



wwPDB X-ray Structure Validation Summary Report ⓘ

Apr 25, 2026 – 02:02 PM EDT

PDB ID : 5DYT / pdb_00005dyt
Title : Crystal structure of human butyrylcholinesterase in complex with N-((1-benzylpiperidin-3-yl)methyl)-N-methylnaphthalene-2-sulfonamide
Authors : Coquelle, N.; Brus, B.; Colletier, J.P.
Deposited on : 2015-09-25
Resolution : 2.55 Å(reported)

This is a wwPDB X-ray Structure 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/XrayValidationReportHelp>

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:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

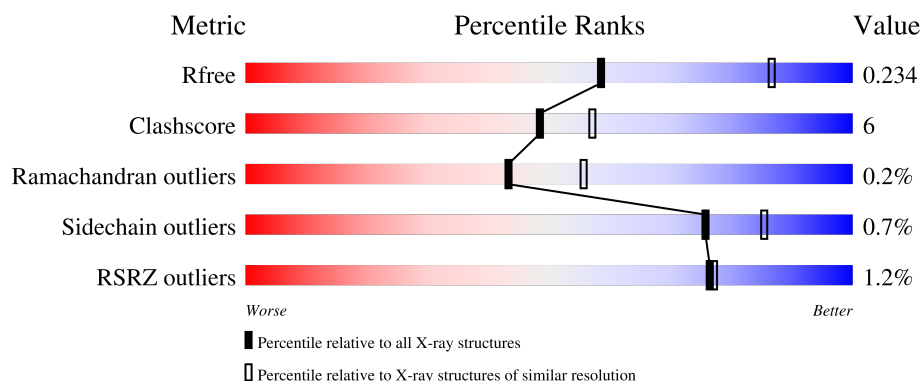
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

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.



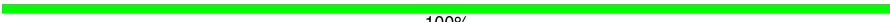
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1091 (2.54-2.54)
Clashscore	190562	1120 (2.54-2.54)
Ramachandran outliers	187476	1106 (2.54-2.54)
Sidechain outliers	187428	1106 (2.54-2.54)
RSRZ outliers	180081	1091 (2.54-2.54)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower 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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	530	87% 13%
1	B	530	84% 15%
2	C	3	33% 67%
2	E	3	100%
2	G	3	67% 33%

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Mol	Chain	Length	Quality of chain
3	D	2	 100%
3	F	2	 50% 50%
3	H	2	 100%
4	I	2	 50% 50%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	NAG	E	1	X	-	-	-
2	NAG	E	2	X	-	-	-
2	FUC	E	3	X	-	-	-
2	NAG	G	2	X	-	-	-
2	FUC	G	3	X	-	-	-
3	NAG	D	2	X	-	-	-
4	FUC	I	2	X	-	-	-
5	NAG	A	602	X	-	-	-
5	NAG	B	607	X	-	-	-
9	UNX	A	610	-	-	X	-

2 Entry composition [i](#)

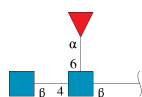
There are 12 unique types of molecules in this entry. The entry contains 9063 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, 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 Cholinesterase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	527	Total	C	N	O	S	0	3	0
			4210	2717	710	768	15			
1	B	525	Total	C	N	O	S	0	0	0
			4160	2688	697	760	15			

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	3	Total	C	N	O	0	0	0
			38	22	2	14			
2	E	3	Total	C	N	O	0	0	0
			38	22	2	14			
2	G	3	Total	C	N	O	0	0	0
			38	22	2	14			

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	D	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	F	2	Total	C	N	O	0	0	0
			28	16	2	10			

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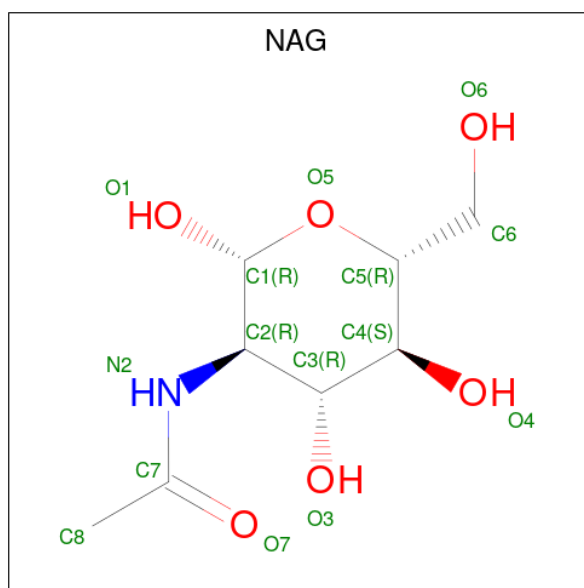
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	H	2	Total	C	N	O	0	0	0
			28	16	2	10			

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	I	2	Total	C	N	O	0	0	0
			24	14	1	9			

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



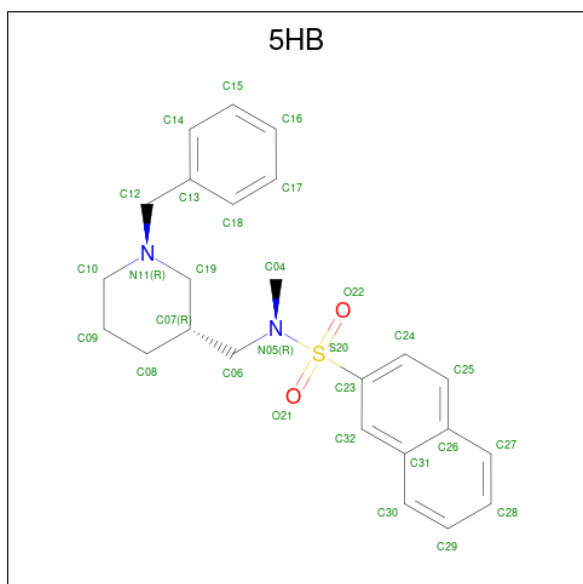
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	B	1	Total	C	N	O	0	0
			14	8	1	5		
5	B	1	Total	C	N	O	0	0
			14	8	1	5		

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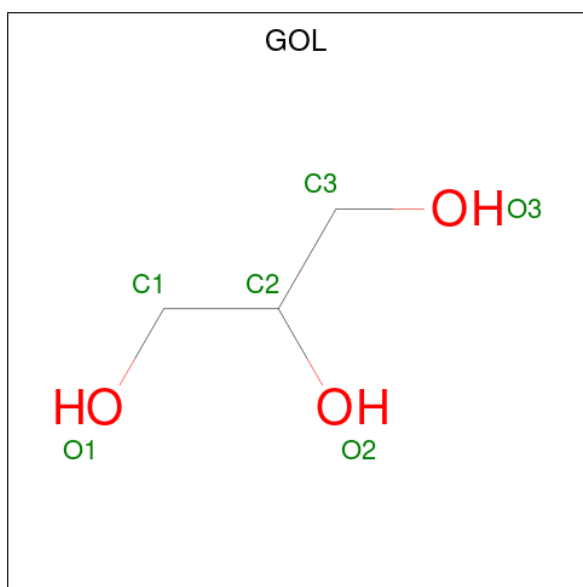
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	B	1	Total	C	N	O	0	0
			14	8	1	5		
5	B	1	Total	C	N	O	0	0
			14	8	1	5		
5	B	1	Total	C	N	O	0	0
			14	8	1	5		
5	B	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 6 is N-[[[(3R)-1-benzylpiperidin-3-yl]methyl]-N-methylnaphthalene-2-sulfonamide (CCD ID: 5HB) (formula: C₂₄H₂₈N₂O₂S).



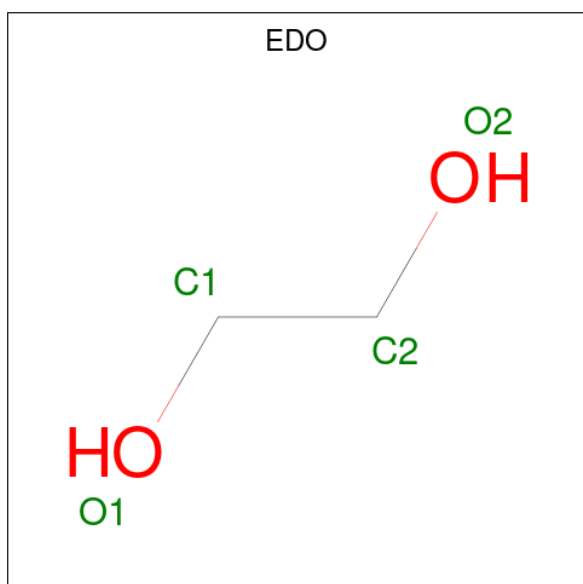
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	A	1	Total	C	N	O	S	0	0
			29	24	2	2	1		
6	B	1	Total	C	N	O	S	0	0
			29	24	2	2	1		

- Molecule 7 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			6	3	3		
7	A	1	Total	C	O	0	0
			6	3	3		
7	A	1	Total	C	O	0	0
			6	3	3		
7	B	1	Total	C	O	0	0
			6	3	3		
7	B	1	Total	C	O	0	0
			6	3	3		

- Molecule 8 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).

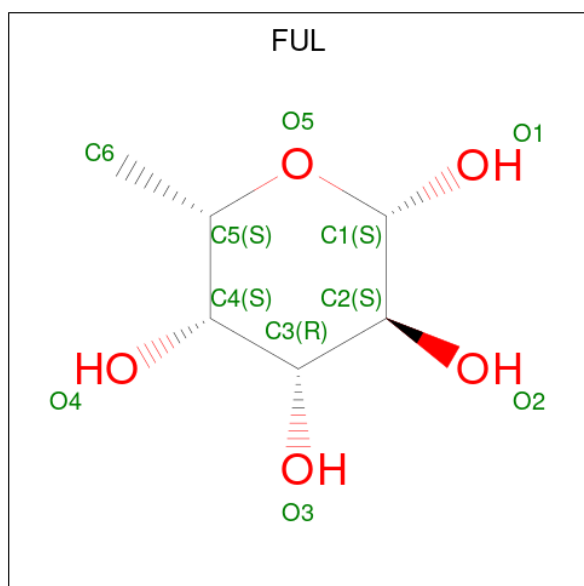


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	1	Total C O 4 2 2	0	0
8	B	1	Total C O 4 2 2	0	0
8	B	1	Total C O 4 2 2	0	0
8	B	1	Total C O 4 2 2	0	0

- Molecule 9 is UNKNOWN LIGAND (CCD ID: UNX) (formula: X).

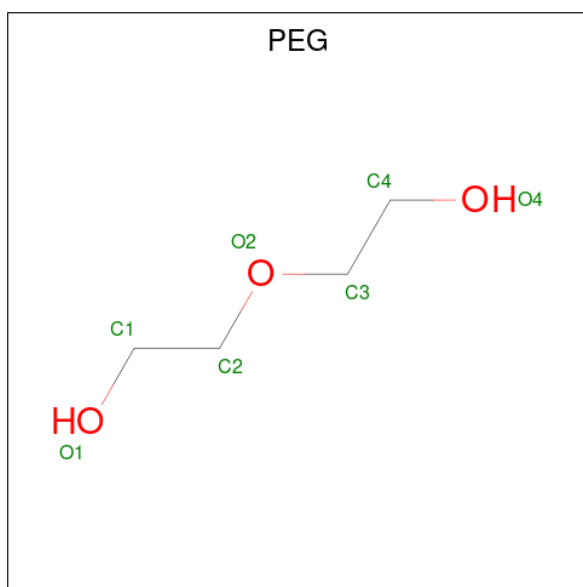
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	3	Total X 3 3	0	0
9	B	3	Total X 3 3	0	0

- Molecule 10 is beta-L-fucopyranose (CCD ID: FUL) (formula: C₆H₁₂O₅).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	B	1	Total C O 10 6 4	0	0

- Molecule 11 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: C₄H₁₀O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
11	B	1	Total	C	O	0	0
			7	4	3		

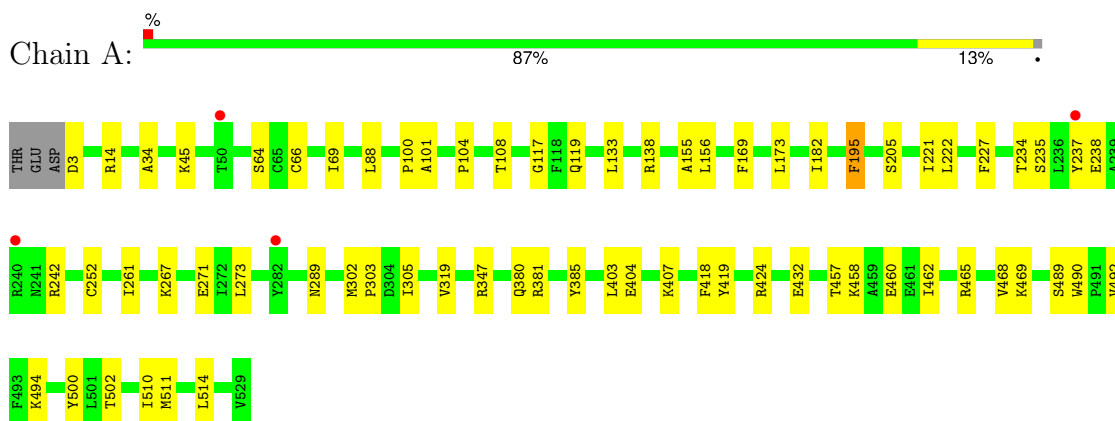
- Molecule 12 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	A	118	Total	O	0	0
			118	118		
12	B	114	Total	O	0	0
			114	114		

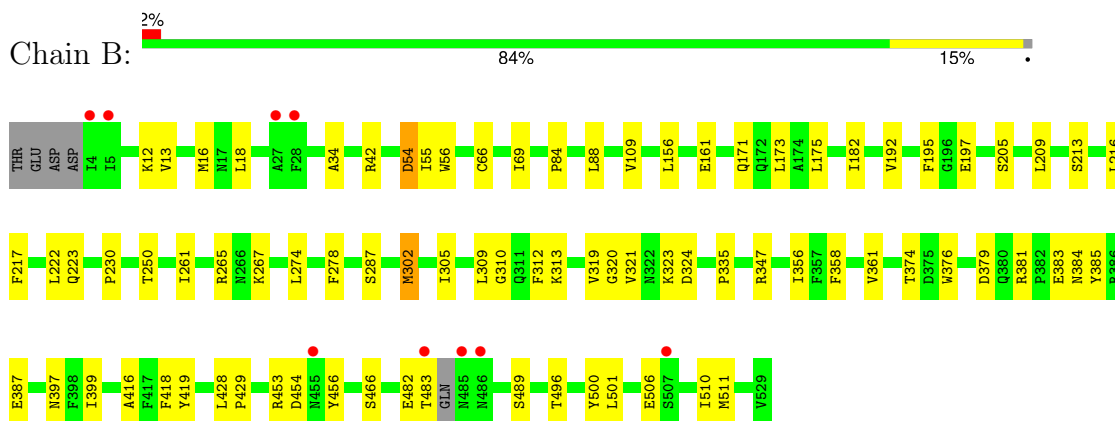
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron 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 dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). 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: Cholinesterase



- Molecule 1: Cholinesterase



- Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain E:  100%

MAG1
MAG2
FUC3

- Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain G:  67% 33%

MAG1
MAG2
FUC3

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

Chain D:  100%

MAG1
MAG2

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

Chain F:  50% 50%

MAG1
MAG2

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

Chain H:  100%

MAG1
MAG2

- Molecule 4: alpha-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain I:  50% 50%

MAG1
FUC2

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	76.47Å 80.23Å 231.28Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.12 – 2.55 46.12 – 2.55	Depositor EDS
% Data completeness (in resolution range)	99.6 (46.12-2.55) 99.6 (46.12-2.55)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.21 (at 2.54Å)	Xtriage
Refinement program	PHENIX (1.10_2155: ???)	Depositor
R, R_{free}	0.179 , 0.232 0.182 , 0.234	Depositor DCC
R_{free} test set	1415 reflections (2.99%)	wwPDB-VP
Wilson B-factor (Å ²)	56.5	Xtriage
Anisotropy	0.323	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 47.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.024 for k,h,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	9063	wwPDB-VP
Average B, all atoms (Å ²)	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.38% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

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: FUL, PEG, NAG, FUC, CSO, EDO, UNX, 5HB, GOL

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	0.37	0/4331	0.56	0/5879
1	B	0.36	0/4270	0.55	0/5796
All	All	0.37	0/8601	0.56	0/11675

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	A	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	155	ALA	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	4210	0	4103	41	1
1	B	4160	0	4034	52	1
2	C	38	0	34	0	0
2	E	38	0	34	0	0
2	G	38	0	34	0	0
3	D	28	0	25	0	0
3	F	28	0	25	1	0
3	H	28	0	24	0	0
4	I	24	0	22	0	0
5	A	28	0	26	0	0
5	B	84	0	78	1	0
6	A	29	0	0	0	0
6	B	29	0	0	0	0
7	A	18	0	24	0	0
7	B	12	0	16	1	0
8	A	4	0	6	0	0
8	B	12	0	18	0	0
9	A	3	0	0	2	0
9	B	3	0	0	1	0
10	B	10	0	10	1	0
11	B	7	0	10	2	0
12	A	118	0	0	5	0
12	B	114	0	0	2	0
All	All	9063	0	8523	96	1

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 96 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:217:PHE:O	1:B:313:LYS:NZ	2.06	0.89
1:B:12:LYS:HB2	1:B:55:ILE:HD12	1.62	0.82
1:B:109:VAL:HB	1:B:192:VAL:HG12	1.58	0.82
1:B:192:VAL:HG23	1:B:217:PHE:HA	1.62	0.81
9:A:608:UNX:UNK	9:A:610:UNX:UNK	1.26	0.77

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:237:TYR:OH	1:B:453:ARG:O[1_545]	2.12	0.08

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 X-ray entries followed by that with respect to entries of similar resolution.

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	527/530 (99%)	504 (96%)	23 (4%)	0	100	100
1	B	520/530 (98%)	495 (95%)	23 (4%)	2 (0%)	30	39
All	All	1047/1060 (99%)	999 (95%)	46 (4%)	2 (0%)	43	56

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	54	ASP
1	B	506	GLU

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 X-ray entries followed by that with respect to entries of similar resolution.

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	451/454 (99%)	449 (100%)	2 (0%)	84	90
1	B	442/454 (97%)	438 (99%)	4 (1%)	70	82
All	All	893/908 (98%)	887 (99%)	6 (1%)	76	85

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

Mol	Chain	Res	Type
1	B	302	MET
1	B	466	SER
1	B	496	THR
1	A	195	PHE
1	A	108	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 10 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	214	HIS
1	B	397	ASN
1	B	479	ASN
1	A	517	GLN
1	B	10	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues 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	$\# Z > 2$
1	CSO	A	66	1	3,6,7	0.46	0	1,6,8	0.60	0
1	CSO	B	66	1	3,6,7	0.61	0	1,6,8	0.43	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
1	CSO	A	66	1	-	0/1/5/7	-
1	CSO	B	66	1	-	0/1/5/7	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	66	CSO	1	0
1	B	66	CSO	1	0

5.5 Carbohydrates [i](#)

17 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	C	1	2,1	14,14,15	0.27	0	17,19,21	0.50	0
2	NAG	C	2	2	14,14,15	0.74	1 (7%)	17,19,21	0.85	1 (5%)
2	FUC	C	3	2	10,10,11	1.88	3 (30%)	14,14,16	0.56	0
3	NAG	D	1	3,1	14,14,15	0.52	0	17,19,21	0.82	0
3	NAG	D	2	3	14,14,15	0.73	0	17,19,21	0.56	0
2	NAG	E	1	2,1	14,14,15	0.28	0	17,19,21	0.97	1 (5%)
2	NAG	E	2	2	14,14,15	0.73	1 (7%)	17,19,21	0.86	1 (5%)
2	FUC	E	3	2	10,10,11	1.84	3 (30%)	14,14,16	1.54	4 (28%)
3	NAG	F	1	3,1	14,14,15	0.27	0	17,19,21	0.67	1 (5%)
3	NAG	F	2	3	14,14,15	0.84	1 (7%)	17,19,21	0.90	1 (5%)
2	NAG	G	1	2,1	14,14,15	0.54	0	17,19,21	0.44	0
2	NAG	G	2	2	14,14,15	0.30	0	17,19,21	0.38	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	FUC	G	3	2	10,10,11	1.80	3 (30%)	14,14,16	1.02	1 (7%)
3	NAG	H	1	3,1	14,14,15	0.46	0	17,19,21	0.64	0
3	NAG	H	2	3	14,14,15	0.26	0	17,19,21	0.50	0
4	NAG	I	1	4,1	14,14,15	0.41	0	17,19,21	0.68	0
4	FUC	I	2	4	10,10,11	1.70	3 (30%)	14,14,16	1.01	1 (7%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	C	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	C	2	2	-	1/6/23/26	0/1/1/1
2	FUC	C	3	2	-	-	0/1/1/1
3	NAG	D	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	D	2	3	1/1/5/7	4/6/23/26	0/1/1/1
2	NAG	E	1	2,1	1/1/5/7	4/6/23/26	0/1/1/1
2	NAG	E	2	2	1/1/5/7	3/6/23/26	0/1/1/1
2	FUC	E	3	2	1/1/4/5	-	0/1/1/1
3	NAG	F	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	F	2	3	-	2/6/23/26	0/1/1/1
2	NAG	G	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	G	2	2	1/1/5/7	2/6/23/26	0/1/1/1
2	FUC	G	3	2	1/1/4/5	-	0/1/1/1
3	NAG	H	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	H	2	3	-	2/6/23/26	0/1/1/1
4	NAG	I	1	4,1	-	1/6/23/26	0/1/1/1
4	FUC	I	2	4	1/1/4/5	-	0/1/1/1

The worst 5 of 15 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	3	FUC	O5-C1	-3.22	1.38	1.43
2	C	3	FUC	O5-C1	-3.04	1.38	1.43
4	I	2	FUC	O5-C1	-2.97	1.38	1.43
2	G	3	FUC	O5-C1	-2.94	1.38	1.43
3	F	2	NAG	O5-C1	2.84	1.48	1.43

The worst 5 of 11 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
2	E	2	NAG	C1-O5-C5	3.15	116.41	112.19
2	C	2	NAG	C1-O5-C5	3.06	116.29	112.19
3	F	2	NAG	C1-O5-C5	3.06	116.28	112.19
2	E	3	FUC	C3-C4-C5	2.78	114.04	109.81
2	E	1	NAG	C1-O5-C5	2.66	115.75	112.19

5 of 7 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	E	1	NAG	C1
2	E	2	NAG	C1
2	E	3	FUC	C1
2	G	2	NAG	C1
2	G	3	FUC	C1

5 of 27 torsion outliers are listed below:

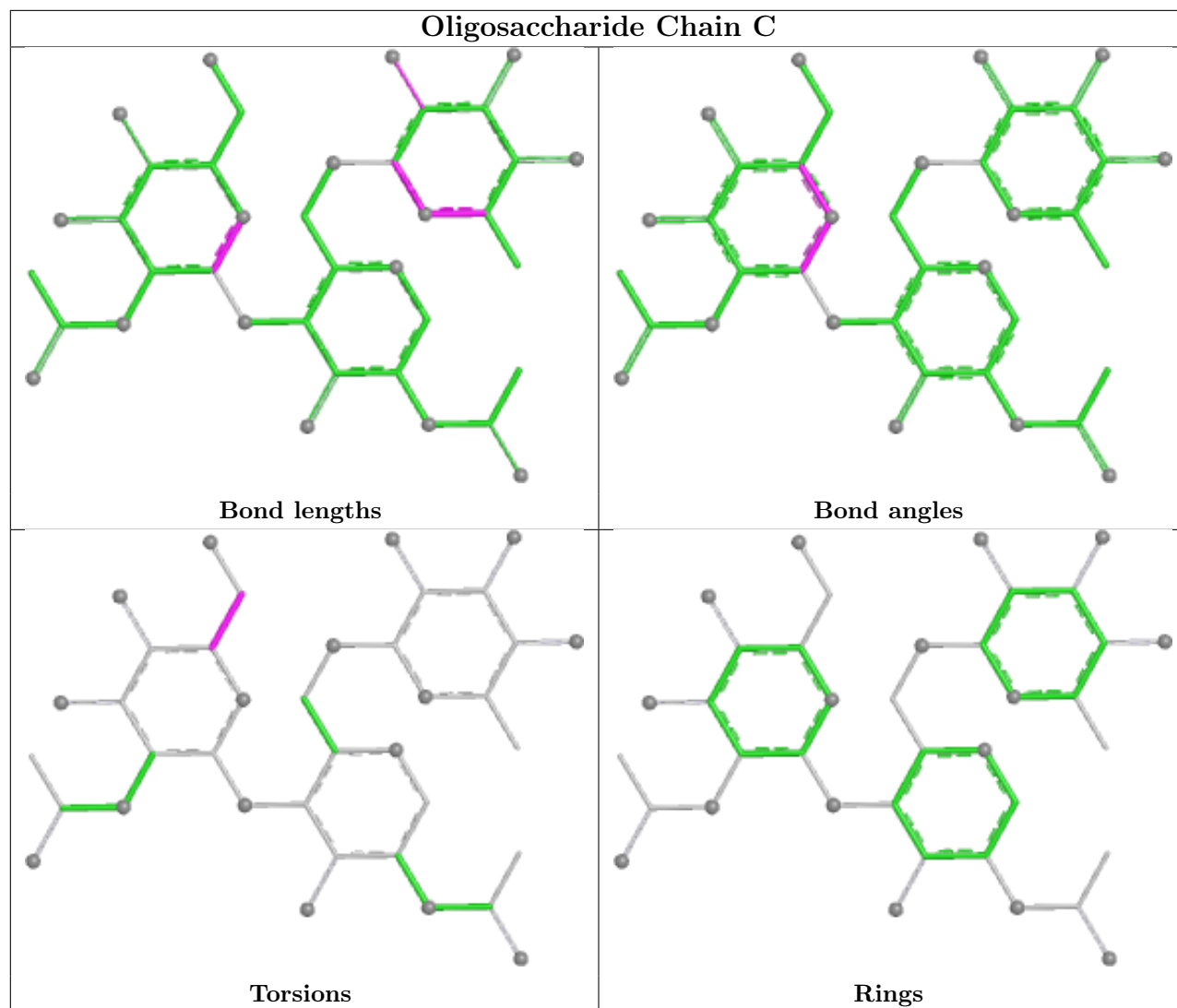
Mol	Chain	Res	Type	Atoms
2	E	2	NAG	C4-C5-C6-O6
2	E	1	NAG	O5-C5-C6-O6
2	G	1	NAG	O5-C5-C6-O6
3	H	1	NAG	C4-C5-C6-O6
2	E	2	NAG	O5-C5-C6-O6

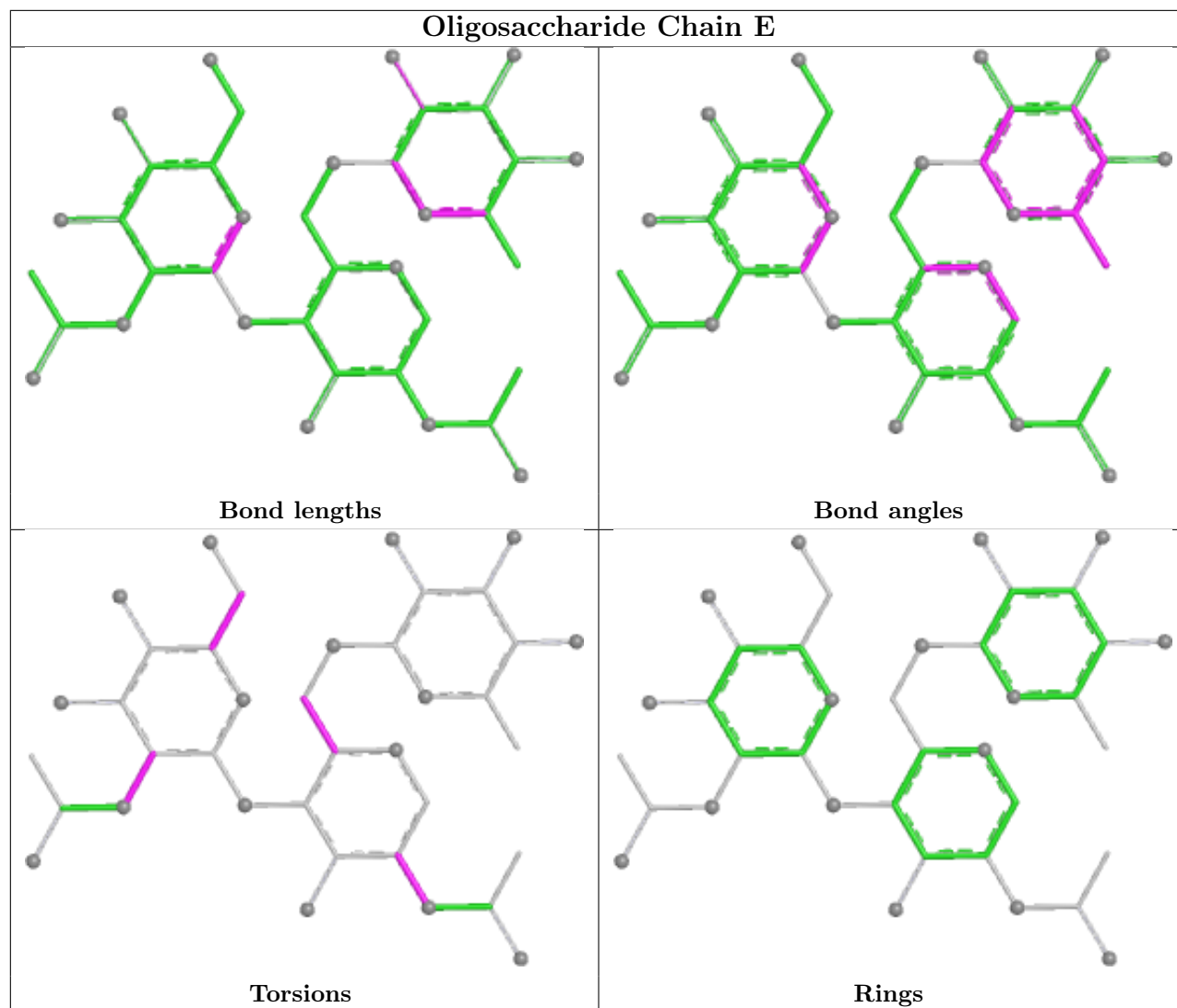
There are no ring outliers.

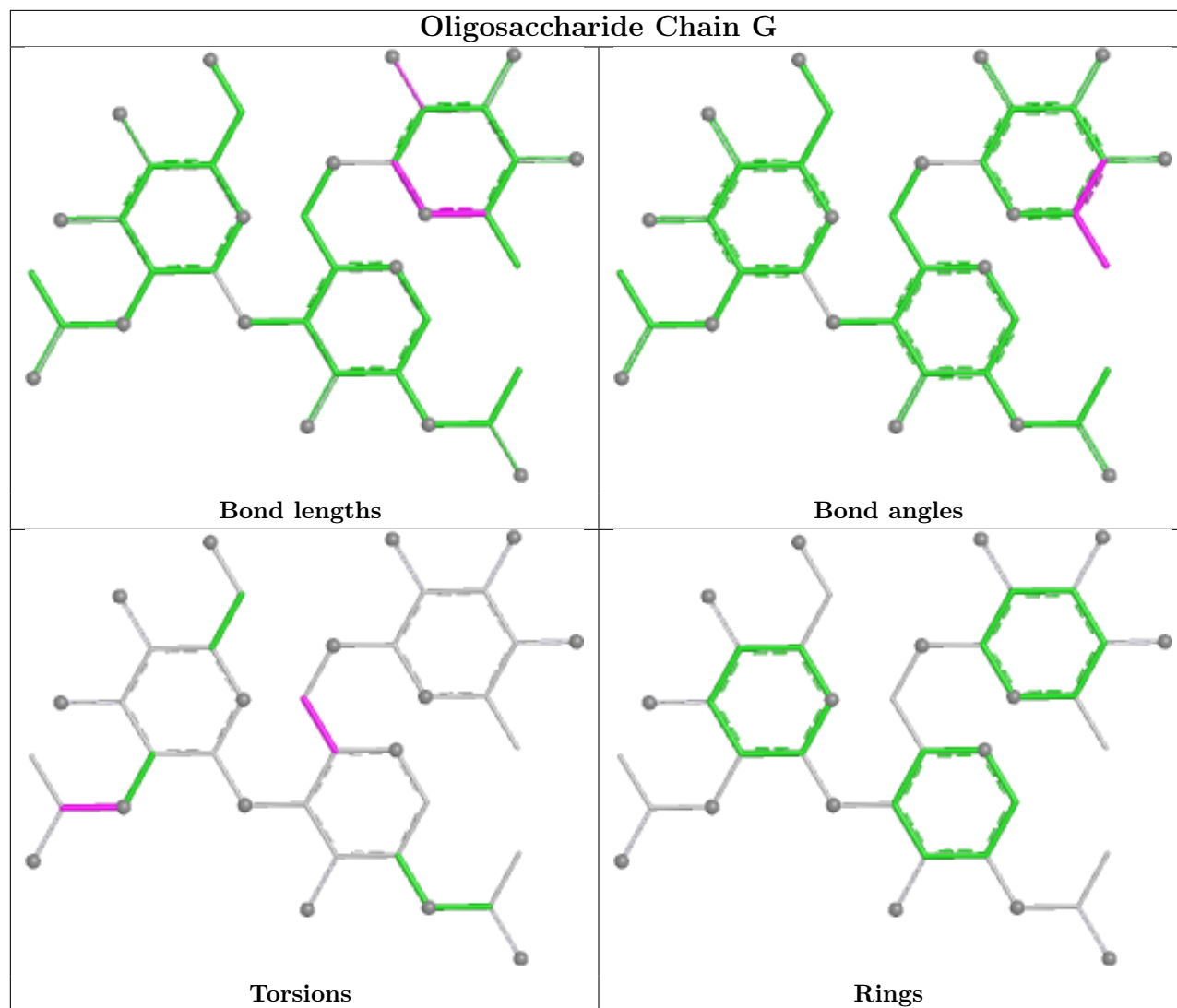
1 monomer is involved in 1 short contact:

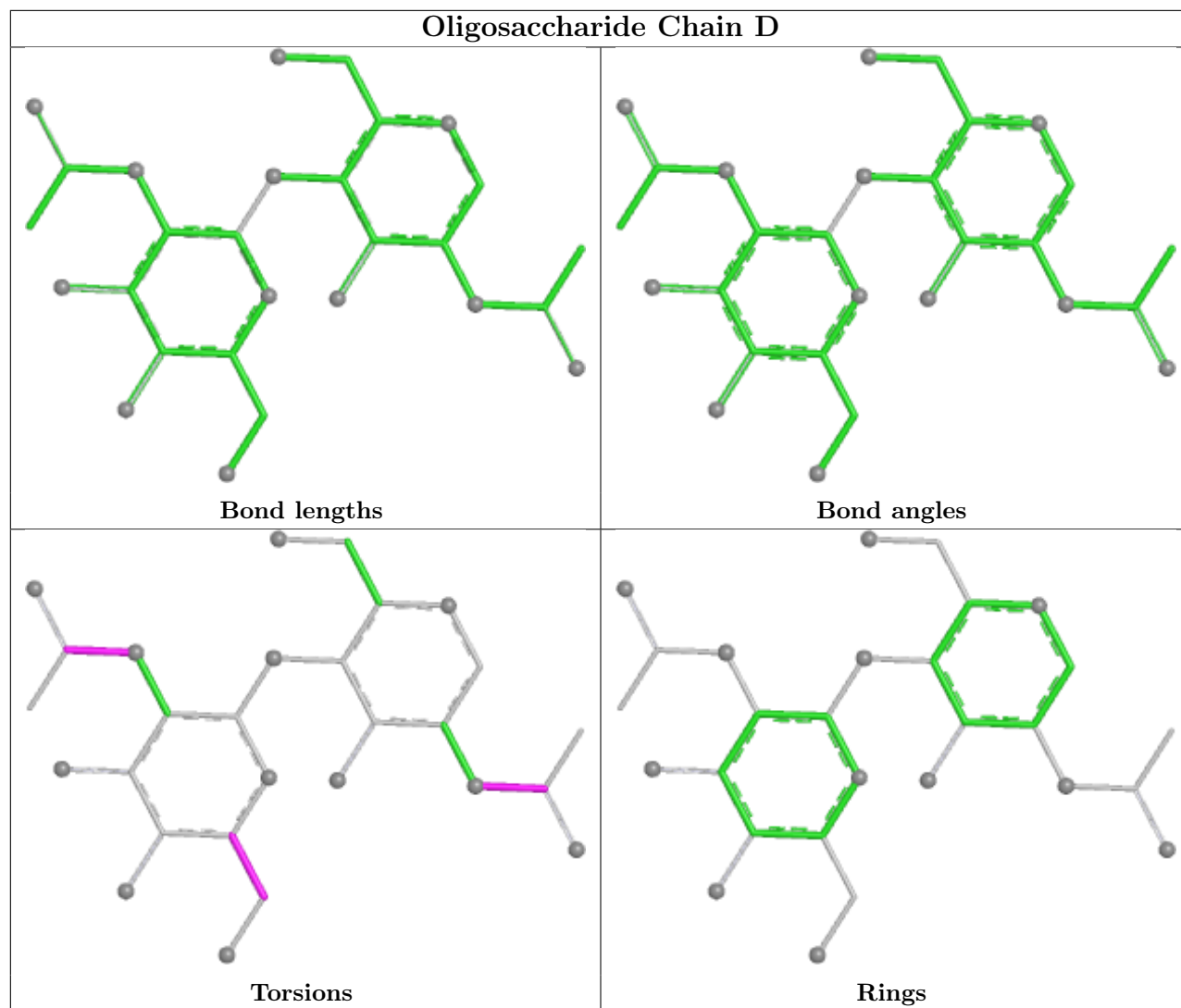
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	F	2	NAG	1	0

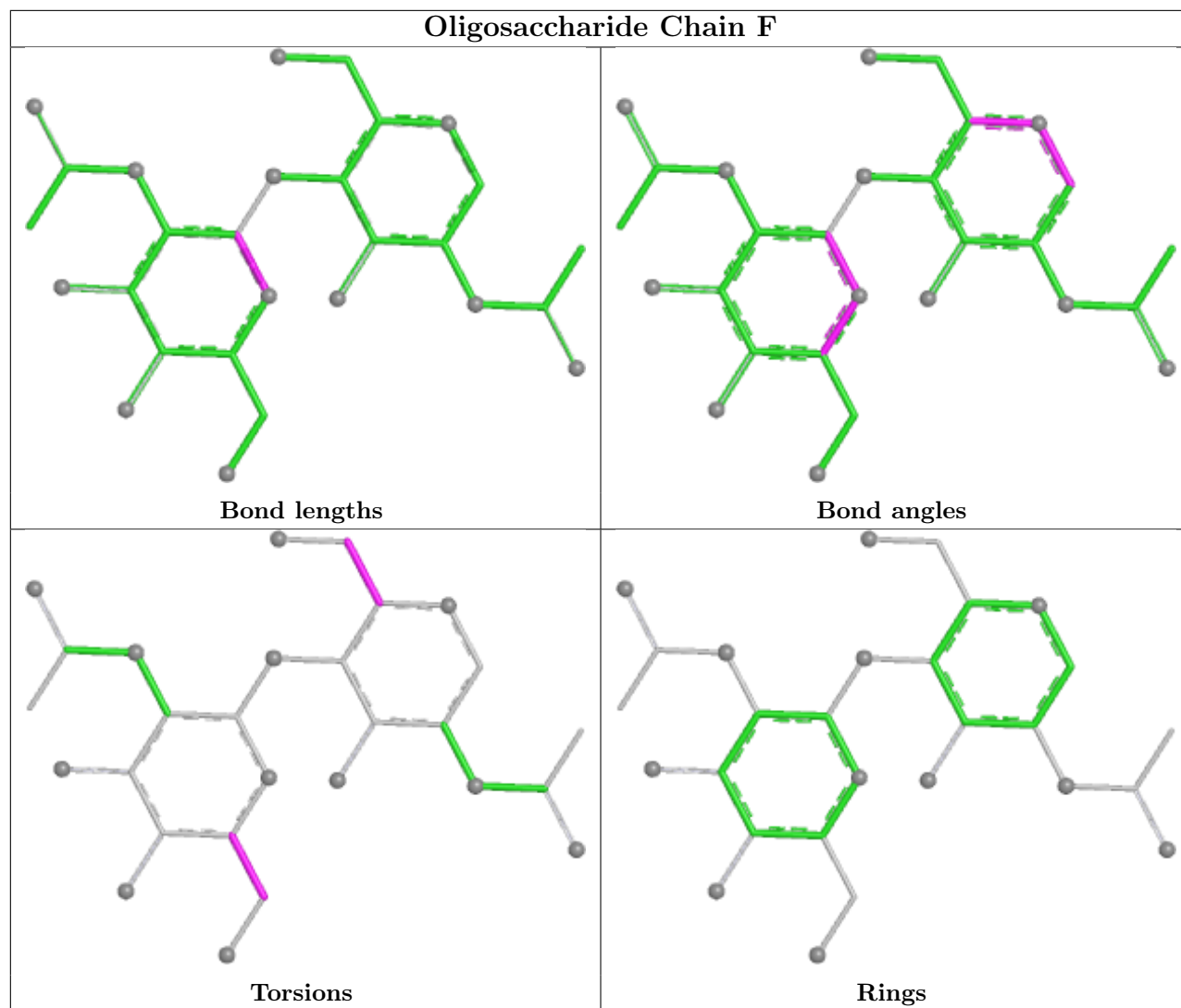
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

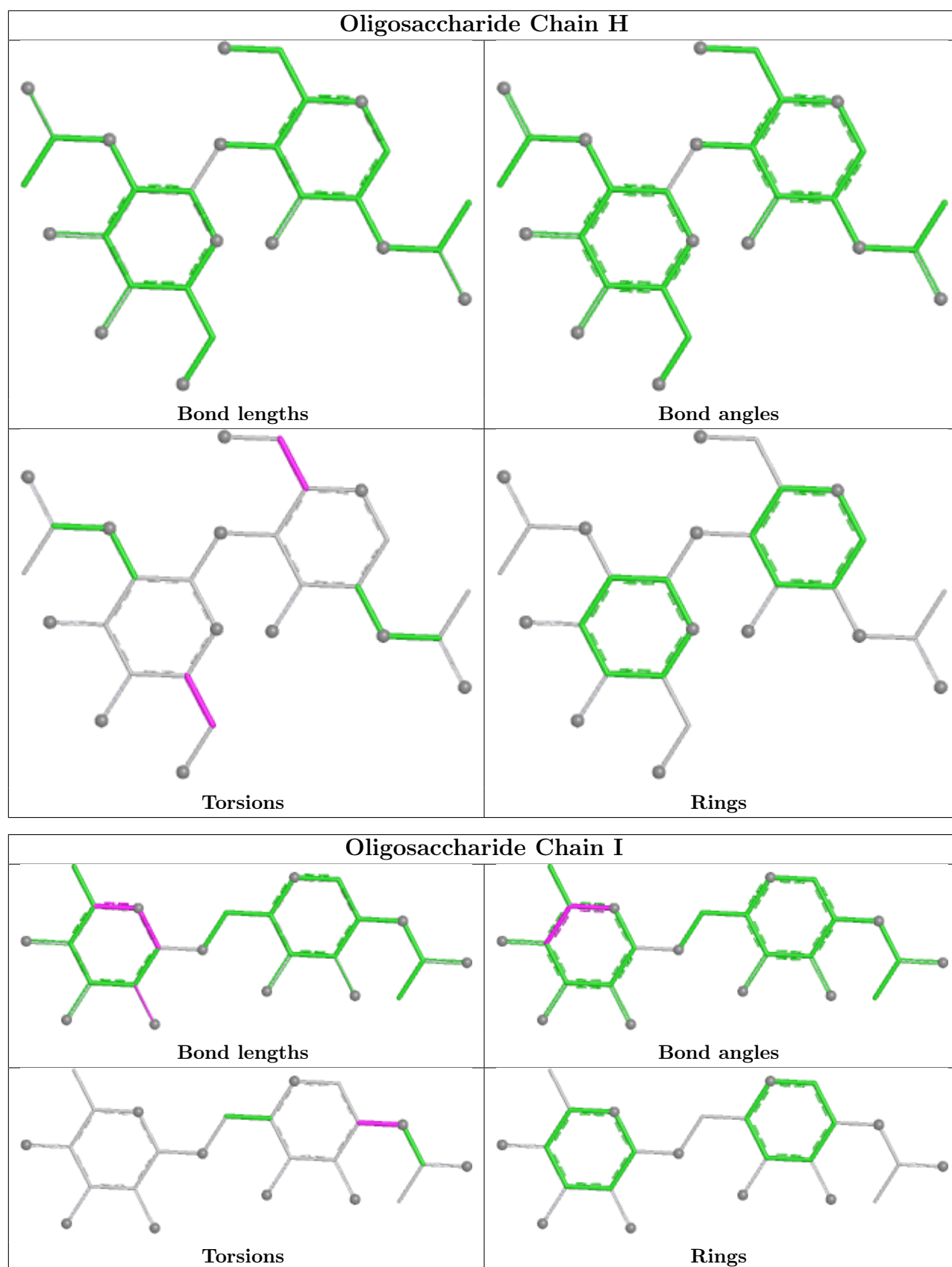












5.6 Ligand geometry

Of 27 ligands modelled in this entry, 6 are unknown - leaving 21 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
8	EDO	B	613	-	3,3,3	1.30	0	2,2,2	1.33	0
5	NAG	B	607	1	14,14,15	0.50	0	17,19,21	1.04	1 (5%)
6	5HB	B	608	-	31,32,32	2.94	4 (12%)	41,45,45	1.77	4 (9%)
6	5HB	A	603	-	31,32,32	2.96	3 (9%)	41,45,45	1.64	4 (9%)
7	GOL	A	606	-	5,5,5	0.47	0	5,5,5	0.22	0
5	NAG	B	602	1	14,14,15	0.47	0	17,19,21	0.46	0
5	NAG	B	603	1	14,14,15	0.44	0	17,19,21	1.50	3 (17%)
7	GOL	A	605	-	5,5,5	0.54	0	5,5,5	0.54	0
7	GOL	B	610	-	5,5,5	0.42	0	5,5,5	0.73	0
8	EDO	B	611	-	3,3,3	0.58	0	2,2,2	0.01	0
5	NAG	A	602	1	14,14,15	0.51	0	17,19,21	1.07	1 (5%)
8	EDO	A	607	-	3,3,3	0.62	0	2,2,2	0.36	0
5	NAG	A	601	1	14,14,15	0.66	0	17,19,21	0.48	0
7	GOL	A	604	-	5,5,5	0.34	0	5,5,5	0.45	0
8	EDO	B	612	-	3,3,3	1.72	1 (33%)	2,2,2	1.53	0
7	GOL	B	609	-	5,5,5	0.37	0	5,5,5	0.29	0
5	NAG	B	601	1	14,14,15	0.93	2 (14%)	17,19,21	1.12	1 (5%)
5	NAG	B	606	1	14,14,15	0.50	0	17,19,21	0.64	1 (5%)
10	FUL	B	604	-	10,10,11	1.74	3 (30%)	14,14,16	1.69	2 (14%)
11	PEG	B	617	-	6,6,6	0.48	0	5,5,5	0.89	0
5	NAG	B	605	1	14,14,15	0.44	0	17,19,21	0.80	1 (5%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	EDO	B	613	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	B	607	1	1/1/5/7	2/6/23/26	0/1/1/1
6	5HB	B	608	-	-	14/20/30/30	0/4/4/4
6	5HB	A	603	-	-	10/20/30/30	0/4/4/4
7	GOL	A	606	-	-	2/4/4/4	-
5	NAG	B	602	1	-	4/6/23/26	0/1/1/1
5	NAG	B	603	1	-	2/6/23/26	0/1/1/1
7	GOL	A	605	-	-	4/4/4/4	-
7	GOL	B	610	-	-	2/4/4/4	-
8	EDO	B	611	-	-	0/1/1/1	-
5	NAG	A	602	1	1/1/5/7	4/6/23/26	0/1/1/1
8	EDO	A	607	-	-	1/1/1/1	-
5	NAG	A	601	1	-	2/6/23/26	0/1/1/1
7	GOL	A	604	-	-	0/4/4/4	-
8	EDO	B	612	-	-	0/1/1/1	-
7	GOL	B	609	-	-	0/4/4/4	-
5	NAG	B	601	1	-	3/6/23/26	0/1/1/1
5	NAG	B	606	1	-	2/6/23/26	0/1/1/1
10	FUL	B	604	-	-	-	0/1/1/1
11	PEG	B	617	-	-	1/4/4/4	-
5	NAG	B	605	1	-	2/6/23/26	0/1/1/1

The worst 5 of 13 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	603	5HB	O22-S20	10.38	1.54	1.43
6	B	608	5HB	O21-S20	9.79	1.54	1.43
6	A	603	5HB	O21-S20	9.79	1.54	1.43
6	B	608	5HB	O22-S20	9.57	1.53	1.43
6	A	603	5HB	C12-C13	-6.93	1.38	1.51

The worst 5 of 18 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	608	5HB	O21-S20-N05	6.63	114.94	107.02
6	A	603	5HB	O21-S20-N05	6.10	114.30	107.02
6	B	608	5HB	O22-S20-O21	-5.80	110.54	119.59
6	A	603	5HB	O22-S20-O21	-4.94	111.89	119.59
10	B	604	FUL	C1-C2-C3	4.54	116.26	109.64

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	A	602	NAG	C1
5	B	607	NAG	C1

5 of 55 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	603	NAG	C1-C2-N2-C7
6	A	603	5HB	C07-C06-N05-S20
6	A	603	5HB	C04-N05-S20-C23
6	A	603	5HB	N05-C06-C07-C19
6	B	608	5HB	C07-C06-N05-C04

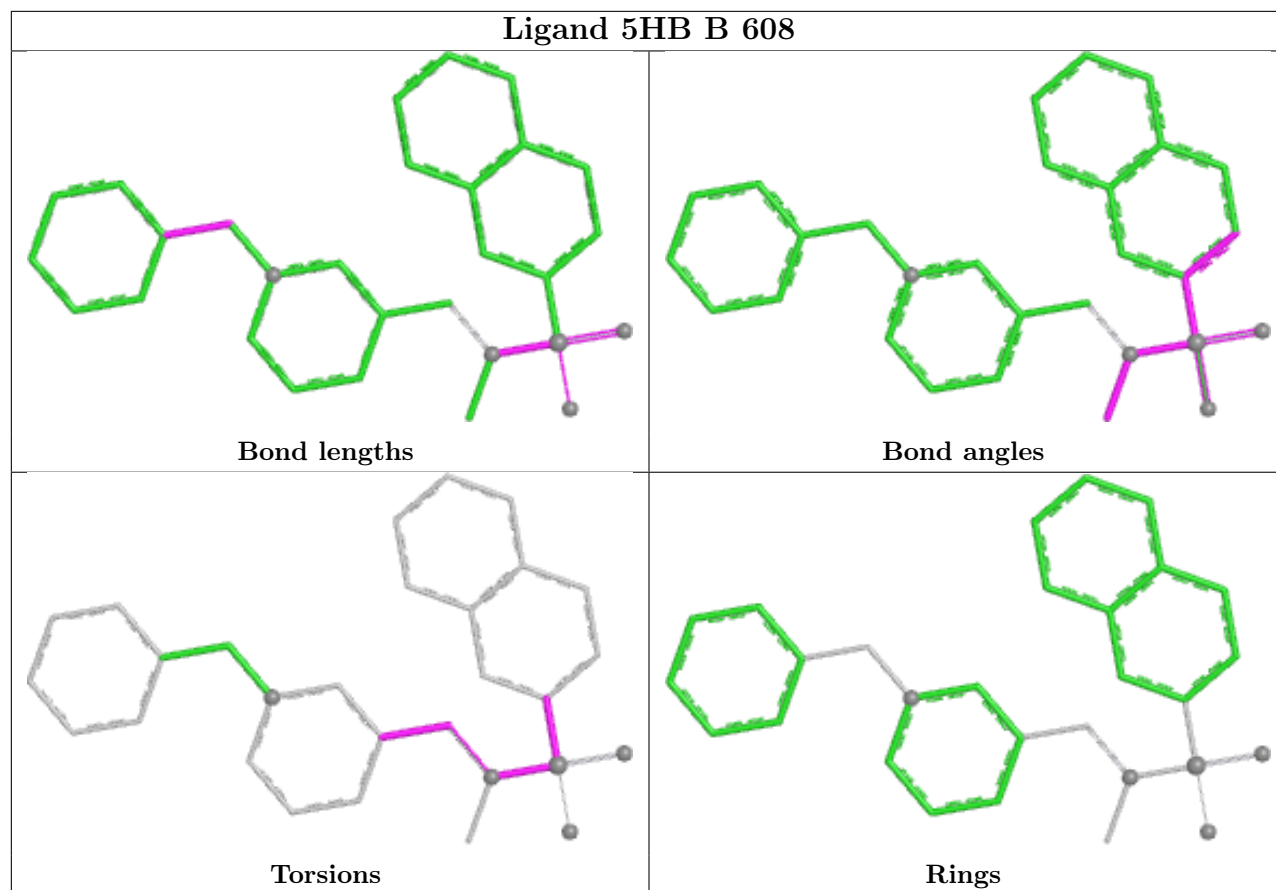
There are no ring outliers.

4 monomers are involved in 5 short contacts:

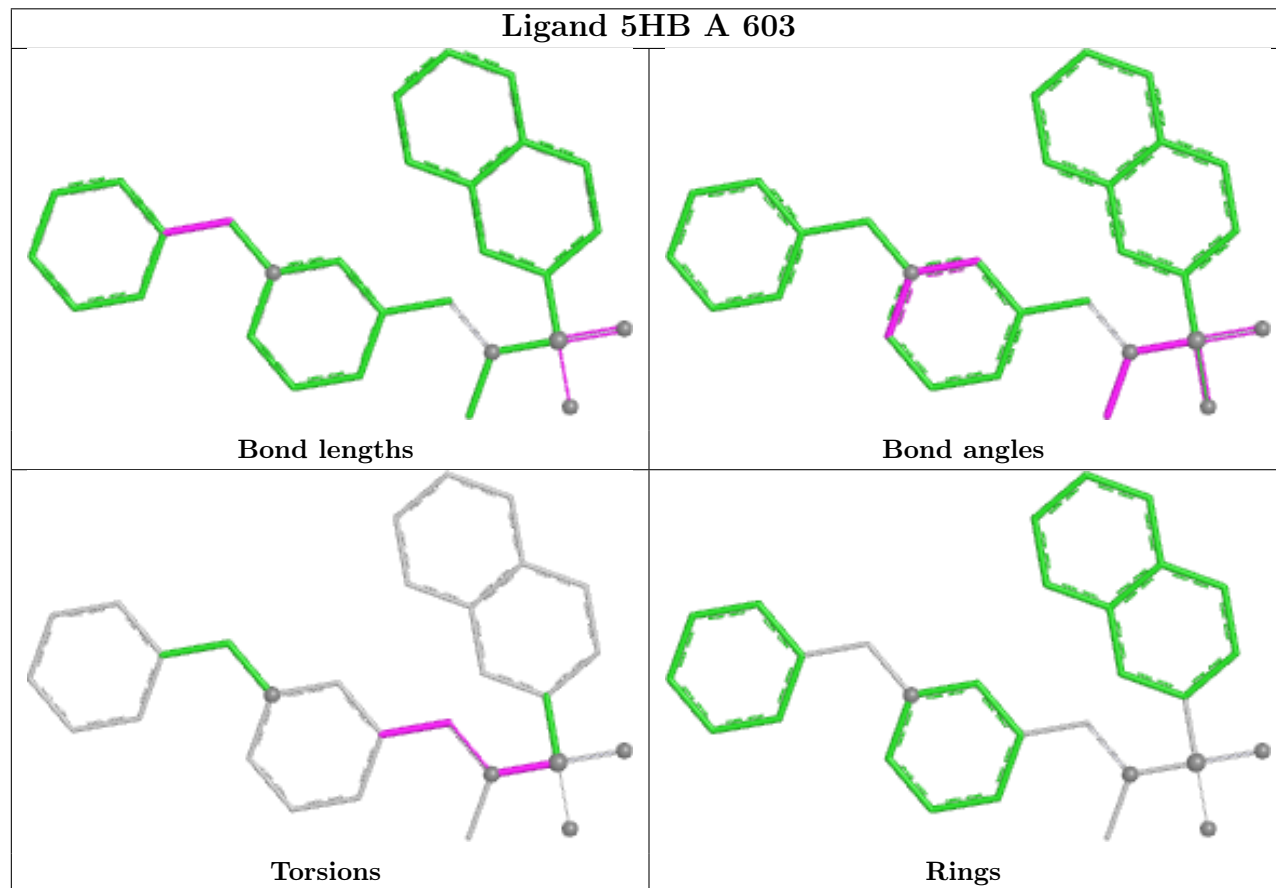
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	B	610	GOL	1	0
5	B	606	NAG	1	0
10	B	604	FUL	1	0
11	B	617	PEG	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 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 5HB B 608



Ligand 5HB A 603



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 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	526/530 (99%)	-0.33	4 (0%) 82 84	24, 50, 82, 133	3 (0%)
1	B	524/530 (98%)	-0.16	9 (1%) 69 69	32, 53, 93, 149	1 (0%)
All	All	1050/1060 (99%)	-0.25	13 (1%) 76 77	24, 52, 88, 149	4 (0%)

The worst 5 of 13 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	4	ILE	4.2
1	B	485	ASN	4.1
1	B	486	ASN	4.0
1	B	507	SER	3.2
1	B	483	THR	2.7

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q < 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
1	CSO	B	66	7/8	0.95	0.09	36,38,56,57	0
1	CSO	A	66	7/8	0.99	0.04	43,46,56,57	0

6.3 Carbohydrates [i](#)

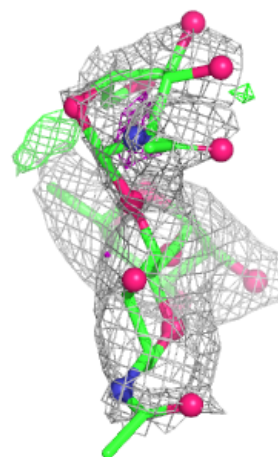
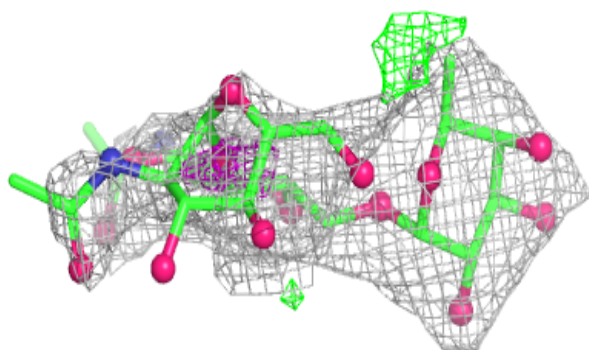
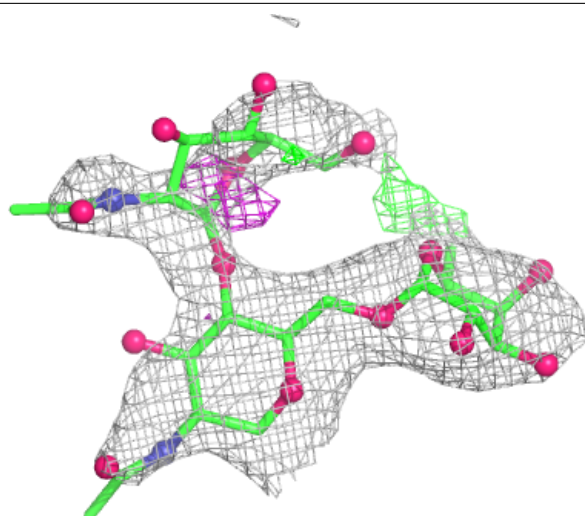
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q < 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	NAG	G	2	14/15	0.19	0.15	127,131,133,133	0
4	FUC	I	2	10/11	0.47	0.17	129,131,133,133	0
2	NAG	E	1	14/15	0.49	0.13	106,116,118,124	0
2	NAG	C	2	14/15	0.50	0.15	117,119,123,124	0
4	NAG	I	1	14/15	0.55	0.17	100,108,119,126	0
2	FUC	C	3	10/11	0.55	0.12	103,108,111,113	0
2	FUC	G	3	10/11	0.57	0.18	114,117,119,120	0
2	NAG	G	1	14/15	0.58	0.12	102,113,116,122	0
2	NAG	E	2	14/15	0.59	0.15	126,129,137,139	0
3	NAG	H	2	14/15	0.62	0.14	105,114,119,121	0
3	NAG	F	2	14/15	0.69	0.16	73,83,90,93	0
2	NAG	C	1	14/15	0.70	0.13	95,101,106,112	0
3	NAG	D	2	14/15	0.70	0.14	100,106,115,115	0
3	NAG	H	1	14/15	0.79	0.13	86,96,108,111	0
3	NAG	F	1	14/15	0.83	0.12	65,73,78,78	0
2	FUC	E	3	10/11	0.84	0.13	111,114,115,116	0
3	NAG	D	1	14/15	0.88	0.09	68,76,83,92	0

The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

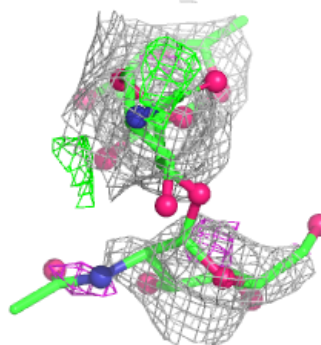
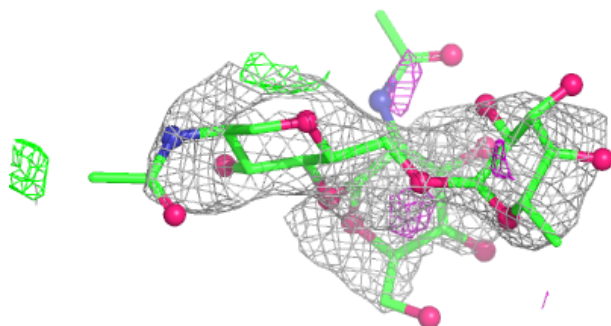
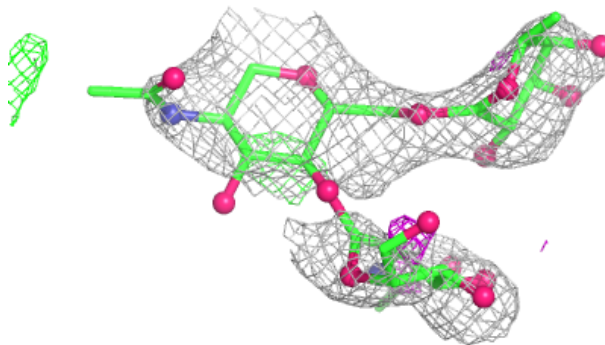
Electron density around Chain C:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



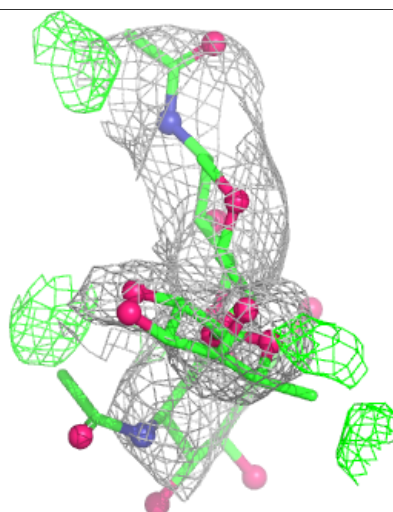
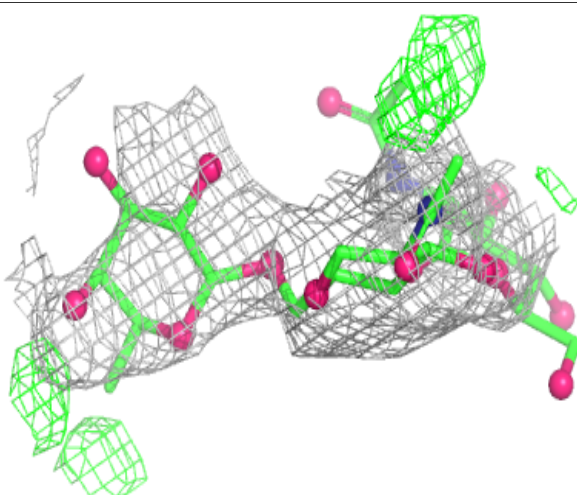
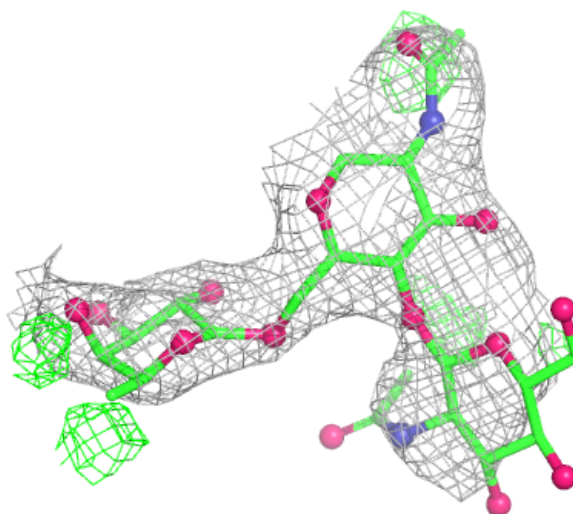
Electron density around Chain E:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



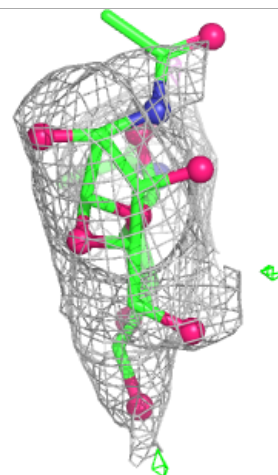
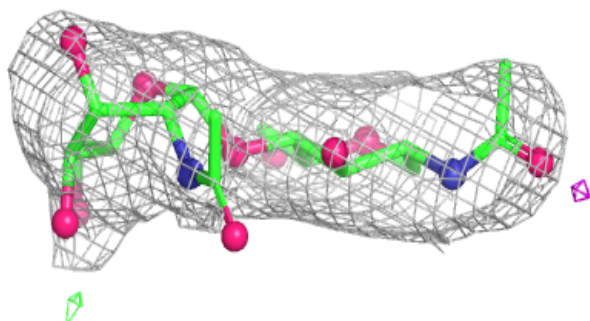
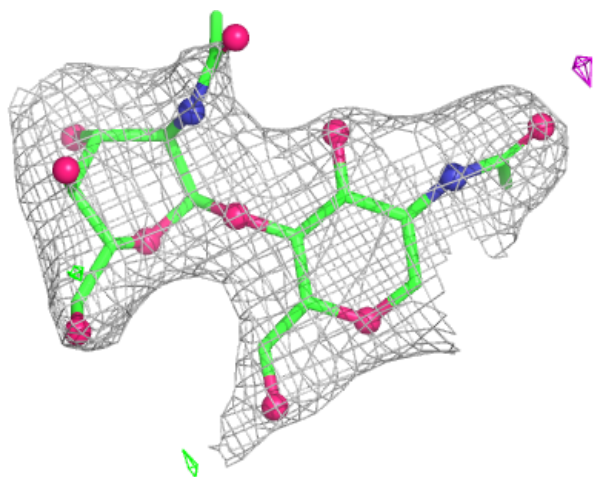
Electron density around Chain G:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



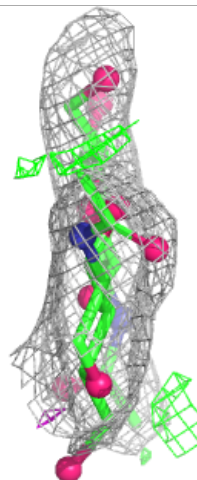
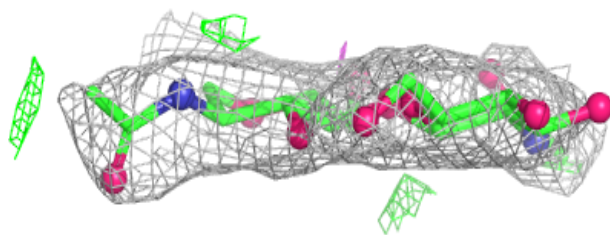
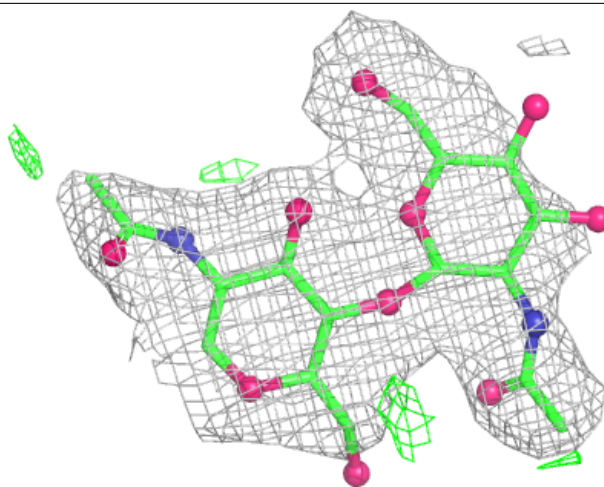
Electron density around Chain D:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



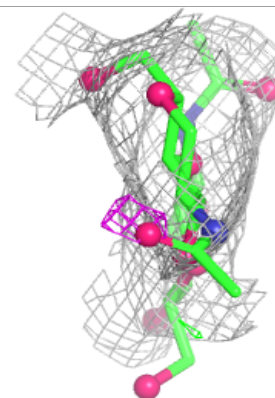
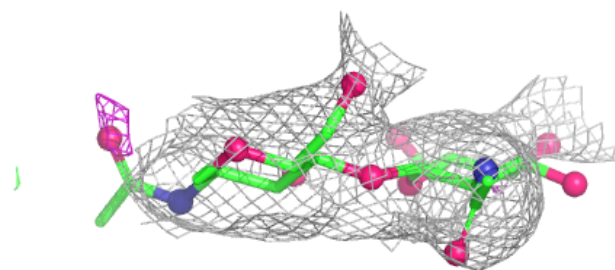
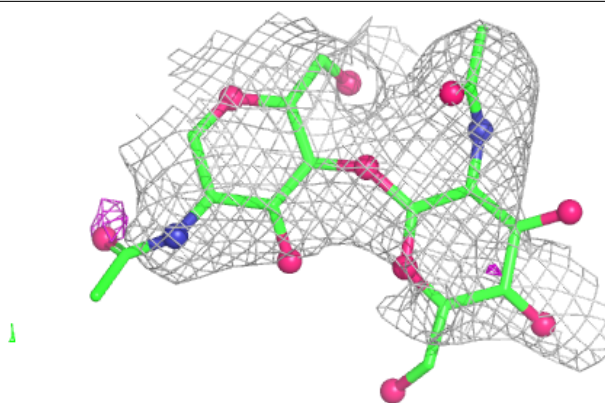
Electron density around Chain F:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

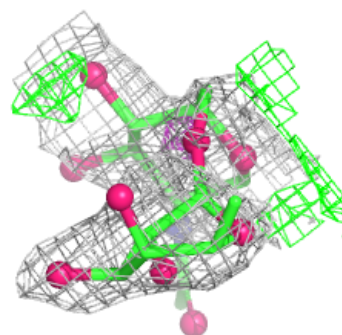
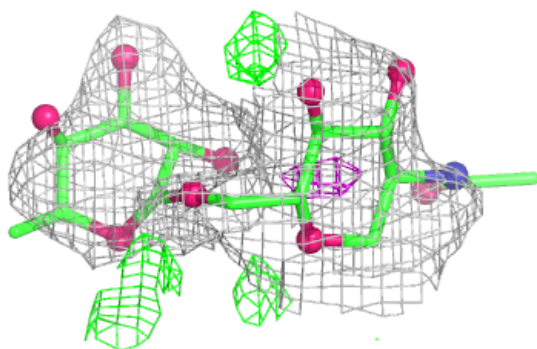
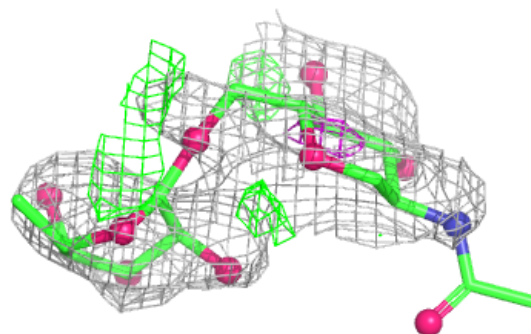


Electron density around Chain H:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around Chain I:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.4 Ligands

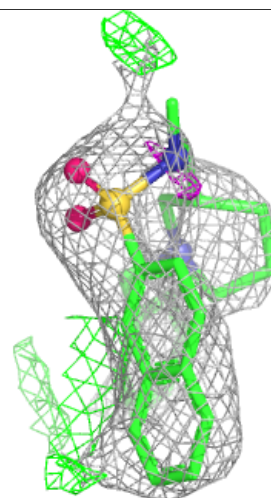
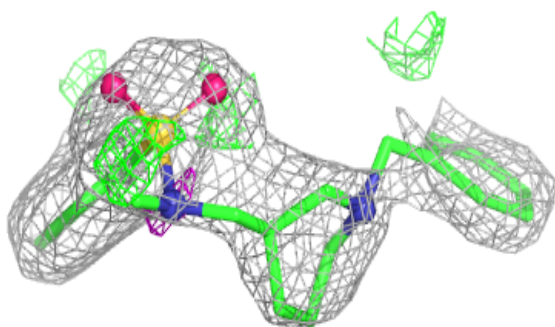
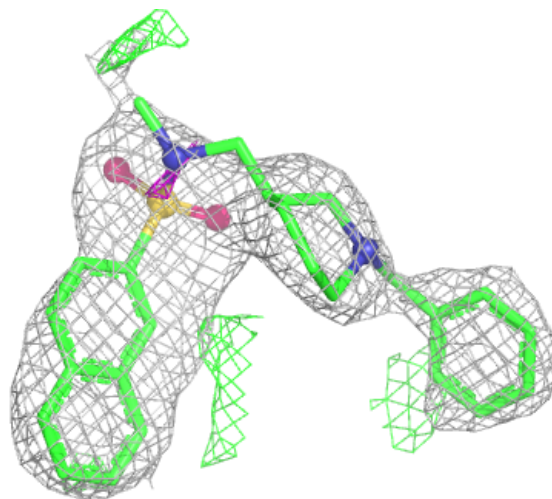
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	NAG	B	601	14/15	0.45	0.17	105,114,121,122	0
8	EDO	B	613	4/4	0.49	0.20	80,81,83,84	0
5	NAG	B	603	14/15	0.55	0.15	97,100,109,110	0
5	NAG	B	602	14/15	0.55	0.15	96,113,122,123	0
5	NAG	B	607	14/15	0.56	0.16	96,111,115,117	0
5	NAG	A	601	14/15	0.63	0.13	76,91,96,99	0
8	EDO	B	611	4/4	0.74	0.19	67,71,75,76	0
8	EDO	B	612	4/4	0.77	0.22	82,83,84,87	0
5	NAG	B	605	14/15	0.77	0.14	103,108,112,113	0
10	FUL	B	604	10/11	0.77	0.18	96,103,105,105	0
9	UNX	A	609	1/1	0.78	0.35	65,65,65,65	0
8	EDO	A	607	4/4	0.80	0.21	75,77,78,78	0
9	UNX	B	615	1/1	0.82	0.58	73,73,73,73	0
5	NAG	A	602	14/15	0.82	0.11	74,79,84,84	0
7	GOL	B	610	6/6	0.84	0.17	78,83,87,93	0
9	UNX	B	614	1/1	0.86	0.39	62,62,62,62	0
9	UNX	A	610	1/1	0.88	0.28	66,66,66,66	0
5	NAG	B	606	14/15	0.88	0.09	67,74,82,83	0
6	5HB	B	608	29/29	0.89	0.17	60,82,89,89	0
7	GOL	A	606	6/6	0.89	0.13	78,83,87,91	0
11	PEG	B	617	7/7	0.89	0.19	75,83,87,87	0
7	GOL	A	605	6/6	0.90	0.22	64,73,77,78	0
7	GOL	A	604	6/6	0.91	0.10	76,79,81,82	0
7	GOL	B	609	6/6	0.92	0.10	60,65,74,77	0
6	5HB	A	603	29/29	0.92	0.17	55,90,95,95	0
9	UNX	A	608	1/1	0.95	0.23	82,82,82,82	0
9	UNX	B	616	1/1	0.99	0.20	64,64,64,64	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

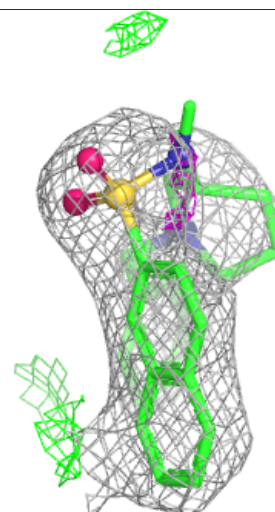
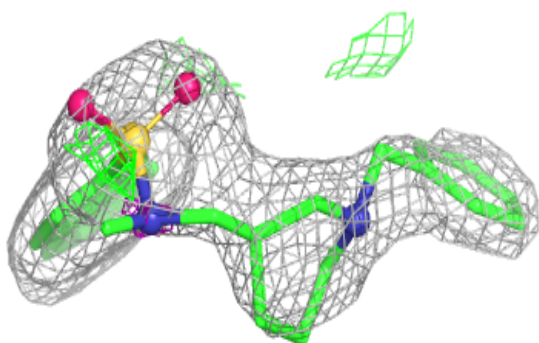
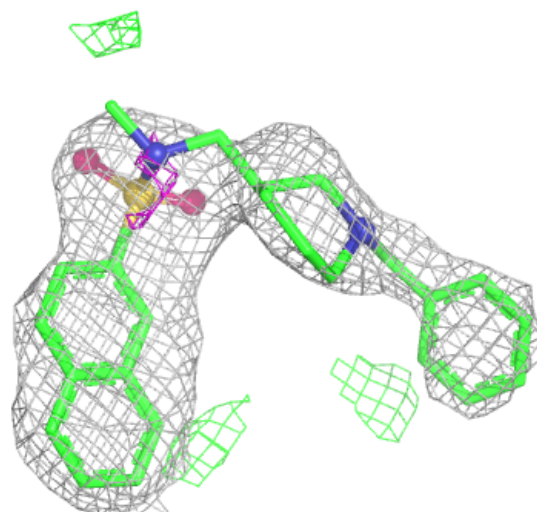
Electron density around 5HB B 608:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around 5HB A 603:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.