Full wwPDB EM Validation Report ⓘ

Nov 28, 2022 – 10:17 AM EST

PDB ID	:	7SCO
EMDB ID	:	EMD-25040
Title	:	Structure of H1 influenza hemagglutinin bound to Fab 310-39G10
Authors	:	Torrents de la Pena, A.; Ward, A.B.
Deposited on	:	2021-09-28
Resolution	:	3.37 Å(reported)

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

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

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

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

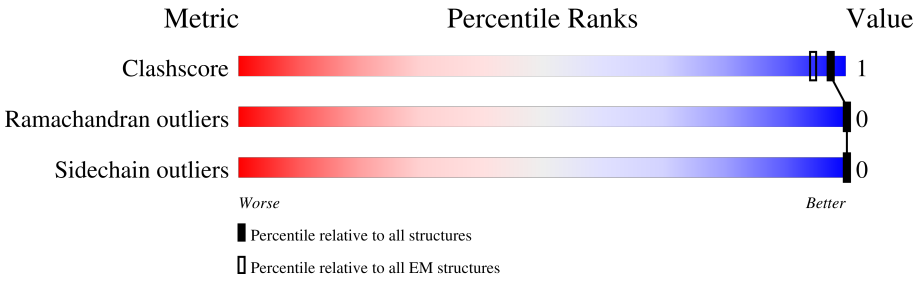
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.37 Å.

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



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

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

Mol	Chain	Length	Quality of chain
1	A	322	5% 95% 5%
1	C	322	5% 96% .
1	G	322	6% 96% .
2	B	231	6% 70% . 26%
2	D	231	7% 71% . 26%
2	I	231	7% 71% . 26%
3	E	119	11% 94% 6%
3	H	119	8% 93% 7%

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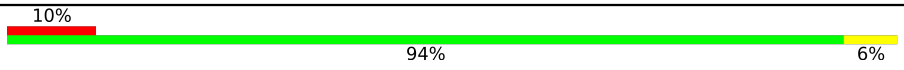
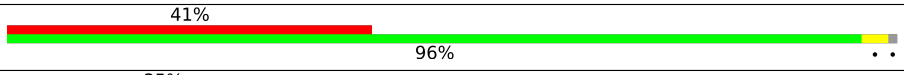
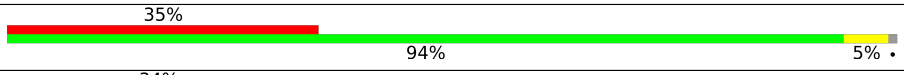
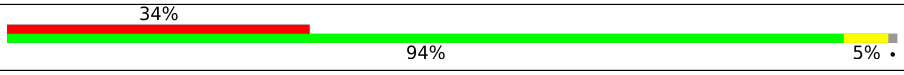
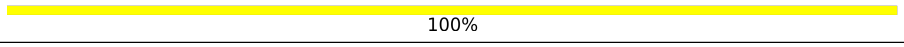
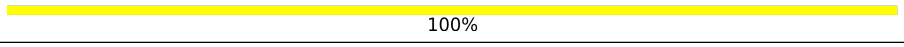
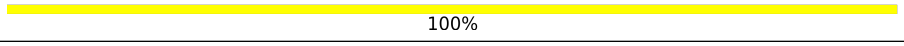
Mol	Chain	Length	Quality of chain
3	J	119	
4	F	108	
4	K	108	
4	L	108	
5	M	2	
5	N	2	
5	O	2	

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 17130 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 Hemagglutinin HA1 chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	322	Total	C	N	O	S	0	0
			2530	1601	436	482	11		
1	C	322	Total	C	N	O	S	0	0
			2530	1601	436	482	11		
1	G	322	Total	C	N	O	S	0	0
			2530	1601	436	482	11		

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	169	VAL	ALA	conflict	UNP Q289M7
A	190	ASN	ASP	conflict	UNP Q289M7
A	225	ASP	ASN	conflict	UNP Q289M7
A	255	TRP	ARG	conflict	UNP Q289M7
C	169	VAL	ALA	conflict	UNP Q289M7
C	190	ASN	ASP	conflict	UNP Q289M7
C	225	ASP	ASN	conflict	UNP Q289M7
C	255	TRP	ARG	conflict	UNP Q289M7
G	169	VAL	ALA	conflict	UNP Q289M7
G	190	ASN	ASP	conflict	UNP Q289M7
G	225	ASP	ASN	conflict	UNP Q289M7
G	255	TRP	ARG	conflict	UNP Q289M7

- Molecule 2 is a protein called Hemagglutinin HA2 chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	171	Total	C	N	O	S	0	0
			1382	863	238	274	7		
2	D	171	Total	C	N	O	S	0	0
			1382	863	238	274	7		
2	I	171	Total	C	N	O	S	0	0
			1382	863	238	274	7		

There are 159 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	327	ARG	-	expression tag	UNP Q289M7
B	328	GLU	-	expression tag	UNP Q289M7
B	329	THR	-	expression tag	UNP Q289M7
B	508	TYR	-	expression tag	UNP Q289M7
B	509	ILE	-	expression tag	UNP Q289M7
B	510	PRO	-	expression tag	UNP Q289M7
B	511	GLU	-	expression tag	UNP Q289M7
B	512	ALA	-	expression tag	UNP Q289M7
B	513	PRO	-	expression tag	UNP Q289M7
B	514	ARG	-	expression tag	UNP Q289M7
B	515	ASP	-	expression tag	UNP Q289M7
B	516	GLY	-	expression tag	UNP Q289M7
B	517	GLN	-	expression tag	UNP Q289M7
B	518	ALA	-	expression tag	UNP Q289M7
B	519	TYR	-	expression tag	UNP Q289M7
B	520	VAL	-	expression tag	UNP Q289M7
B	521	ARG	-	expression tag	UNP Q289M7
B	522	LYS	-	expression tag	UNP Q289M7
B	523	ASP	-	expression tag	UNP Q289M7
B	524	GLY	-	expression tag	UNP Q289M7
B	525	GLU	-	expression tag	UNP Q289M7
B	526	TRP	-	expression tag	UNP Q289M7
B	527	VAL	-	expression tag	UNP Q289M7
B	528	LEU	-	expression tag	UNP Q289M7
B	529	LEU	-	expression tag	UNP Q289M7
B	530	SER	-	expression tag	UNP Q289M7
B	531	THR	-	expression tag	UNP Q289M7
B	532	PHE	-	expression tag	UNP Q289M7
B	533	LEU	-	expression tag	UNP Q289M7
B	534	GLY	-	expression tag	UNP Q289M7
B	535	SER	-	expression tag	UNP Q289M7
B	536	GLY	-	expression tag	UNP Q289M7
B	537	LEU	-	expression tag	UNP Q289M7
B	538	ASN	-	expression tag	UNP Q289M7
B	539	ASP	-	expression tag	UNP Q289M7
B	540	ILE	-	expression tag	UNP Q289M7
B	541	PHE	-	expression tag	UNP Q289M7
B	542	GLU	-	expression tag	UNP Q289M7
B	543	ALA	-	expression tag	UNP Q289M7
B	544	GLN	-	expression tag	UNP Q289M7
B	545	LYS	-	expression tag	UNP Q289M7
B	546	ILE	-	expression tag	UNP Q289M7

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Chain	Residue	Modelled	Actual	Comment	Reference
B	547	GLU	-	expression tag	UNP Q289M7
B	548	TRP	-	expression tag	UNP Q289M7
B	549	HIS	-	expression tag	UNP Q289M7
B	550	GLU	-	expression tag	UNP Q289M7
B	551	GLY	-	expression tag	UNP Q289M7
B	552	HIS	-	expression tag	UNP Q289M7
B	553	HIS	-	expression tag	UNP Q289M7
B	554	HIS	-	expression tag	UNP Q289M7
B	555	HIS	-	expression tag	UNP Q289M7
B	556	HIS	-	expression tag	UNP Q289M7
B	557	HIS	-	expression tag	UNP Q289M7
D	327	ARG	-	expression tag	UNP Q289M7
D	328	GLU	-	expression tag	UNP Q289M7
D	329	THR	-	expression tag	UNP Q289M7
D	508	TYR	-	expression tag	UNP Q289M7
D	509	ILE	-	expression tag	UNP Q289M7
D	510	PRO	-	expression tag	UNP Q289M7
D	511	GLU	-	expression tag	UNP Q289M7
D	512	ALA	-	expression tag	UNP Q289M7
D	513	PRO	-	expression tag	UNP Q289M7
D	514	ARG	-	expression tag	UNP Q289M7
D	515	ASP	-	expression tag	UNP Q289M7
D	516	GLY	-	expression tag	UNP Q289M7
D	517	GLN	-	expression tag	UNP Q289M7
D	518	ALA	-	expression tag	UNP Q289M7
D	519	TYR	-	expression tag	UNP Q289M7
D	520	VAL	-	expression tag	UNP Q289M7
D	521	ARG	-	expression tag	UNP Q289M7
D	522	LYS	-	expression tag	UNP Q289M7
D	523	ASP	-	expression tag	UNP Q289M7
D	524	GLY	-	expression tag	UNP Q289M7
D	525	GLU	-	expression tag	UNP Q289M7
D	526	TRP	-	expression tag	UNP Q289M7
D	527	VAL	-	expression tag	UNP Q289M7
D	528	LEU	-	expression tag	UNP Q289M7
D	529	LEU	-	expression tag	UNP Q289M7
D	530	SER	-	expression tag	UNP Q289M7
D	531	THR	-	expression tag	UNP Q289M7
D	532	PHE	-	expression tag	UNP Q289M7
D	533	LEU	-	expression tag	UNP Q289M7
D	534	GLY	-	expression tag	UNP Q289M7
D	535	SER	-	expression tag	UNP Q289M7

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Chain	Residue	Modelled	Actual	Comment	Reference
D	536	GLY	-	expression tag	UNP Q289M7
D	537	LEU	-	expression tag	UNP Q289M7
D	538	ASN	-	expression tag	UNP Q289M7
D	539	ASP	-	expression tag	UNP Q289M7
D	540	ILE	-	expression tag	UNP Q289M7
D	541	PHE	-	expression tag	UNP Q289M7
D	542	GLU	-	expression tag	UNP Q289M7
D	543	ALA	-	expression tag	UNP Q289M7
D	544	GLN	-	expression tag	UNP Q289M7
D	545	LYS	-	expression tag	UNP Q289M7
D	546	ILE	-	expression tag	UNP Q289M7
D	547	GLU	-	expression tag	UNP Q289M7
D	548	TRP	-	expression tag	UNP Q289M7
D	549	HIS	-	expression tag	UNP Q289M7
D	550	GLU	-	expression tag	UNP Q289M7
D	551	GLY	-	expression tag	UNP Q289M7
D	552	HIS	-	expression tag	UNP Q289M7
D	553	HIS	-	expression tag	UNP Q289M7
D	554	HIS	-	expression tag	UNP Q289M7
D	555	HIS	-	expression tag	UNP Q289M7
D	556	HIS	-	expression tag	UNP Q289M7
D	557	HIS	-	expression tag	UNP Q289M7
I	327	ARG	-	expression tag	UNP Q289M7
I	328	GLU	-	expression tag	UNP Q289M7
I	329	THR	-	expression tag	UNP Q289M7
I	508	TYR	-	expression tag	UNP Q289M7
I	509	ILE	-	expression tag	UNP Q289M7
I	510	PRO	-	expression tag	UNP Q289M7
I	511	GLU	-	expression tag	UNP Q289M7
I	512	ALA	-	expression tag	UNP Q289M7
I	513	PRO	-	expression tag	UNP Q289M7
I	514	ARG	-	expression tag	UNP Q289M7
I	515	ASP	-	expression tag	UNP Q289M7
I	516	GLY	-	expression tag	UNP Q289M7
I	517	GLN	-	expression tag	UNP Q289M7
I	518	ALA	-	expression tag	UNP Q289M7
I	519	TYR	-	expression tag	UNP Q289M7
I	520	VAL	-	expression tag	UNP Q289M7
I	521	ARG	-	expression tag	UNP Q289M7
I	522	LYS	-	expression tag	UNP Q289M7
I	523	ASP	-	expression tag	UNP Q289M7
I	524	GLY	-	expression tag	UNP Q289M7

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Chain	Residue	Modelled	Actual	Comment	Reference
I	525	GLU	-	expression tag	UNP Q289M7
I	526	TRP	-	expression tag	UNP Q289M7
I	527	VAL	-	expression tag	UNP Q289M7
I	528	LEU	-	expression tag	UNP Q289M7
I	529	LEU	-	expression tag	UNP Q289M7
I	530	SER	-	expression tag	UNP Q289M7
I	531	THR	-	expression tag	UNP Q289M7
I	532	PHE	-	expression tag	UNP Q289M7
I	533	LEU	-	expression tag	UNP Q289M7
I	534	GLY	-	expression tag	UNP Q289M7
I	535	SER	-	expression tag	UNP Q289M7
I	536	GLY	-	expression tag	UNP Q289M7
I	537	LEU	-	expression tag	UNP Q289M7
I	538	ASN	-	expression tag	UNP Q289M7
I	539	ASP	-	expression tag	UNP Q289M7
I	540	ILE	-	expression tag	UNP Q289M7
I	541	PHE	-	expression tag	UNP Q289M7
I	542	GLU	-	expression tag	UNP Q289M7
I	543	ALA	-	expression tag	UNP Q289M7
I	544	GLN	-	expression tag	UNP Q289M7
I	545	LYS	-	expression tag	UNP Q289M7
I	546	ILE	-	expression tag	UNP Q289M7
I	547	GLU	-	expression tag	UNP Q289M7
I	548	TRP	-	expression tag	UNP Q289M7
I	549	HIS	-	expression tag	UNP Q289M7
I	550	GLU	-	expression tag	UNP Q289M7
I	551	GLY	-	expression tag	UNP Q289M7
I	552	HIS	-	expression tag	UNP Q289M7
I	553	HIS	-	expression tag	UNP Q289M7
I	554	HIS	-	expression tag	UNP Q289M7
I	555	HIS	-	expression tag	UNP Q289M7
I	556	HIS	-	expression tag	UNP Q289M7
I	557	HIS	-	expression tag	UNP Q289M7

- Molecule 3 is a protein called 310-39G10 Fab, Heavy Chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	H	119	Total	C	N	O	S	0	0
			900	566	152	178	4		
3	E	119	Total	C	N	O	S	0	0
			900	566	152	178	4		
3	J	119	Total	C	N	O	S	0	0
			900	566	152	178	4		

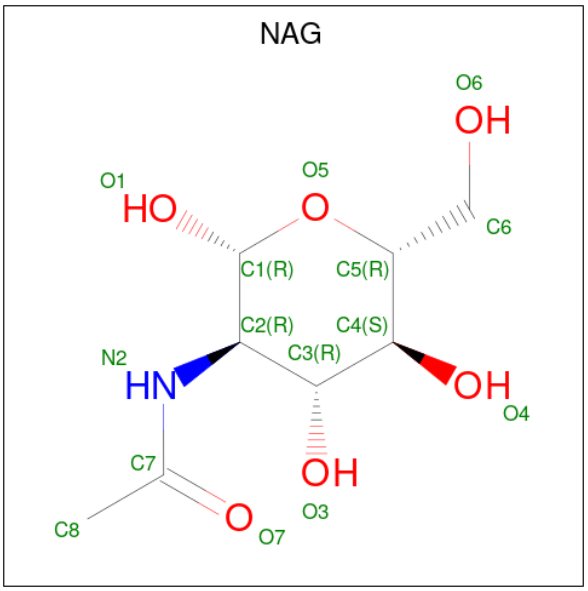
- Molecule 4 is a protein called 310-39G10 Fab, Light Chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	L	107	Total	C	N	O	S	0	0
			814	511	140	161	2		
4	F	107	Total	C	N	O	S	0	0
			814	511	140	161	2		
4	K	107	Total	C	N	O	S	0	0
			814	511	140	161	2		

- Molecule 5 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

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

- Molecule 6 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).

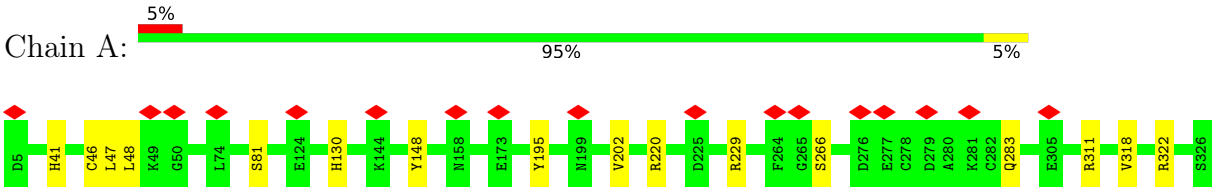


Mol	Chain	Residues	Atoms				AltConf
6	A	1	Total	C	N	O	0
			56	32	4	20	
6	A	1	Total	C	N	O	0
			56	32	4	20	
6	A	1	Total	C	N	O	0
			56	32	4	20	
6	A	1	Total	C	N	O	0
			56	32	4	20	
6	C	1	Total	C	N	O	0
			56	32	4	20	
6	C	1	Total	C	N	O	0
			56	32	4	20	
6	C	1	Total	C	N	O	0
			56	32	4	20	
6	C	1	Total	C	N	O	0
			56	32	4	20	
6	G	1	Total	C	N	O	0
			56	32	4	20	
6	G	1	Total	C	N	O	0
			56	32	4	20	
6	G	1	Total	C	N	O	0
			56	32	4	20	
6	G	1	Total	C	N	O	0
			56	32	4	20	

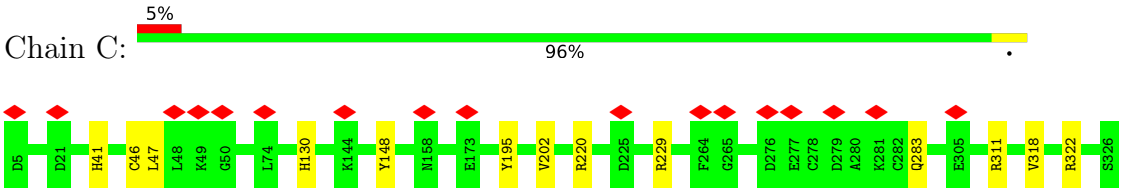
3 Residue-property plots (i)

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.

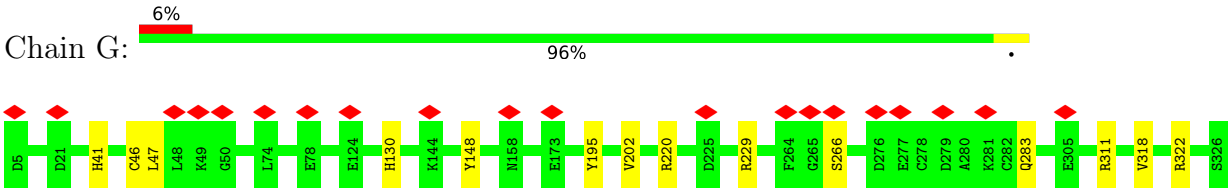
• Molecule 1: Hemagglutinin HA1 chain



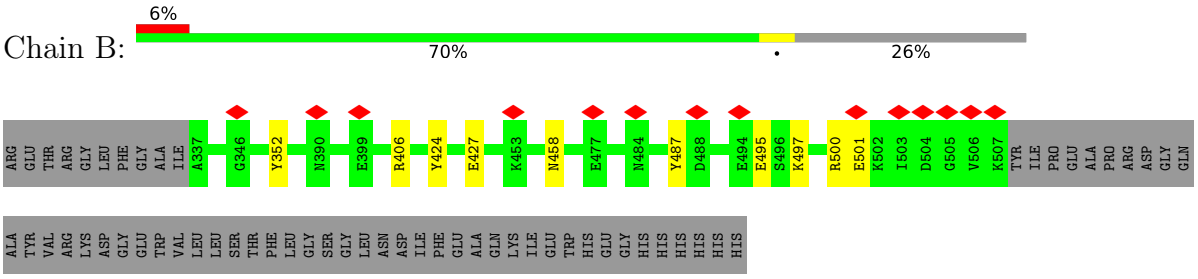
• Molecule 1: Hemagglutinin HA1 chain



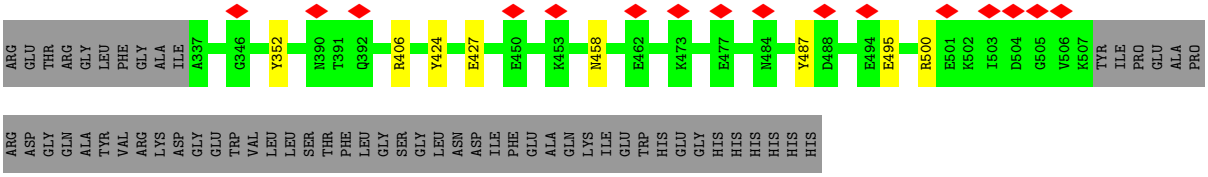
• Molecule 1: Hemagglutinin HA1 chain



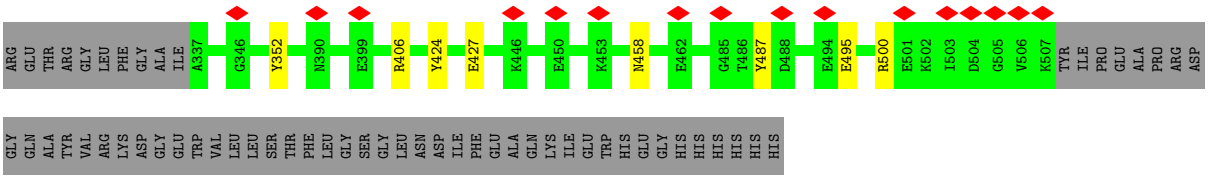
• Molecule 2: Hemagglutinin HA2 chain



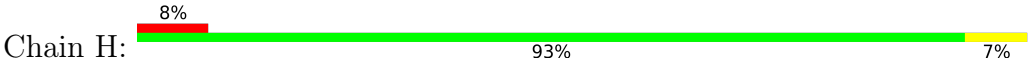
• Molecule 2: Hemagglutinin HA2 chain

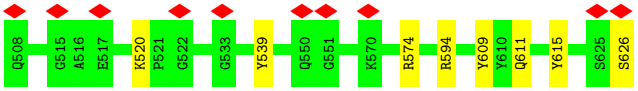


• Molecule 2: Hemagglutinin HA2 chain

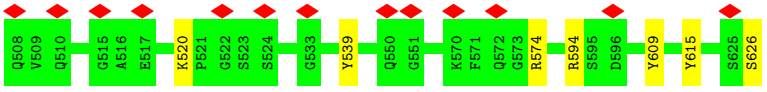


• Molecule 3: 310-39G10 Fab, Heavy Chain

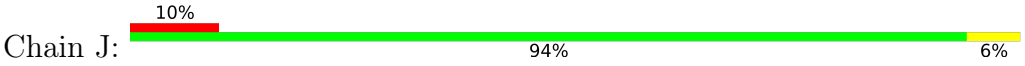


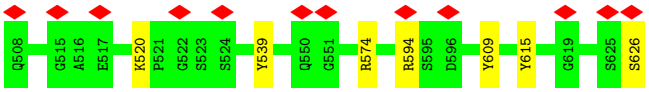


• Molecule 3: 310-39G10 Fab, Heavy Chain

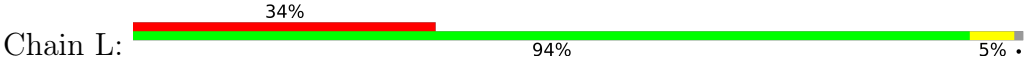


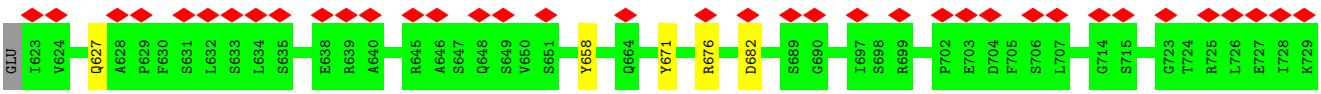
• Molecule 3: 310-39G10 Fab, Heavy Chain



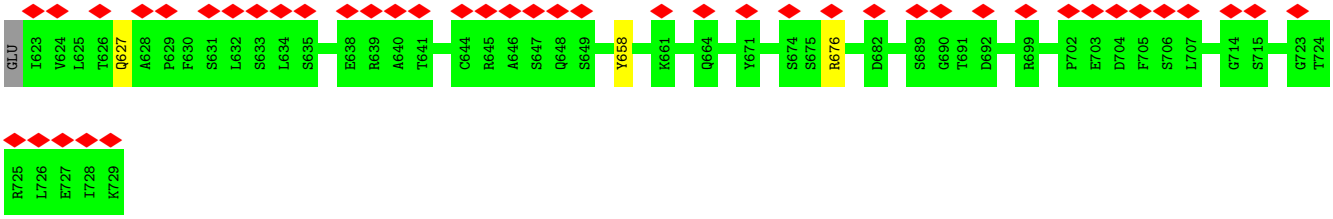


• Molecule 4: 310-39G10 Fab, Light Chain

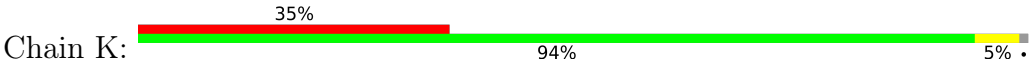


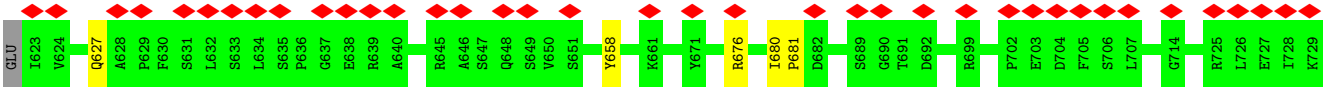


• Molecule 4: 310-39G10 Fab, Light Chain

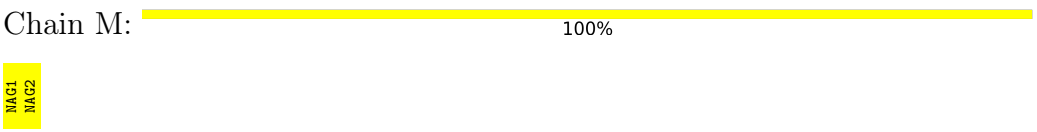


• Molecule 4: 310-39G10 Fab, Light Chain

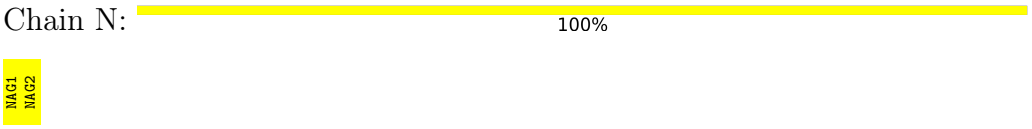




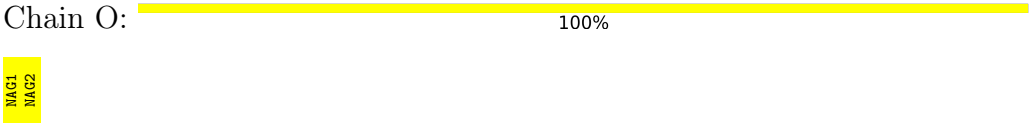
• Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



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



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



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C3	Depositor
Number of particles used	135198	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/Å^2$)	49.88	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	36000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.085	Depositor
Minimum map value	-0.053	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.0145	Depositor
Map size (Å)	368.0, 368.0, 368.0	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.15, 1.15, 1.15	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	1.18	9/2598 (0.3%)	0.96	6/3541 (0.2%)
1	C	1.18	8/2598 (0.3%)	0.96	6/3541 (0.2%)
1	G	1.18	9/2598 (0.3%)	0.96	6/3541 (0.2%)
2	B	1.21	5/1408 (0.4%)	0.88	3/1891 (0.2%)
2	D	1.21	5/1408 (0.4%)	0.88	3/1891 (0.2%)
2	I	1.21	5/1408 (0.4%)	0.88	3/1891 (0.2%)
3	E	1.09	1/921 (0.1%)	0.98	6/1250 (0.5%)
3	H	1.09	1/921 (0.1%)	0.98	6/1250 (0.5%)
3	J	1.08	0/921	0.98	6/1250 (0.5%)
4	F	1.05	1/833 (0.1%)	0.98	2/1128 (0.2%)
4	K	1.05	1/833 (0.1%)	0.98	2/1128 (0.2%)
4	L	1.05	1/833 (0.1%)	0.98	2/1128 (0.2%)
All	All	1.15	46/17280 (0.3%)	0.95	51/23430 (0.2%)

All (46) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	130	HIS	CB-CG	-8.06	1.35	1.50
1	C	130	HIS	CB-CG	-8.03	1.35	1.50
1	A	130	HIS	CB-CG	-8.03	1.35	1.50
2	I	352	TYR	CB-CG	-7.49	1.40	1.51
2	D	352	TYR	CB-CG	-7.45	1.40	1.51
2	B	352	TYR	CB-CG	-7.42	1.40	1.51
1	G	148	TYR	CG-CD2	-6.93	1.30	1.39
1	C	148	TYR	CG-CD2	-6.91	1.30	1.39
1	A	148	TYR	CG-CD2	-6.84	1.30	1.39
1	A	283	GLN	CG-CD	-6.66	1.35	1.51
1	G	283	GLN	CG-CD	-6.66	1.35	1.51
1	C	283	GLN	CG-CD	-6.66	1.35	1.51
2	D	427	GLU	CD-OE2	-6.38	1.18	1.25
2	B	427	GLU	CD-OE2	-6.37	1.18	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	I	427	GLU	CD-OE2	-6.36	1.18	1.25
1	A	148	TYR	CE2-CZ	-6.12	1.30	1.38
1	G	148	TYR	CE2-CZ	-6.10	1.30	1.38
1	C	148	TYR	CE2-CZ	-6.09	1.30	1.38
1	C	318	VAL	CB-CG2	-5.73	1.40	1.52
1	G	318	VAL	CB-CG2	-5.70	1.40	1.52
1	A	318	VAL	CB-CG2	-5.69	1.41	1.52
2	B	352	TYR	CZ-OH	-5.42	1.28	1.37
2	I	352	TYR	CZ-OH	-5.41	1.28	1.37
1	G	195	TYR	CG-CD2	-5.39	1.32	1.39
2	D	352	TYR	CZ-OH	-5.38	1.28	1.37
1	A	195	TYR	CG-CD2	-5.34	1.32	1.39
1	C	195	TYR	CG-CD2	-5.33	1.32	1.39
1	A	202	VAL	CB-CG2	-5.33	1.41	1.52
1	C	202	VAL	CB-CG2	-5.31	1.41	1.52
1	A	41	HIS	CB-CG	-5.29	1.40	1.50
1	C	41	HIS	CB-CG	-5.29	1.40	1.50
1	G	202	VAL	CB-CG2	-5.29	1.41	1.52
1	G	41	HIS	CB-CG	-5.28	1.40	1.50
2	D	495	GLU	CD-OE1	-5.23	1.19	1.25
4	L	627	GLN	CG-CD	-5.21	1.39	1.51
2	I	495	GLU	CD-OE1	-5.20	1.20	1.25
4	F	627	GLN	CG-CD	-5.20	1.39	1.51
2	D	352	TYR	CD2-CE2	-5.17	1.31	1.39
4	K	627	GLN	CG-CD	-5.17	1.39	1.51
2	I	352	TYR	CD2-CE2	-5.16	1.31	1.39
2	B	495	GLU	CD-OE1	-5.16	1.20	1.25
2	B	352	TYR	CD2-CE2	-5.11	1.31	1.39
1	A	266	SER	CB-OG	-5.08	1.35	1.42
3	H	609	TYR	CG-CD2	-5.06	1.32	1.39
1	G	266	SER	CB-OG	-5.06	1.35	1.42
3	E	609	TYR	CG-CD2	-5.01	1.32	1.39

All (51) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	J	574	ARG	NE-CZ-NH2	-9.15	115.73	120.30
3	E	574	ARG	NE-CZ-NH2	-9.04	115.78	120.30
3	H	574	ARG	NE-CZ-NH2	-9.02	115.79	120.30
1	G	311	ARG	NE-CZ-NH2	-8.19	116.20	120.30
1	C	311	ARG	NE-CZ-NH2	-8.10	116.25	120.30
1	A	311	ARG	NE-CZ-NH2	-8.07	116.26	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	G	148	TYR	CB-CG-CD2	-7.59	116.44	121.00
1	C	148	TYR	CB-CG-CD2	-7.54	116.47	121.00
1	A	148	TYR	CB-CG-CD2	-7.52	116.49	121.00
4	L	676	ARG	NE-CZ-NH2	-7.30	116.65	120.30
4	F	676	ARG	NE-CZ-NH2	-7.30	116.65	120.30
4	K	676	ARG	NE-CZ-NH2	-7.25	116.67	120.30
3	J	574	ARG	NE-CZ-NH1	7.14	123.87	120.30
3	E	574	ARG	NE-CZ-NH1	7.12	123.86	120.30
3	H	574	ARG	NE-CZ-NH1	7.05	123.82	120.30
2	D	406	ARG	NE-CZ-NH2	-6.81	116.89	120.30
2	B	406	ARG	NE-CZ-NH2	-6.80	116.90	120.30
2	I	406	ARG	NE-CZ-NH2	-6.77	116.91	120.30
1	C	322	ARG	NE-CZ-NH2	-6.63	116.98	120.30
1	A	322	ARG	NE-CZ-NH2	-6.55	117.02	120.30
3	J	594	ARG	NE-CZ-NH2	-6.50	117.05	120.30
3	E	594	ARG	NE-CZ-NH2	-6.49	117.05	120.30
1	G	322	ARG	NE-CZ-NH2	-6.46	117.07	120.30
3	H	594	ARG	NE-CZ-NH2	-6.39	117.11	120.30
3	E	615	TYR	CB-CG-CD2	-6.26	117.24	121.00
3	H	615	TYR	CB-CG-CD2	-6.22	117.27	121.00
3	J	615	TYR	CB-CG-CD2	-6.20	117.28	121.00
1	C	229	ARG	NE-CZ-NH2	-6.06	117.27	120.30
1	A	229	ARG	NE-CZ-NH2	-6.00	117.30	120.30
1	G	229	ARG	NE-CZ-NH2	-5.95	117.33	120.30
3	H	609	TYR	CB-CG-CD2	-5.64	117.61	121.00
3	E	609	TYR	CB-CG-CD2	-5.63	117.62	121.00
3	J	609	TYR	CB-CG-CD2	-5.63	117.62	121.00
2	B	424	TYR	CB-CG-CD1	-5.55	117.67	121.00
2	I	424	TYR	CB-CG-CD1	-5.53	117.68	121.00
2	D	424	TYR	CB-CG-CD1	-5.46	117.72	121.00
1	A	220	ARG	NE-CZ-NH1	5.40	123.00	120.30
2	D	487	TYR	CB-CG-CD2	-5.40	117.76	121.00
1	G	220	ARG	NE-CZ-NH1	5.40	123.00	120.30
1	C	220	ARG	NE-CZ-NH1	5.37	122.99	120.30
1	G	311	ARG	NE-CZ-NH1	5.36	122.98	120.30
2	B	487	TYR	CB-CG-CD2	-5.35	117.79	121.00
1	A	311	ARG	NE-CZ-NH1	5.29	122.95	120.30
2	I	487	TYR	CB-CG-CD2	-5.26	117.84	121.00
1	C	311	ARG	NE-CZ-NH1	5.25	122.92	120.30
4	K	658	TYR	CB-CG-CD2	-5.18	117.89	121.00
4	L	658	TYR	CB-CG-CD2	-5.16	117.91	121.00
4	F	658	TYR	CB-CG-CD2	-5.13	117.92	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	H	539	TYR	CB-CG-CD1	-5.10	117.94	121.00
3	E	539	TYR	CB-CG-CD1	-5.06	117.96	121.00
3	J	539	TYR	CB-CG-CD1	-5.06	117.96	121.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2530	0	2438	3	0
1	C	2530	0	2438	1	0
1	G	2530	0	2438	1	0
2	B	1382	0	1312	2	0
2	D	1382	0	1312	1	0
2	I	1382	0	1312	1	0
3	E	900	0	874	1	0
3	H	900	0	874	5	0
3	J	900	0	874	1	0
4	F	814	0	793	0	0
4	K	814	0	793	1	0
4	L	814	0	793	5	0
5	M	28	0	25	0	0
5	N	28	0	25	0	0
5	O	28	0	25	0	0
6	A	56	0	52	0	0
6	C	56	0	52	0	0
6	G	56	0	52	0	0
All	All	17130	0	16482	18	0

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

All (18) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:611:GLN:OE1	4:L:671:TYR:OH	1.88	0.91
3:H:611:GLN:OE1	4:L:671:TYR:CZ	2.31	0.84
2:B:497:LYS:HE2	2:B:501:GLU:OE2	1.97	0.63
3:H:611:GLN:CD	4:L:671:TYR:OH	2.40	0.60
3:E:520:LYS:NZ	3:E:626:SER:OXT	2.46	0.48
3:H:520:LYS:NZ	3:H:626:SER:OXT	2.46	0.47
3:H:611:GLN:CD	4:L:671:TYR:HH	2.16	0.47
1:A:46:CYS:SG	1:A:47:LEU:N	2.88	0.46
3:J:520:LYS:NZ	3:J:626:SER:OXT	2.46	0.46
1:C:46:CYS:SG	1:C:47:LEU:N	2.88	0.45
1:G:46:CYS:SG	1:G:47:LEU:N	2.88	0.45
1:A:48:LEU:HD23	1:A:81:SER:OG	2.18	0.43
4:L:682:ASP:OD1	4:L:682:ASP:N	2.51	0.43
2:D:458:ASN:O	2:D:500:ARG:NH1	2.54	0.41
4:K:680:ILE:HA	4:K:681:PRO:HD3	1.91	0.41
1:A:48:LEU:HB3	1:A:81:SER:OG	2.21	0.41
2:I:458:ASN:O	2:I:500:ARG:NH1	2.54	0.41
2:B:458:ASN:O	2:B:500:ARG:NH1	2.54	0.41

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	320/322 (99%)	316 (99%)	4 (1%)	0	100	100
1	C	320/322 (99%)	316 (99%)	4 (1%)	0	100	100
1	G	320/322 (99%)	316 (99%)	4 (1%)	0	100	100
2	B	169/231 (73%)	167 (99%)	2 (1%)	0	100	100
2	D	169/231 (73%)	167 (99%)	2 (1%)	0	100	100
2	I	169/231 (73%)	167 (99%)	2 (1%)	0	100	100
3	E	117/119 (98%)	116 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	H	117/119 (98%)	116 (99%)	1 (1%)	0	100	100
3	J	117/119 (98%)	116 (99%)	1 (1%)	0	100	100
4	F	105/108 (97%)	102 (97%)	3 (3%)	0	100	100
4	K	105/108 (97%)	102 (97%)	3 (3%)	0	100	100
4	L	105/108 (97%)	102 (97%)	3 (3%)	0	100	100
All	All	2133/2340 (91%)	2103 (99%)	30 (1%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	283/283 (100%)	283 (100%)	0	100	100
1	C	283/283 (100%)	283 (100%)	0	100	100
1	G	283/283 (100%)	283 (100%)	0	100	100
2	B	149/198 (75%)	149 (100%)	0	100	100
2	D	149/198 (75%)	149 (100%)	0	100	100
2	I	149/198 (75%)	149 (100%)	0	100	100
3	E	97/97 (100%)	97 (100%)	0	100	100
3	H	97/97 (100%)	97 (100%)	0	100	100
3	J	97/97 (100%)	97 (100%)	0	100	100
4	F	90/91 (99%)	90 (100%)	0	100	100
4	K	90/91 (99%)	90 (100%)	0	100	100
4	L	90/91 (99%)	90 (100%)	0	100	100
All	All	1857/2007 (92%)	1857 (100%)	0	100	100

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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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)

6 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
5	NAG	M	1	1,5	14,14,15	2.09	6 (42%)	17,19,21	1.01	1 (5%)
5	NAG	M	2	5	14,14,15	1.89	5 (35%)	17,19,21	0.92	1 (5%)
5	NAG	N	1	1,5	14,14,15	2.10	5 (35%)	17,19,21	1.01	1 (5%)
5	NAG	N	2	5	14,14,15	1.90	5 (35%)	17,19,21	0.92	1 (5%)
5	NAG	O	1	1,5	14,14,15	2.10	5 (35%)	17,19,21	1.01	1 (5%)
5	NAG	O	2	5	14,14,15	1.90	5 (35%)	17,19,21	0.92	1 (5%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	M	1	1,5	-	0/6/23/26	0/1/1/1
5	NAG	M	2	5	-	0/6/23/26	0/1/1/1
5	NAG	N	1	1,5	-	0/6/23/26	0/1/1/1
5	NAG	N	2	5	-	0/6/23/26	0/1/1/1
5	NAG	O	1	1,5	-	0/6/23/26	0/1/1/1
5	NAG	O	2	5	-	0/6/23/26	0/1/1/1

All (31) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	N	1	NAG	C1-C2	5.25	1.60	1.52
5	M	1	NAG	C1-C2	5.23	1.60	1.52
5	O	1	NAG	C1-C2	5.19	1.60	1.52
5	N	2	NAG	C1-C2	4.19	1.58	1.52
5	O	2	NAG	C1-C2	4.16	1.58	1.52
5	M	2	NAG	C1-C2	4.16	1.58	1.52
5	N	2	NAG	O5-C5	3.16	1.49	1.43
5	O	2	NAG	O5-C5	3.15	1.49	1.43
5	M	2	NAG	O5-C5	3.10	1.49	1.43
5	O	1	NAG	O5-C5	2.73	1.49	1.43
5	N	1	NAG	O5-C5	2.69	1.48	1.43
5	M	1	NAG	O5-C5	2.68	1.48	1.43
5	N	2	NAG	C4-C5	2.44	1.58	1.53
5	O	1	NAG	O5-C1	2.43	1.47	1.43
5	M	2	NAG	C4-C5	2.42	1.58	1.53
5	O	2	NAG	C4-C5	2.42	1.58	1.53
5	N	1	NAG	O5-C1	2.41	1.47	1.43
5	M	2	NAG	C3-C2	2.37	1.57	1.52
5	M	1	NAG	O5-C1	2.36	1.47	1.43
5	N	2	NAG	C3-C2	2.33	1.57	1.52
5	O	2	NAG	C3-C2	2.31	1.57	1.52
5	O	1	NAG	C3-C2	2.29	1.57	1.52
5	N	1	NAG	C3-C2	2.28	1.57	1.52
5	M	1	NAG	C3-C2	2.28	1.57	1.52
5	O	1	NAG	C2-N2	2.19	1.50	1.46
5	N	1	NAG	C2-N2	2.15	1.50	1.46
5	M	1	NAG	C2-N2	2.15	1.50	1.46
5	O	2	NAG	C4-C3	2.09	1.57	1.52
5	N	2	NAG	C4-C3	2.05	1.57	1.52
5	M	2	NAG	C4-C3	2.05	1.57	1.52
5	M	1	NAG	C4-C5	2.00	1.57	1.53

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	M	1	NAG	C8-C7-N2	2.10	119.66	116.10
5	O	1	NAG	C8-C7-N2	2.09	119.64	116.10
5	N	1	NAG	C8-C7-N2	2.09	119.64	116.10
5	M	2	NAG	C8-C7-N2	2.07	119.60	116.10
5	N	2	NAG	C8-C7-N2	2.07	119.60	116.10
5	O	2	NAG	C8-C7-N2	2.05	119.58	116.10

There are no chirality outliers.

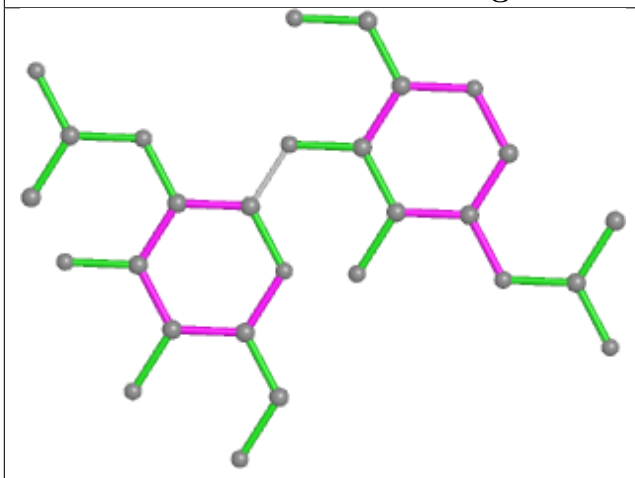
There are no torsion outliers.

There are no ring outliers.

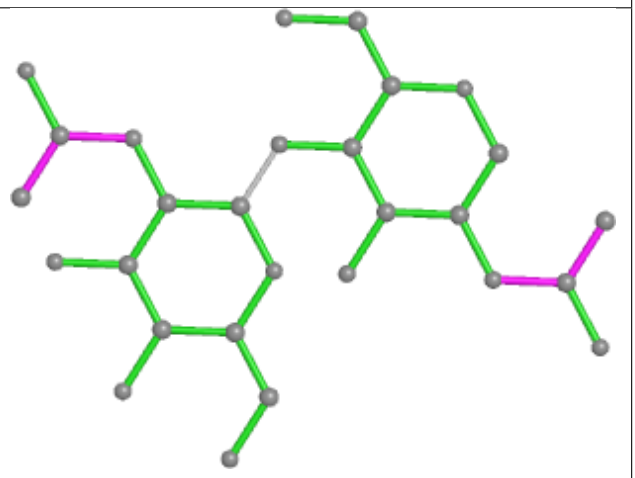
No monomer is involved in short contacts.

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

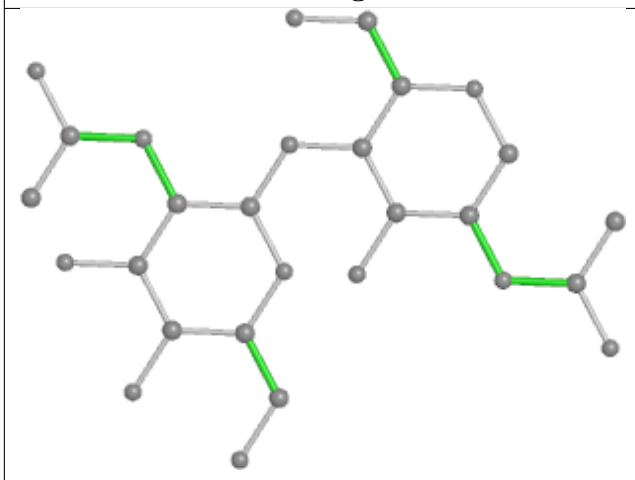
Oligosaccharide Chain M



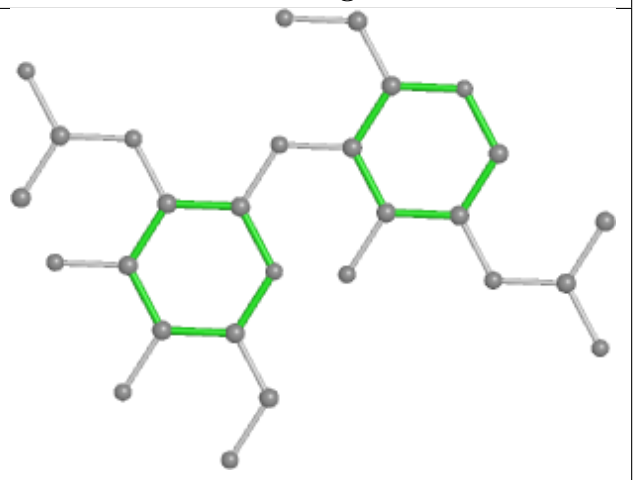
Bond lengths



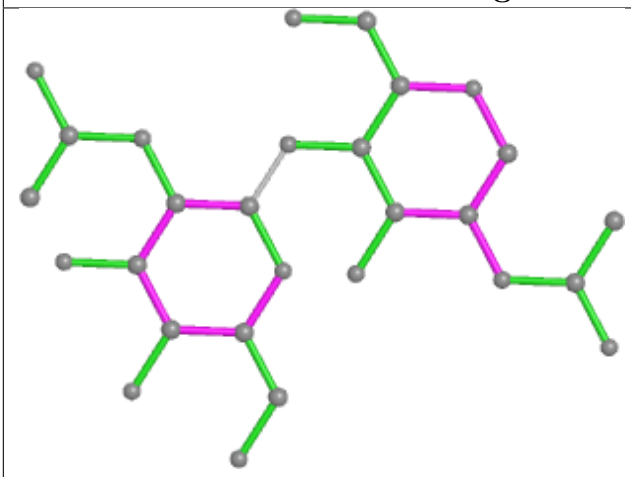
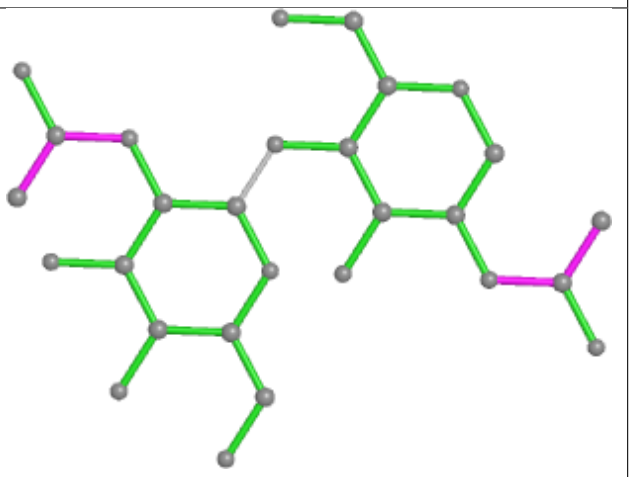
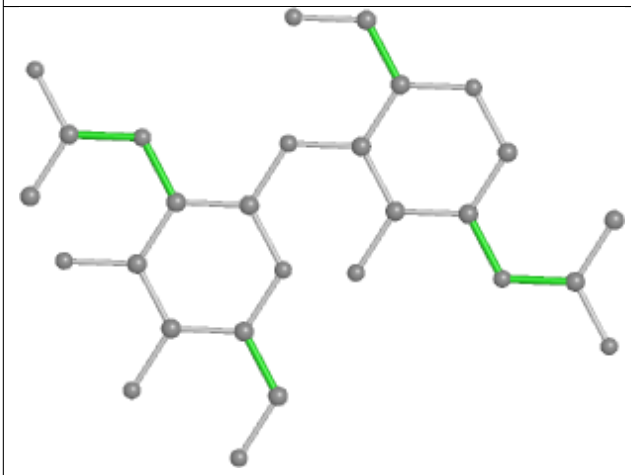
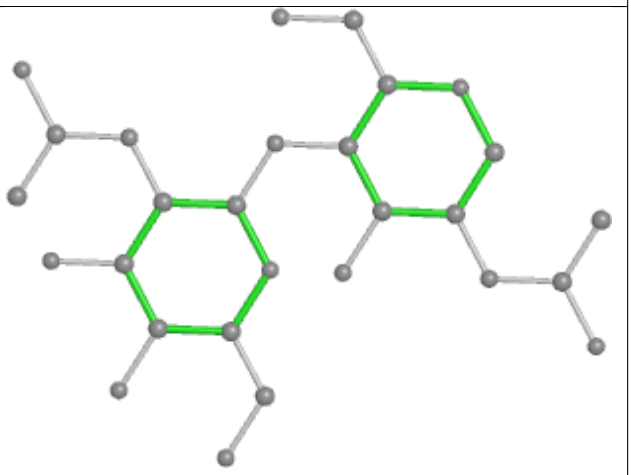
Bond angles

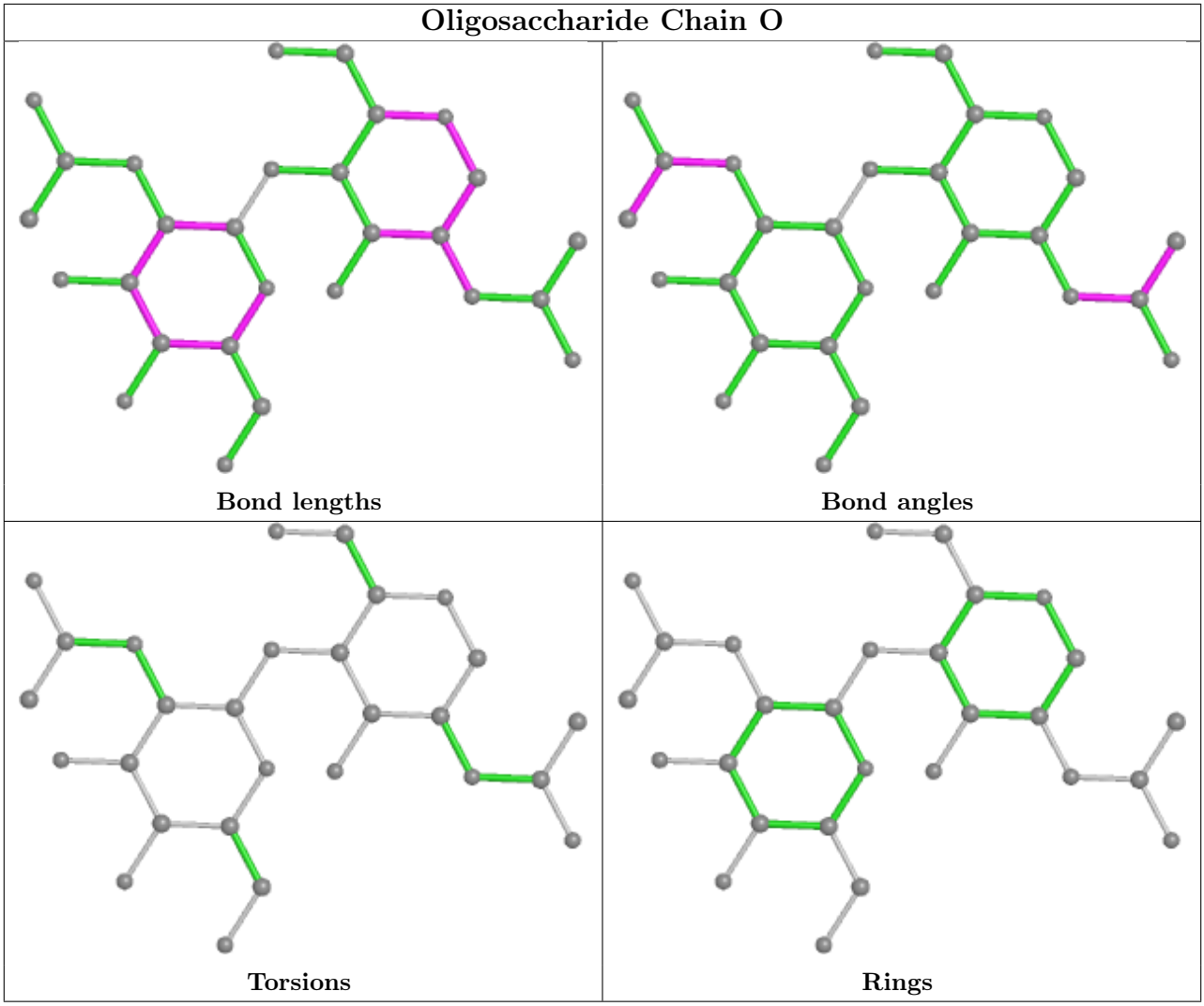


Torsions



Rings

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



5.6 Ligand geometry (i)

12 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
6	NAG	A	401	1	14,14,15	2.14	6 (42%)	17,19,21	1.06	1 (5%)
6	NAG	G	401	1	14,14,15	2.15	6 (42%)	17,19,21	1.05	1 (5%)
6	NAG	A	402	1	14,14,15	2.18	5 (35%)	17,19,21	0.99	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
6	NAG	C	403	1	14,14,15	2.16	5 (35%)	17,19,21	0.92	1 (5%)
6	NAG	C	404	1	14,14,15	2.19	5 (35%)	17,19,21	1.10	2 (11%)
6	NAG	A	404	1	14,14,15	2.21	6 (42%)	17,19,21	1.10	2 (11%)
6	NAG	G	404	1	14,14,15	2.20	6 (42%)	17,19,21	1.11	2 (11%)
6	NAG	C	401	1	14,14,15	2.14	6 (42%)	17,19,21	1.06	1 (5%)
6	NAG	A	403	1	14,14,15	2.16	5 (35%)	17,19,21	0.93	1 (5%)
6	NAG	G	402	1	14,14,15	2.17	5 (35%)	17,19,21	1.00	1 (5%)
6	NAG	G	403	1	14,14,15	2.16	5 (35%)	17,19,21	0.93	1 (5%)
6	NAG	C	402	1	14,14,15	2.19	5 (35%)	17,19,21	0.99	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
6	NAG	A	401	1	-	0/6/23/26	0/1/1/1
6	NAG	G	401	1	-	0/6/23/26	0/1/1/1
6	NAG	A	402	1	-	0/6/23/26	0/1/1/1
6	NAG	C	403	1	-	0/6/23/26	0/1/1/1
6	NAG	C	404	1	-	0/6/23/26	0/1/1/1
6	NAG	A	404	1	-	0/6/23/26	0/1/1/1
6	NAG	G	404	1	-	0/6/23/26	0/1/1/1
6	NAG	C	401	1	-	0/6/23/26	0/1/1/1
6	NAG	A	403	1	-	0/6/23/26	0/1/1/1
6	NAG	G	402	1	-	0/6/23/26	0/1/1/1
6	NAG	G	403	1	-	0/6/23/26	0/1/1/1
6	NAG	C	402	1	-	0/6/23/26	0/1/1/1

All (65) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	404	NAG	C1-C2	5.68	1.60	1.52
6	G	404	NAG	C1-C2	5.64	1.60	1.52
6	C	404	NAG	C1-C2	5.62	1.60	1.52
6	C	402	NAG	C1-C2	5.51	1.60	1.52
6	A	403	NAG	C1-C2	5.51	1.60	1.52
6	C	403	NAG	C1-C2	5.49	1.60	1.52
6	G	401	NAG	C1-C2	5.48	1.60	1.52
6	G	403	NAG	C1-C2	5.47	1.60	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	C	401	NAG	C1-C2	5.46	1.60	1.52
6	A	401	NAG	C1-C2	5.46	1.60	1.52
6	G	402	NAG	C1-C2	5.44	1.60	1.52
6	A	402	NAG	C1-C2	5.43	1.60	1.52
6	C	402	NAG	O5-C5	3.24	1.50	1.43
6	A	402	NAG	O5-C5	3.23	1.50	1.43
6	G	402	NAG	O5-C5	3.20	1.49	1.43
6	A	403	NAG	O5-C5	3.09	1.49	1.43
6	C	403	NAG	O5-C5	3.08	1.49	1.43
6	G	403	NAG	O5-C5	3.08	1.49	1.43
6	A	404	NAG	O5-C5	3.05	1.49	1.43
6	C	404	NAG	O5-C5	3.04	1.49	1.43
6	C	401	NAG	O5-C5	3.03	1.49	1.43
6	A	401	NAG	O5-C5	3.03	1.49	1.43
6	G	401	NAG	O5-C5	3.00	1.49	1.43
6	G	404	NAG	O5-C5	2.99	1.49	1.43
6	A	402	NAG	O5-C1	2.74	1.48	1.43
6	G	402	NAG	O5-C1	2.72	1.48	1.43
6	C	402	NAG	O5-C1	2.70	1.48	1.43
6	G	404	NAG	O5-C1	2.69	1.48	1.43
6	A	401	NAG	O5-C1	2.67	1.48	1.43
6	C	403	NAG	O5-C1	2.67	1.48	1.43
6	A	404	NAG	O5-C1	2.66	1.48	1.43
6	G	403	NAG	O5-C1	2.66	1.48	1.43
6	G	401	NAG	O5-C1	2.66	1.48	1.43
6	C	404	NAG	O5-C1	2.65	1.48	1.43
6	C	401	NAG	O5-C1	2.65	1.47	1.43
6	A	403	NAG	O5-C1	2.63	1.47	1.43
6	A	402	NAG	C3-C2	2.48	1.57	1.52
6	C	402	NAG	C3-C2	2.46	1.57	1.52
6	G	402	NAG	C3-C2	2.43	1.57	1.52
6	A	404	NAG	C3-C2	2.40	1.57	1.52
6	G	404	NAG	C3-C2	2.36	1.57	1.52
6	C	404	NAG	C3-C2	2.36	1.57	1.52
6	G	403	NAG	C3-C2	2.31	1.57	1.52
6	A	403	NAG	C3-C2	2.26	1.57	1.52
6	C	403	NAG	C3-C2	2.26	1.57	1.52
6	G	401	NAG	C3-C2	2.25	1.57	1.52
6	C	401	NAG	C3-C2	2.25	1.57	1.52
6	A	401	NAG	C3-C2	2.21	1.57	1.52
6	C	403	NAG	C4-C5	2.20	1.57	1.53
6	G	403	NAG	C4-C5	2.20	1.57	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	403	NAG	C4-C5	2.19	1.57	1.53
6	G	404	NAG	C4-C5	2.19	1.57	1.53
6	C	404	NAG	C4-C5	2.18	1.57	1.53
6	A	404	NAG	C4-C5	2.17	1.57	1.53
6	A	402	NAG	C4-C5	2.17	1.57	1.53
6	C	402	NAG	C4-C5	2.15	1.57	1.53
6	G	402	NAG	C4-C5	2.13	1.57	1.53
6	A	401	NAG	C2-N2	2.06	1.49	1.46
6	G	401	NAG	C2-N2	2.06	1.49	1.46
6	G	401	NAG	C4-C5	2.04	1.57	1.53
6	C	401	NAG	C4-C5	2.04	1.57	1.53
6	A	404	NAG	C2-N2	2.03	1.49	1.46
6	G	404	NAG	C2-N2	2.02	1.49	1.46
6	A	401	NAG	C4-C5	2.01	1.57	1.53
6	C	401	NAG	C2-N2	2.00	1.49	1.46

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	C	404	NAG	C8-C7-N2	2.70	120.67	116.10
6	G	404	NAG	C8-C7-N2	2.70	120.67	116.10
6	A	404	NAG	C8-C7-N2	2.67	120.61	116.10
6	A	401	NAG	C8-C7-N2	2.33	120.04	116.10
6	C	401	NAG	C8-C7-N2	2.32	120.02	116.10
6	G	402	NAG	C8-C7-N2	2.31	120.01	116.10
6	A	402	NAG	C8-C7-N2	2.29	119.97	116.10
6	G	401	NAG	C8-C7-N2	2.28	119.97	116.10
6	C	402	NAG	C8-C7-N2	2.28	119.96	116.10
6	G	404	NAG	O7-C7-C8	-2.24	117.90	122.06
6	C	404	NAG	O7-C7-C8	-2.20	117.97	122.06
6	A	404	NAG	O7-C7-C8	-2.20	117.97	122.06
6	A	403	NAG	C8-C7-N2	2.03	119.54	116.10
6	G	403	NAG	C8-C7-N2	2.03	119.53	116.10
6	C	403	NAG	C8-C7-N2	2.00	119.49	116.10

There are no chirality outliers.

There are no torsion outliers.

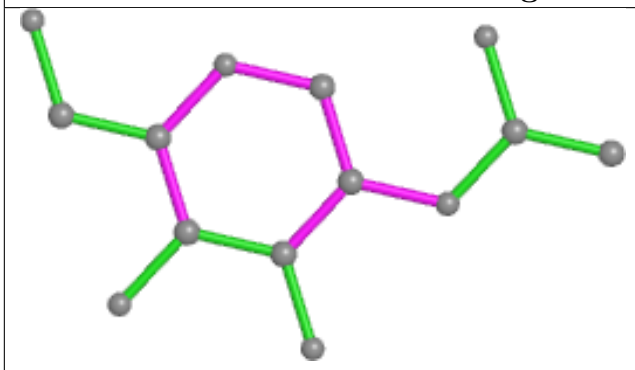
There are no ring outliers.

No monomer is involved in short contacts.

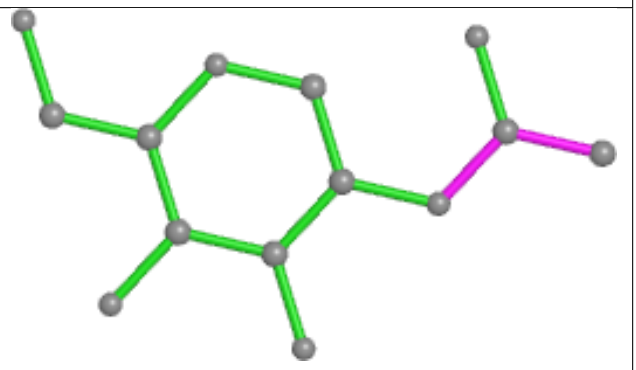
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In

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.

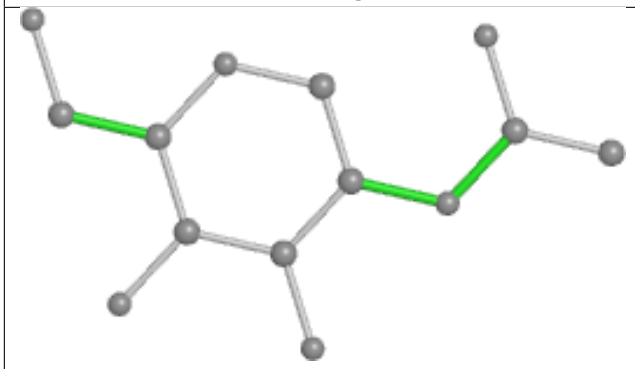
Ligand NAG A 401



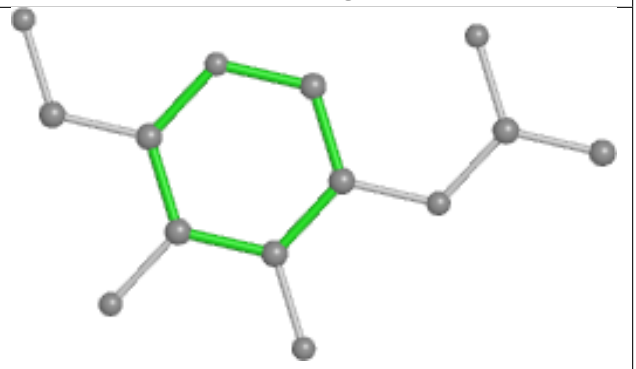
Bond lengths



Bond angles

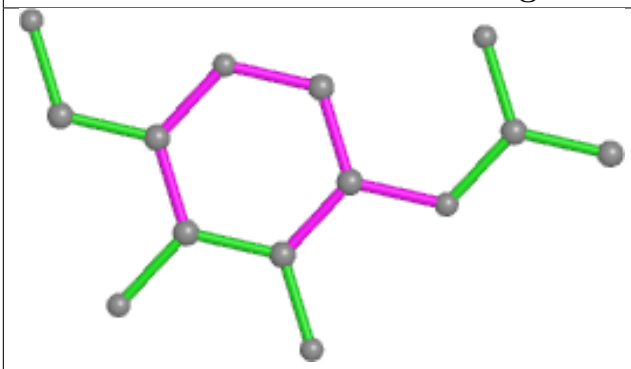


Torsions

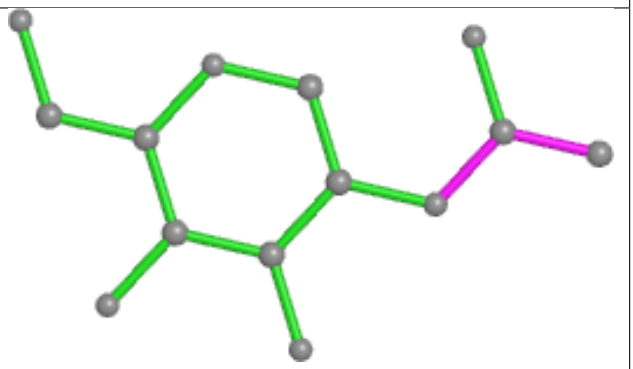


Rings

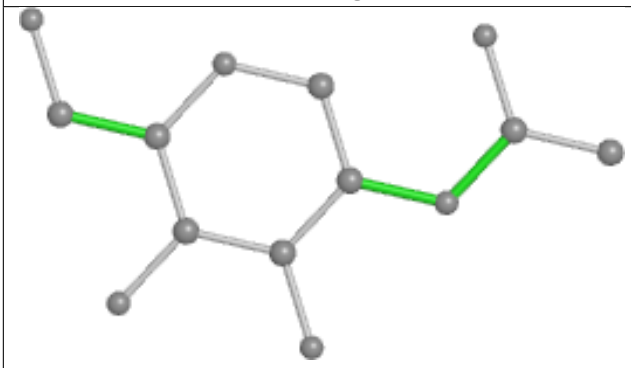
Ligand NAG G 401



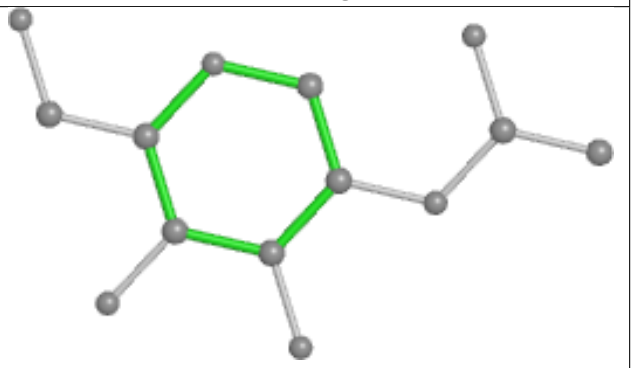
Bond lengths



Bond angles

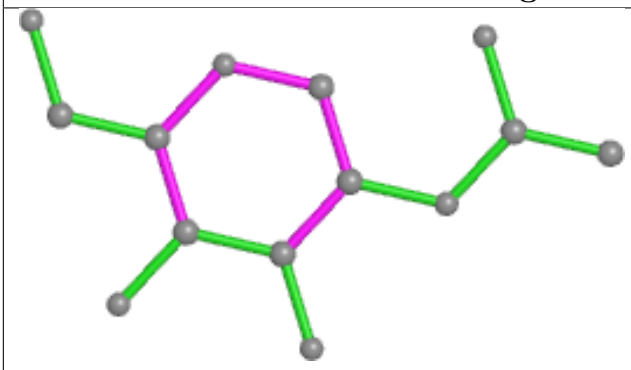


Torsions

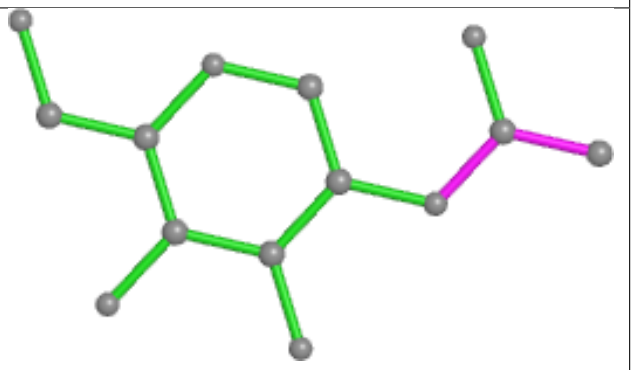


Rings

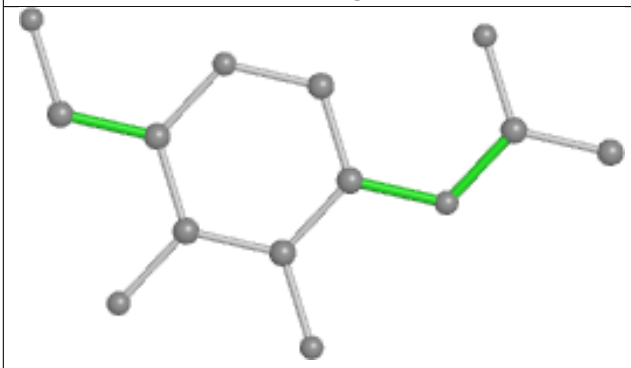
Ligand NAG A 402



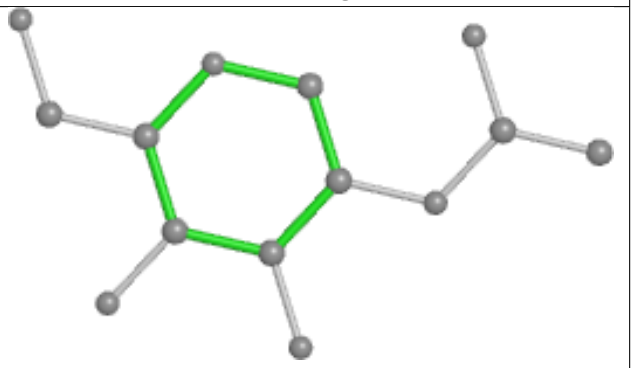
Bond lengths



Bond angles

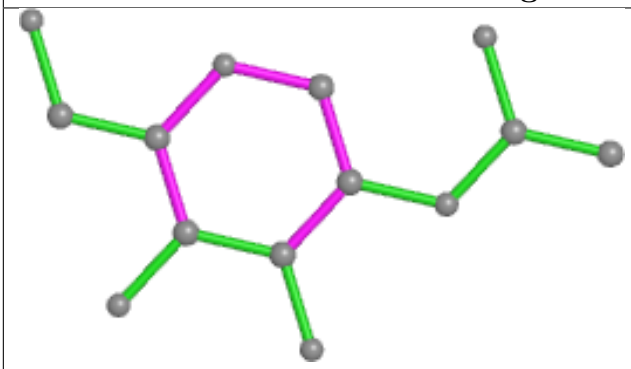


Torsions

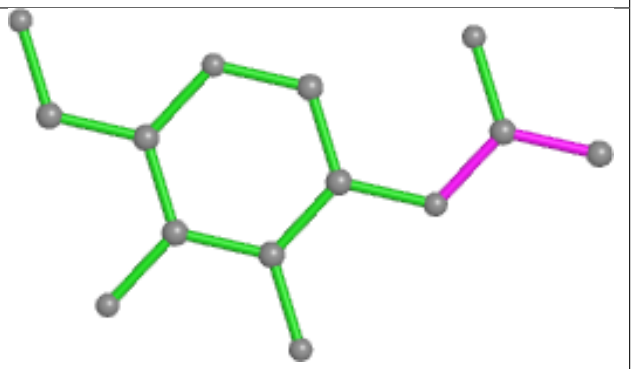


Rings

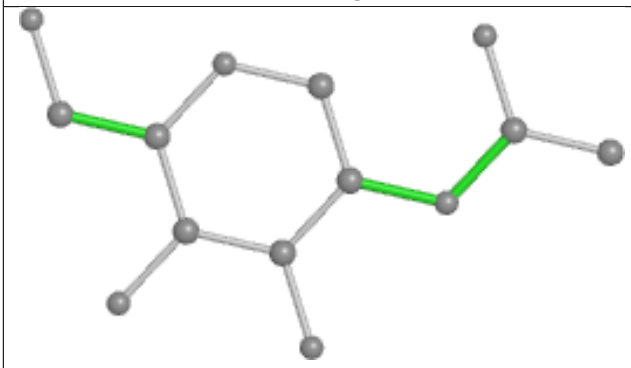
Ligand NAG C 403



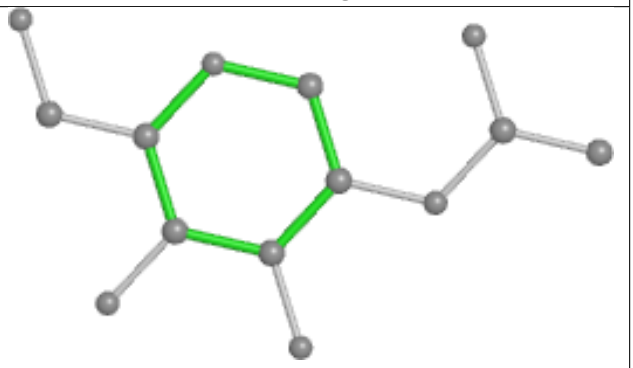
Bond lengths



Bond angles

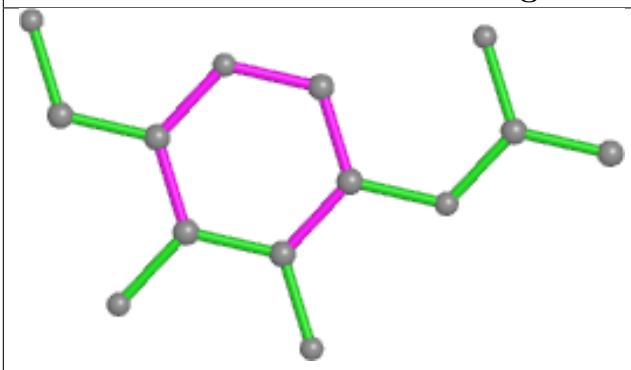


Torsions

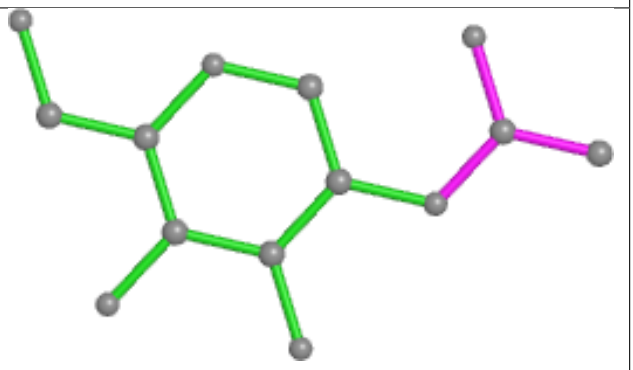


Rings

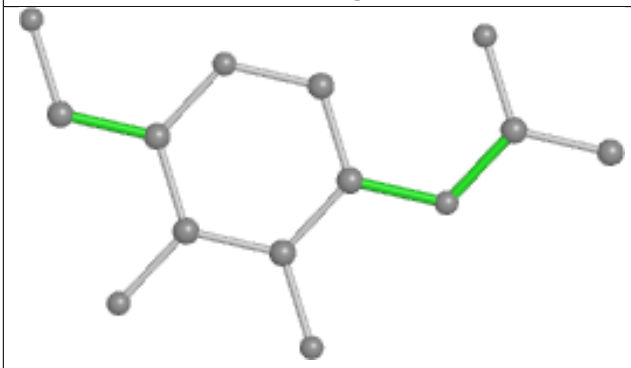
Ligand NAG C 404



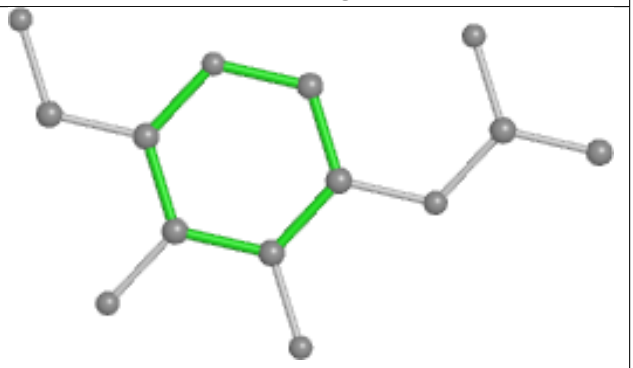
Bond lengths



Bond angles

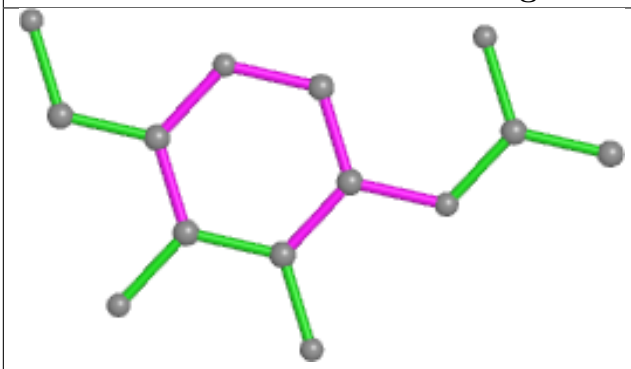


Torsions

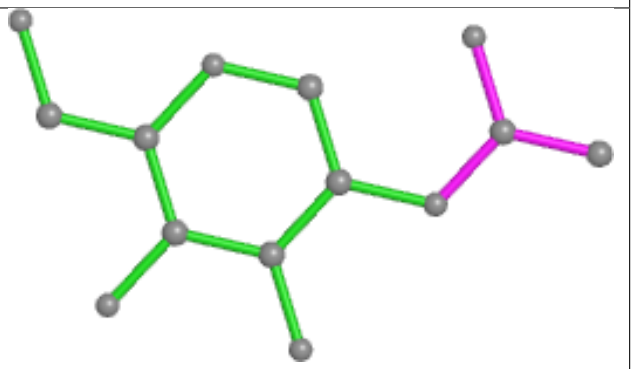


Rings

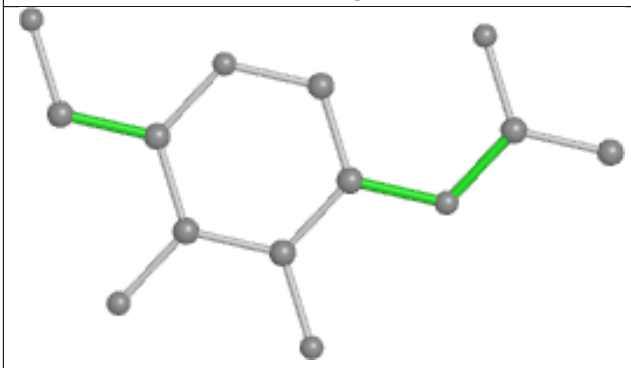
Ligand NAG A 404



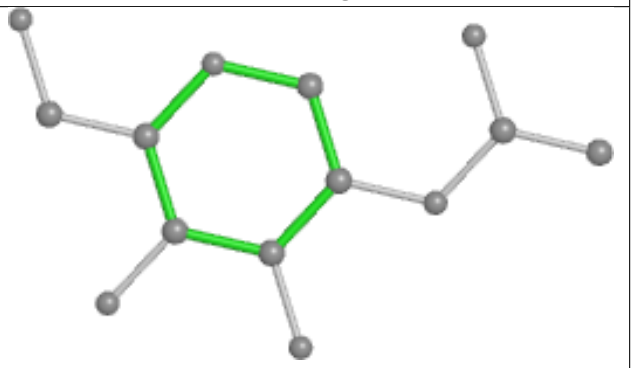
Bond lengths



Bond angles

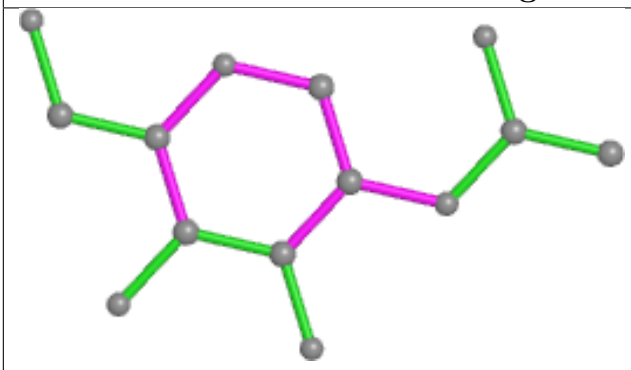


Torsions

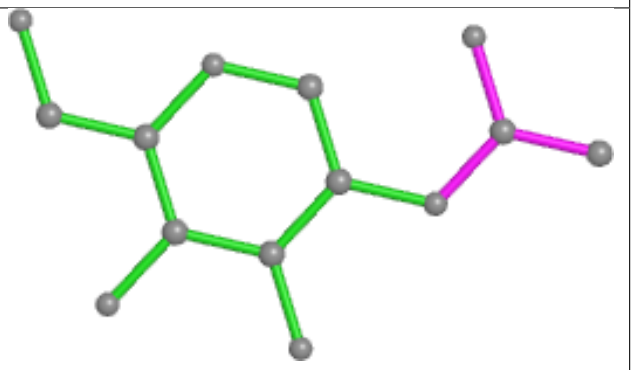


Rings

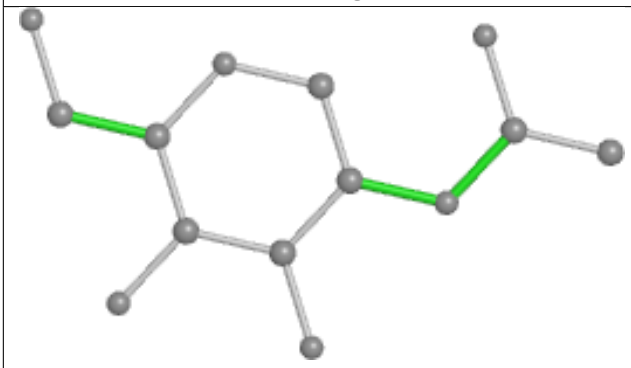
Ligand NAG G 404



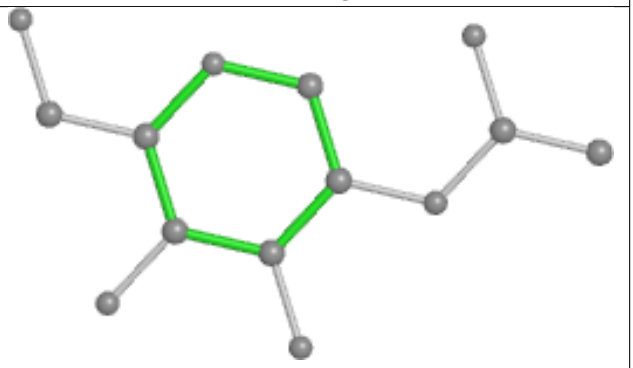
Bond lengths



Bond angles

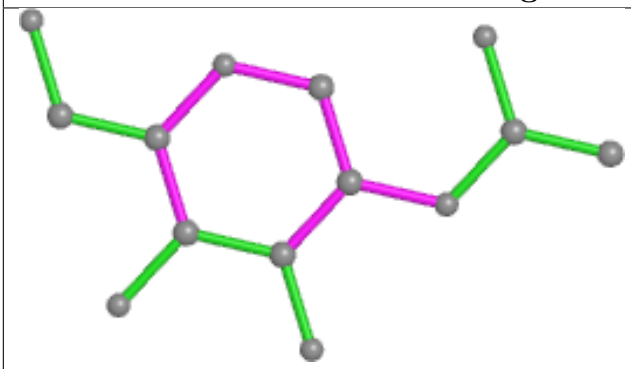


Torsions

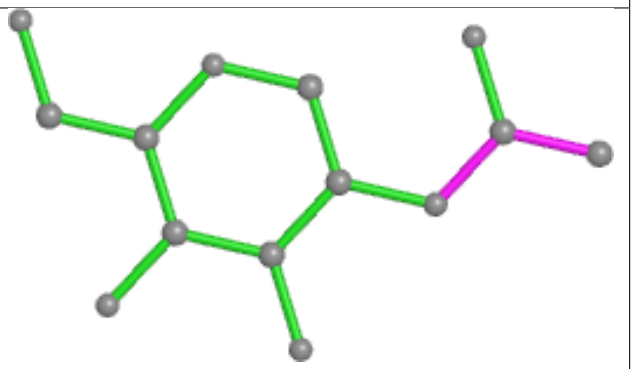


Rings

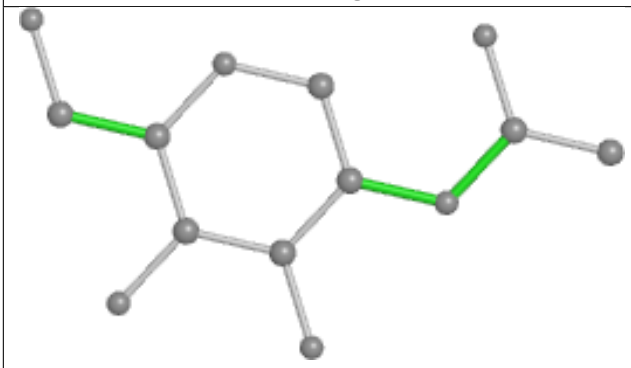
Ligand NAG C 401



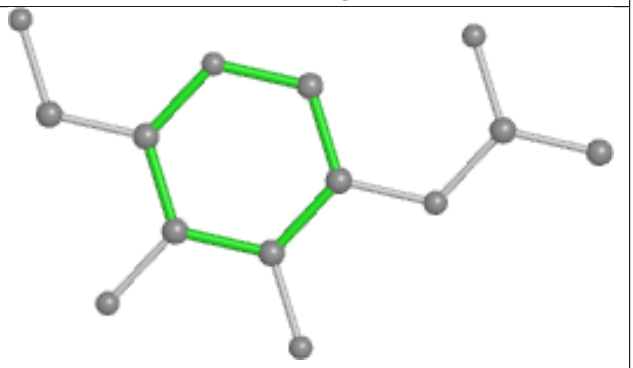
Bond lengths



Bond angles

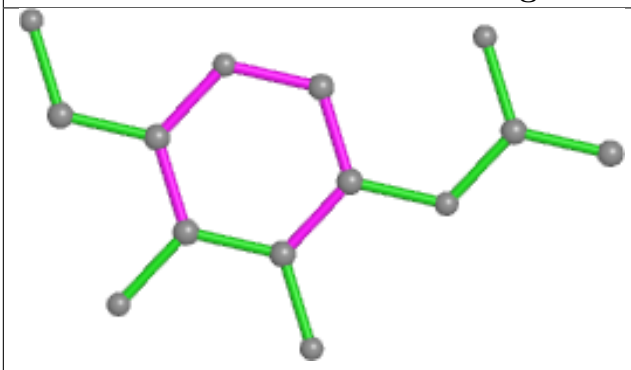


Torsions

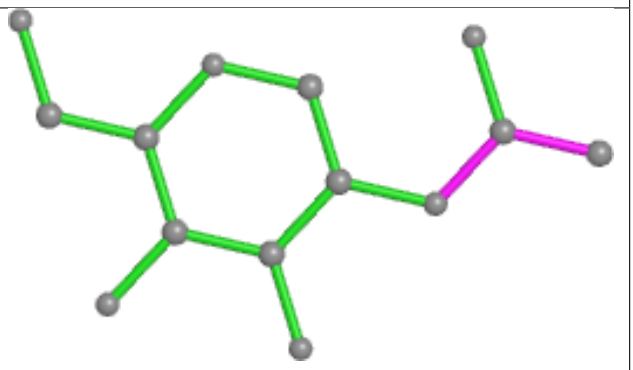


Rings

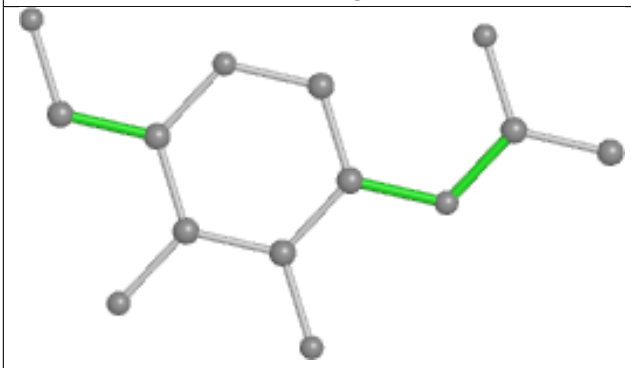
Ligand NAG A 403



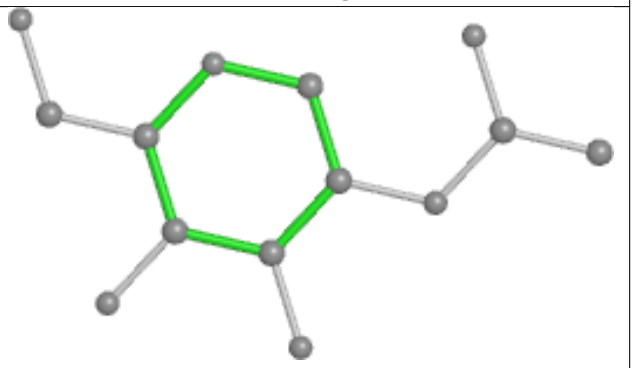
Bond lengths



Bond angles

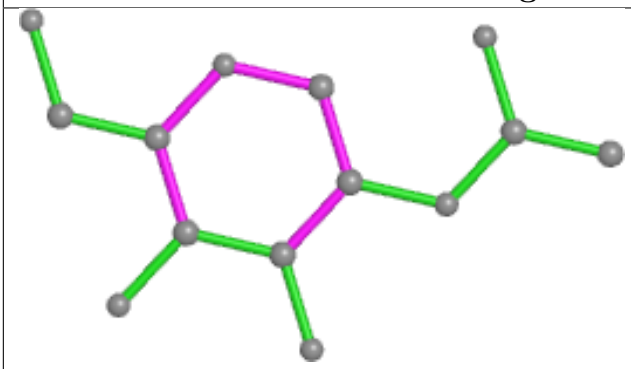


Torsions

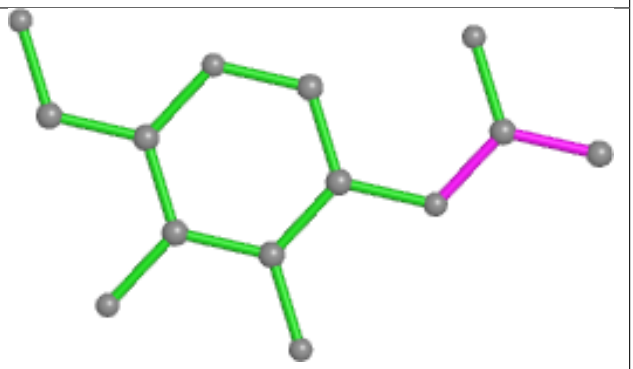


Rings

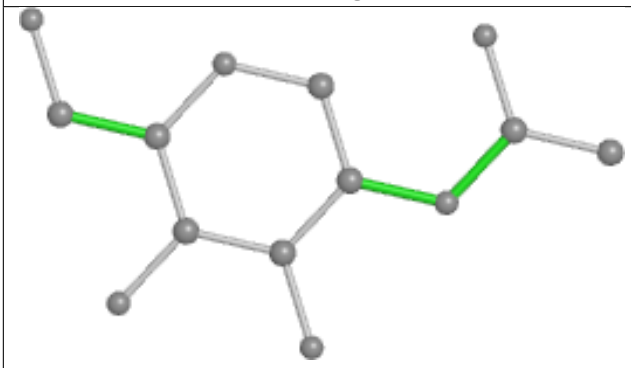
Ligand NAG G 402



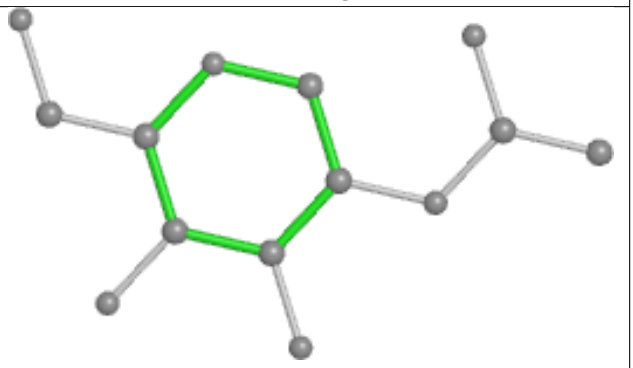
Bond lengths



Bond angles

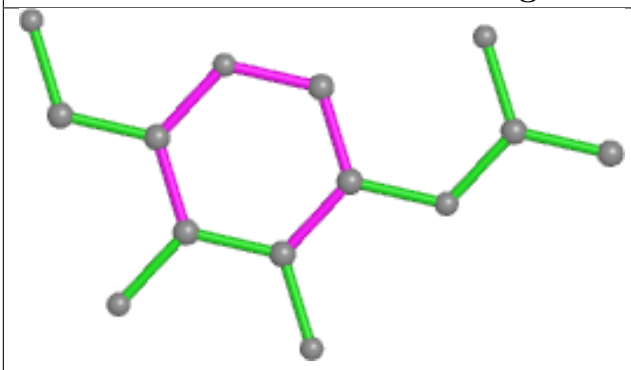


Torsions

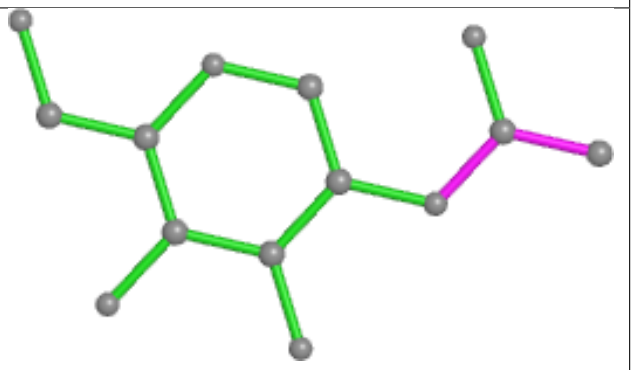


Rings

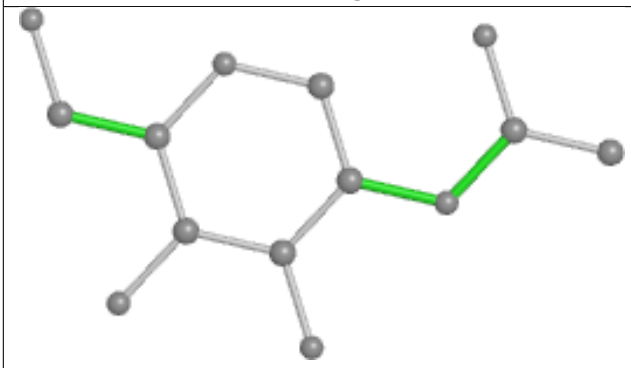
Ligand NAG G 403



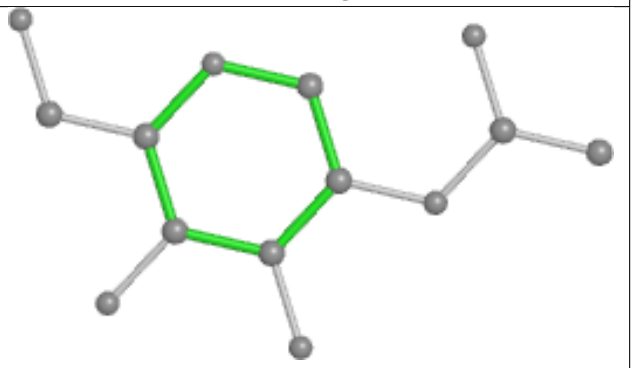
Bond lengths



Bond angles

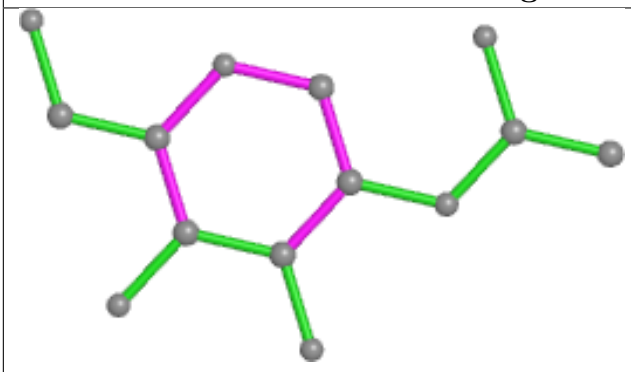


Torsions

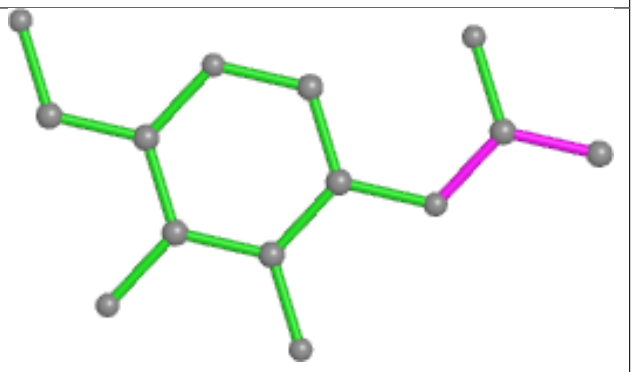


Rings

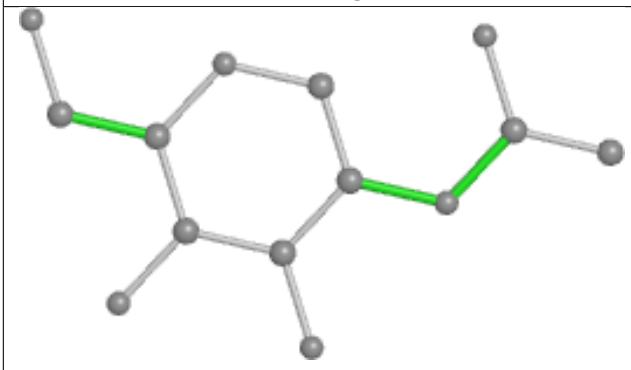
Ligand NAG C 402



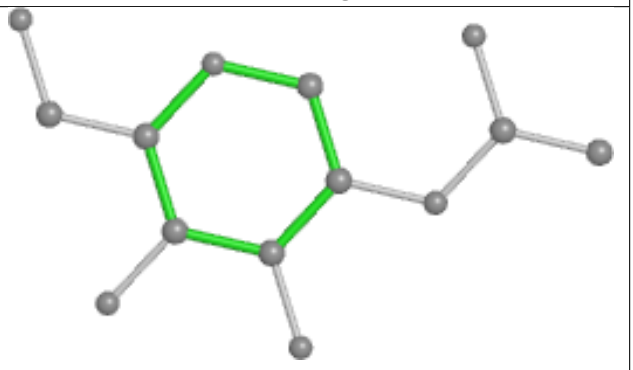
Bond lengths



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.

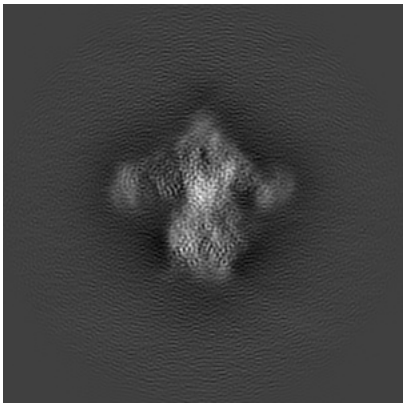
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-25040. These allow visual inspection of the internal detail of the map and identification of artifacts.

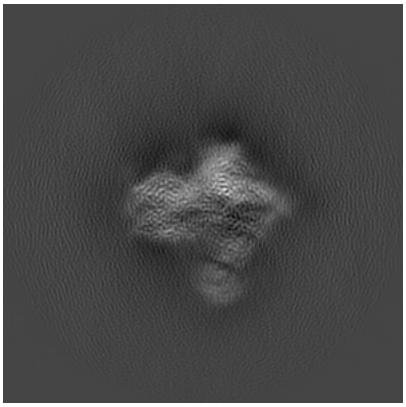
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

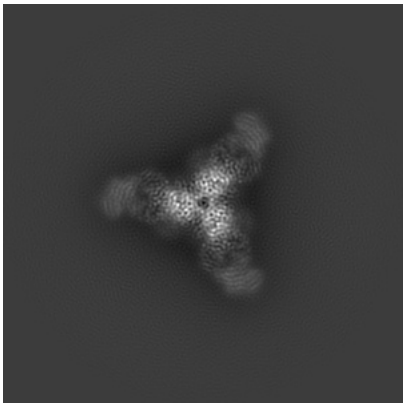
6.1.1 Primary map



X



Y

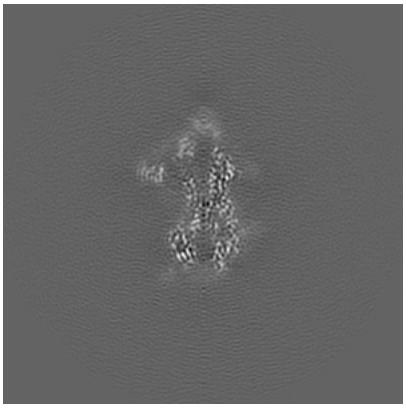


Z

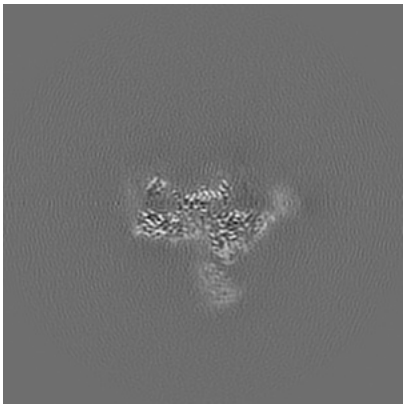
The images above show the map projected in three orthogonal directions.

6.2 Central slices

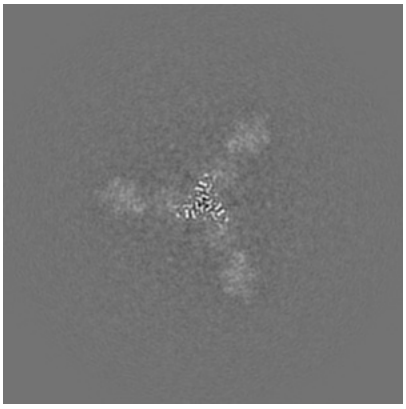
6.2.1 Primary map



X Index: 160



Y Index: 160

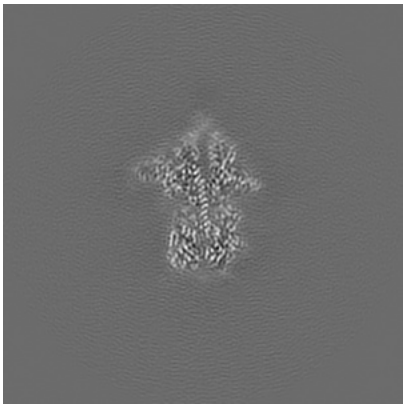


Z Index: 160

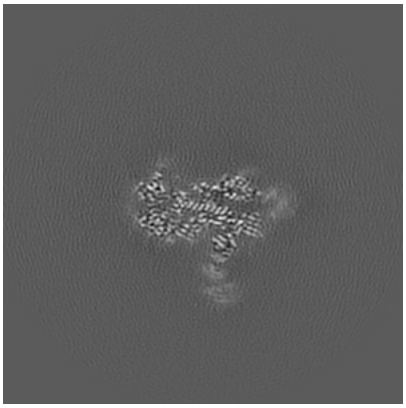
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

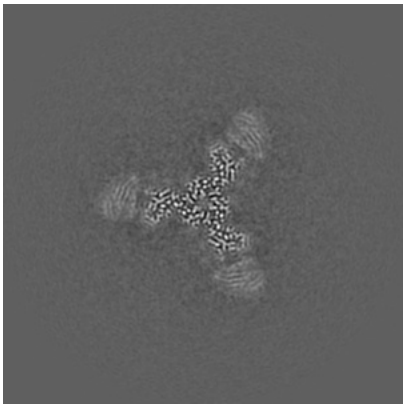
6.3.1 Primary map



X Index: 167



Y Index: 154



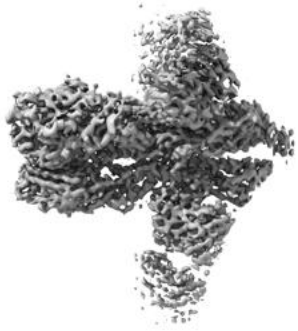
Z Index: 175

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

6.4 Orthogonal surface views (i)

6.4.1 Primary map

X



Y

Z

The images above show the 3D surface view of the map at the recommended contour level 0.0145. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

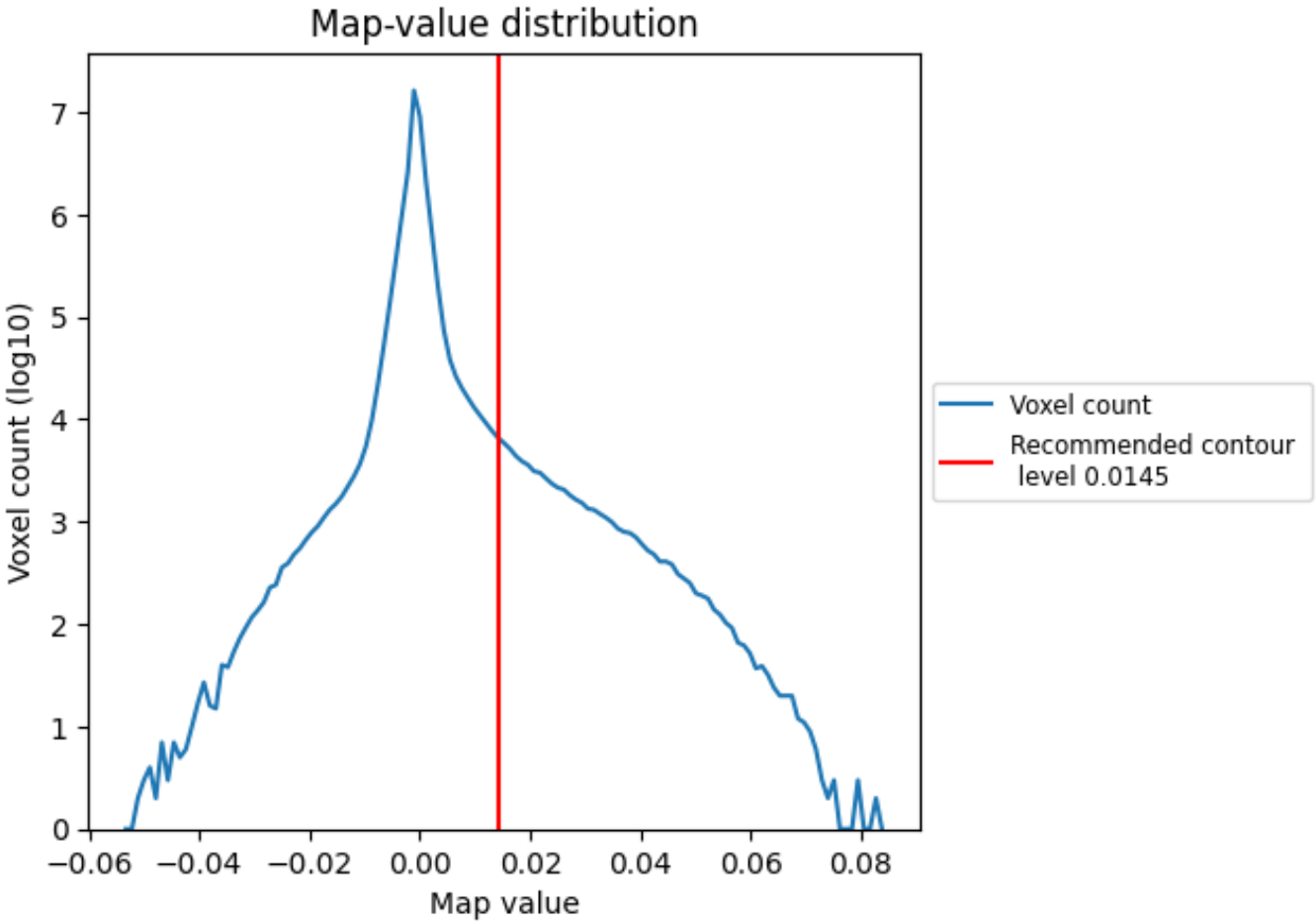
6.5 Mask visualisation (i)

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

7 Map analysis

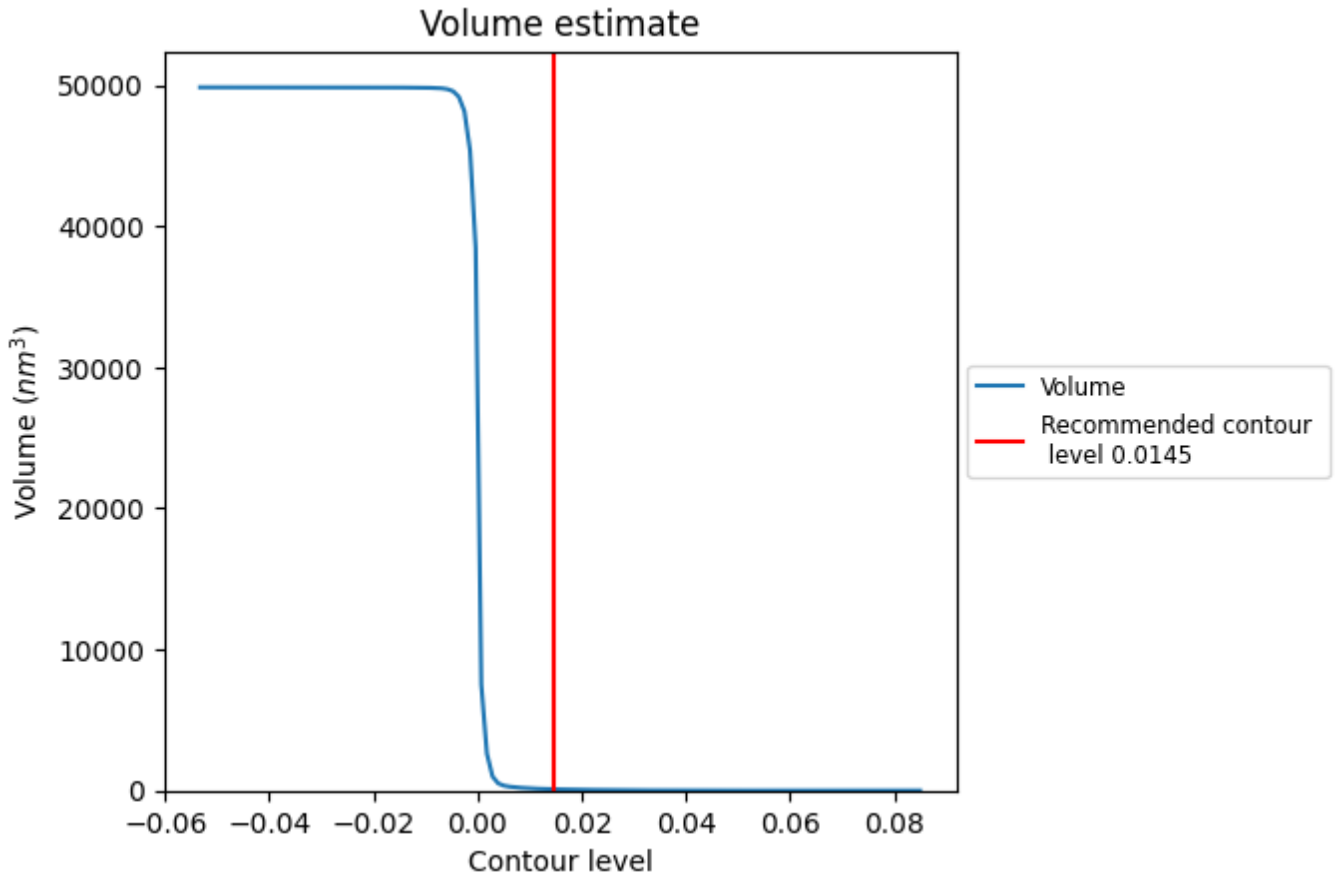
This section contains the results of statistical analysis of the map.

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.

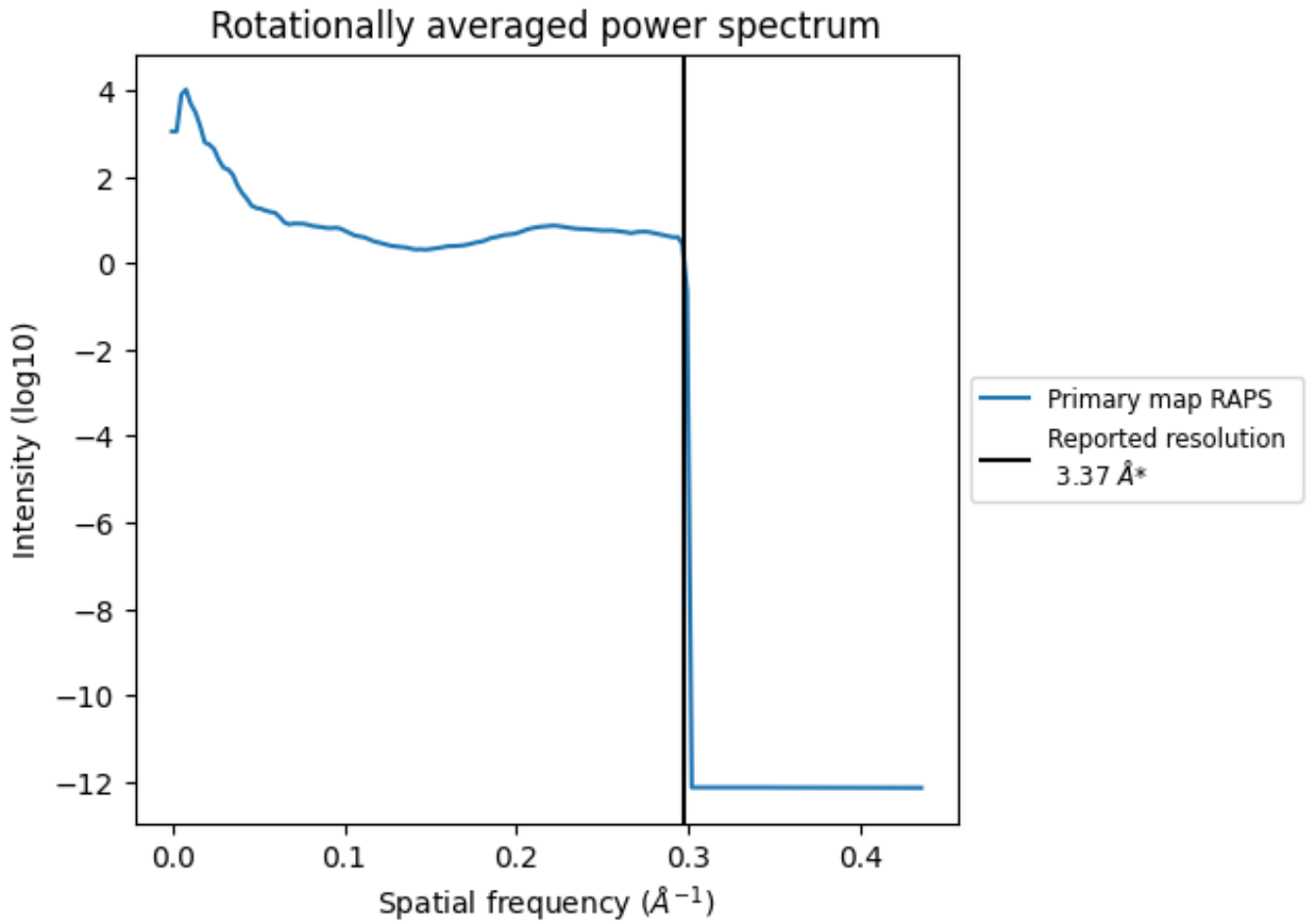
7.2 Volume estimate (i)



The volume at the recommended contour level is 95 nm^3; this corresponds to an approximate mass of 86 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)

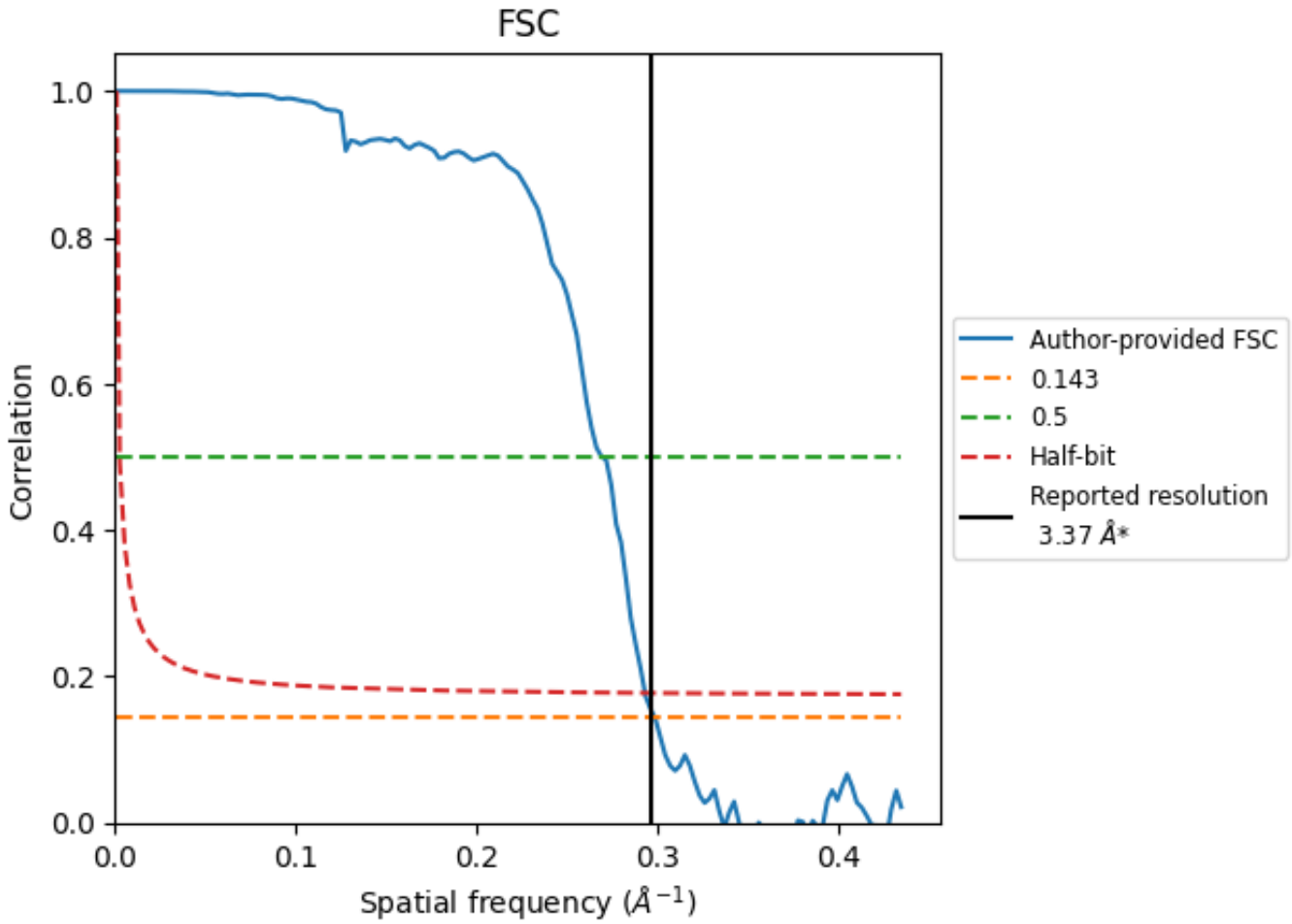


*Reported resolution corresponds to spatial frequency of 0.297 Å^{-1}

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 0.297 Å^{-1}

8.2 Resolution estimates (i)

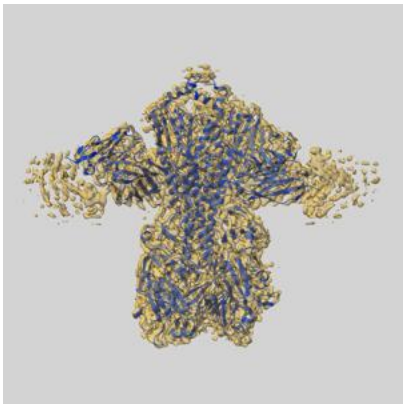
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.37	-	-
Author-provided FSC curve	3.35	3.71	3.41
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

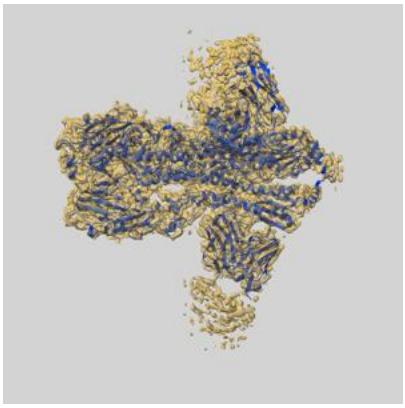
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-25040 and PDB model 7SCO. Per-residue inclusion information can be found in section 3 on page 11.

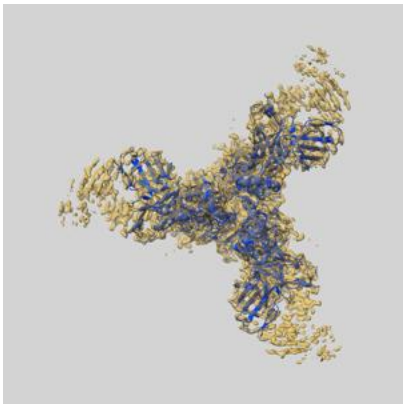
9.1 Map-model overlay



X



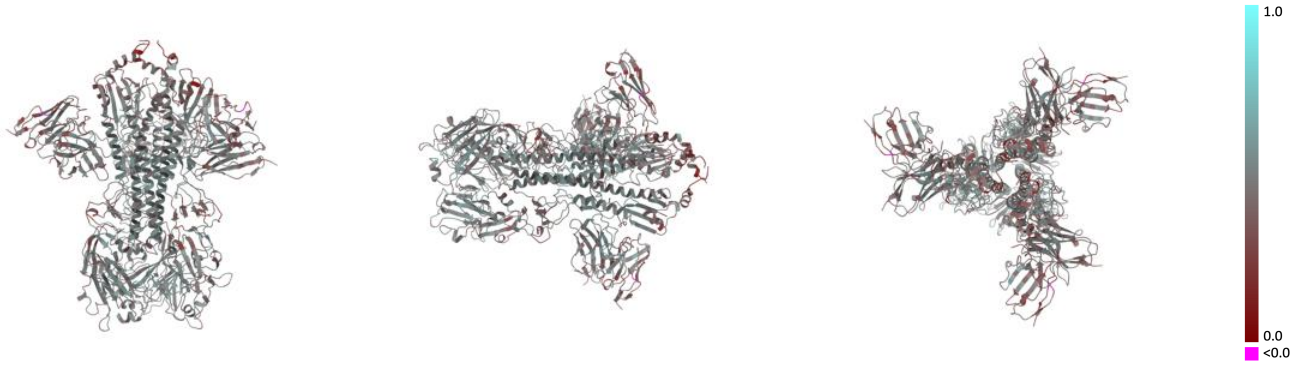
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0145 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

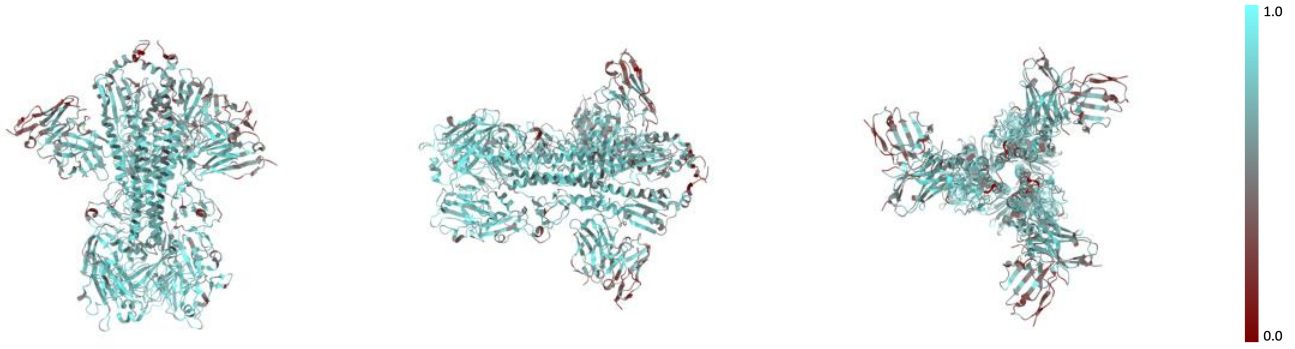
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

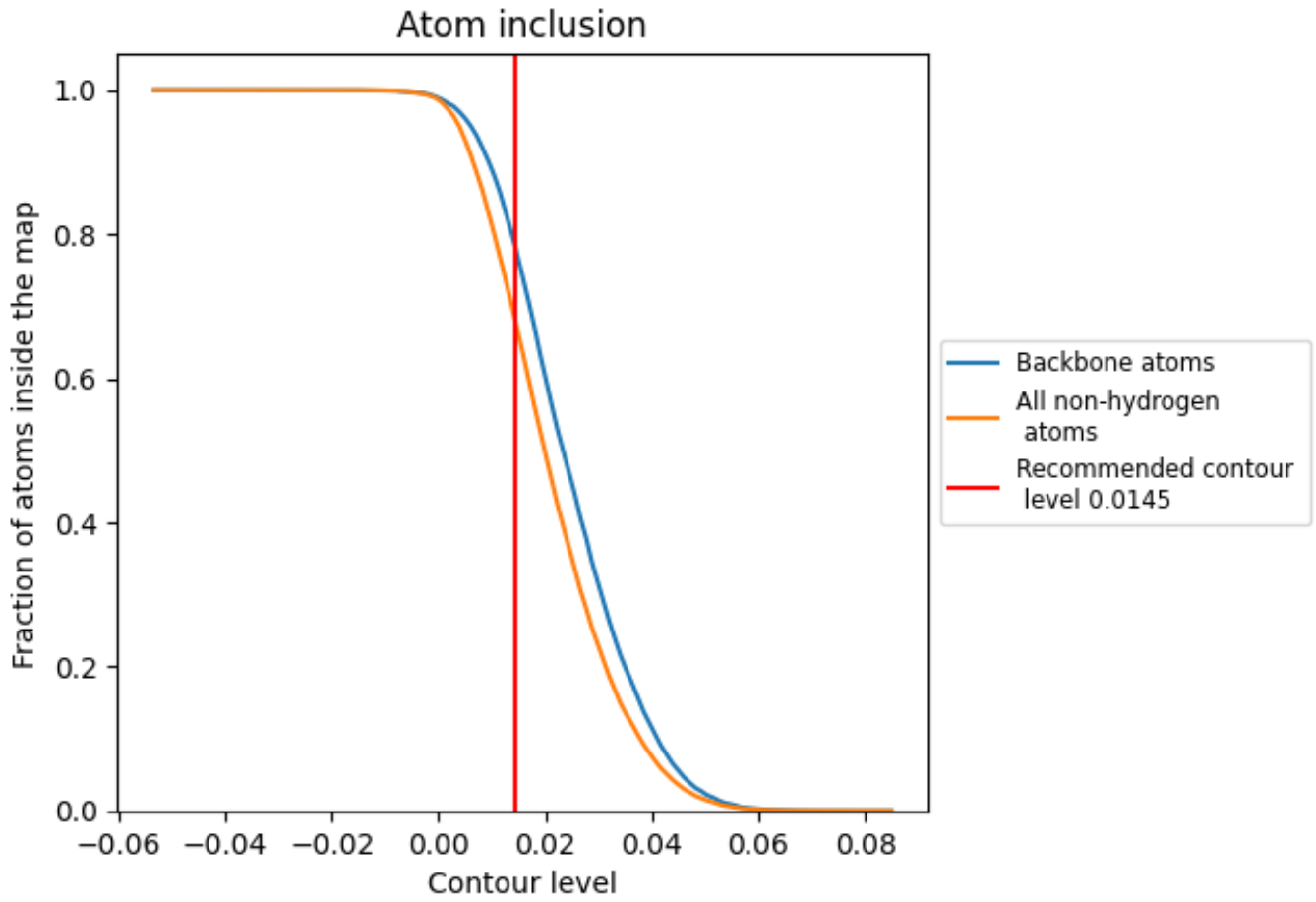
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0145).

9.4 Atom inclusion (i)



At the recommended contour level, 78% of all backbone atoms, 68% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.0145) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6780	0.4510
A	0.7262	0.4710
B	0.6997	0.4620
C	0.7250	0.4660
D	0.6836	0.4500
E	0.6792	0.4510
F	0.4912	0.3880
G	0.7230	0.4640
H	0.6940	0.4670
I	0.6865	0.4510
J	0.6769	0.4540
K	0.5113	0.3880
L	0.5113	0.3970
M	0.6429	0.4320
N	0.5714	0.4360
O	0.6071	0.4220