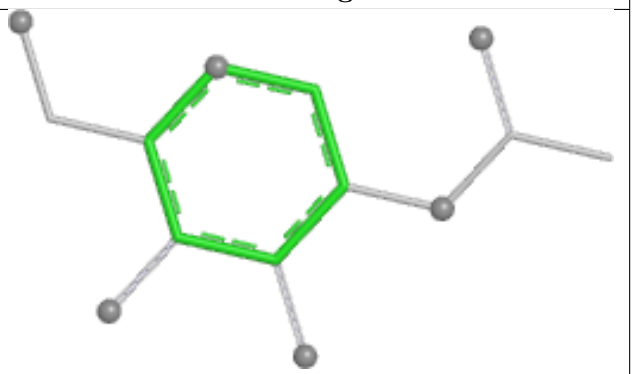
Bond lengths



Bond angles

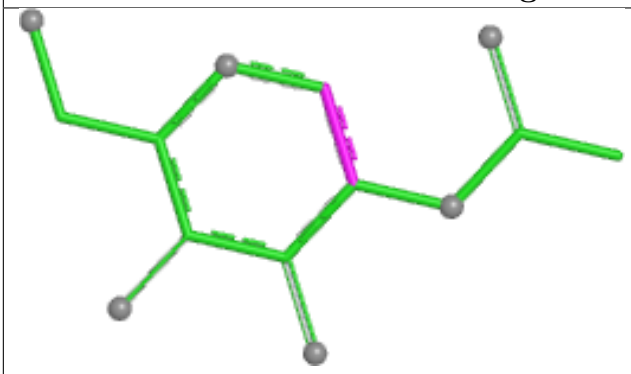


Torsions

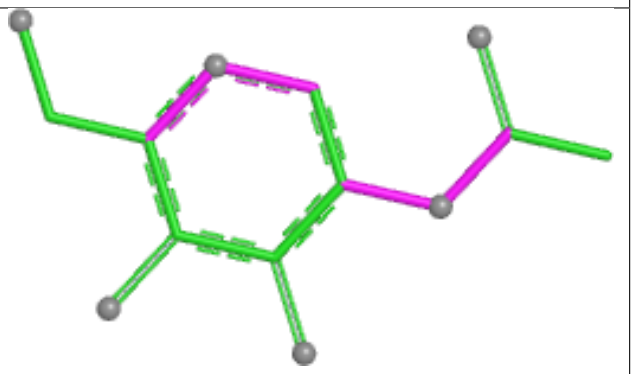


Rings

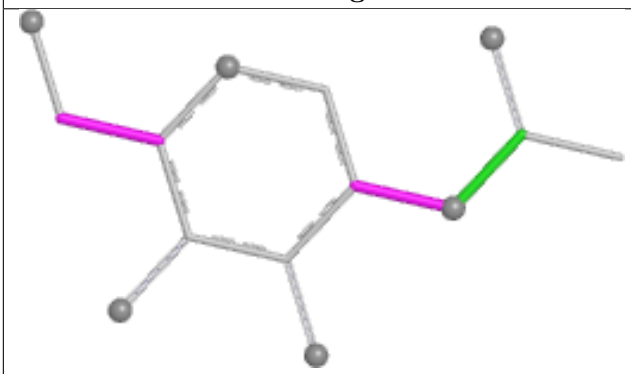
Ligand NAG A 604



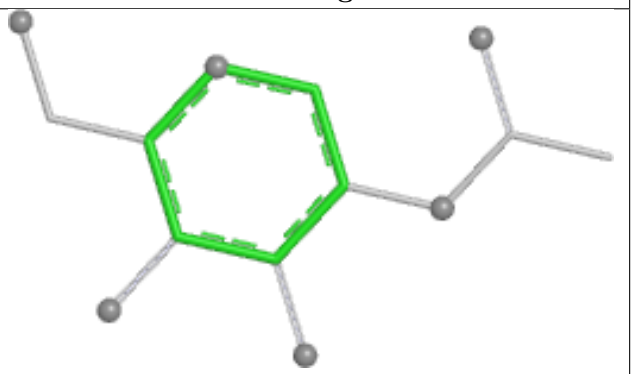
Bond lengths



Bond angles

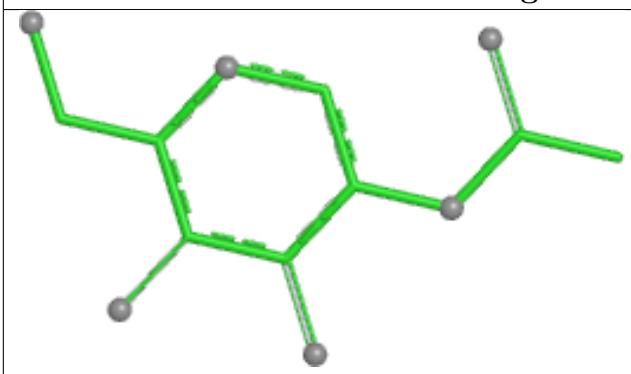


Torsions

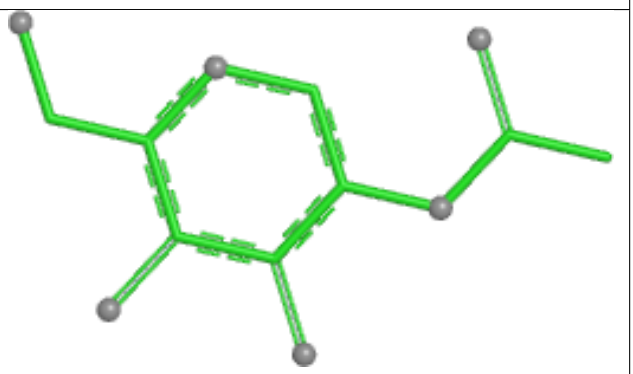


Rings

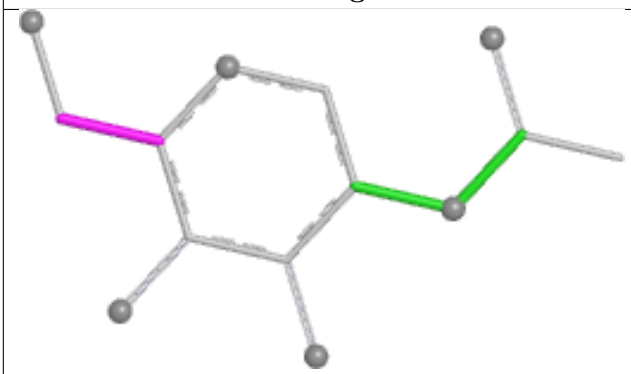
Ligand NAG B 605



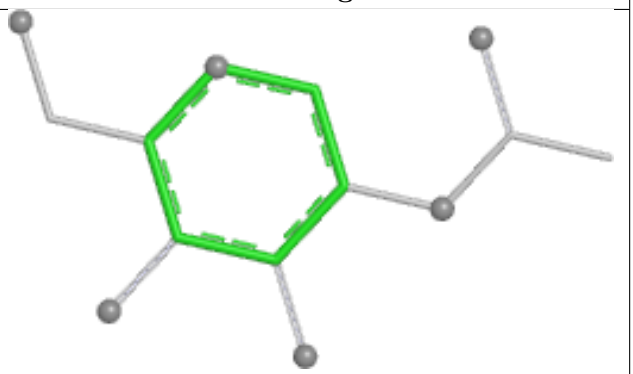
Bond lengths



Bond angles

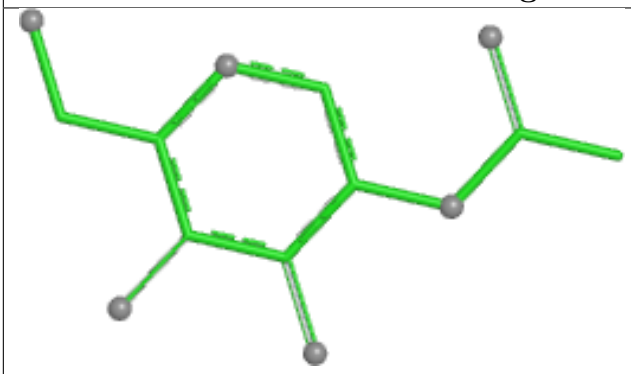


Torsions

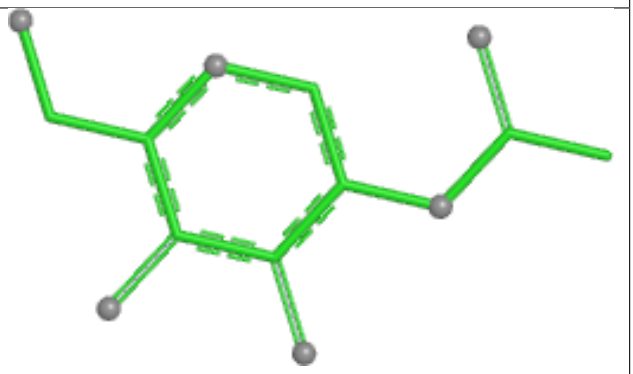


Rings

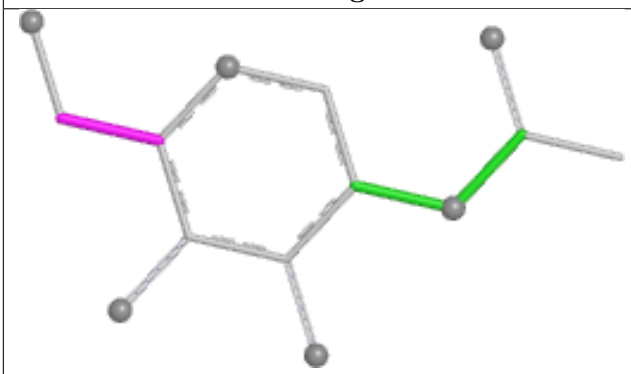
Ligand NAG A 606



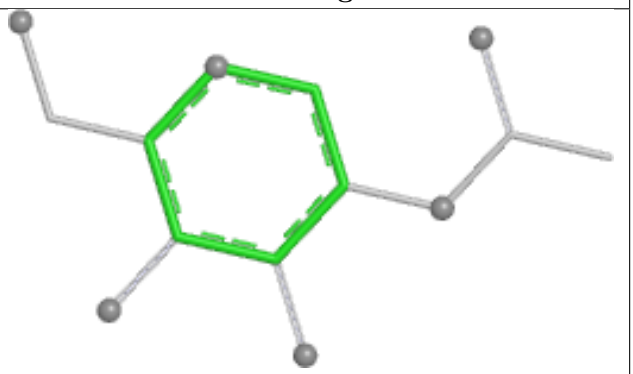
Bond lengths



Bond angles

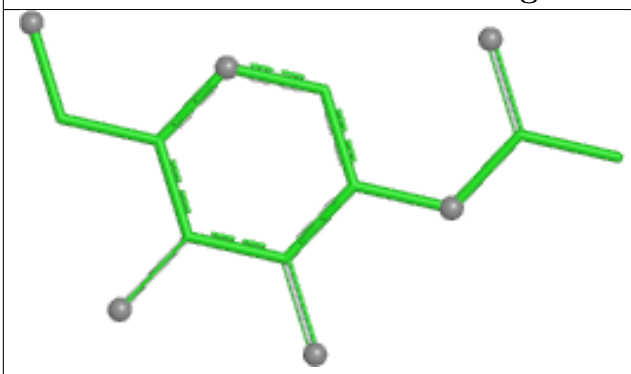


Torsions

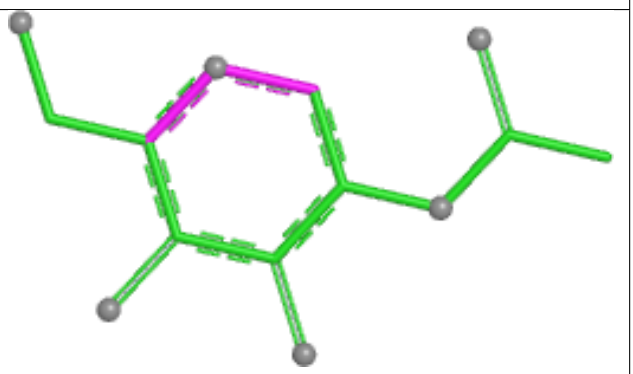


Rings

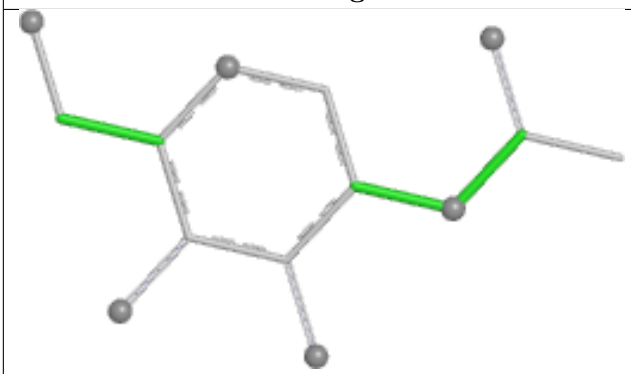
Ligand NAG C 608



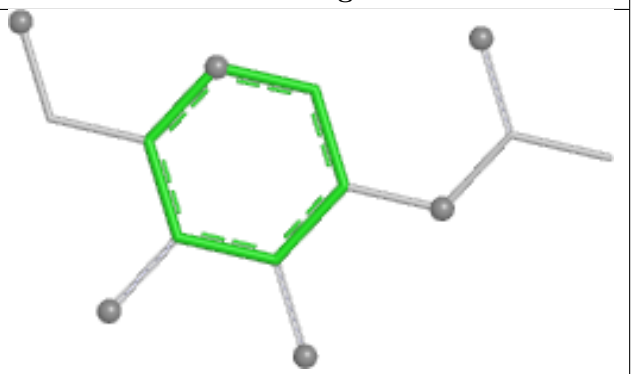
Bond lengths



Bond angles

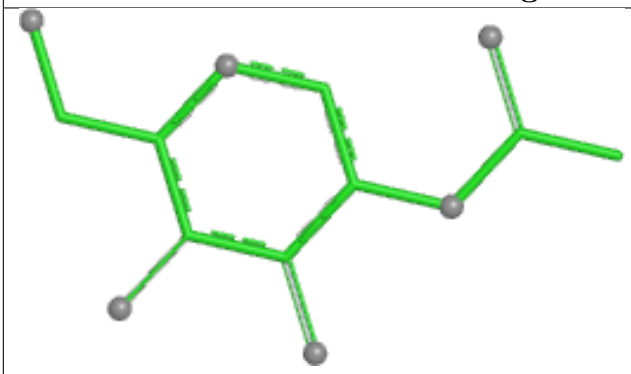


Torsions

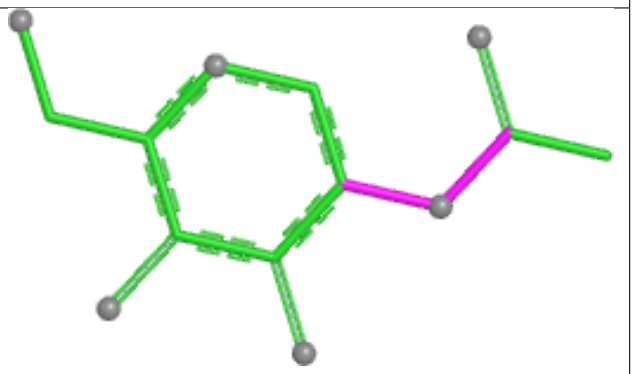


Rings

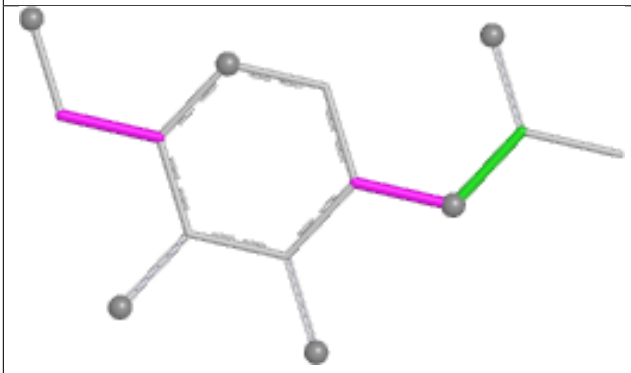
Ligand NAG B 603



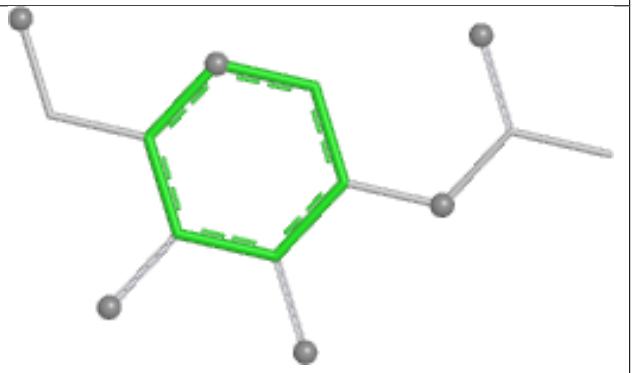
Bond lengths



Bond angles

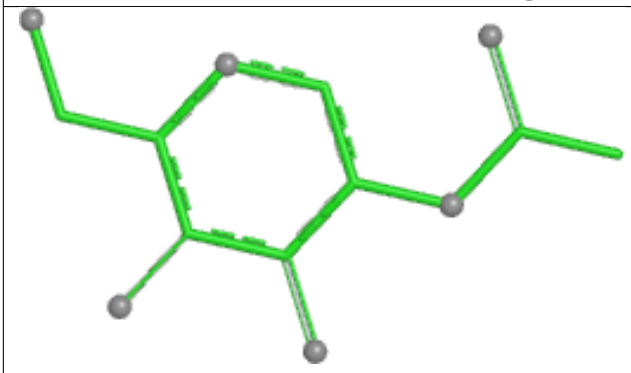


Torsions

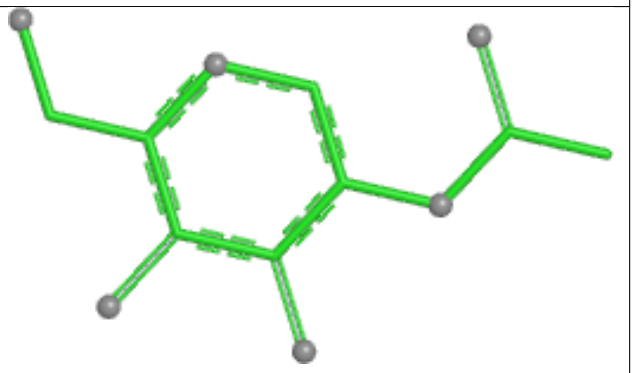


Rings

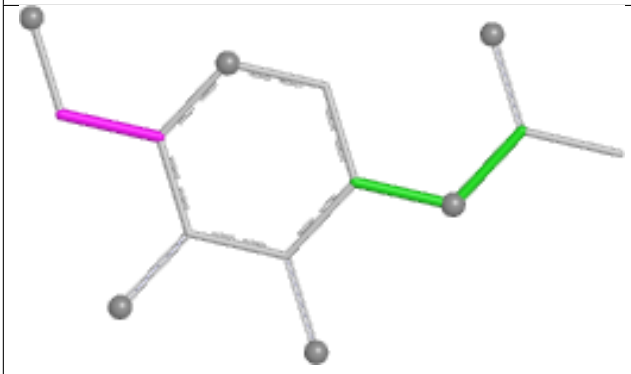
Ligand NAG C 607



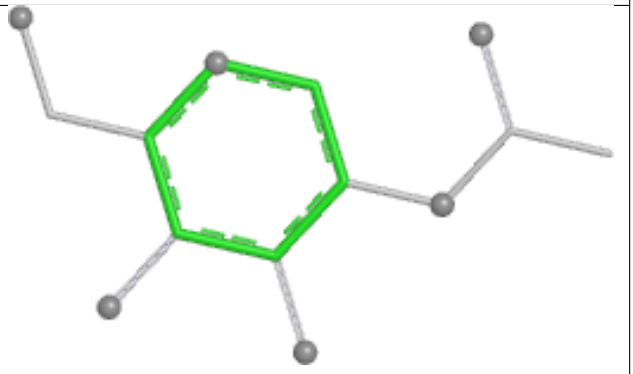
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

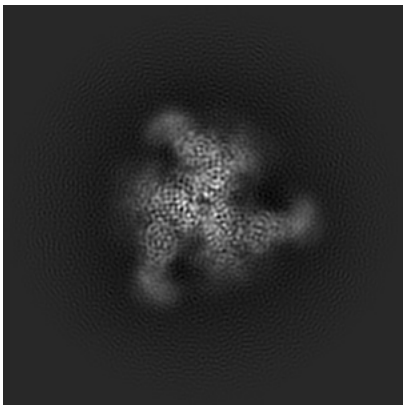
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-43879. These allow visual inspection of the internal detail of the map and identification of artifacts.

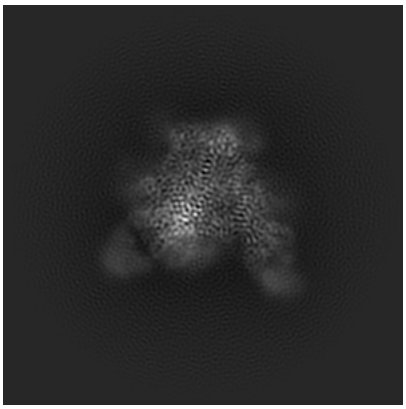
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

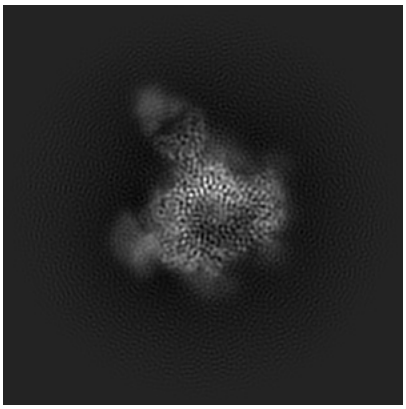
6.1.1 Primary map



X

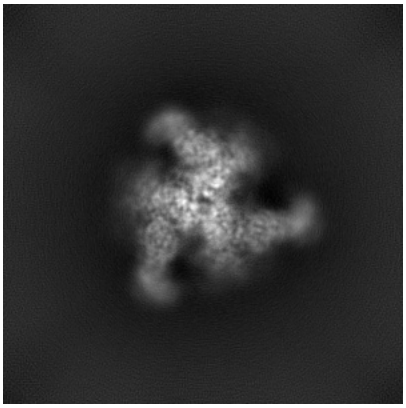


Y

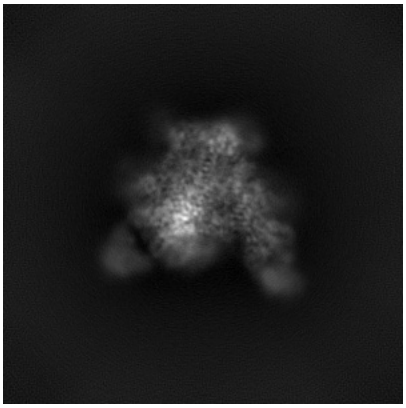


Z

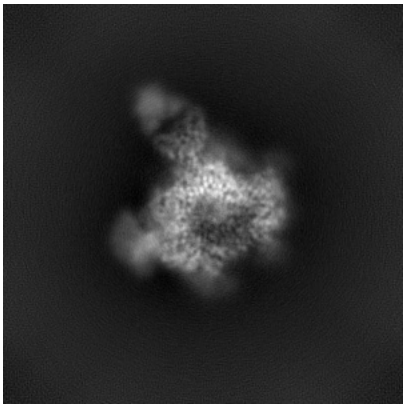
6.1.2 Raw map



X



Y

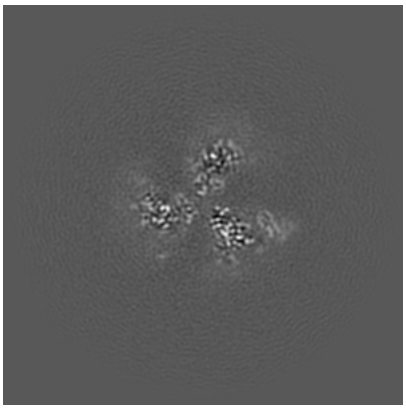


Z

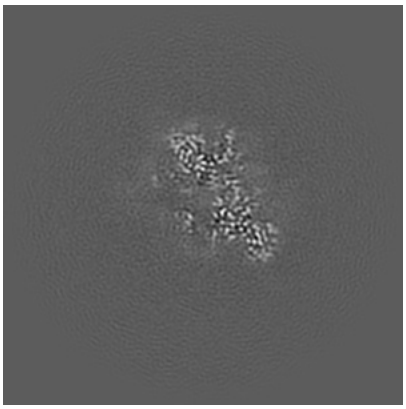
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

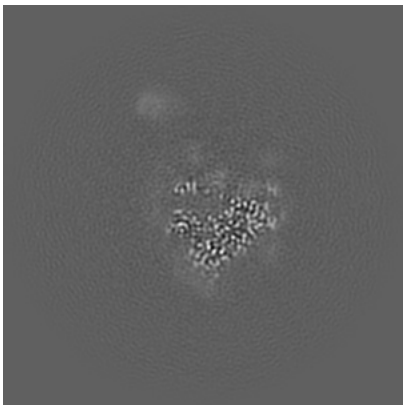
6.2.1 Primary map



X Index: 160

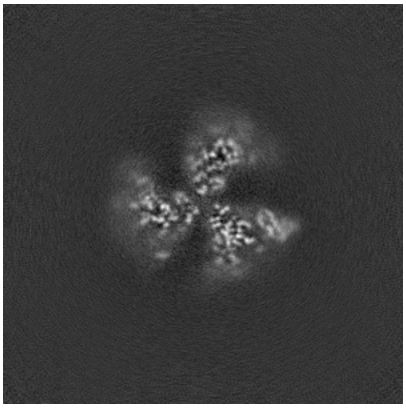


Y Index: 160

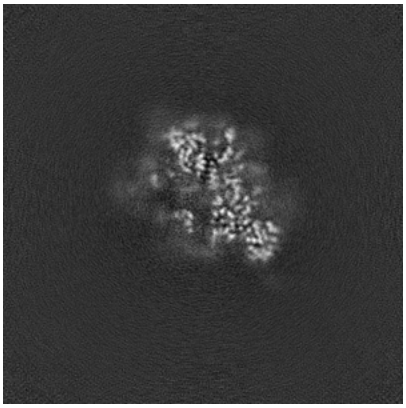


Z Index: 160

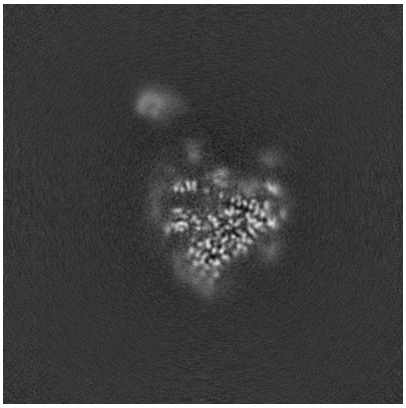
6.2.2 Raw map



X Index: 160



Y Index: 160

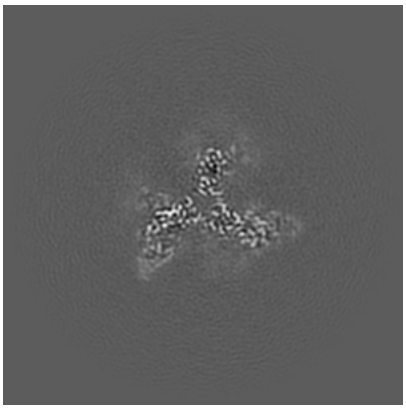


Z Index: 160

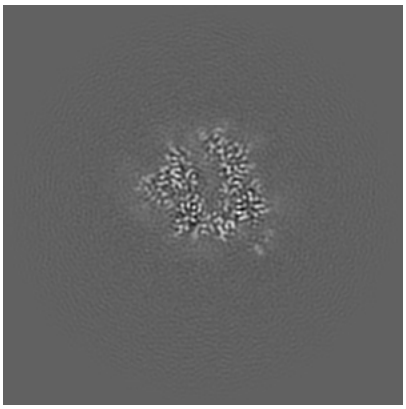
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

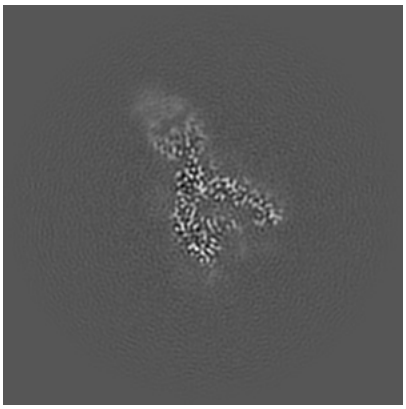
6.3.1 Primary map



X Index: 152

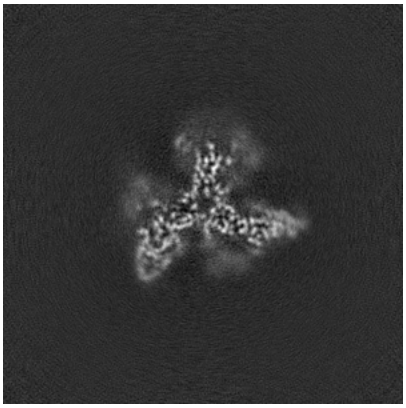


Y Index: 171

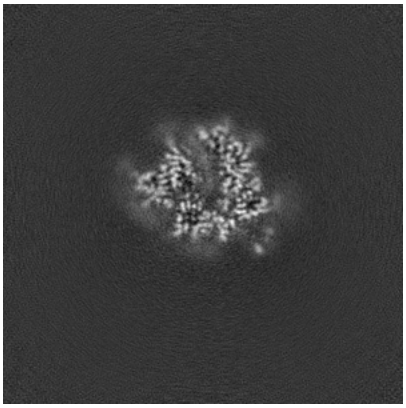


Z Index: 148

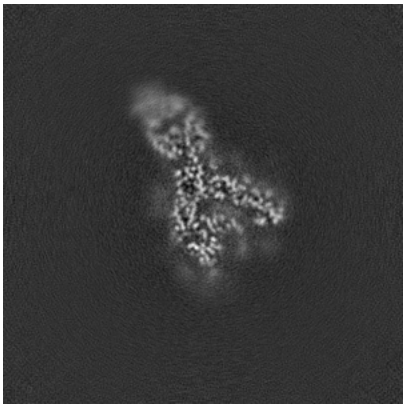
6.3.2 Raw map



X Index: 149



Y Index: 172

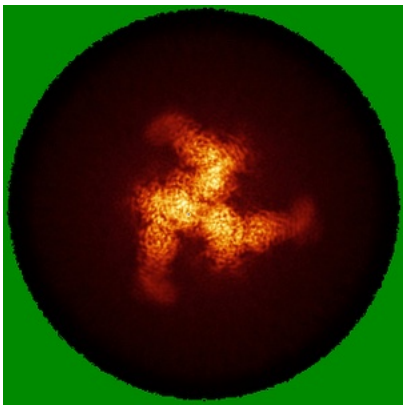


Z Index: 148

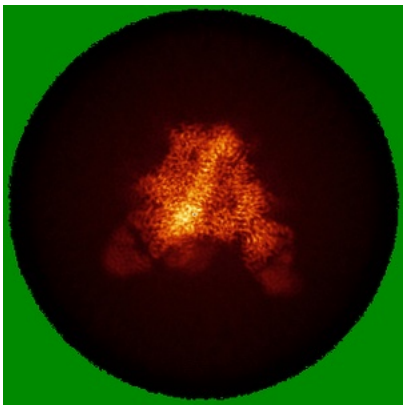
The images above show the largest variance slices of the map in three orthogonal directions.

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

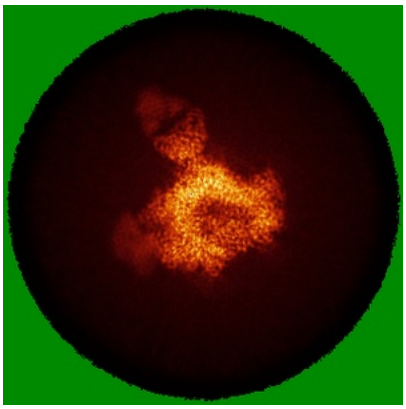
6.4.1 Primary map



X

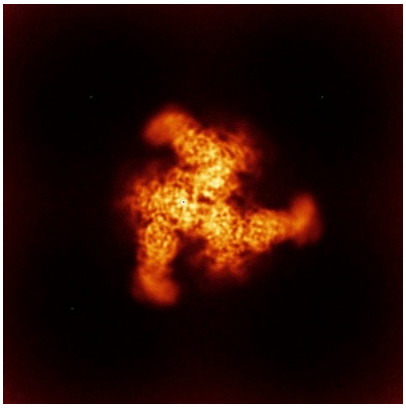


Y

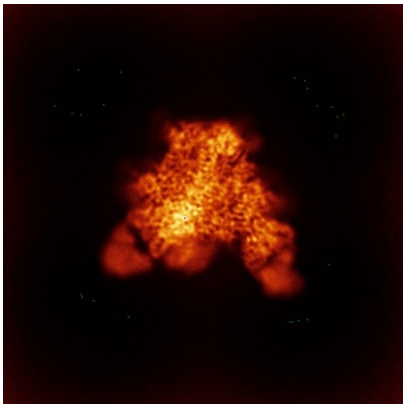


Z

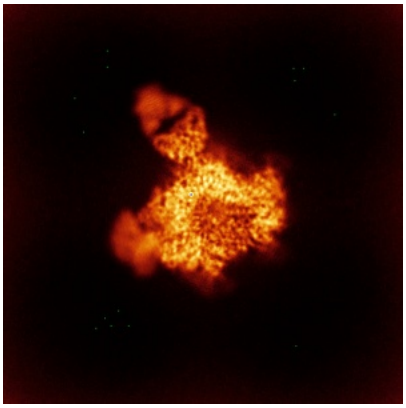
6.4.2 Raw map



X



Y

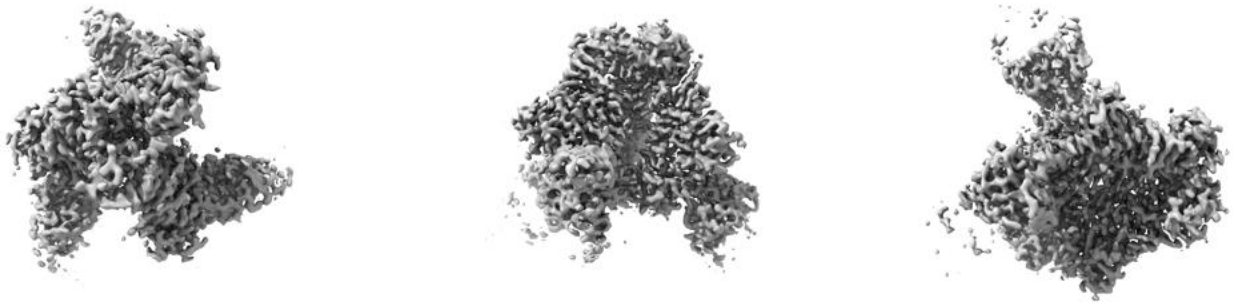


Z

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

6.5 Orthogonal surface views (i)

6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.2. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map

X Y Z

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

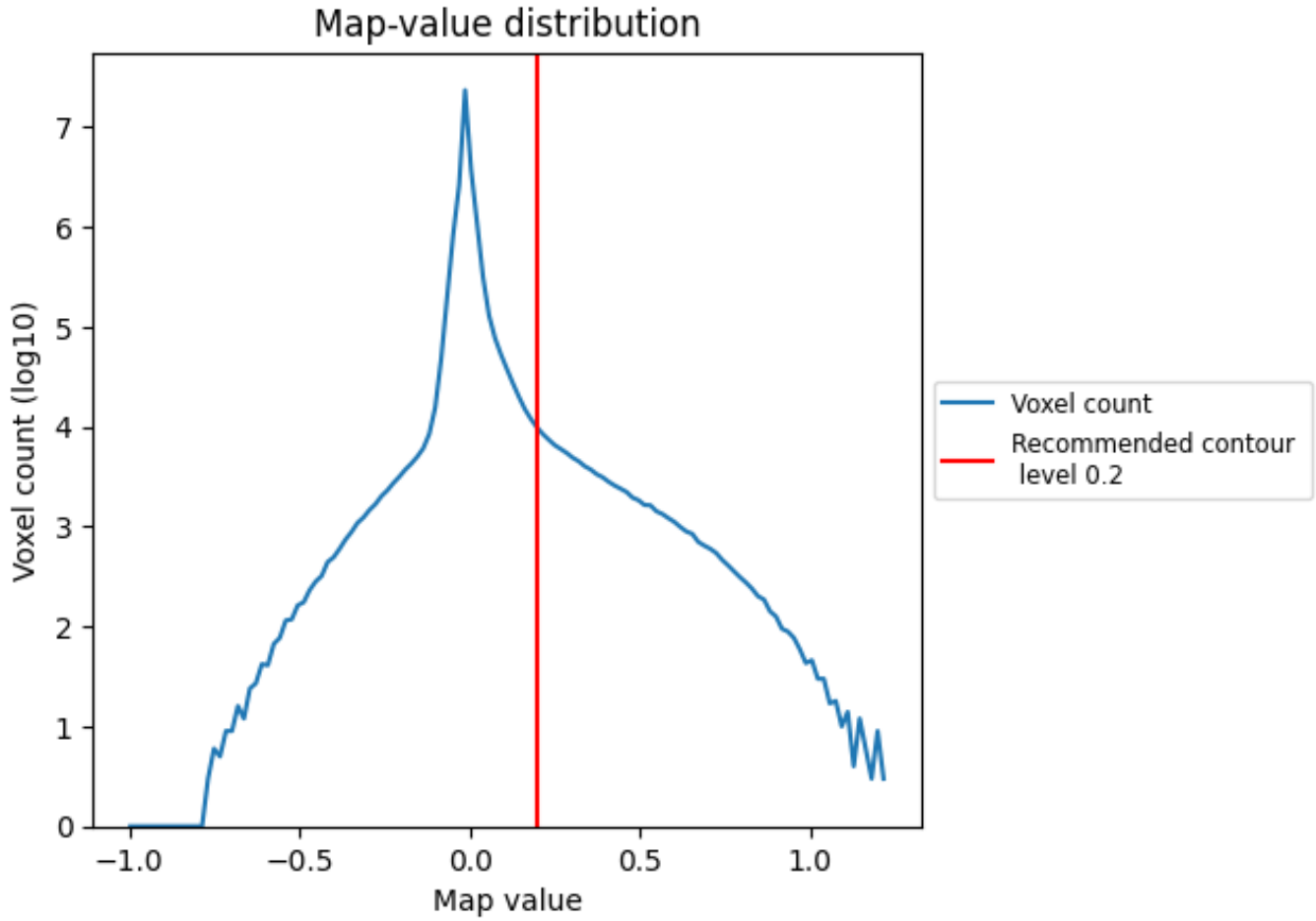
6.6 Mask visualisation (i)

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

7 Map analysis

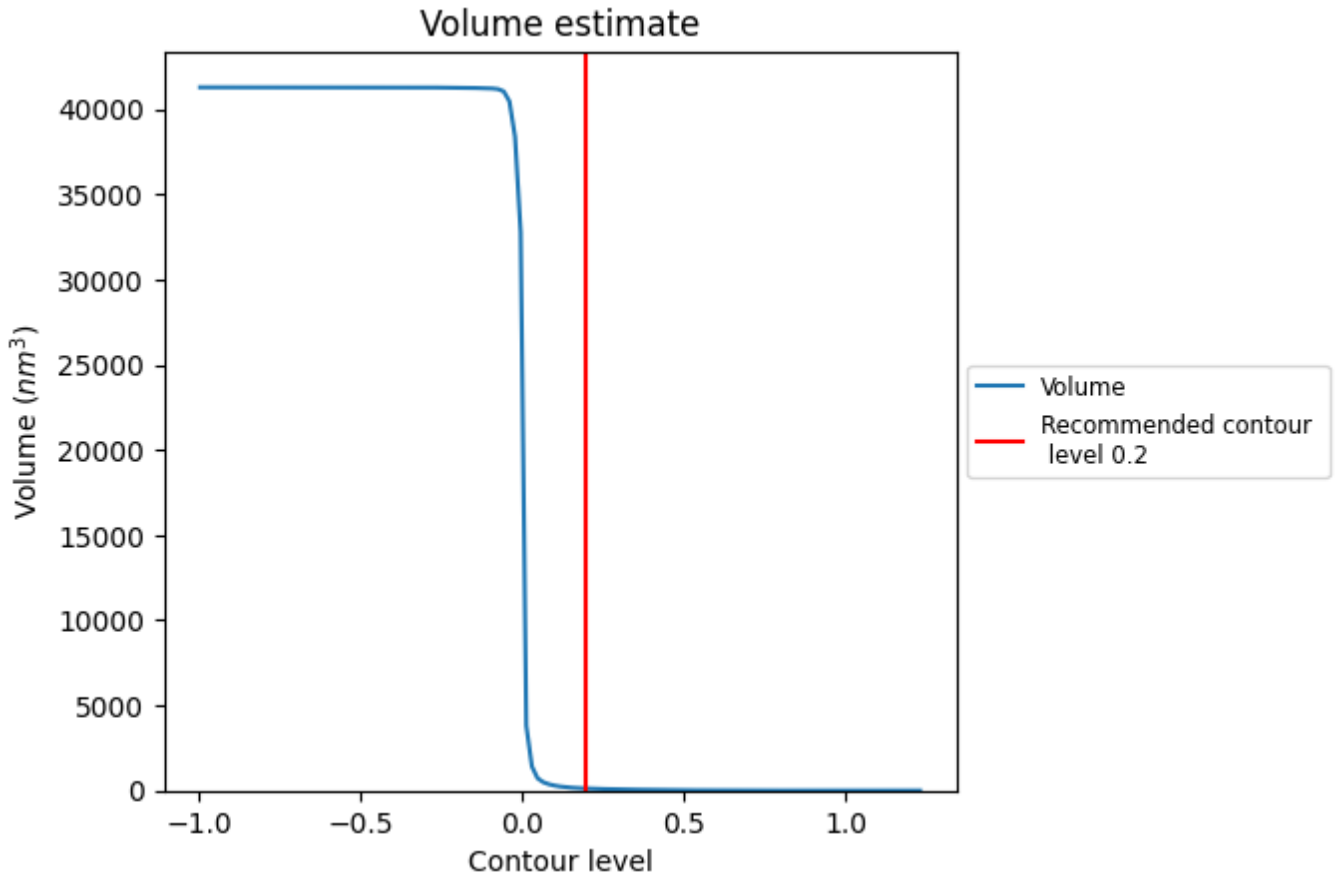
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

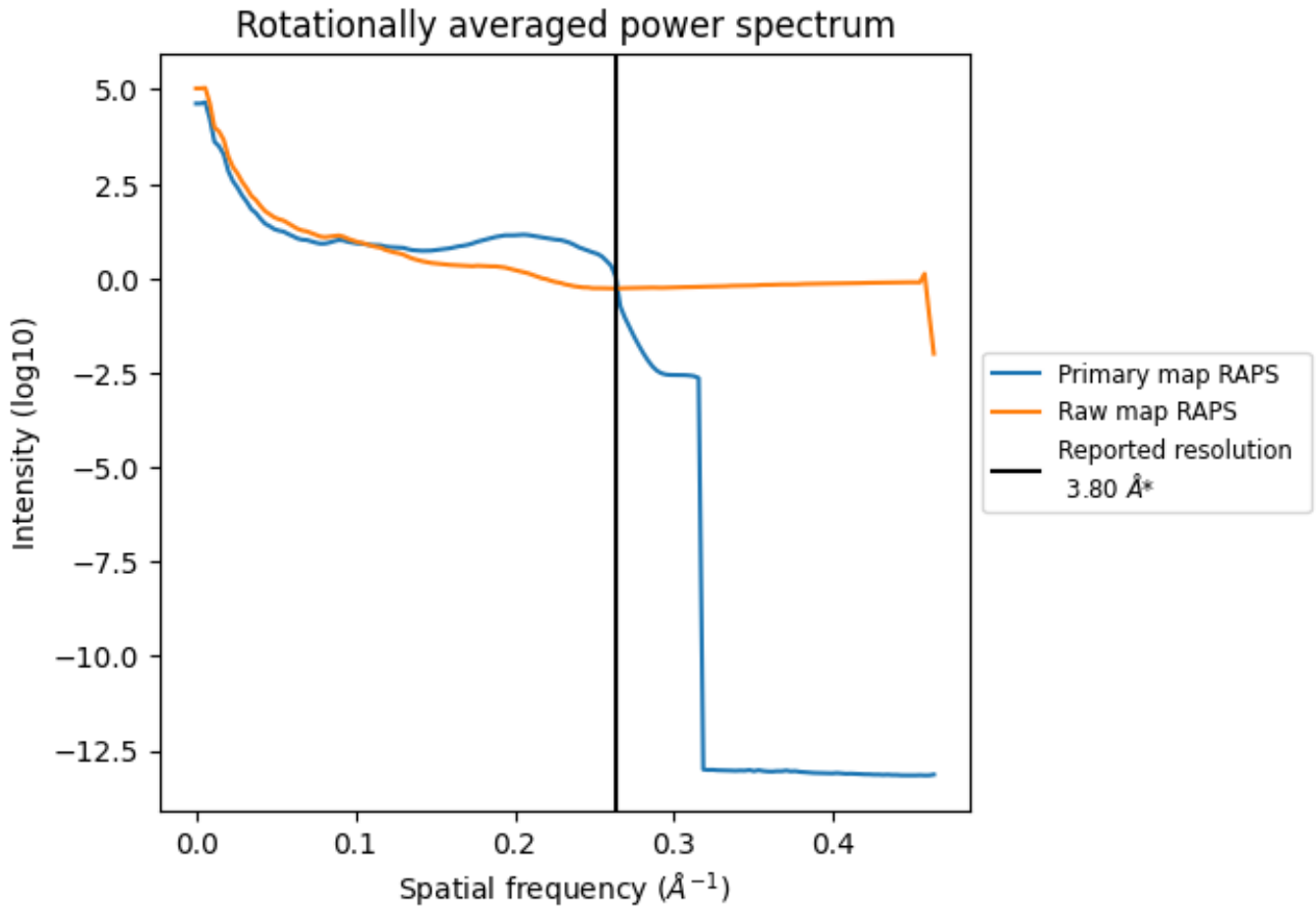
7.2 Volume estimate



The volume at the recommended contour level is 121 nm^3; this corresponds to an approximate mass of 110 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)

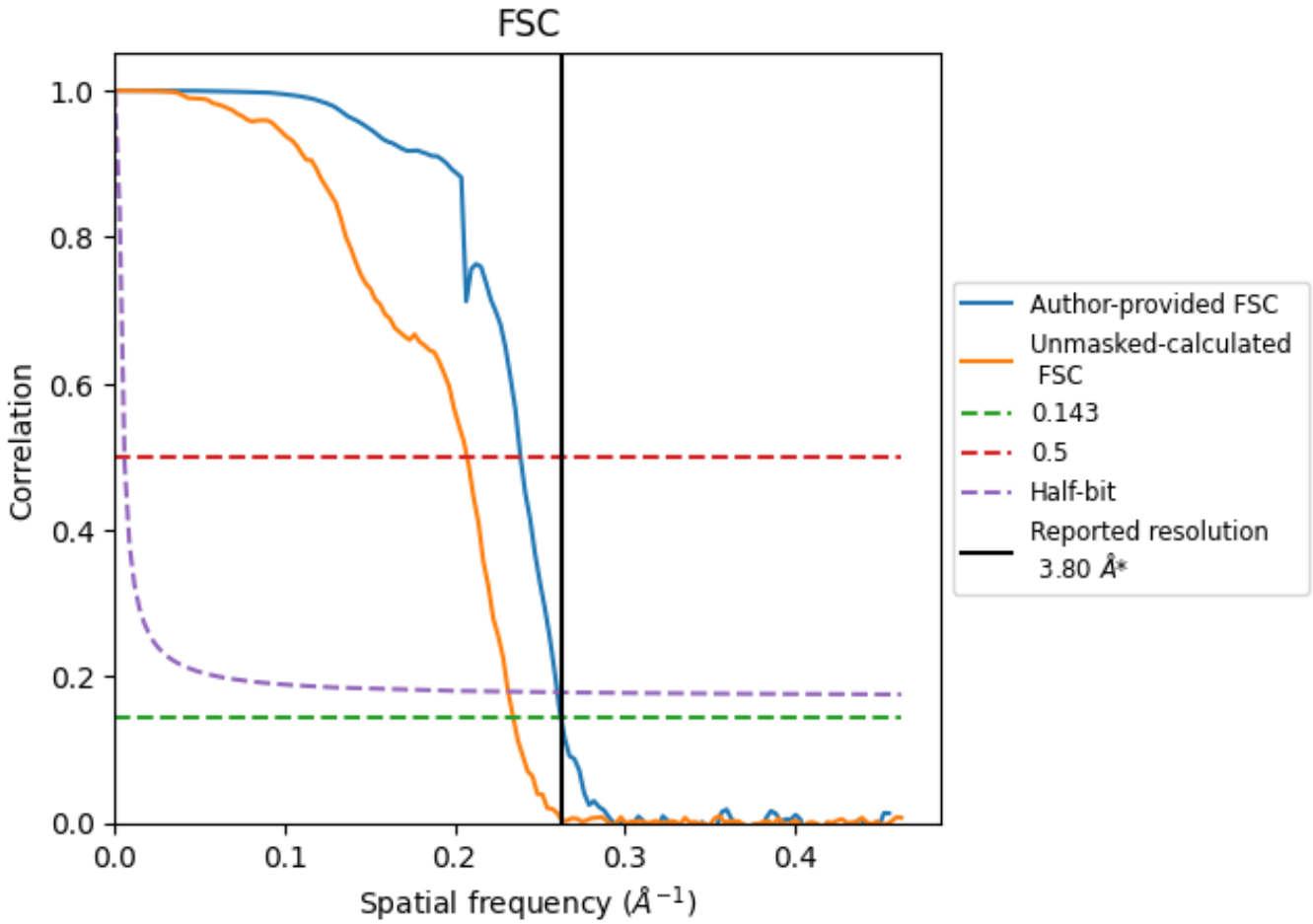


*Reported resolution corresponds to spatial frequency of 0.263 $Å^{-1}$

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 0.263 Å^{-1}

8.2 Resolution estimates (i)

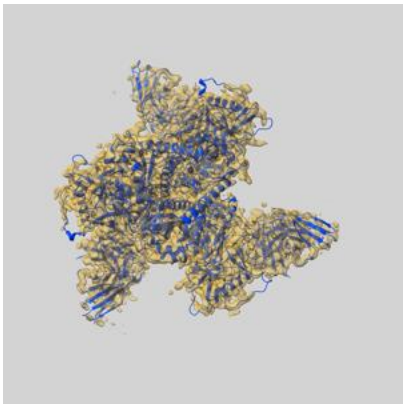
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.80	-	-
Author-provided FSC curve	3.81	4.19	3.84
Unmasked-calculated*	4.26	4.82	4.32

*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 4.26 differs from the reported value 3.8 by more than 10 %

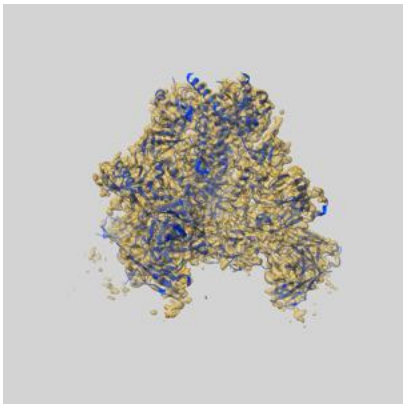
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-43879 and PDB model 9AUG. Per-residue inclusion information can be found in section 3 on page 19.

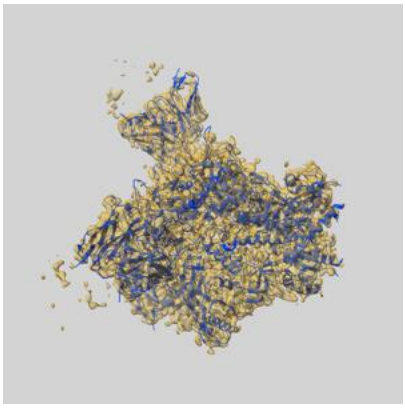
9.1 Map-model overlay



X



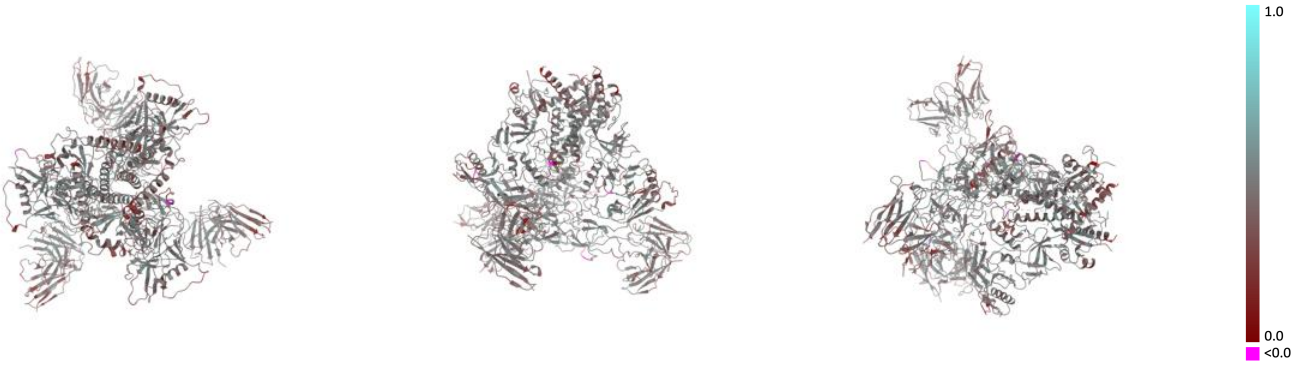
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.2 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.

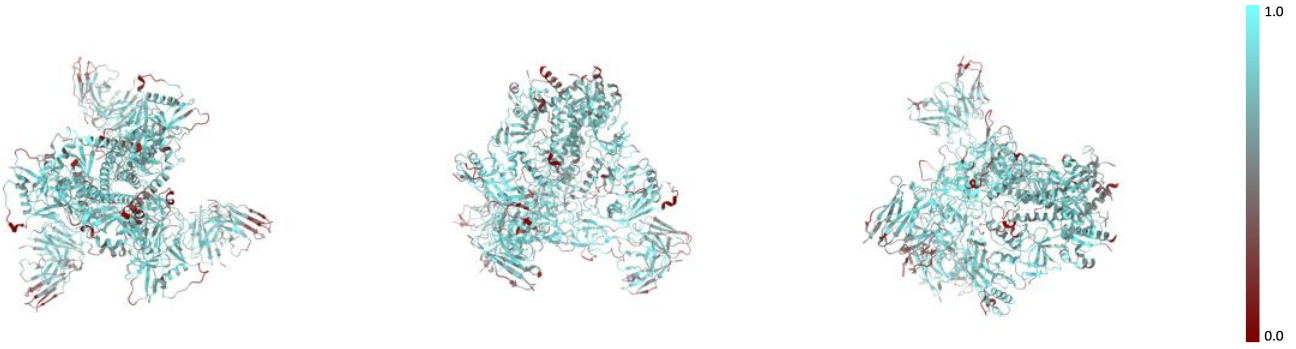
9.2 Q-score mapped to coordinate model (i)



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.

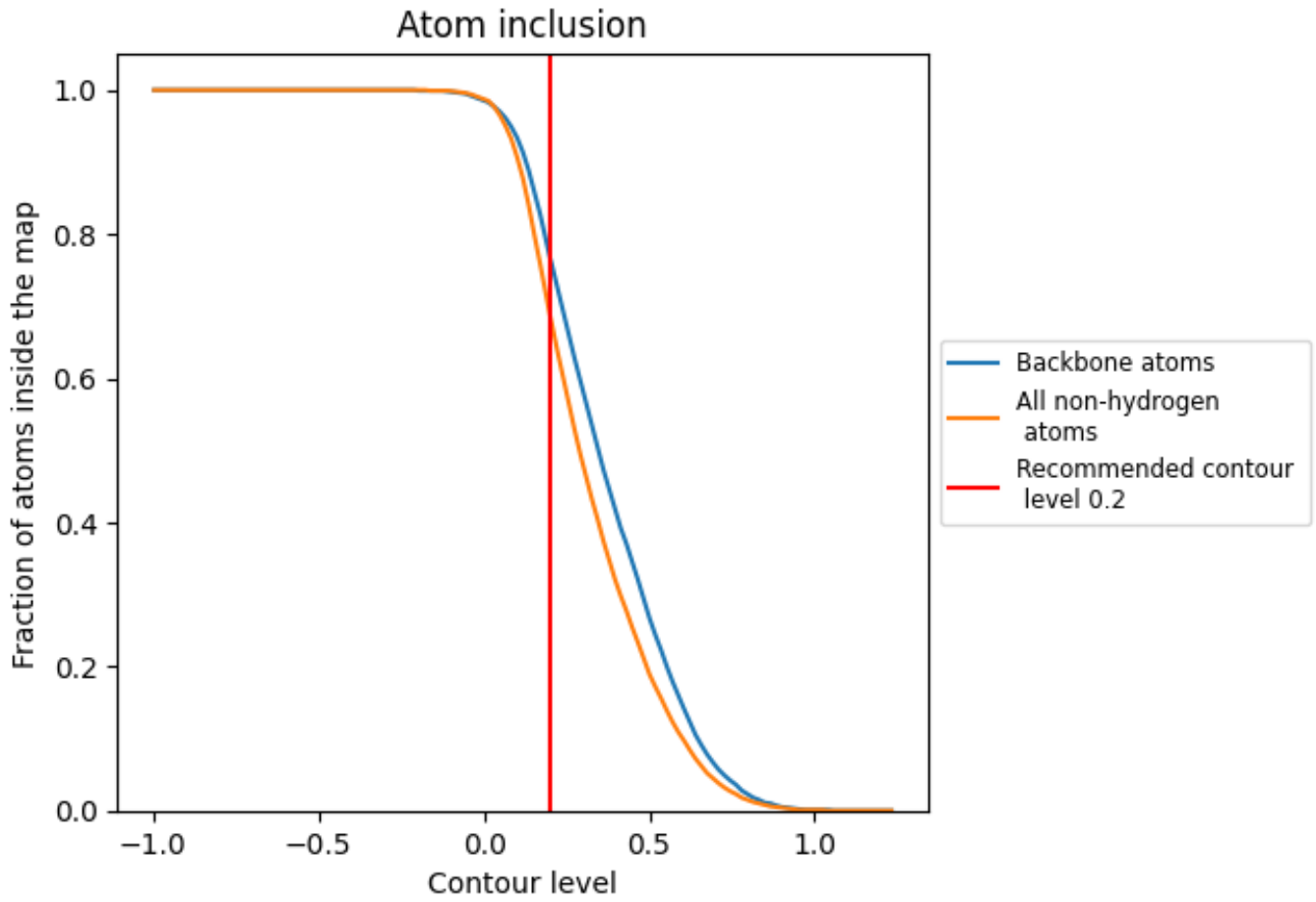
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.2).

9.4 Atom inclusion (i)



At the recommended contour level, 77% of all backbone atoms, 69% 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 (0.2) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6870	0.4360
A	0.7320	0.4580
B	0.6940	0.4400
C	0.7220	0.4520
D	0.7300	0.4360
E	0.6420	0.4090
F	0.6640	0.4050
G	0.7540	0.4530
H	0.6950	0.4280
I	0.7330	0.4430
J	0.5380	0.3880
K	0.5150	0.3820
L	0.5570	0.3960
M	0.7050	0.4490
N	0.6700	0.4420
O	0.6670	0.4850
P	0.7500	0.5080
Q	0.2860	0.3140
R	0.5570	0.4420
S	0.6810	0.4460
T	0.5900	0.4660
U	0.7140	0.4180
V	0.2860	0.2270
W	0.7380	0.4750
X	0.6490	0.4540
Y	0.6150	0.4350
Z	0.7140	0.4720
a	0.3570	0.2650