wwPDB EM Validation Summary Report

Nov 12, 2024 – 03:30 AM JST

PDB ID	:	8XLV
EMDB ID	:	EMD-38460
Title	:	Cryo-EM structure of SARS-CoV-2 Omicron BA.2.86 spike protein(6P), 1-RBD-up state
Authors	:	Li, L.J.; Gu, Y.H.; Shi, K.Y.; Qi, J.X.; Gao, G.F.
Deposited on	:	2023-12-26
Resolution	:	3.07 Å(reported)

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

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

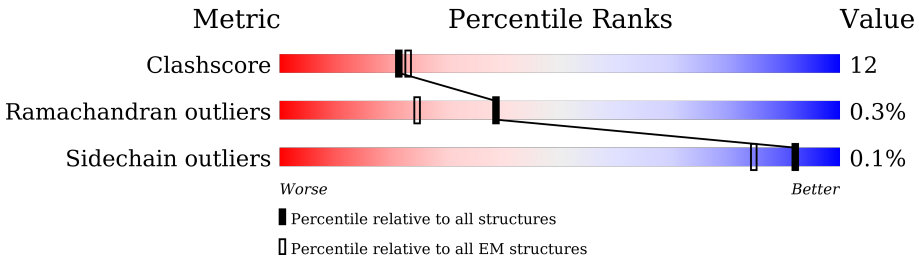
EMDB validation analysis	:	0.0.1.dev113
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

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 3.07 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	1191	7% 63% 22% 15%
1	B	1191	14% 60% 24% 16%
1	C	1191	64% 21% 15%
2	D	2	100%
2	E	2	50% 50% 50%
2	F	2	50% 50%
2	G	2	50% 50% 50%
2	H	2	100% 50% 50%

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Mol	Chain	Length	Quality of chain
2	I	2	

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 24219 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 Spike glycoprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1011	Total	C	N	O	S	0	0
			7924	5076	1313	1499	36		
1	B	1003	Total	C	N	O	S	0	0
			7867	5038	1303	1490	36		
1	C	1011	Total	C	N	O	S	0	0
			7924	5076	1313	1499	36		

There are 417 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	MET	-	initiating methionine	UNP P0DTC2
A	1	PHE	-	expression tag	UNP P0DTC2
A	2	VAL	-	expression tag	UNP P0DTC2
A	3	PHE	-	expression tag	UNP P0DTC2
A	4	LEU	-	expression tag	UNP P0DTC2
A	5	VAL	-	expression tag	UNP P0DTC2
A	6	LEU	-	expression tag	UNP P0DTC2
A	7	LEU	-	expression tag	UNP P0DTC2
A	8	PRO	-	expression tag	UNP P0DTC2
A	9	LEU	-	expression tag	UNP P0DTC2
A	10	VAL	-	expression tag	UNP P0DTC2
A	11	SER	-	expression tag	UNP P0DTC2
A	12	SER	-	expression tag	UNP P0DTC2
A	13	GLN	-	expression tag	UNP P0DTC2
A	14	CYS	-	expression tag	UNP P0DTC2
A	15	VAL	-	expression tag	UNP P0DTC2
A	16	MET	-	expression tag	UNP P0DTC2
A	17	PRO	-	expression tag	UNP P0DTC2
A	18	LEU	-	expression tag	UNP P0DTC2
A	19	PHE	-	expression tag	UNP P0DTC2
A	20	ASN	-	expression tag	UNP P0DTC2
A	21	LEU	-	expression tag	UNP P0DTC2
A	22	ILE	-	expression tag	UNP P0DTC2
A	23	THR	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	24	THR	-	expression tag	UNP P0DTC2
A	25	THR	-	expression tag	UNP P0DTC2
A	26	GLN	-	expression tag	UNP P0DTC2
A	27	SER	-	expression tag	UNP P0DTC2
A	50	LEU	SER	variant	UNP P0DTC2
A	?	-	HIS	deletion	UNP P0DTC2
A	?	-	VAL	deletion	UNP P0DTC2
A	127	PHE	VAL	variant	UNP P0DTC2
A	143	ASP	GLY	variant	UNP P0DTC2
A	?	-	TYR	deletion	UNP P0DTC2
A	157	SER	PHE	variant	UNP P0DTC2
A	158	GLY	ARG	variant	UNP P0DTC2
A	?	-	ASN	deletion	UNP P0DTC2
A	212	ILE	LEU	variant	UNP P0DTC2
A	213	GLY	VAL	variant	UNP P0DTC2
A	216	PHE	LEU	variant	UNP P0DTC2
A	245	ASN	HIS	variant	UNP P0DTC2
A	264	ASP	ALA	variant	UNP P0DTC2
A	332	VAL	ILE	variant	UNP P0DTC2
A	339	HIS	GLY	variant	UNP P0DTC2
A	356	THR	LYS	variant	UNP P0DTC2
A	371	PHE	SER	variant	UNP P0DTC2
A	373	PRO	SER	variant	UNP P0DTC2
A	375	PHE	SER	variant	UNP P0DTC2
A	376	ALA	THR	variant	UNP P0DTC2
A	403	LYS	ARG	variant	UNP P0DTC2
A	405	ASN	ASP	variant	UNP P0DTC2
A	408	SER	ARG	variant	UNP P0DTC2
A	417	ASN	LYS	variant	UNP P0DTC2
A	440	LYS	ASN	variant	UNP P0DTC2
A	445	HIS	VAL	variant	UNP P0DTC2
A	446	SER	GLY	variant	UNP P0DTC2
A	450	ASP	ASN	variant	UNP P0DTC2
A	452	TRP	LEU	variant	UNP P0DTC2
A	460	LYS	ASN	variant	UNP P0DTC2
A	477	ASN	SER	variant	UNP P0DTC2
A	478	LYS	THR	variant	UNP P0DTC2
A	481	LYS	ASN	variant	UNP P0DTC2
A	?	-	VAL	deletion	UNP P0DTC2
A	483	LYS	GLU	variant	UNP P0DTC2
A	485	PRO	PHE	variant	UNP P0DTC2
A	497	ARG	GLN	variant	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	500	TYR	ASN	variant	UNP P0DTC2
A	504	HIS	TYR	variant	UNP P0DTC2
A	553	LYS	GLU	variant	UNP P0DTC2
A	569	VAL	ALA	variant	UNP P0DTC2
A	613	GLY	ASP	variant	UNP P0DTC2
A	620	SER	PRO	variant	UNP P0DTC2
A	654	TYR	HIS	variant	UNP P0DTC2
A	669	VAL	ILE	variant	UNP P0DTC2
A	678	LYS	ASN	variant	UNP P0DTC2
A	680	ARG	PRO	variant	UNP P0DTC2
A	681	GLY	ARG	engineered mutation	UNP P0DTC2
A	682	SER	ARG	engineered mutation	UNP P0DTC2
A	684	SER	ARG	engineered mutation	UNP P0DTC2
A	763	LYS	ASN	variant	UNP P0DTC2
A	795	TYR	ASP	variant	UNP P0DTC2
A	816	PRO	PHE	engineered mutation	UNP P0DTC2
A	891	PRO	ALA	engineered mutation	UNP P0DTC2
A	898	PRO	ALA	engineered mutation	UNP P0DTC2
A	938	PHE	SER	variant	UNP P0DTC2
A	941	PRO	ALA	engineered mutation	UNP P0DTC2
A	953	HIS	GLN	variant	UNP P0DTC2
A	968	LYS	ASN	variant	UNP P0DTC2
A	985	PRO	LYS	engineered mutation	UNP P0DTC2
A	986	PRO	VAL	engineered mutation	UNP P0DTC2
A	1142	LEU	PRO	variant	UNP P0DTC2
A	1147	GLY	-	expression tag	UNP P0DTC2
A	1148	GLY	-	expression tag	UNP P0DTC2
A	1149	GLY	-	expression tag	UNP P0DTC2
A	1150	SER	-	expression tag	UNP P0DTC2
A	1151	GLY	-	expression tag	UNP P0DTC2
A	1152	GLY	-	expression tag	UNP P0DTC2
A	1153	GLY	-	expression tag	UNP P0DTC2
A	1154	SER	-	expression tag	UNP P0DTC2
A	1155	GLY	-	expression tag	UNP P0DTC2
A	1156	TYR	-	expression tag	UNP P0DTC2
A	1157	ILE	-	expression tag	UNP P0DTC2
A	1158	PRO	-	expression tag	UNP P0DTC2
A	1159	GLU	-	expression tag	UNP P0DTC2
A	1160	ALA	-	expression tag	UNP P0DTC2
A	1161	PRO	-	expression tag	UNP P0DTC2
A	1162	ARG	-	expression tag	UNP P0DTC2
A	1163	ASP	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1164	GLY	-	expression tag	UNP P0DTC2
A	1165	GLN	-	expression tag	UNP P0DTC2
A	1166	ALA	-	expression tag	UNP P0DTC2
A	1167	TYR	-	expression tag	UNP P0DTC2
A	1168	VAL	-	expression tag	UNP P0DTC2
A	1169	ARG	-	expression tag	UNP P0DTC2
A	1170	LYS	-	expression tag	UNP P0DTC2
A	1171	ASP	-	expression tag	UNP P0DTC2
A	1172	GLY	-	expression tag	UNP P0DTC2
A	1173	GLU	-	expression tag	UNP P0DTC2
A	1174	TRP	-	expression tag	UNP P0DTC2
A	1175	VAL	-	expression tag	UNP P0DTC2
A	1176	LEU	-	expression tag	UNP P0DTC2
A	1177	LEU	-	expression tag	UNP P0DTC2
A	1178	SER	-	expression tag	UNP P0DTC2
A	1179	THR	-	expression tag	UNP P0DTC2
A	1180	PHE	-	expression tag	UNP P0DTC2
A	1181	LEU	-	expression tag	UNP P0DTC2
A	1182	GLY	-	expression tag	UNP P0DTC2
A	1183	GLY	-	expression tag	UNP P0DTC2
A	1184	GLY	-	expression tag	UNP P0DTC2
A	1185	SER	-	expression tag	UNP P0DTC2
A	1186	ALA	-	expression tag	UNP P0DTC2
A	1187	TRP	-	expression tag	UNP P0DTC2
A	1188	SER	-	expression tag	UNP P0DTC2
A	1189	HIS	-	expression tag	UNP P0DTC2
A	1190	PRO	-	expression tag	UNP P0DTC2
A	1191	GLN	-	expression tag	UNP P0DTC2
A	1192	PHE	-	expression tag	UNP P0DTC2
A	1193	GLU	-	expression tag	UNP P0DTC2
A	1194	LYS	-	expression tag	UNP P0DTC2
B	0	MET	-	initiating methionine	UNP P0DTC2
B	1	PHE	-	expression tag	UNP P0DTC2
B	2	VAL	-	expression tag	UNP P0DTC2
B	3	PHE	-	expression tag	UNP P0DTC2
B	4	LEU	-	expression tag	UNP P0DTC2
B	5	VAL	-	expression tag	UNP P0DTC2
B	6	LEU	-	expression tag	UNP P0DTC2
B	7	LEU	-	expression tag	UNP P0DTC2
B	8	PRO	-	expression tag	UNP P0DTC2
B	9	LEU	-	expression tag	UNP P0DTC2
B	10	VAL	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	11	SER	-	expression tag	UNP P0DTC2
B	12	SER	-	expression tag	UNP P0DTC2
B	13	GLN	-	expression tag	UNP P0DTC2
B	14	CYS	-	expression tag	UNP P0DTC2
B	15	VAL	-	expression tag	UNP P0DTC2
B	16	MET	-	expression tag	UNP P0DTC2
B	17	PRO	-	expression tag	UNP P0DTC2
B	18	LEU	-	expression tag	UNP P0DTC2
B	19	PHE	-	expression tag	UNP P0DTC2
B	20	ASN	-	expression tag	UNP P0DTC2
B	21	LEU	-	expression tag	UNP P0DTC2
B	22	ILE	-	expression tag	UNP P0DTC2
B	23	THR	-	expression tag	UNP P0DTC2
B	24	THR	-	expression tag	UNP P0DTC2
B	25	THR	-	expression tag	UNP P0DTC2
B	26	GLN	-	expression tag	UNP P0DTC2
B	27	SER	-	expression tag	UNP P0DTC2
B	50	LEU	SER	variant	UNP P0DTC2
B	?	-	HIS	deletion	UNP P0DTC2
B	?	-	VAL	deletion	UNP P0DTC2
B	127	PHE	VAL	variant	UNP P0DTC2
B	143	ASP	GLY	variant	UNP P0DTC2
B	?	-	TYR	deletion	UNP P0DTC2
B	157	SER	PHE	variant	UNP P0DTC2
B	158	GLY	ARG	variant	UNP P0DTC2
B	?	-	ASN	deletion	UNP P0DTC2
B	212	ILE	LEU	variant	UNP P0DTC2
B	213	GLY	VAL	variant	UNP P0DTC2
B	216	PHE	LEU	variant	UNP P0DTC2
B	245	ASN	HIS	variant	UNP P0DTC2
B	264	ASP	ALA	variant	UNP P0DTC2
B	332	VAL	ILE	variant	UNP P0DTC2
B	339	HIS	GLY	variant	UNP P0DTC2
B	356	THR	LYS	variant	UNP P0DTC2
B	371	PHE	SER	variant	UNP P0DTC2
B	373	PRO	SER	variant	UNP P0DTC2
B	375	PHE	SER	variant	UNP P0DTC2
B	376	ALA	THR	variant	UNP P0DTC2
B	403	LYS	ARG	variant	UNP P0DTC2
B	405	ASN	ASP	variant	UNP P0DTC2
B	408	SER	ARG	variant	UNP P0DTC2
B	417	ASN	LYS	variant	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	440	LYS	ASN	variant	UNP P0DTC2
B	445	HIS	VAL	variant	UNP P0DTC2
B	446	SER	GLY	variant	UNP P0DTC2
B	450	ASP	ASN	variant	UNP P0DTC2
B	452	TRP	LEU	variant	UNP P0DTC2
B	460	LYS	ASN	variant	UNP P0DTC2
B	477	ASN	SER	variant	UNP P0DTC2
B	478	LYS	THR	variant	UNP P0DTC2
B	481	LYS	ASN	variant	UNP P0DTC2
B	?	-	VAL	deletion	UNP P0DTC2
B	483	LYS	GLU	variant	UNP P0DTC2
B	485	PRO	PHE	variant	UNP P0DTC2
B	497	ARG	GLN	variant	UNP P0DTC2
B	500	TYR	ASN	variant	UNP P0DTC2
B	504	HIS	TYR	variant	UNP P0DTC2
B	553	LYS	GLU	variant	UNP P0DTC2
B	569	VAL	ALA	variant	UNP P0DTC2
B	613	GLY	ASP	variant	UNP P0DTC2
B	620	SER	PRO	variant	UNP P0DTC2
B	654	TYR	HIS	variant	UNP P0DTC2
B	669	VAL	ILE	variant	UNP P0DTC2
B	678	LYS	ASN	variant	UNP P0DTC2
B	680	ARG	PRO	variant	UNP P0DTC2
B	681	GLY	ARG	engineered mutation	UNP P0DTC2
B	682	SER	ARG	engineered mutation	UNP P0DTC2
B	684	SER	ARG	engineered mutation	UNP P0DTC2
B	763	LYS	ASN	variant	UNP P0DTC2
B	795	TYR	ASP	variant	UNP P0DTC2
B	816	PRO	PHE	engineered mutation	UNP P0DTC2
B	891	PRO	ALA	engineered mutation	UNP P0DTC2
B	898	PRO	ALA	engineered mutation	UNP P0DTC2
B	938	PHE	SER	variant	UNP P0DTC2
B	941	PRO	ALA	engineered mutation	UNP P0DTC2
B	953	HIS	GLN	variant	UNP P0DTC2
B	968	LYS	ASN	variant	UNP P0DTC2
B	985	PRO	LYS	engineered mutation	UNP P0DTC2
B	986	PRO	VAL	engineered mutation	UNP P0DTC2
B	1142	LEU	PRO	variant	UNP P0DTC2
B	1147	GLY	-	expression tag	UNP P0DTC2
B	1148	GLY	-	expression tag	UNP P0DTC2
B	1149	GLY	-	expression tag	UNP P0DTC2
B	1150	SER	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1151	GLY	-	expression tag	UNP P0DTC2
B	1152	GLY	-	expression tag	UNP P0DTC2
B	1153	GLY	-	expression tag	UNP P0DTC2
B	1154	SER	-	expression tag	UNP P0DTC2
B	1155	GLY	-	expression tag	UNP P0DTC2
B	1156	TYR	-	expression tag	UNP P0DTC2
B	1157	ILE	-	expression tag	UNP P0DTC2
B	1158	PRO	-	expression tag	UNP P0DTC2
B	1159	GLU	-	expression tag	UNP P0DTC2
B	1160	ALA	-	expression tag	UNP P0DTC2
B	1161	PRO	-	expression tag	UNP P0DTC2
B	1162	ARG	-	expression tag	UNP P0DTC2
B	1163	ASP	-	expression tag	UNP P0DTC2
B	1164	GLY	-	expression tag	UNP P0DTC2
B	1165	GLN	-	expression tag	UNP P0DTC2
B	1166	ALA	-	expression tag	UNP P0DTC2
B	1167	TYR	-	expression tag	UNP P0DTC2
B	1168	VAL	-	expression tag	UNP P0DTC2
B	1169	ARG	-	expression tag	UNP P0DTC2
B	1170	LYS	-	expression tag	UNP P0DTC2
B	1171	ASP	-	expression tag	UNP P0DTC2
B	1172	GLY	-	expression tag	UNP P0DTC2
B	1173	GLU	-	expression tag	UNP P0DTC2
B	1174	TRP	-	expression tag	UNP P0DTC2
B	1175	VAL	-	expression tag	UNP P0DTC2
B	1176	LEU	-	expression tag	UNP P0DTC2
B	1177	LEU	-	expression tag	UNP P0DTC2
B	1178	SER	-	expression tag	UNP P0DTC2
B	1179	THR	-	expression tag	UNP P0DTC2
B	1180	PHE	-	expression tag	UNP P0DTC2
B	1181	LEU	-	expression tag	UNP P0DTC2
B	1182	GLY	-	expression tag	UNP P0DTC2
B	1183	GLY	-	expression tag	UNP P0DTC2
B	1184	GLY	-	expression tag	UNP P0DTC2
B	1185	SER	-	expression tag	UNP P0DTC2
B	1186	ALA	-	expression tag	UNP P0DTC2
B	1187	TRP	-	expression tag	UNP P0DTC2
B	1188	SER	-	expression tag	UNP P0DTC2
B	1189	HIS	-	expression tag	UNP P0DTC2
B	1190	PRO	-	expression tag	UNP P0DTC2
B	1191	GLN	-	expression tag	UNP P0DTC2
B	1192	PHE	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1193	GLU	-	expression tag	UNP P0DTC2
B	1194	LYS	-	expression tag	UNP P0DTC2
C	0	MET	-	initiating methionine	UNP P0DTC2
C	1	PHE	-	expression tag	UNP P0DTC2
C	2	VAL	-	expression tag	UNP P0DTC2
C	3	PHE	-	expression tag	UNP P0DTC2
C	4	LEU	-	expression tag	UNP P0DTC2
C	5	VAL	-	expression tag	UNP P0DTC2
C	6	LEU	-	expression tag	UNP P0DTC2
C	7	LEU	-	expression tag	UNP P0DTC2
C	8	PRO	-	expression tag	UNP P0DTC2
C	9	LEU	-	expression tag	UNP P0DTC2
C	10	VAL	-	expression tag	UNP P0DTC2
C	11	SER	-	expression tag	UNP P0DTC2
C	12	SER	-	expression tag	UNP P0DTC2
C	13	GLN	-	expression tag	UNP P0DTC2
C	14	CYS	-	expression tag	UNP P0DTC2
C	15	VAL	-	expression tag	UNP P0DTC2
C	16	MET	-	expression tag	UNP P0DTC2
C	17	PRO	-	expression tag	UNP P0DTC2
C	18	LEU	-	expression tag	UNP P0DTC2
C	19	PHE	-	expression tag	UNP P0DTC2
C	20	ASN	-	expression tag	UNP P0DTC2
C	21	LEU	-	expression tag	UNP P0DTC2
C	22	ILE	-	expression tag	UNP P0DTC2
C	23	THR	-	expression tag	UNP P0DTC2
C	24	THR	-	expression tag	UNP P0DTC2
C	25	THR	-	expression tag	UNP P0DTC2
C	26	GLN	-	expression tag	UNP P0DTC2
C	27	SER	-	expression tag	UNP P0DTC2
C	50	LEU	SER	variant	UNP P0DTC2
C	?	-	HIS	deletion	UNP P0DTC2
C	?	-	VAL	deletion	UNP P0DTC2
C	127	PHE	VAL	variant	UNP P0DTC2
C	143	ASP	GLY	variant	UNP P0DTC2
C	?	-	TYR	deletion	UNP P0DTC2
C	157	SER	PHE	variant	UNP P0DTC2
C	158	GLY	ARG	variant	UNP P0DTC2
C	?	-	ASN	deletion	UNP P0DTC2
C	212	ILE	LEU	variant	UNP P0DTC2
C	213	GLY	VAL	variant	UNP P0DTC2
C	216	PHE	LEU	variant	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	245	ASN	HIS	variant	UNP P0DTC2
C	264	ASP	ALA	variant	UNP P0DTC2
C	332	VAL	ILE	variant	UNP P0DTC2
C	339	HIS	GLY	variant	UNP P0DTC2
C	356	THR	LYS	variant	UNP P0DTC2
C	371	PHE	SER	variant	UNP P0DTC2
C	373	PRO	SER	variant	UNP P0DTC2
C	375	PHE	SER	variant	UNP P0DTC2
C	376	ALA	THR	variant	UNP P0DTC2
C	403	LYS	ARG	variant	UNP P0DTC2
C	405	ASN	ASP	variant	UNP P0DTC2
C	408	SER	ARG	variant	UNP P0DTC2
C	417	ASN	LYS	variant	UNP P0DTC2
C	440	LYS	ASN	variant	UNP P0DTC2
C	445	HIS	VAL	variant	UNP P0DTC2
C	446	SER	GLY	variant	UNP P0DTC2
C	450	ASP	ASN	variant	UNP P0DTC2
C	452	TRP	LEU	variant	UNP P0DTC2
C	460	LYS	ASN	variant	UNP P0DTC2
C	477	ASN	SER	variant	UNP P0DTC2
C	478	LYS	THR	variant	UNP P0DTC2
C	481	LYS	ASN	variant	UNP P0DTC2
C	?	-	VAL	deletion	UNP P0DTC2
C	483	LYS	GLU	variant	UNP P0DTC2
C	485	PRO	PHE	variant	UNP P0DTC2
C	497	ARG	GLN	variant	UNP P0DTC2
C	500	TYR	ASN	variant	UNP P0DTC2
C	504	HIS	TYR	variant	UNP P0DTC2
C	553	LYS	GLU	variant	UNP P0DTC2
C	569	VAL	ALA	variant	UNP P0DTC2
C	613	GLY	ASP	variant	UNP P0DTC2
C	620	SER	PRO	variant	UNP P0DTC2
C	654	TYR	HIS	variant	UNP P0DTC2
C	669	VAL	ILE	variant	UNP P0DTC2
C	678	LYS	ASN	variant	UNP P0DTC2
C	680	ARG	PRO	variant	UNP P0DTC2
C	681	GLY	ARG	engineered mutation	UNP P0DTC2
C	682	SER	ARG	engineered mutation	UNP P0DTC2
C	684	SER	ARG	engineered mutation	UNP P0DTC2
C	763	LYS	ASN	variant	UNP P0DTC2
C	795	TYR	ASP	variant	UNP P0DTC2
C	816	PRO	PHE	engineered mutation	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	891	PRO	ALA	engineered mutation	UNP P0DTC2
C	898	PRO	ALA	engineered mutation	UNP P0DTC2
C	938	PHE	SER	variant	UNP P0DTC2
C	941	PRO	ALA	engineered mutation	UNP P0DTC2
C	953	HIS	GLN	variant	UNP P0DTC2
C	968	LYS	ASN	variant	UNP P0DTC2
C	985	PRO	LYS	engineered mutation	UNP P0DTC2
C	986	PRO	VAL	engineered mutation	UNP P0DTC2
C	1142	LEU	PRO	variant	UNP P0DTC2
C	1147	GLY	-	expression tag	UNP P0DTC2
C	1148	GLY	-	expression tag	UNP P0DTC2
C	1149	GLY	-	expression tag	UNP P0DTC2
C	1150	SER	-	expression tag	UNP P0DTC2
C	1151	GLY	-	expression tag	UNP P0DTC2
C	1152	GLY	-	expression tag	UNP P0DTC2
C	1153	GLY	-	expression tag	UNP P0DTC2
C	1154	SER	-	expression tag	UNP P0DTC2
C	1155	GLY	-	expression tag	UNP P0DTC2
C	1156	TYR	-	expression tag	UNP P0DTC2
C	1157	ILE	-	expression tag	UNP P0DTC2
C	1158	PRO	-	expression tag	UNP P0DTC2
C	1159	GLU	-	expression tag	UNP P0DTC2
C	1160	ALA	-	expression tag	UNP P0DTC2
C	1161	PRO	-	expression tag	UNP P0DTC2
C	1162	ARG	-	expression tag	UNP P0DTC2
C	1163	ASP	-	expression tag	UNP P0DTC2
C	1164	GLY	-	expression tag	UNP P0DTC2
C	1165	GLN	-	expression tag	UNP P0DTC2
C	1166	ALA	-	expression tag	UNP P0DTC2
C	1167	TYR	-	expression tag	UNP P0DTC2
C	1168	VAL	-	expression tag	UNP P0DTC2
C	1169	ARG	-	expression tag	UNP P0DTC2
C	1170	LYS	-	expression tag	UNP P0DTC2
C	1171	ASP	-	expression tag	UNP P0DTC2
C	1172	GLY	-	expression tag	UNP P0DTC2
C	1173	GLU	-	expression tag	UNP P0DTC2
C	1174	TRP	-	expression tag	UNP P0DTC2
C	1175	VAL	-	expression tag	UNP P0DTC2
C	1176	LEU	-	expression tag	UNP P0DTC2
C	1177	LEU	-	expression tag	UNP P0DTC2
C	1178	SER	-	expression tag	UNP P0DTC2
C	1179	THR	-	expression tag	UNP P0DTC2

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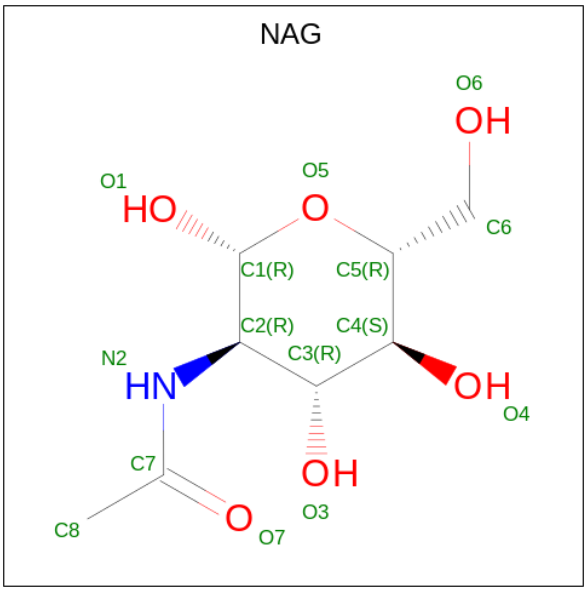
Chain	Residue	Modelled	Actual	Comment	Reference
C	1180	PHE	-	expression tag	UNP P0DTC2
C	1181	LEU	-	expression tag	UNP P0DTC2
C	1182	GLY	-	expression tag	UNP P0DTC2
C	1183	GLY	-	expression tag	UNP P0DTC2
C	1184	GLY	-	expression tag	UNP P0DTC2
C	1185	SER	-	expression tag	UNP P0DTC2
C	1186	ALA	-	expression tag	UNP P0DTC2
C	1187	TRP	-	expression tag	UNP P0DTC2
C	1188	SER	-	expression tag	UNP P0DTC2
C	1189	HIS	-	expression tag	UNP P0DTC2
C	1190	PRO	-	expression tag	UNP P0DTC2
C	1191	GLN	-	expression tag	UNP P0DTC2
C	1192	PHE	-	expression tag	UNP P0DTC2
C	1193	GLU	-	expression tag	UNP P0DTC2
C	1194	LYS	-	expression tag	UNP P0DTC2

- Molecule 2 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
2	D	2	Total	C	N	O	0	0
			28	16	2	10		
2	E	2	Total	C	N	O	0	0
			28	16	2	10		
2	F	2	Total	C	N	O	0	0
			28	16	2	10		
2	G	2	Total	C	N	O	0	0
			28	16	2	10		
2	H	2	Total	C	N	O	0	0
			28	16	2	10		
2	I	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 3 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
3	A	1	Total	C	N	O	0
			14	8	1	5	
3	A	1	Total	C	N	O	0
			14	8	1	5	
3	A	1	Total	C	N	O	0
			14	8	1	5	
3	A	1	Total	C	N	O	0
			14	8	1	5	
3	A	1	Total	C	N	O	0
			14	8	1	5	
3	A	1	Total	C	N	O	0
			14	8	1	5	
3	A	1	Total	C	N	O	0
			14	8	1	5	
3	A	1	Total	C	N	O	0
			14	8	1	5	
3	A	1	Total	C	N	O	0
			14	8	1	5	
3	B	1	Total	C	N	O	0
			14	8	1	5	
3	B	1	Total	C	N	O	0
			14	8	1	5	
3	B	1	Total	C	N	O	0
			14	8	1	5	
3	B	1	Total	C	N	O	0
			14	8	1	5	
3	B	1	Total	C	N	O	0
			14	8	1	5	

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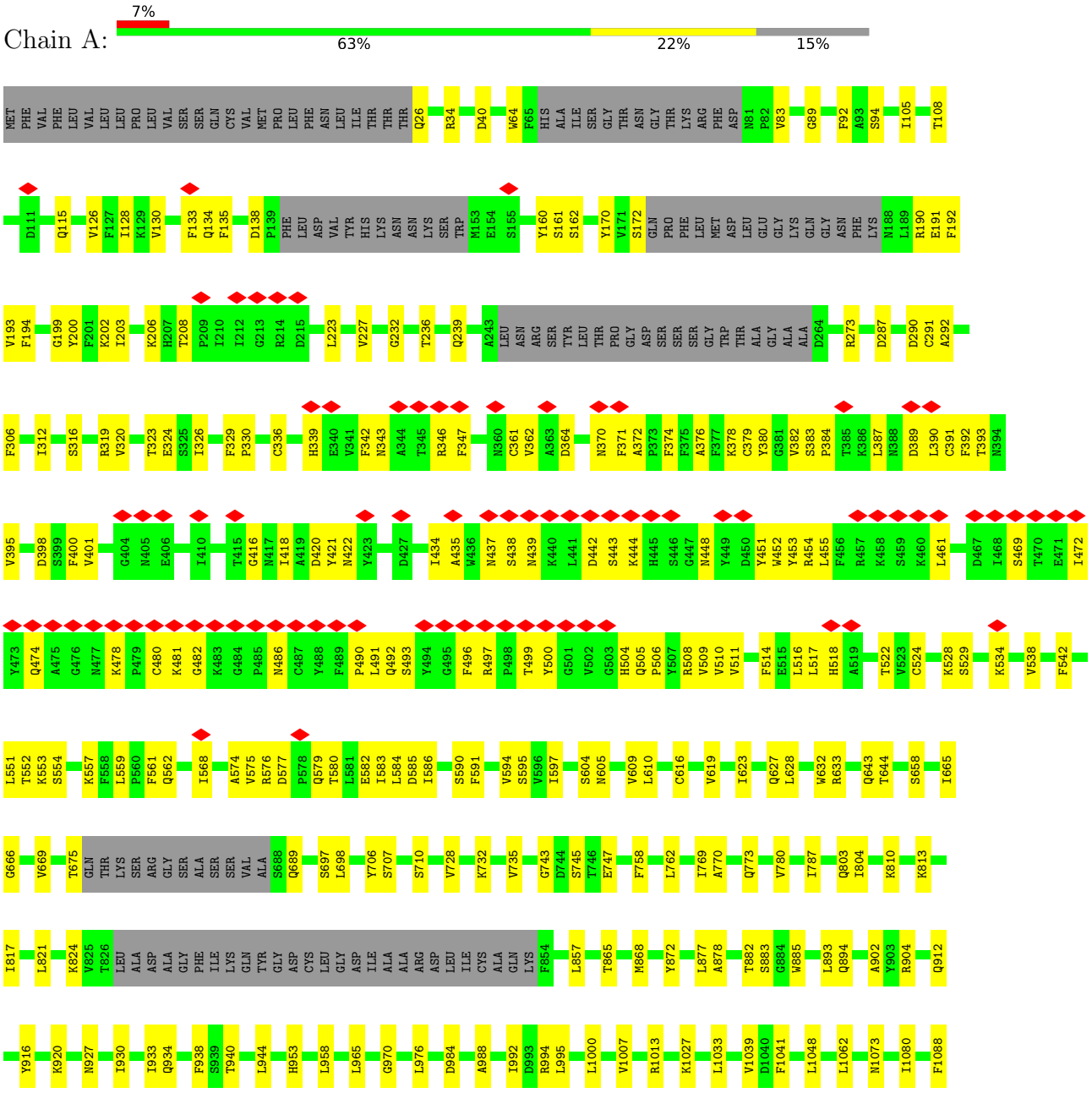
Mol	Chain	Residues	Atoms				AltConf
3	B	1	Total	C	N	O	0
			14	8	1	5	
3	B	1	Total	C	N	O	0
			14	8	1	5	
3	B	1	Total	C	N	O	0
			14	8	1	5	
3	B	1	Total	C	N	O	0
			14	8	1	5	
3	C	1	Total	C	N	O	0
			14	8	1	5	
3	C	1	Total	C	N	O	0
			14	8	1	5	
3	C	1	Total	C	N	O	0
			14	8	1	5	
3	C	1	Total	C	N	O	0
			14	8	1	5	
3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

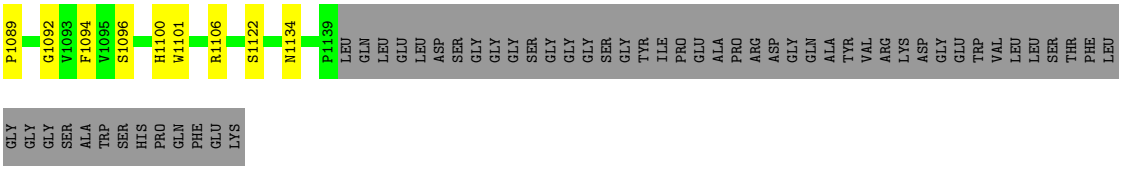
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Spike glycoprotein

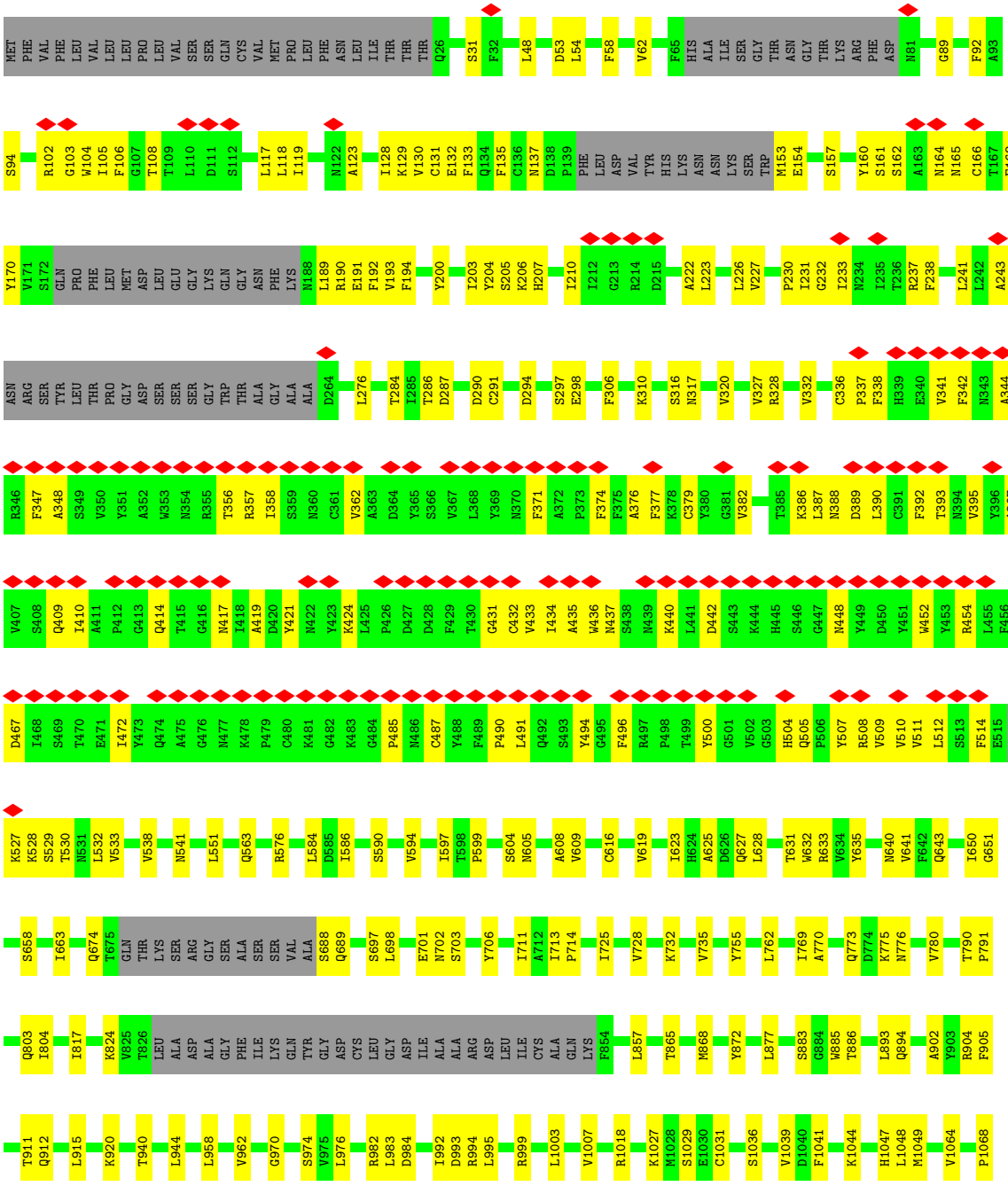
Chain A:

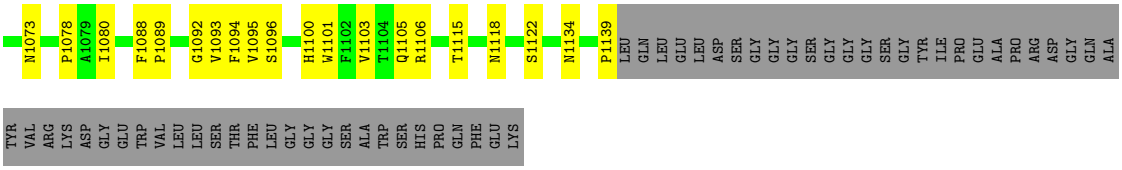




• Molecule 1: Spike glycoprotein

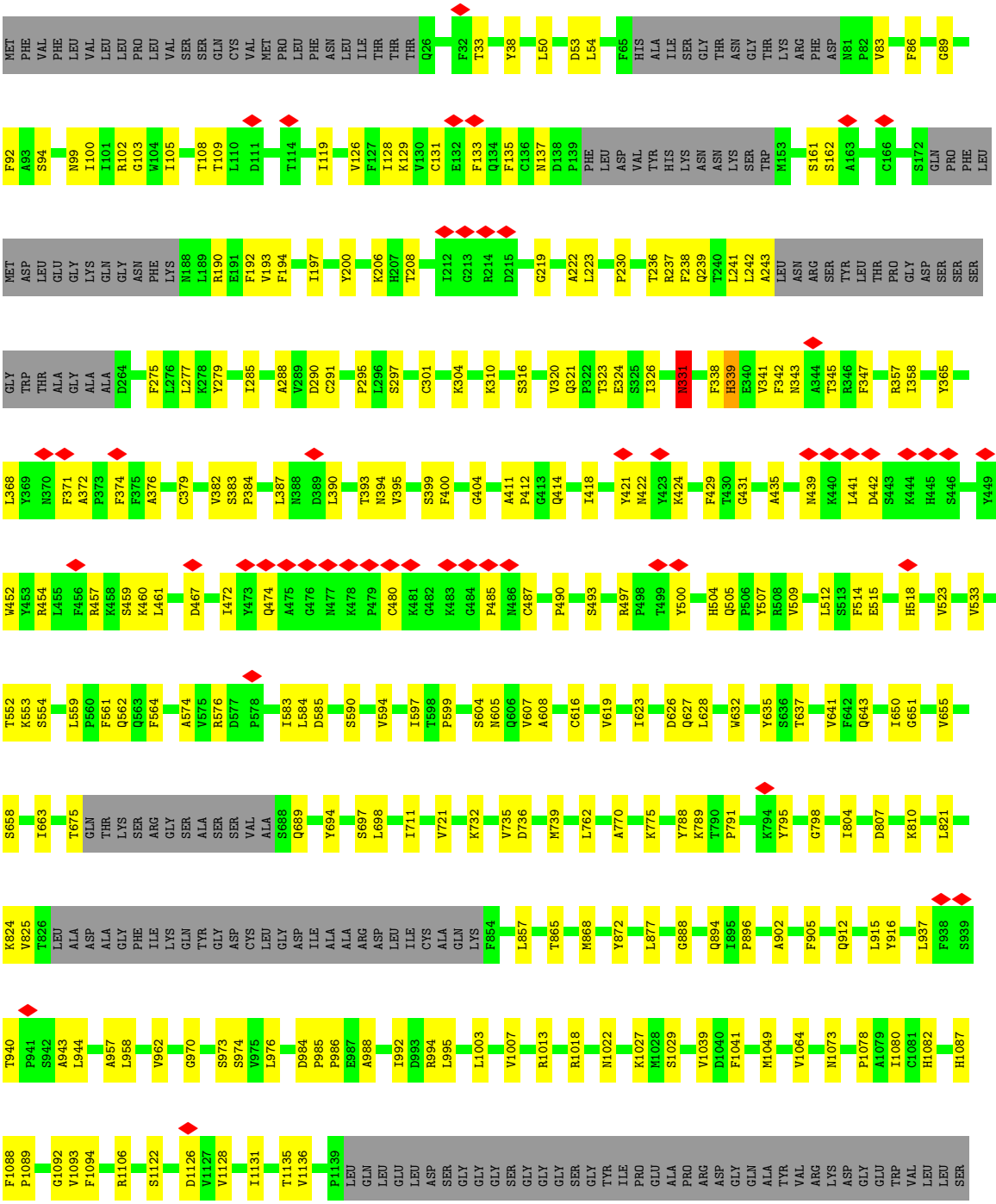
Chain B:





• Molecule 1: Spike glycoprotein

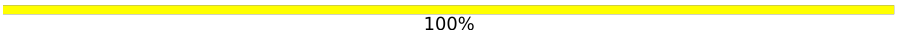
Chain C:



THR PHE LEU GLY GLY GLY SER ALA TRP SER HIS PRO GLN PHE GLU LYS

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

Chain D:



NAG1 NAG2

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

Chain E:

NAG1 NAG2

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

Chain F:

NAG1 NAG2

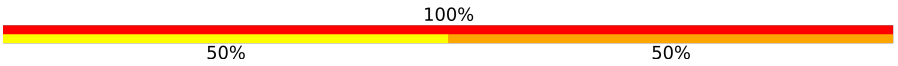
• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain G:

NAG1 NAG2

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

Chain H:



NAG1 NAG2

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

Chain I:

NAG1
NAG2

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	242344	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 ($e^-/Å^2$)	60	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	2.204	Depositor
Minimum map value	-0.002	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.027	Depositor
Recommended contour level	0.05	Depositor
Map size (Å)	334.5, 334.5, 334.5	wwPDB
Map dimensions	500, 500, 500	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.669, 0.669, 0.669	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.28	0/8117	0.49	0/11049
1	B	0.26	0/8057	0.48	0/10963
1	C	0.27	0/8117	0.50	2/11049 (0.0%)
All	All	0.27	0/24291	0.49	2/33061 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	279	TYR	N-CA-CB	-8.19	95.86	110.60
1	C	279	TYR	CA-CB-CG	5.07	123.03	113.40

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	7924	0	7730	190	0
1	B	7867	0	7667	212	0
1	C	7924	0	7728	184	0
2	D	28	0	25	2	0
2	E	28	0	25	0	0
2	F	28	0	25	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	G	28	0	25	0	0
2	H	28	0	25	3	0
2	I	28	0	25	0	0
3	A	126	0	117	11	0
3	B	126	0	117	10	0
3	C	84	0	78	0	0
All	All	24219	0	23587	552	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 12.

The worst 5 of 552 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:431:GLY:HA3	1:B:512:LEU:O	1.61	0.99
1:A:374:PHE:HZ	3:A:1209:NAG:H81	1.26	0.99
1:A:393:THR:HG21	1:A:518:HIS:HB2	1.45	0.96
1:A:516:LEU:HD23	1:B:982:ARG:CZ	1.98	0.92
1:A:374:PHE:CZ	3:A:1209:NAG:H81	2.05	0.91

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	997/1191 (84%)	925 (93%)	70 (7%)	2 (0%)	44 72
1	B	987/1191 (83%)	909 (92%)	76 (8%)	2 (0%)	44 72
1	C	997/1191 (84%)	907 (91%)	86 (9%)	4 (0%)	30 60
All	All	2981/3573 (83%)	2741 (92%)	232 (8%)	8 (0%)	38 66

5 of 8 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	160	TYR
1	A	160	TYR
1	C	331	ASN
1	C	342	PHE
1	A	522	THR

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	888/1031 (86%)	888 (100%)	0	100	100
1	B	882/1031 (86%)	882 (100%)	0	100	100
1	C	888/1031 (86%)	886 (100%)	2 (0%)	92	96
All	All	2658/3093 (86%)	2656 (100%)	2 (0%)	92	97

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	331	ASN
1	C	339	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 8 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	912	GLN
1	C	643	GLN
1	C	339	HIS
1	C	321	GLN
1	C	439	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)

12 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	$\#\|Z\| > 2$
2	NAG	D	1	1,2	14,14,15	0.27	0	17,19,21	0.51	0
2	NAG	D	2	2	14,14,15	0.22	0	17,19,21	0.40	0
2	NAG	E	1	1,2	14,14,15	0.40	0	17,19,21	0.73	0
2	NAG	E	2	2	14,14,15	0.37	0	17,19,21	1.01	1 (5%)
2	NAG	F	1	1,2	14,14,15	0.39	0	17,19,21	0.64	0
2	NAG	F	2	2	14,14,15	0.38	0	17,19,21	0.90	1 (5%)
2	NAG	G	1	1,2	14,14,15	0.37	0	17,19,21	0.99	1 (5%)
2	NAG	G	2	2	14,14,15	0.37	0	17,19,21	0.65	0
2	NAG	H	1	1,2	14,14,15	0.38	0	17,19,21	0.99	1 (5%)
2	NAG	H	2	2	14,14,15	0.36	0	17,19,21	0.95	1 (5%)
2	NAG	I	1	1,2	14,14,15	0.39	0	17,19,21	0.34	0
2	NAG	I	2	2	14,14,15	0.38	0	17,19,21	0.98	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
2	NAG	D	1	1,2	-	3/6/23/26	0/1/1/1
2	NAG	D	2	2	-	2/6/23/26	0/1/1/1
2	NAG	E	1	1,2	-	1/6/23/26	0/1/1/1
2	NAG	E	2	2	-	1/6/23/26	0/1/1/1
2	NAG	F	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	F	2	2	-	1/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	G	1	1,2	-	3/6/23/26	0/1/1/1
2	NAG	G	2	2	-	3/6/23/26	0/1/1/1
2	NAG	H	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	H	2	2	-	3/6/23/26	0/1/1/1
2	NAG	I	1	1,2	-	1/6/23/26	0/1/1/1
2	NAG	I	2	2	-	3/6/23/26	0/1/1/1

There are no bond length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	2	NAG	C2-N2-C7	3.32	127.62	122.90
2	F	2	NAG	C2-N2-C7	3.30	127.61	122.90
2	I	2	NAG	C2-N2-C7	3.24	127.52	122.90
2	G	1	NAG	C2-N2-C7	3.12	127.34	122.90
2	H	2	NAG	C2-N2-C7	2.92	127.06	122.90

There are no chirality outliers.

5 of 25 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	G	1	NAG	C3-C2-N2-C7
2	G	1	NAG	C8-C7-N2-C2
2	G	1	NAG	O7-C7-N2-C2
2	G	2	NAG	C8-C7-N2-C2
2	G	2	NAG	O7-C7-N2-C2

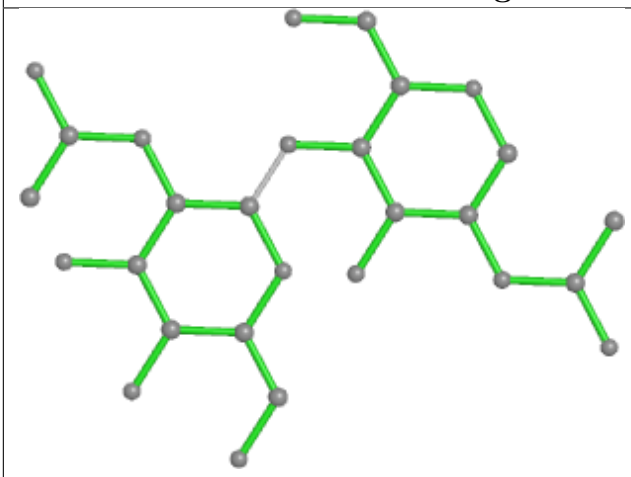
There are no ring outliers.

3 monomers are involved in 5 short contacts:

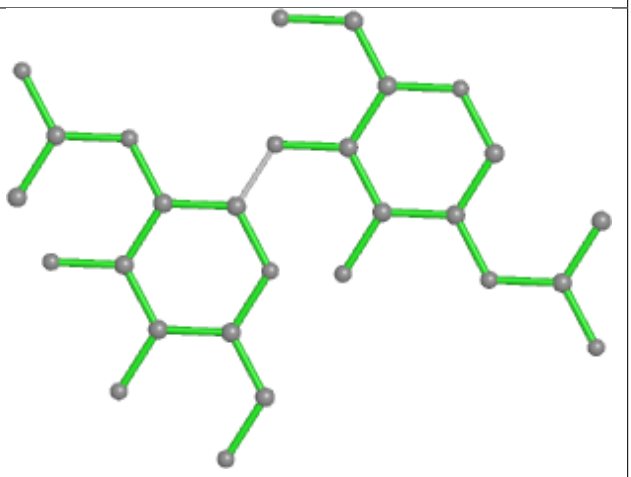
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	1	NAG	2	0
2	D	2	NAG	2	0
2	H	1	NAG	3	0

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

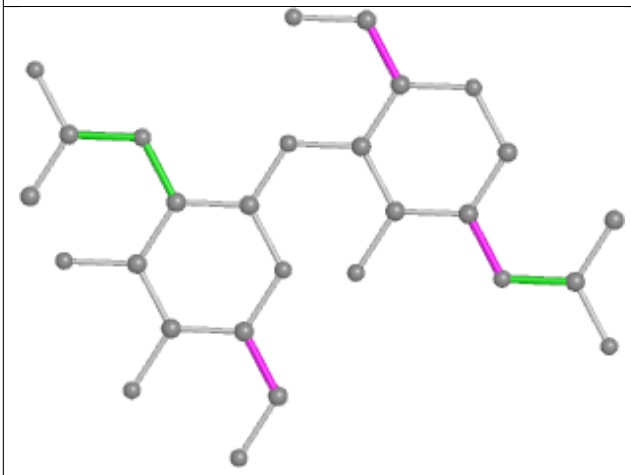
Oligosaccharide Chain D



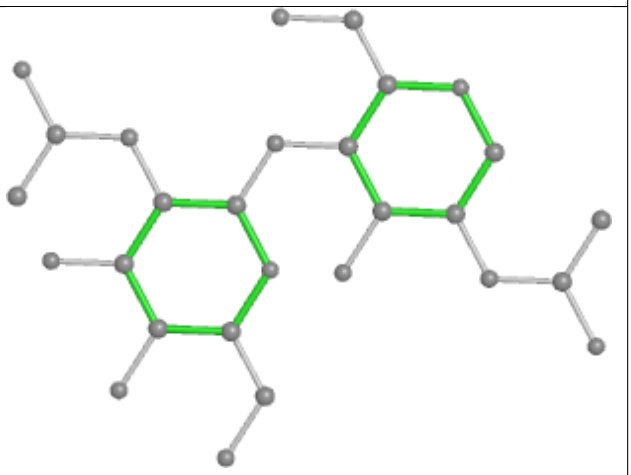
Bond lengths



Bond angles

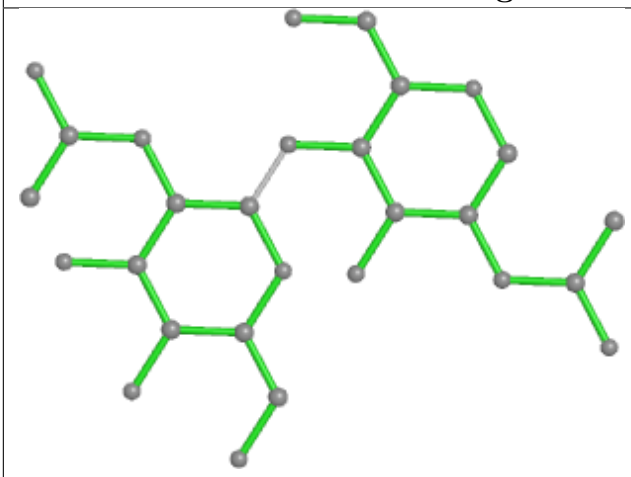


Torsions

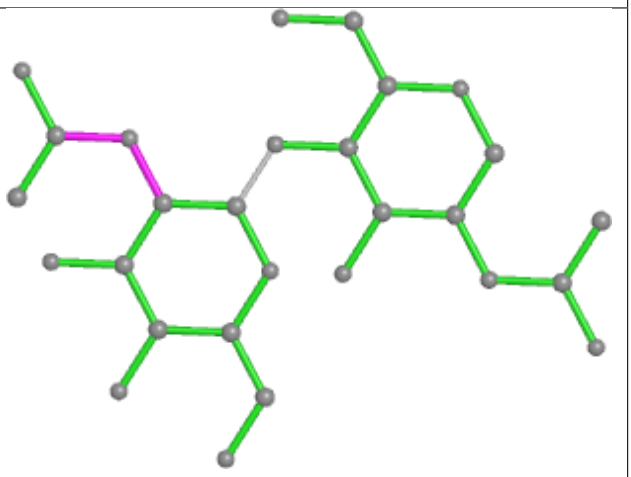


Rings

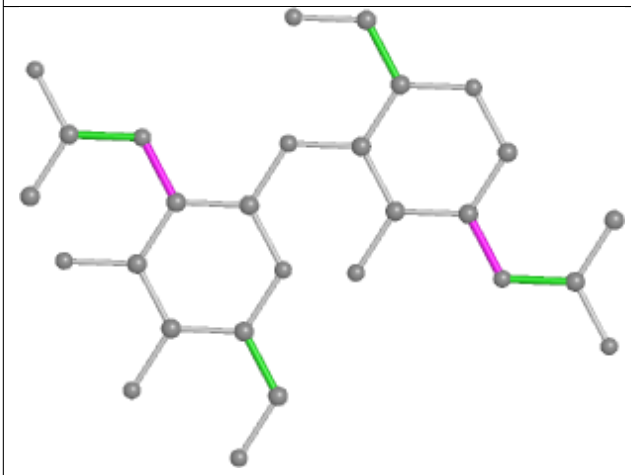
Oligosaccharide Chain E



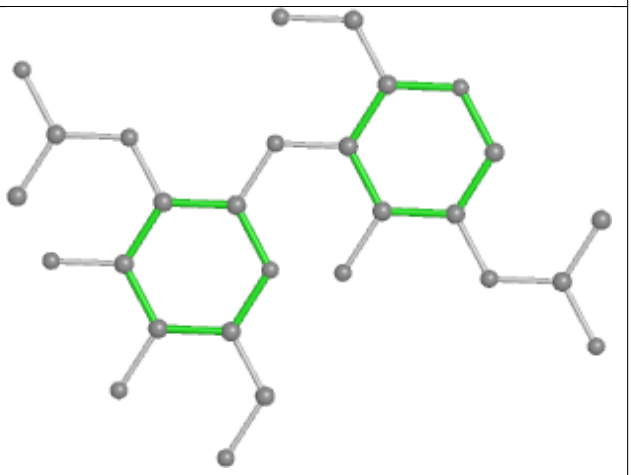
Bond lengths



Bond angles

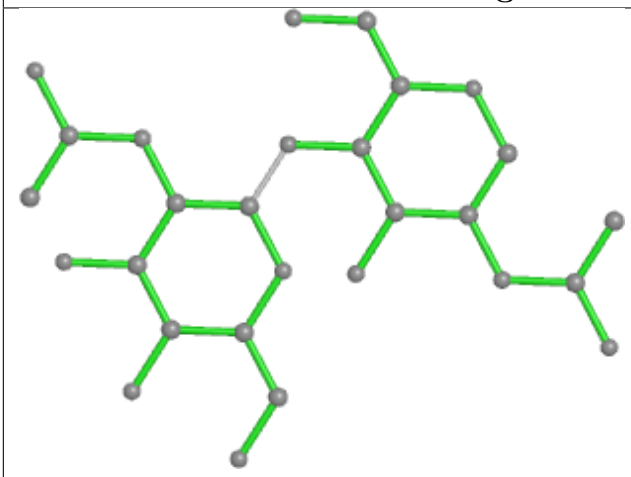


Torsions

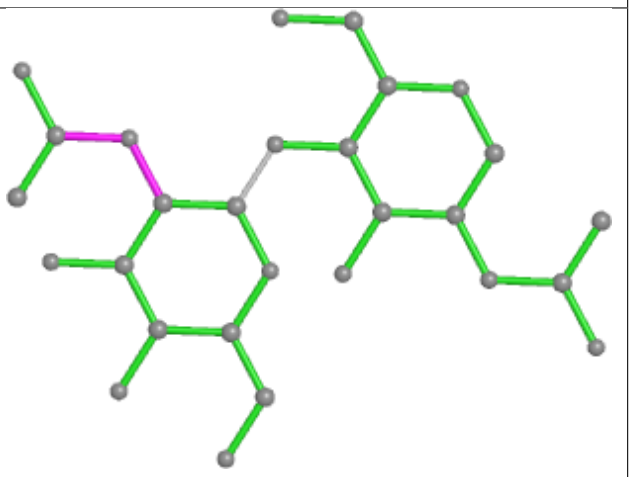


Rings

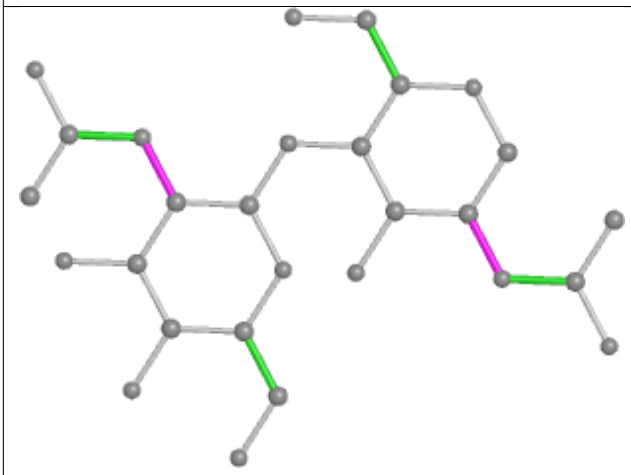
Oligosaccharide Chain F



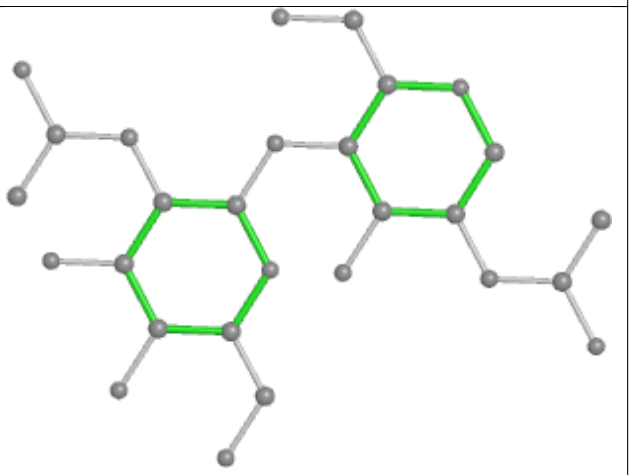
Bond lengths



Bond angles

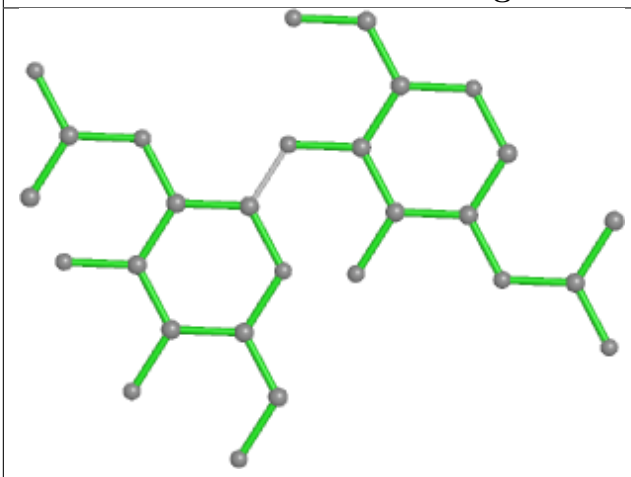


Torsions

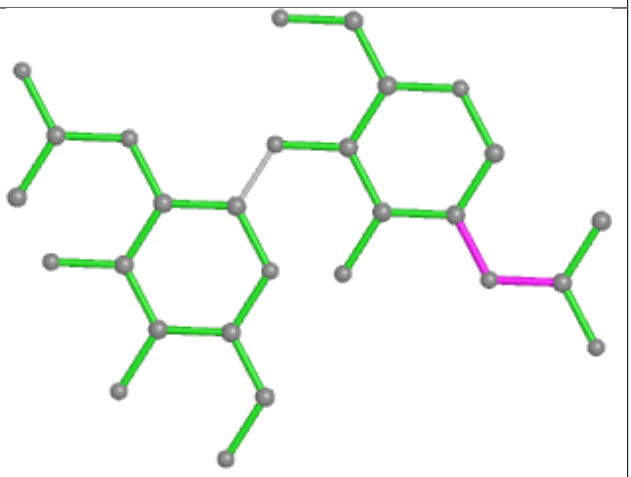


Rings

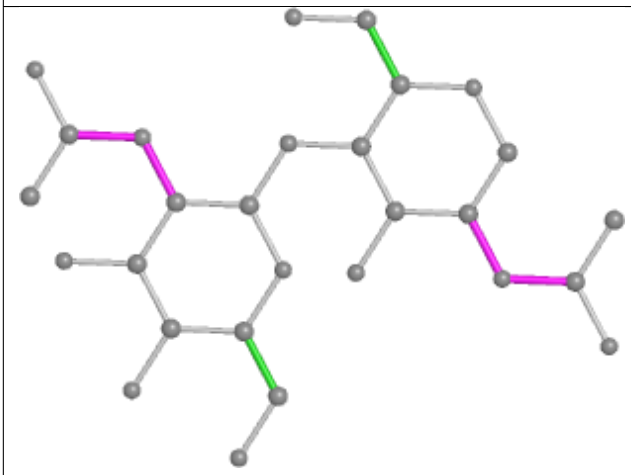
Oligosaccharide Chain G



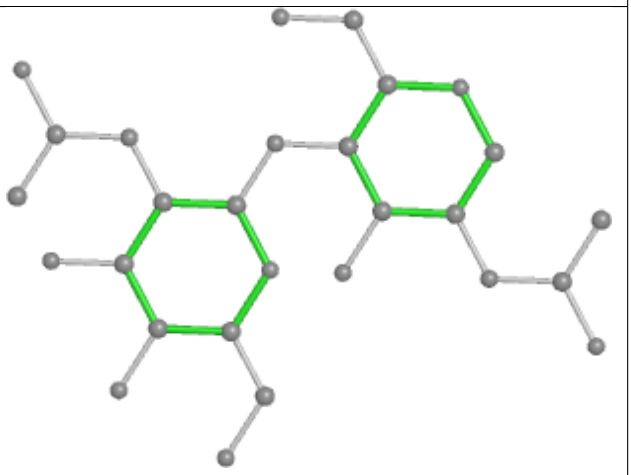
Bond lengths



Bond angles

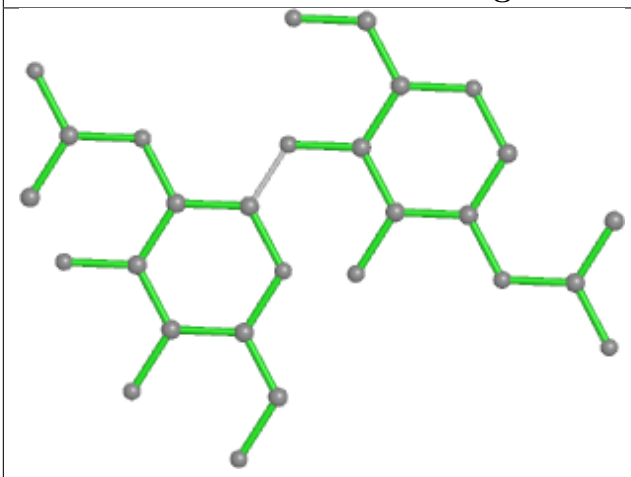


Torsions

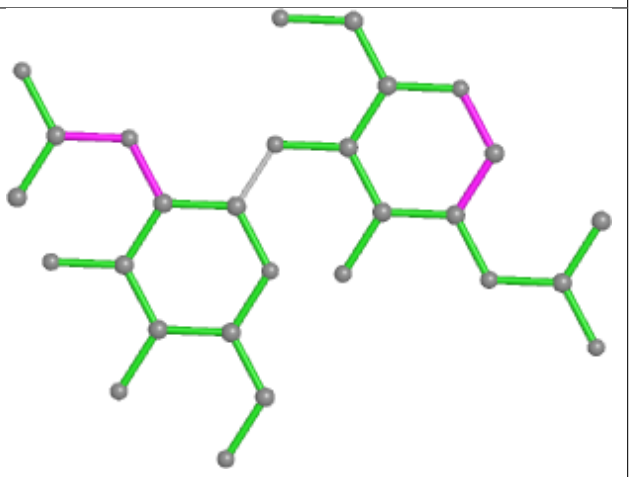


Rings

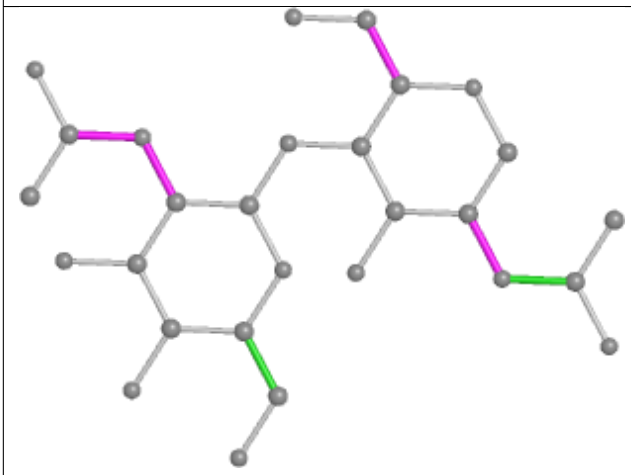
Oligosaccharide Chain H



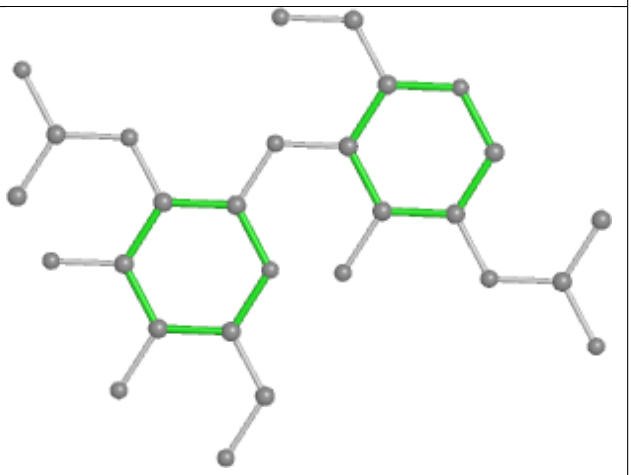
Bond lengths



Bond angles

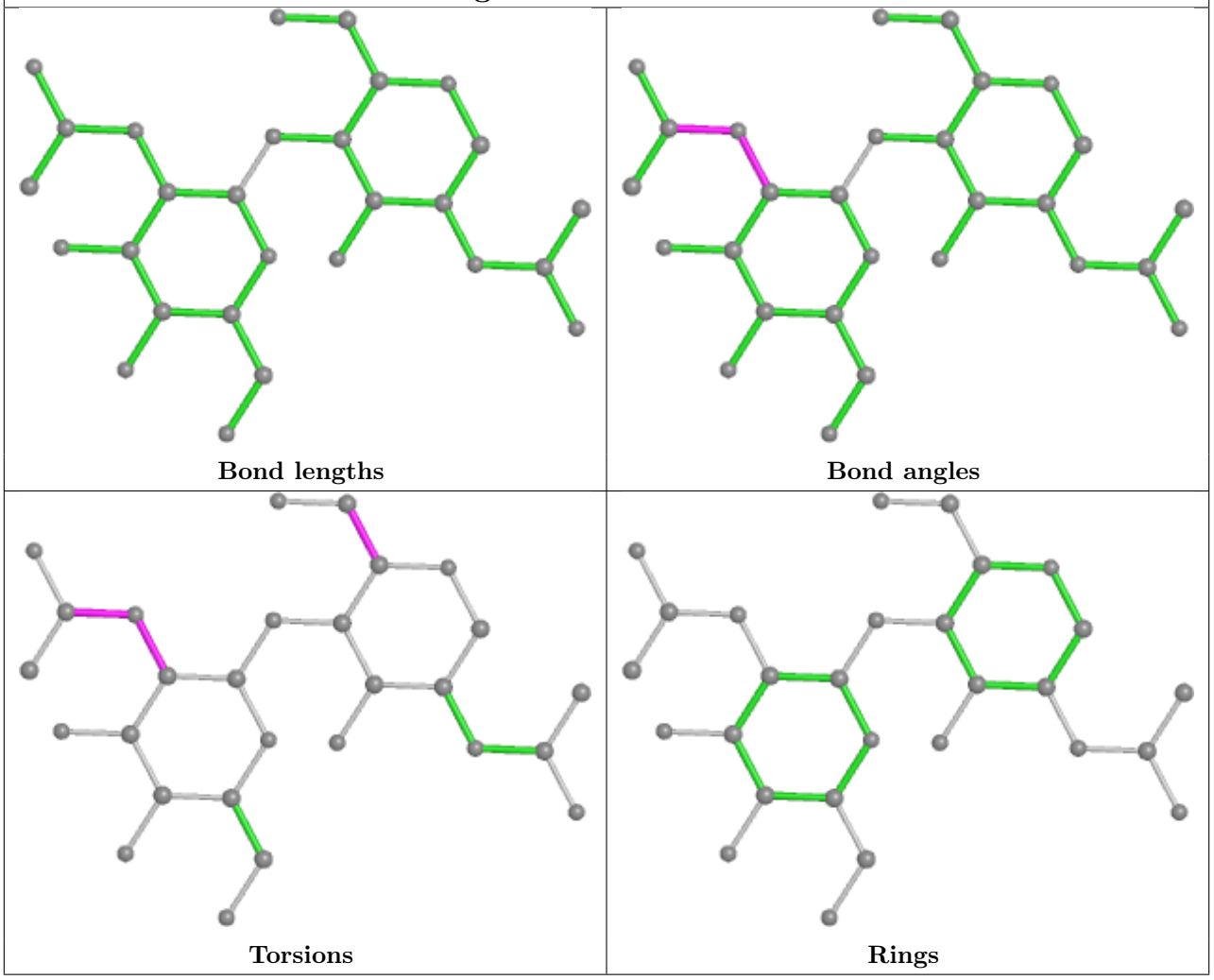


Torsions



Rings

Oligosaccharide Chain I



5.6 Ligand geometry (i)

24 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	$\#\|Z\| > 2$
3	NAG	C	1203	1	14,14,15	0.25	0	17,19,21	0.52	0
3	NAG	A	1201	1	14,14,15	0.20	0	17,19,21	0.45	0
3	NAG	A	1203	1	14,14,15	0.24	0	17,19,21	0.52	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	NAG	B	1209	1	14,14,15	0.31	0	17,19,21	1.07	1 (5%)
3	NAG	B	1201	1	14,14,15	0.41	0	17,19,21	0.36	0
3	NAG	C	1205	1	14,14,15	0.25	0	17,19,21	0.60	0
3	NAG	B	1207	1	14,14,15	0.39	0	17,19,21	0.45	0
3	NAG	B	1206	1	14,14,15	0.21	0	17,19,21	0.44	0
3	NAG	B	1208	1	14,14,15	0.29	0	17,19,21	1.40	2 (11%)
3	NAG	A	1204	1	14,14,15	0.39	0	17,19,21	0.88	1 (5%)
3	NAG	B	1203	1	14,14,15	0.42	0	17,19,21	0.43	0
3	NAG	B	1204	1	14,14,15	0.29	0	17,19,21	0.40	0
3	NAG	B	1205	1	14,14,15	0.25	0	17,19,21	0.48	0
3	NAG	A	1209	1	14,14,15	0.29	0	17,19,21	0.66	0
3	NAG	A	1205	1	14,14,15	0.23	0	17,19,21	0.56	0
3	NAG	A	1207	1	14,14,15	0.40	0	17,19,21	0.96	2 (11%)
3	NAG	A	1208	1	14,14,15	0.42	0	17,19,21	0.64	0
3	NAG	C	1206	1	14,14,15	0.28	0	17,19,21	0.53	0
3	NAG	A	1206	1	14,14,15	0.23	0	17,19,21	0.45	0
3	NAG	C	1201	1	14,14,15	0.18	0	17,19,21	0.39	0
3	NAG	C	1204	1	14,14,15	0.24	0	17,19,21	0.36	0
3	NAG	A	1202	1	14,14,15	0.21	0	17,19,21	0.44	0
3	NAG	C	1202	1	14,14,15	0.20	0	17,19,21	0.45	0
3	NAG	B	1202	1	14,14,15	0.15	0	17,19,21	0.48	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
3	NAG	C	1203	1	-	3/6/23/26	0/1/1/1
3	NAG	A	1201	1	-	0/6/23/26	0/1/1/1
3	NAG	A	1203	1	-	3/6/23/26	0/1/1/1
3	NAG	B	1209	1	-	0/6/23/26	0/1/1/1
3	NAG	B	1201	1	-	1/6/23/26	0/1/1/1
3	NAG	C	1205	1	-	3/6/23/26	0/1/1/1
3	NAG	B	1207	1	-	1/6/23/26	0/1/1/1
3	NAG	B	1206	1	-	0/6/23/26	0/1/1/1
3	NAG	B	1208	1	-	0/6/23/26	0/1/1/1
3	NAG	A	1204	1	-	1/6/23/26	0/1/1/1
3	NAG	B	1203	1	-	0/6/23/26	0/1/1/1
3	NAG	B	1204	1	-	3/6/23/26	0/1/1/1
3	NAG	B	1205	1	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	A	1209	1	-	1/6/23/26	0/1/1/1
3	NAG	A	1205	1	-	2/6/23/26	0/1/1/1
3	NAG	A	1207	1	-	5/6/23/26	0/1/1/1
3	NAG	A	1208	1	-	3/6/23/26	0/1/1/1
3	NAG	C	1206	1	-	0/6/23/26	0/1/1/1
3	NAG	A	1206	1	-	2/6/23/26	0/1/1/1
3	NAG	C	1201	1	-	1/6/23/26	0/1/1/1
3	NAG	C	1204	1	-	4/6/23/26	0/1/1/1
3	NAG	A	1202	1	-	3/6/23/26	0/1/1/1
3	NAG	C	1202	1	-	4/6/23/26	0/1/1/1
3	NAG	B	1202	1	-	4/6/23/26	0/1/1/1

There are no bond length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	1208	NAG	C2-N2-C7	-3.38	118.09	122.90
3	B	1208	NAG	C4-C3-C2	-3.25	106.26	111.02
3	A	1204	NAG	C2-N2-C7	2.76	126.83	122.90
3	B	1209	NAG	C4-C3-C2	-2.68	107.09	111.02
3	A	1207	NAG	C1-C2-N2	2.68	115.06	110.49

There are no chirality outliers.

5 of 46 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1207	NAG	C3-C2-N2-C7
3	A	1207	NAG	C8-C7-N2-C2
3	A	1207	NAG	O7-C7-N2-C2
3	A	1208	NAG	C8-C7-N2-C2
3	A	1208	NAG	O7-C7-N2-C2

There are no ring outliers.

11 monomers are involved in 21 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	1209	NAG	2	0
3	B	1207	NAG	1	0
3	B	1208	NAG	3	0

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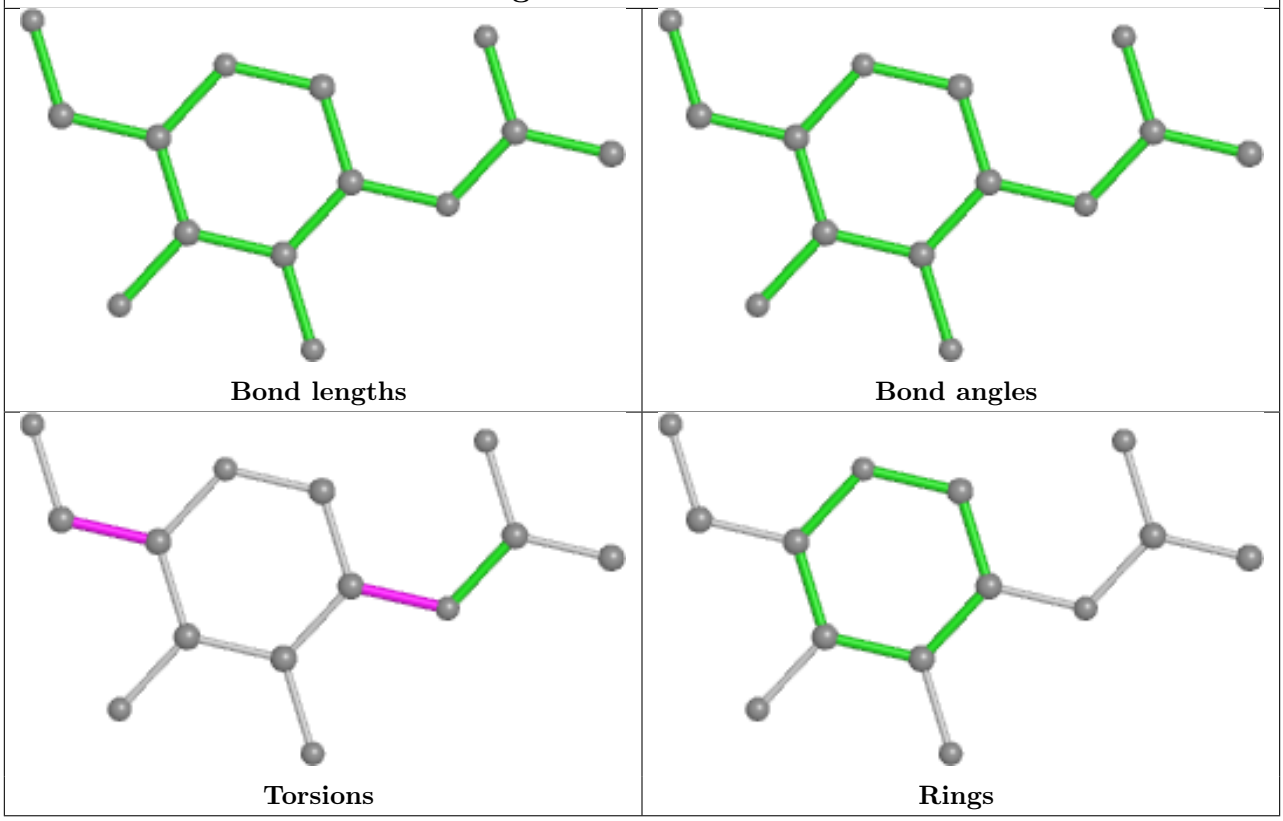
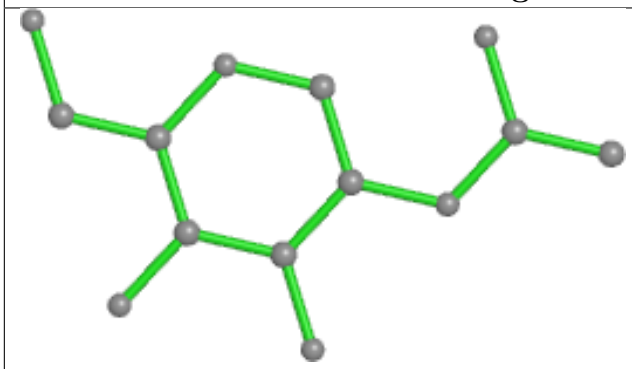
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1204	NAG	1	0
3	B	1204	NAG	1	0
3	B	1205	NAG	1	0
3	A	1209	NAG	6	0
3	A	1205	NAG	1	0
3	A	1207	NAG	1	0
3	A	1208	NAG	2	0
3	B	1202	NAG	2	0

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.

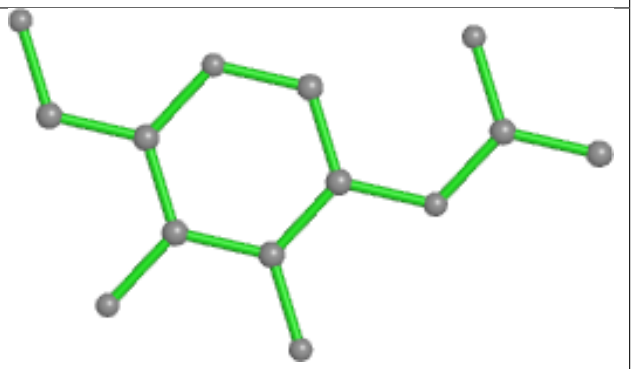
Ligand NAG C 1203



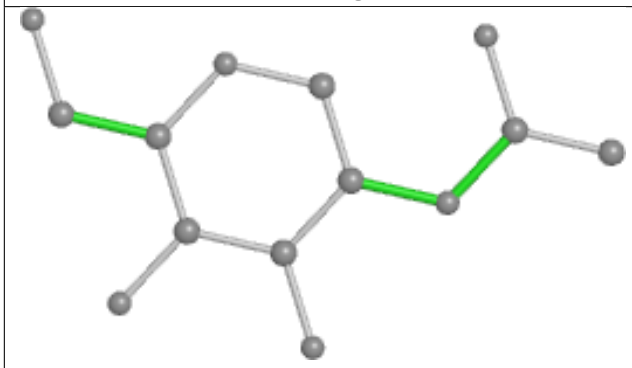
Ligand NAG A 1201



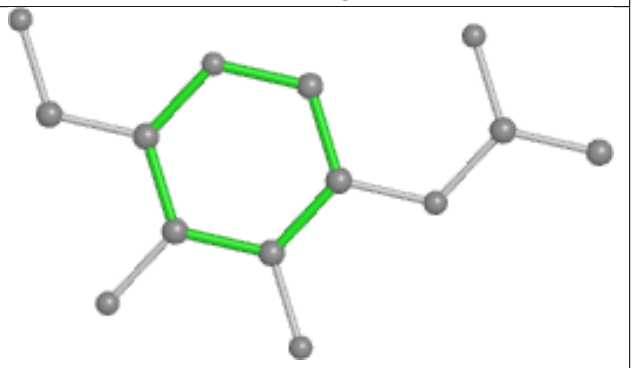
Bond lengths



Bond angles

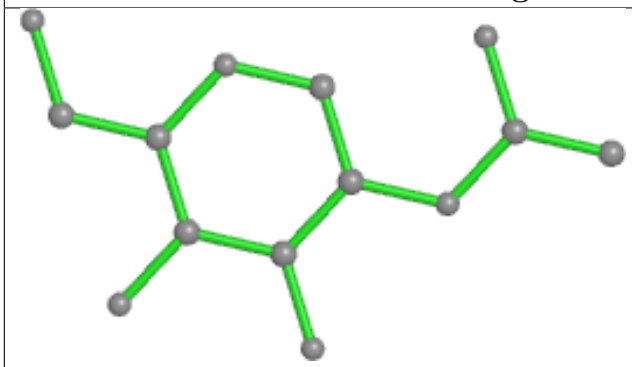


Torsions

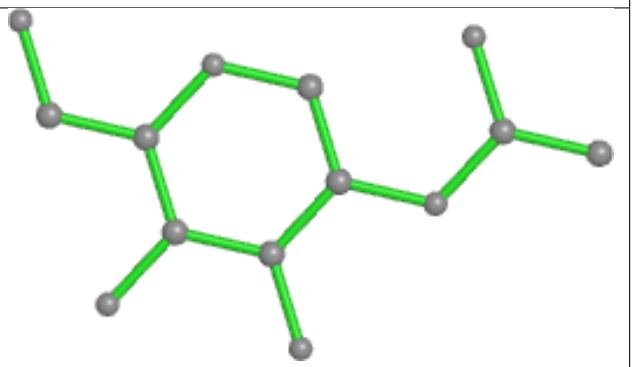


Rings

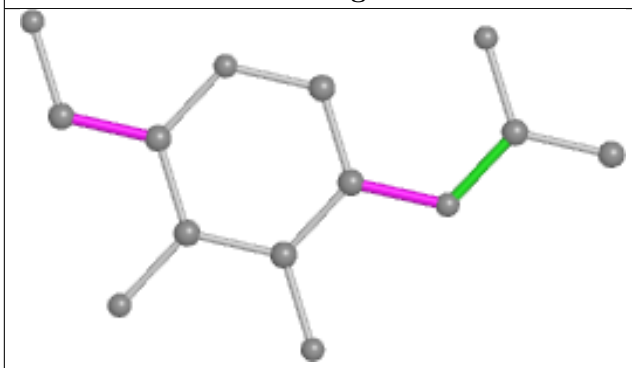
Ligand NAG A 1203



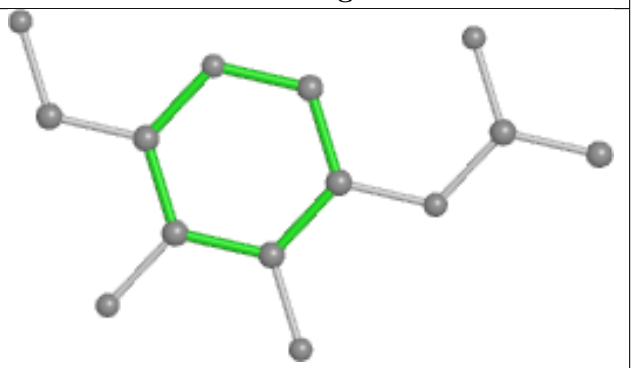
Bond lengths



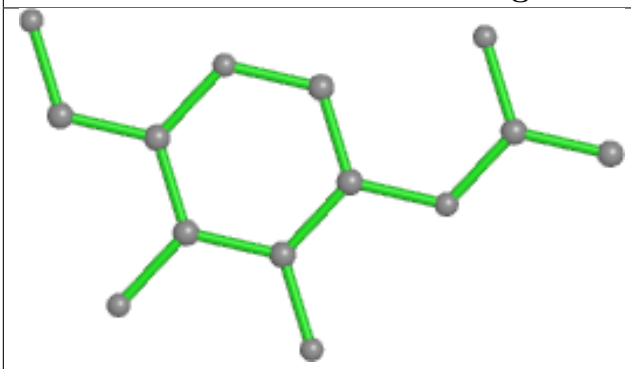
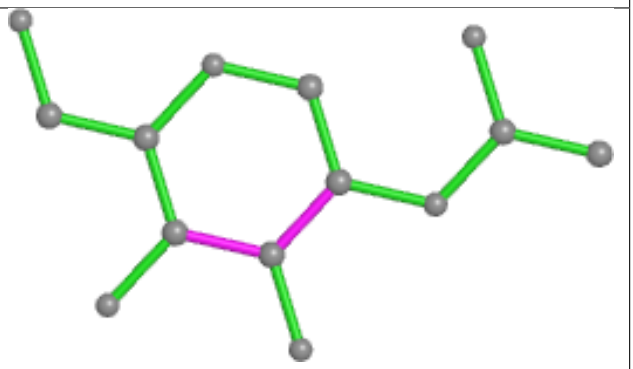
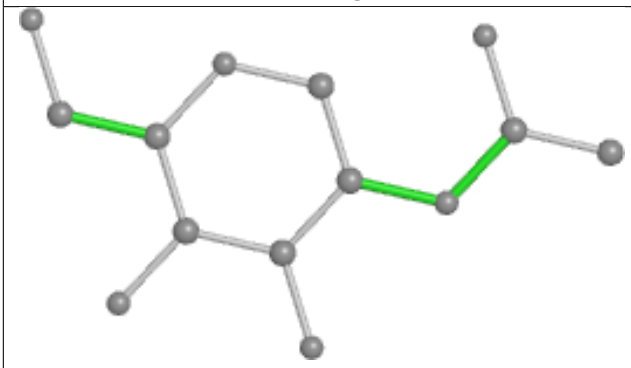
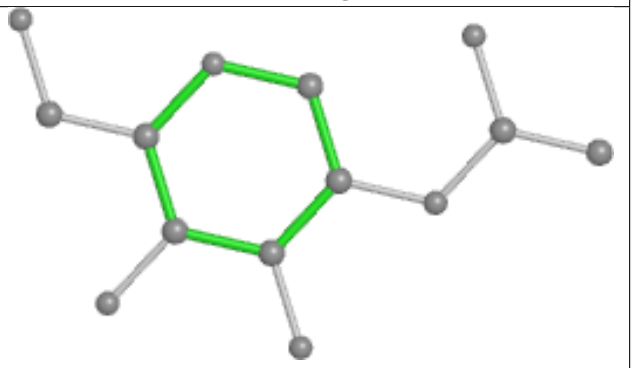
Bond angles



Torsions



Rings

Ligand NAG B 1209	
	
Bond lengths	Bond angles
	
Torsions	Rings

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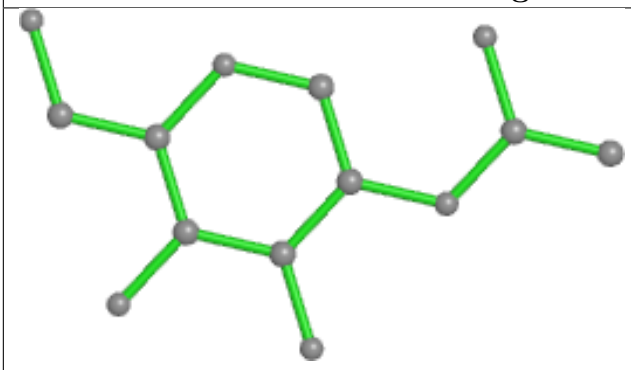
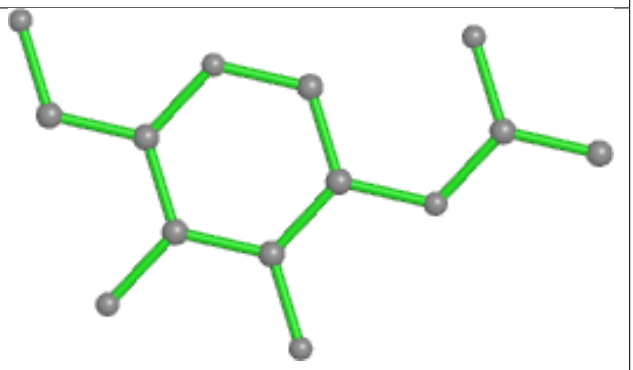
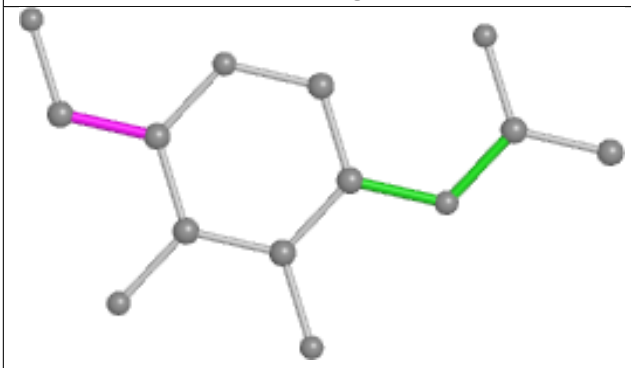
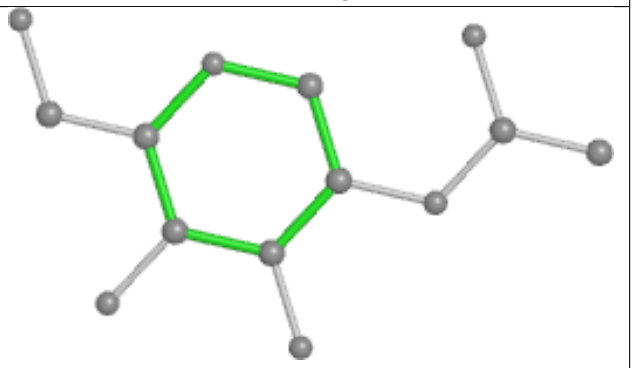
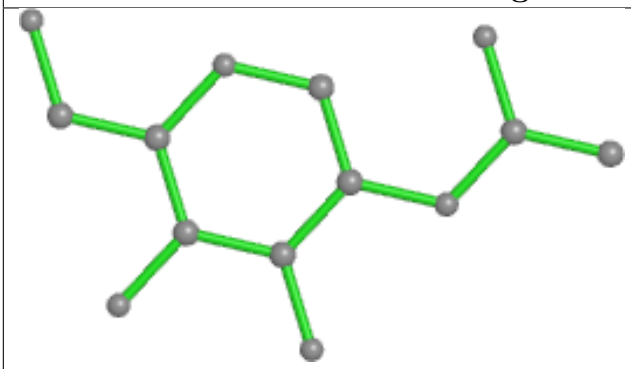
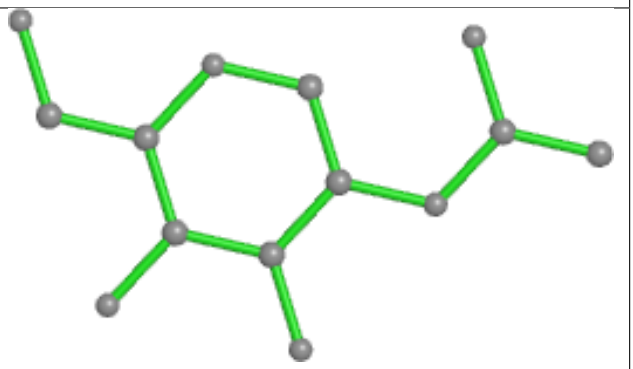
	
Bond lengths	Bond angles
	
Torsions	Rings

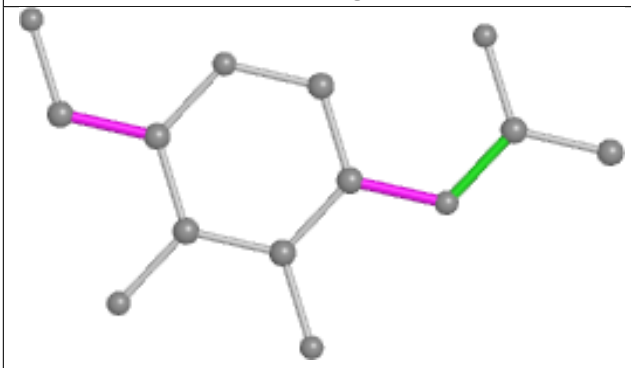
Ligand NAG C 1205



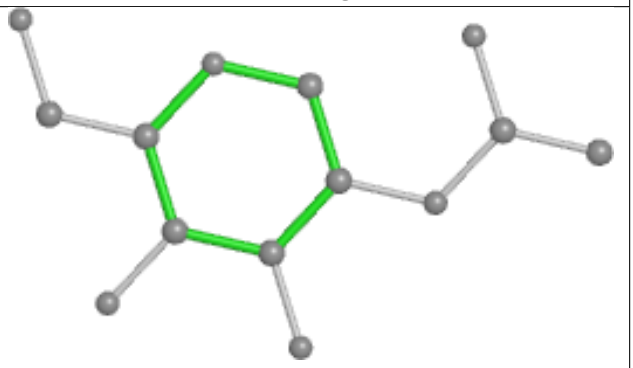
Bond lengths



Bond angles

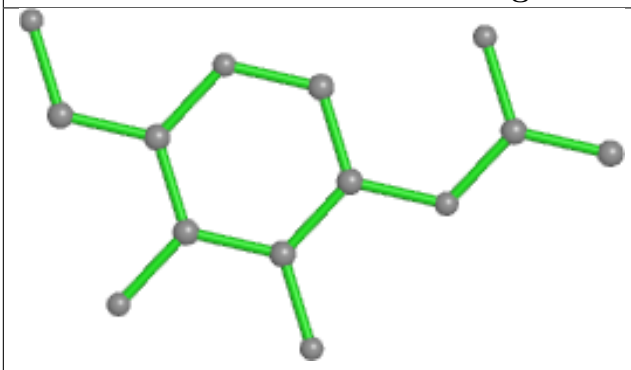


Torsions

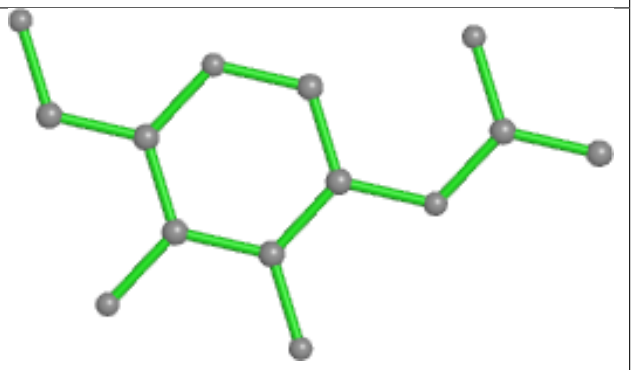


Rings

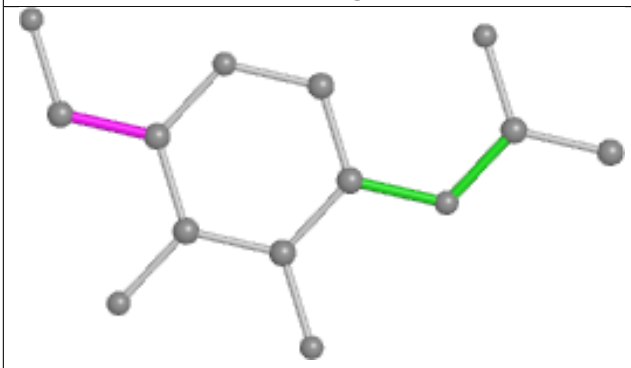
Ligand NAG B 1207



Bond lengths



Bond angles



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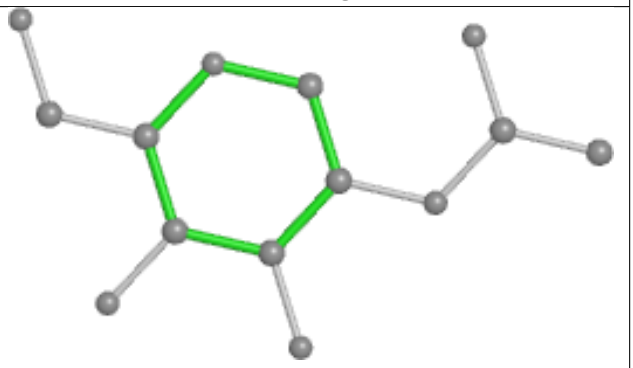
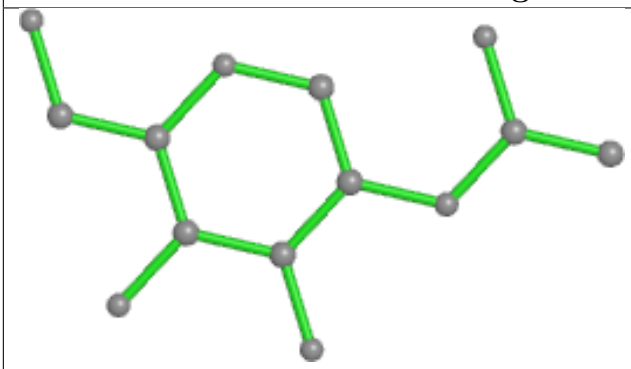
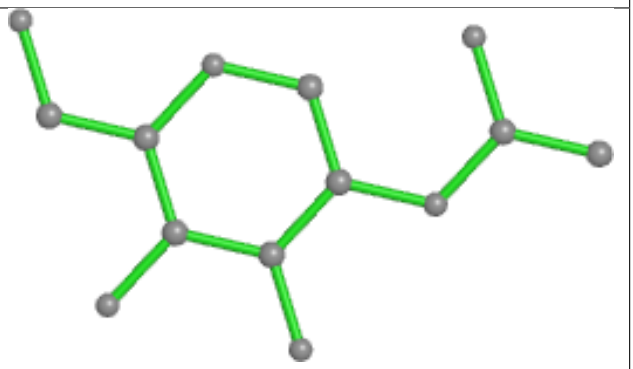
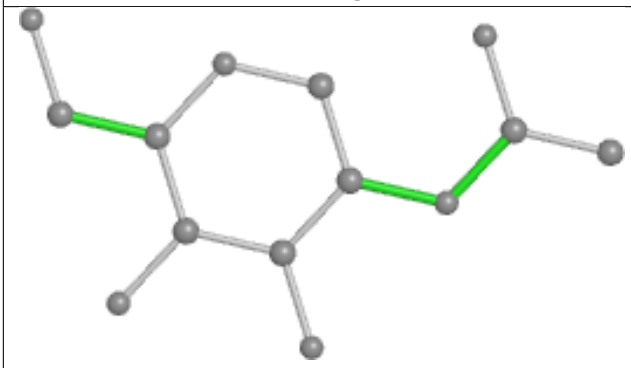
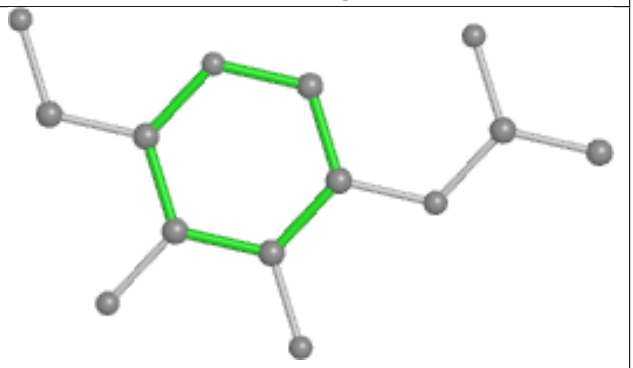


Rings

Ligand NAG B 1206	
	
Bond lengths	Bond angles
	
Torsions	Rings

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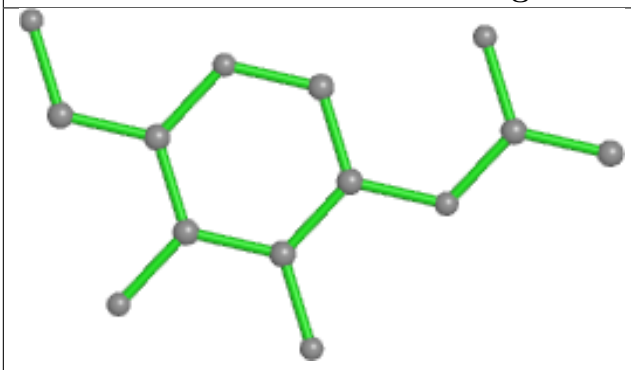
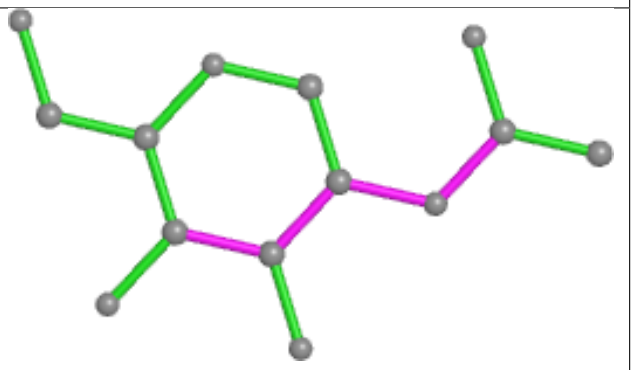
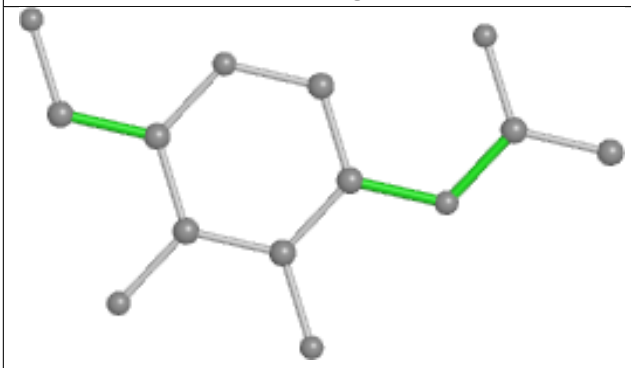
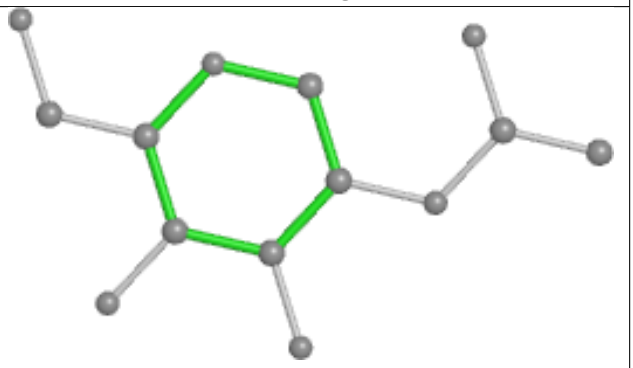
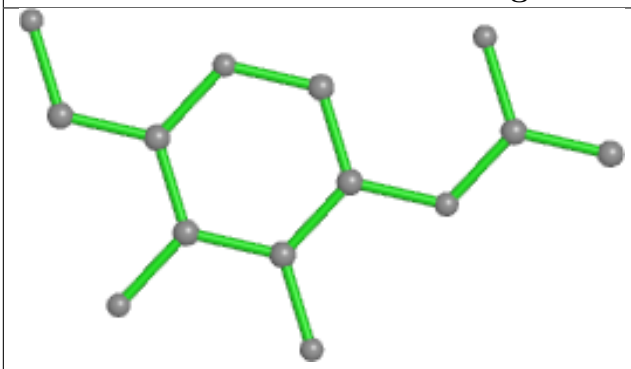
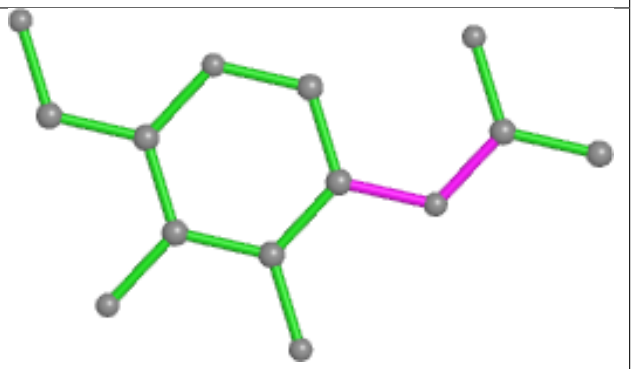
	
Bond lengths	Bond angles
	
Torsions	Rings

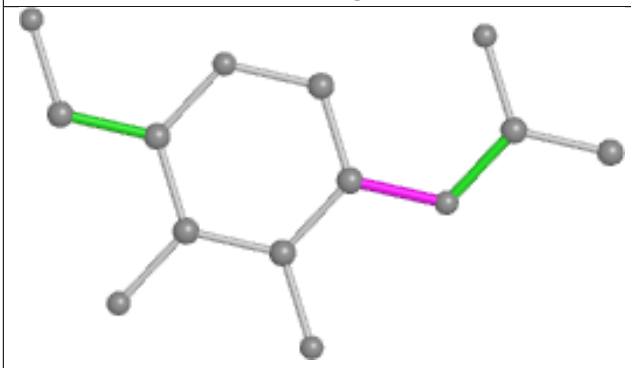
Ligand NAG A 1204



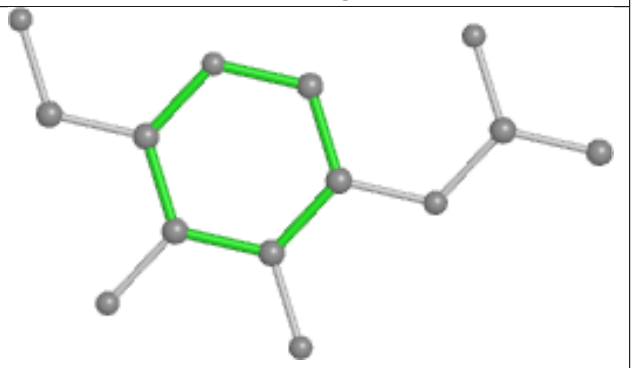
Bond lengths



Bond angles

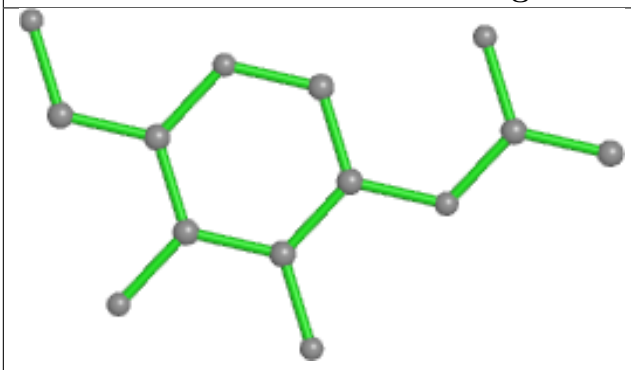


Torsions

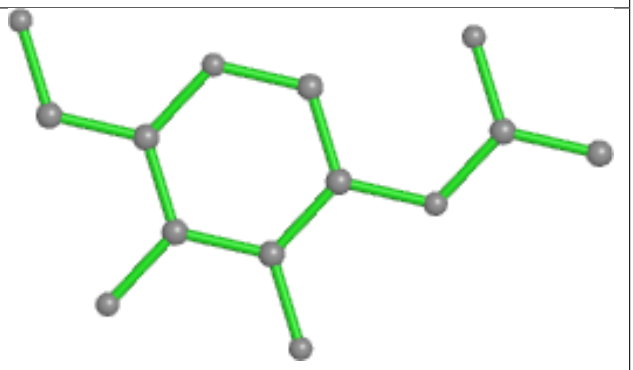


Rings

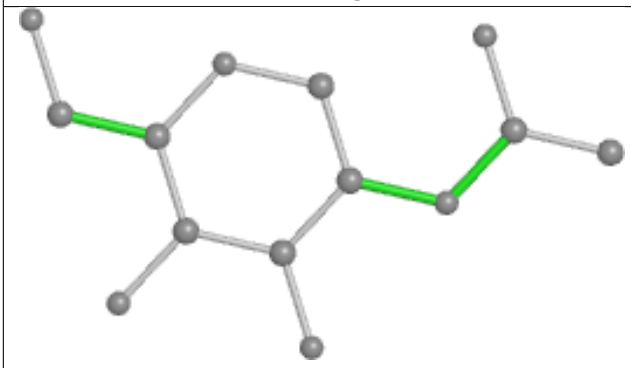
Ligand NAG B 1203



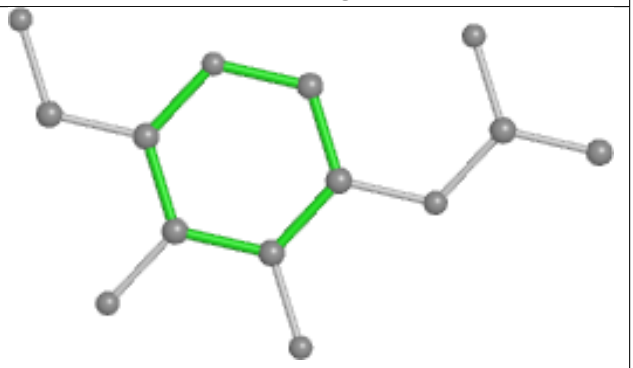
Bond lengths



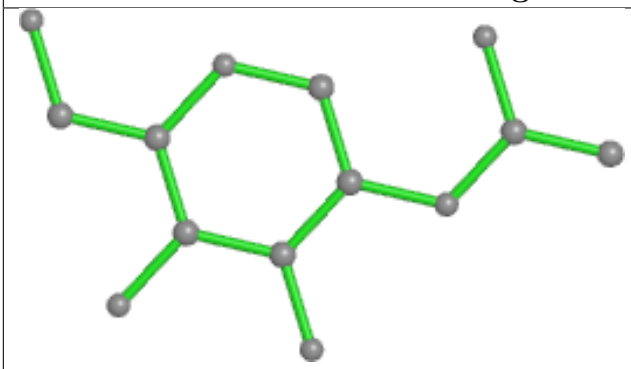
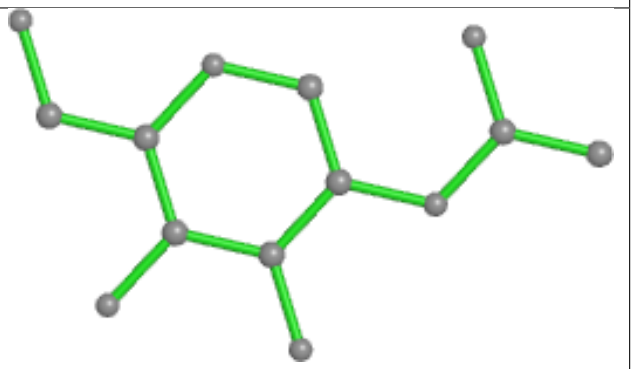
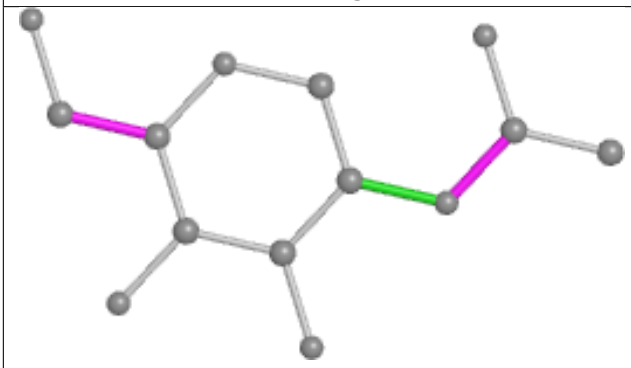
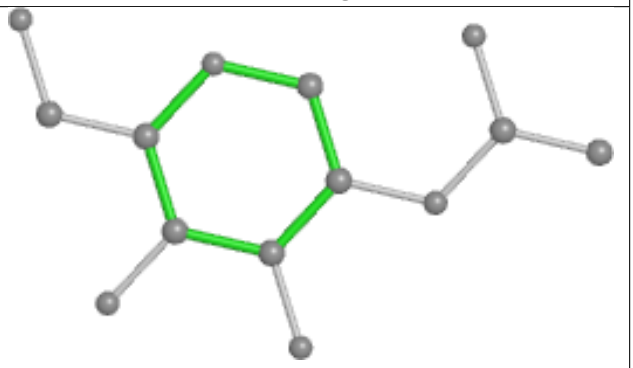
Bond angles

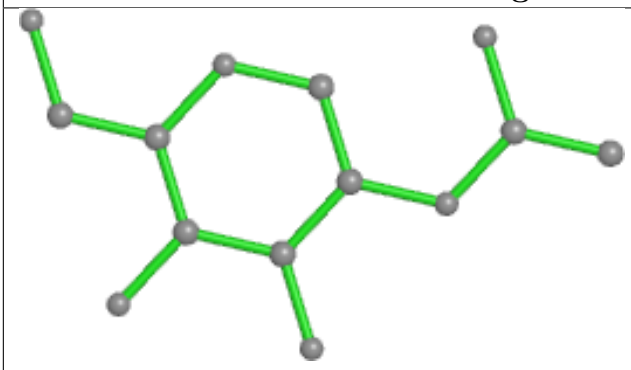
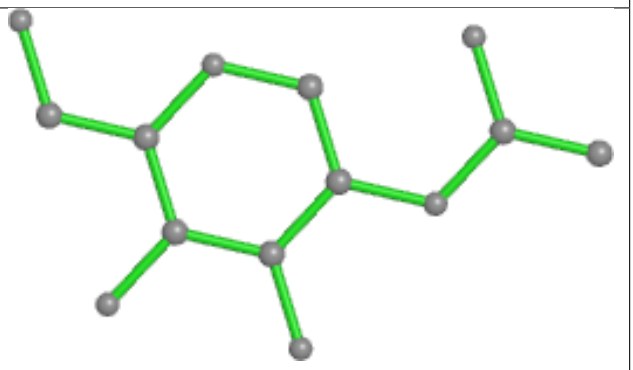
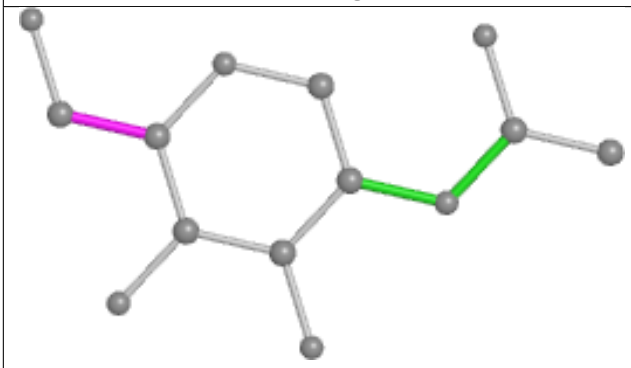
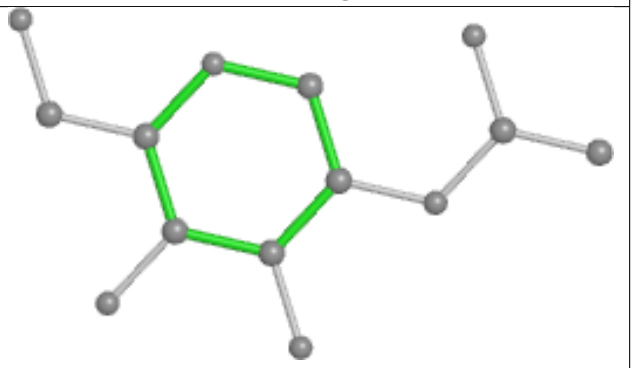


Torsions

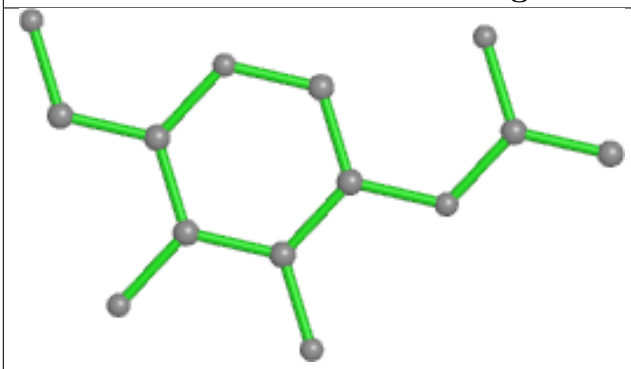


Rings

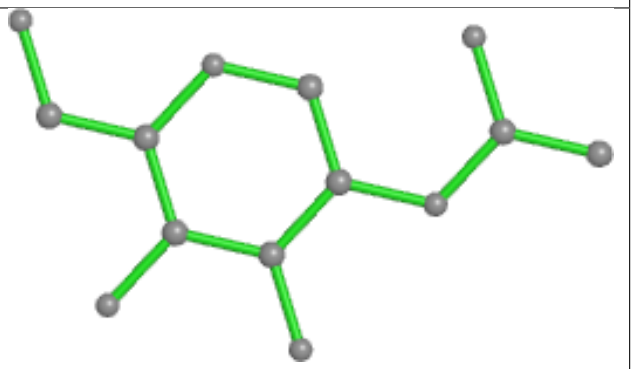
Ligand NAG B 1204	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand NAG B 1205	
	
Bond lengths	Bond angles
	
Torsions	Rings

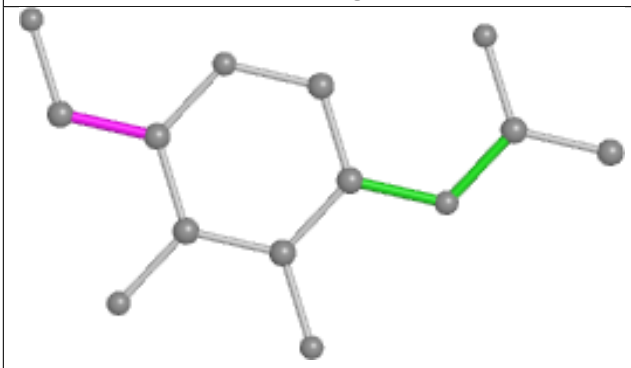
Ligand NAG A 1209



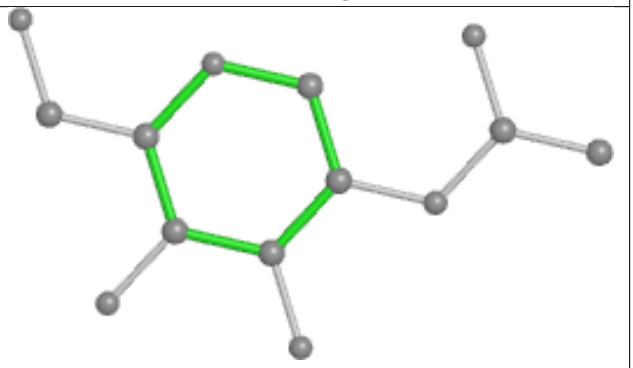
Bond lengths



Bond angles

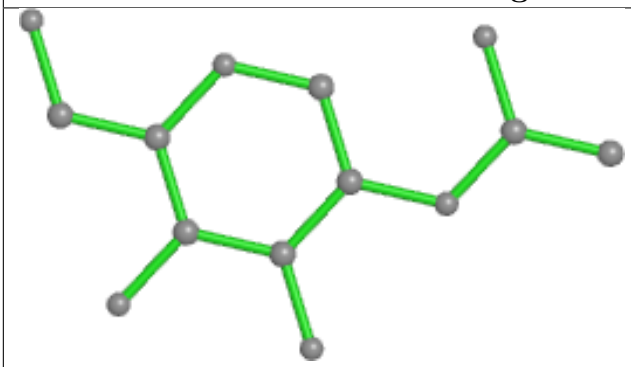


Torsions

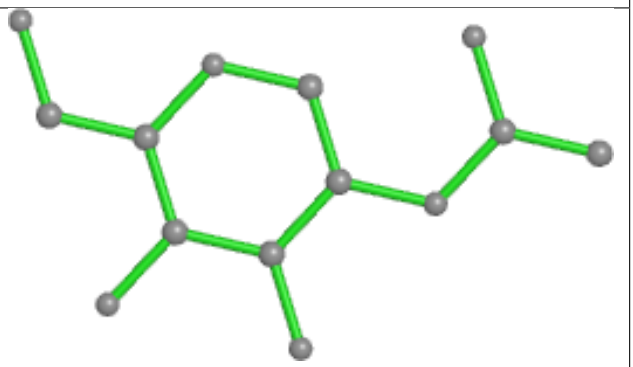


Rings

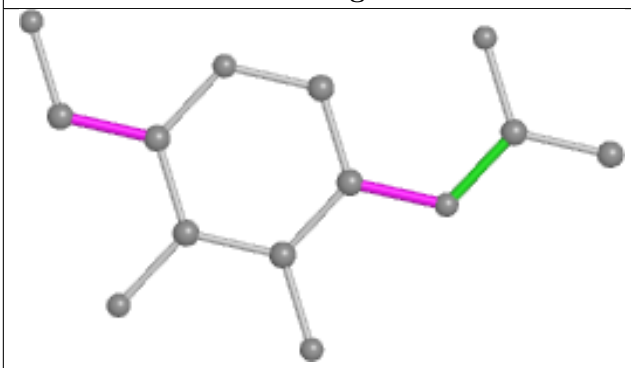
Ligand NAG A 1205



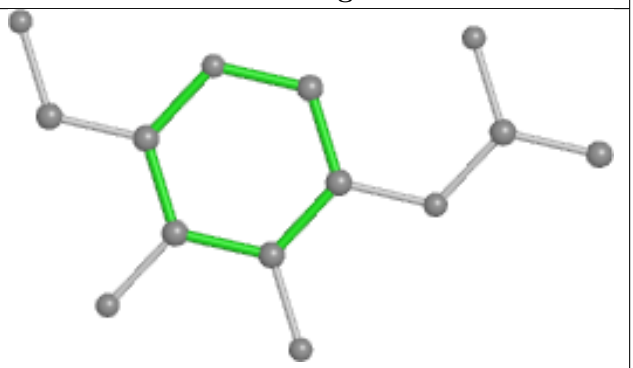
Bond lengths



Bond angles

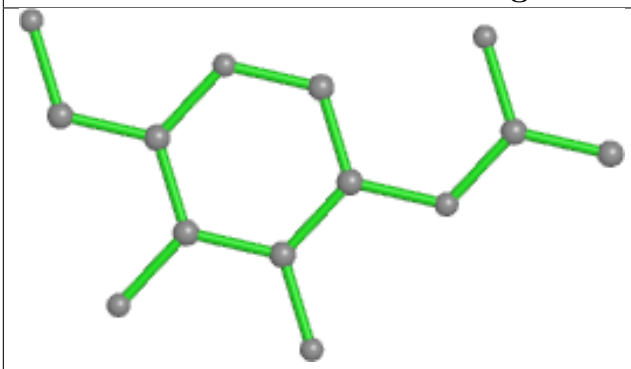


Torsions

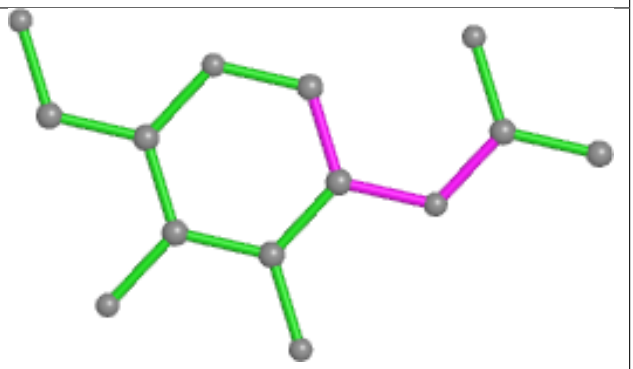


Rings

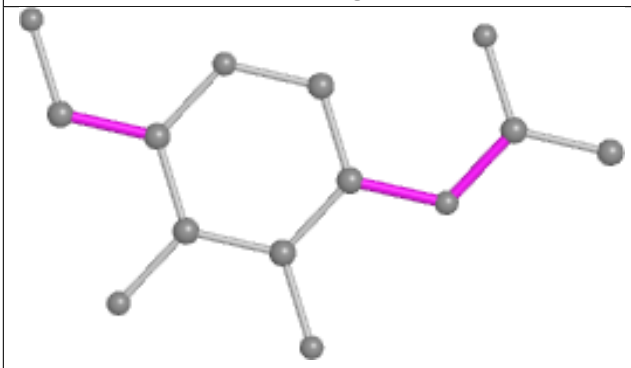
Ligand NAG A 1207



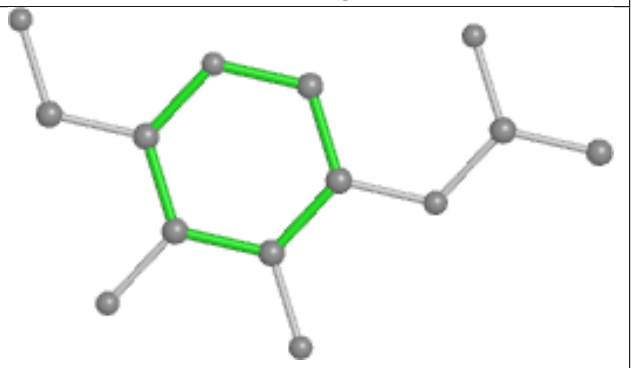
Bond lengths



Bond angles

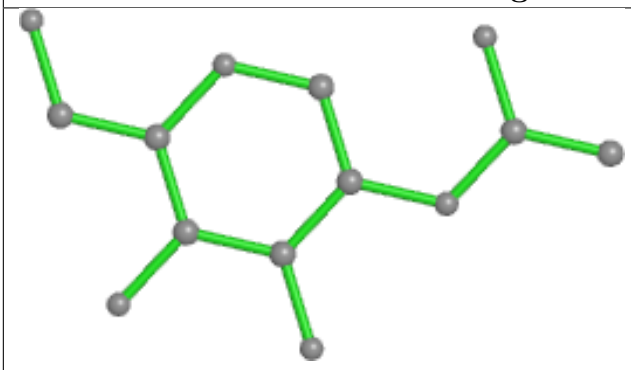


Torsions

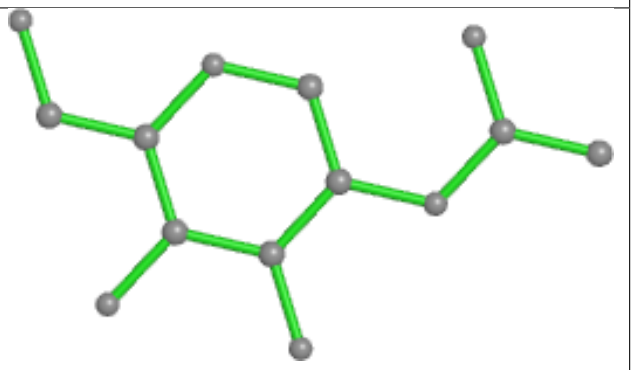


Rings

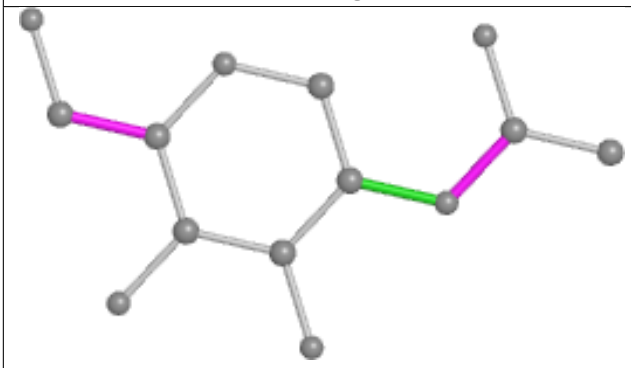
Ligand NAG A 1208



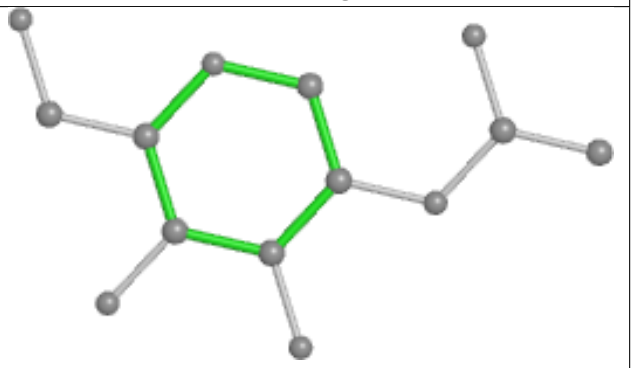
Bond lengths



Bond angles

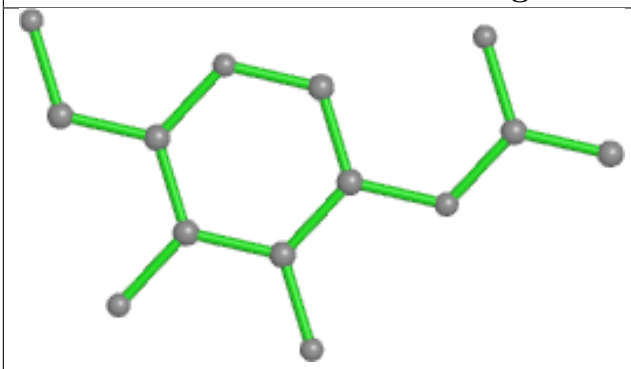


Torsions

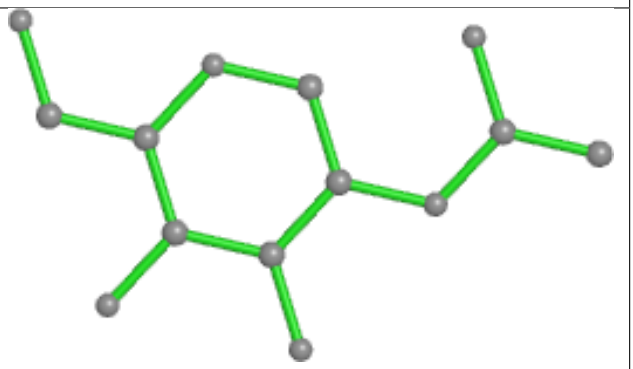


Rings

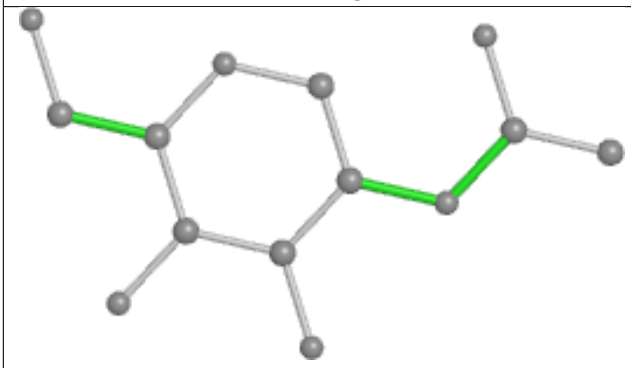
Ligand NAG C 1206



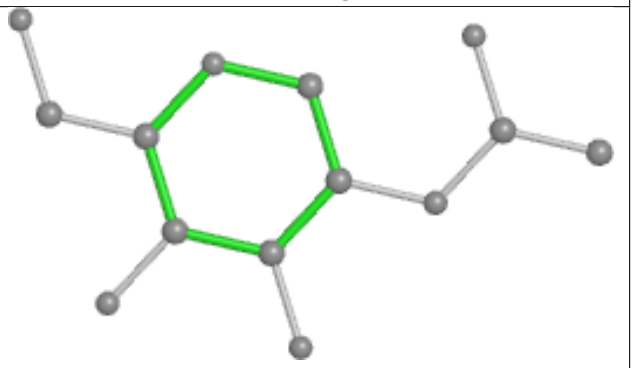
Bond lengths



Bond angles

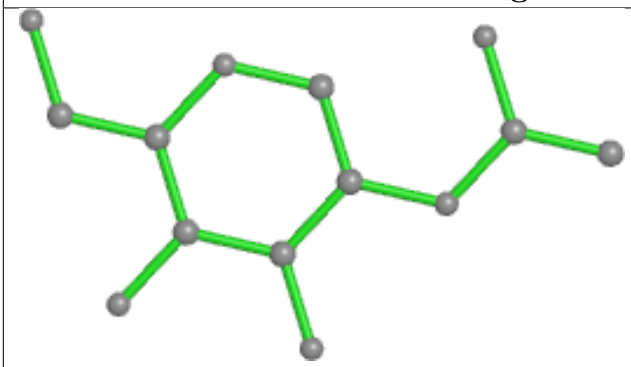


Torsions

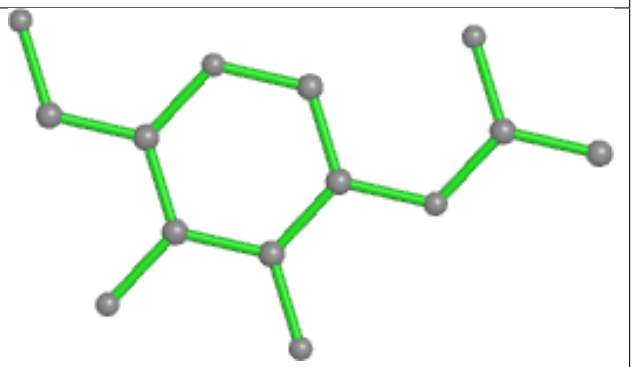


Rings

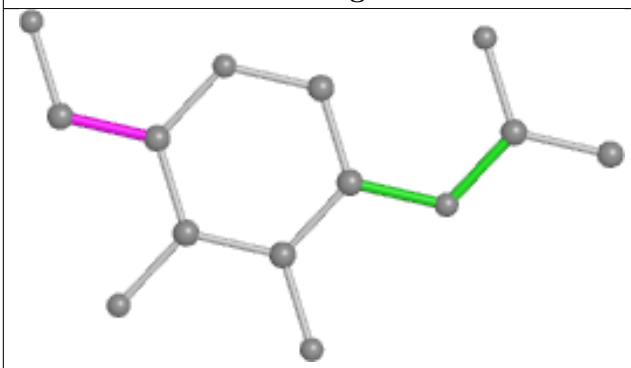
Ligand NAG A 1206



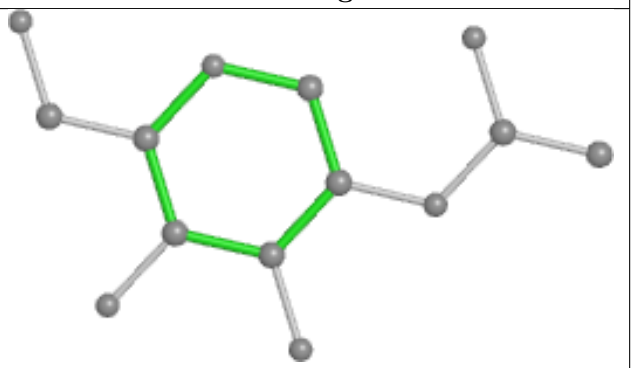
Bond lengths



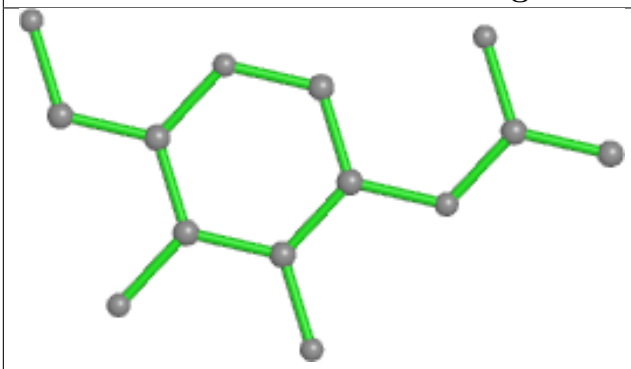
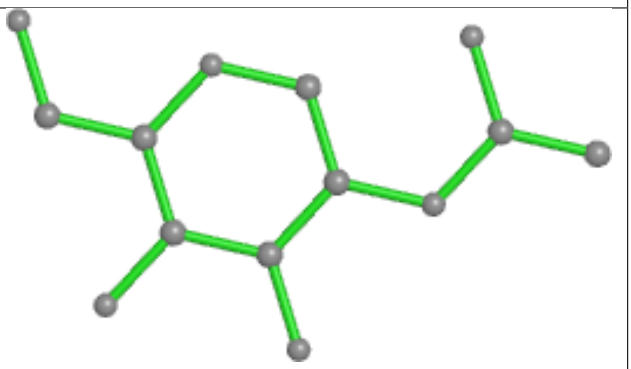
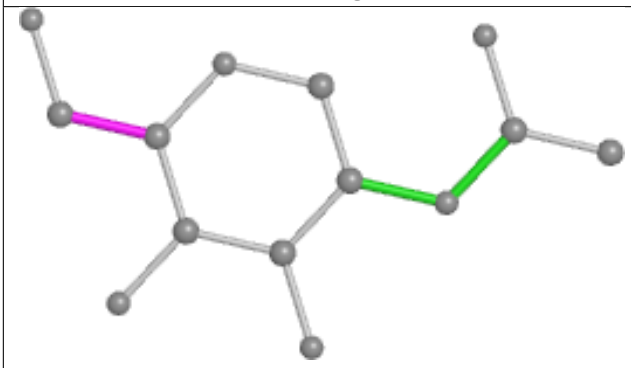
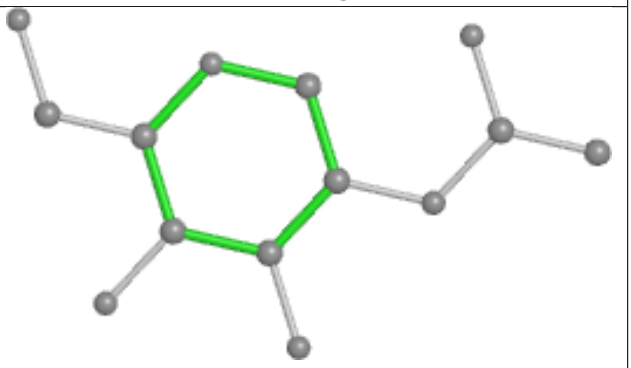
Bond angles

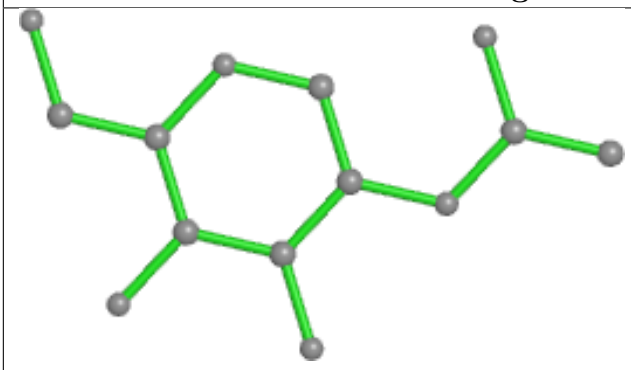
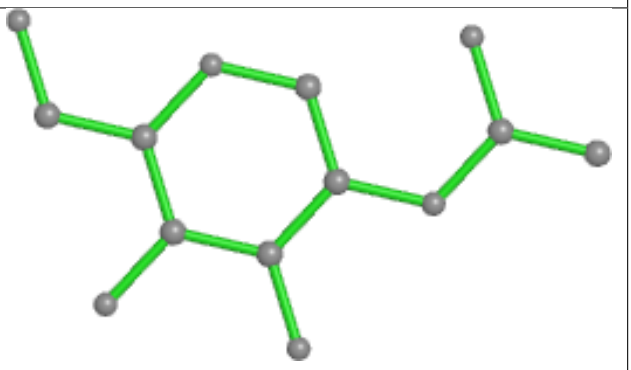
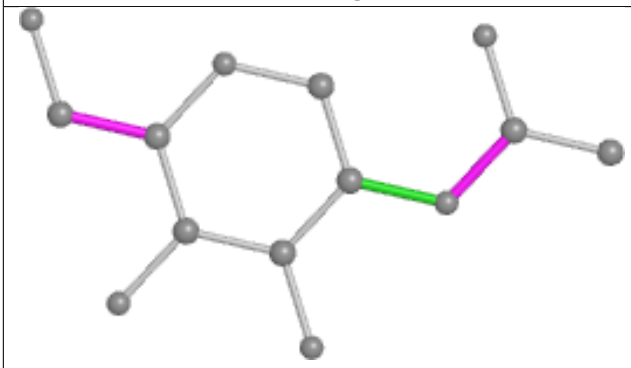
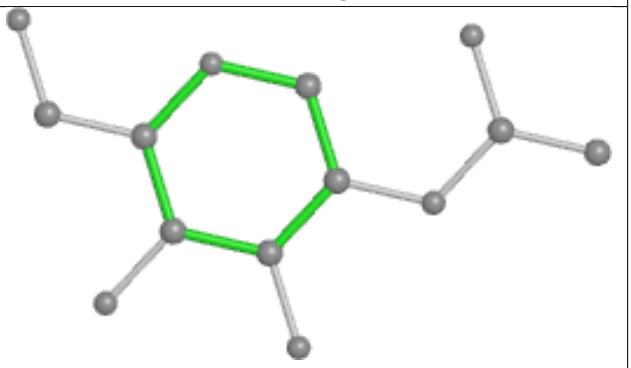


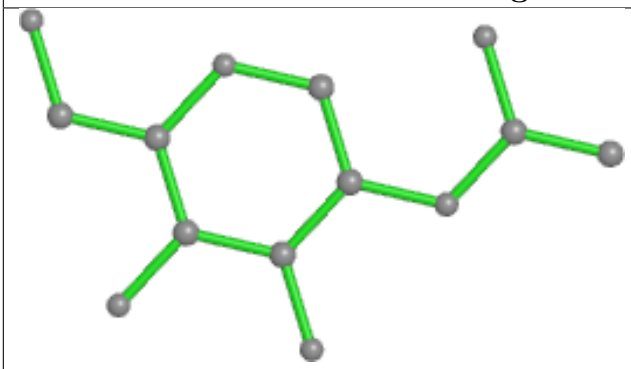
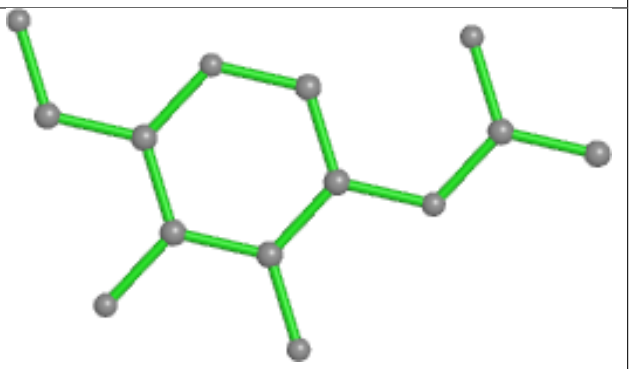
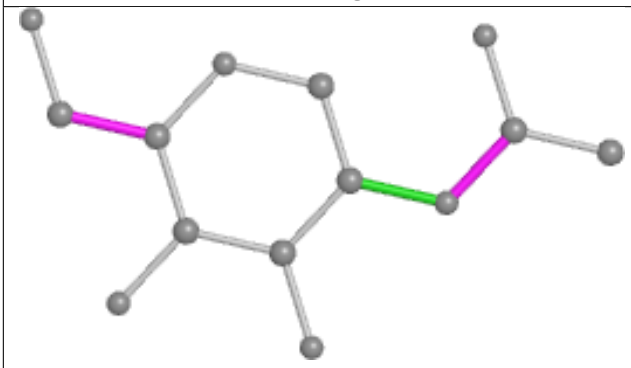
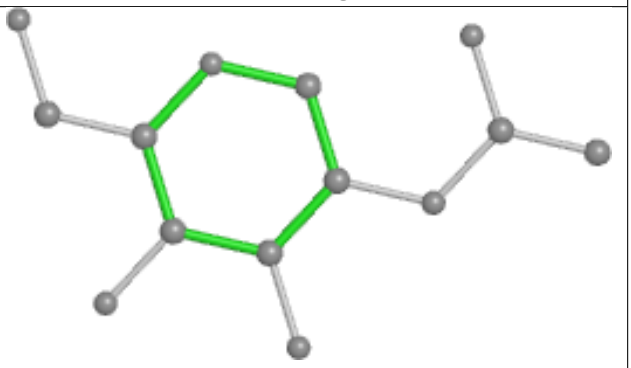
Torsions

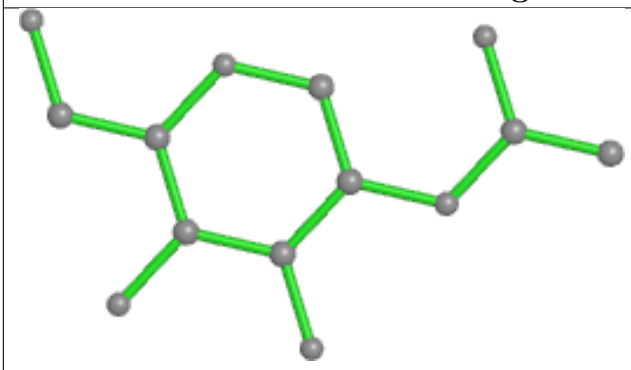
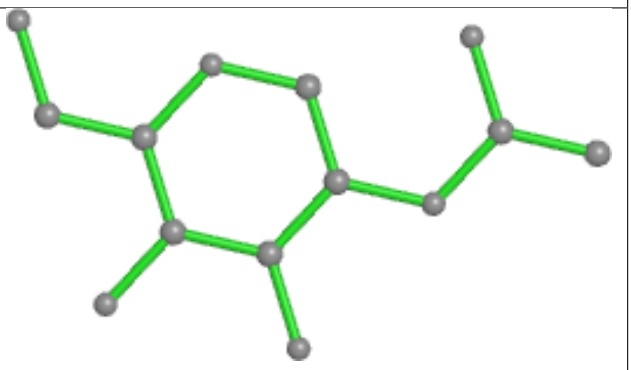
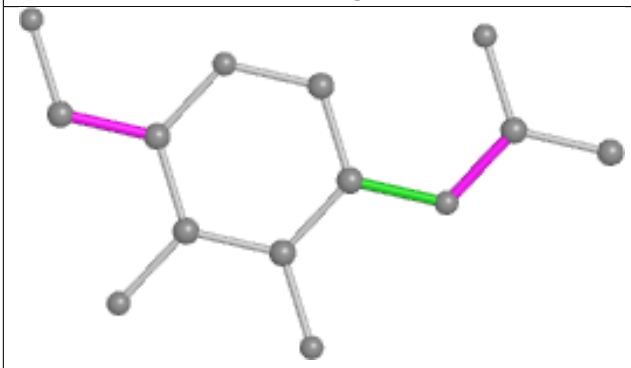
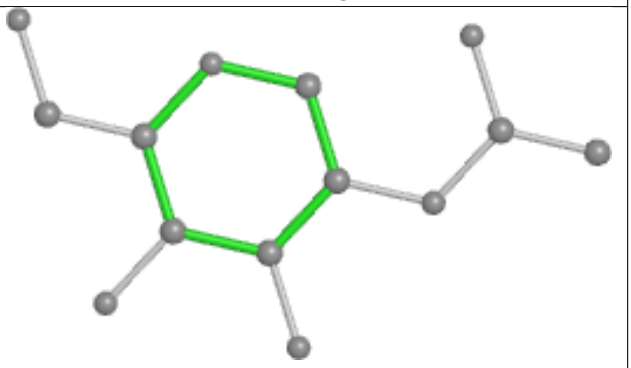


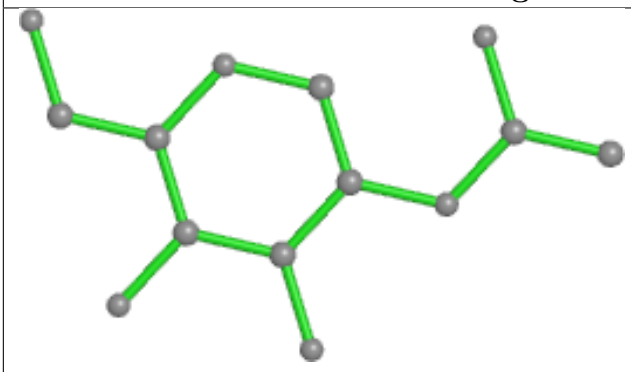
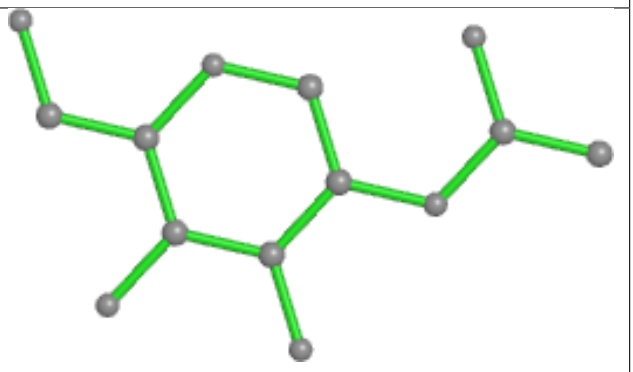
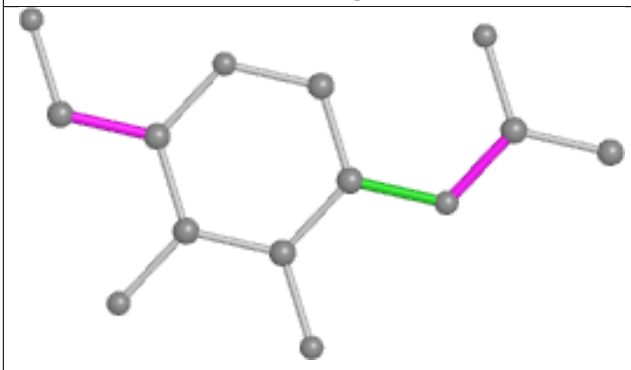
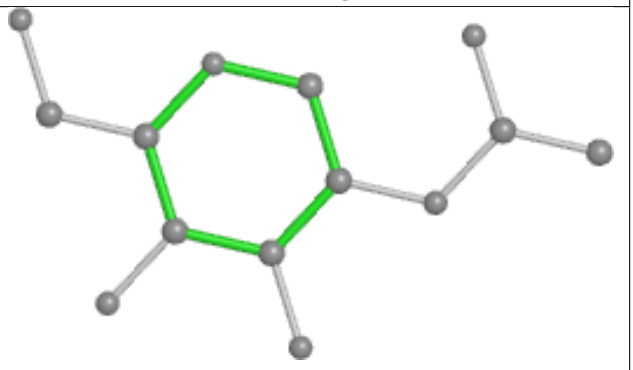
Rings

Ligand NAG C 1201	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand NAG C 1204	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand NAG A 1202	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand NAG C 1202	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand NAG B 1202	
 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

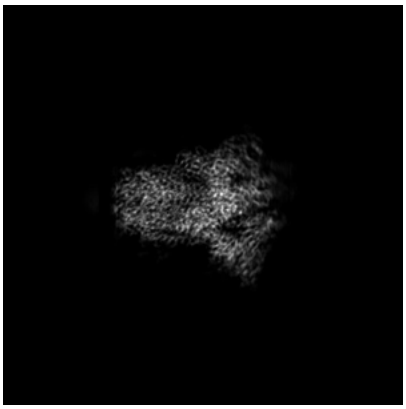
This section contains visualisations of the EMDB entry EMD-38460. These allow visual inspection of the internal detail of the map and identification of artifacts.

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.

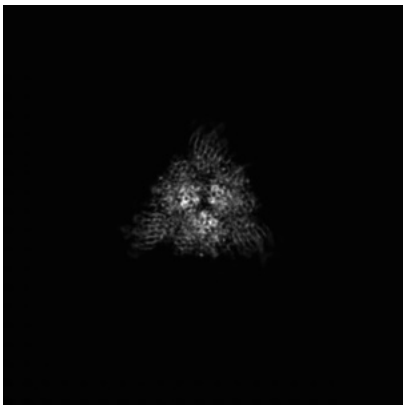
6.1 Orthogonal projections

6.1.1 Primary map

X

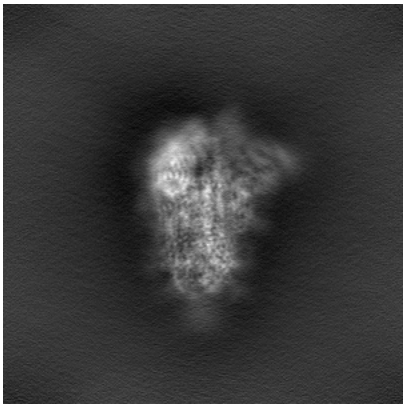


Y

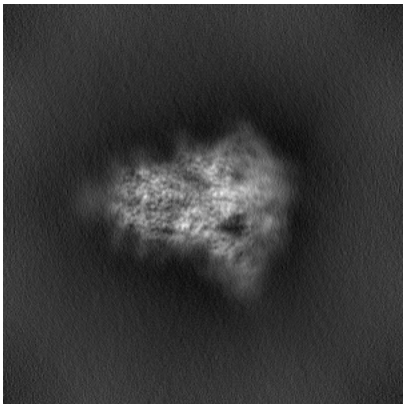


Z

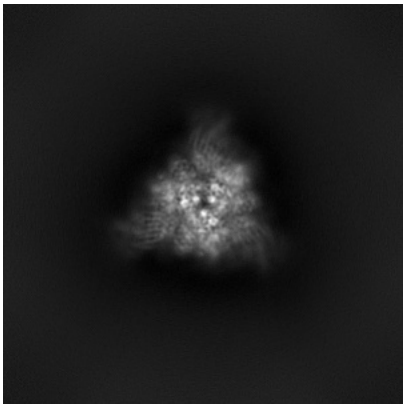
6.1.2 Raw map



X



Y



Z

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

6.2 Central slices (i)

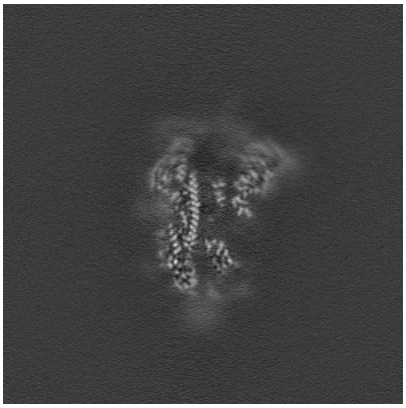
6.2.1 Primary map

X Index: 250

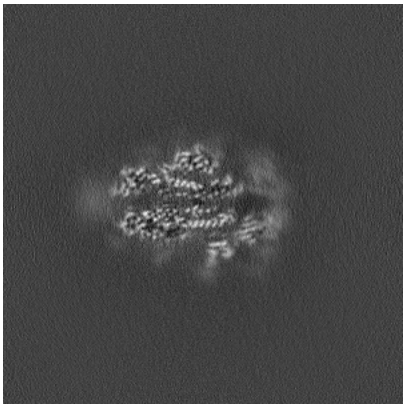
Y Index: 250

Z Index: 250

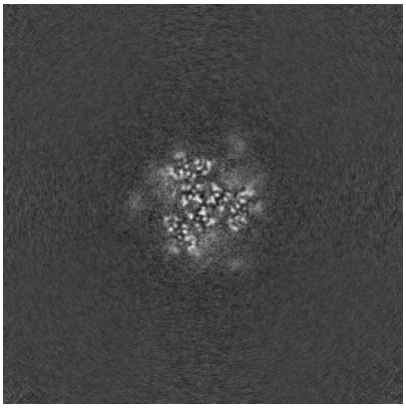
6.2.2 Raw map



X Index: 250



Y Index: 250



Z Index: 250

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

6.3 Largest variance slices (i)

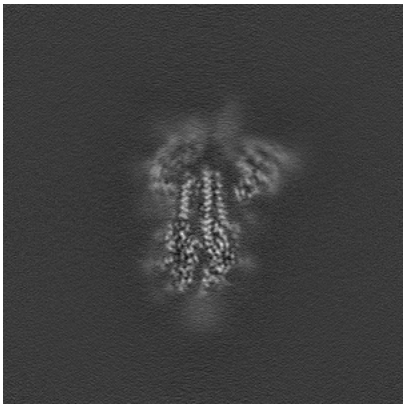
6.3.1 Primary map

X Index: 266

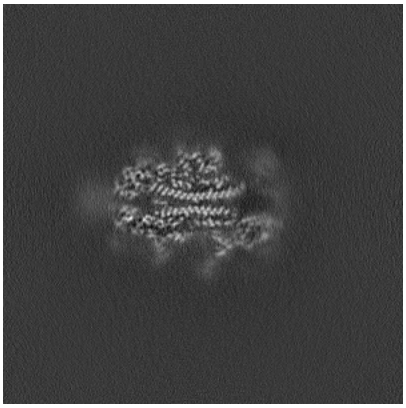
Y Index: 254

Z Index: 266

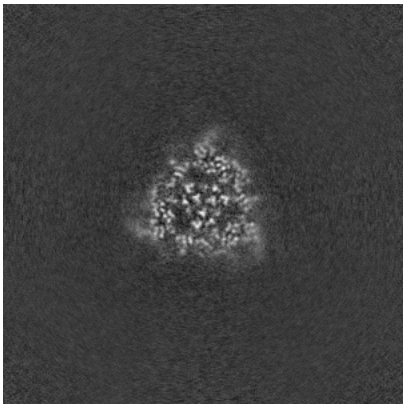
6.3.2 Raw map



X Index: 262



Y Index: 255

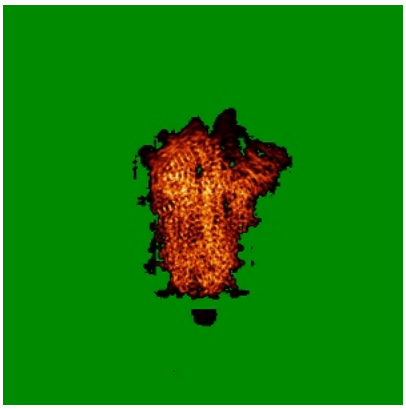


Z Index: 266

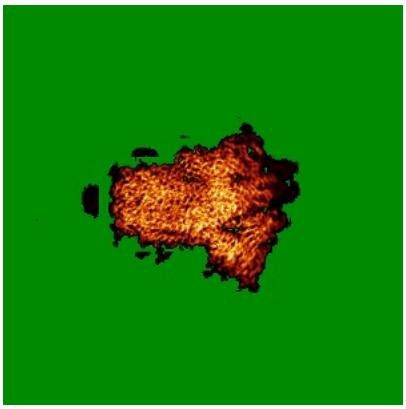
The images above show the largest variance slices of the map in three orthogonal directions.

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

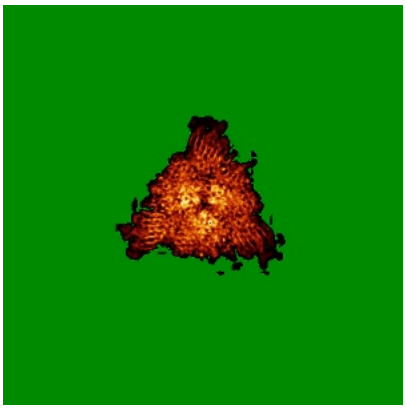
6.4.1 Primary map



X

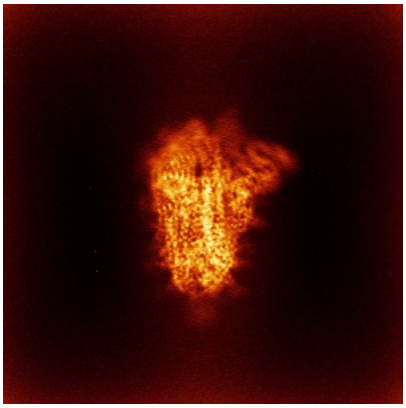


Y

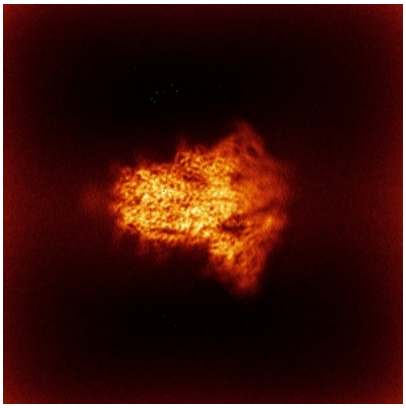


Z

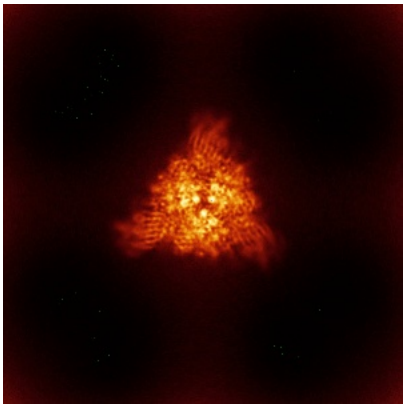
6.4.2 Raw map



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 0.05. 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.

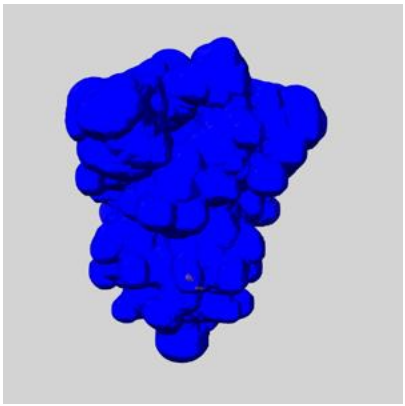
6.6 Mask visualisation

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

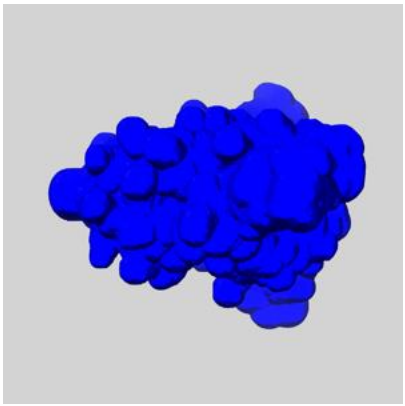
A mask typically either:

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

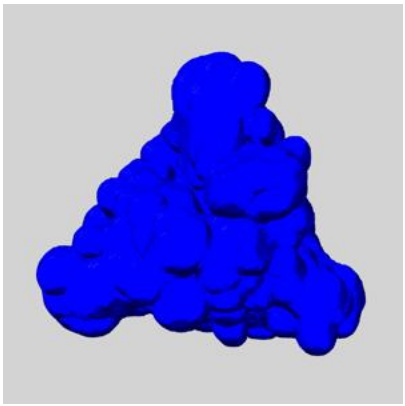
6.6.1 emd_38460_msk_1.map



X



Y

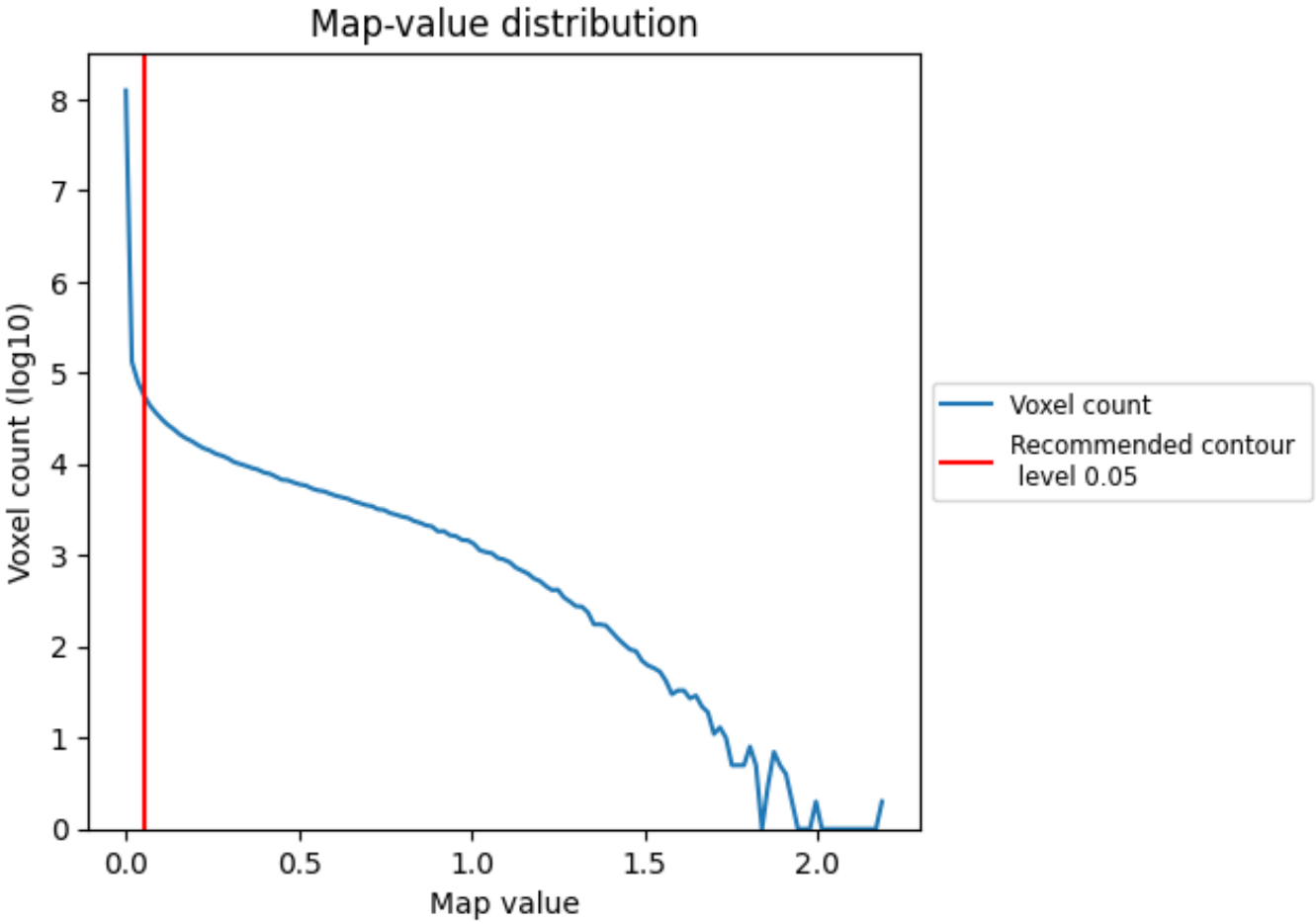


Z

7 Map analysis

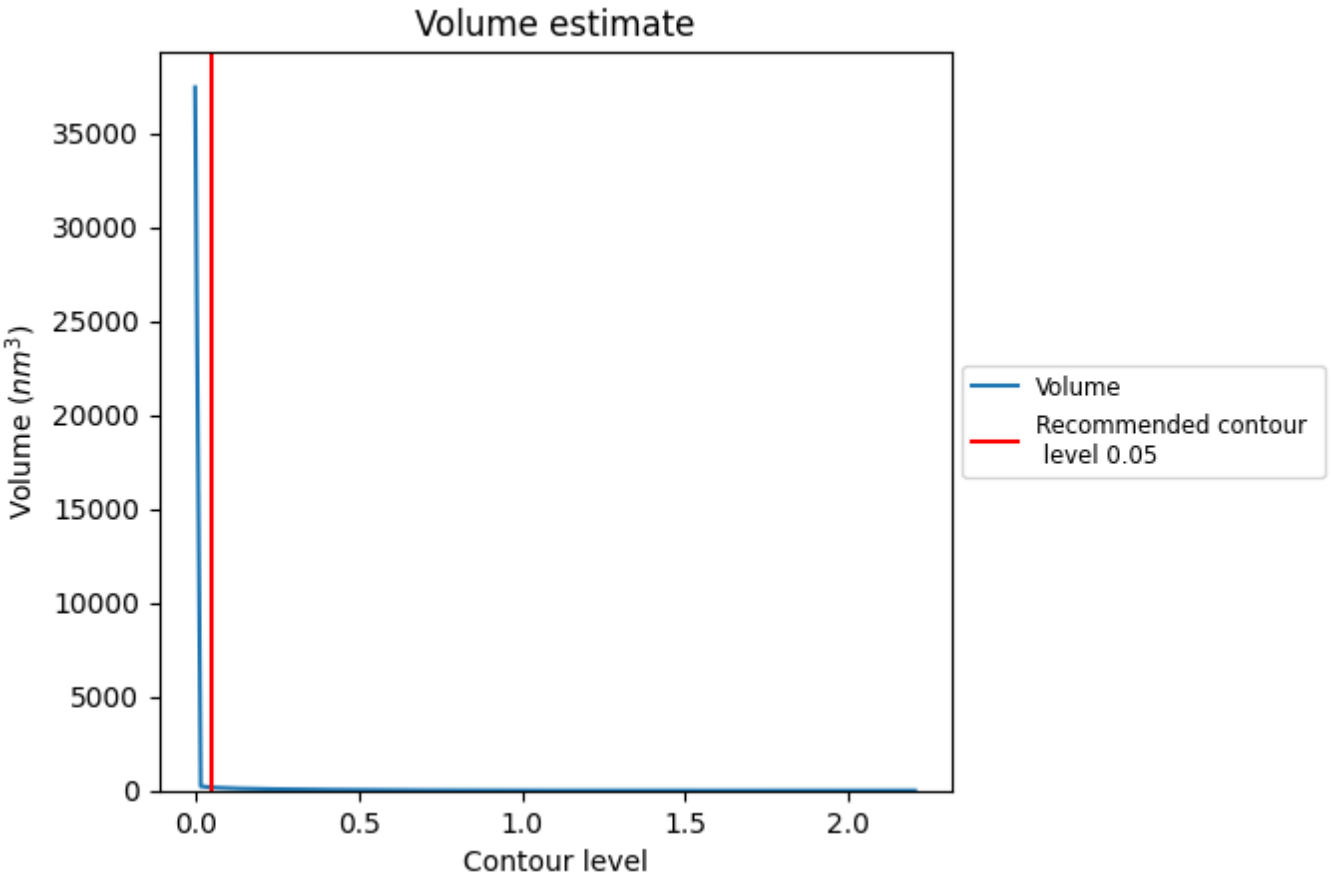
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

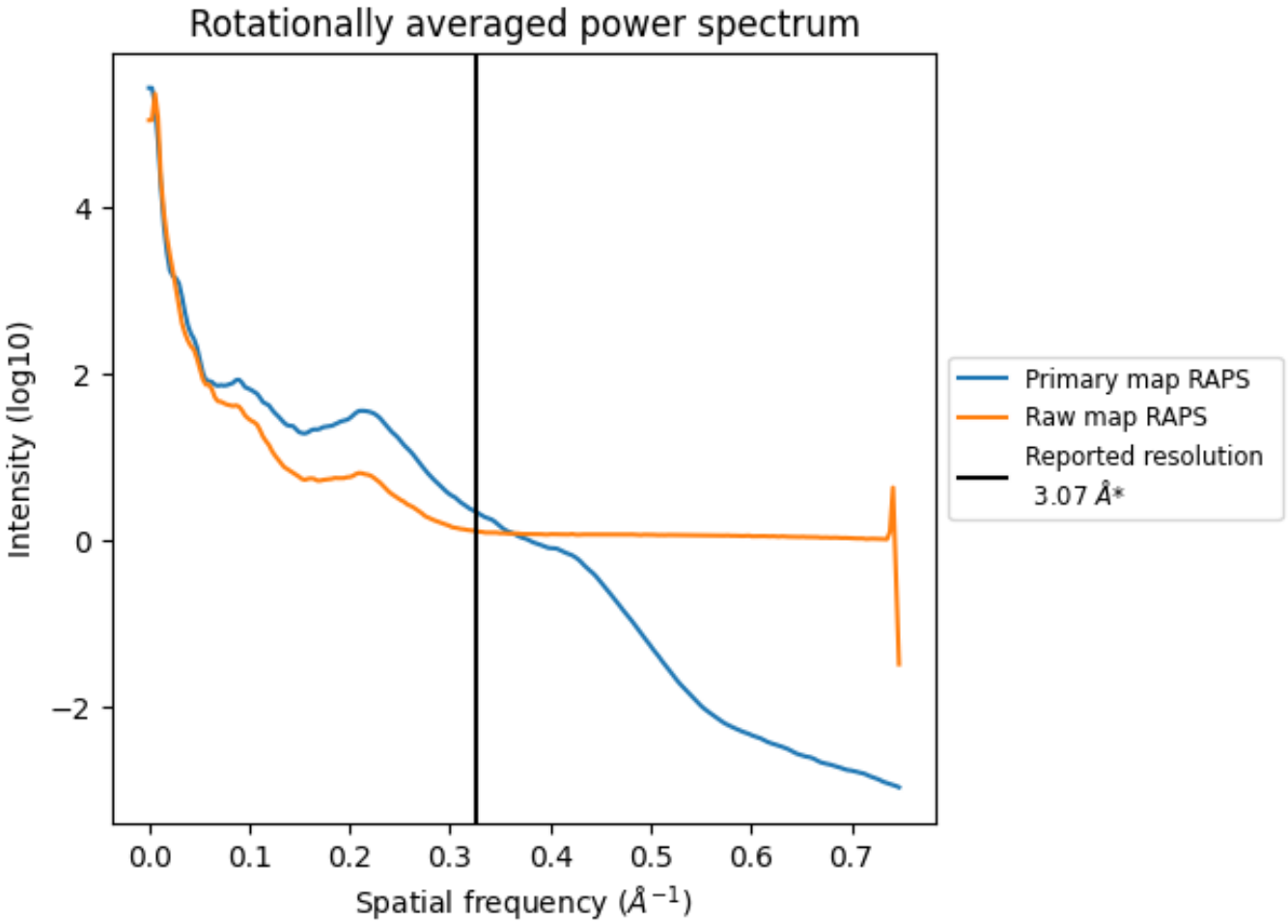
7.2 Volume estimate (i)



The volume at the recommended contour level is 168 nm^3; this corresponds to an approximate mass of 152 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)

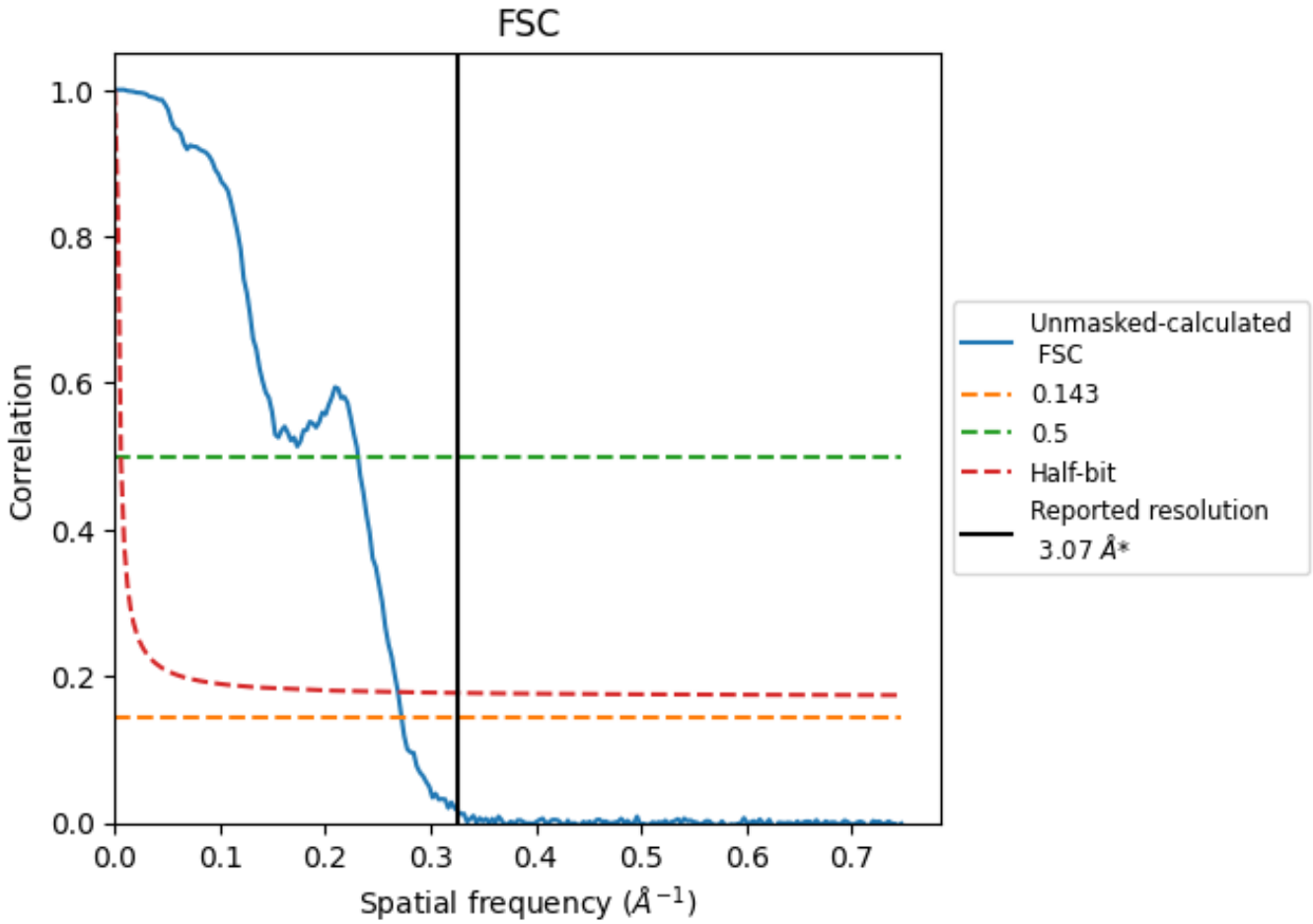


*Reported resolution corresponds to spatial frequency of 0.326 Å^{-1}

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 0.326 Å^{-1}

8.2 Resolution estimates (i)

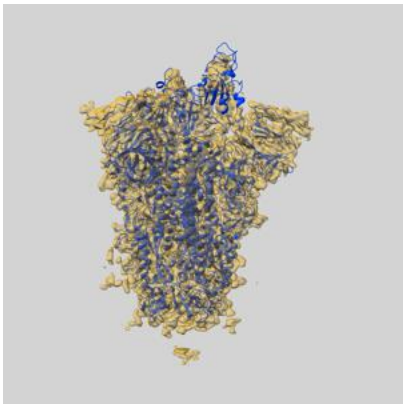
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.07	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.67	4.33	3.72

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.67 differs from the reported value 3.07 by more than 10 %

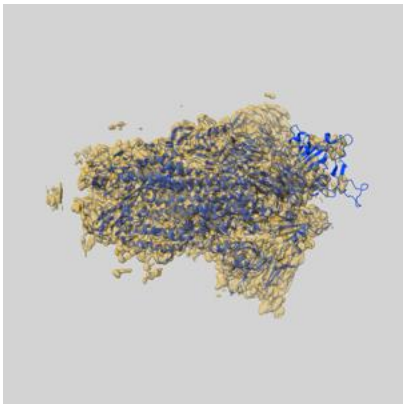
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-38460 and PDB model 8XLV. Per-residue inclusion information can be found in section 3 on page 17.

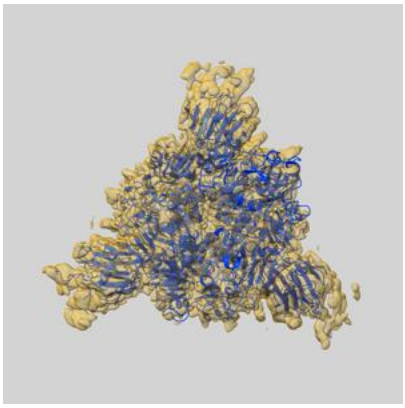
9.1 Map-model overlay



X



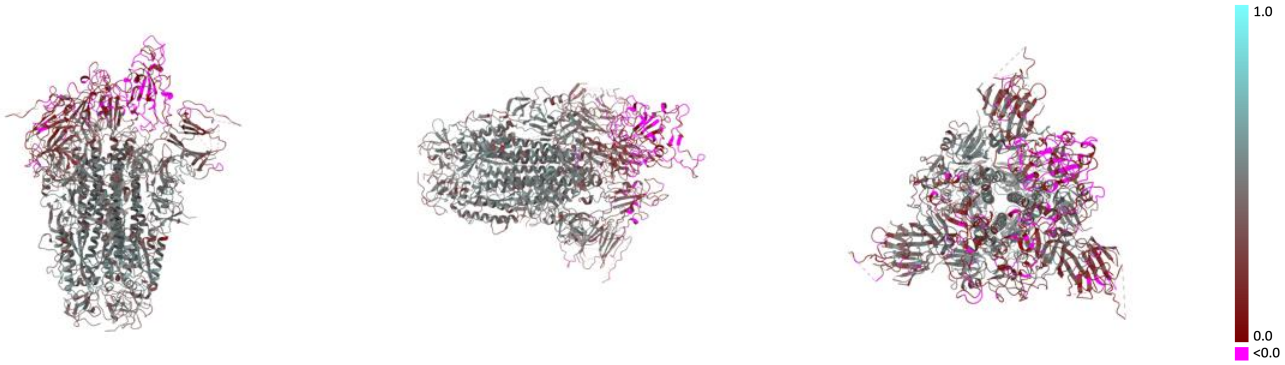
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.05 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

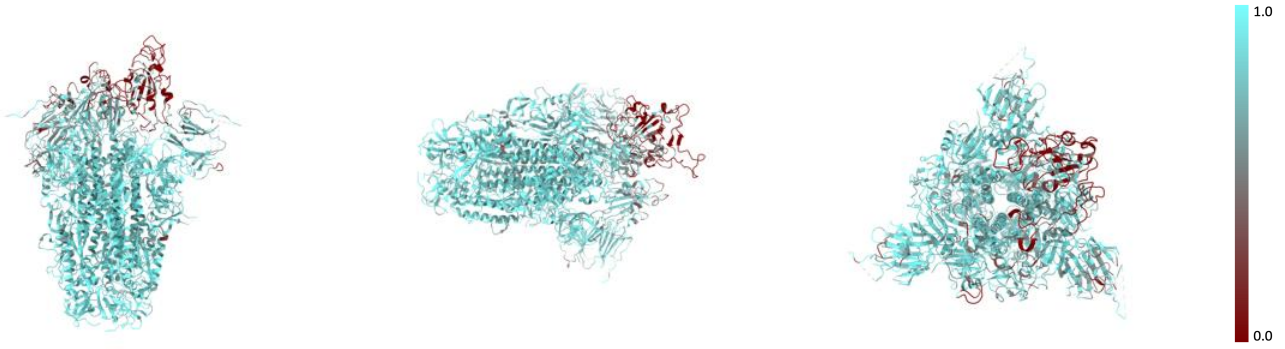
9.2 Q-score mapped to coordinate model



X Y Z

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

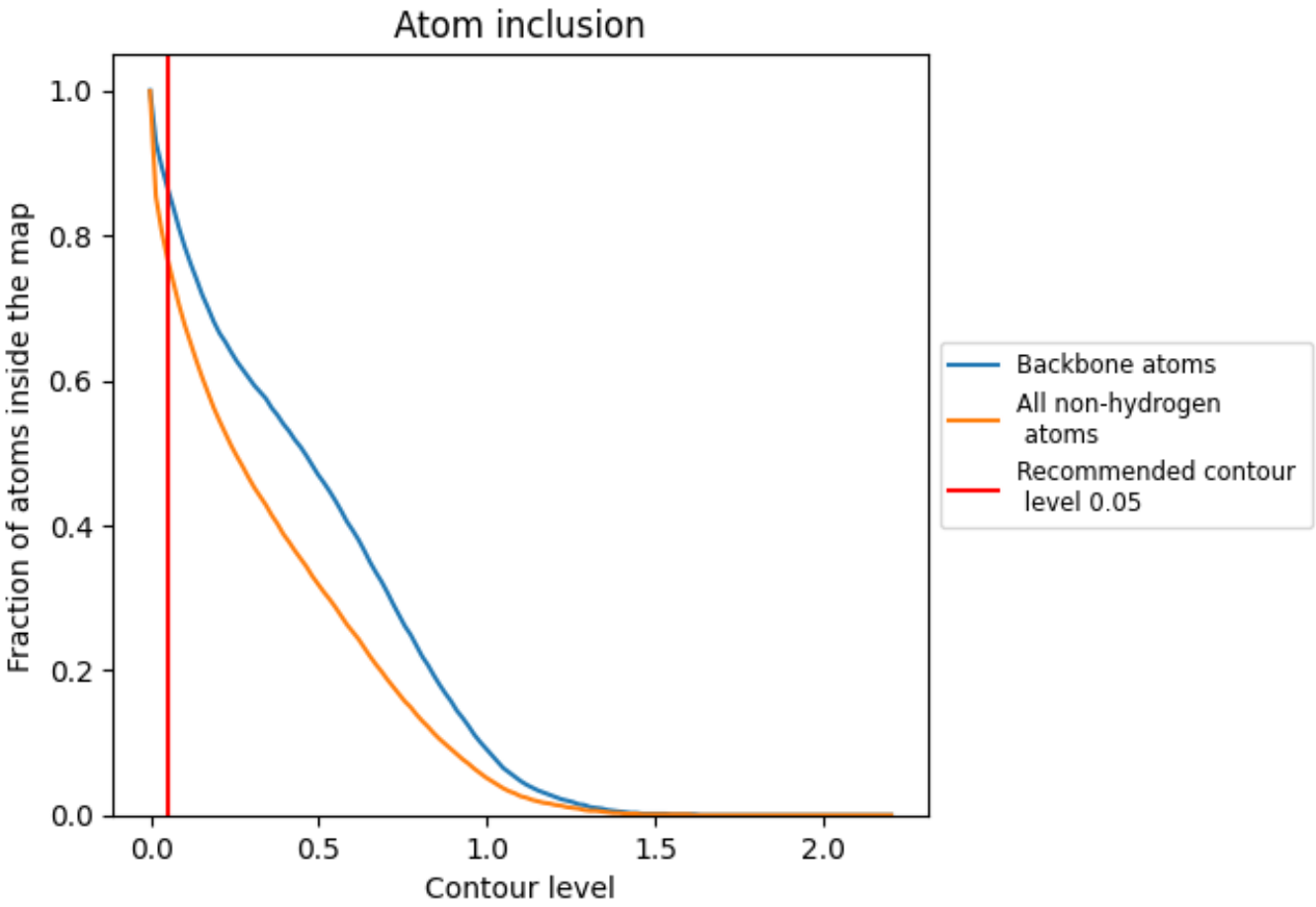
9.3 Atom inclusion mapped to coordinate model



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.05).

9.4 Atom inclusion (i)



At the recommended contour level, 87% of all backbone atoms, 77% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.05) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7680	0.3540
A	0.7850	0.3620
B	0.7190	0.3290
C	0.8070	0.3750
D	0.7860	0.4150
E	0.5710	0.2450
F	0.7140	0.3820
G	0.2140	-0.0050
H	0.0710	0.1470
I	0.2500	0.0110