wwPDB EM Validation Summary Report (i)

Jul 25, 2023 – 12:16 PM EDT

PDB ID	:	7TCN
EMDB ID	:	EMD-25814
Title	:	Cryo-EM structure of CH235.12 in complex with HIV-1 Env trimer CH505T F.N279K.SOSIP.664 with high-mannose glycans
Authors	:	Manne, K.; Henderson, R.; Acharya, P.
Deposited on	:	2021-12-27
Resolution	:	4.10 Å(reported)
Based on initial models	:	6UDA, 5F96

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 (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

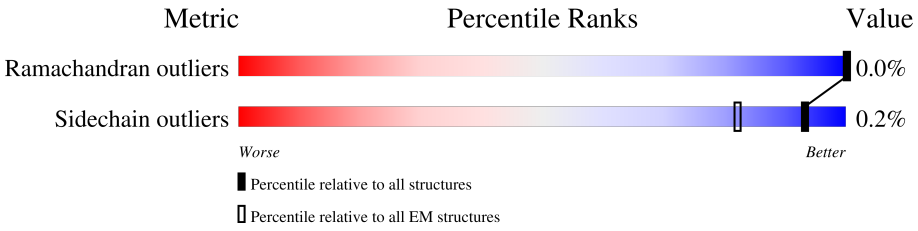
EMDB validation analysis	:	0.0.1.dev50
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.34

1 Overall quality at a glance

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

The reported resolution of this entry is 4.10 Å.

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



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

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

Mol	Chain	Length	Quality of chain
1	A	486	5% 88% 12%
1	E	486	6% 90% 10%
1	I	486	6% 90% 10%
2	B	160	7% 76% 24%
2	F	160	6% 75% 24%
2	J	160	7% 76% 24%
3	C	225	11% 97%
3	G	225	12% 97%
3	K	225	12% 97%

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Mol	Chain	Length	Quality of chain
4	D	213	18% 99%
4	H	213	17% 99%
4	L	213	16% 99%
5	0	3	67% 33%
5	M	3	33% 67%
5	N	3	33% 100%
5	e	3	33% 100%
5	j	3	67% 33%
5	v	3	33% 67% 33%
6	4	4	25% 75% 25%
6	R	4	25% 75% 25%
6	n	4	25% 75% 25%
7	h	2	50% 50% 50%
7	y	2	50% 50% 50%

2 Entry composition (i)

There are 9 unique types of molecules in this entry. The entry contains 23747 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Envelope glycoprotein gp160.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	426	Total	C	N	O	S	0	0
			3357	2112	587	632	26		
1	E	438	Total	C	N	O	S	0	0
			3446	2167	603	648	28		
1	I	438	Total	C	N	O	S	0	0
			3446	2167	603	648	28		

There are 108 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	7	MET	-	initiating methionine	UNP M4M0W3
A	8	PRO	-	expression tag	UNP M4M0W3
A	9	MET	-	expression tag	UNP M4M0W3
A	10	GLY	-	expression tag	UNP M4M0W3
A	11	SER	-	expression tag	UNP M4M0W3
A	12	LEU	-	expression tag	UNP M4M0W3
A	13	GLN	-	expression tag	UNP M4M0W3
A	14	PRO	-	expression tag	UNP M4M0W3
A	15	LEU	-	expression tag	UNP M4M0W3
A	16	ALA	-	expression tag	UNP M4M0W3
A	17	THR	-	expression tag	UNP M4M0W3
A	18	LEU	-	expression tag	UNP M4M0W3
A	19	TYR	-	expression tag	UNP M4M0W3
A	20	LEU	-	expression tag	UNP M4M0W3
A	21	LEU	-	expression tag	UNP M4M0W3
A	22	GLY	-	expression tag	UNP M4M0W3
A	23	MET	-	expression tag	UNP M4M0W3
A	24	LEU	-	expression tag	UNP M4M0W3
A	25	VAL	-	expression tag	UNP M4M0W3
A	26	ALA	-	expression tag	UNP M4M0W3
A	27	SER	-	expression tag	UNP M4M0W3
A	28	VAL	-	expression tag	UNP M4M0W3
A	29	LEU	-	expression tag	UNP M4M0W3
A	30	ALA	-	expression tag	UNP M4M0W3

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Chain	Residue	Modelled	Actual	Comment	Reference
A	31	ALA	-	expression tag	UNP M4M0W3
A	32	GLU	-	expression tag	UNP M4M0W3
A	33	ASN	-	expression tag	UNP M4M0W3
A	34	LEU	-	expression tag	UNP M4M0W3
A	64	LYS	GLU	conflict	UNP M4M0W3
A	316	TRP	ALA	conflict	UNP M4M0W3
A	488	LYS	GLU	conflict	UNP M4M0W3
A	489	ILE	VAL	conflict	UNP M4M0W3
A	490	GLU	LYS	conflict	UNP M4M0W3
A	498	ARG	ASN	conflict	UNP M4M0W3
A	499	CYS	ALA	conflict	UNP M4M0W3
A	500	LYS	ARG	conflict	UNP M4M0W3
E	7	MET	-	initiating methionine	UNP M4M0W3
E	8	PRO	-	expression tag	UNP M4M0W3
E	9	MET	-	expression tag	UNP M4M0W3
E	10	GLY	-	expression tag	UNP M4M0W3
E	11	SER	-	expression tag	UNP M4M0W3
E	12	LEU	-	expression tag	UNP M4M0W3
E	13	GLN	-	expression tag	UNP M4M0W3
E	14	PRO	-	expression tag	UNP M4M0W3
E	15	LEU	-	expression tag	UNP M4M0W3
E	16	ALA	-	expression tag	UNP M4M0W3
E	17	THR	-	expression tag	UNP M4M0W3
E	18	LEU	-	expression tag	UNP M4M0W3
E	19	TYR	-	expression tag	UNP M4M0W3
E	20	LEU	-	expression tag	UNP M4M0W3
E	21	LEU	-	expression tag	UNP M4M0W3
E	22	GLY	-	expression tag	UNP M4M0W3
E	23	MET	-	expression tag	UNP M4M0W3
E	24	LEU	-	expression tag	UNP M4M0W3
E	25	VAL	-	expression tag	UNP M4M0W3
E	26	ALA	-	expression tag	UNP M4M0W3
E	27	SER	-	expression tag	UNP M4M0W3
E	28	VAL	-	expression tag	UNP M4M0W3
E	29	LEU	-	expression tag	UNP M4M0W3
E	30	ALA	-	expression tag	UNP M4M0W3
E	31	ALA	-	expression tag	UNP M4M0W3
E	32	GLU	-	expression tag	UNP M4M0W3
E	33	ASN	-	expression tag	UNP M4M0W3
E	34	LEU	-	expression tag	UNP M4M0W3
E	64	LYS	GLU	conflict	UNP M4M0W3
E	316	TRP	ALA	conflict	UNP M4M0W3

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Chain	Residue	Modelled	Actual	Comment	Reference
E	488	LYS	GLU	conflict	UNP M4M0W3
E	489	ILE	VAL	conflict	UNP M4M0W3
E	490	GLU	LYS	conflict	UNP M4M0W3
E	498	ARG	ASN	conflict	UNP M4M0W3
E	499	CYS	ALA	conflict	UNP M4M0W3
E	500	LYS	ARG	conflict	UNP M4M0W3
I	7	MET	-	initiating methionine	UNP M4M0W3
I	8	PRO	-	expression tag	UNP M4M0W3
I	9	MET	-	expression tag	UNP M4M0W3
I	10	GLY	-	expression tag	UNP M4M0W3
I	11	SER	-	expression tag	UNP M4M0W3
I	12	LEU	-	expression tag	UNP M4M0W3
I	13	GLN	-	expression tag	UNP M4M0W3
I	14	PRO	-	expression tag	UNP M4M0W3
I	15	LEU	-	expression tag	UNP M4M0W3
I	16	ALA	-	expression tag	UNP M4M0W3
I	17	THR	-	expression tag	UNP M4M0W3
I	18	LEU	-	expression tag	UNP M4M0W3
I	19	TYR	-	expression tag	UNP M4M0W3
I	20	LEU	-	expression tag	UNP M4M0W3
I	21	LEU	-	expression tag	UNP M4M0W3
I	22	GLY	-	expression tag	UNP M4M0W3
I	23	MET	-	expression tag	UNP M4M0W3
I	24	LEU	-	expression tag	UNP M4M0W3
I	25	VAL	-	expression tag	UNP M4M0W3
I	26	ALA	-	expression tag	UNP M4M0W3
I	27	SER	-	expression tag	UNP M4M0W3
I	28	VAL	-	expression tag	UNP M4M0W3
I	29	LEU	-	expression tag	UNP M4M0W3
I	30	ALA	-	expression tag	UNP M4M0W3
I	31	ALA	-	expression tag	UNP M4M0W3
I	32	GLU	-	expression tag	UNP M4M0W3
I	33	ASN	-	expression tag	UNP M4M0W3
I	34	LEU	-	expression tag	UNP M4M0W3
I	64	LYS	GLU	conflict	UNP M4M0W3
I	316	TRP	ALA	conflict	UNP M4M0W3
I	488	LYS	GLU	conflict	UNP M4M0W3
I	489	ILE	VAL	conflict	UNP M4M0W3
I	490	GLU	LYS	conflict	UNP M4M0W3
I	498	ARG	ASN	conflict	UNP M4M0W3
I	499	CYS	ALA	conflict	UNP M4M0W3
I	500	LYS	ARG	conflict	UNP M4M0W3

- Molecule 2 is a protein called Glycoprotein 41.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	122	Total	C	N	O	S	0	0
			969	611	167	185	6		
2	F	122	Total	C	N	O	S	0	0
			969	611	167	185	6		
2	J	122	Total	C	N	O	S	0	0
			969	611	167	185	6		

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	505	GLY	-	expression tag	UNP Q2N0S5
B	506	ARG	-	expression tag	UNP Q2N0S5
B	507	ARG	-	expression tag	UNP Q2N0S5
B	508	ARG	-	expression tag	UNP Q2N0S5
B	509	ARG	-	expression tag	UNP Q2N0S5
B	510	ARG	-	expression tag	UNP Q2N0S5
B	559	PRO	ILE	conflict	UNP Q2N0S5
B	605	CYS	THR	conflict	UNP Q2N0S5
F	505	GLY	-	expression tag	UNP Q2N0S5
F	506	ARG	-	expression tag	UNP Q2N0S5
F	507	ARG	-	expression tag	UNP Q2N0S5
F	508	ARG	-	expression tag	UNP Q2N0S5
F	509	ARG	-	expression tag	UNP Q2N0S5
F	510	ARG	-	expression tag	UNP Q2N0S5
F	559	PRO	ILE	conflict	UNP Q2N0S5
F	605	CYS	THR	conflict	UNP Q2N0S5
J	505	GLY	-	expression tag	UNP Q2N0S5
J	506	ARG	-	expression tag	UNP Q2N0S5
J	507	ARG	-	expression tag	UNP Q2N0S5
J	508	ARG	-	expression tag	UNP Q2N0S5
J	509	ARG	-	expression tag	UNP Q2N0S5
J	510	ARG	-	expression tag	UNP Q2N0S5
J	559	PRO	ILE	conflict	UNP Q2N0S5
J	605	CYS	THR	conflict	UNP Q2N0S5

- Molecule 3 is a protein called CH235.12 Fab Heavy Chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	220	Total	C	N	O	S	0	0
			1677	1061	287	320	9		
3	G	220	Total	C	N	O	S	0	0
			1677	1061	287	320	9		

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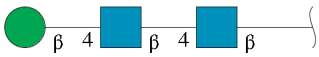
Mol	Chain	Residues	Atoms					AltConf	Trace
3	K	220	Total	C	N	O	S	0	0
			1677	1061	287	320	9		

- Molecule 4 is a protein called CH235.12 Fab Light Chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	211	Total	C	N	O	S	0	0
			1635	1022	285	324	4		
4	H	211	Total	C	N	O	S	0	0
			1635	1022	285	324	4		
4	L	211	Total	C	N	O	S	0	0
			1635	1022	285	324	4		

- Molecule 5 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
5	0	3	Total	C	N	O	0	0
			39	22	2	15		
5	M	3	Total	C	N	O	0	0
			39	22	2	15		
5	N	3	Total	C	N	O	0	0
			39	22	2	15		
5	e	3	Total	C	N	O	0	0
			39	22	2	15		
5	j	3	Total	C	N	O	0	0
			39	22	2	15		
5	v	3	Total	C	N	O	0	0
			39	22	2	15		

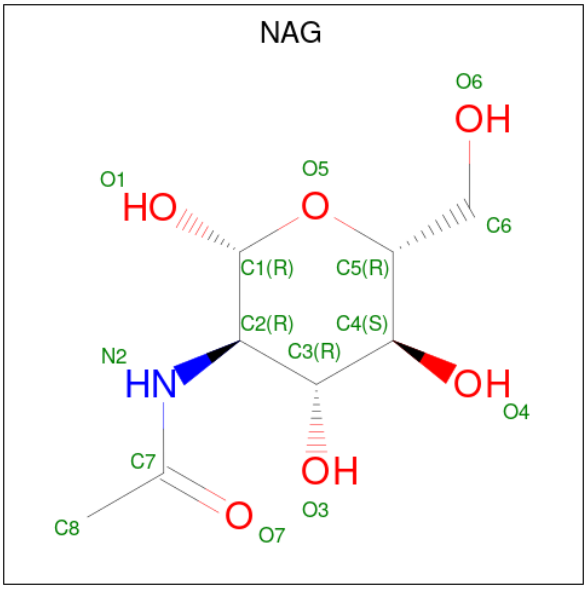
- Molecule 6 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

Mol	Chain	Residues	Atoms	AltConf	Trace
6	4	4	Total C N O 50 28 2 20	0	0
6	R	4	Total C N O 50 28 2 20	0	0
6	n	4	Total C N O 50 28 2 20	0	0

- Molecule 7 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
7	h	2	Total C N O 28 16 2 10	0	0
7	y	2	Total C N O 28 16 2 10	0	0

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

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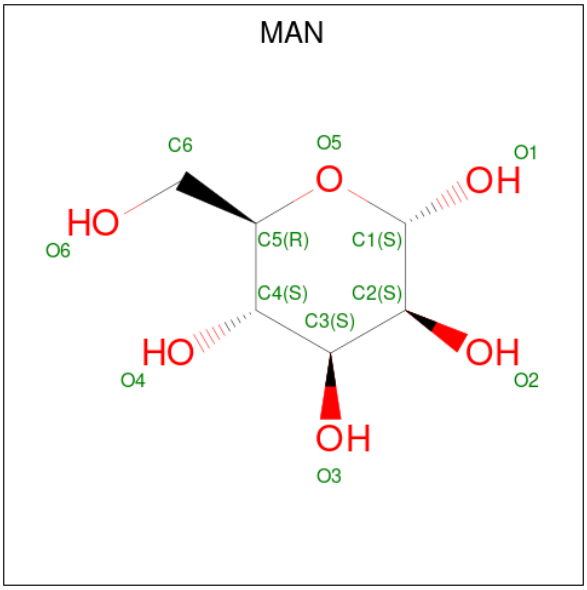
Mol	Chain	Residues	Atoms				AltConf
8	A	1	Total	C	N	O	0
			14	8	1	5	
8	A	1	Total	C	N	O	0
			14	8	1	5	
8	A	1	Total	C	N	O	0
			14	8	1	5	
8	A	1	Total	C	N	O	0
			14	8	1	5	
8	E	1	Total	C	N	O	0
			14	8	1	5	
8	E	1	Total	C	N	O	0
			14	8	1	5	
8	E	1	Total	C	N	O	0
			14	8	1	5	
8	E	1	Total	C	N	O	0
			14	8	1	5	
8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

- Molecule 9 is alpha-D-mannopyranose (three-letter code: MAN) (formula: $C_6H_{12}O_6$) (labeled as "Ligand of Interest" by depositor).



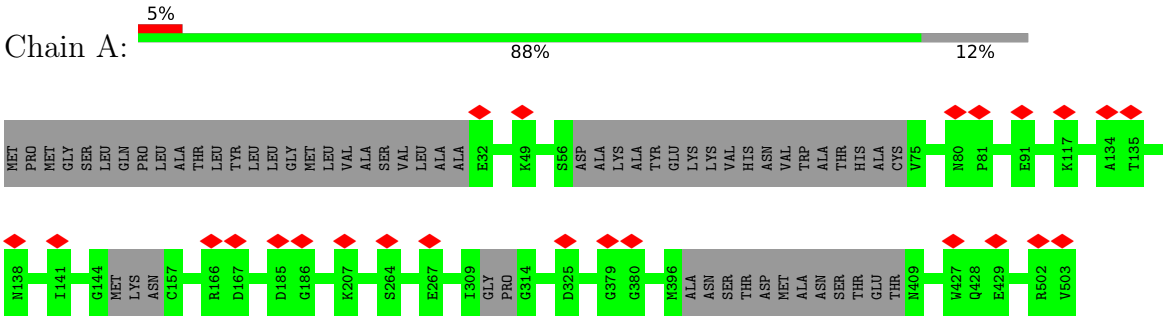
Mol	Chain	Residues	Atoms			AltConf
9	C	1	Total	C	O	0
			11	6	5	
9	G	1	Total	C	O	0
			11	6	5	
9	K	1	Total	C	O	0
			11	6	5	

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.

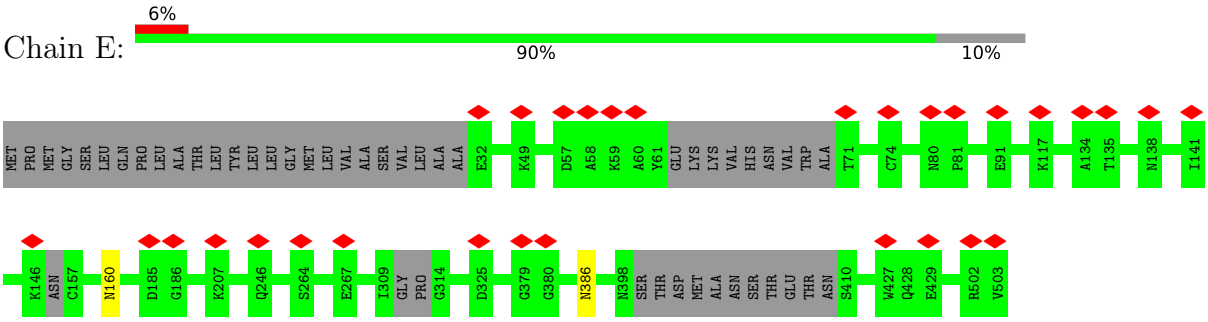
• Molecule 1: Envelope glycoprotein gp160

Chain A:



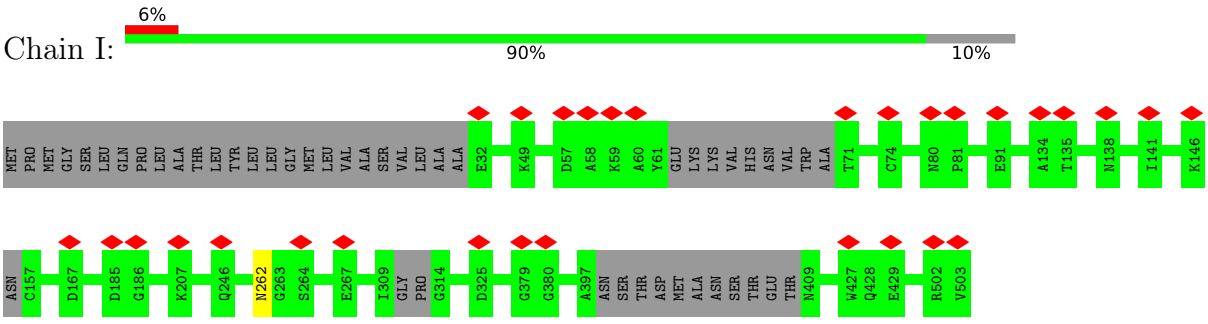
• Molecule 1: Envelope glycoprotein gp160

Chain E:



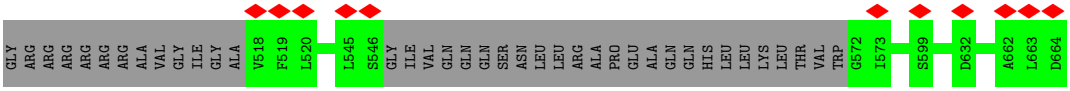
• Molecule 1: Envelope glycoprotein gp160

Chain I:

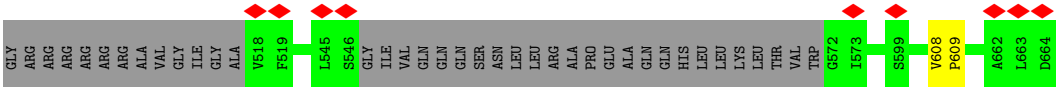


• Molecule 2: Glycoprotein 41

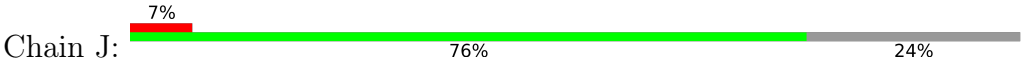
Chain B:

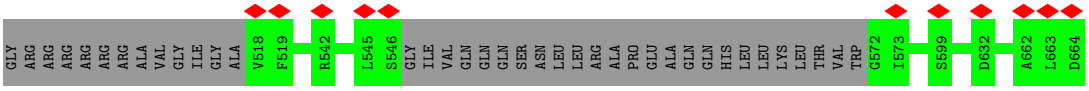


• Molecule 2: Glycoprotein 41

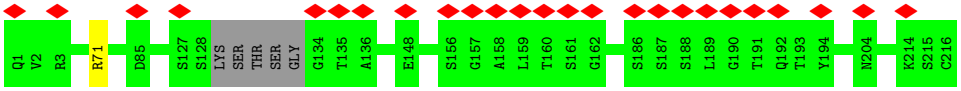


• Molecule 2: Glycoprotein 41

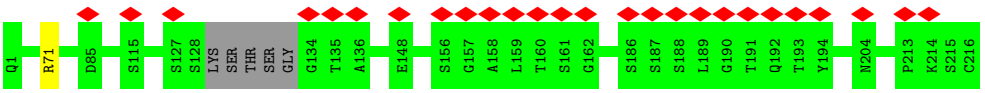




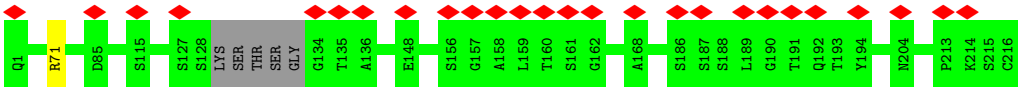
• Molecule 3: CH235.12 Fab Heavy Chain



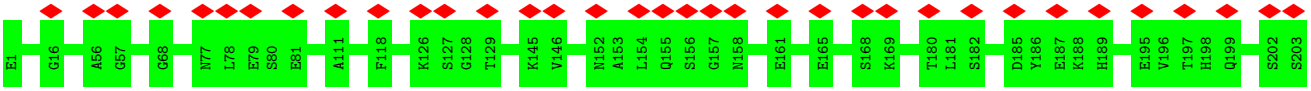
• Molecule 3: CH235.12 Fab Heavy Chain

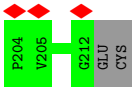


• Molecule 3: CH235.12 Fab Heavy Chain



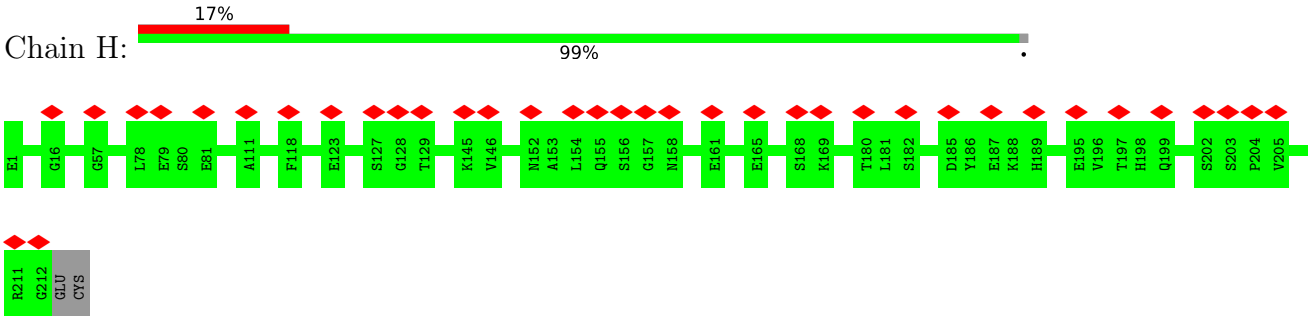
• Molecule 4: CH235.12 Fab Light Chain





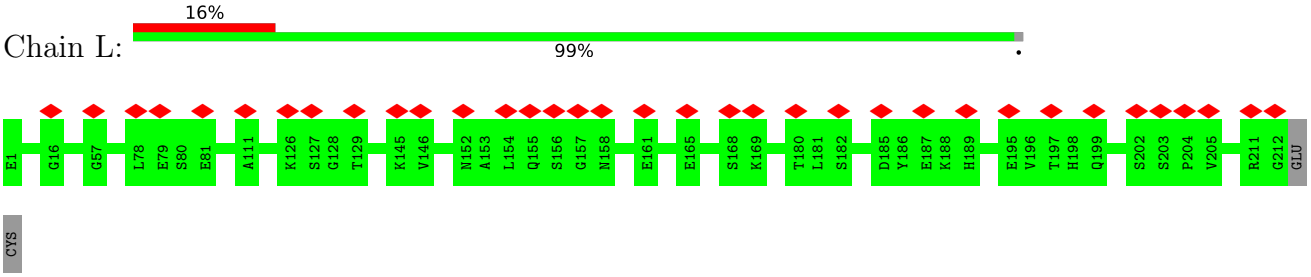
• Molecule 4: CH235.12 Fab Light Chain

Chain H:



• Molecule 4: CH235.12 Fab Light Chain

Chain L:



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

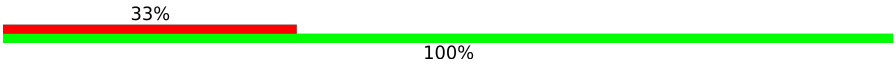
Chain 0:

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

Chain M:

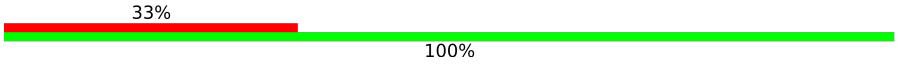
• Molecule 5: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain N:



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

Chain e:



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

Chain j:

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

Chain v:

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

Chain 4:

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

Chain R:

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

Chain n:

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

Chain h:

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

Chain y:

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	53398	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 ($e^-/Å^2$)	66.71	Depositor
Minimum defocus (nm)	750	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	3.037	Depositor
Minimum map value	-0.587	Depositor
Average map value	0.004	Depositor
Map value standard deviation	0.127	Depositor
Recommended contour level	1.0	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: BMA, NAG, MAN

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.28	0/3421	0.59	0/4636
1	E	0.28	0/3512	0.61	0/4758
1	I	0.28	0/3512	0.59	0/4758
2	B	0.30	0/985	0.59	0/1334
2	F	0.35	0/985	0.62	0/1334
2	J	0.29	0/985	0.58	0/1334
3	C	0.30	0/1720	0.60	0/2341
3	G	0.31	0/1720	0.64	0/2341
3	K	0.30	0/1720	0.62	0/2341
4	D	0.28	0/1671	0.61	0/2272
4	H	0.28	0/1671	0.61	0/2272
4	L	0.28	0/1671	0.60	0/2272
All	All	0.29	0/23573	0.60	0/31993

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	F	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	F	609	PRO	Peptide

5.2 Too-close contacts

Due to software issues we are unable to calculate clashes - this section is therefore empty.

5.3 Torsion angles

5.3.1 Protein backbone

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	416/486 (86%)	395 (95%)	21 (5%)	0	100	100
1	E	428/486 (88%)	405 (95%)	23 (5%)	0	100	100
1	I	428/486 (88%)	402 (94%)	26 (6%)	0	100	100
2	B	118/160 (74%)	109 (92%)	9 (8%)	0	100	100
2	F	118/160 (74%)	108 (92%)	9 (8%)	1 (1%)	19	58
2	J	118/160 (74%)	111 (94%)	7 (6%)	0	100	100
3	C	216/225 (96%)	204 (94%)	12 (6%)	0	100	100
3	G	216/225 (96%)	206 (95%)	10 (5%)	0	100	100
3	K	216/225 (96%)	200 (93%)	16 (7%)	0	100	100
4	D	209/213 (98%)	194 (93%)	15 (7%)	0	100	100
4	H	209/213 (98%)	193 (92%)	16 (8%)	0	100	100
4	L	209/213 (98%)	196 (94%)	13 (6%)	0	100	100
All	All	2901/3252 (89%)	2723 (94%)	177 (6%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	F	608	VAL

5.3.2 Protein sidechains

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	384/432 (89%)	384 (100%)	0	100 100
1	E	392/432 (91%)	390 (100%)	2 (0%)	88 93
1	I	392/432 (91%)	391 (100%)	1 (0%)	92 95
2	B	105/135 (78%)	105 (100%)	0	100 100
2	F	105/135 (78%)	105 (100%)	0	100 100
2	J	105/135 (78%)	105 (100%)	0	100 100
3	C	184/188 (98%)	183 (100%)	1 (0%)	88 93
3	G	184/188 (98%)	183 (100%)	1 (0%)	88 93
3	K	184/188 (98%)	183 (100%)	1 (0%)	88 93
4	D	182/184 (99%)	182 (100%)	0	100 100
4	H	182/184 (99%)	182 (100%)	0	100 100
4	L	182/184 (99%)	182 (100%)	0	100 100
All	All	2581/2817 (92%)	2575 (100%)	6 (0%)	93 96

5 of 6 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	G	71	ARG
1	I	262	ASN
3	K	71	ARG
1	E	160	ASN
3	C	71	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	160	ASN
3	K	164	HIS
4	L	137	ASN

5.3.3 RNA

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)

34 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	0	1	5,1	14,14,15	0.97	1 (7%)	17,19,21	0.90	1 (5%)
5	NAG	0	2	5	14,14,15	0.29	0	17,19,21	0.58	0
5	BMA	0	3	5	11,11,12	0.53	0	15,15,17	0.92	0
6	NAG	4	1	6,1	14,14,15	0.23	0	17,19,21	0.47	0
6	NAG	4	2	6	14,14,15	0.26	0	17,19,21	0.45	0
6	BMA	4	3	6	11,11,12	0.65	0	15,15,17	0.89	0
6	MAN	4	4	6	11,11,12	0.55	0	15,15,17	1.12	2 (13%)
5	NAG	M	1	5,1	14,14,15	0.63	1 (7%)	17,19,21	0.78	1 (5%)
5	NAG	M	2	5	14,14,15	0.42	0	17,19,21	1.24	1 (5%)
5	BMA	M	3	5	11,11,12	0.64	0	15,15,17	0.73	0
5	NAG	N	1	5,1	14,14,15	0.33	0	17,19,21	0.45	0
5	NAG	N	2	5	14,14,15	0.18	0	17,19,21	0.51	0
5	BMA	N	3	5	11,11,12	0.53	0	15,15,17	0.72	0
6	NAG	R	1	6,1	14,14,15	0.28	0	17,19,21	0.46	0
6	NAG	R	2	6	14,14,15	0.25	0	17,19,21	0.45	0
6	BMA	R	3	6	11,11,12	0.70	0	15,15,17	0.81	0
6	MAN	R	4	6	11,11,12	0.53	0	15,15,17	0.98	2 (13%)
5	NAG	e	1	5,1	14,14,15	0.35	0	17,19,21	0.49	0
5	NAG	e	2	5	14,14,15	0.22	0	17,19,21	0.50	0
5	BMA	e	3	5	11,11,12	0.49	0	15,15,17	0.71	0
7	NAG	h	1	7,1	14,14,15	0.44	0	17,19,21	0.87	1 (5%)
7	NAG	h	2	7	14,14,15	0.39	0	17,19,21	0.51	0
5	NAG	j	1	5,1	14,14,15	1.06	1 (7%)	17,19,21	1.17	2 (11%)
5	NAG	j	2	5	14,14,15	0.20	0	17,19,21	0.58	0
5	BMA	j	3	5	11,11,12	0.45	0	15,15,17	0.86	0
6	NAG	n	1	6,1	14,14,15	0.33	0	17,19,21	0.50	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	0.23	0	17,19,21	0.44	0
6	BMA	n	3	6	11,11,12	0.72	0	15,15,17	0.86	0
6	MAN	n	4	6	11,11,12	0.48	0	15,15,17	1.01	2 (13%)
5	NAG	v	1	5,1	14,14,15	0.28	0	17,19,21	0.73	1 (5%)
5	NAG	v	2	5	14,14,15	0.18	0	17,19,21	0.56	0
5	BMA	v	3	5	11,11,12	0.57	0	15,15,17	0.73	0
7	NAG	y	1	7,1	14,14,15	0.75	1 (7%)	17,19,21	1.24	1 (5%)
7	NAG	y	2	7	14,14,15	0.38	0	17,19,21	0.47	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
5	NAG	0	1	5,1	-	3/6/23/26	0/1/1/1
5	NAG	0	2	5	-	1/6/23/26	0/1/1/1
5	BMA	0	3	5	-	0/2/19/22	0/1/1/1
6	NAG	4	1	6,1	-	1/6/23/26	0/1/1/1
6	NAG	4	2	6	-	2/6/23/26	0/1/1/1
6	BMA	4	3	6	-	1/2/19/22	0/1/1/1
6	MAN	4	4	6	-	0/2/19/22	0/1/1/1
5	NAG	M	1	5,1	-	4/6/23/26	0/1/1/1
5	NAG	M	2	5	-	3/6/23/26	0/1/1/1
5	BMA	M	3	5	-	0/2/19/22	0/1/1/1
5	NAG	N	1	5,1	-	1/6/23/26	0/1/1/1
5	NAG	N	2	5	-	1/6/23/26	0/1/1/1
5	BMA	N	3	5	-	0/2/19/22	0/1/1/1
6	NAG	R	1	6,1	-	1/6/23/26	0/1/1/1
6	NAG	R	2	6	-	2/6/23/26	0/1/1/1
6	BMA	R	3	6	-	0/2/19/22	0/1/1/1
6	MAN	R	4	6	-	1/2/19/22	0/1/1/1
5	NAG	e	1	5,1	-	0/6/23/26	0/1/1/1
5	NAG	e	2	5	-	1/6/23/26	0/1/1/1
5	BMA	e	3	5	-	0/2/19/22	0/1/1/1
7	NAG	h	1	7,1	-	0/6/23/26	0/1/1/1
7	NAG	h	2	7	-	1/6/23/26	0/1/1/1
5	NAG	j	1	5,1	-	2/6/23/26	0/1/1/1
5	NAG	j	2	5	-	2/6/23/26	0/1/1/1
5	BMA	j	3	5	-	2/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	NAG	n	1	6,1	-	4/6/23/26	0/1/1/1
6	NAG	n	2	6	-	2/6/23/26	0/1/1/1
6	BMA	n	3	6	-	2/2/19/22	0/1/1/1
6	MAN	n	4	6	-	2/2/19/22	0/1/1/1
5	NAG	v	1	5,1	-	2/6/23/26	0/1/1/1
5	NAG	v	2	5	-	1/6/23/26	0/1/1/1
5	BMA	v	3	5	-	0/2/19/22	0/1/1/1
7	NAG	y	1	7,1	-	0/6/23/26	0/1/1/1
7	NAG	y	2	7	-	1/6/23/26	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	j	1	NAG	O5-C1	-3.75	1.37	1.43
5	0	1	NAG	O5-C1	-3.46	1.38	1.43
5	M	1	NAG	O5-C1	-2.15	1.40	1.43
7	y	1	NAG	C1-C2	2.08	1.55	1.52

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	y	1	NAG	C1-O5-C5	4.40	118.16	112.19
6	4	4	MAN	C1-O5-C5	3.13	116.44	112.19
5	M	2	NAG	C3-C4-C5	3.06	115.69	110.24
7	h	1	NAG	C1-O5-C5	3.03	116.29	112.19
5	j	1	NAG	C3-C4-C5	3.00	115.58	110.24

There are no chirality outliers.

5 of 43 torsion outliers are listed below:

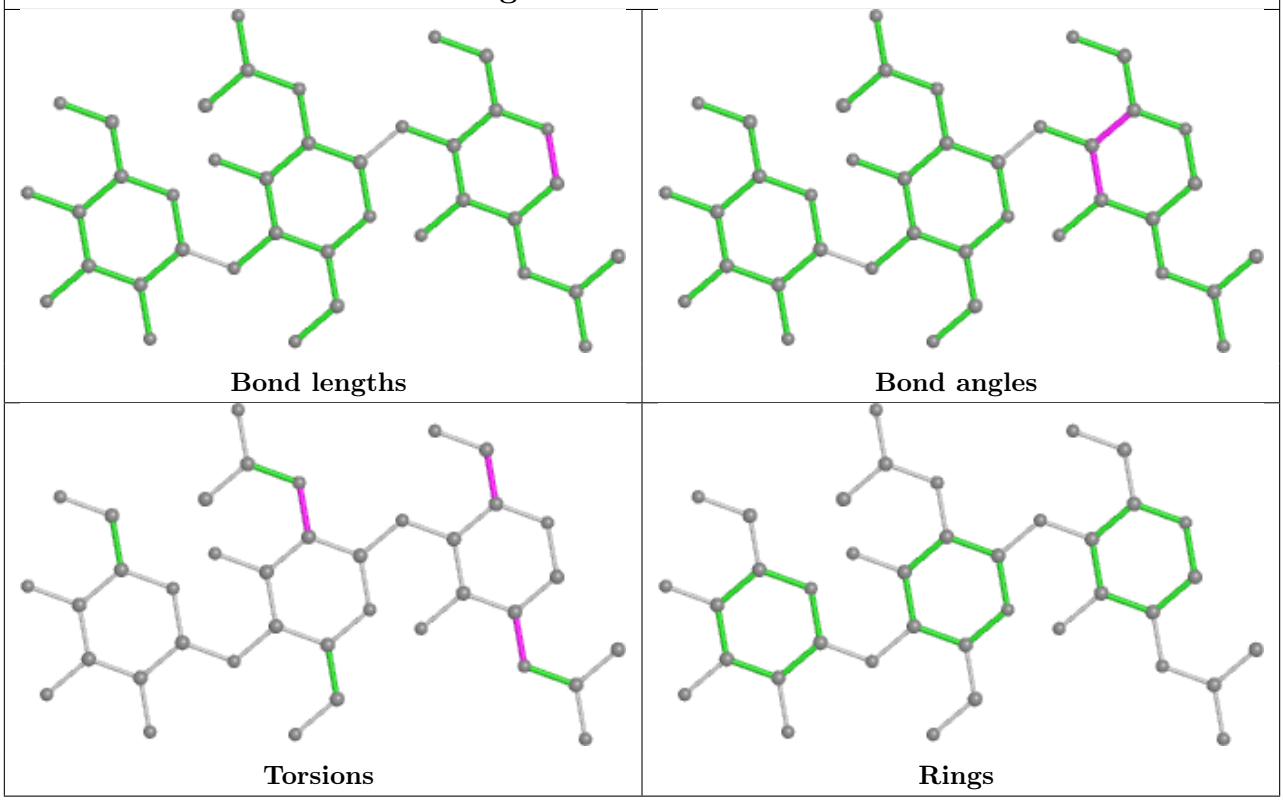
Mol	Chain	Res	Type	Atoms
5	M	2	NAG	C4-C5-C6-O6
5	M	1	NAG	O5-C5-C6-O6
6	n	2	NAG	O5-C5-C6-O6
6	R	2	NAG	O5-C5-C6-O6
5	M	1	NAG	C4-C5-C6-O6

There are no ring outliers.

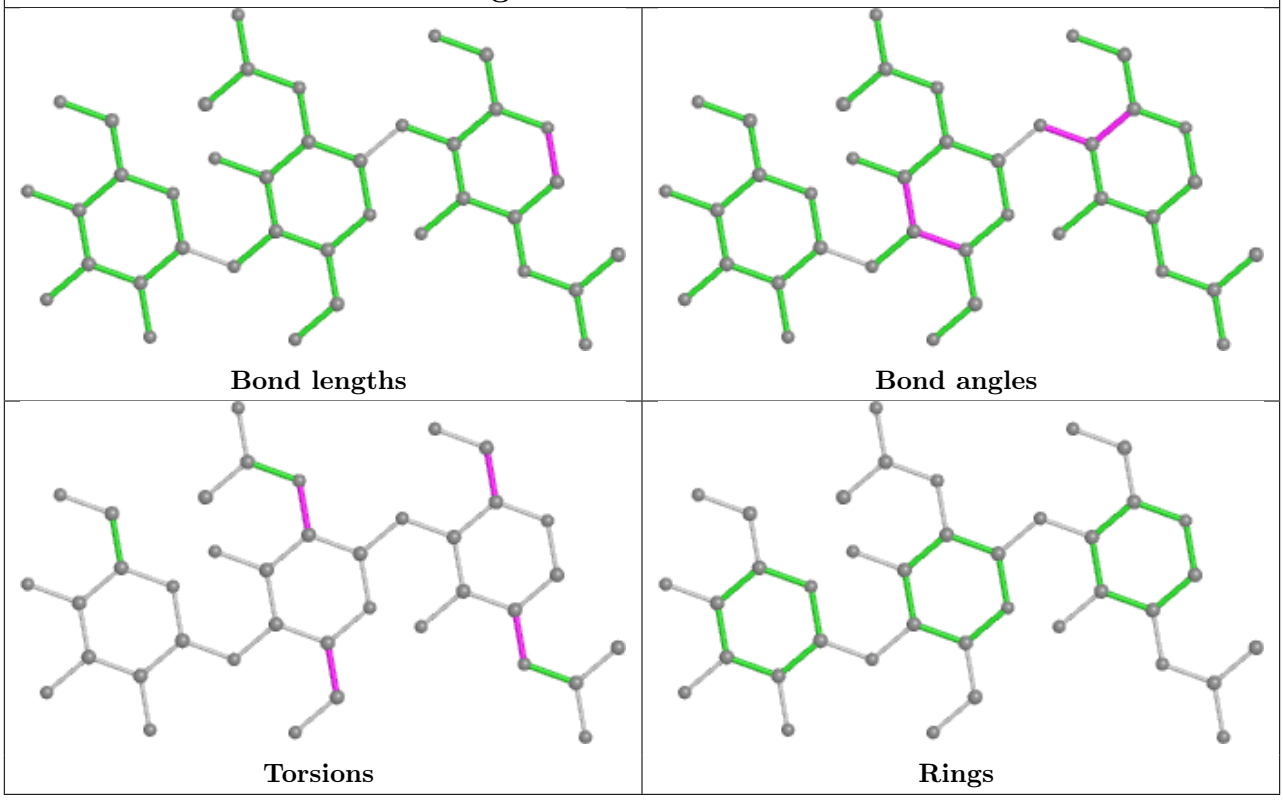
No monomer is involved in short contacts.

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

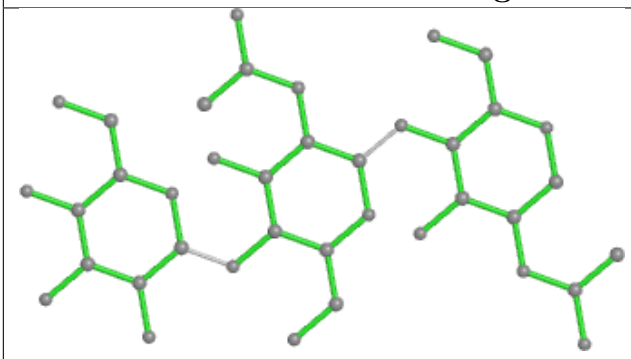
Oligosaccharide Chain 0



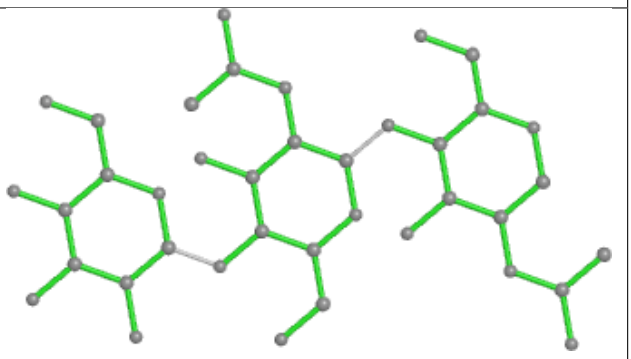
Oligosaccharide Chain M



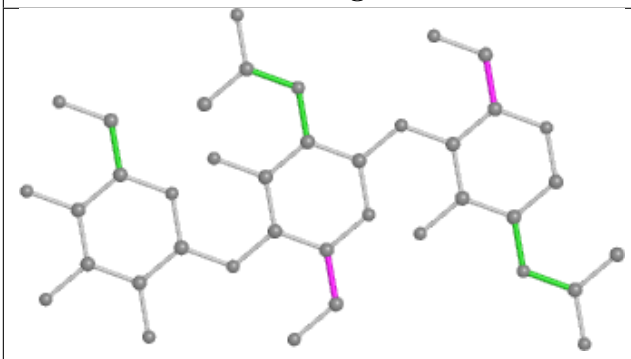
Oligosaccharide Chain N



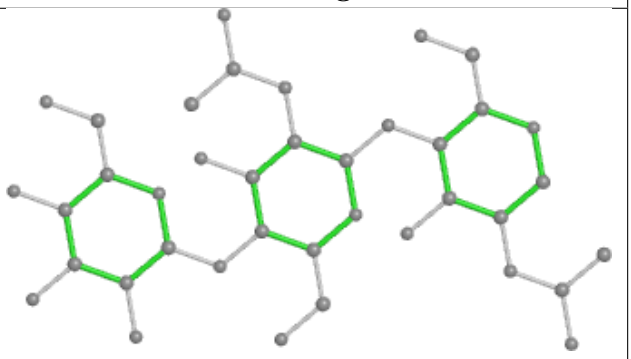
Bond lengths



Bond angles

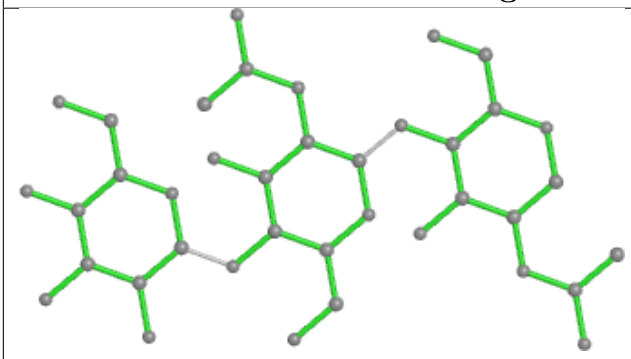


Torsions

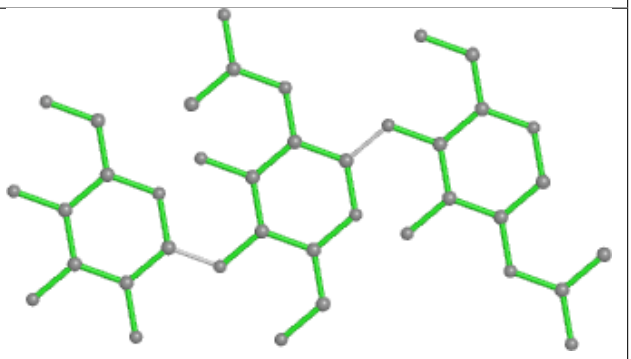


Rings

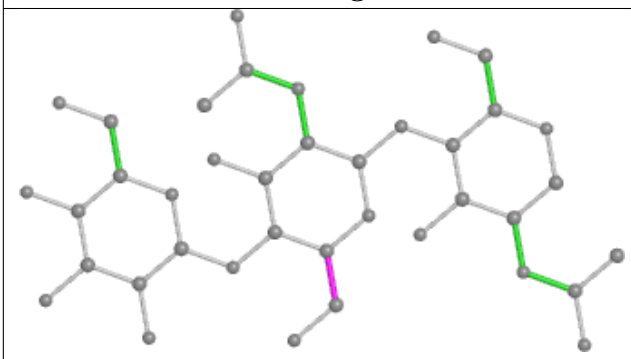
Oligosaccharide Chain e



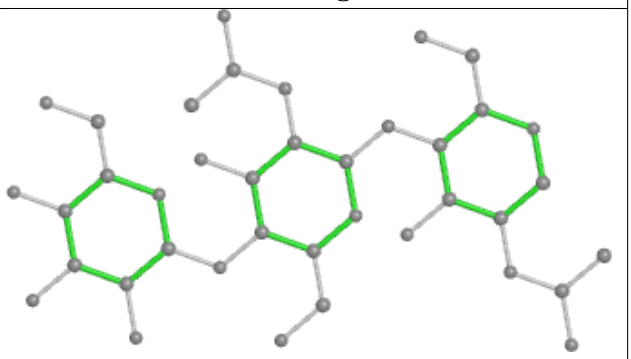
Bond lengths



Bond angles

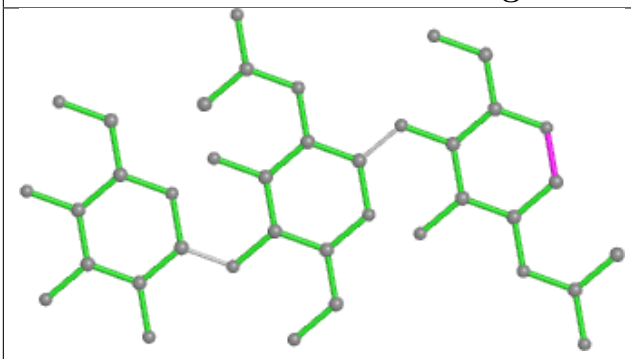


Torsions

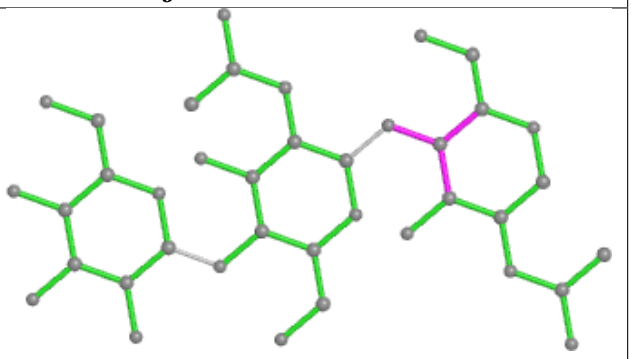


Rings

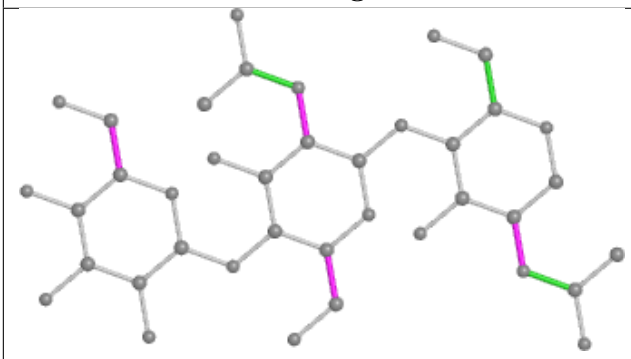
Oligosaccharide Chain j



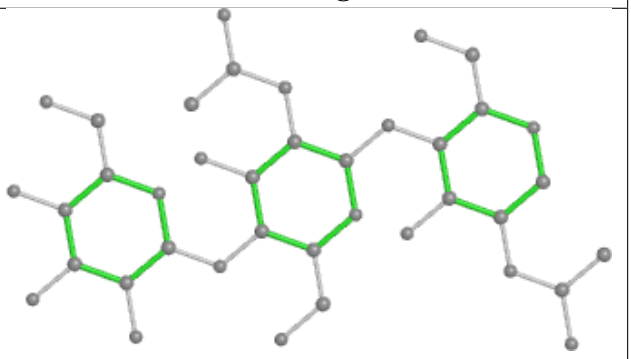
Bond lengths



Bond angles

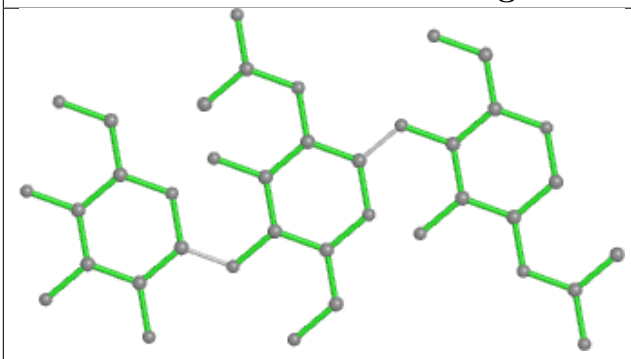


Torsions

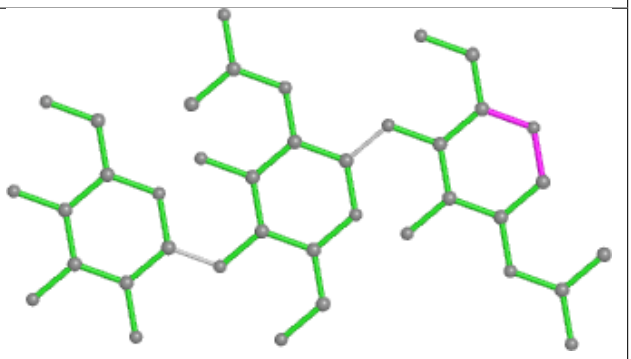


Rings

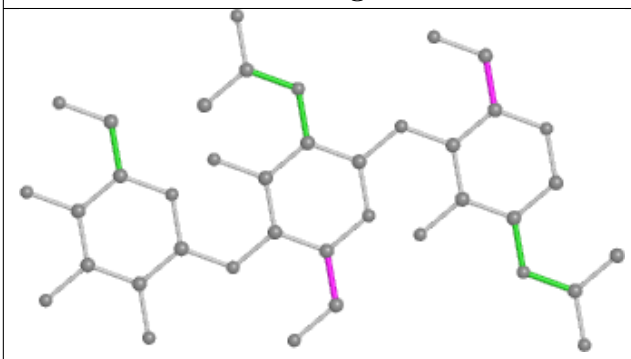
Oligosaccharide Chain v



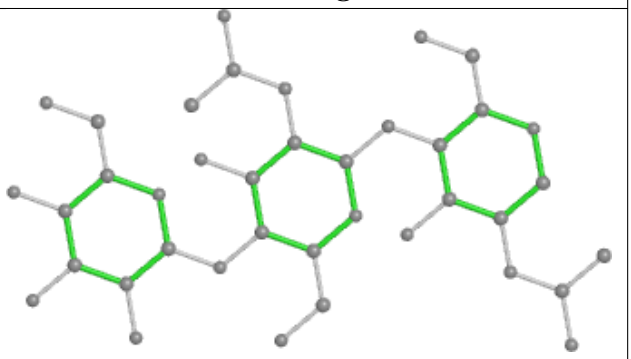
Bond lengths



Bond angles

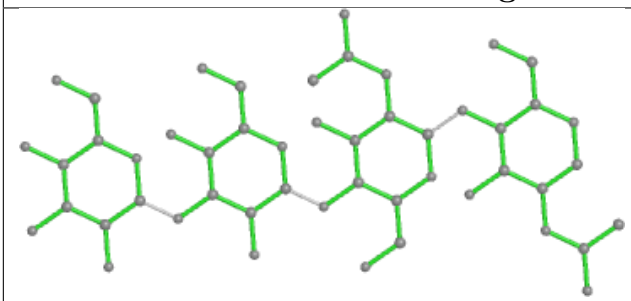


Torsions

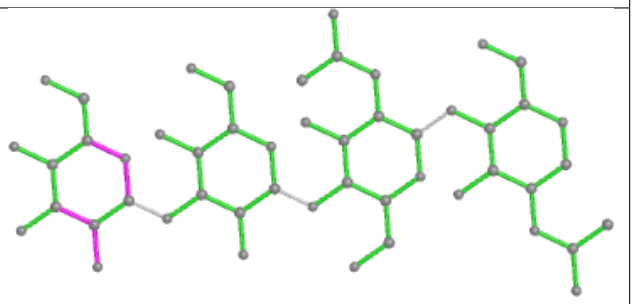


Rings

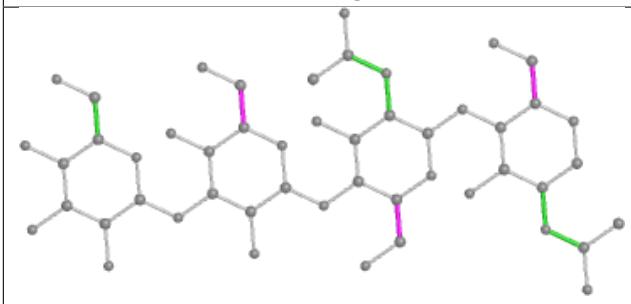
Oligosaccharide Chain 4



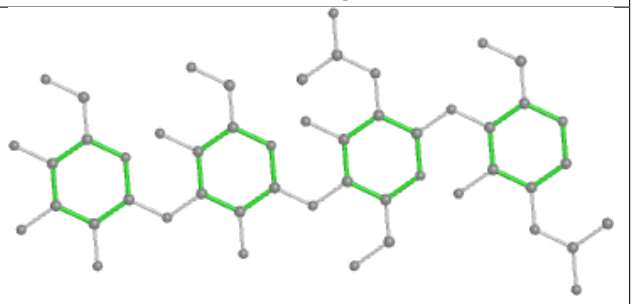
Bond lengths



Bond angles

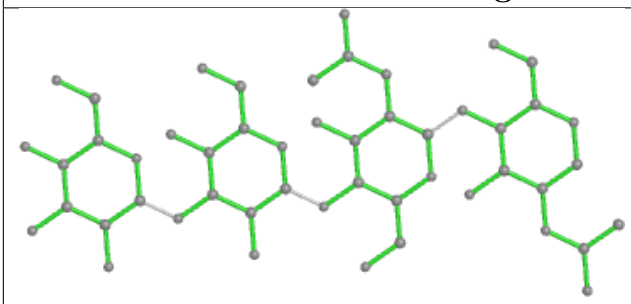


Torsions

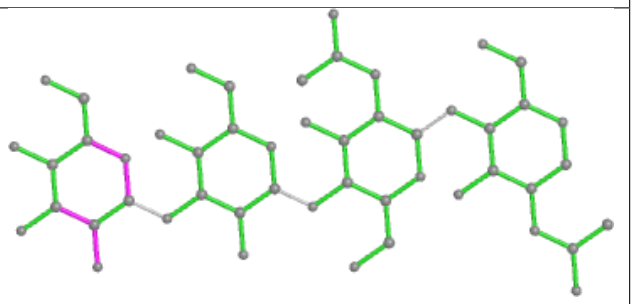


Rings

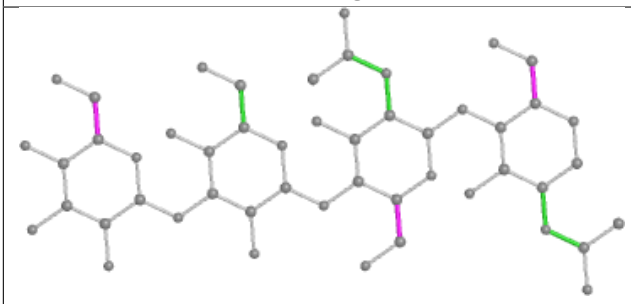
Oligosaccharide Chain R



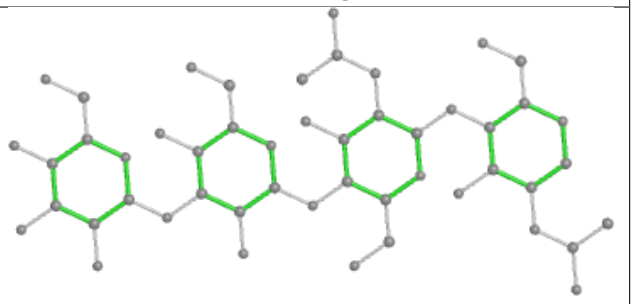
Bond lengths



Bond angles

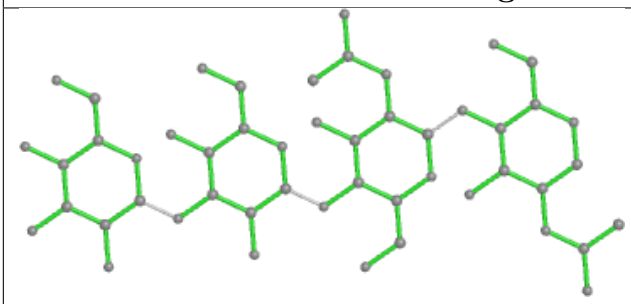


Torsions

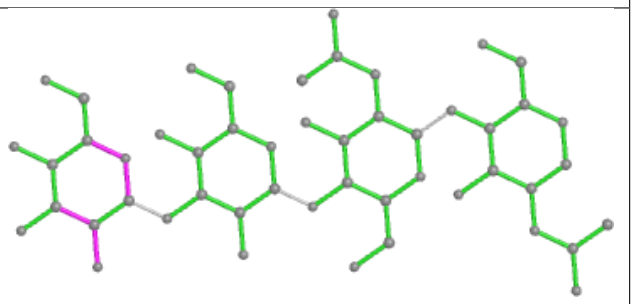


Rings

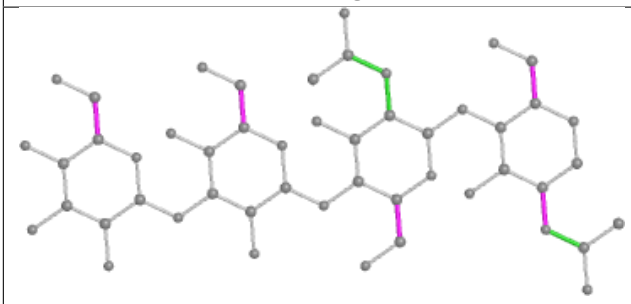
Oligosaccharide Chain n



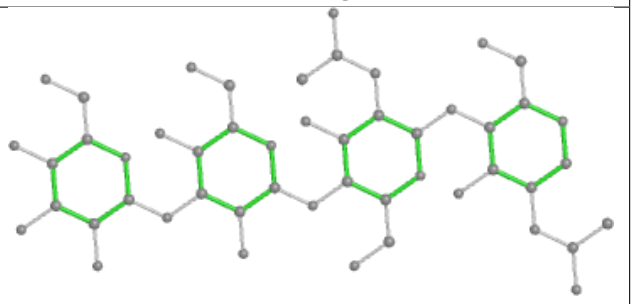
Bond lengths



Bond angles

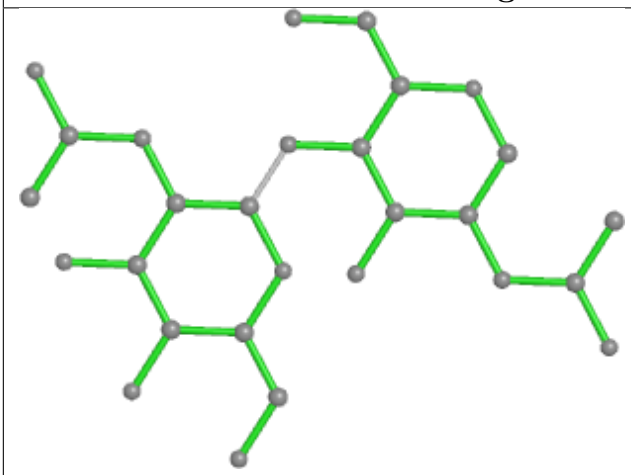


Torsions

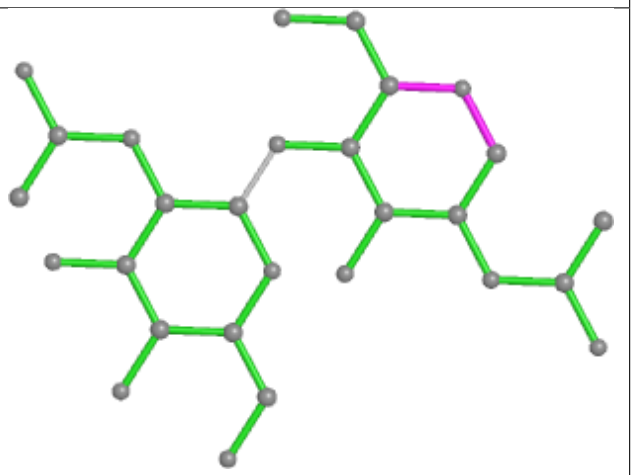


Rings

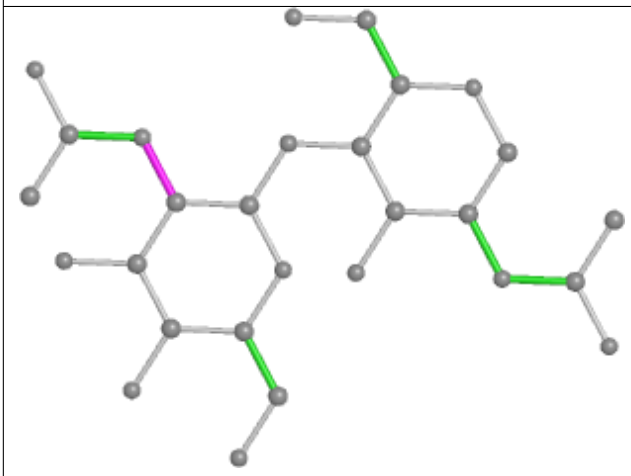
Oligosaccharide Chain h



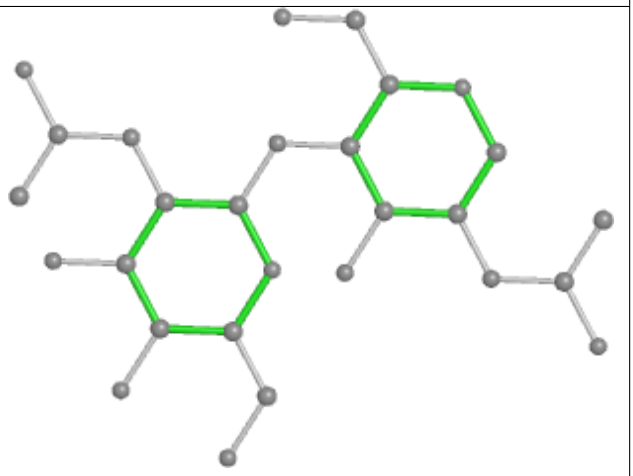
Bond lengths



Bond angles

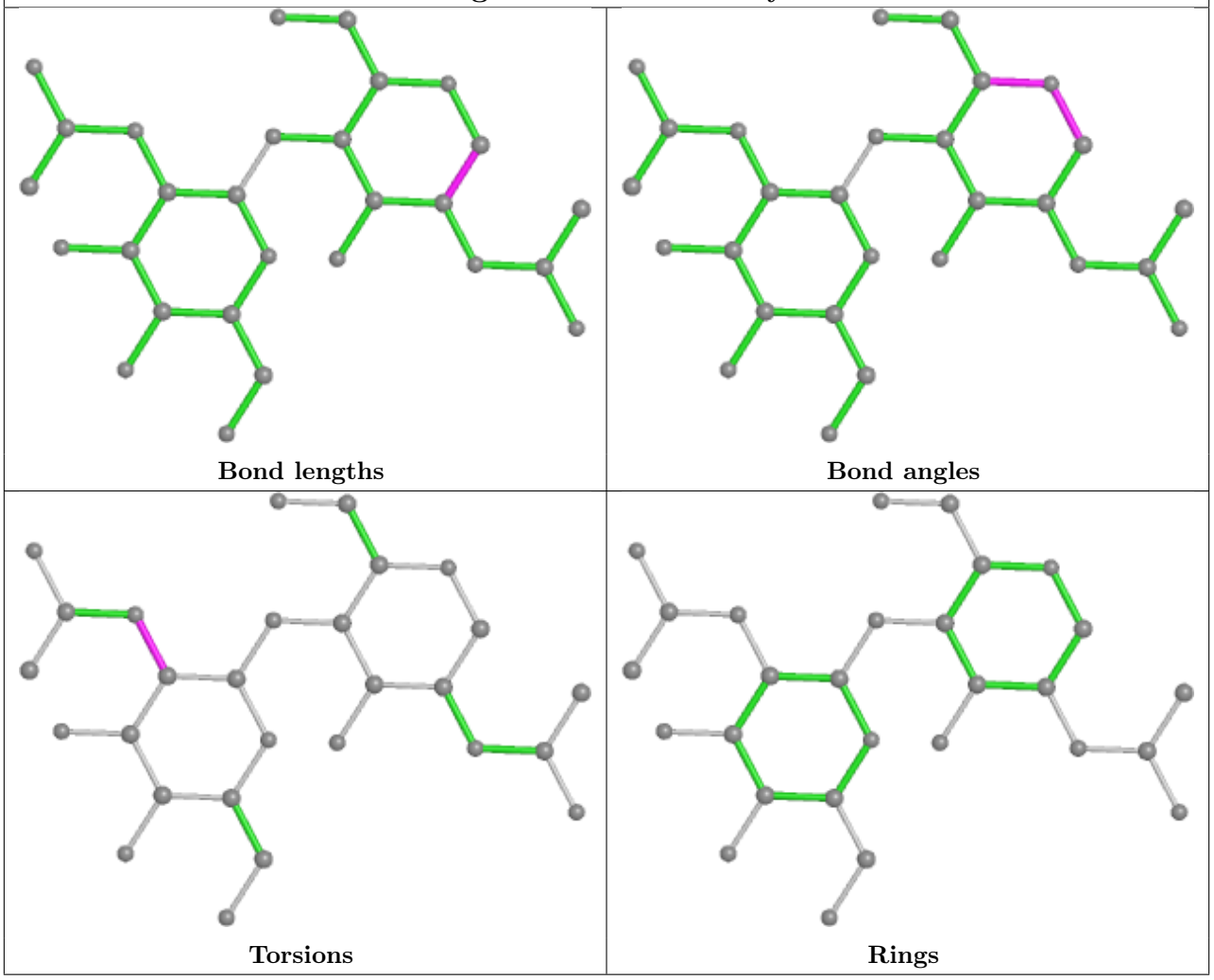


Torsions



Rings

Oligosaccharide Chain y



5.6 Ligand geometry (i)

16 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	$\#\|Z\| > 2$
8	NAG	A	604	-	14,14,15	0.22	0	17,19,21	0.40	0
8	NAG	E	602	-	14,14,15	0.21	0	17,19,21	0.41	0
8	NAG	I	601	-	14,14,15	0.37	0	17,19,21	0.96	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
8	NAG	I	604	1	14,14,15	0.27	0	17,19,21	0.41	0
9	MAN	K	301	-	11,11,12	0.71	0	15,15,17	1.15	2 (13%)
9	MAN	C	301	-	11,11,12	0.75	1 (9%)	15,15,17	1.06	2 (13%)
8	NAG	I	603	-	14,14,15	0.17	0	17,19,21	0.42	0
8	NAG	A	603	-	14,14,15	0.28	0	17,19,21	0.37	0
8	NAG	A	601	1	14,14,15	0.32	0	17,19,21	0.37	0
8	NAG	A	605	1	14,14,15	0.22	0	17,19,21	0.40	0
8	NAG	E	604	1	14,14,15	0.24	0	17,19,21	0.43	0
8	NAG	I	602	-	14,14,15	0.21	0	17,19,21	0.40	0
8	NAG	A	602	-	14,14,15	0.25	0	17,19,21	0.35	0
9	MAN	G	301	-	11,11,12	0.66	0	15,15,17	1.02	1 (6%)
8	NAG	E	603	-	14,14,15	0.21	0	17,19,21	0.41	0
8	NAG	E	601	-	14,14,15	0.37	0	17,19,21	0.96	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
8	NAG	A	604	-	-	3/6/23/26	0/1/1/1
8	NAG	E	602	-	-	3/6/23/26	0/1/1/1
8	NAG	I	601	-	-	5/6/23/26	0/1/1/1
8	NAG	I	604	1	-	1/6/23/26	0/1/1/1
9	MAN	K	301	-	-	2/2/19/22	0/1/1/1
9	MAN	C	301	-	-	2/2/19/22	0/1/1/1
8	NAG	I	603	-	-	3/6/23/26	0/1/1/1
8	NAG	A	603	-	-	2/6/23/26	0/1/1/1
8	NAG	A	601	1	-	4/6/23/26	0/1/1/1
8	NAG	A	605	1	-	2/6/23/26	0/1/1/1
8	NAG	E	604	1	-	2/6/23/26	0/1/1/1
8	NAG	I	602	-	-	1/6/23/26	0/1/1/1
8	NAG	A	602	-	-	2/6/23/26	0/1/1/1
9	MAN	G	301	-	-	0/2/19/22	0/1/1/1
8	NAG	E	603	-	-	2/6/23/26	0/1/1/1
8	NAG	E	601	-	-	4/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	C	301	MAN	O5-C1	-2.16	1.40	1.43

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	E	601	NAG	C2-N2-C7	3.18	127.43	122.90
8	I	601	NAG	C2-N2-C7	3.12	127.35	122.90
9	K	301	MAN	O2-C2-C3	-2.42	105.29	110.14
9	G	301	MAN	O2-C2-C3	-2.42	105.30	110.14
9	C	301	MAN	O2-C2-C3	-2.31	105.52	110.14

There are no chirality outliers.

5 of 38 torsion outliers are listed below:

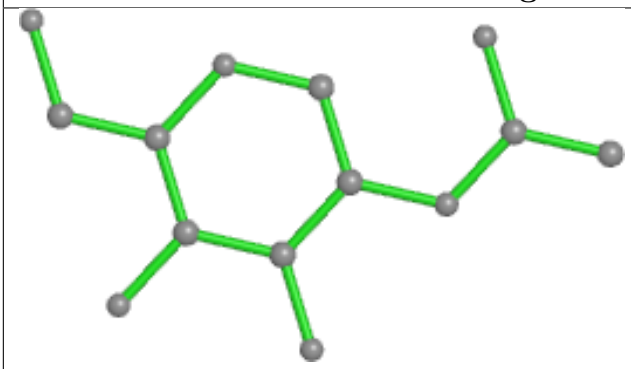
Mol	Chain	Res	Type	Atoms
8	A	605	NAG	O5-C5-C6-O6
8	I	601	NAG	C4-C5-C6-O6
8	A	602	NAG	O5-C5-C6-O6
8	A	601	NAG	C1-C2-N2-C7
8	E	604	NAG	O5-C5-C6-O6

There are no ring outliers.

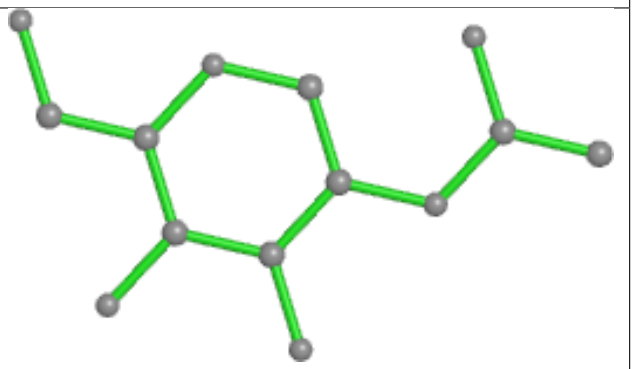
No monomer is involved in short contacts.

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

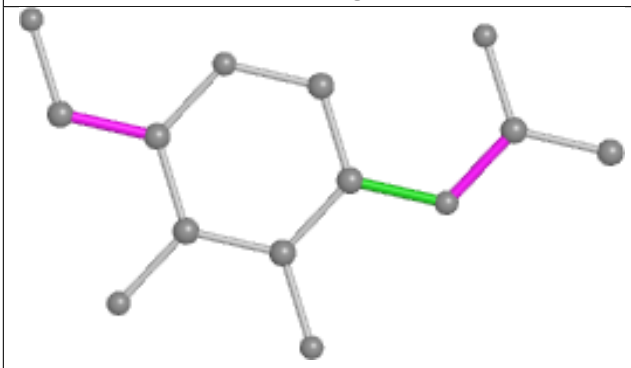
Ligand NAG A 604



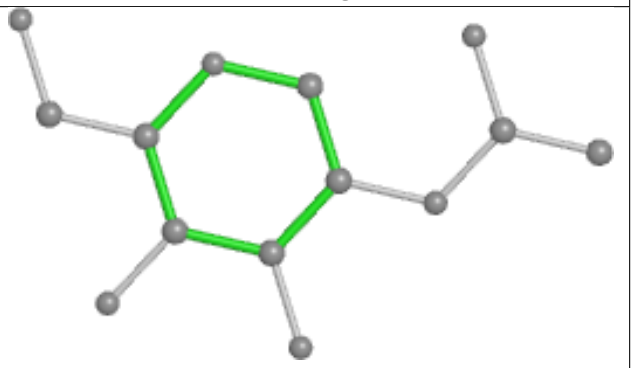
Bond lengths



Bond angles

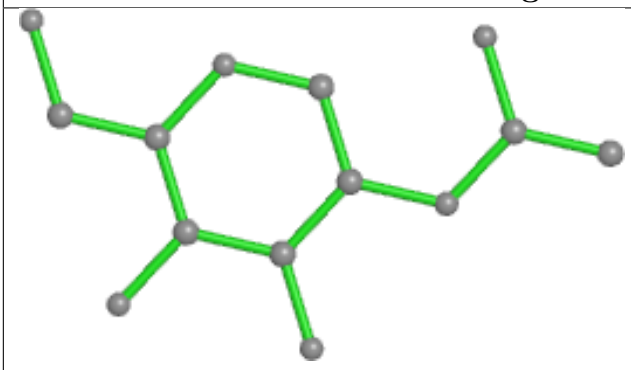


Torsions

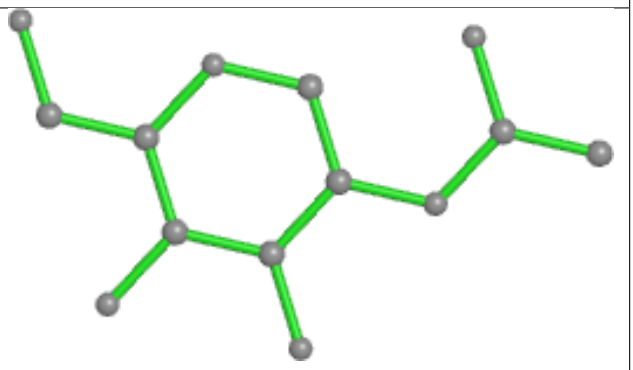


Rings

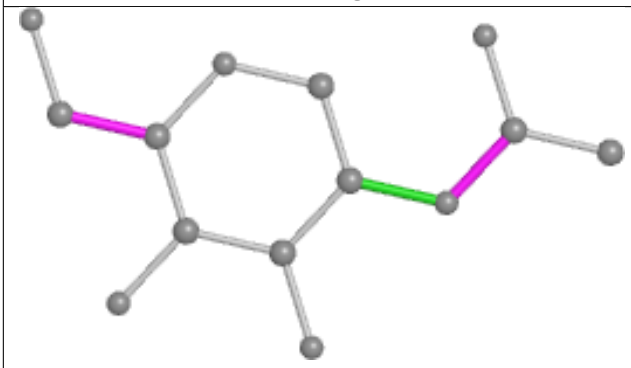
Ligand NAG E 602



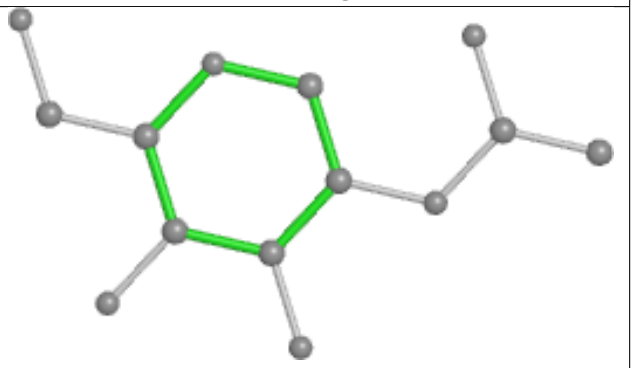
Bond lengths



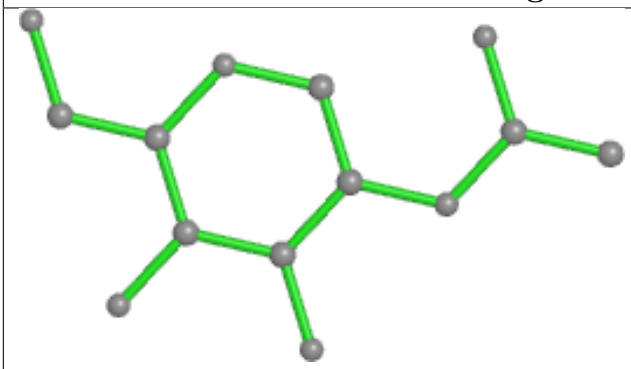
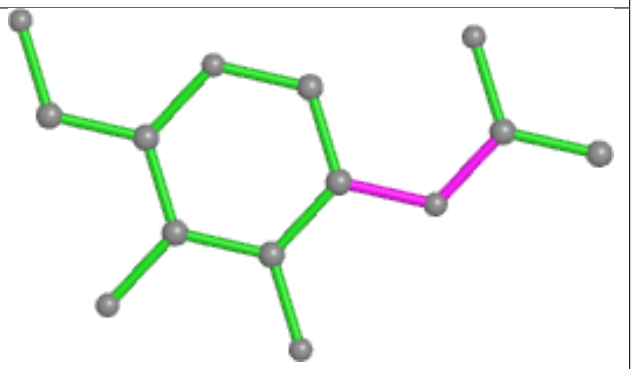
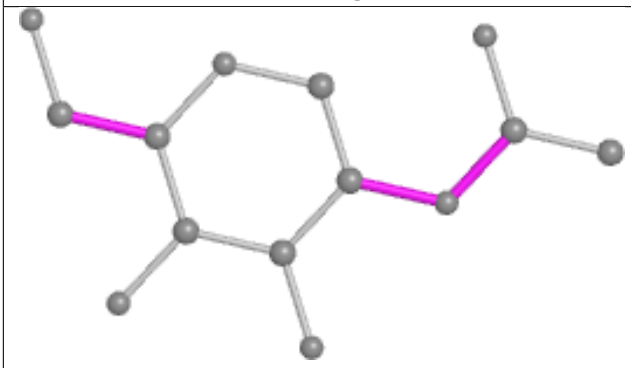
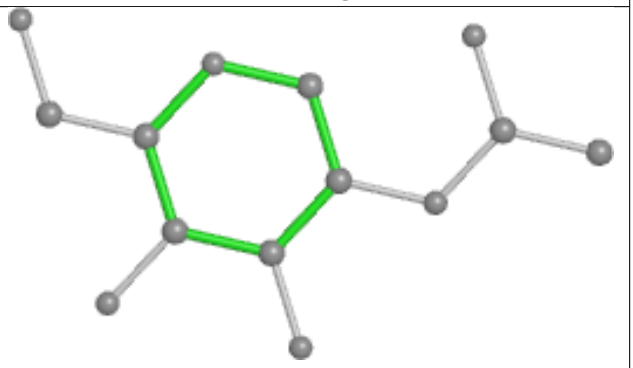
Bond angles

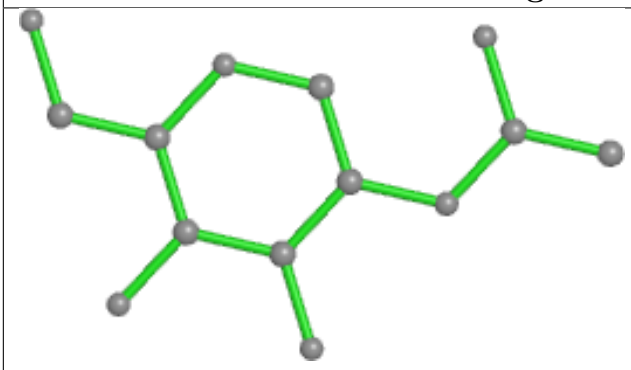
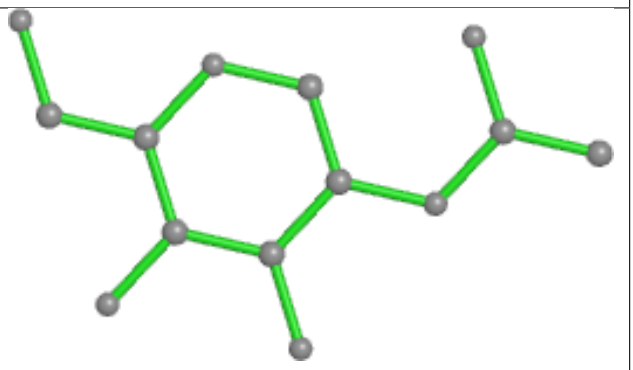
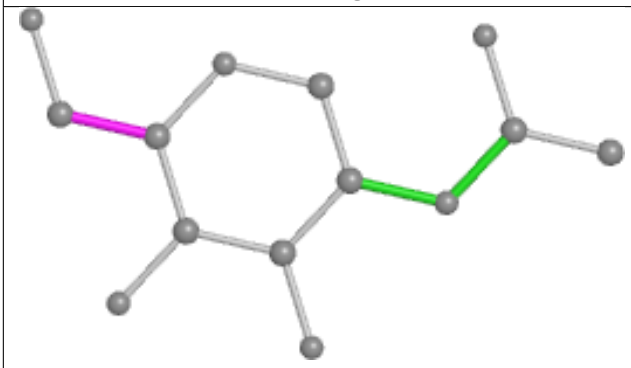
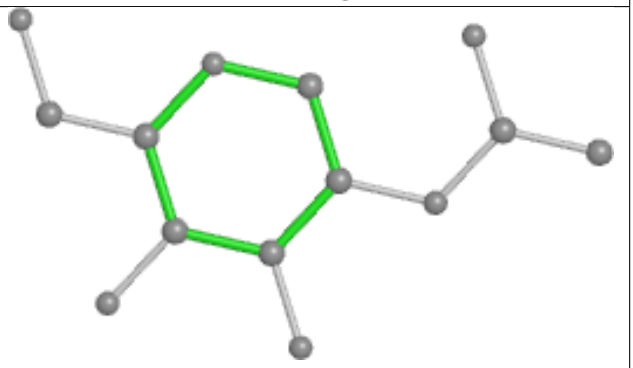


Torsions

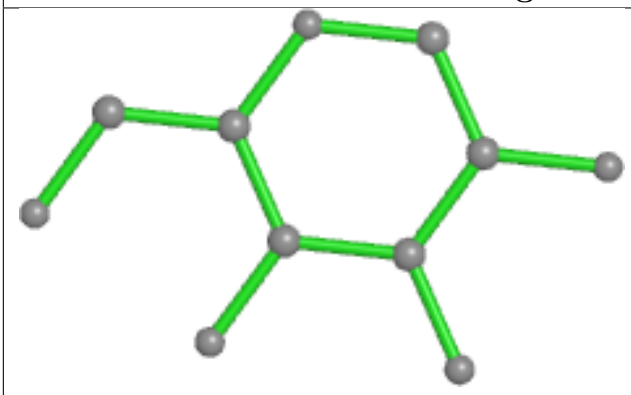


Rings

Ligand NAG I 601	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand NAG I 604	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand MAN K 301



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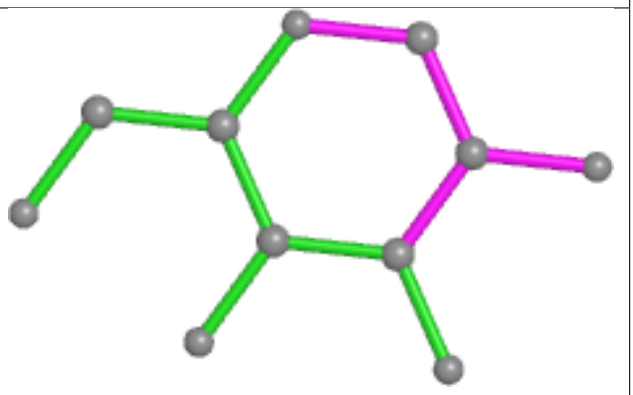

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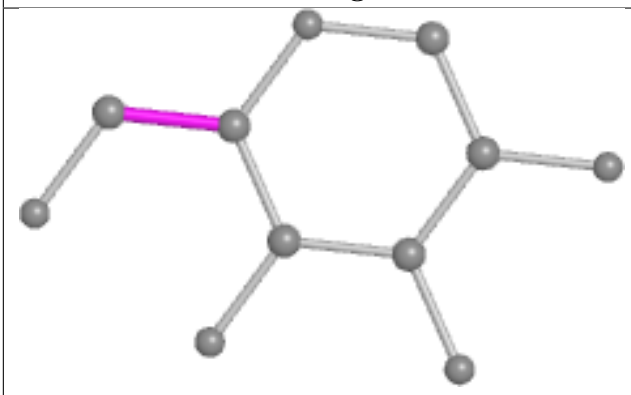

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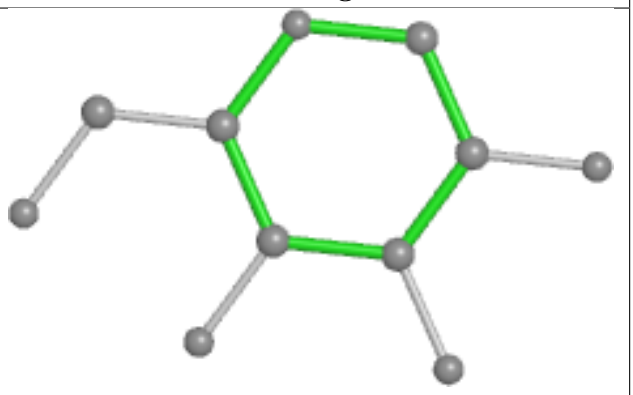
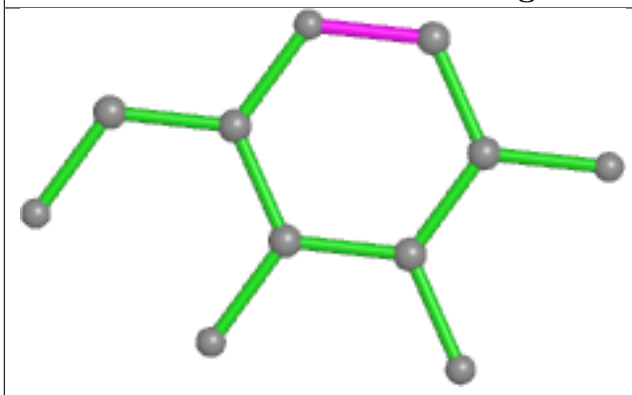


Rings

Ligand MAN C 301



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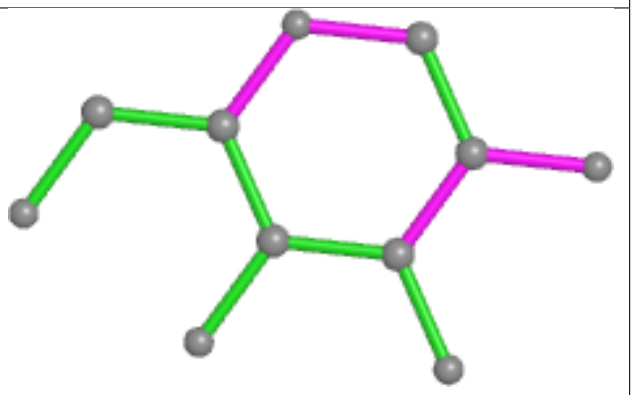
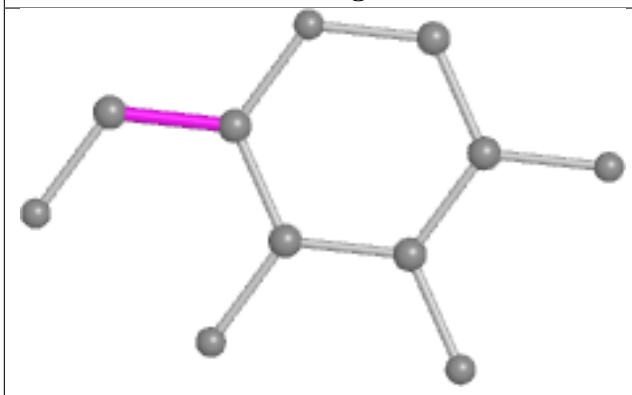


Bond angles



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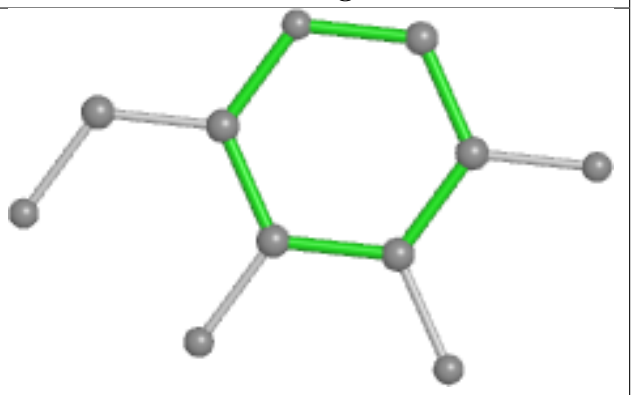
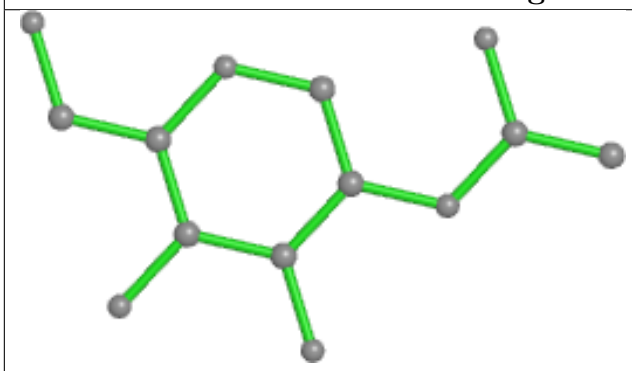
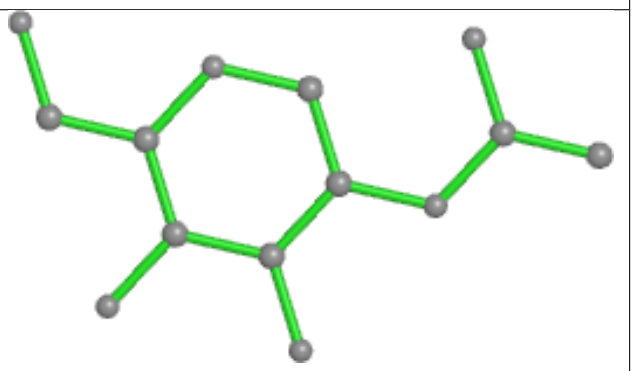


Rings

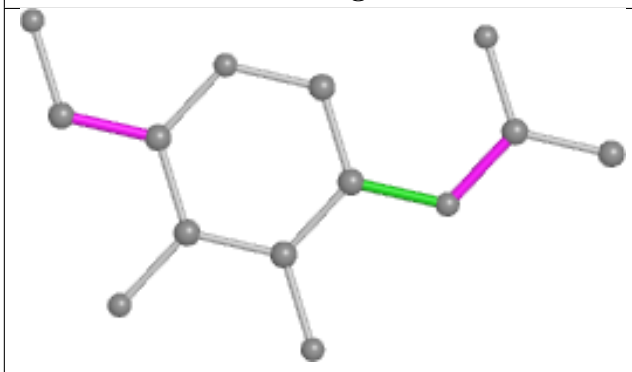
Ligand NAG I 603



Bond lengths



Bond angles



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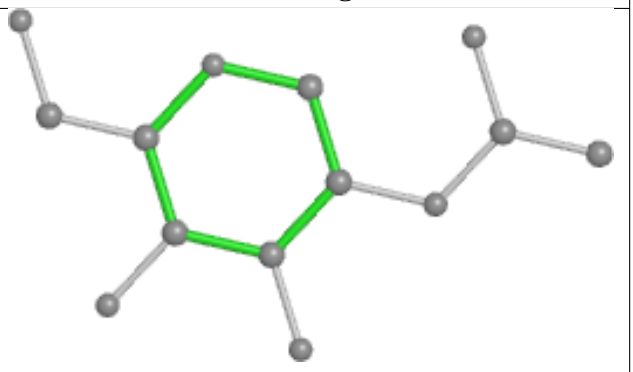
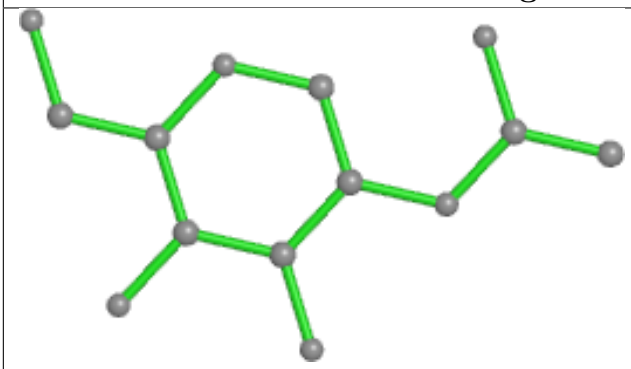


Rings

Ligand NAG A 603



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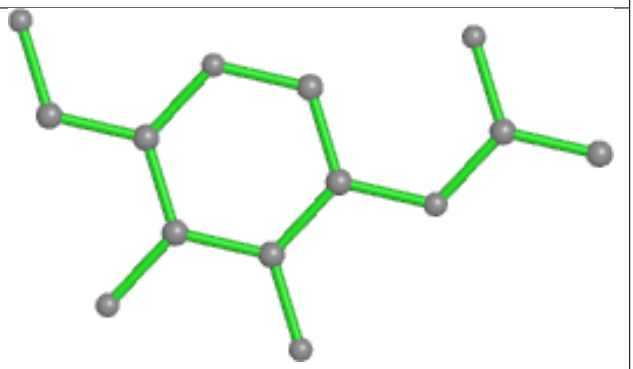
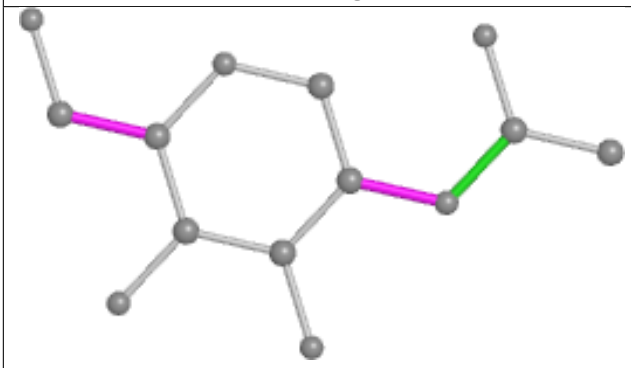
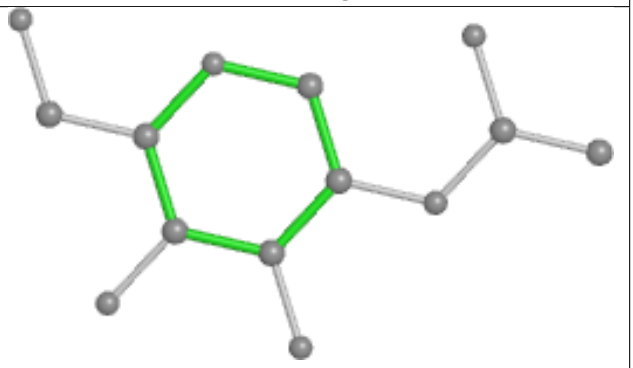


Bond angles

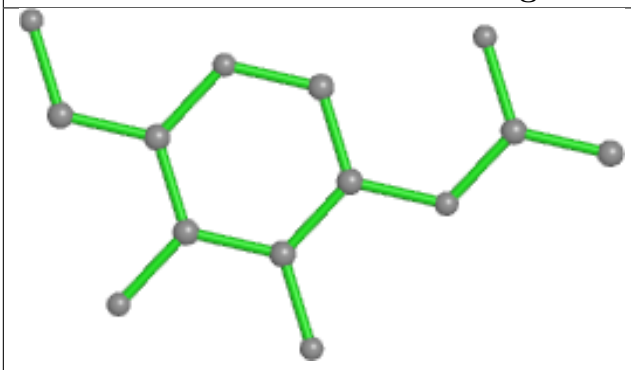


Torsions



Rings

Ligand NAG A 601



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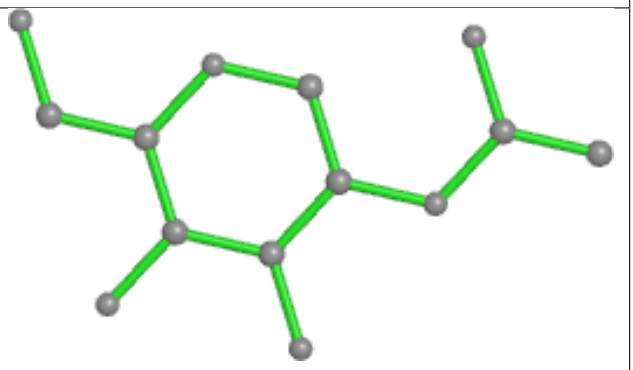
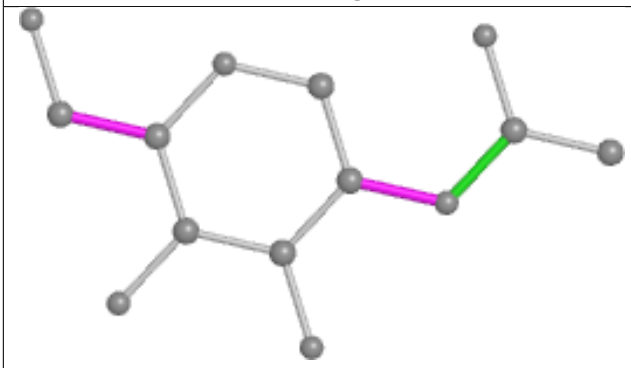


Bond angles



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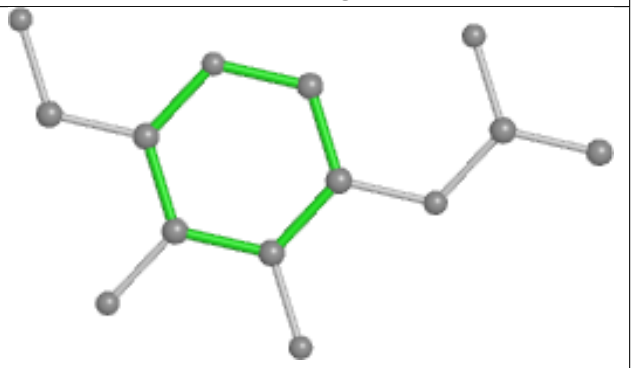
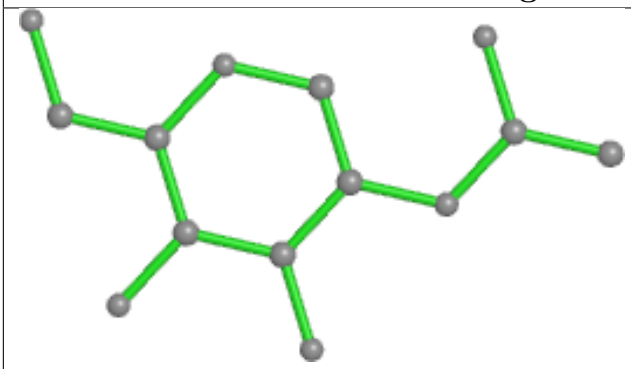
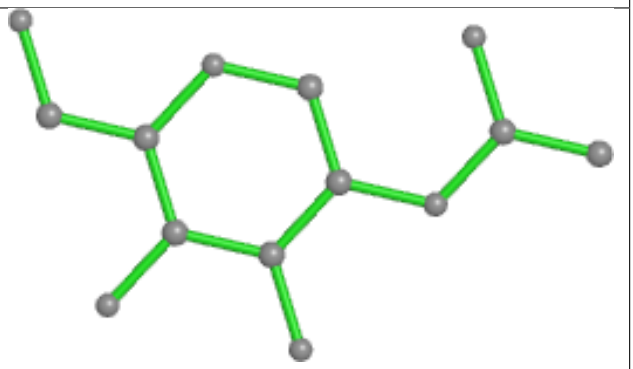


Rings

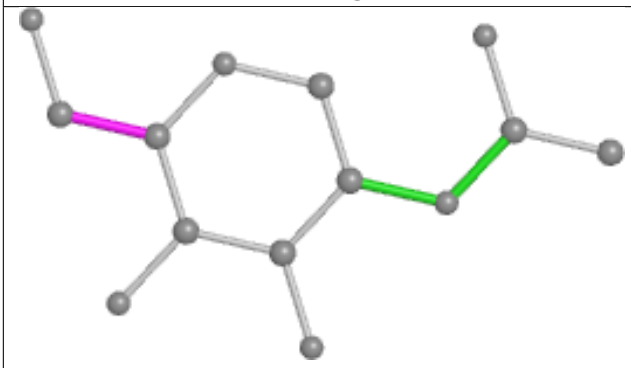
Ligand NAG A 605



Bond lengths



Bond angles



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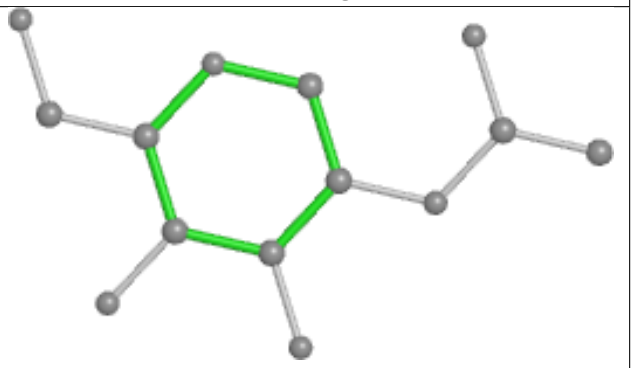
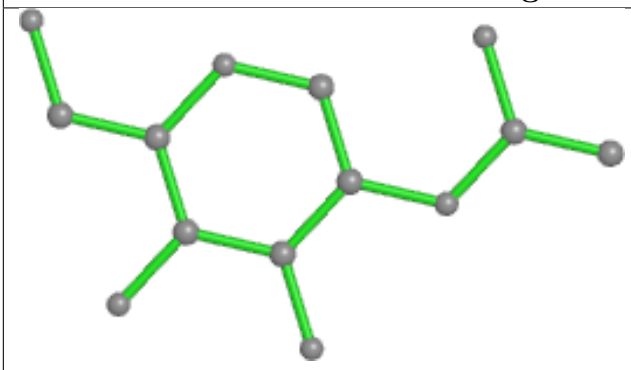


Rings

Ligand NAG E 604



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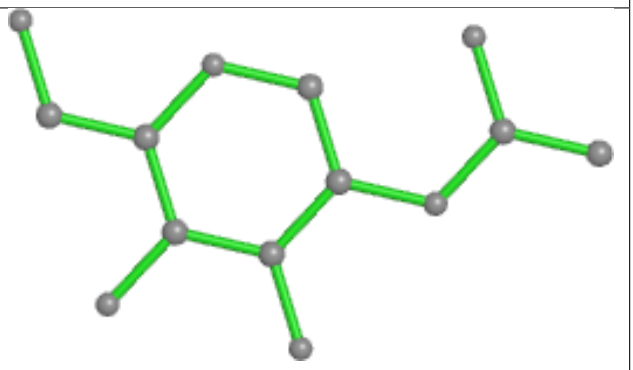
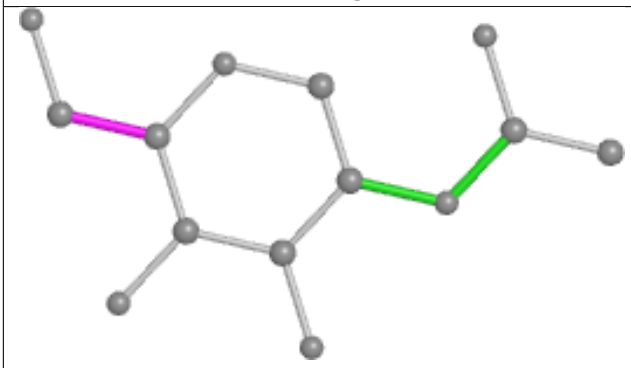
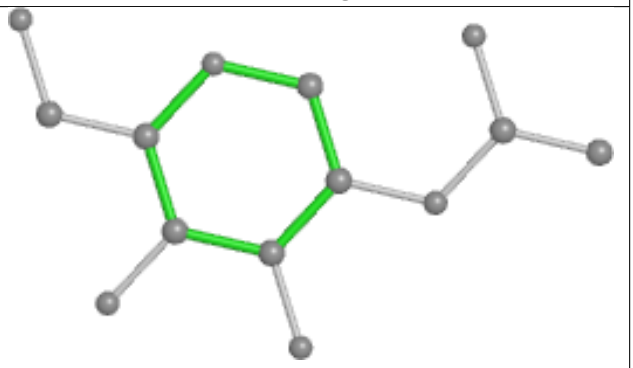


Bond angles

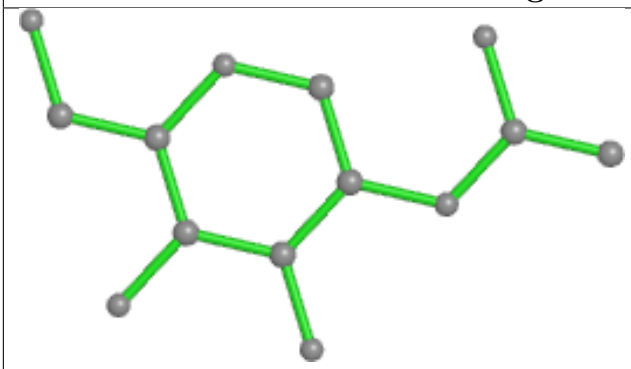


Torsions



Rings

Ligand NAG I 602



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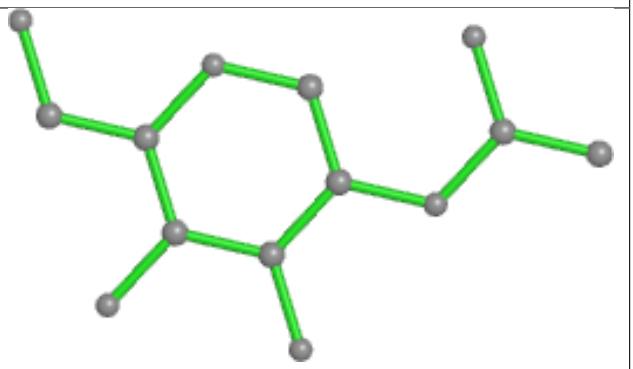
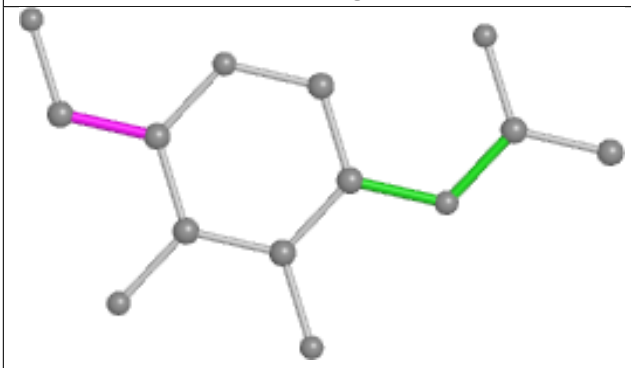


Bond angles



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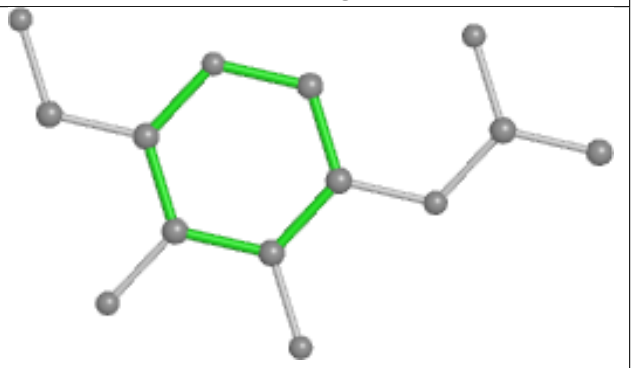
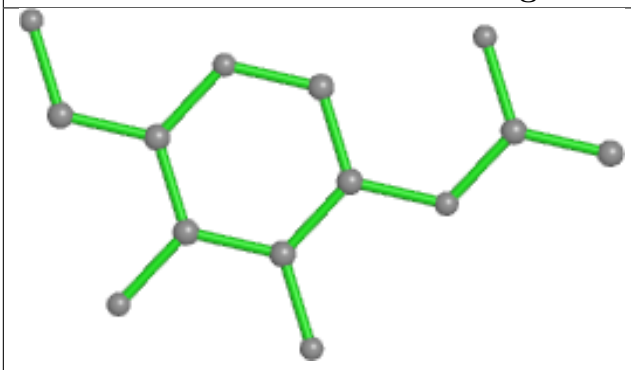
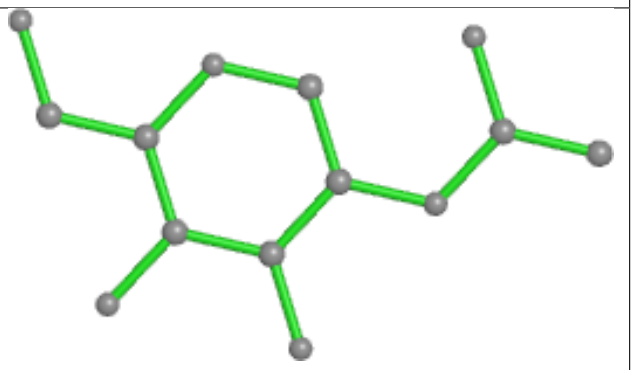


Rings

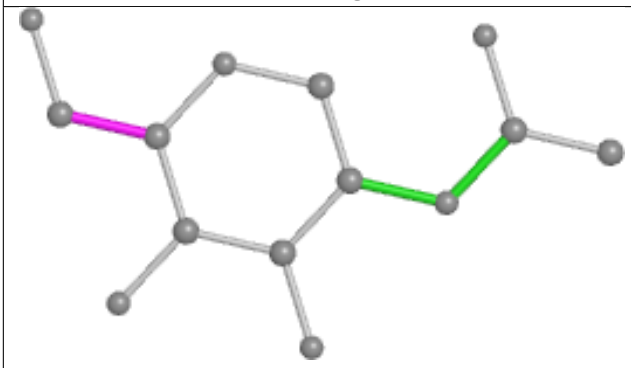
Ligand NAG A 602



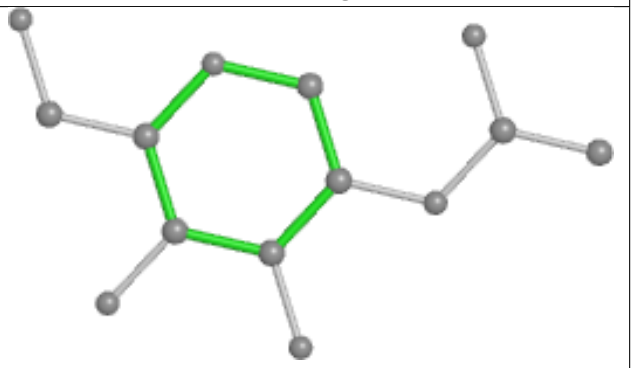
Bond lengths



Bond angles

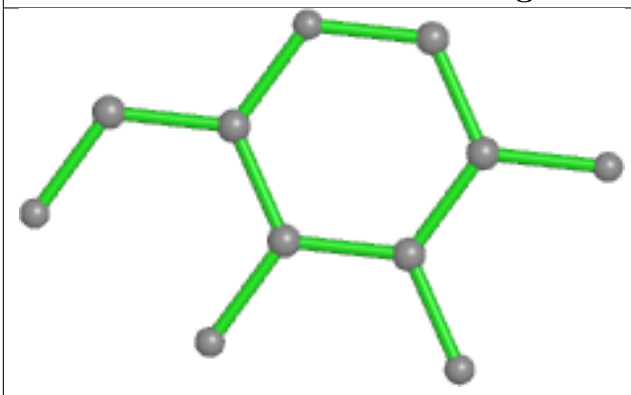


Torsions

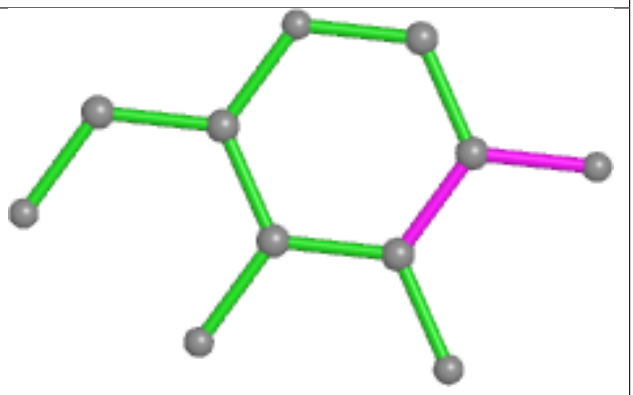


Rings

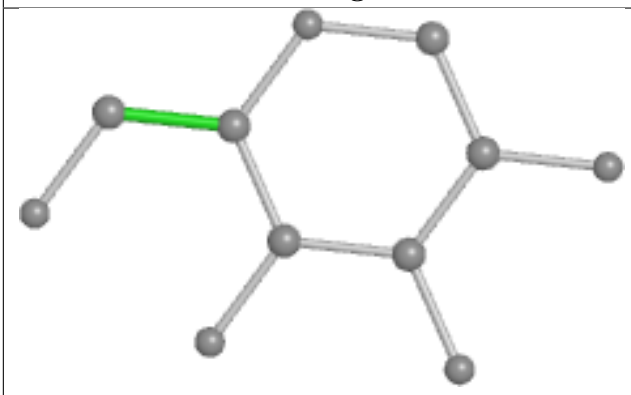
Ligand MAN G 301



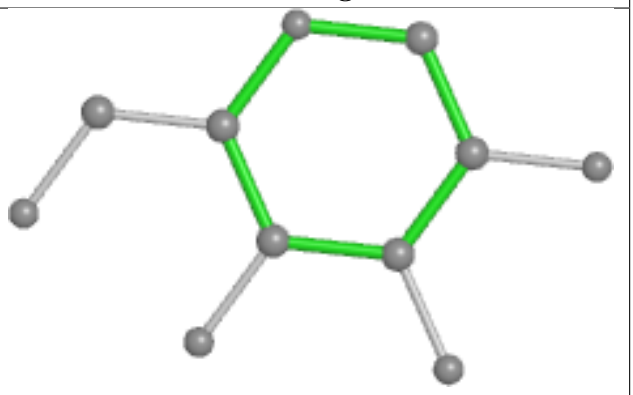
Bond lengths



Bond angles

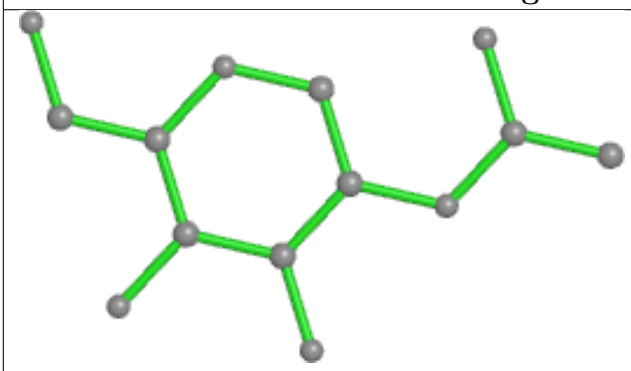


Torsions

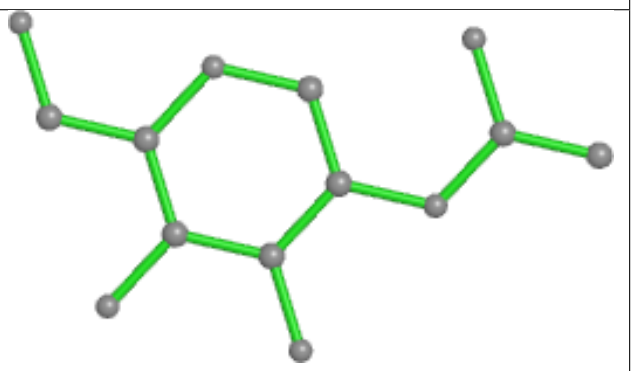


Rings

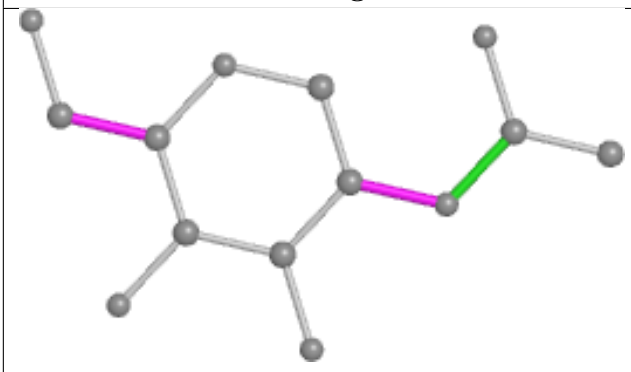
Ligand NAG E 603



Bond lengths



Bond angles



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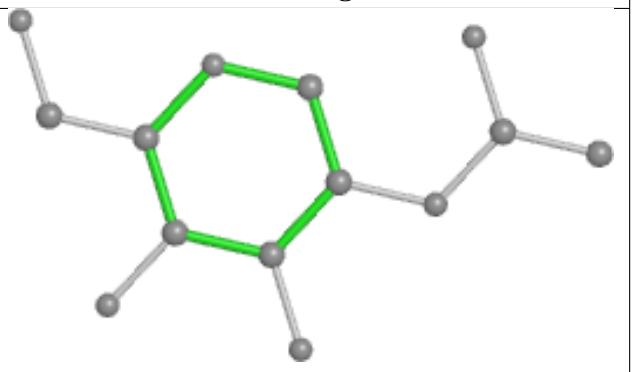
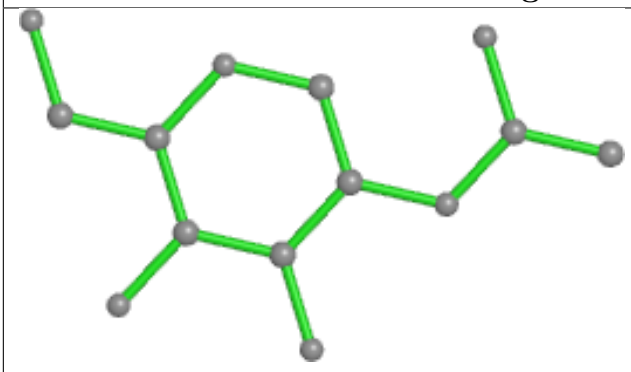
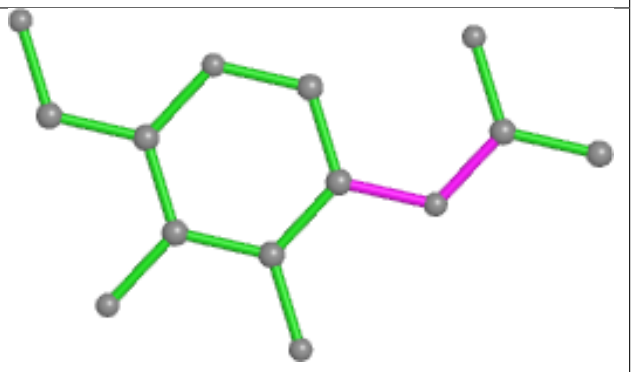


Rings

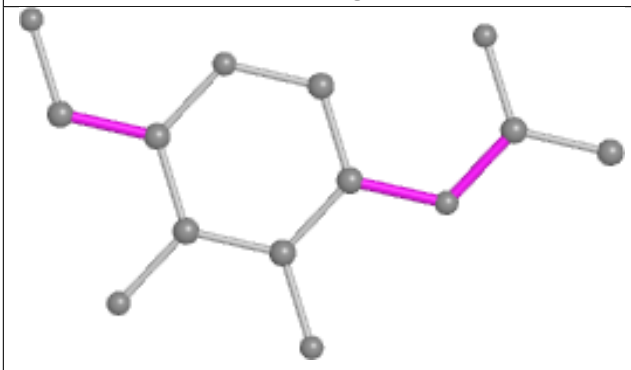
Ligand NAG E 601



Bond lengths



Bond angles



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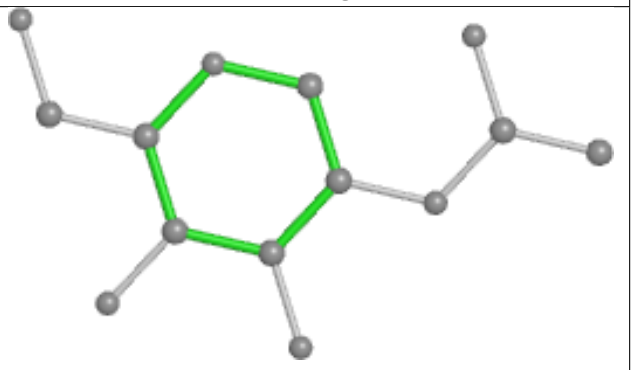


Rings

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.

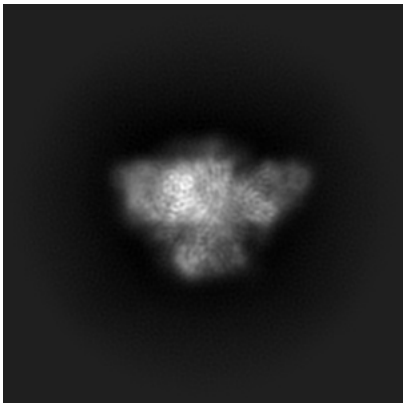
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-25814. These allow visual inspection of the internal detail of the map and identification of artifacts.

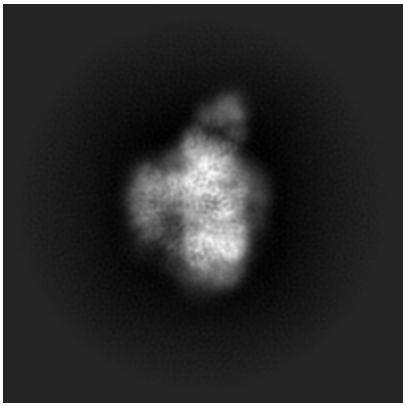
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

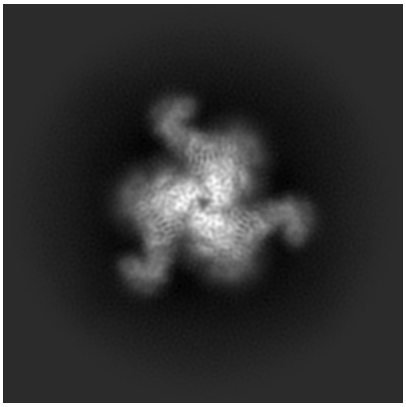
6.1.1 Primary map



X



Y

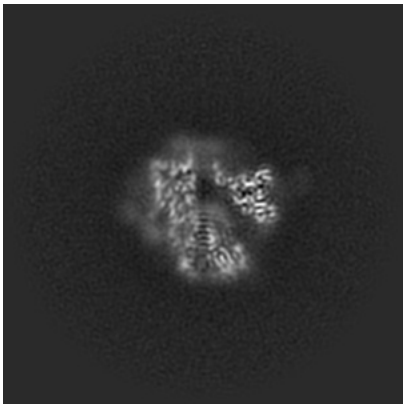


Z

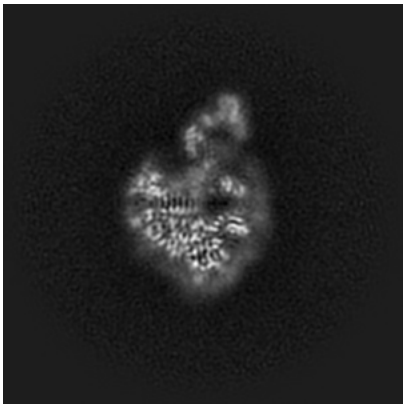
The images above show the map projected in three orthogonal directions.

6.2 Central slices

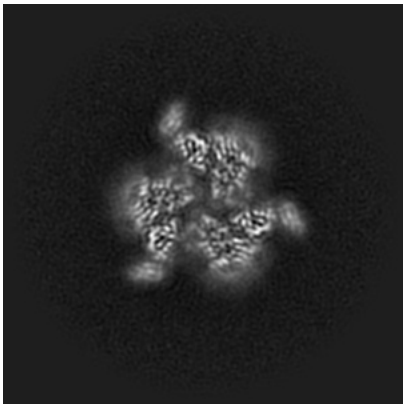
6.2.1 Primary map



X Index: 160



Y Index: 160

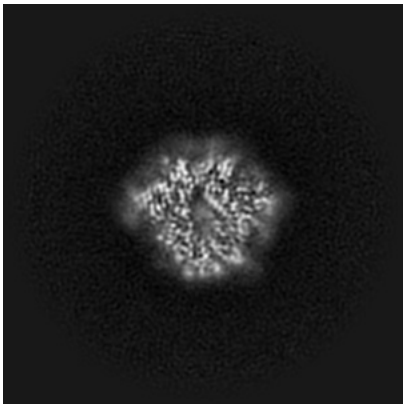


Z Index: 160

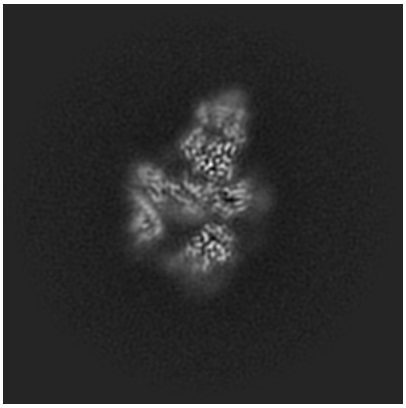
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

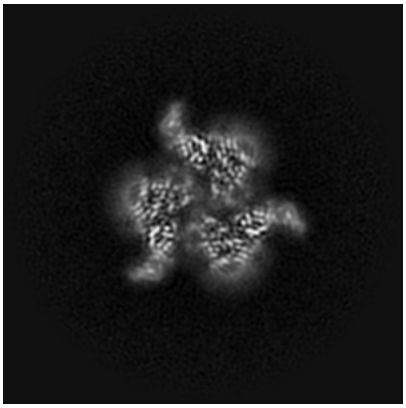
6.3.1 Primary map



X Index: 170



Y Index: 144

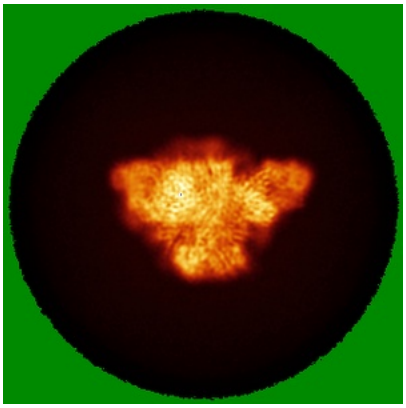


Z Index: 159

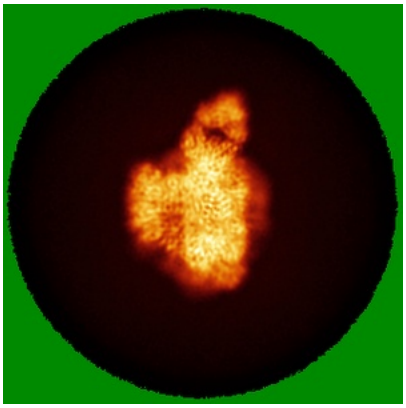
The images above show the largest variance slices of the map in three orthogonal directions.

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

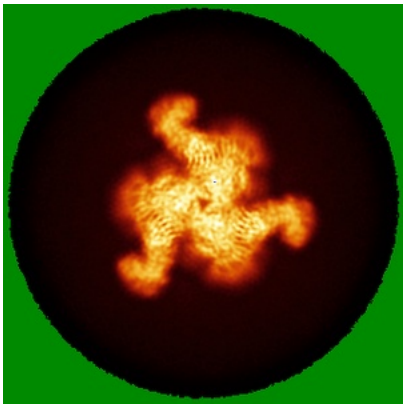
6.4.1 Primary map



X



Y



Z

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 1.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

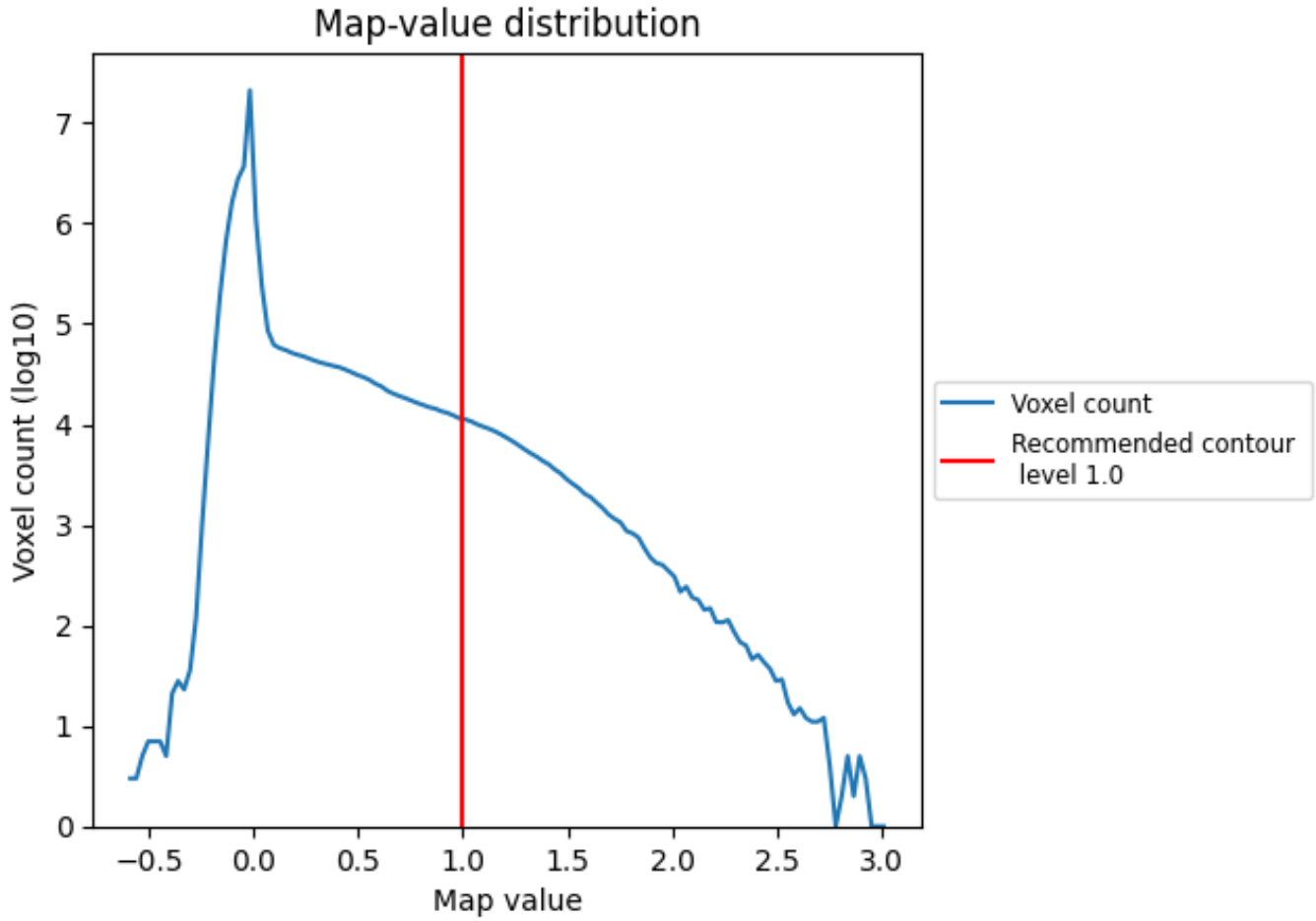
6.6 Mask visualisation (i)

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

7 Map analysis

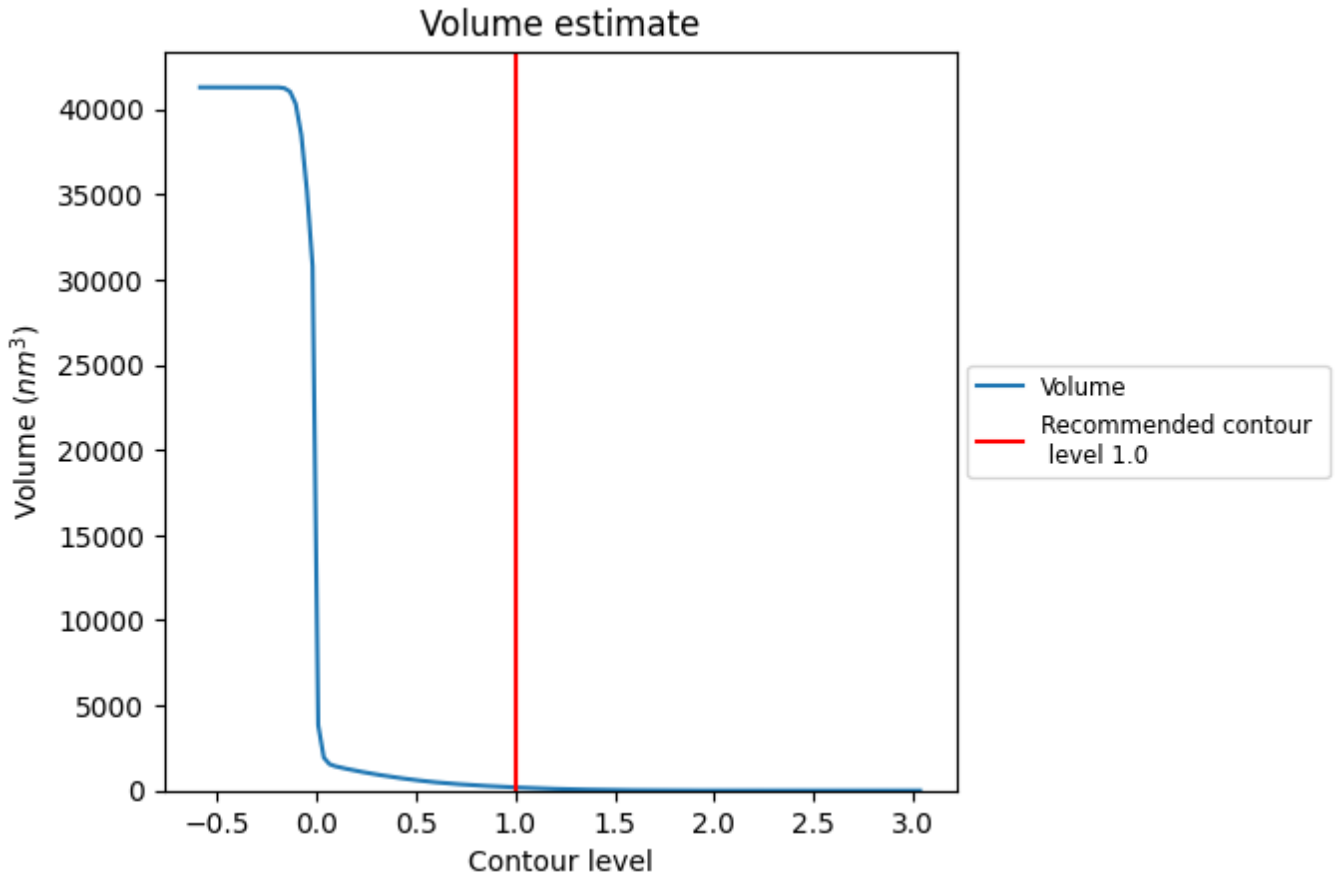
This section contains the results of statistical analysis of the map.

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.

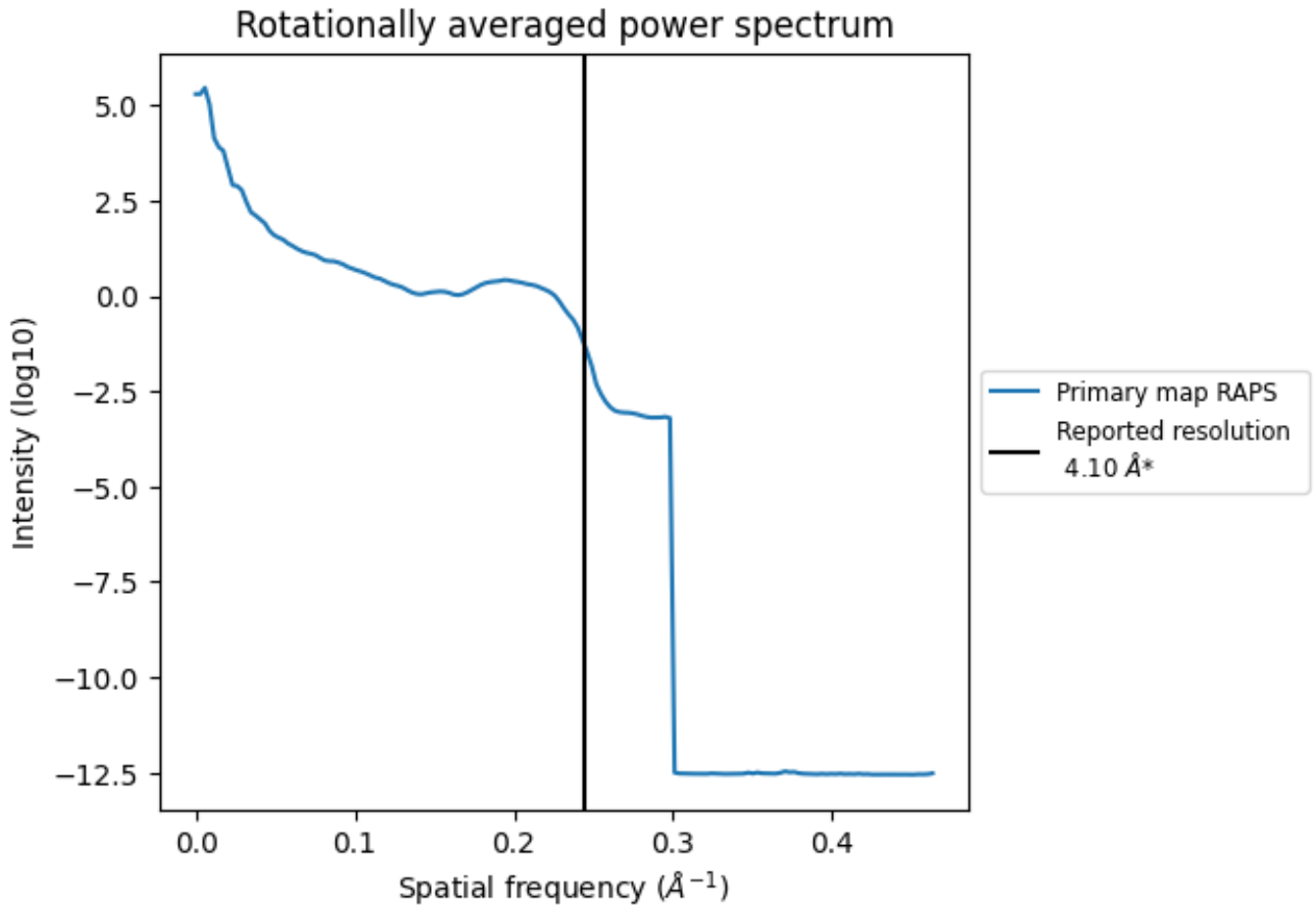
7.2 Volume estimate (i)



The volume at the recommended contour level is 186 nm^3; this corresponds to an approximate mass of 168 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 0.244 $Å^{-1}$

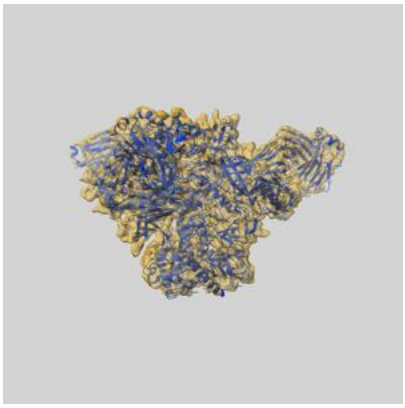
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

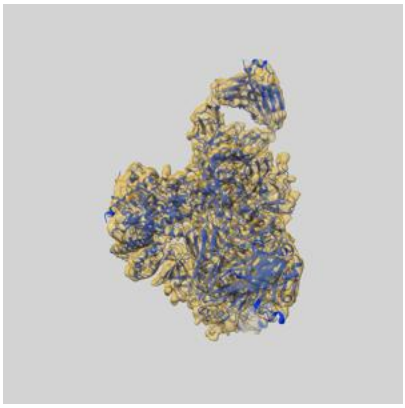
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-25814 and PDB model 7TCN. Per-residue inclusion information can be found in section 3 on page 12.

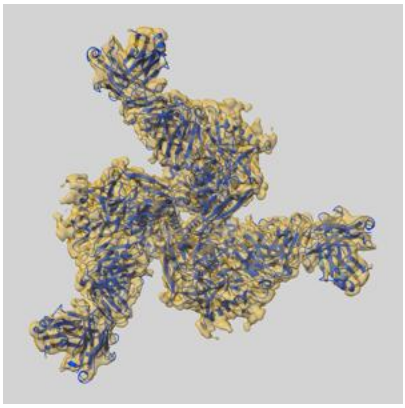
9.1 Map-model overlay



X



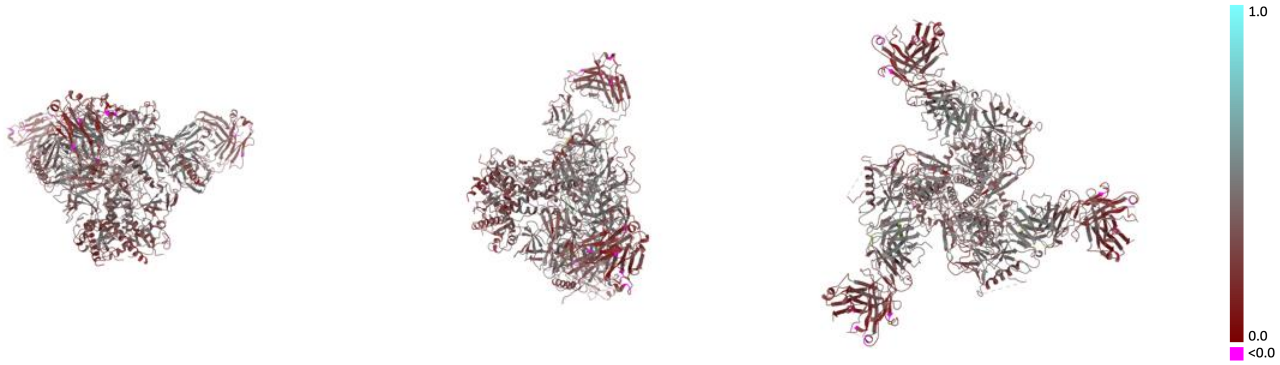
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 1.0 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.

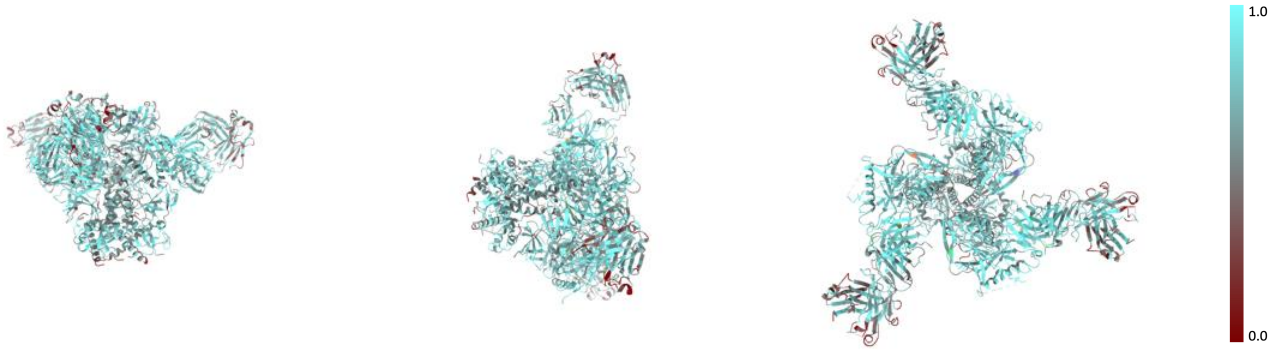
9.2 Q-score mapped to coordinate model



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.

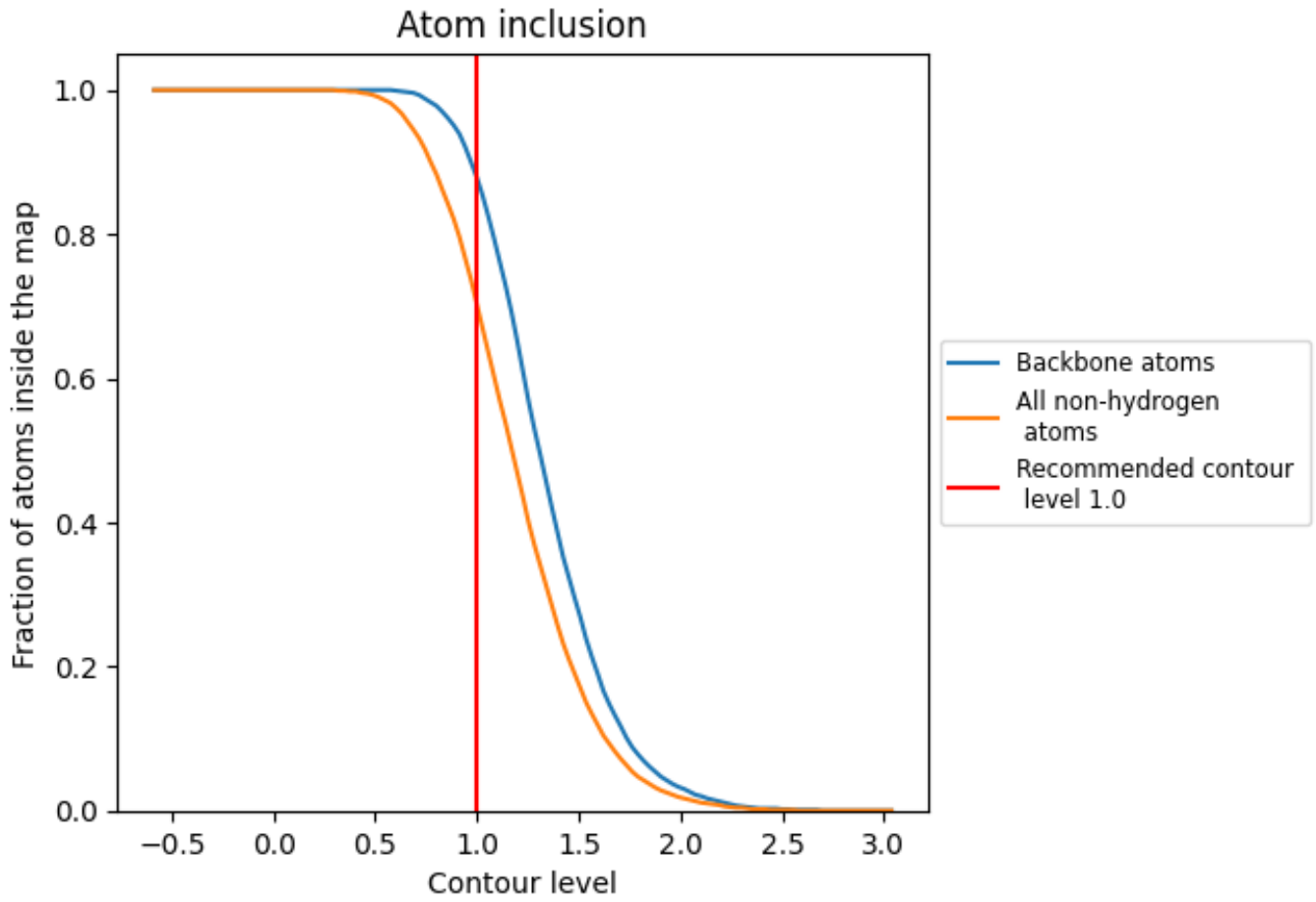
9.3 Atom inclusion mapped to coordinate model



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 (1.0).

9.4 Atom inclusion (i)



At the recommended contour level, 88% of all backbone atoms, 70% 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 (1.0) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7020	0.3460
0	0.5640	0.3680
4	0.7000	0.4220
A	0.7340	0.3770
B	0.6740	0.2960
C	0.7180	0.3610
D	0.6600	0.3040
E	0.7260	0.3700
F	0.6800	0.2950
G	0.7090	0.3600
H	0.6560	0.2990
I	0.7280	0.3730
J	0.6680	0.3000
K	0.7180	0.3590
L	0.6650	0.3050
M	0.6410	0.2760
N	0.4360	0.4140
R	0.7000	0.4370
e	0.4100	0.3910
h	0.5710	0.3160
j	0.5640	0.3310
n	0.6800	0.4220
v	0.4100	0.3950
y	0.4640	0.2490