wwPDB EM Validation Summary Report (i)

Oct 18, 2026 – 12:39 PM JST

PDB ID	:	43EI / pdb_000043ei
EMDB ID	:	EMD-81815
Title	:	cryo-EM structure of the extracellular domain of Anopheles stephensi IR8a-IR75k receptor in complex with octanoic acid
Authors	:	Xu, L.; Pan, X.J.
Deposited on	:	2026-06-28
Resolution	:	2.55 Å(reported)
Based on initial model	:	.

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:

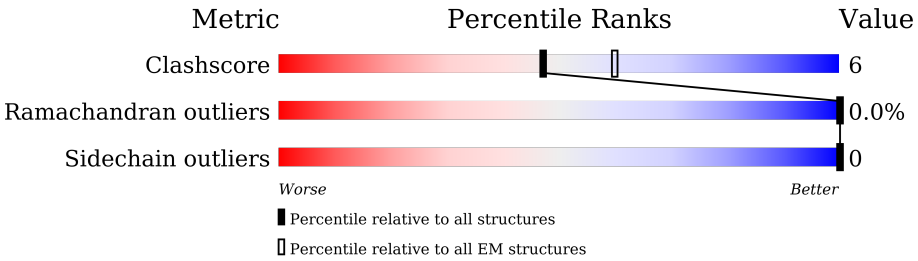
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.2
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.51

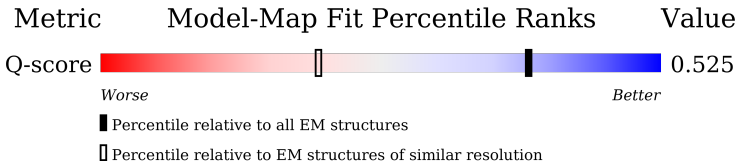
1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.55 Å.

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





Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	7475 (2.05 - 3.05)

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	927	9% 57% 12% 30%
1	B	927	10% 58% 12% 31%
2	C	657	• 59% 10% 30%
2	D	657	• 59% 10% 31%

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Mol	Chain	Length	Quality of chain
3	E	3	67% 33%
3	H	3	67% 33%
4	F	2	100%
4	G	2	50% 50%
4	I	2	100%
4	J	2	50% 50%

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 18117 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 Ionotropic receptor coreceptor Ir8a.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	645	5155	3281	866	984	24	0	0
1	B	644	5144	3274	865	981	24	0	0

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	62	LEU	PHE	conflict	UNP A0A182YLZ0
A	81	GLN	ARG	conflict	UNP A0A182YLZ0
A	106	SER	GLY	conflict	UNP A0A182YLZ0
A	160	VAL	ALA	conflict	UNP A0A182YLZ0
A	174	ASP	GLU	conflict	UNP A0A182YLZ0
A	275	VAL	ILE	conflict	UNP A0A182YLZ0
A	294	ALA	SER	conflict	UNP A0A182YLZ0
A	300	GLU	GLN	conflict	UNP A0A182YLZ0
A	343	VAL	ILE	conflict	UNP A0A182YLZ0
A	810	ALA	THR	conflict	UNP A0A182YLZ0
B	62	LEU	PHE	conflict	UNP A0A182YLZ0
B	81	GLN	ARG	conflict	UNP A0A182YLZ0
B	106	SER	GLY	conflict	UNP A0A182YLZ0
B	160	VAL	ALA	conflict	UNP A0A182YLZ0
B	174	ASP	GLU	conflict	UNP A0A182YLZ0
B	275	VAL	ILE	conflict	UNP A0A182YLZ0
B	294	ALA	SER	conflict	UNP A0A182YLZ0
B	300	GLU	GLN	conflict	UNP A0A182YLZ0
B	343	VAL	ILE	conflict	UNP A0A182YLZ0
B	810	ALA	THR	conflict	UNP A0A182YLZ0

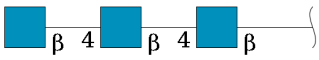
- Molecule 2 is a protein called Ionotropic glutamate receptor C-terminal domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	C	457	3721	2364	667	680	10	0	0
2	D	456	3713	2360	666	677	10	0	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	189	ALA	PRO	conflict	UNP A0A182XYX5
C	231	HIS	GLN	conflict	UNP A0A182XYX5
C	241	ILE	VAL	conflict	UNP A0A182XYX5
D	189	ALA	PRO	conflict	UNP A0A182XYX5
D	231	HIS	GLN	conflict	UNP A0A182XYX5
D	241	ILE	VAL	conflict	UNP A0A182XYX5

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



Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
3	E	3	42	24	3	15	0	0
3	H	3	42	24	3	15	0	0

- Molecule 4 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
			Total	C	N	O		
4	F	2	28	16	2	10	0	0
4	G	2	28	16	2	10	0	0
4	I	2	28	16	2	10	0	0

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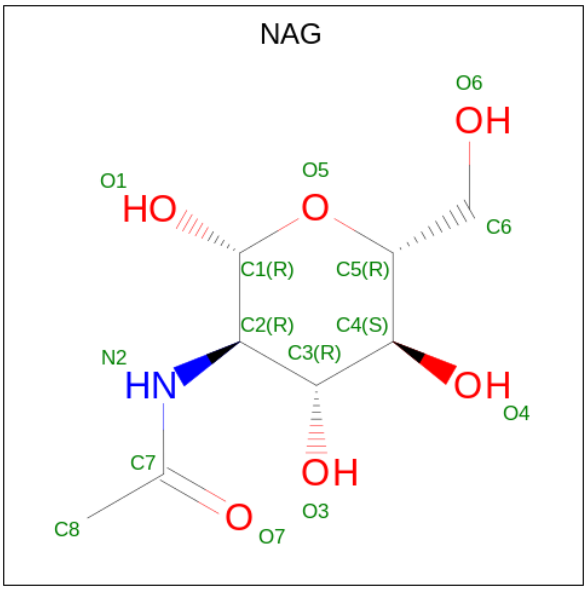
Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
4	J	2	28	16	2	10	0	0

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$) (labeled as "Ligand of Interest" by depositor).



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

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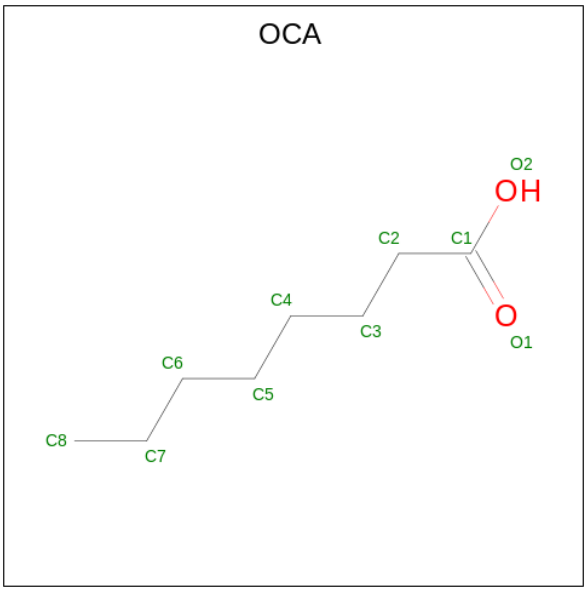
Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
5	D	1	14	8	1	5	0
5	D	1	14	8	1	5	0

- Molecule 6 is OCTANOIC ACID (CAPRYLIC ACID) (CCD ID: OCA) (formula: $C_8H_{16}O_2$) (labeled as "Ligand of Interest" by depositor).



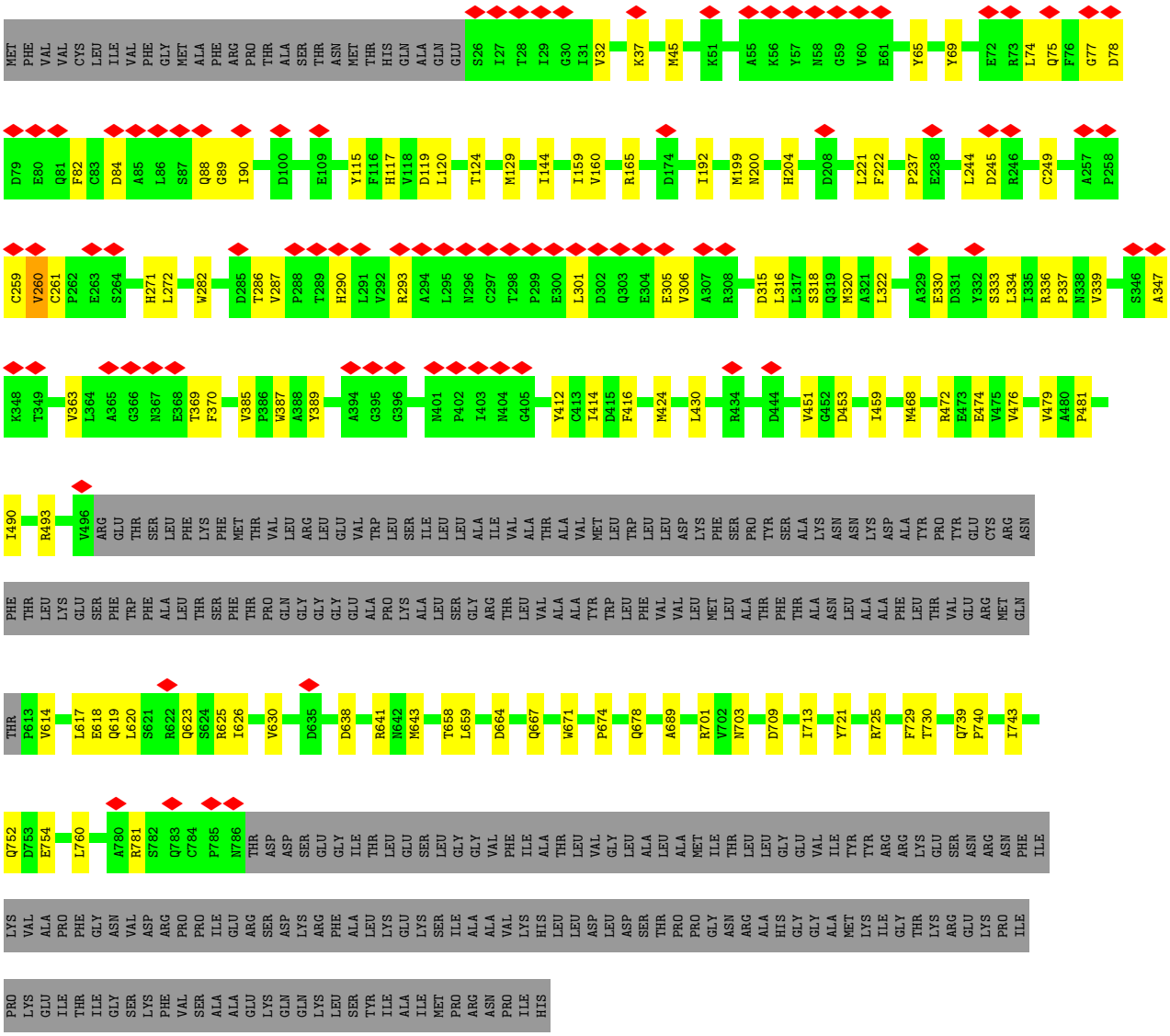
Mol	Chain	Residues	Atoms				AltConf
			Total	C	O		
6	C	1	10	8	2		0
6	D	1	10	8	2		0

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: Ionotropic receptor coreceptor Ir8a

Chain A: 9% 57% 12% 30%



• Molecule 1: Ionotropic receptor coreceptor Ir8a

Chain B: 10% 58% 12% 31%

MET PHE VAL VAL CYS LEU ILE VAL PHE GLY MET ALA PHE ARG PRO THR ALA SER THR ASN MET THR HIS GLN ALA GLN GLU S26 I27 T28 I29 G30 M45 D48 K51 A55 K56 Y57 N58 G59 V60 E61 E72 R73 L74 Q75 F76 G77 D78 D79 E80 Q81 F82 C83 D84

A85 L86 S87 Q88 D100 S106 E109 T110 D119 L120 T124 K127 L128 M129 L157 R165 D174 I192 V193 A194 M197 Q198 M199 N200 D208 L221 F222 L225 Q226 T227 D228 H232 E233 D234 L243 L244 D245 R246 Q255 S256 A257 P258 C259

V260 C261 P262 E263 S264 F265 D266 H269 V270 H271 L272 V275 L276 I279 W282 D285 T286 V287 P288 T289 H290 L291 V292 R293 A294 L295 N296 C297 T298 P299 E300 L301 D302 Q303 E304 E305 V306 A307 R308 L316 I328 D331 Y332 S333 P337 N338 V339 S346 A347 K348

T349 N350 G354 V363 L364 A365 G366 N367 E368 T369 A394 G395 G396 K397 V398 N401 PRO I403 N404 G405 C413 I414 M424 L430 R434 D442 P443 D444 G445 R446 V451 G452 D453 I459 I463 A464 S465 M468 R472 V476 V479 A480 P481

R493 V496 ARG GLU THR SER LEU PHE LYS PHE MET THR VAL LEU ARG LEU GLU VAL TRP LEU SER ILE LEU LEU ALA ILE VAL ALA THR ALA VAL MET LEU TRP LEU LEU ASP LYS PHE SER PRO TYR SER ALA LYS ASN ASN LYS ASP ALA TYR PRO TYR GLU CYS ARG ASN PHE THR

LEU LYS GLU SER PHE TRP PHE ALA LEU THR SER PHE THR PRO GLN GLY GLY GLY GLU ALA PRO LYS ALA LEU SER GLY ARG THR LEU VAL ALA ALA TYR TRP LEU PHE VAL VAL LEU MET LEU ALA THR PHE THR ALA ASN LEU ALA ALA PHE LEU THR VAL GLU ARG MET GLN THR P613

V614 Q619 R622 Q623 S624 R625 I626 V630 V631 K632 D635 M643 T658 L659 W671 P674 E677 A689 R701 V702 N703 L706 D709 I713 Q739 P740 Y741 Q752 D753 E754 L760 Q783 C784 P785 N786 THR ASP ASP SER GLU GLY ILE

THR LEU GLU SER LEU GLY GLY VAL PHE ILE ALA THR LEU VAL GLY LEU ALA LEU ALA MET ILE THR LEU LEU GLY GLU VAL ILE TYR TYR ARG ARG LYS GLU SER ASN ARG ASN PHE ILE LYS VAL ALA PRO PHE GLY ASN VAL ASP ARG PRO PRO ILE GLU ARG SER ASP LYS ARG PHE

ALA LEU LYS GLU LYS SER ILE ALA ALA VAL LYS HIS LEU LEU ASP LEU ASP SER THR PRO PRO GLY ASN ARG ALA HIS GLY GLY ALA MET LYS ILE GLY THR LYS ARG GLU LYS PRO ILE PRO LYS GLU ILE THR ILE GLY SER LYS PHE VAL SER ALA ALA GLU LYS GLN GLN LYS LEU

SER TYR ILE ALA ILE MET PRO ARG ASN PRO ILE HIS

- Molecule 2: Ionotropic glutamate receptor C-terminal domain-containing protein

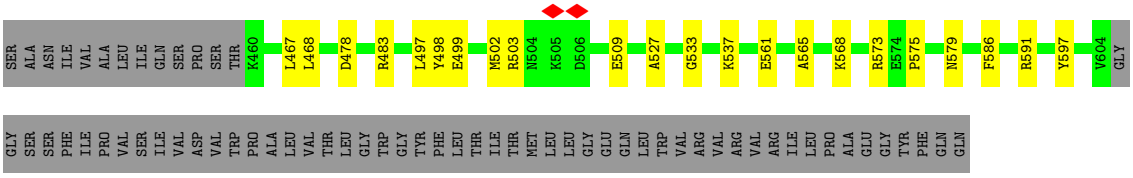
Chain C: 59% 10% 30%

MET SER ARG ILE LEU GLN PRO GLN PRO SER ALA TRP LEU VAL PHE LEU ILE ILE VAL HIS THR GLY SER GLY MET SER ALA ASN ILE PRO PRO SER PRO THR V35 L36 D37 L40 A41 A42 D51 R52 Q55 W62 A65 L70 F83 V84 R85 D90 Q93

Q101 I104 C112 T123 Q124 R131 L139 E140 A141 G142 T143 W147 E152 Y153 P154 E157 L161 N165 R186 G190 T191 S192 S193 P194 P195 G196 P197 V198 Y199 Q208 T217 V222 D252 H257 R263 A275 W288 G289

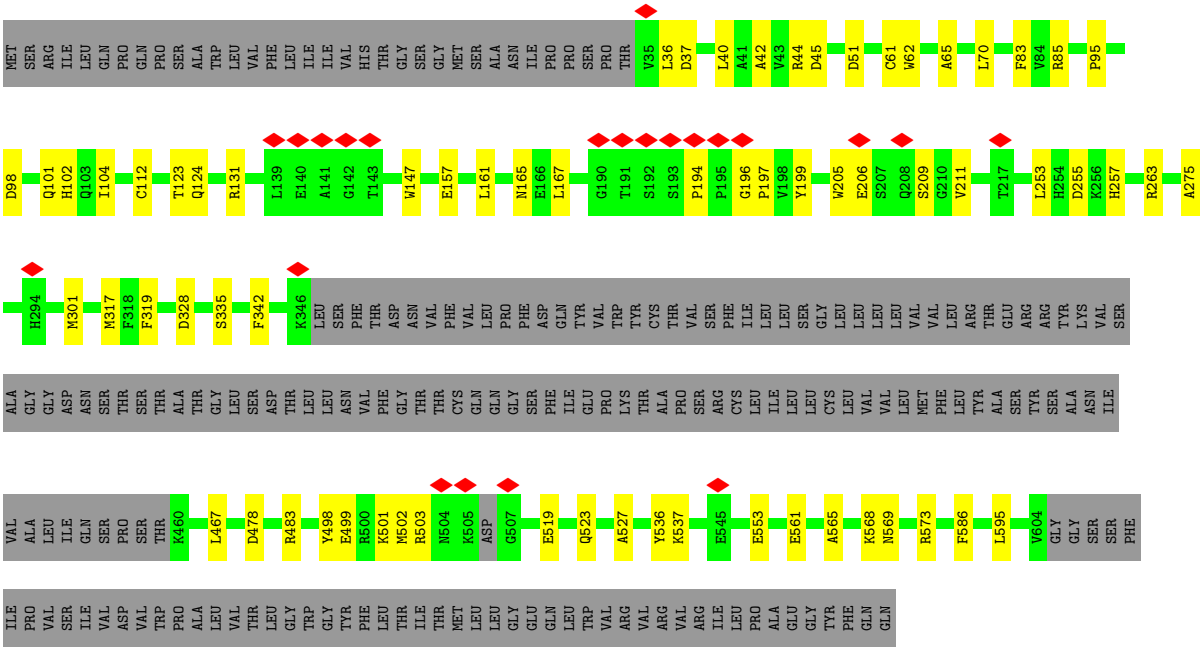
H294 N299 G300 M301 V302 G303 E304 L309 M317 F318 F319 S335 F342 K346 LEU SER PHE THR ASP ASN VAL PHE GLY THR THR CYS GLN GLN GLY SER PHE ILE GLU PRO LYS THR ALA PRO SER ARG CYS LEU ILE LEU LEU SER GLY LEU LEU LEU VAL VAL LEU ARG THR GLU ARG ARG

TYR LYS VAL SER ALA GLY GLY ASP ASN SER THR SER THR ALA THR GLY LEU SER ASP THR LEU LEU ASN VAL PHE GLY THR THR CYS GLN GLN GLY SER PHE ILE GLU PRO LYS THR ALA PRO SER ARG CYS LEU ILE LEU LEU CYS LEU VAL VAL LEU MET PHE LEU TYR ALA SER TYR



• Molecule 2: Ionotropic glutamate receptor C-terminal domain-containing protein

Chain D:



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

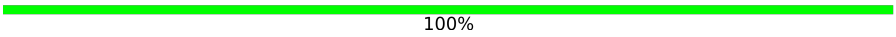
Chain E:

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

Chain H:

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

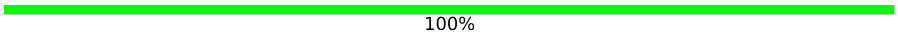
Chain F:



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

Chain G:

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

Chain I: 

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

Chain J:

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	109623	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50.0	Depositor
Minimum defocus (nm)	1100	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	0.289	Depositor
Minimum map value	-0.153	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.0573	Depositor
Map size (Å)	411.84, 411.84, 411.84	wwPDB
Map dimensions	440, 440, 440	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.936, 0.936, 0.936	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

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

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	0.10	0/5272	0.29	0/7167
1	B	0.11	0/5259	0.30	0/7147
2	C	0.10	0/3808	0.27	0/5167
2	D	0.08	0/3799	0.25	0/5153
All	All	0.10	0/18138	0.28	0/24634

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
1	B	0	2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	263	GLU	Peptide
1	B	264	SER	Peptide

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	5155	0	5010	75	0
1	B	5144	0	4998	74	0
2	C	3721	0	3684	45	0
2	D	3713	0	3679	42	0
3	E	42	0	37	1	0
3	H	42	0	37	1	0
4	F	28	0	25	0	0
4	G	28	0	25	1	0
4	I	28	0	25	0	0
4	J	28	0	25	2	0
5	A	56	0	52	1	0
5	B	56	0	52	0	0
5	C	28	0	26	0	0
5	D	28	0	26	0	0
6	C	10	0	15	2	0
6	D	10	0	15	0	0
All	All	18117	0	17731	215	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 6.

The worst 5 of 215 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:330:GLU:HB3	1:A:333:SER:HB3	1.62	0.79
1:A:479:VAL:HG12	1:A:481:PRO:HD2	1.66	0.78
1:B:479:VAL:HG12	1:B:481:PRO:HD2	1.69	0.73
2:D:51:ASP:O	2:D:131:ARG:NH1	2.20	0.73
2:C:252:ASP:O	2:C:263:ARG:NH2	2.23	0.71

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	641/927 (69%)	606 (94%)	34 (5%)	1 (0%)	43	56
1	B	638/927 (69%)	608 (95%)	30 (5%)	0	100	100
2	C	453/657 (69%)	437 (96%)	16 (4%)	0	100	100
2	D	450/657 (68%)	432 (96%)	18 (4%)	0	100	100
All	All	2182/3168 (69%)	2083 (96%)	98 (4%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	260	VAL

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	564/802 (70%)	564 (100%)	0	100	100
1	B	562/802 (70%)	562 (100%)	0	100	100
2	C	406/582 (70%)	406 (100%)	0	100	100
2	D	405/582 (70%)	405 (100%)	0	100	100
All	All	1937/2768 (70%)	1937 (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. 5 of 15 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	254	GLN
2	D	321	GLN
1	B	255	GLN
2	D	589	GLN
2	C	504	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

14 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	$\#\|Z\| > 2$
3	NAG	E	1	2,3	14,14,15	0.22	0	17,19,21	0.51	0
3	NAG	E	2	3	14,14,15	0.21	0	17,19,21	0.46	0
3	NAG	E	3	3	14,14,15	0.24	0	17,19,21	0.42	0
4	NAG	F	1	2,4	14,14,15	0.22	0	17,19,21	0.44	0
4	NAG	F	2	4	14,14,15	0.23	0	17,19,21	0.39	0
4	NAG	G	1	1,4	14,14,15	0.25	0	17,19,21	0.49	0
4	NAG	G	2	4	14,14,15	0.26	0	17,19,21	0.40	0
3	NAG	H	1	2,3	14,14,15	0.23	0	17,19,21	0.52	0
3	NAG	H	2	3	14,14,15	0.22	0	17,19,21	0.44	0
3	NAG	H	3	3	14,14,15	0.23	0	17,19,21	0.41	0
4	NAG	I	1	2,4	14,14,15	0.24	0	17,19,21	0.44	0
4	NAG	I	2	4	14,14,15	0.23	0	17,19,21	0.40	0
4	NAG	J	1	1,4	14,14,15	0.26	0	17,19,21	0.46	0
4	NAG	J	2	4	14,14,15	0.27	0	17,19,21	0.39	0

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

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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	E	2	3	-	2/6/23/26	0/1/1/1
3	NAG	E	3	3	-	2/6/23/26	0/1/1/1
4	NAG	F	1	2,4	-	1/6/23/26	0/1/1/1
4	NAG	F	2	4	-	1/6/23/26	0/1/1/1
4	NAG	G	1	1,4	-	4/6/23/26	0/1/1/1
4	NAG	G	2	4	-	2/6/23/26	0/1/1/1
3	NAG	H	1	2,3	-	0/6/23/26	0/1/1/1
3	NAG	H	2	3	-	2/6/23/26	0/1/1/1
3	NAG	H	3	3	-	2/6/23/26	0/1/1/1
4	NAG	I	1	2,4	-	2/6/23/26	0/1/1/1
4	NAG	I	2	4	-	2/6/23/26	0/1/1/1
4	NAG	J	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	J	2	4	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 24 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	E	3	NAG	C4-C5-C6-O6
3	H	3	NAG	C4-C5-C6-O6
4	G	2	NAG	O5-C5-C6-O6
3	E	3	NAG	O5-C5-C6-O6
3	H	3	NAG	O5-C5-C6-O6

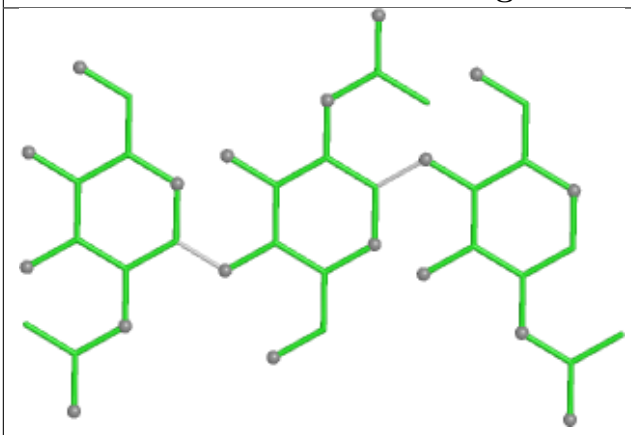
There are no ring outliers.

4 monomers are involved in 5 short contacts:

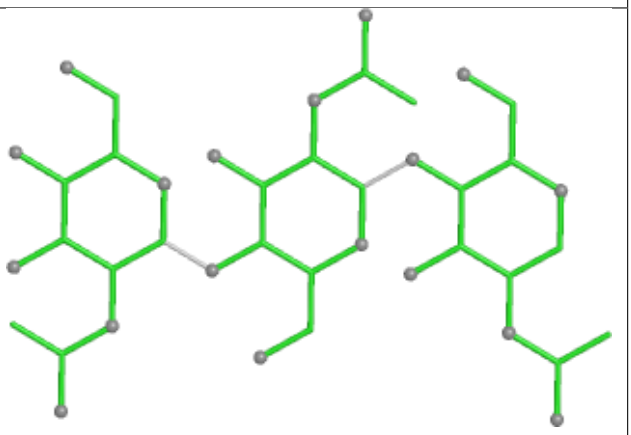
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	G	1	NAG	1	0
3	E	1	NAG	1	0
4	J	1	NAG	2	0
3	H	1	NAG	1	0

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

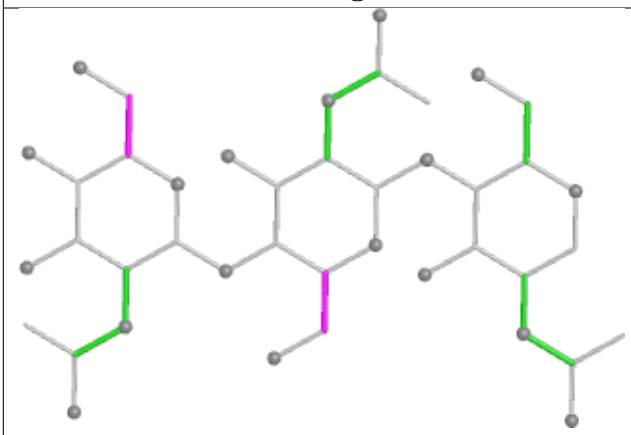
Oligosaccharide Chain E



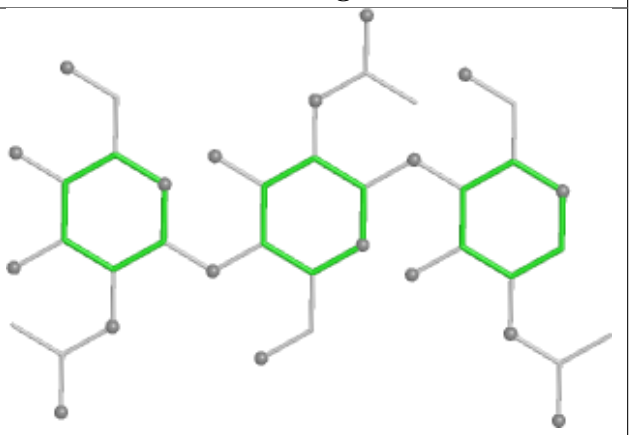
Bond lengths



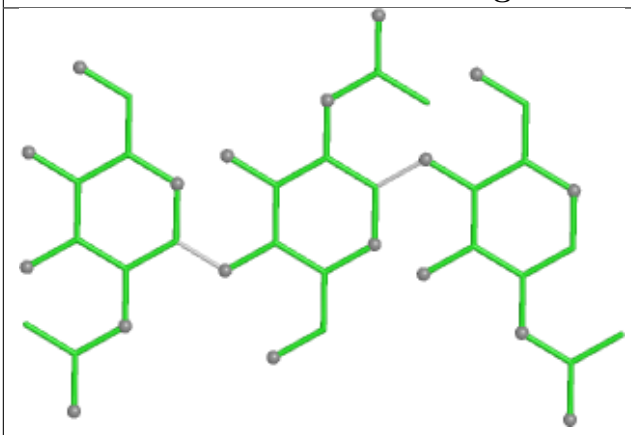
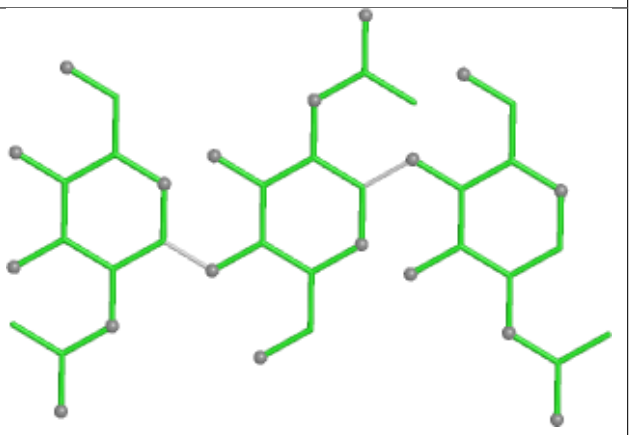
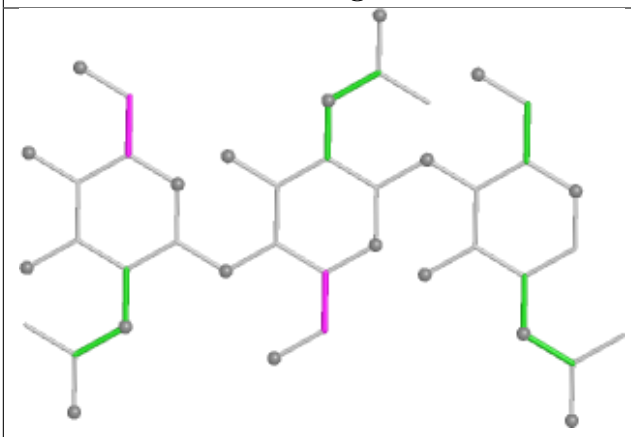
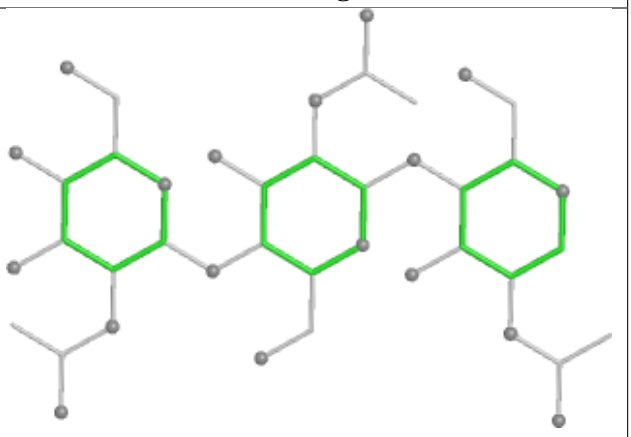
Bond angles



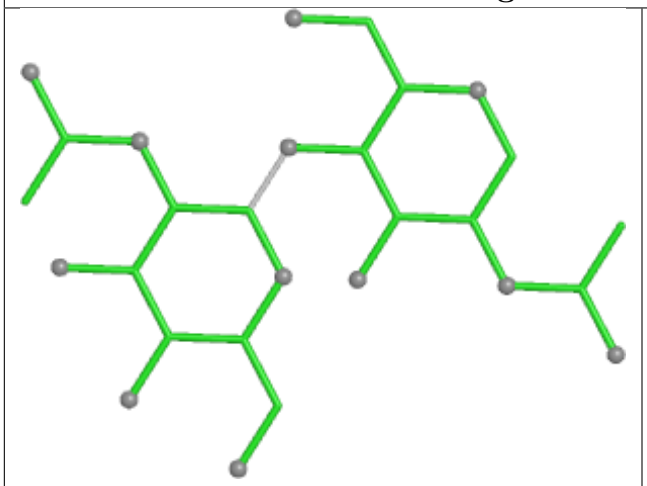
Torsions



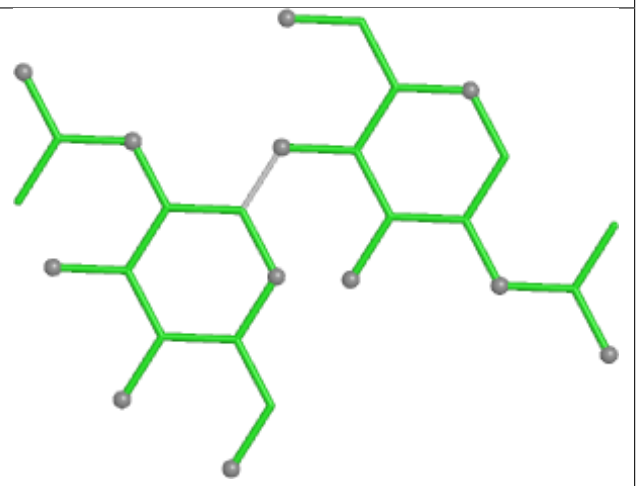
Rings

Oligosaccharide Chain H	
 Bond lengths	 Bond angles
 Torsions	 Rings

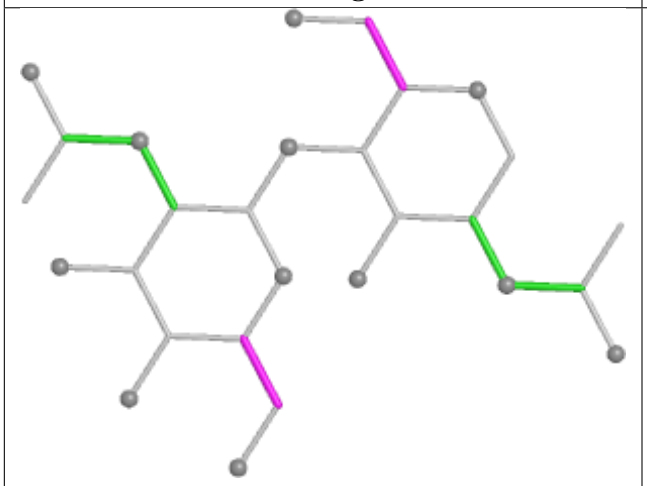
Oligosaccharide Chain F



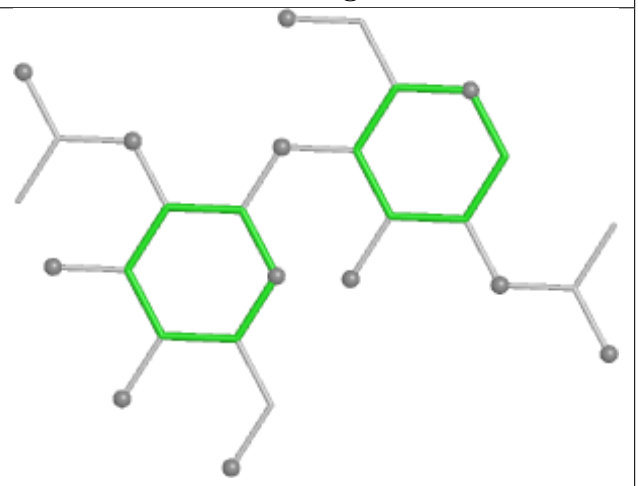
Bond lengths



Bond angles

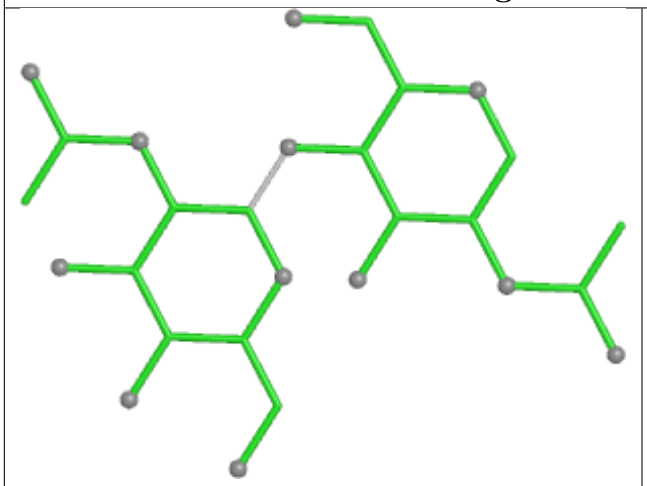


Torsions

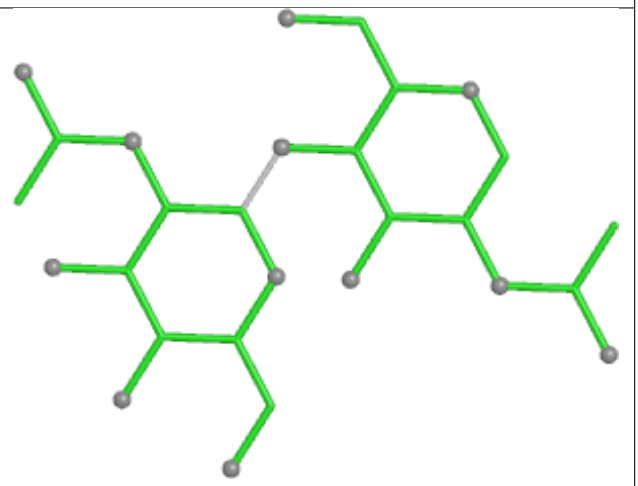


Rings

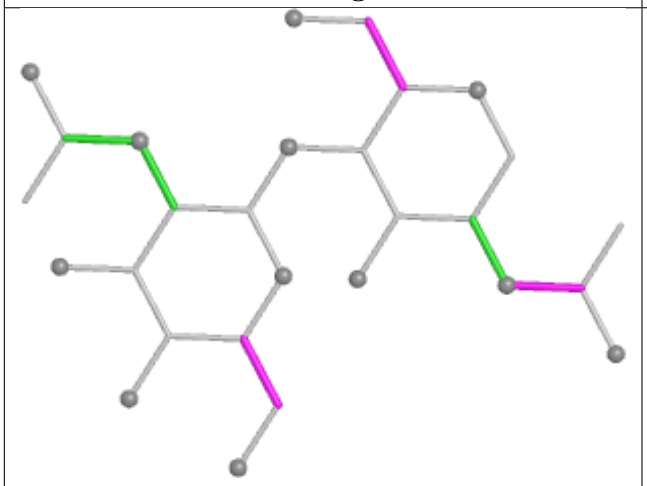
Oligosaccharide Chain G



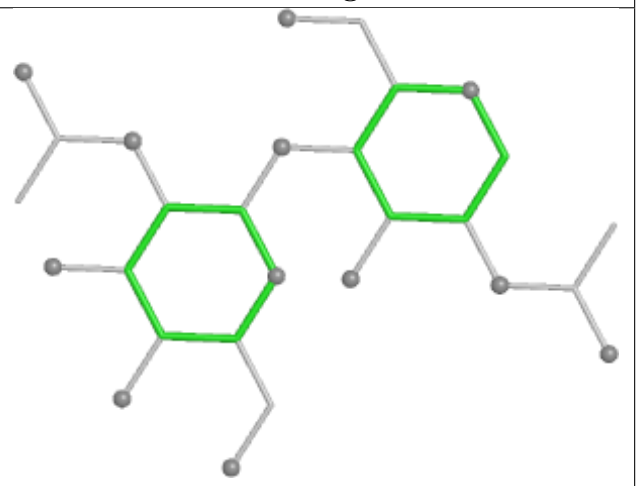
Bond lengths



Bond angles

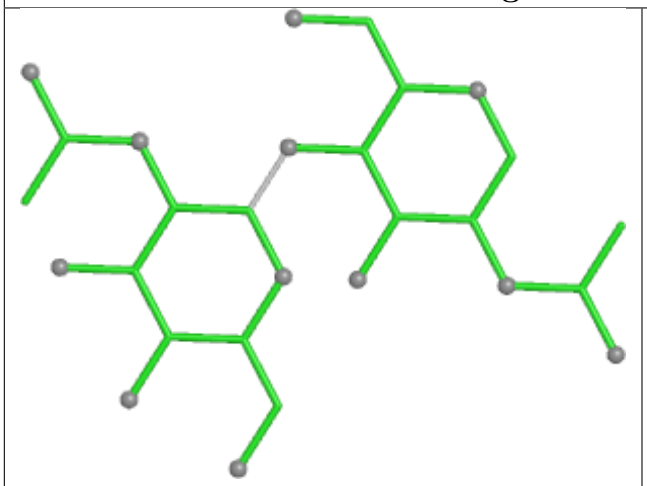


Torsions

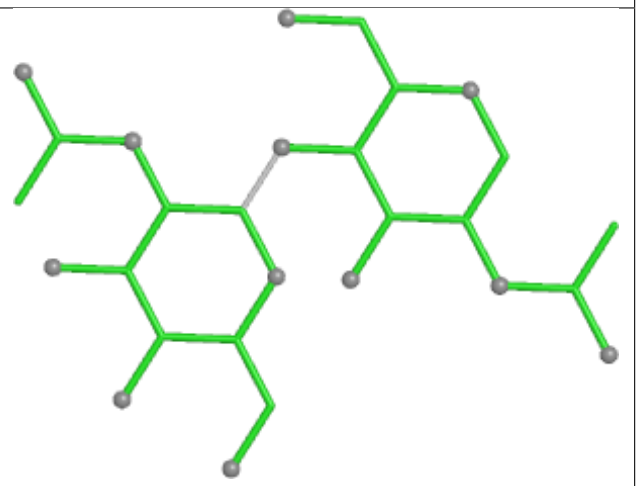


Rings

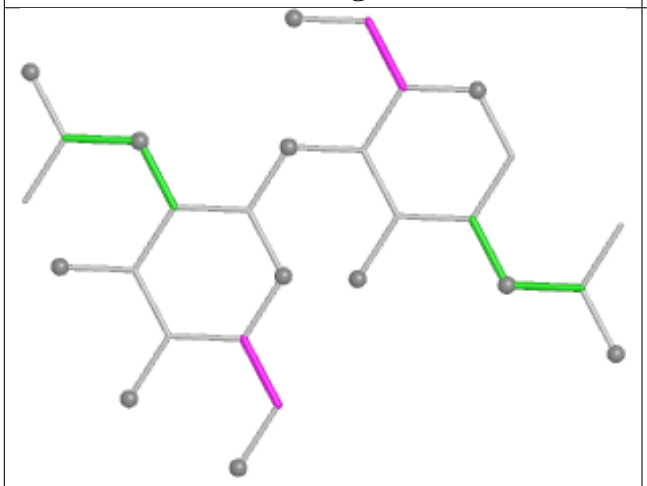
Oligosaccharide Chain I



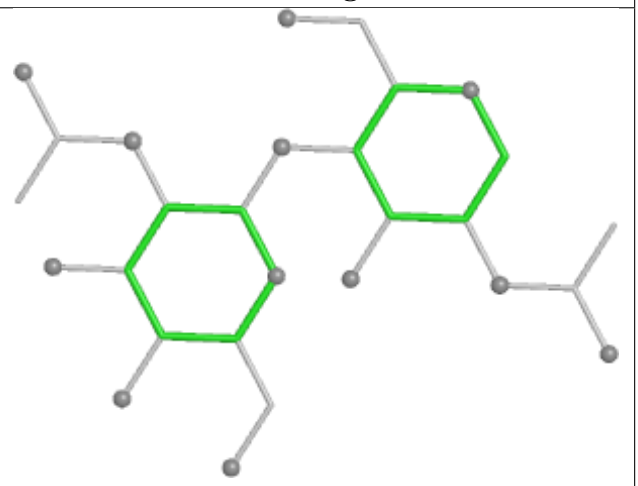
Bond lengths



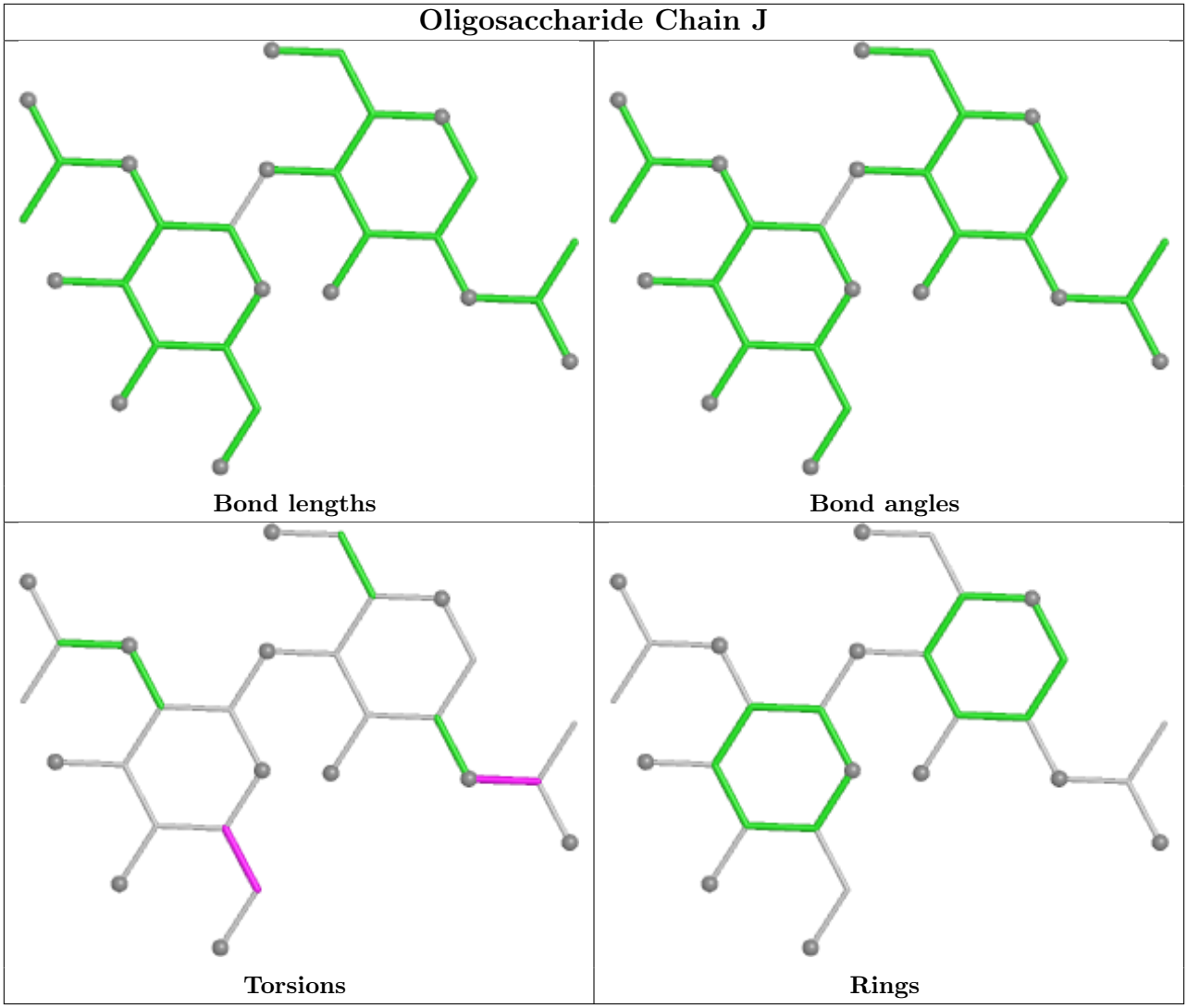
Bond angles



Torsions



Rings



5.6 Ligand geometry (i)

14 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	$\#\|Z\| > 2$
5	NAG	C	703	2	14,14,15	0.23	0	17,19,21	0.42	0
5	NAG	A	1004	1	14,14,15	0.24	0	17,19,21	0.44	0
6	OCA	C	701	-	9,9,9	0.74	0	9,9,9	1.20	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
5	NAG	B	1004	1	14,14,15	0.26	0	17,19,21	0.33	0
5	NAG	D	703	2	14,14,15	0.23	0	17,19,21	0.42	0
5	NAG	A	1003	1	14,14,15	0.24	0	17,19,21	0.45	0
5	NAG	A	1001	1	14,14,15	0.26	0	17,19,21	0.36	0
5	NAG	B	1001	1	14,14,15	0.38	0	17,19,21	0.44	0
5	NAG	A	1002	1	14,14,15	0.33	0	17,19,21	0.41	0
5	NAG	B	1003	1	14,14,15	0.23	0	17,19,21	0.44	0
5	NAG	D	702	2	14,14,15	0.23	0	17,19,21	0.41	0
5	NAG	C	702	2	14,14,15	0.23	0	17,19,21	0.42	0
6	OCA	D	701	-	9,9,9	0.75	0	9,9,9	1.23	0
5	NAG	B	1002	1	14,14,15	0.25	0	17,19,21	0.40	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	C	703	2	-	0/6/23/26	0/1/1/1
5	NAG	A	1004	1	-	1/6/23/26	0/1/1/1
6	OCA	C	701	-	-	2/7/7/7	-
5	NAG	B	1004	1	-	0/6/23/26	0/1/1/1
5	NAG	D	703	2	-	0/6/23/26	0/1/1/1
5	NAG	A	1003	1	-	2/6/23/26	0/1/1/1
5	NAG	A	1001	1	-	0/6/23/26	0/1/1/1
5	NAG	B	1001	1	-	2/6/23/26	0/1/1/1
5	NAG	A	1002	1	-	3/6/23/26	0/1/1/1
5	NAG	B	1003	1	-	1/6/23/26	0/1/1/1
5	NAG	D	702	2	-	2/6/23/26	0/1/1/1
5	NAG	C	702	2	-	2/6/23/26	0/1/1/1
6	OCA	D	701	-	-	1/7/7/7	-
5	NAG	B	1002	1	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 18 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	1002	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
5	A	1003	NAG	O5-C5-C6-O6
5	C	702	NAG	O5-C5-C6-O6
5	D	702	NAG	O5-C5-C6-O6
5	B	1002	NAG	C4-C5-C6-O6

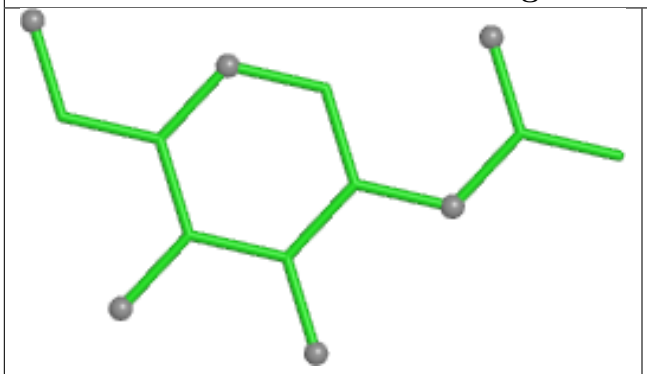
There are no ring outliers.

2 monomers are involved in 3 short contacts:

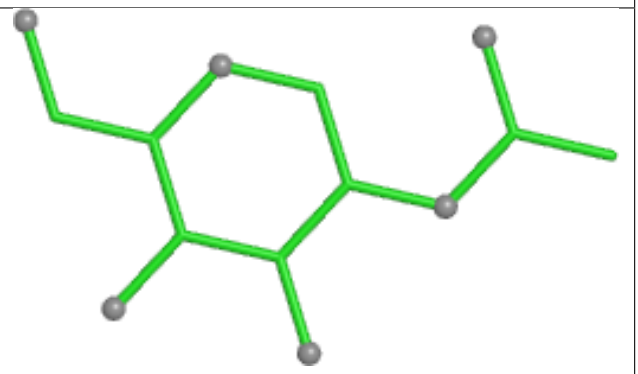
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	C	701	OCA	2	0
5	A	1002	NAG	1	0

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

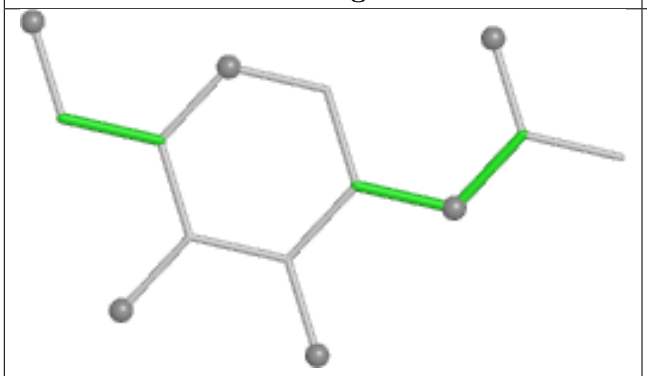
Ligand NAG C 703



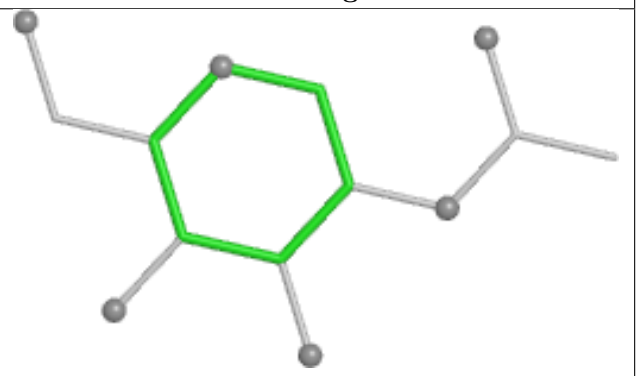
Bond lengths



Bond angles

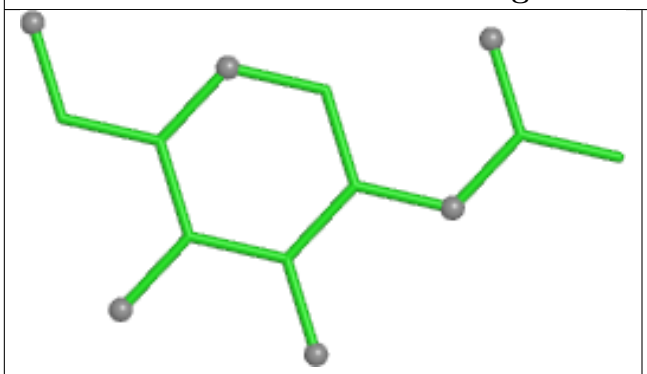


Torsions

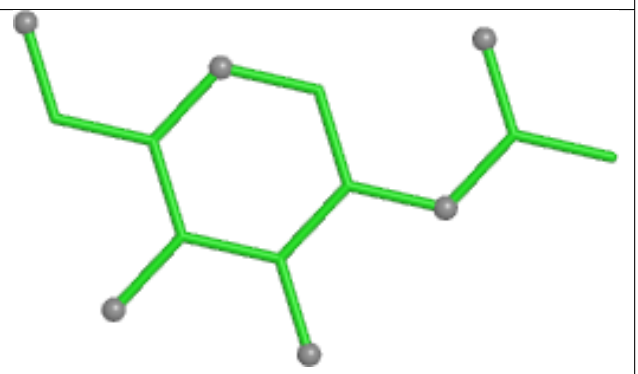


Rings

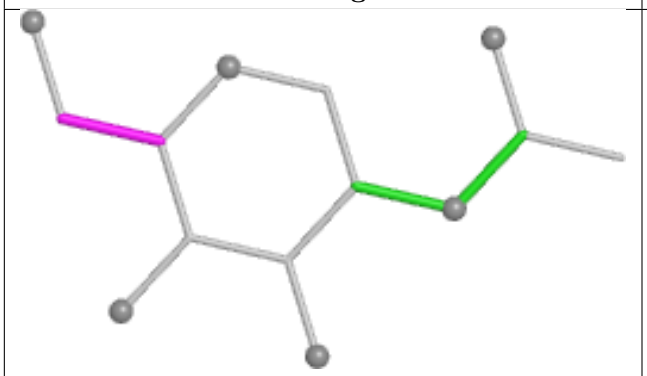
Ligand NAG A 1004



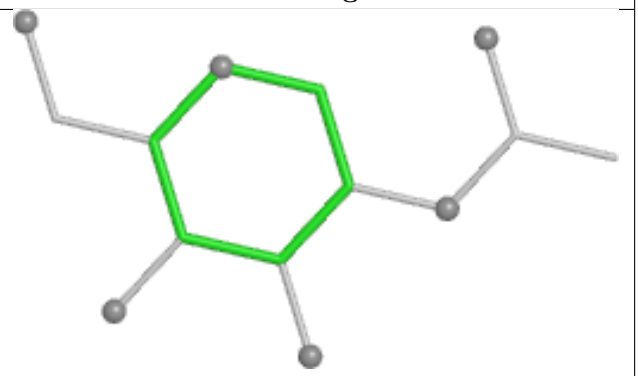
Bond lengths



Bond angles

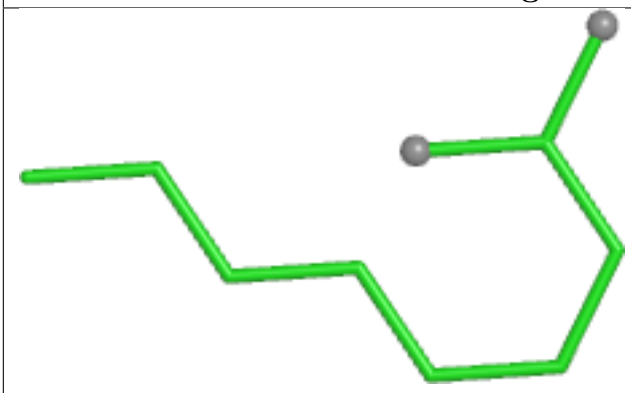


Torsions

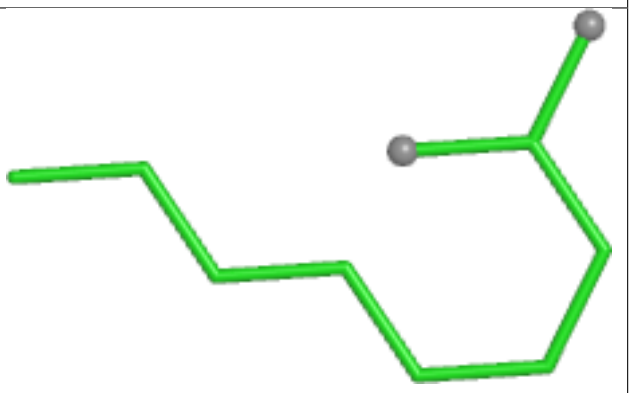


Rings

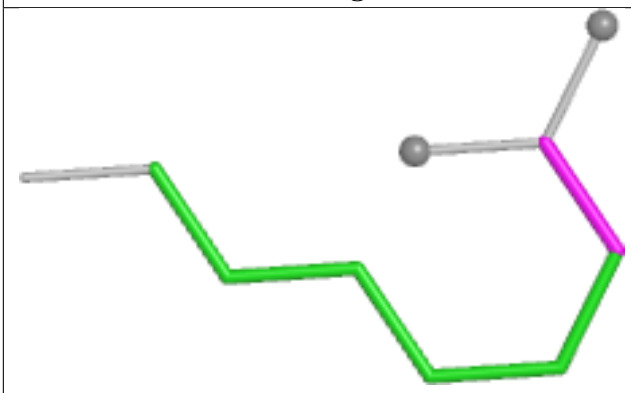
Ligand OCA C 701



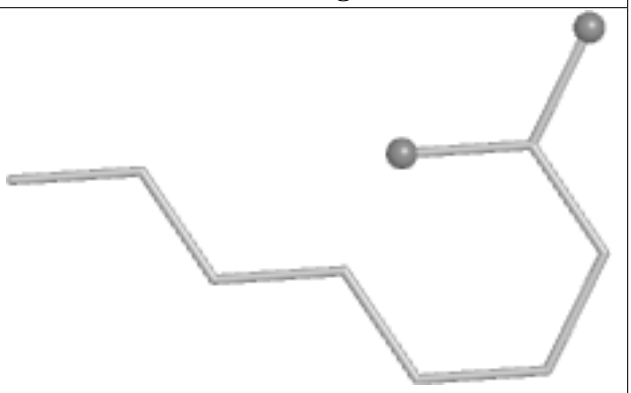
Bond lengths



Bond angles

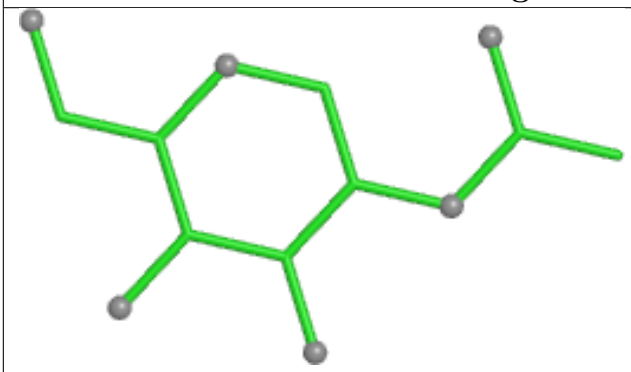


Torsions

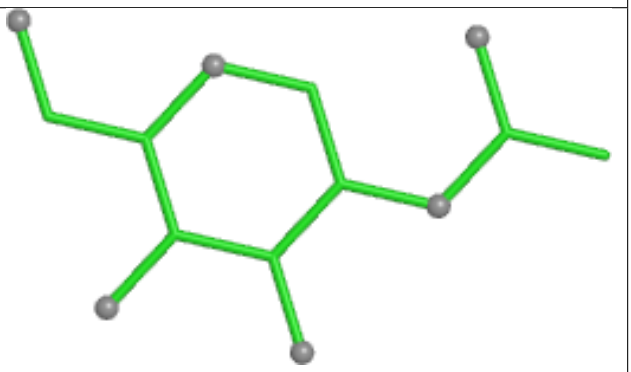


Rings

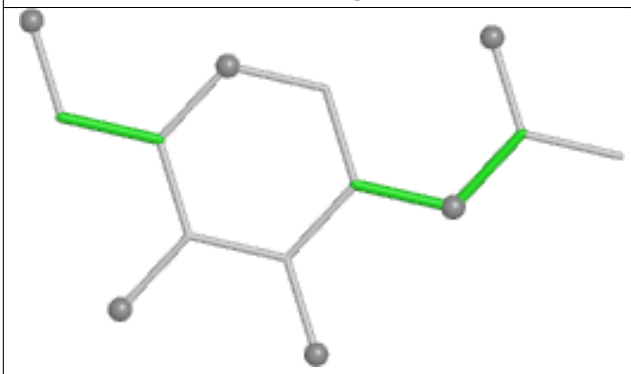
Ligand NAG B 1004



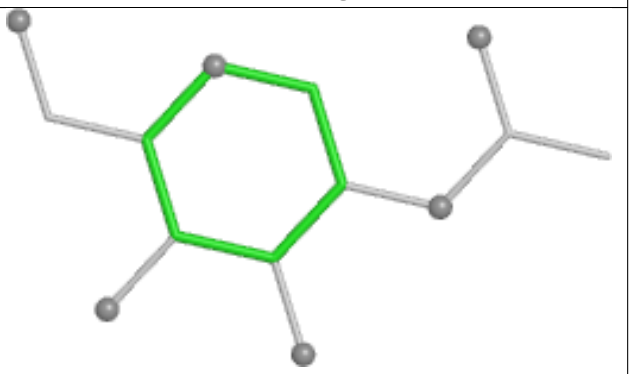
Bond lengths



Bond angles

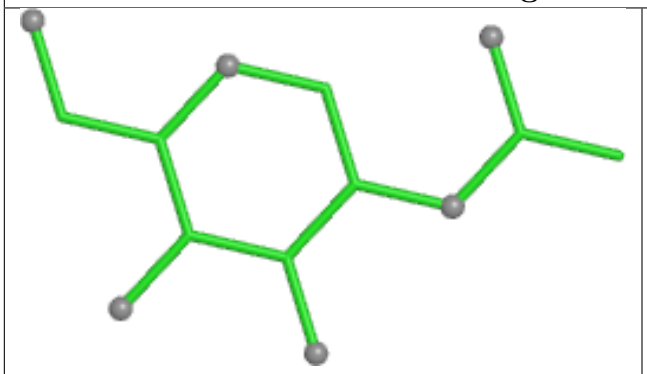


Torsions

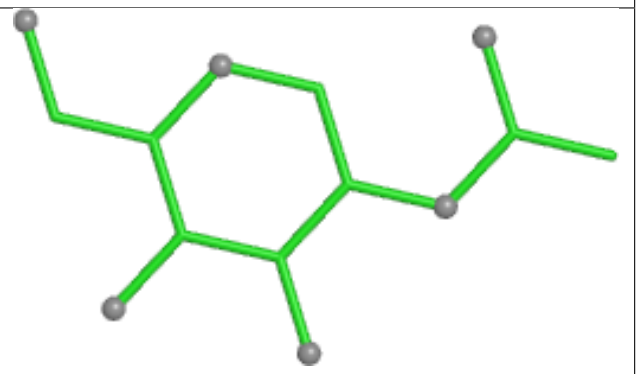


Rings

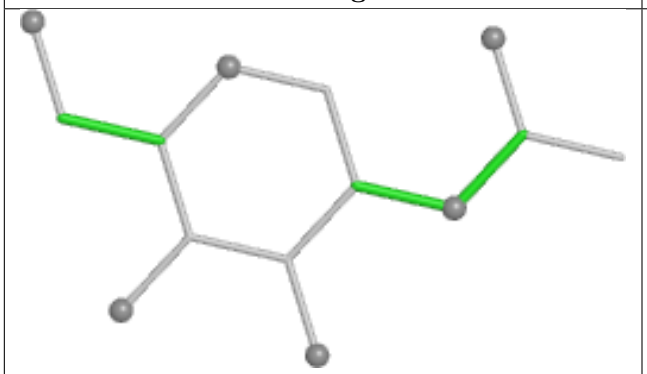
Ligand NAG D 703



Bond lengths



Bond angles



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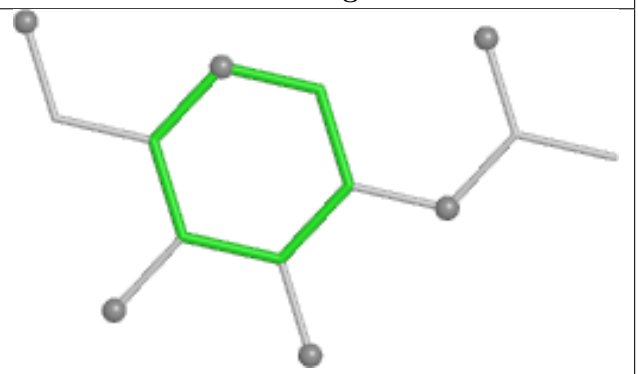
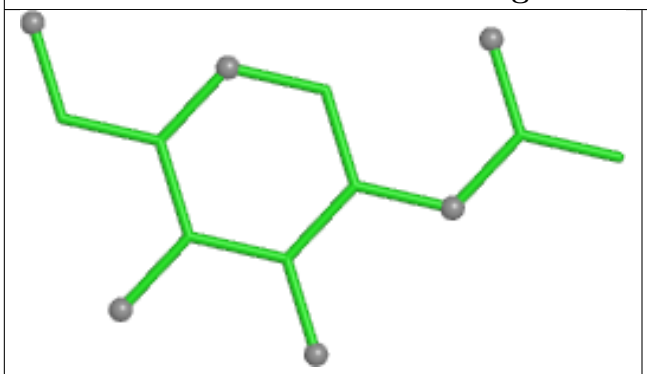
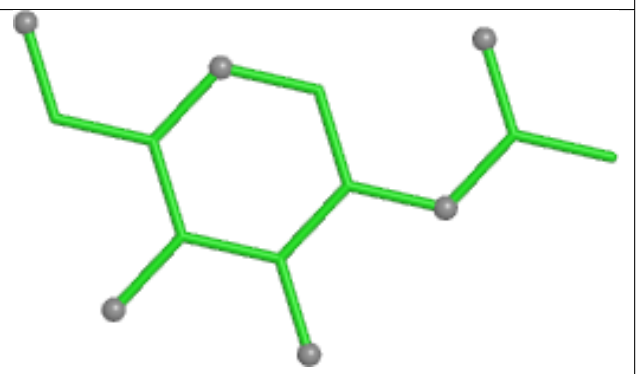


Rings

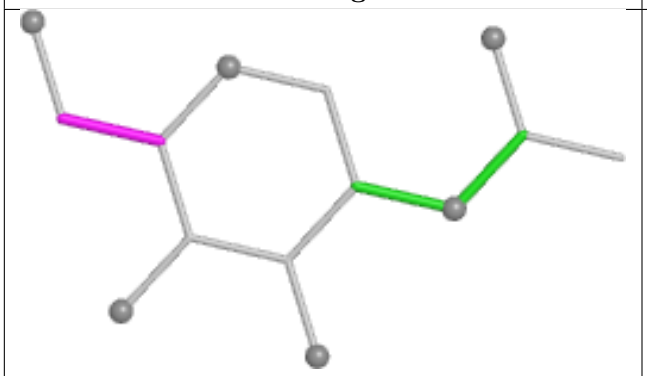
Ligand NAG A 1003



Bond lengths



Bond angles



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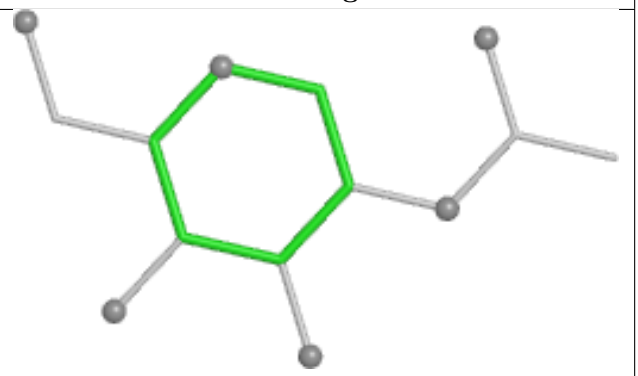
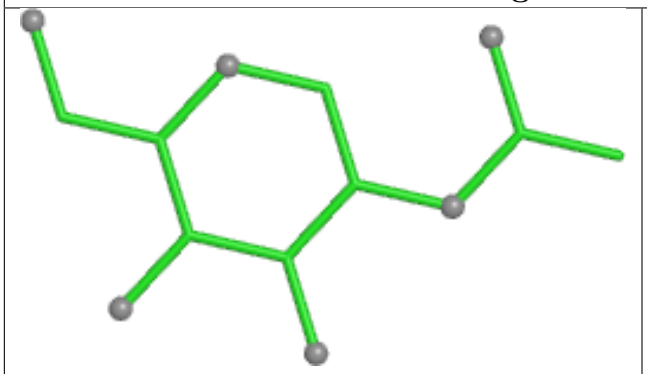
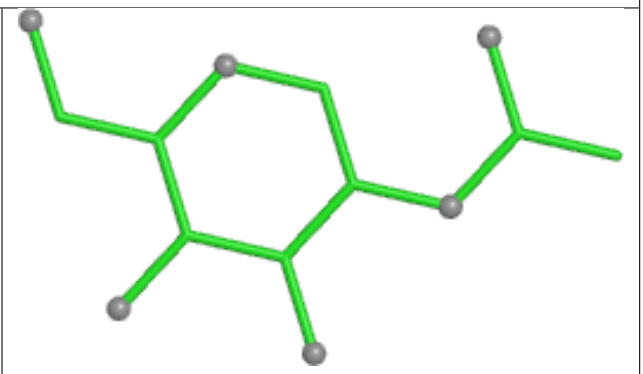


Rings

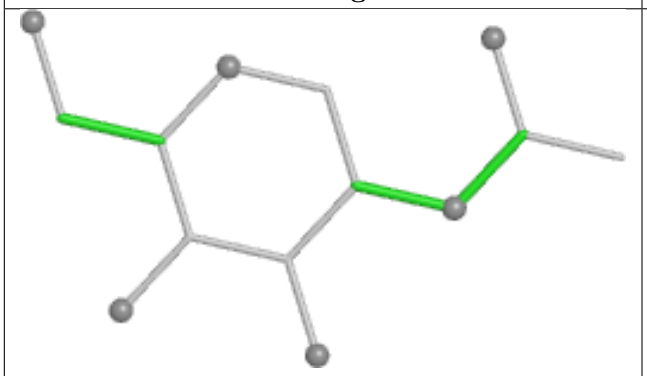
Ligand NAG A 1001



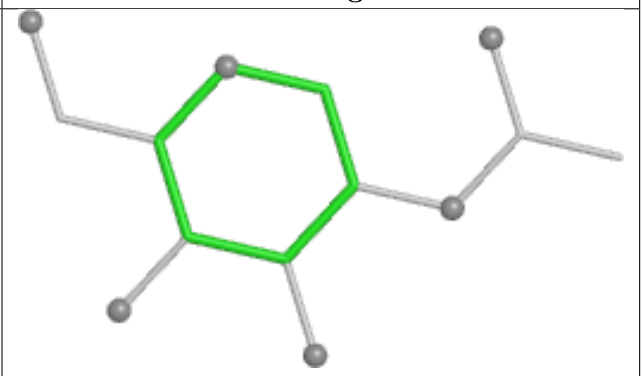
Bond lengths



Bond angles

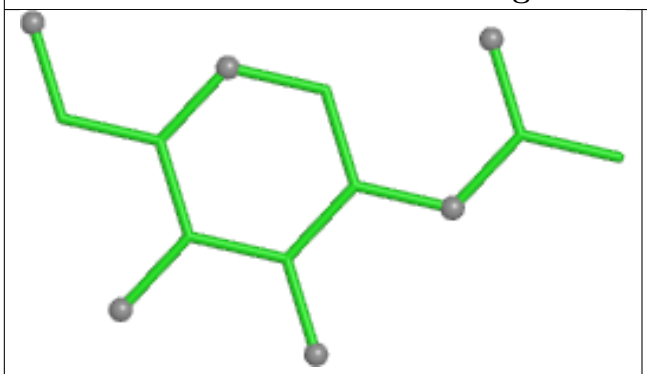


Torsions

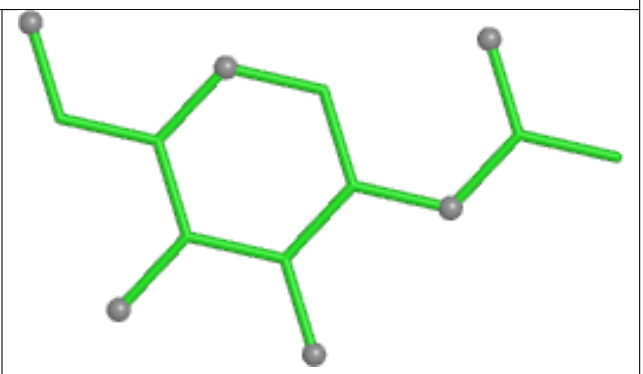


Rings

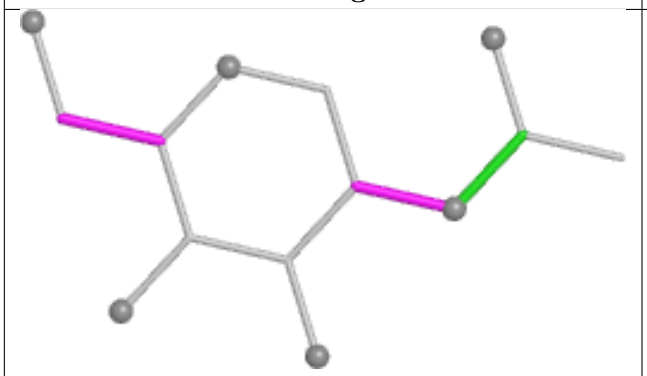
Ligand NAG B 1001



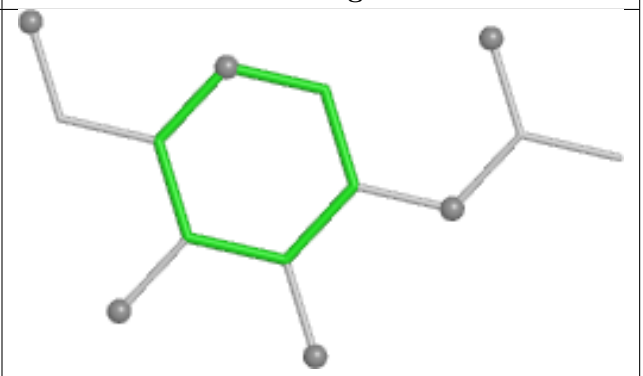
Bond lengths



Bond angles

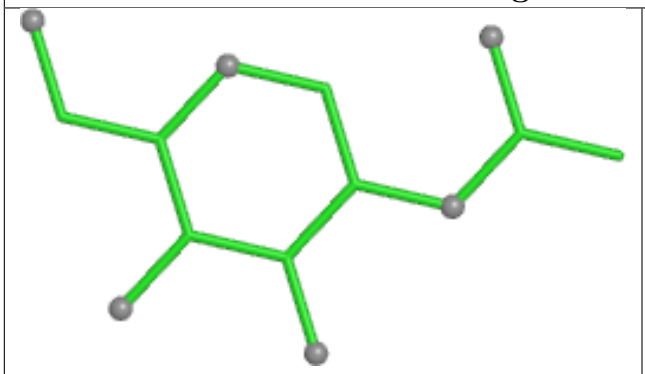


Torsions

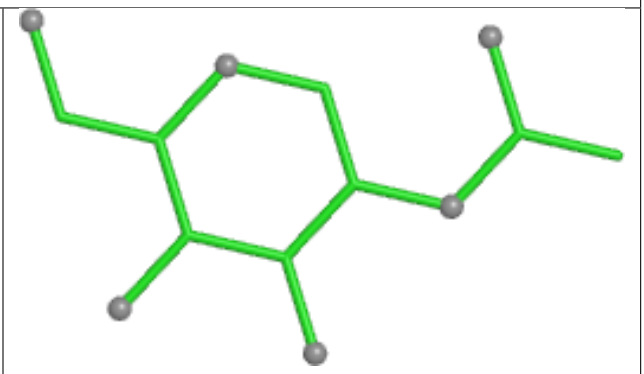


Rings

Ligand NAG A 1002



Bond lengths



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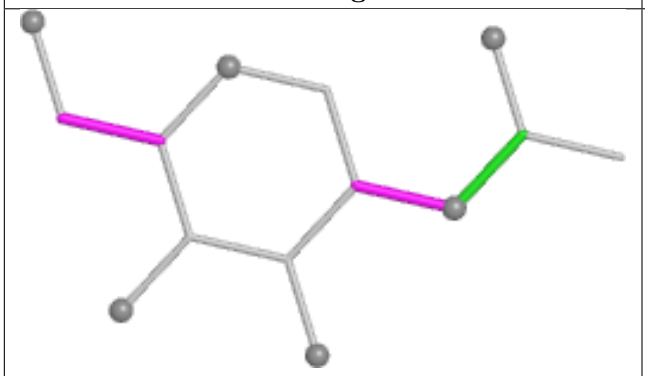

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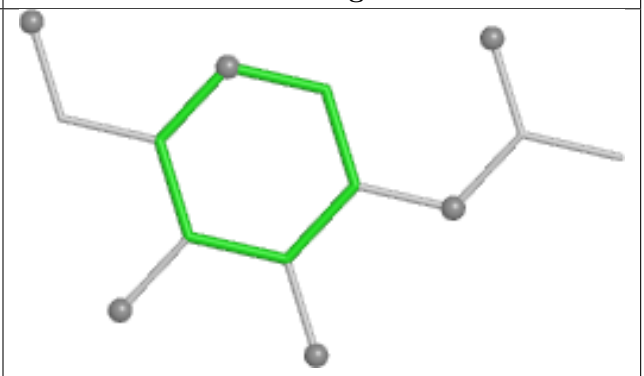
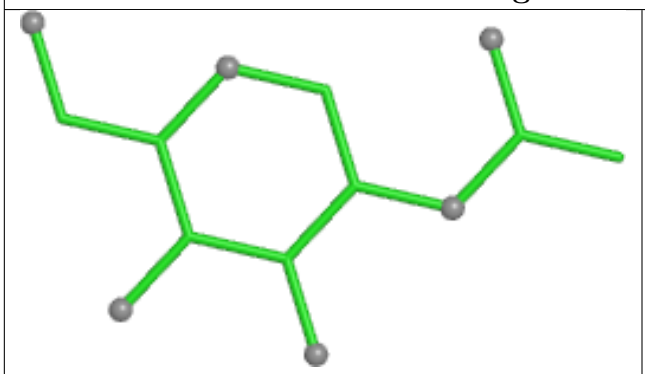
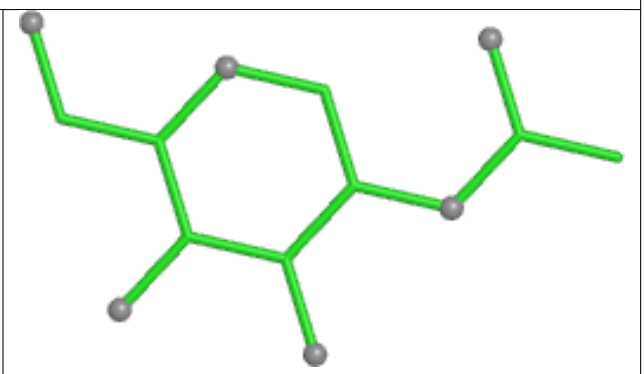


Rings

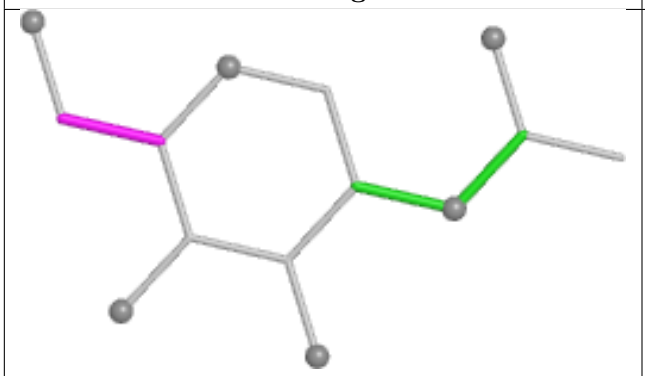
Ligand NAG B 1003



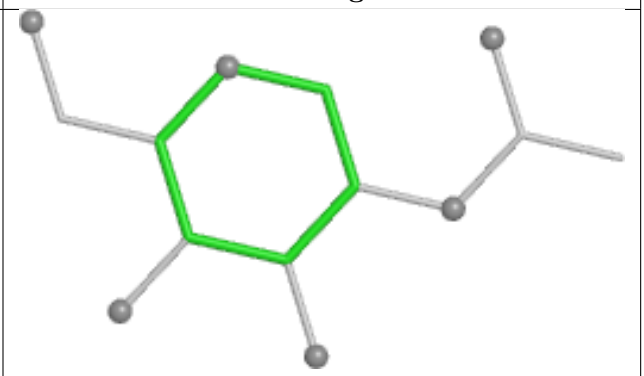
Bond lengths



Bond angles

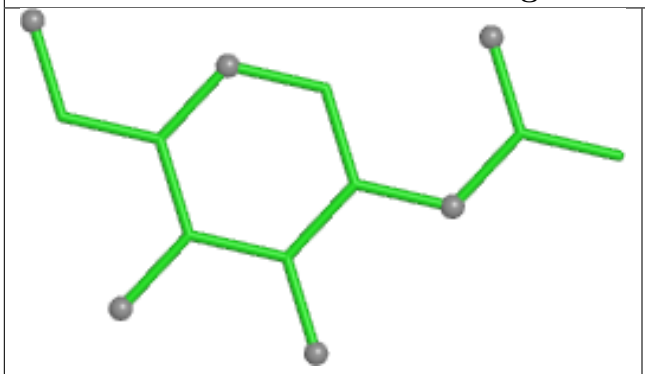


Torsions



Rings

Ligand NAG D 702



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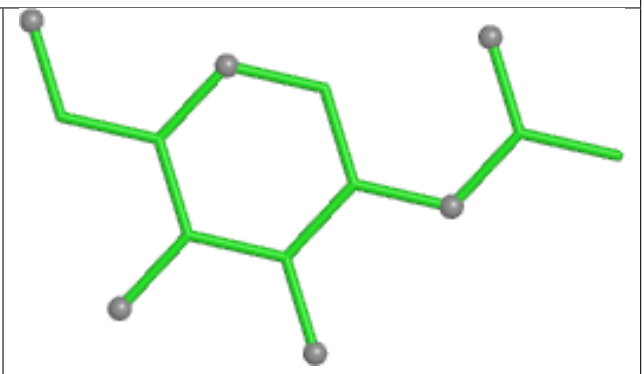
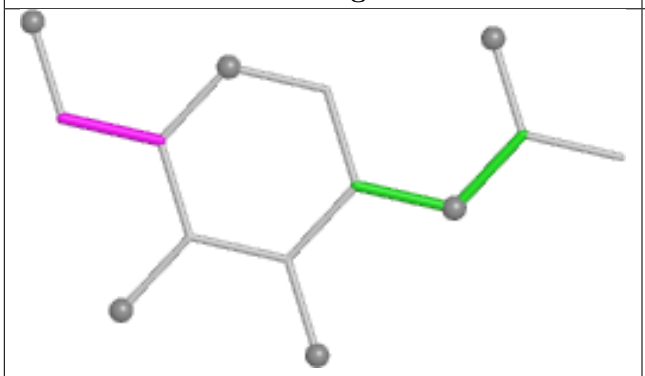
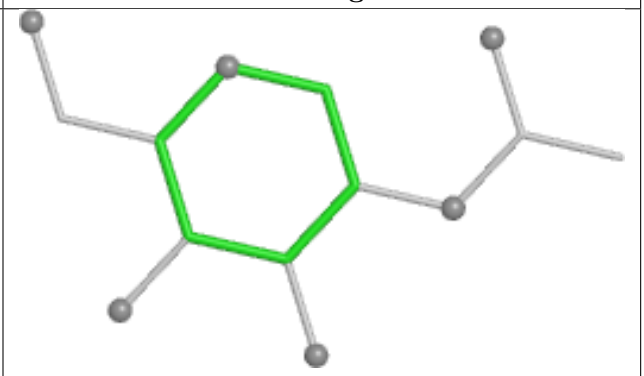


Bond angles

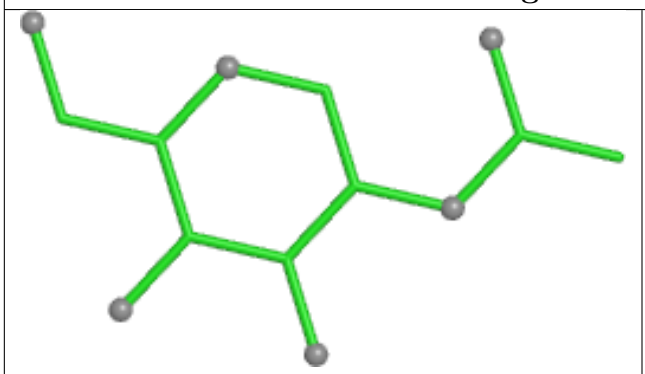


Torsions

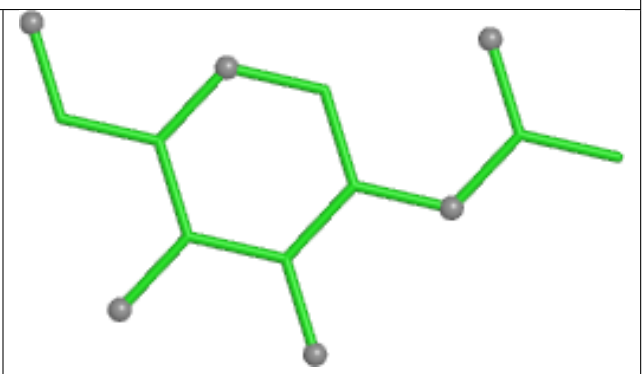


Rings

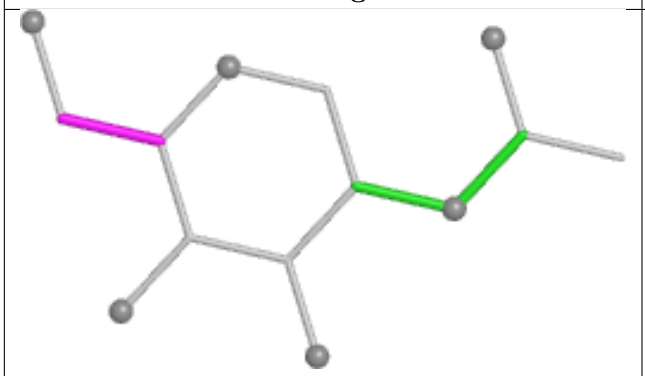
Ligand NAG C 702



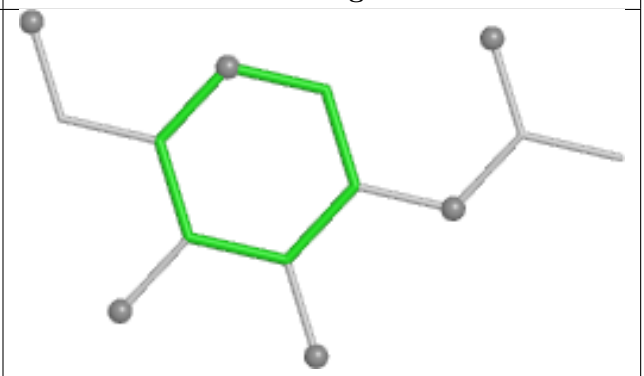
Bond lengths



Bond angles

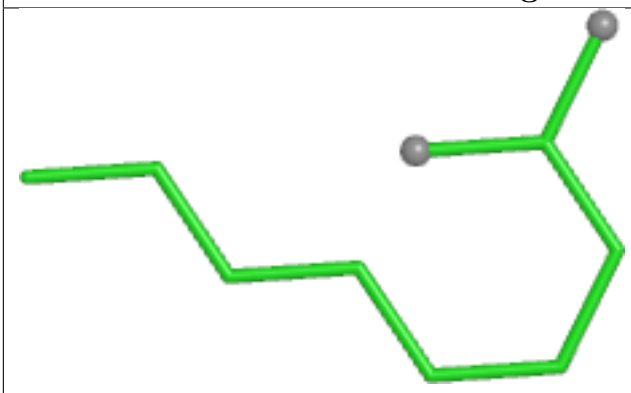


Torsions

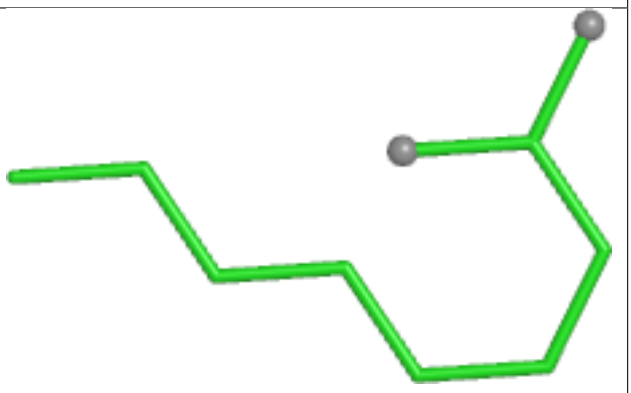


Rings

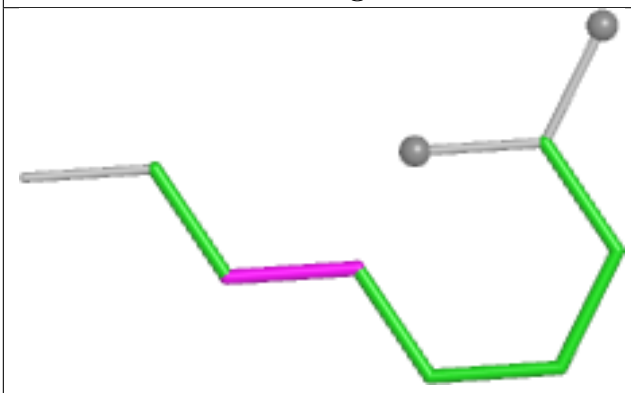
Ligand OCA D 701



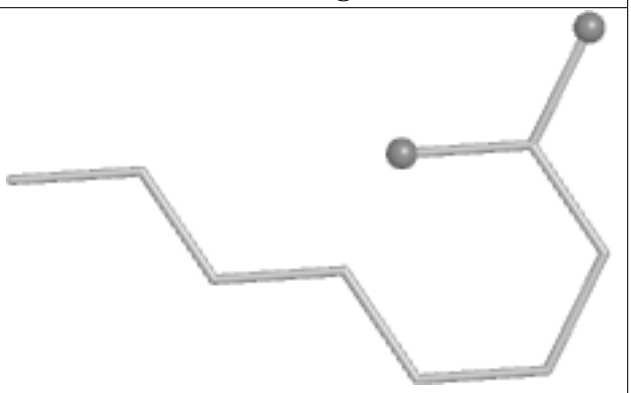
Bond lengths



Bond angles

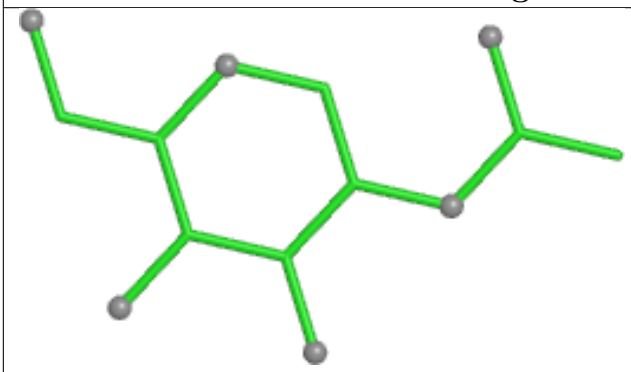


Torsions

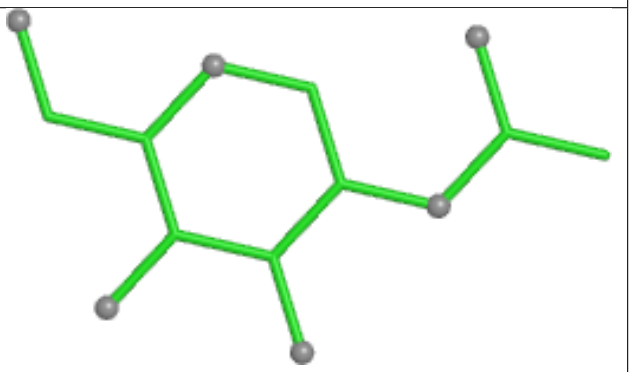


Rings

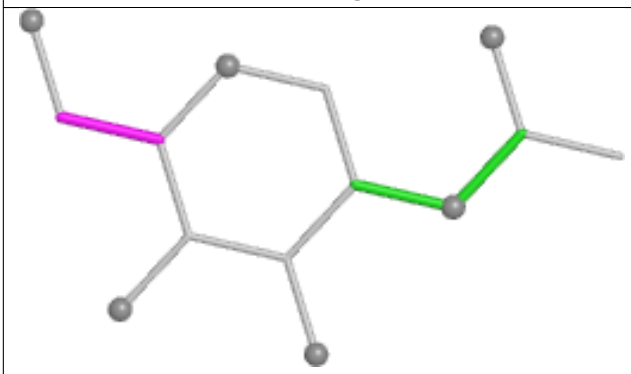
Ligand NAG B 1002



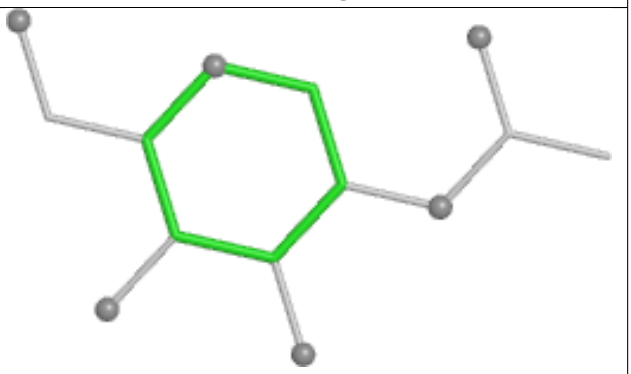
Bond lengths



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.

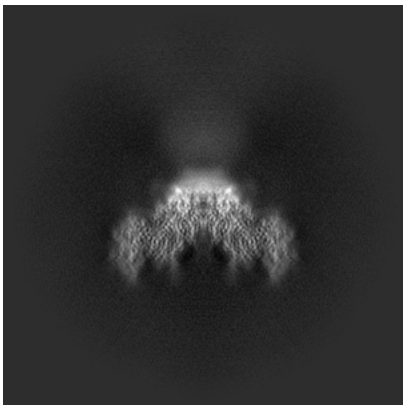
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-81815. These allow visual inspection of the internal detail of the map and identification of artifacts.

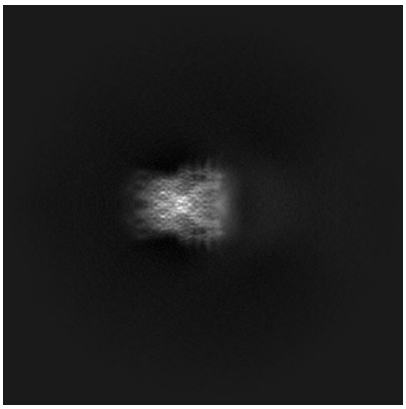
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections (i)

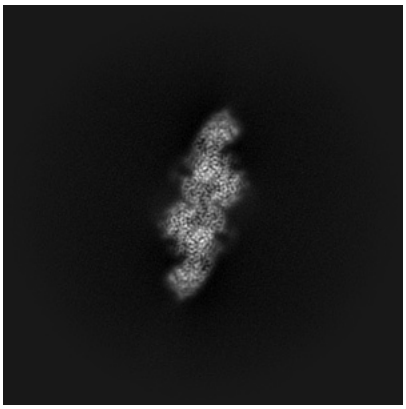
6.1.1 Primary map



X

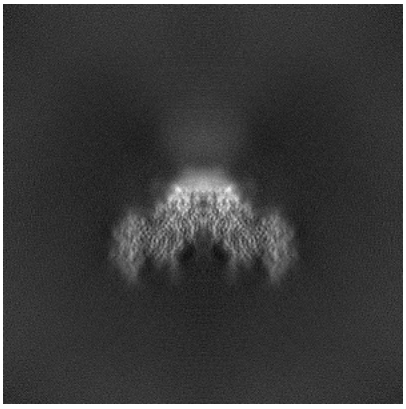


Y

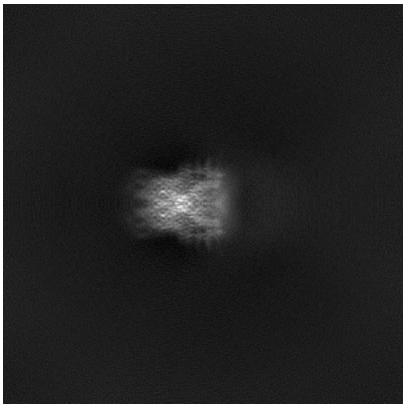


Z

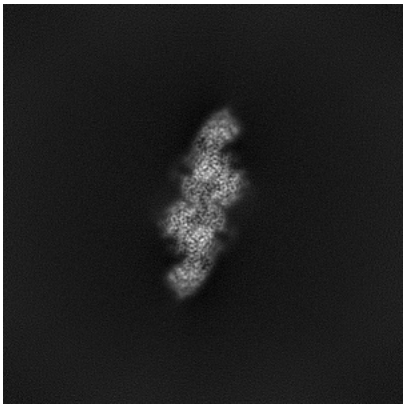
6.1.2 Raw map



X



Y

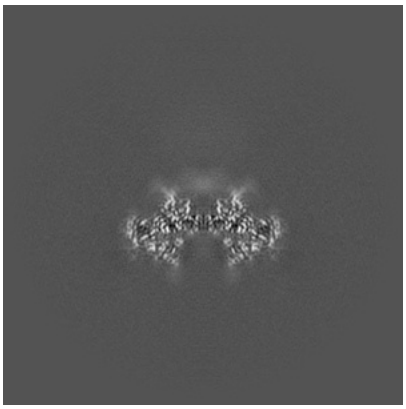


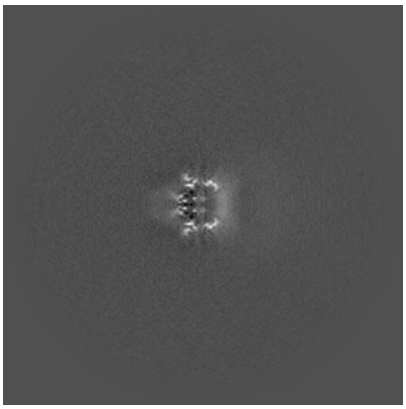
Z

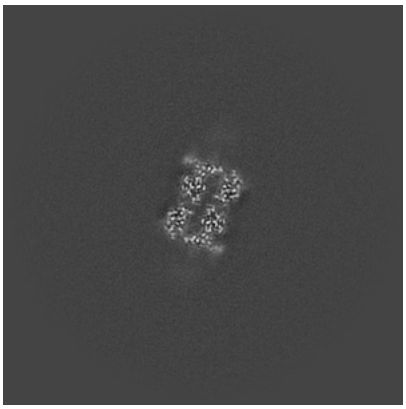
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

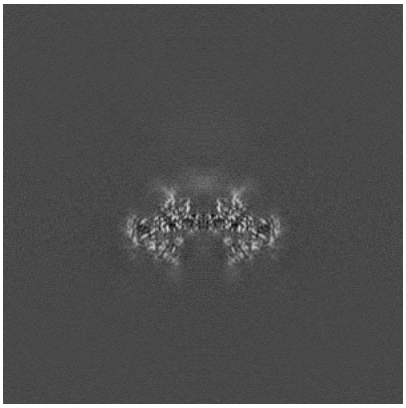
6.2.1 Primary map

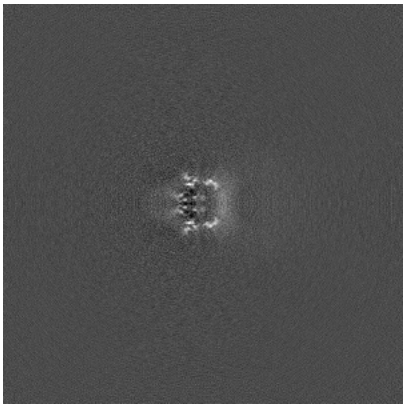

X Index: 220

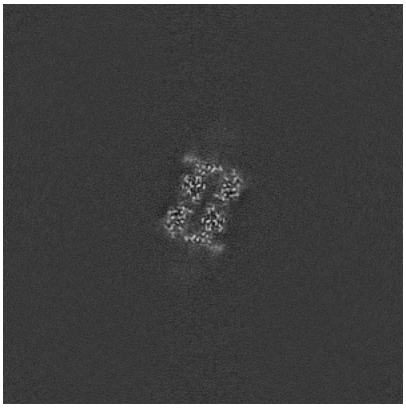

Y Index: 220


Z Index: 220

6.2.2 Raw map


X Index: 220

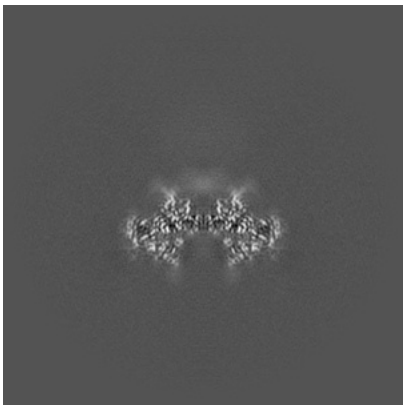

Y Index: 220


Z Index: 220

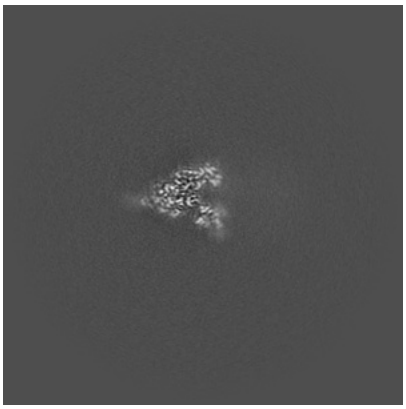
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

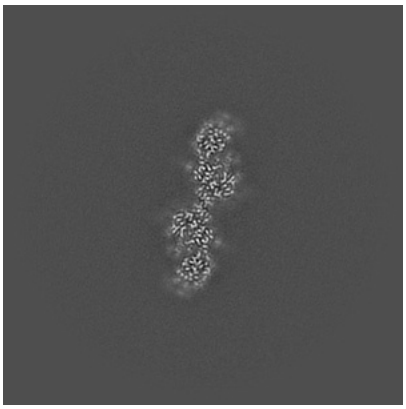
6.3.1 Primary map



X Index: 220

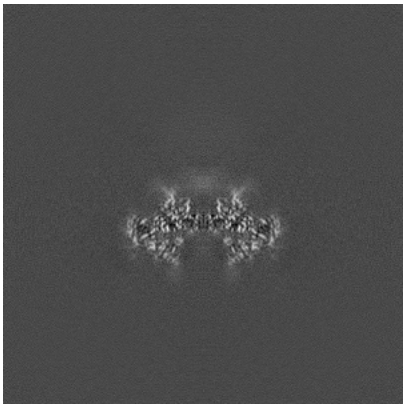


Y Index: 248

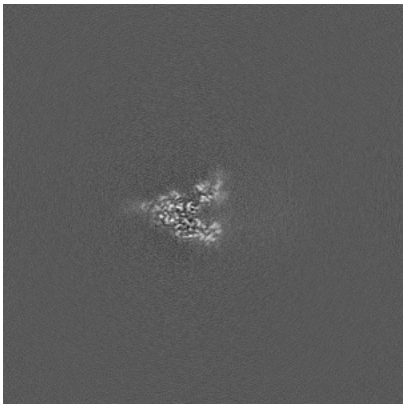


Z Index: 194

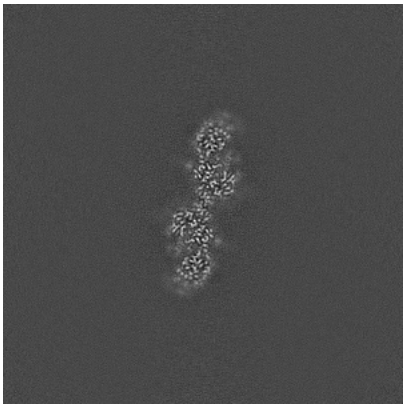
6.3.2 Raw map



X Index: 220



Y Index: 192

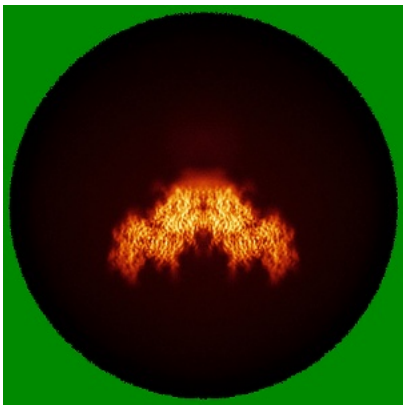


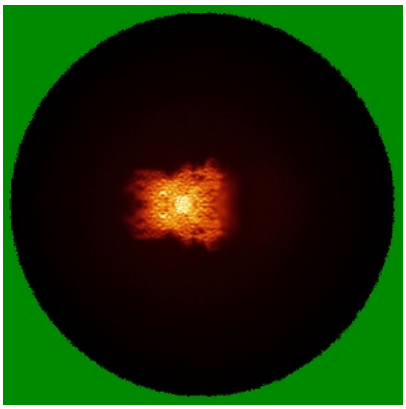
Z Index: 194

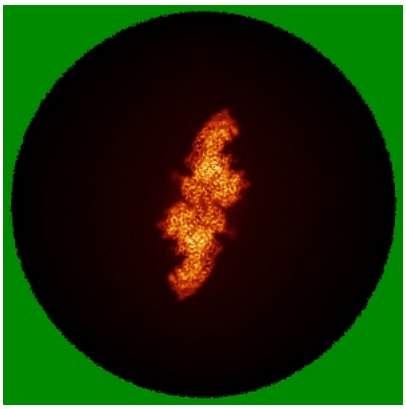
The images above show the largest variance slices of the map in three orthogonal directions.

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

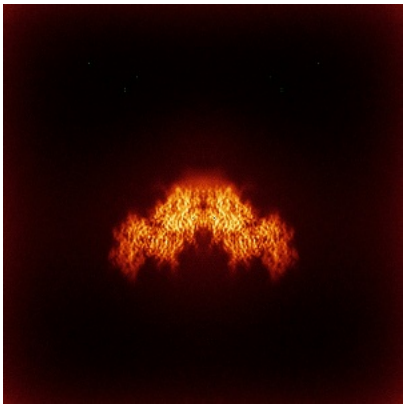
6.4.1 Primary map

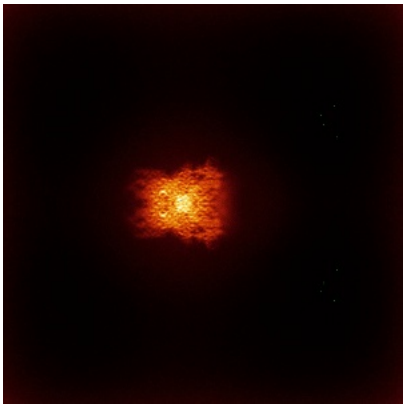

X

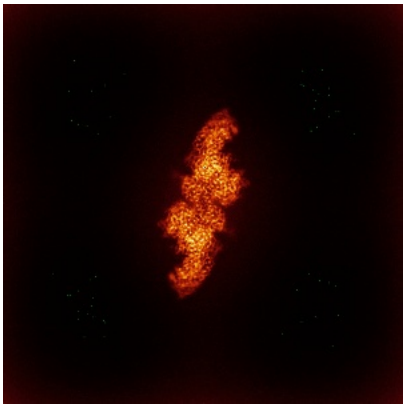

Y


Z

6.4.2 Raw map


X

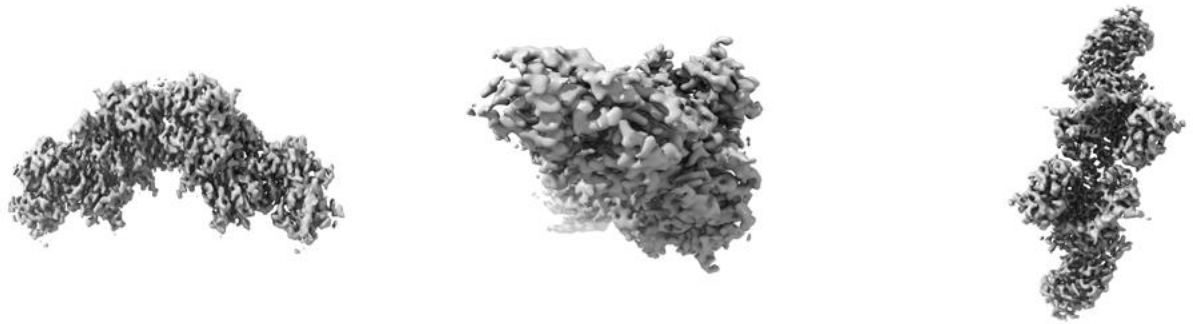

Y


Z

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

6.5 Orthogonal surface views (i)

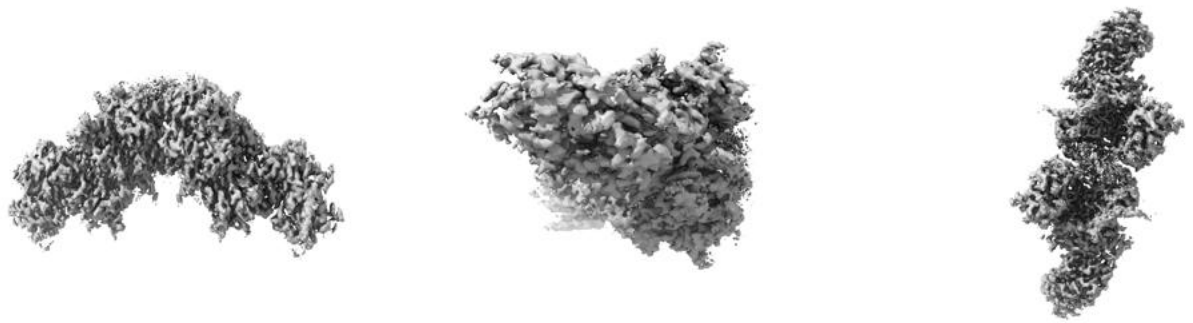
6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.0573. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X Y Z

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

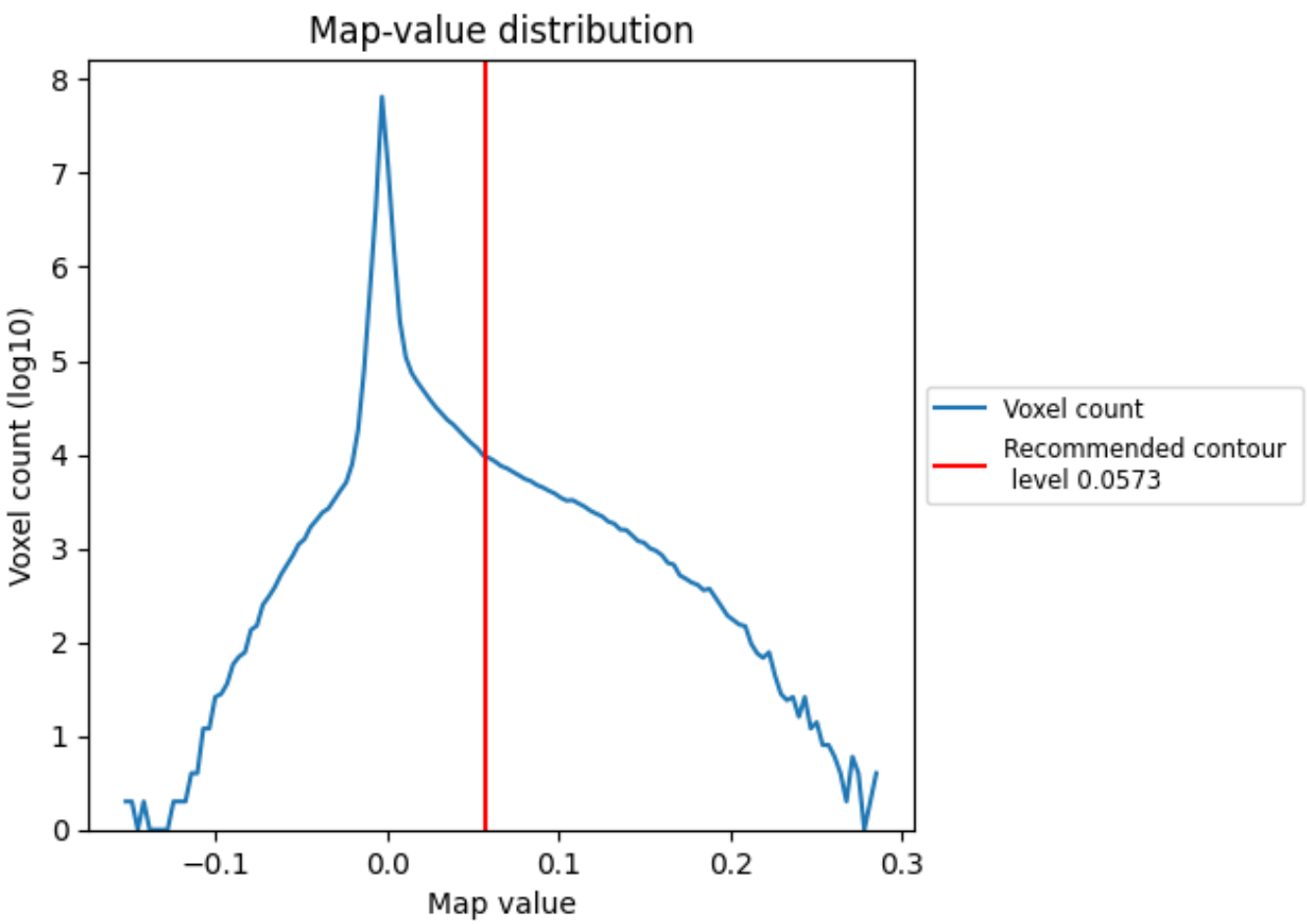
6.6 Mask visualisation (i)

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

7 Map analysis (i)

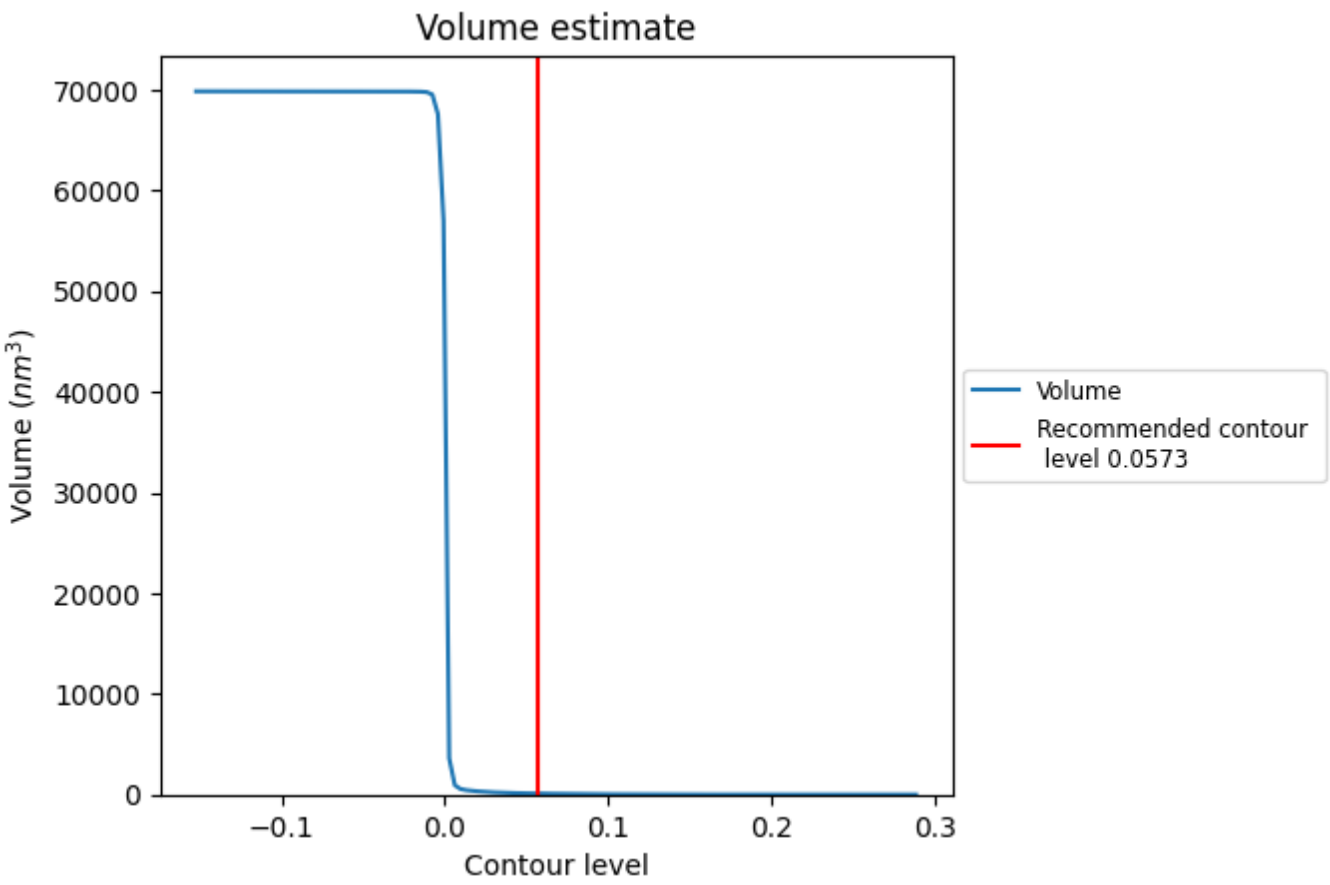
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution (i)



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

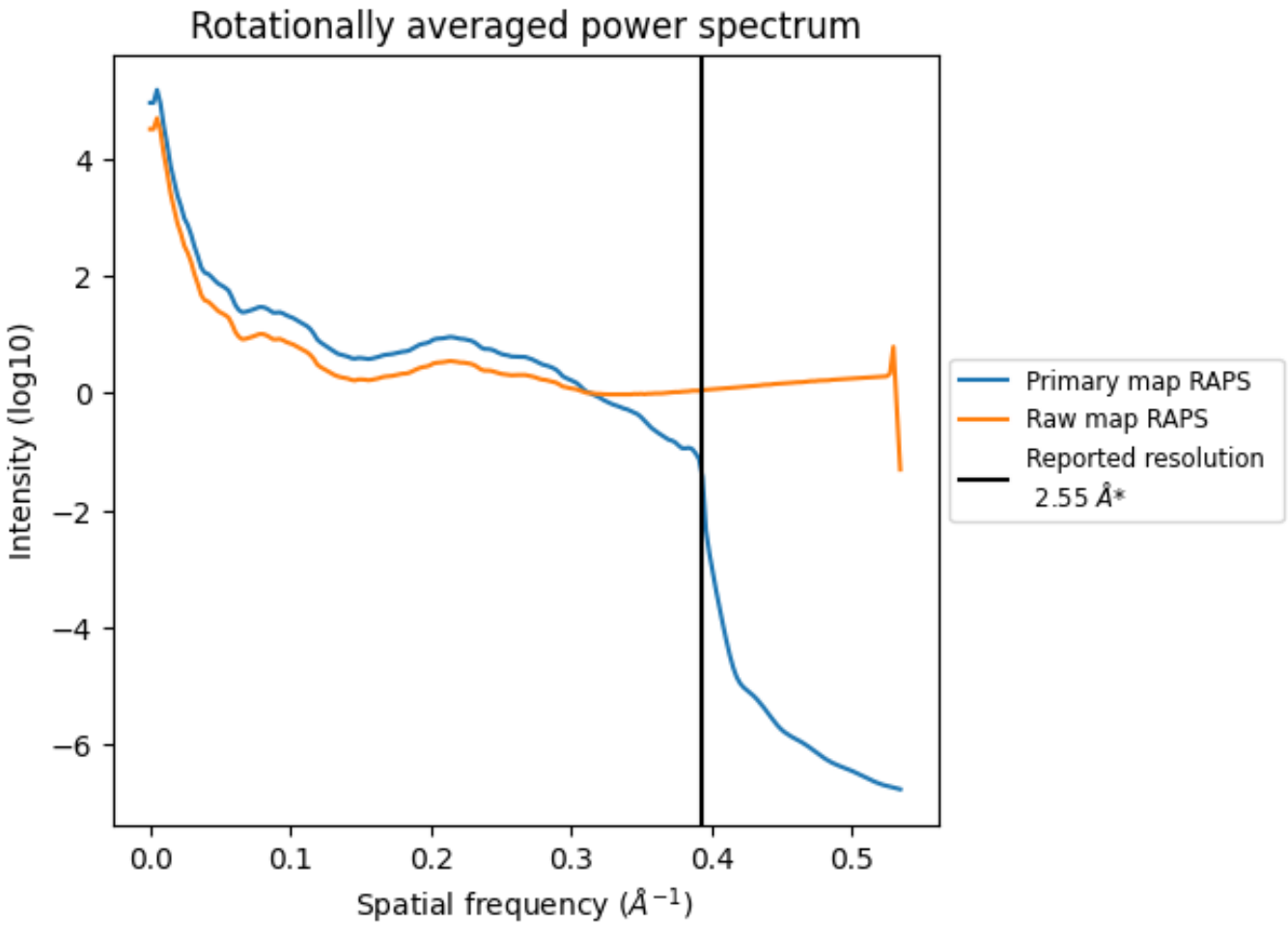
7.2 Volume estimate (i)



The volume at the recommended contour level is 99 nm^3; this corresponds to an approximate mass of 89 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)

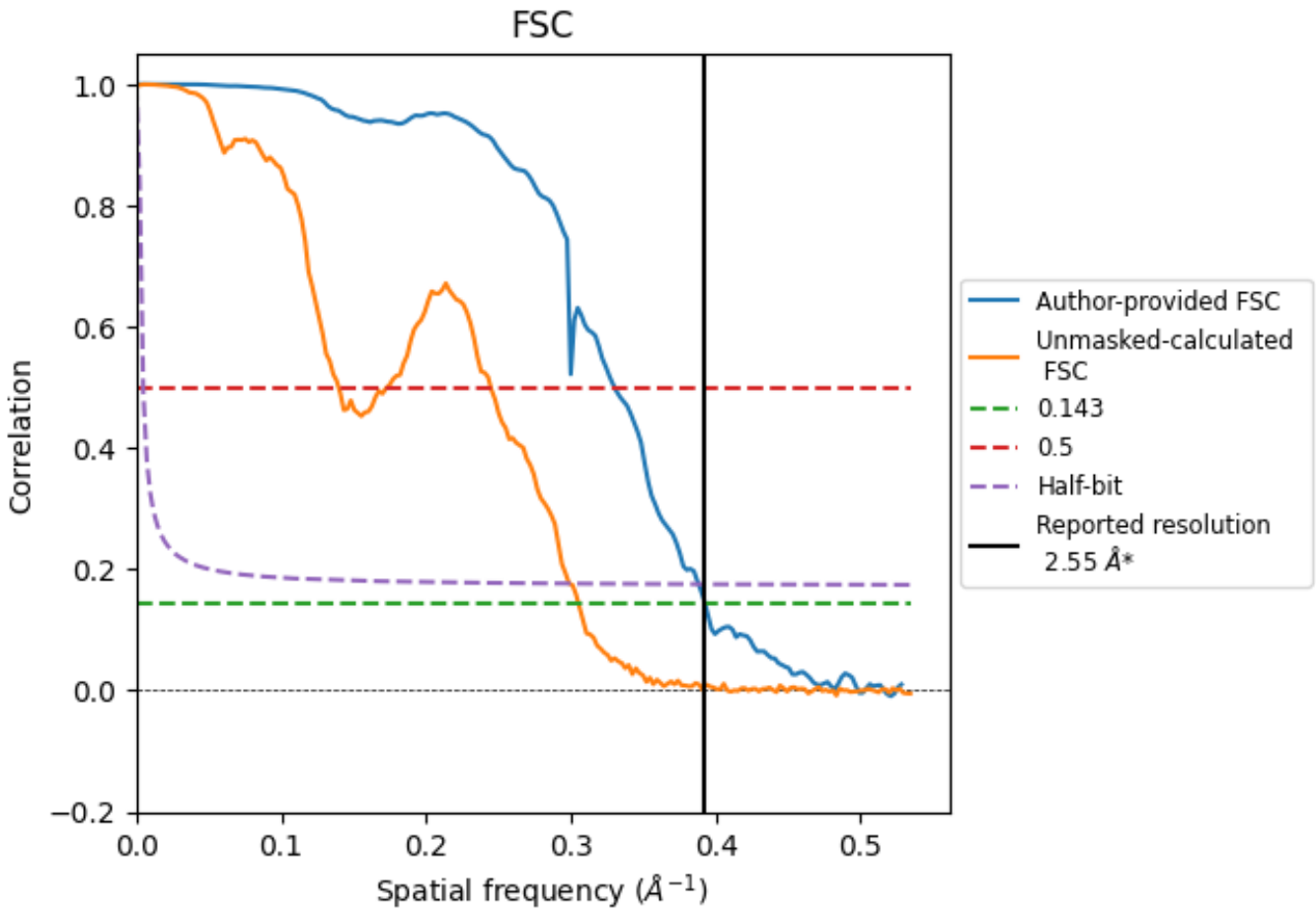


*Reported resolution corresponds to spatial frequency of 0.392 Å^{-1}

8 Fourier-Shell correlation (i)

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

8.1 FSC (i)



*Reported resolution corresponds to spatial frequency of 0.392 Å^{-1}

8.2 Resolution estimates (i)

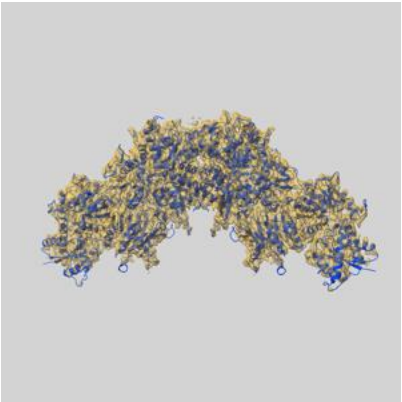
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.55	-	-
Author-provided FSC curve	2.55	3.03	2.58
Unmasked-calculated*	3.28	7.16	3.35

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.28 differs from the reported value 2.55 by more than 10 %

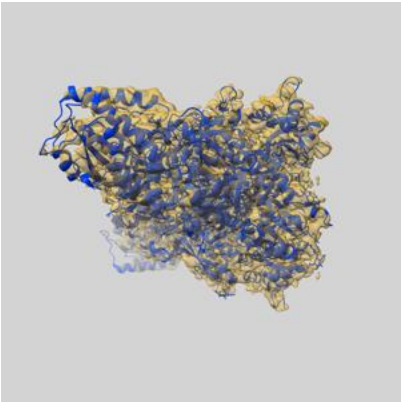
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-81815 and PDB model 43EI. Per-residue inclusion information can be found in section 3 on page 8.

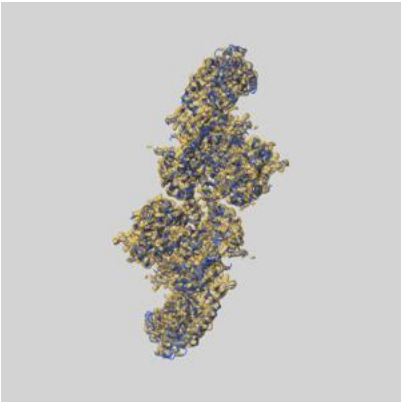
9.1 Map-model overlay (i)



X



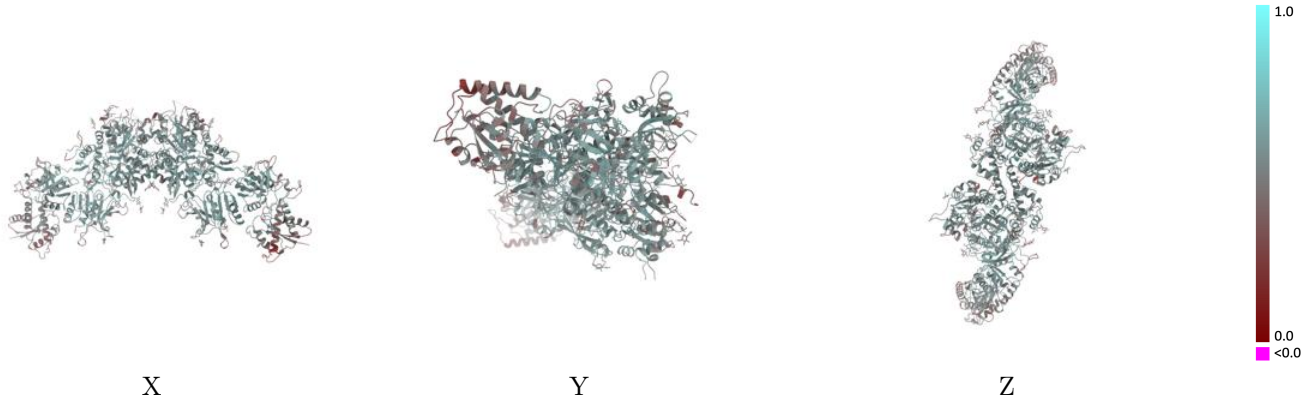
Y



Z

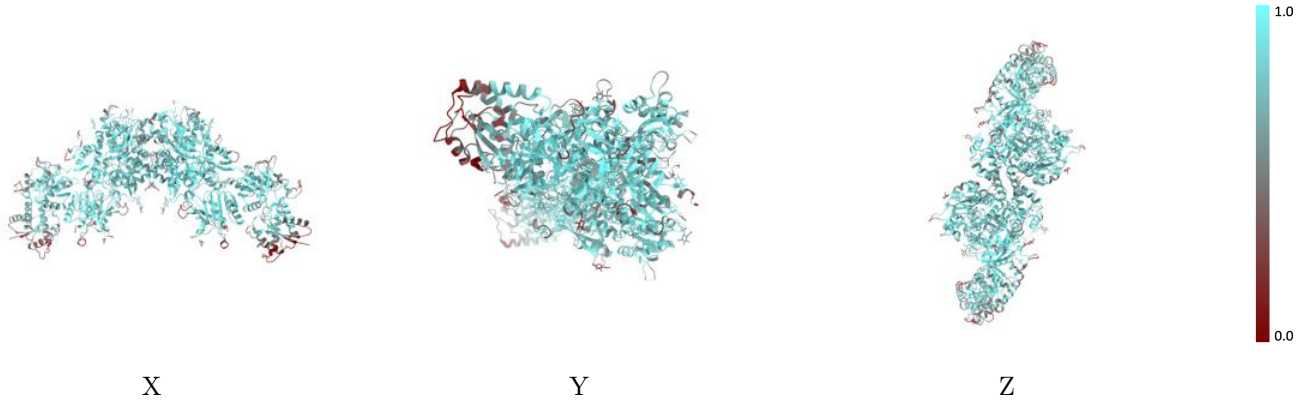
The images above show the 3D surface view of the map at the recommended contour level 0.0573 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model (i)



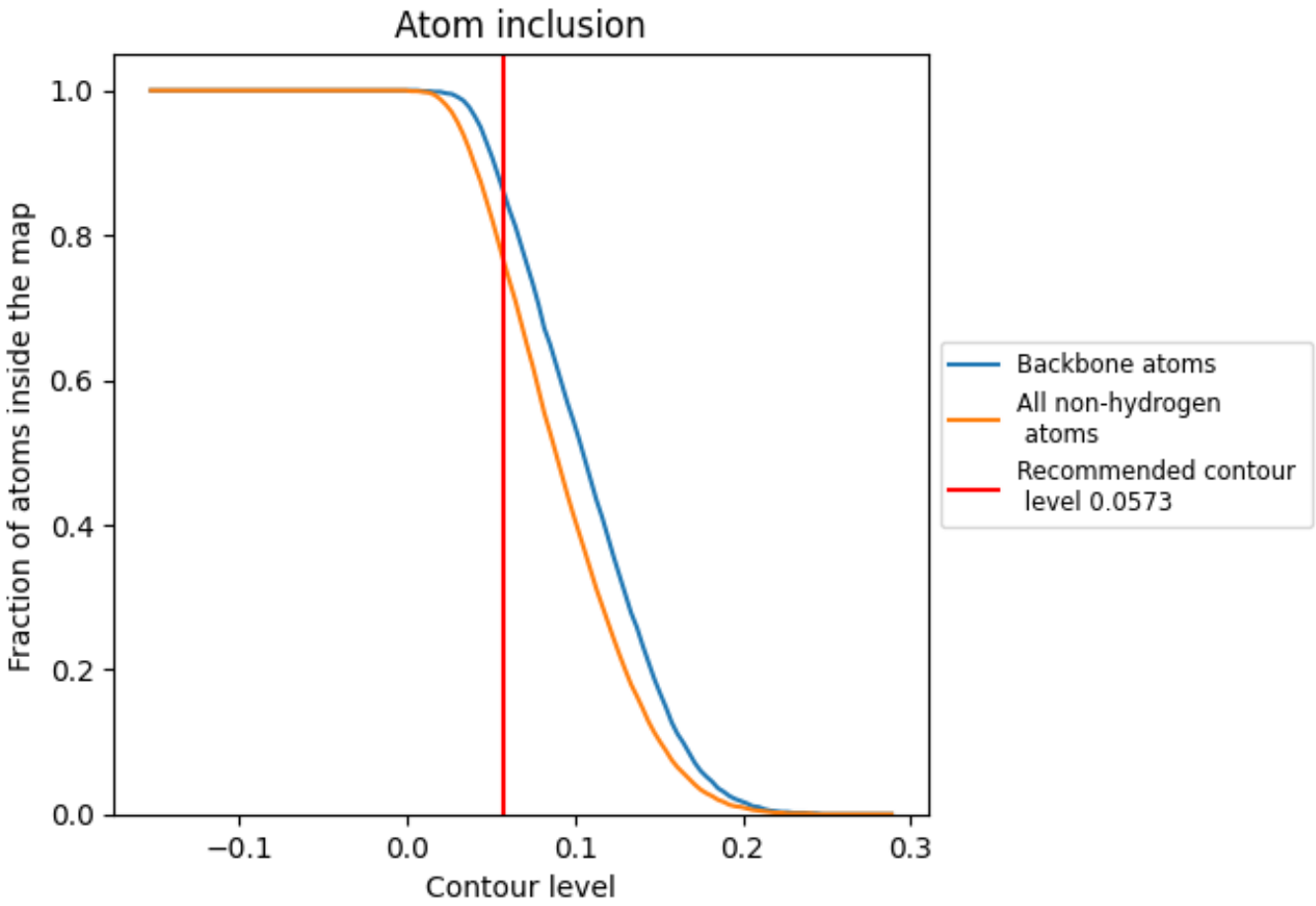
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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



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 (0.0573).

9.4 Atom inclusion (i)



At the recommended contour level, 86% of all backbone atoms, 77% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.0573) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7670	0.5250
A	0.7330	0.5110
B	0.7340	0.5110
C	0.8140	0.5460
D	0.8190	0.5480
E	0.6670	0.4850
F	0.6430	0.4960
G	0.6790	0.4650
H	0.6910	0.4920
I	0.6070	0.4990
J	0.6430	0.4550