Full wwPDB X-ray Structure Validation Report ⓘ

Apr 20, 2024 – 02:00 pm BST

PDB ID	:	5DYT
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 Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/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:

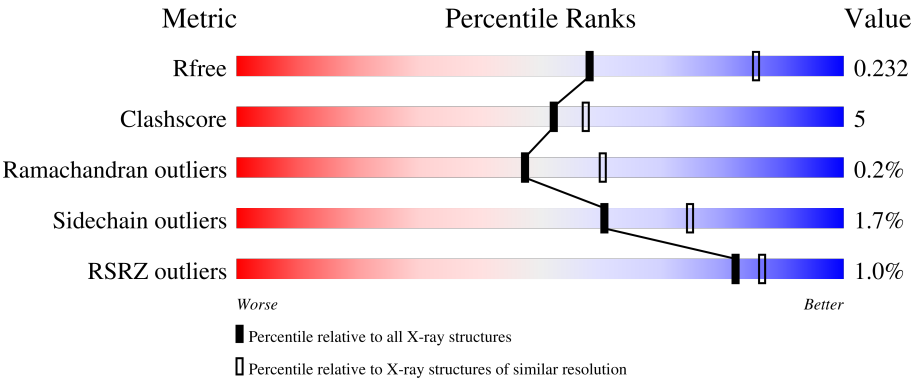
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1 Overall quality at a glance (i)

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}	130704	1284 (2.56-2.52)
Clashscore	141614	1332 (2.56-2.52)
Ramachandran outliers	138981	1315 (2.56-2.52)
Sidechain outliers	138945	1315 (2.56-2.52)
RSRZ outliers	127900	1272 (2.56-2.52)

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 <=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	% 86% 13% .
1	B	530	% 83% 16% .
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	-	-	X
2	FUC	E	3	X	-	-	-
2	NAG	G	2	X	-	-	X
2	FUC	G	3	X	-	-	-
3	NAG	D	2	X	-	-	-
4	FUC	I	2	X	-	-	-
5	NAG	A	610	X	-	-	-
5	NAG	B	611	X	-	-	-
9	UNX	A	623	-	-	X	-

2 Entry composition

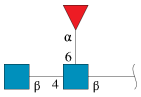
There are 12 unique types of molecules in this entry. The entry contains 9063 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

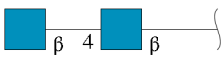
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	527	Total	C	N	O	S	0	3	0
			4210	2717	710	768	15			
1	B	525	Total	C	N	O	S	0	0	0
			4160	2688	697	760	15			

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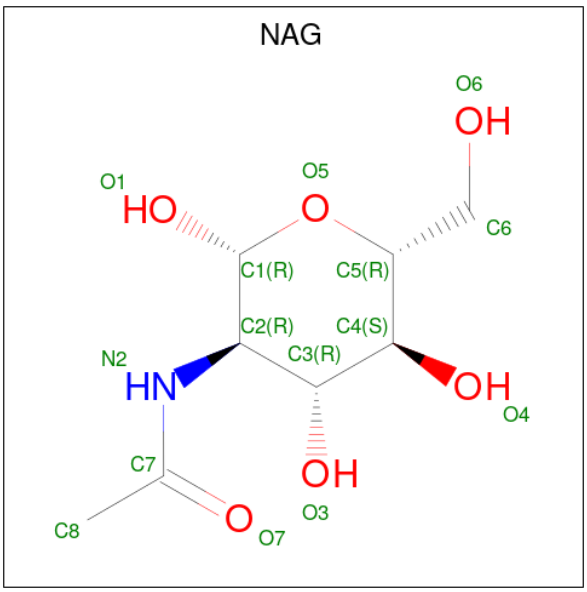
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
3	H	2	Total C N O 28 16 2 10	0	0	0

- 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 24 14 1 9	0	0	0

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

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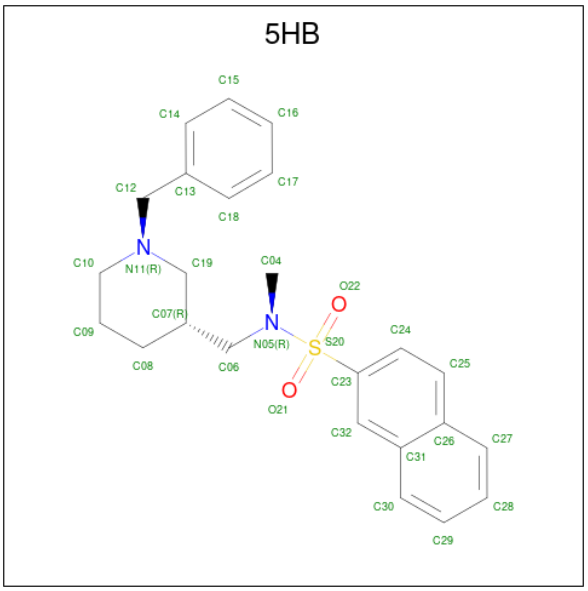
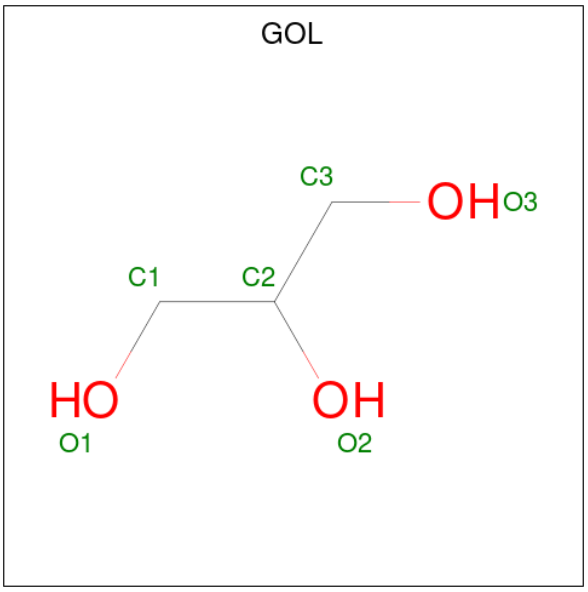
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	1	Total C N O 14 8 1 5	0	0
5	B	1	Total C N O 14 8 1 5	0	0
5	B	1	Total C N O 14 8 1 5	0	0
5	B	1	Total C N O 14 8 1 5	0	0

- Molecule 6 is N-{[(3R)-1-benzylpiperidin-3-yl]methyl}-N-methylnaphthalene-2-sulfonamide (three-letter code: 5HB) (formula: $C_{24}H_{28}N_2O_2S$).



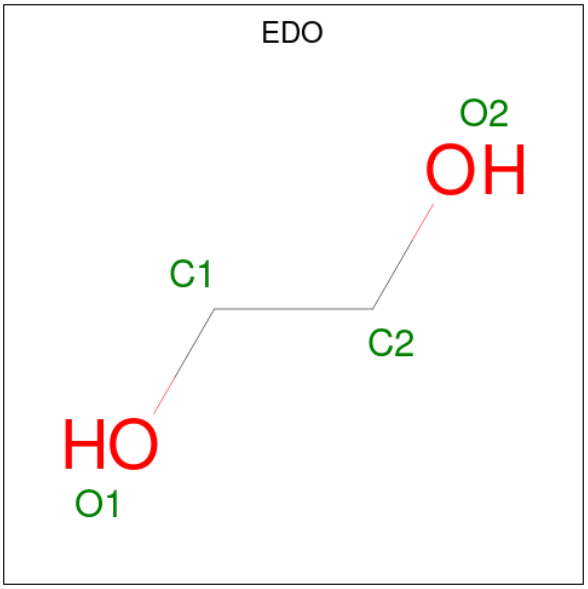
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C N O S 29 24 2 2 1	0	0
6	B	1	Total C N O S 29 24 2 2 1	0	0

- Molecule 7 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 8 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).

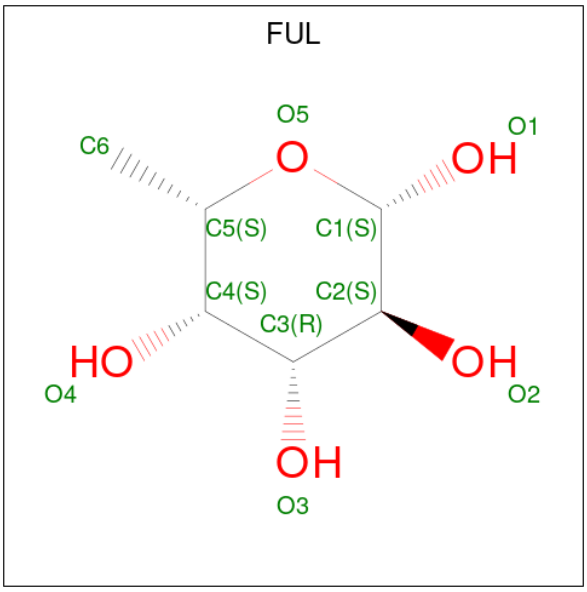


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	1	Total C O 4 2 2	0	0
8	B	1	Total C O 4 2 2	0	0
8	B	1	Total C O 4 2 2	0	0
8	B	1	Total C O 4 2 2	0	0

- Molecule 9 is UNKNOWN ATOM OR ION (three-letter code: UNX) (formula: X).

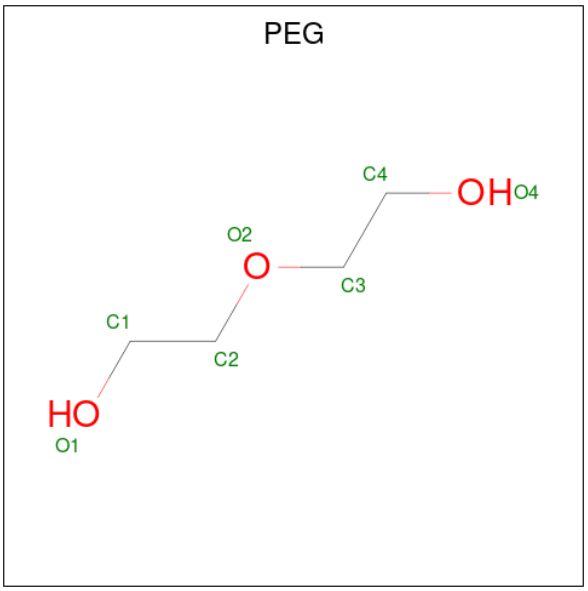
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	3	Total X 3 3	0	0
9	B	3	Total X 3 3	0	0

- Molecule 10 is beta-L-fucopyranose (three-letter code: FUL) (formula: $C_6H_{12}O_5$).



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

- Molecule 11 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



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

- Molecule 12 is water.

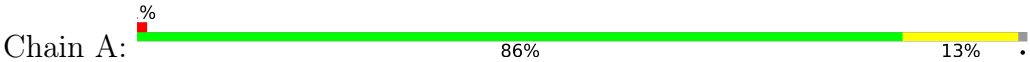
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
12	A	118	Total O 118 118	0	0
12	B	114	Total O 114 114	0	0

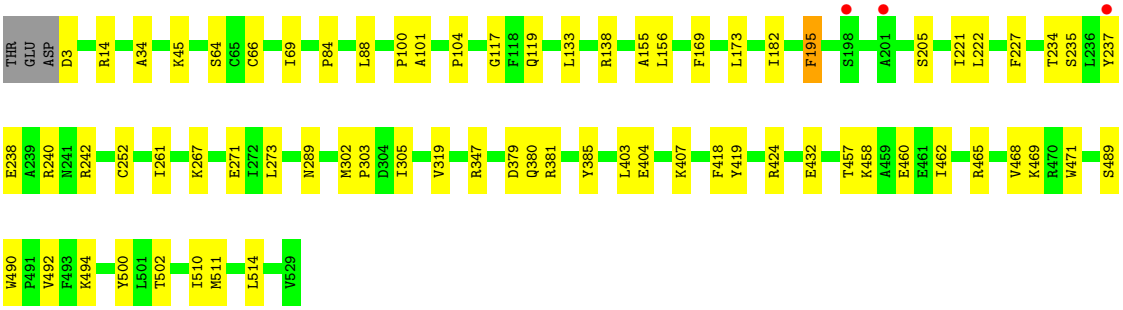
3 Residue-property plots (i)

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 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

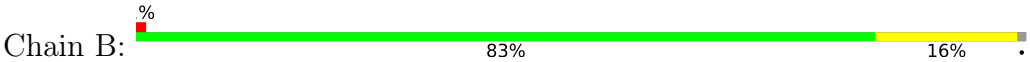
Chain A:

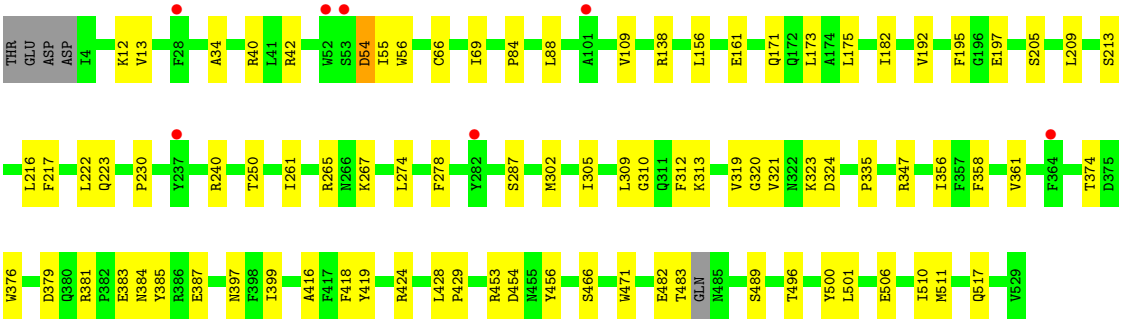




• Molecule 1: Cholinesterase

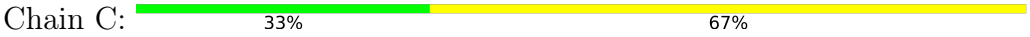
Chain B:





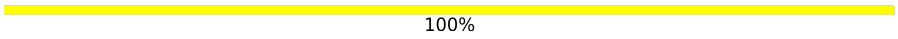
• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain C:



• 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:

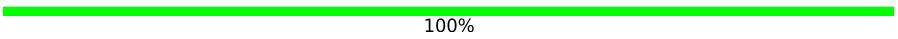


• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain G:

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

Chain D:

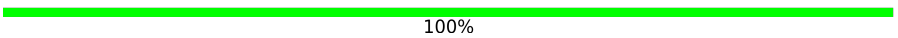


• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain F:

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

Chain H:



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

Chain I:

4 Data and refinement statistics (i)

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 46.91 – 2.55	Depositor EDS
% Data completeness (in resolution range)	99.6 (46.12-2.55) 99.7 (46.91-2.55)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.21 (at 2.54Å)	Xtriage
Refinement program	PHENIX (1.10_2155: ???)	Depositor
R, R_{free}	0.179 , 0.232 0.179 , 0.232	Depositor DCC
R_{free} test set	1415 reflections (3.00%)	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)	0.31 , 48.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: FUC, FUL, CSO, GOL, PEG, UNX, 5HB, NAG, EDO

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	0.44	0/4331	0.60	0/5879
1	B	0.43	0/4270	0.58	0/5796
All	All	0.43	0/8601	0.59	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

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	42	1
1	B	4160	0	4034	50	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	95	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 5.

All (95) 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:621:UNX:UNK	9:A:623:UNX:UNK	1.26	0.77
1:A:100:PRO:HG2	1:A:104:PRO:HG3	1.68	0.76
1:A:458:LYS:O	1:A:462:ILE:HD12	1.89	0.71
1:B:161:GLU:OE1	1:B:265:ARG:NH1	2.24	0.70
9:B:618:UNX:UNK	9:B:620:UNX:UNK	1.36	0.69
1:A:3:ASP:N	12:A:702:HOH:O	2.29	0.65
1:B:250:THR:HB	1:B:267:LYS:HE2	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:494:LYS:NZ	12:A:701:HOH:O	2.26	0.64
1:B:428:LEU:HA	11:B:621:PEG:H42	1.80	0.64
5:B:608:NAG:O6	12:B:701:HOH:O	2.16	0.61
1:B:34:ALA:HB2	1:B:173:LEU:HD23	1.83	0.61
1:B:429:PRO:HD3	11:B:621:PEG:H31	1.83	0.61
1:A:3:ASP:OD2	1:A:14:ARG:NH1	2.34	0.60
1:B:381:ARG:NH2	1:B:387:GLU:OE1	2.34	0.60
1:A:502:THR:HG21	1:A:511:MET:CE	2.32	0.59
1:B:381:ARG:NH1	1:B:383:GLU:OE2	2.36	0.59
1:A:404:GLU:HG2	12:A:802:HOH:O	2.04	0.58
1:B:69:ILE:HD11	1:B:88:LEU:HD11	1.83	0.58
1:B:54:ASP:O	1:B:55:ILE:HD13	2.04	0.57
1:B:335:PRO:HD3	1:B:356:ILE:HD12	1.87	0.56
1:A:101:ALA:O	1:A:138[B]:ARG:NH2	2.39	0.56
1:B:500:TYR:CZ	1:B:511:MET:HB2	2.41	0.56
1:A:45:LYS:HD2	1:A:169:PHE:CD2	2.42	0.55
1:B:42:ARG:O	1:B:265:ARG:NH2	2.40	0.55
1:B:13:VAL:HG12	1:B:56:TRP:HB3	1.89	0.55
1:B:192:VAL:CG2	1:B:217:PHE:HA	2.35	0.53
1:A:227:PHE:CD1	1:A:303:PRO:HB2	2.43	0.53
1:A:34:ALA:HB2	1:A:173:LEU:HD23	1.91	0.52
9:A:622:UNX:UNK	9:A:623:UNX:UNK	1.54	0.52
1:A:319:VAL:O	1:A:418:PHE:HA	2.10	0.52
1:A:156:LEU:HD12	1:A:261:ILE:HD11	1.92	0.52
1:B:482:GLU:HG2	1:B:483:THR:H	1.75	0.51
1:B:323:LYS:HE2	1:B:324:ASP:OD2	2.10	0.51
1:B:428:LEU:HD12	1:B:429:PRO:HD2	1.93	0.51
1:B:156:LEU:HD12	1:B:261:ILE:HD11	1.91	0.50
1:A:492:VAL:HG13	1:B:274:LEU:HD13	1.94	0.50
1:A:465[B]:ARG:NH2	12:A:710:HOH:O	2.43	0.50
1:A:502:THR:HG21	1:A:511:MET:HE3	1.93	0.50
1:B:319:VAL:O	1:B:418:PHE:HA	2.12	0.50
1:A:302:MET:HB2	1:A:305:ILE:HD12	1.94	0.49
1:A:502:THR:HG21	1:A:511:MET:HE2	1.94	0.49
1:A:457:THR:OG1	1:A:460:GLU:HG3	2.12	0.49
1:A:424:ARG:NH1	1:A:432:GLU:HA	2.28	0.48
1:B:287:SER:HA	7:B:614:GOL:H32	1.95	0.48
1:A:238:GLU:O	1:A:242:ARG:HG3	2.13	0.48
1:A:195:PHE:HB3	1:A:221:ILE:HB	1.95	0.48
1:B:419:TYR:HA	1:B:501:LEU:O	2.14	0.48
1:B:230:PRO:HG2	1:B:397:ASN:HD22	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:500:TYR:CE1	1:B:511:MET:HB2	2.49	0.47
1:B:84:PRO:HG2	1:B:88:LEU:HD21	1.96	0.47
1:B:171:GLN:O	1:B:175:LEU:HG	2.15	0.47
1:B:209:LEU:HD23	1:B:312:PHE:HB3	1.97	0.46
1:A:419:TYR:HB3	1:A:490:TRP:CZ2	2.50	0.46
1:A:234:THR:HG22	1:A:235:SER:O	2.15	0.45
1:B:321:VAL:HG11	1:B:399:ILE:HA	1.99	0.45
1:B:347:ARG:HB2	1:B:385:TYR:CZ	2.51	0.45
1:B:109:VAL:HG21	1:B:182:ILE:HG12	1.98	0.45
1:B:278:PHE:O	10:B:606:FUL:O4	2.33	0.45
1:B:374:THR:HG22	1:B:376:TRP:CZ2	2.51	0.45
1:A:289:ASN:ND2	12:A:719:HOH:O	2.50	0.45
1:B:310:GLY:HA2	1:B:312:PHE:CE2	2.52	0.44
1:B:320:GLY:HA3	1:B:419:TYR:CE2	2.52	0.44
1:A:182:ILE:HD12	1:A:182:ILE:HA	1.92	0.44
1:A:380:GLN:HA	1:A:381:ARG:C	2.37	0.44
1:A:469:LYS:HB2	1:A:469:LYS:HE2	1.75	0.43
1:A:133:LEU:HD23	1:A:468:VAL:HG13	2.00	0.43
1:B:205:SER:HB3	1:B:222:LEU:HD21	2.01	0.43
1:A:227:PHE:CE1	1:A:303:PRO:HB2	2.54	0.43
1:B:213:SER:HA	1:B:216:LEU:HD12	2.01	0.43
1:A:403:LEU:O	1:A:407:LYS:HG3	2.19	0.42
1:A:64:SER:HB2	1:A:88:LEU:HD23	2.01	0.42
1:A:500:TYR:CE1	1:A:514:LEU:HB2	2.55	0.42
1:A:205:SER:HB3	1:A:222:LEU:HD21	2.01	0.42
1:B:379:ASP:OD1	1:B:379:ASP:N	2.41	0.42
1:B:428:LEU:HD12	1:B:429:PRO:CD	2.51	0.41
1:A:117:GLY:O	1:A:119:GLN:HG2	2.20	0.41
1:A:347:ARG:HB2	1:A:385:TYR:CZ	2.56	0.41
1:A:156:LEU:CD1	1:A:261:ILE:HD11	2.51	0.41
1:A:252:CYS:SG	1:A:267:LYS:HE3	2.61	0.41
1:B:489:SER:O	1:B:510:ILE:HD11	2.21	0.41
1:A:66:CSO:HB2	1:A:273:LEU:HD11	2.03	0.41
1:B:197:GLU:HA	1:B:223:GLN:O	2.21	0.41
1:B:416:ALA:N	12:B:705:HOH:O	2.39	0.41
1:B:66:CSO:OD	3:F:2:NAG:H82	2.20	0.40
1:B:305:ILE:HG22	1:B:309:LEU:HD22	2.03	0.40
1:B:376:TRP:CH2	1:B:384:ASN:HB3	2.55	0.40
1:A:69:ILE:HD11	1:A:88:LEU:HD11	2.03	0.40
1:B:358:PHE:HB3	1:B:361:VAL:CG2	2.51	0.40
1:B:454:ASP:O	1:B:456:TYR:N	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:267:LYS:HD2	1:A:271:GLU:HG2	2.04	0.40
1:A:489:SER:O	1:A:510:ILE:HD11	2.22	0.40

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%)	34	46
All	All	1047/1060 (99%)	999 (95%)	46 (4%)	2 (0%)	47	60

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%)	446 (99%)	5 (1%)	73 83
1	B	442/454 (97%)	432 (98%)	10 (2%)	50 65
All	All	893/908 (98%)	878 (98%)	15 (2%)	60 75

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	84	PRO
1	A	195	PHE
1	A	240	ARG
1	A	379	ASP
1	A	471	TRP
1	B	40	ARG
1	B	138	ARG
1	B	195	PHE
1	B	240	ARG
1	B	302	MET
1	B	424	ARG
1	B	466	SER
1	B	471	TRP
1	B	496	THR
1	B	517	GLN

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

Mol	Chain	Res	Type
1	A	311	GLN
1	B	10	ASN
1	B	397	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)

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	0,6,8	-	-
1	CSO	B	66	1	3,6,7	0.60	0	0,6,8	-	-

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	0.26	0	17,19,21	0.49	0
2	NAG	C	2	2	14,14,15	0.74	1 (7%)	17,19,21	0.83	1 (5%)
2	FUC	C	3	2	10,10,11	1.91	5 (50%)	14,14,16	0.59	0
3	NAG	D	1	3,1	14,14,15	0.53	0	17,19,21	0.81	0
3	NAG	D	2	3	14,14,15	0.71	0	17,19,21	0.55	0
2	NAG	E	1	2,1	14,14,15	0.26	0	17,19,21	0.94	1 (5%)
2	NAG	E	2	2	14,14,15	0.73	1 (7%)	17,19,21	0.84	1 (5%)
2	FUC	E	3	2	10,10,11	1.89	4 (40%)	14,14,16	1.74	4 (28%)
3	NAG	F	1	3,1	14,14,15	0.26	0	17,19,21	0.65	1 (5%)
3	NAG	F	2	3	14,14,15	0.86	1 (7%)	17,19,21	0.88	1 (5%)
2	NAG	G	1	2,1	14,14,15	0.51	0	17,19,21	0.44	0
2	NAG	G	2	2	14,14,15	0.30	0	17,19,21	0.36	0
2	FUC	G	3	2	10,10,11	1.83	3 (30%)	14,14,16	1.06	1 (7%)
3	NAG	H	1	3,1	14,14,15	0.46	0	17,19,21	0.61	0
3	NAG	H	2	3	14,14,15	0.25	0	17,19,21	0.48	0
4	NAG	I	1	1,4	14,14,15	0.42	0	17,19,21	0.65	0
4	FUC	I	2	4	10,10,11	1.74	2 (20%)	14,14,16	1.03	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	3/6/23/26	0/1/1/1
2	NAG	E	2	2	1/1/5/7	4/6/23/26	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

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

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	3	FUC	O5-C1	-3.40	1.38	1.43
2	C	3	FUC	O5-C1	-3.21	1.38	1.43
4	I	2	FUC	O5-C1	-3.14	1.38	1.43
2	G	3	FUC	O5-C1	-3.11	1.38	1.43
3	F	2	NAG	O5-C1	2.98	1.48	1.43
2	C	3	FUC	O2-C2	-2.34	1.38	1.43
2	E	3	FUC	O2-C2	-2.31	1.38	1.43
2	C	2	NAG	O5-C1	2.29	1.47	1.43
2	G	3	FUC	O5-C5	-2.28	1.38	1.43
2	C	3	FUC	O5-C5	-2.20	1.38	1.43
2	E	2	NAG	O5-C1	2.19	1.47	1.43
4	I	2	FUC	O2-C2	-2.14	1.38	1.43
2	G	3	FUC	O2-C2	-2.08	1.38	1.43
2	E	3	FUC	O3-C3	-2.07	1.38	1.43
2	E	3	FUC	O5-C5	-2.05	1.39	1.43
2	C	3	FUC	O3-C3	-2.05	1.38	1.43
2	C	3	FUC	C2-C3	-2.02	1.49	1.52

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	3	FUC	O5-C1-C2	-3.76	104.97	110.77
2	E	2	NAG	C1-O5-C5	3.11	116.41	112.19
2	C	2	NAG	C1-O5-C5	3.02	116.29	112.19
3	F	2	NAG	C1-O5-C5	3.02	116.28	112.19
2	E	3	FUC	C3-C4-C5	2.74	114.04	109.77
2	E	1	NAG	C1-O5-C5	2.63	115.75	112.19
4	I	2	FUC	O5-C5-C4	2.59	114.16	109.52
2	E	3	FUC	O5-C5-C4	2.52	114.04	109.52
3	F	1	NAG	C1-O5-C5	2.31	115.33	112.19
2	G	3	FUC	C6-C5-C4	-2.11	109.18	113.07
2	E	3	FUC	C6-C5-C4	-2.04	109.30	113.07

All (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
3	D	2	NAG	C1
4	I	2	FUC	C1

All (26) torsion outliers are listed below:

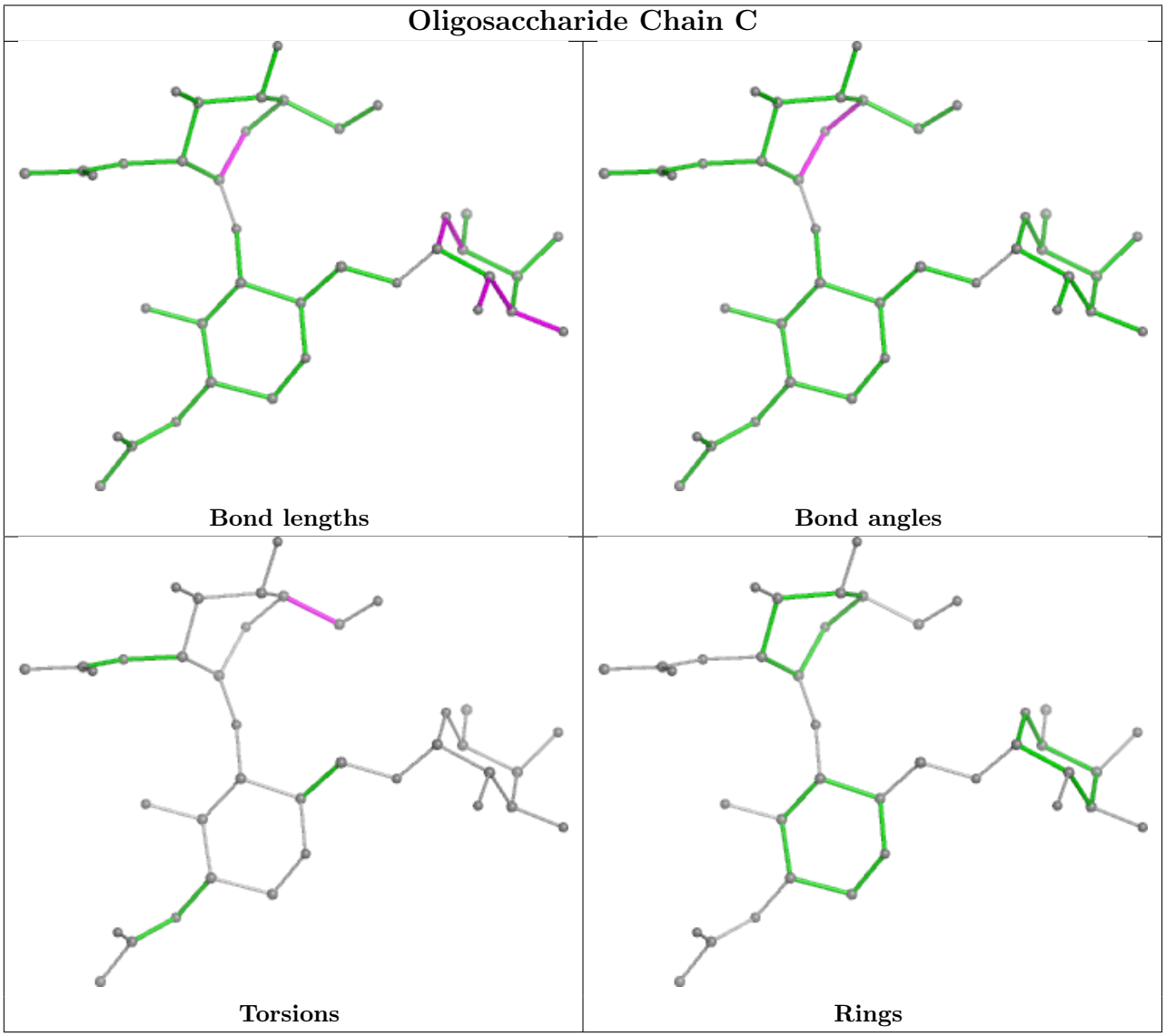
Mol	Chain	Res	Type	Atoms
2	E	2	NAG	C4-C5-C6-O6
2	E	1	NAG	O5-C5-C6-O6
2	G	1	NAG	O5-C5-C6-O6
3	H	1	NAG	C4-C5-C6-O6
2	E	2	NAG	O5-C5-C6-O6
3	D	2	NAG	O5-C5-C6-O6
3	D	2	NAG	C4-C5-C6-O6
2	G	1	NAG	C4-C5-C6-O6
2	G	2	NAG	C8-C7-N2-C2
2	G	2	NAG	O7-C7-N2-C2
3	D	1	NAG	C8-C7-N2-C2
3	D	1	NAG	O7-C7-N2-C2
3	D	2	NAG	C8-C7-N2-C2
3	D	2	NAG	O7-C7-N2-C2
3	H	2	NAG	C4-C5-C6-O6
3	F	2	NAG	C4-C5-C6-O6
2	E	1	NAG	C4-C5-C6-O6
3	H	1	NAG	O5-C5-C6-O6
3	F	1	NAG	C4-C5-C6-O6
3	F	2	NAG	O5-C5-C6-O6
3	H	2	NAG	O5-C5-C6-O6
2	C	2	NAG	O5-C5-C6-O6
3	F	1	NAG	O5-C5-C6-O6
2	E	2	NAG	C1-C2-N2-C7
2	E	1	NAG	C3-C2-N2-C7
2	E	2	NAG	C3-C2-N2-C7

There are no ring outliers.

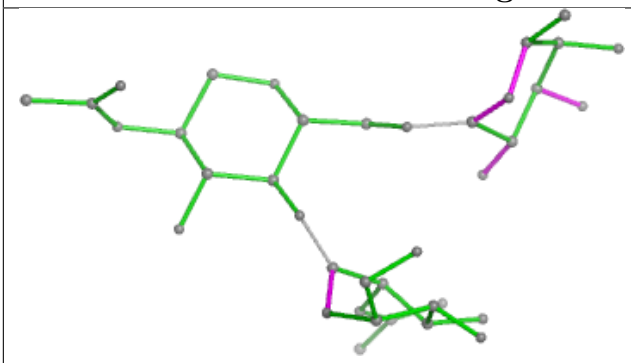
1 monomer is involved in 1 short contact:

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

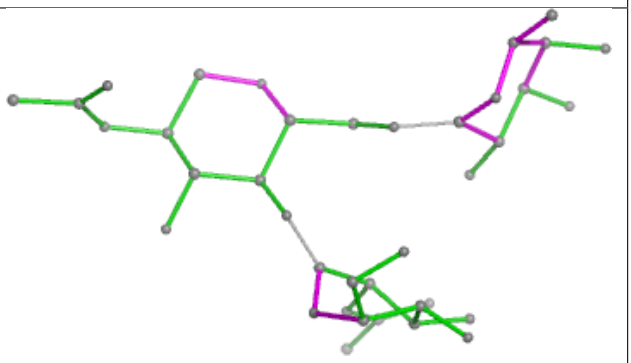
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.



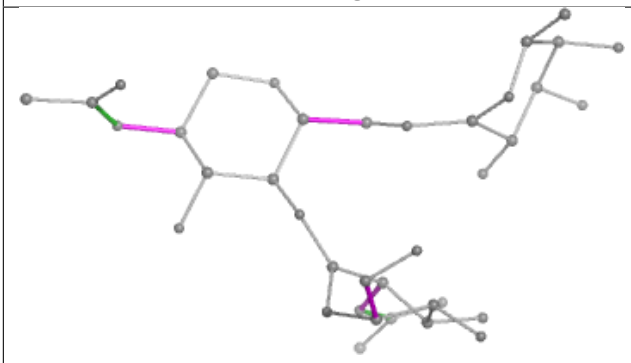
Oligosaccharide Chain E



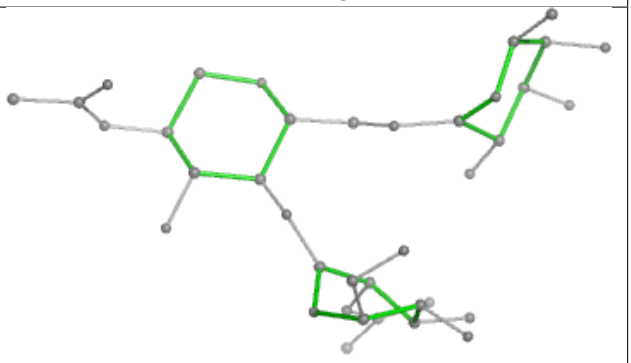
Bond lengths



Bond angles

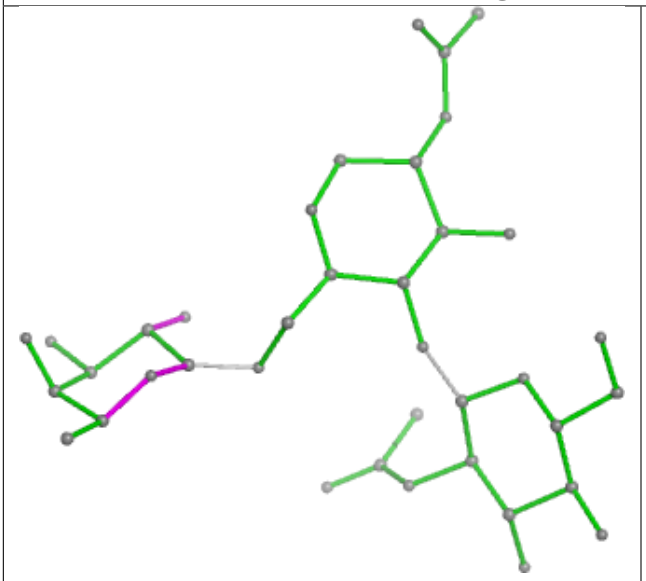


Torsions

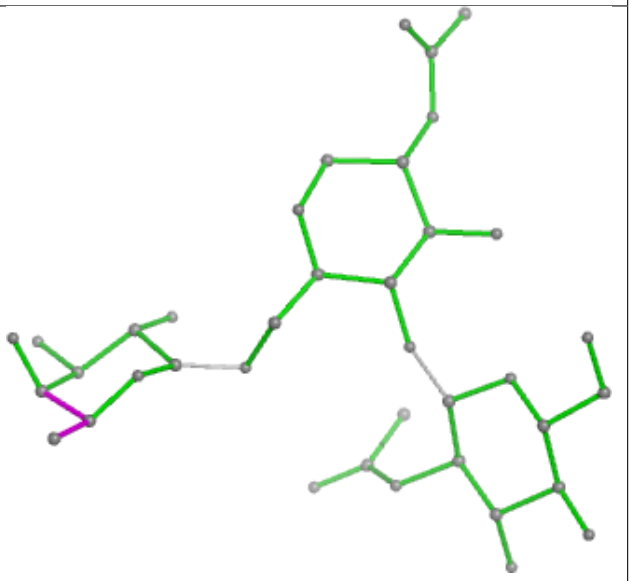


Rings

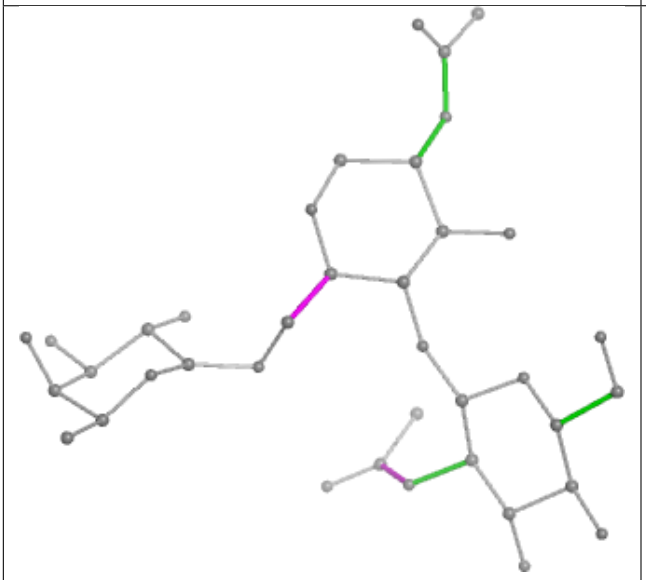
Oligosaccharide Chain G



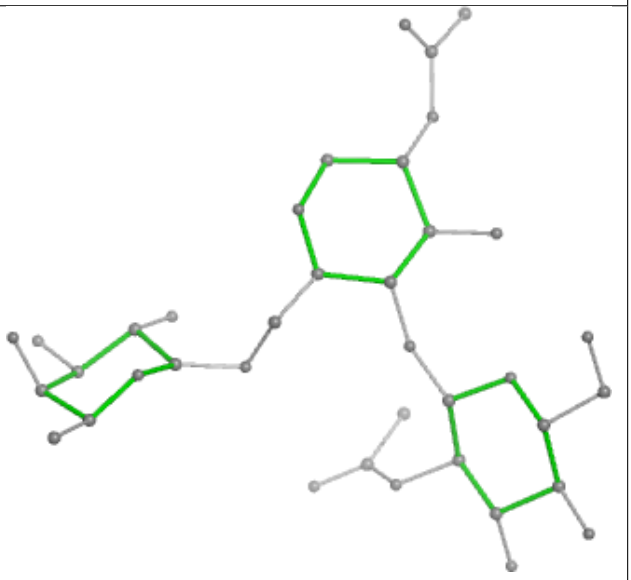
Bond lengths



Bond angles

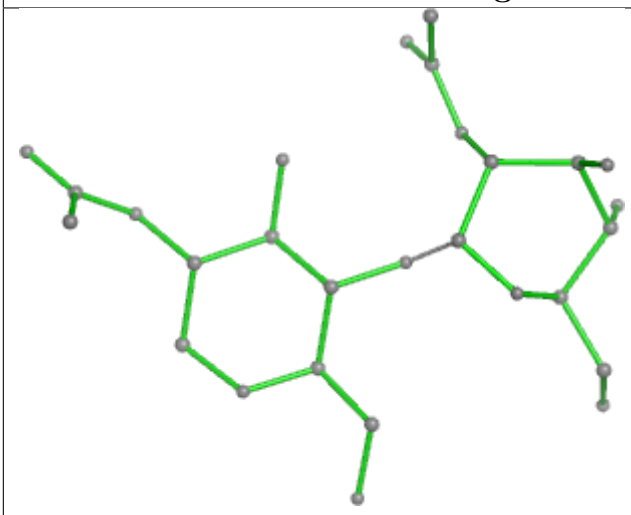


Torsions

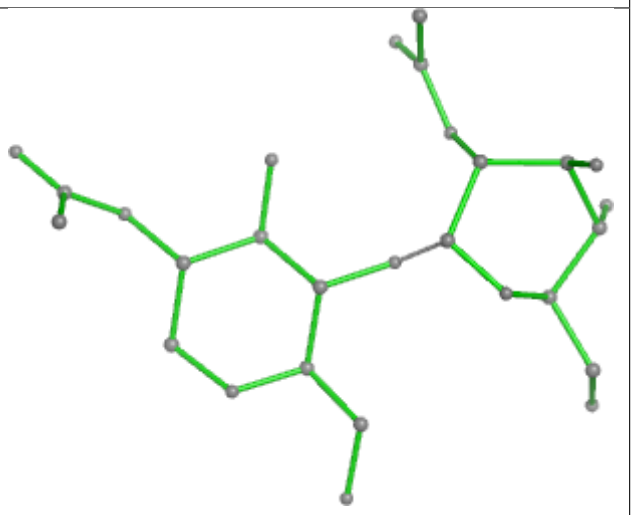


Rings

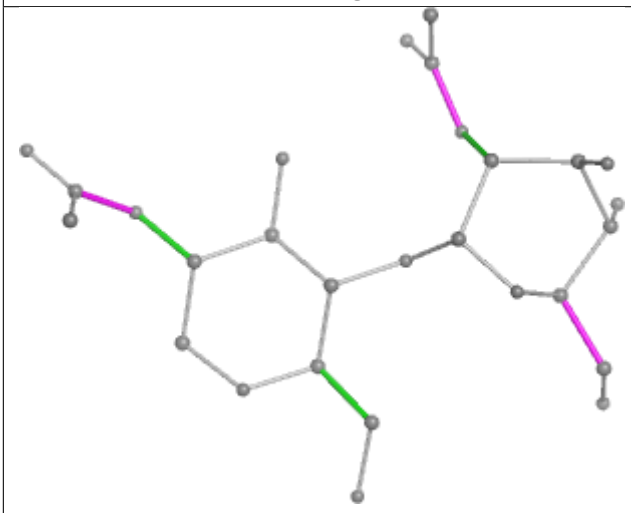
Oligosaccharide Chain D



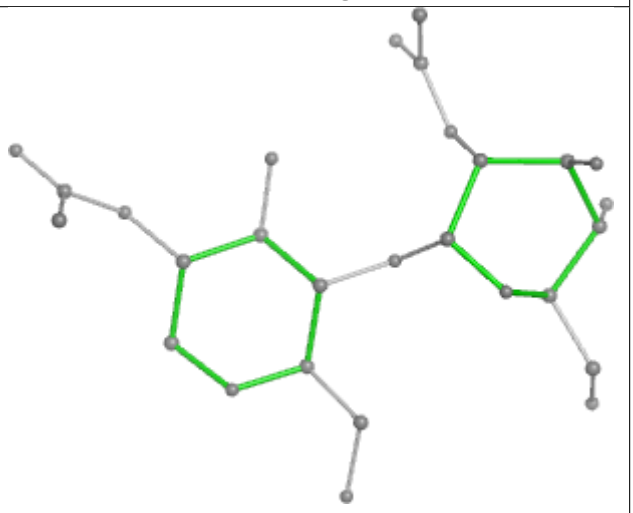
Bond lengths



Bond angles

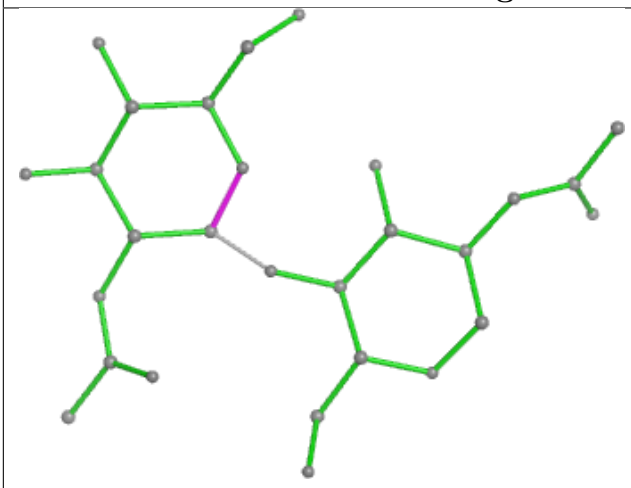


Torsions

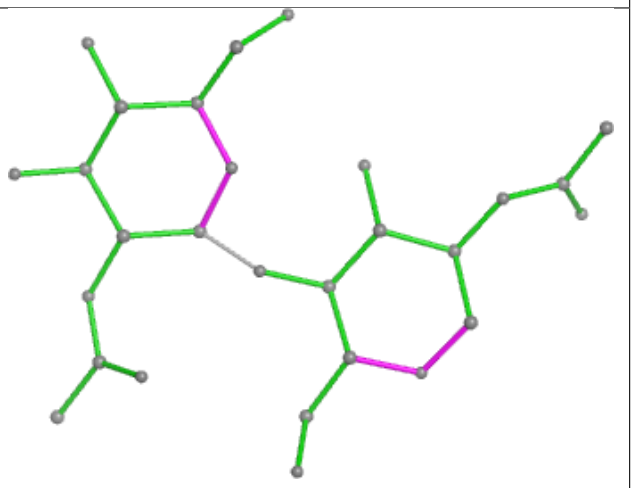


Rings

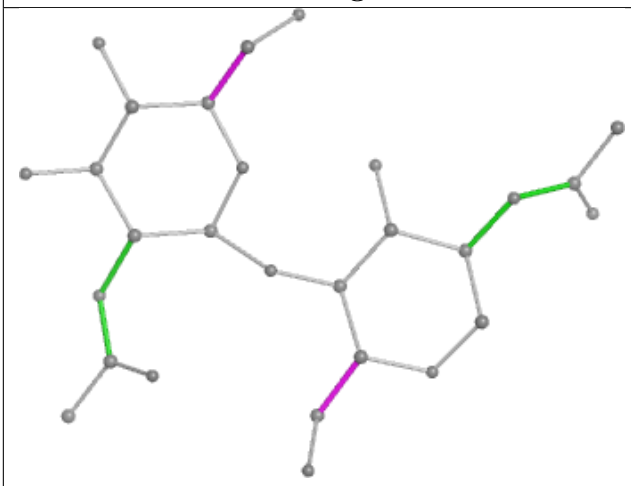
Oligosaccharide Chain F



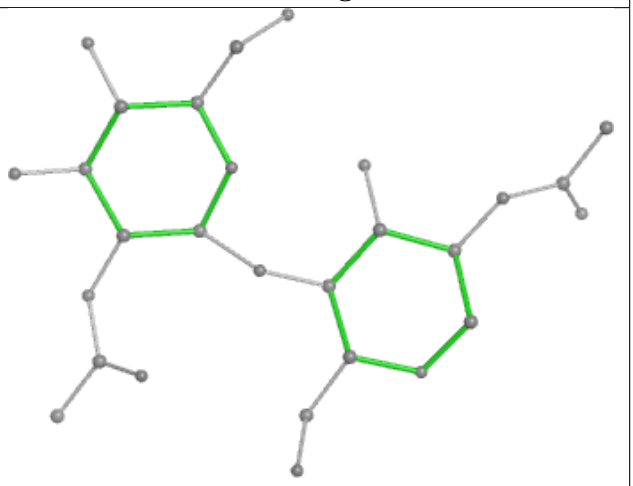
Bond lengths



Bond angles

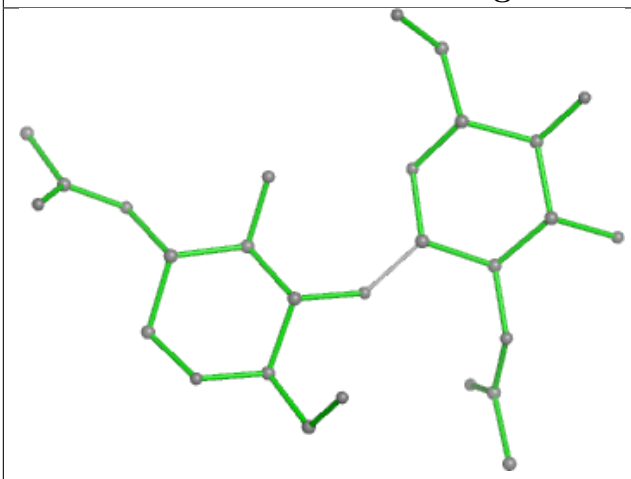


Torsions

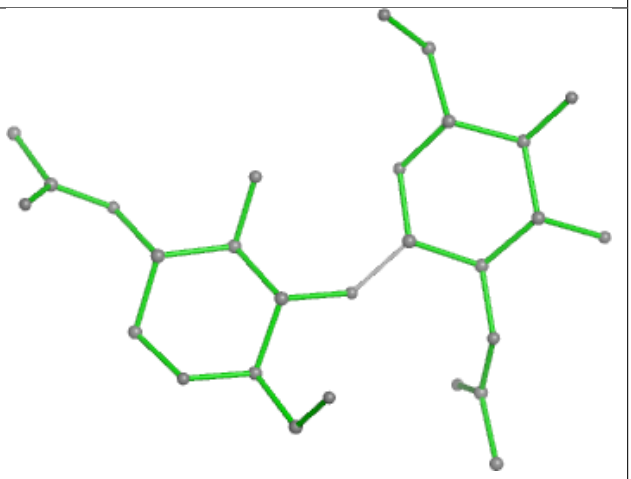


Rings

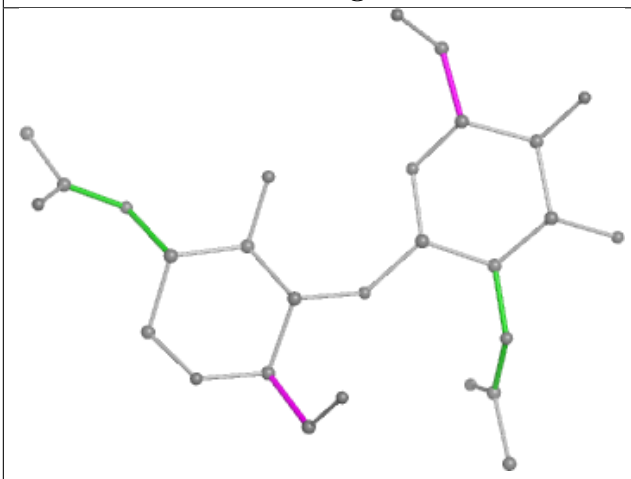
Oligosaccharide Chain H



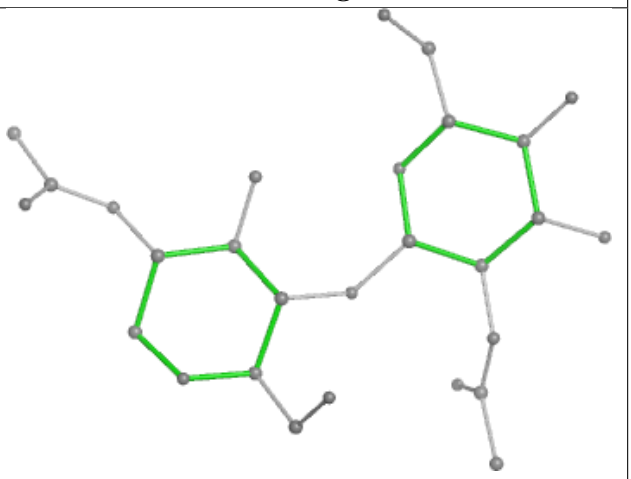
Bond lengths



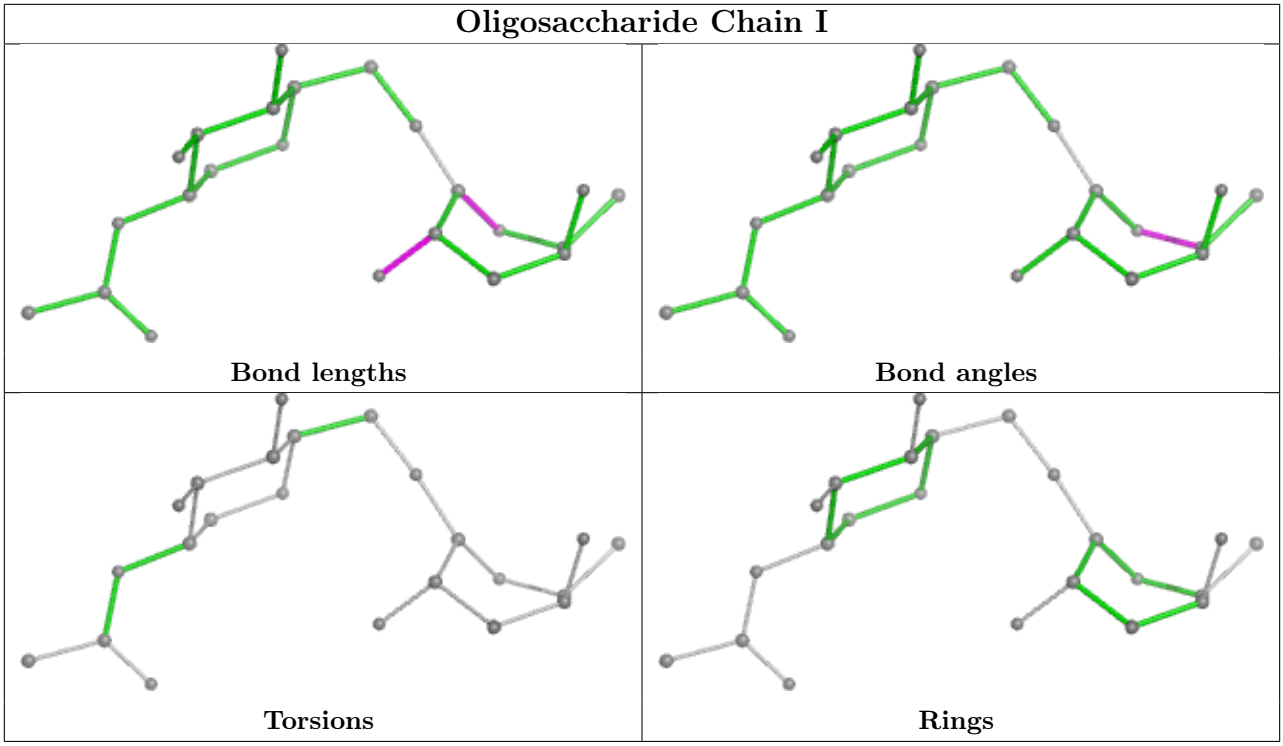
Bond angles



Torsions



Rings



5.6 Ligand geometry (i)

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	$\#\|Z\| > 2$
7	GOL	A	618	-	5,5,5	0.53	0	5,5,5	0.52	0
11	PEG	B	621	-	6,6,6	0.47	0	5,5,5	0.90	0
5	NAG	B	607	1	14,14,15	0.43	0	17,19,21	0.78	1 (5%)
8	EDO	B	616	-	3,3,3	1.76	1 (33%)	2,2,2	1.56	0
6	5HB	A	616	-	31,32,32	2.87	3 (9%)	41,45,45	1.59	4 (9%)
5	NAG	B	608	1	14,14,15	0.50	0	17,19,21	0.62	1 (5%)
8	EDO	A	620	-	3,3,3	0.66	0	2,2,2	0.43	0
5	NAG	B	611	1	14,14,15	0.51	0	17,19,21	1.02	1 (5%)
5	NAG	A	601	1	14,14,15	0.64	0	17,19,21	0.47	0
7	GOL	A	617	-	5,5,5	0.34	0	5,5,5	0.43	0
5	NAG	B	603	1	14,14,15	0.41	0	17,19,21	1.43	3 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
7	GOL	A	619	-	5,5,5	0.46	0	5,5,5	0.22	0
6	5HB	B	612	-	31,32,32	2.85	4 (12%)	41,45,45	1.72	4 (9%)
7	GOL	B	613	-	5,5,5	0.36	0	5,5,5	0.27	0
8	EDO	B	617	-	3,3,3	1.30	0	2,2,2	1.34	0
8	EDO	B	615	-	3,3,3	0.61	0	2,2,2	0.06	0
5	NAG	B	602	1	14,14,15	0.45	0	17,19,21	0.44	0
5	NAG	A	610	1	14,14,15	0.53	0	17,19,21	1.05	1 (5%)
5	NAG	B	601	1	14,14,15	0.93	1 (7%)	17,19,21	1.10	1 (5%)
7	GOL	B	614	-	5,5,5	0.40	0	5,5,5	0.69	0
10	FUL	B	606	-	10,10,11	1.76	3 (30%)	14,14,16	1.88	2 (14%)

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
7	GOL	A	618	-	-	4/4/4/4	-
11	PEG	B	621	-	-	1/4/4/4	-
5	NAG	B	607	1	-	2/6/23/26	0/1/1/1
8	EDO	B	616	-	-	0/1/1/1	-
6	5HB	A	616	-	-	9/20/30/30	0/4/4/4
5	NAG	B	608	1	-	2/6/23/26	0/1/1/1
8	EDO	A	620	-	-	1/1/1/1	-
5	NAG	B	611	1	1/1/5/7	2/6/23/26	0/1/1/1
5	NAG	A	601	1	-	2/6/23/26	0/1/1/1
7	GOL	A	617	-	-	0/4/4/4	-
5	NAG	B	603	1	-	2/6/23/26	0/1/1/1
7	GOL	A	619	-	-	2/4/4/4	-
6	5HB	B	612	-	-	14/20/30/30	0/4/4/4
7	GOL	B	613	-	-	0/4/4/4	-
8	EDO	B	617	-	-	0/1/1/1	-
8	EDO	B	615	-	-	0/1/1/1	-
5	NAG	B	602	1	-	3/6/23/26	0/1/1/1
5	NAG	A	610	1	1/1/5/7	4/6/23/26	0/1/1/1
5	NAG	B	601	1	-	3/6/23/26	0/1/1/1
7	GOL	B	614	-	-	2/4/4/4	-
10	FUL	B	606	-	-	-	0/1/1/1

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	616	5HB	O22-S20	9.98	1.54	1.43
6	B	612	5HB	O21-S20	9.41	1.54	1.43
6	A	616	5HB	O21-S20	9.41	1.54	1.43
6	B	612	5HB	O22-S20	9.19	1.53	1.43
6	A	616	5HB	C12-C13	-6.98	1.38	1.51
6	B	612	5HB	C12-C13	-6.75	1.39	1.51
6	B	612	5HB	S20-N05	4.11	1.74	1.63
10	B	606	FUL	O5-C1	-3.18	1.38	1.43
5	B	601	NAG	O5-C1	2.82	1.48	1.43
10	B	606	FUL	O2-C2	-2.32	1.38	1.43
8	B	616	EDO	O1-C1	2.21	1.53	1.42
10	B	606	FUL	O5-C5	-2.18	1.38	1.43

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	B	612	5HB	O21-S20-N05	6.32	114.94	107.05
6	A	616	5HB	O21-S20-N05	5.81	114.30	107.05
6	B	612	5HB	O22-S20-O21	-5.54	110.54	119.52
10	B	606	FUL	C1-C2-C3	5.37	116.26	109.67
6	A	616	5HB	O22-S20-O21	-4.71	111.89	119.52
5	B	601	NAG	C1-O5-C5	3.98	117.58	112.19
5	A	610	NAG	C1-O5-C5	3.90	117.47	112.19
5	B	611	NAG	C1-O5-C5	3.89	117.47	112.19
5	B	603	NAG	C2-N2-C7	3.41	127.76	122.90
5	B	603	NAG	C1-O5-C5	3.17	116.48	112.19
5	B	603	NAG	C1-C2-N2	2.75	115.18	110.49
10	B	606	FUL	C2-C3-C4	2.33	114.92	110.89
6	A	616	5HB	C10-N11-C19	2.30	113.04	109.52
5	B	607	NAG	C1-O5-C5	2.24	115.23	112.19
6	A	616	5HB	C04-N05-S20	-2.24	110.39	116.23
6	B	612	5HB	C24-C23-S20	-2.16	117.48	119.76
6	B	612	5HB	C04-N05-S20	-2.10	110.74	116.23
5	B	608	NAG	C1-O5-C5	2.02	114.92	112.19

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	A	610	NAG	C1
5	B	611	NAG	C1

All (53) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	603	NAG	C1-C2-N2-C7
6	A	616	5HB	C07-C06-N05-S20
6	A	616	5HB	C04-N05-S20-C23
6	B	612	5HB	C07-C06-N05-S20
6	B	612	5HB	N05-C06-C07-C08
6	B	612	5HB	N05-C06-C07-C19
7	A	618	GOL	C1-C2-C3-O3
7	B	614	GOL	O1-C1-C2-C3
5	B	602	NAG	O5-C5-C6-O6
5	B	607	NAG	C4-C5-C6-O6
5	B	607	NAG	O5-C5-C6-O6
5	A	610	NAG	O5-C5-C6-O6
5	A	601	NAG	C8-C7-N2-C2
5	A	601	NAG	O7-C7-N2-C2
5	A	610	NAG	C8-C7-N2-C2
5	A	610	NAG	O7-C7-N2-C2
5	B	601	NAG	C8-C7-N2-C2
5	B	601	NAG	O7-C7-N2-C2
5	A	610	NAG	C4-C5-C6-O6
7	A	619	GOL	O1-C1-C2-O2
6	A	616	5HB	N05-C06-C07-C08
5	B	602	NAG	C4-C5-C6-O6
7	A	618	GOL	O1-C1-C2-C3
7	A	619	GOL	O1-C1-C2-C3
6	A	616	5HB	C04-N05-S20-O21
6	A	616	5HB	C04-N05-S20-O22
6	A	616	5HB	C06-N05-S20-O21
6	B	612	5HB	C04-N05-S20-O21
6	B	612	5HB	C04-N05-S20-O22
6	B	612	5HB	C06-N05-S20-O21
6	B	612	5HB	C06-N05-S20-O22
5	B	608	NAG	O5-C5-C6-O6
7	B	614	GOL	O1-C1-C2-O2
5	B	608	NAG	C4-C5-C6-O6
7	A	618	GOL	O2-C2-C3-O3
5	B	601	NAG	O5-C5-C6-O6
5	B	603	NAG	O5-C5-C6-O6
8	A	620	EDO	O1-C1-C2-O2
6	A	616	5HB	N05-C06-C07-C19
5	B	602	NAG	C3-C2-N2-C7
6	B	612	5HB	C04-N05-S20-C23
6	B	612	5HB	C06-N05-S20-C23

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Mol	Chain	Res	Type	Atoms
5	B	611	NAG	C4-C5-C6-O6
6	B	612	5HB	C24-C23-S20-O22
11	B	621	PEG	O1-C1-C2-O2
6	B	612	5HB	C32-C23-S20-O22
6	A	616	5HB	C06-N05-S20-O22
5	B	611	NAG	O5-C5-C6-O6
6	B	612	5HB	C24-C23-S20-N05
6	B	612	5HB	C07-C06-N05-C04
6	B	612	5HB	C32-C23-S20-N05
6	A	616	5HB	C06-N05-S20-C23
7	A	618	GOL	O1-C1-C2-O2

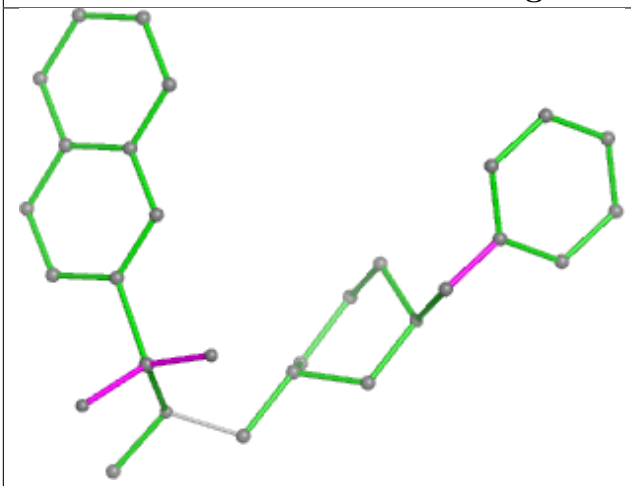
There are no ring outliers.

4 monomers are involved in 5 short contacts:

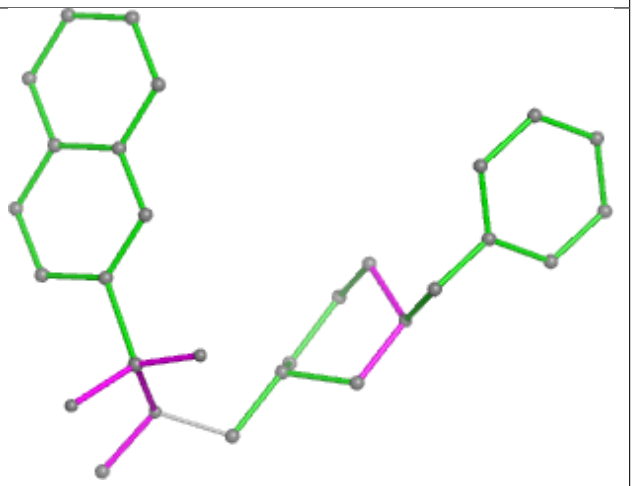
Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	B	621	PEG	2	0
5	B	608	NAG	1	0
7	B	614	GOL	1	0
10	B	606	FUL	1	0

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.

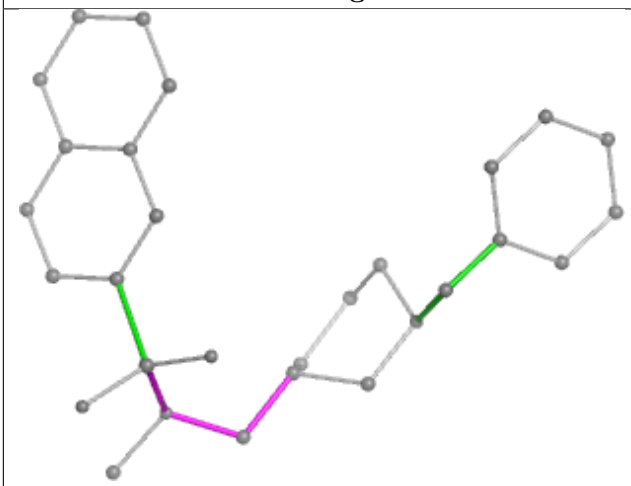
Ligand 5HB A 616



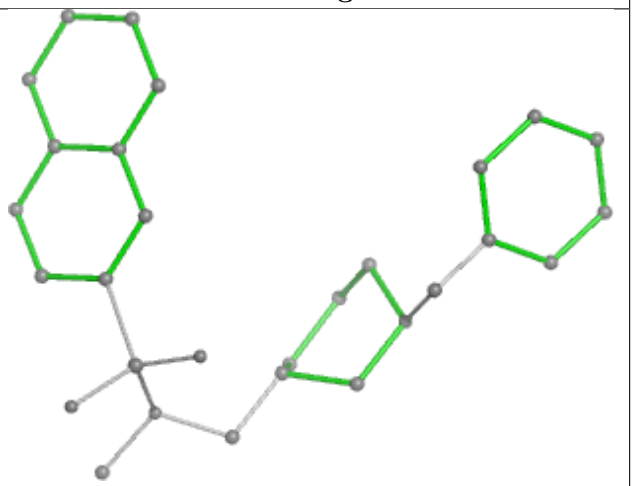
Bond lengths



Bond angles

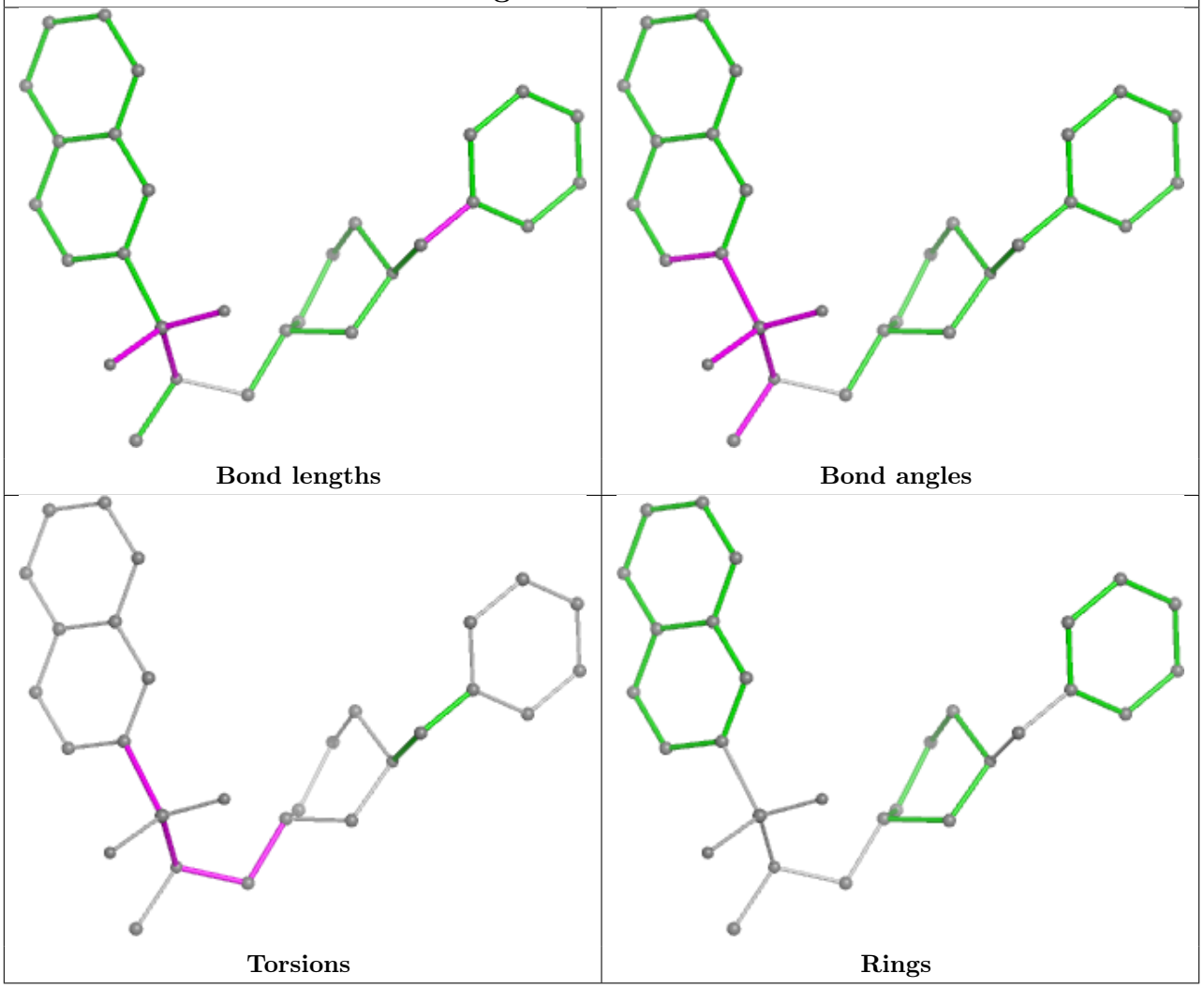


Torsions



Rings

Ligand 5HB B 612



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

6.1 Protein, DNA and RNA chains

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, 95^{th} 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%)	-0.12	3 (0%) 89 92	28, 50, 82, 133	0
1	B	524/530 (98%)	-0.01	7 (1%) 77 82	32, 53, 93, 149	1 (0%)
All	All	1050/1060 (99%)	-0.06	10 (0%) 82 86	28, 52, 88, 149	1 (0%)

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	237	TYR	3.2
1	B	52	TRP	2.7
1	B	282	TYR	2.6
1	A	237	TYR	2.4
1	B	101	ALA	2.4
1	B	364	PHE	2.3
1	A	198	SER	2.2
1	B	53	SER	2.2
1	B	28	PHE	2.2
1	A	201	ALA	2.1

6.2 Non-standard residues in protein, DNA, RNA chains

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, 95^{th} 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	0.97	0.17	36,38,56,57	0
1	CSO	A	66	7/8	0.99	0.11	43,46,56,57	0

6.3 Carbohydrates (i)

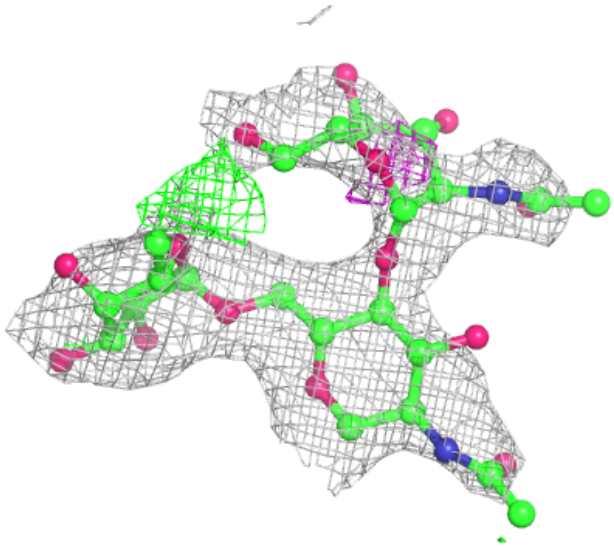
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

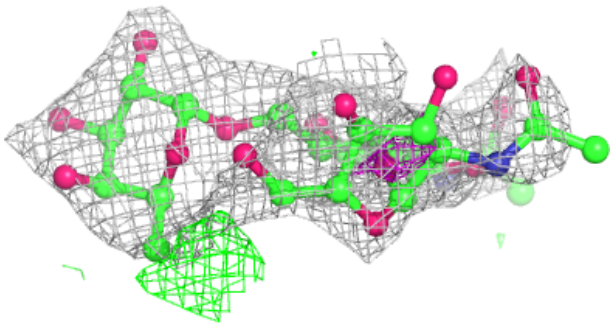
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	NAG	I	1	14/15	0.61	0.33	100,108,119,126	0
2	NAG	C	2	14/15	0.63	0.38	117,119,123,124	0
3	NAG	H	2	14/15	0.71	0.37	105,114,119,121	0
2	FUC	G	3	10/11	0.72	0.37	114,117,119,120	0
2	NAG	E	2	14/15	0.75	0.51	126,129,137,139	0
3	NAG	F	2	14/15	0.77	0.24	73,83,90,93	0
2	NAG	E	1	14/15	0.78	0.28	106,116,118,124	0
4	FUC	I	2	10/11	0.79	0.27	129,131,133,133	0
2	NAG	G	2	14/15	0.80	0.49	127,131,133,133	0
2	NAG	C	1	14/15	0.81	0.25	95,101,106,112	0
3	NAG	D	2	14/15	0.81	0.36	100,106,115,115	0
2	NAG	G	1	14/15	0.82	0.23	102,113,116,122	0
2	FUC	E	3	10/11	0.85	0.41	111,114,115,116	0
3	NAG	F	1	14/15	0.89	0.16	65,73,78,78	0
2	FUC	C	3	10/11	0.90	0.24	103,108,111,113	0
3	NAG	H	1	14/15	0.92	0.29	86,96,108,111	0
3	NAG	D	1	14/15	0.92	0.21	68,76,83,92	0

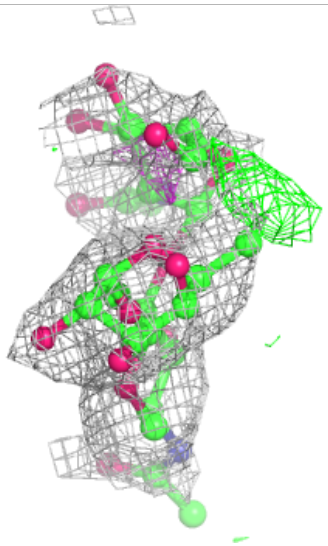
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

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)

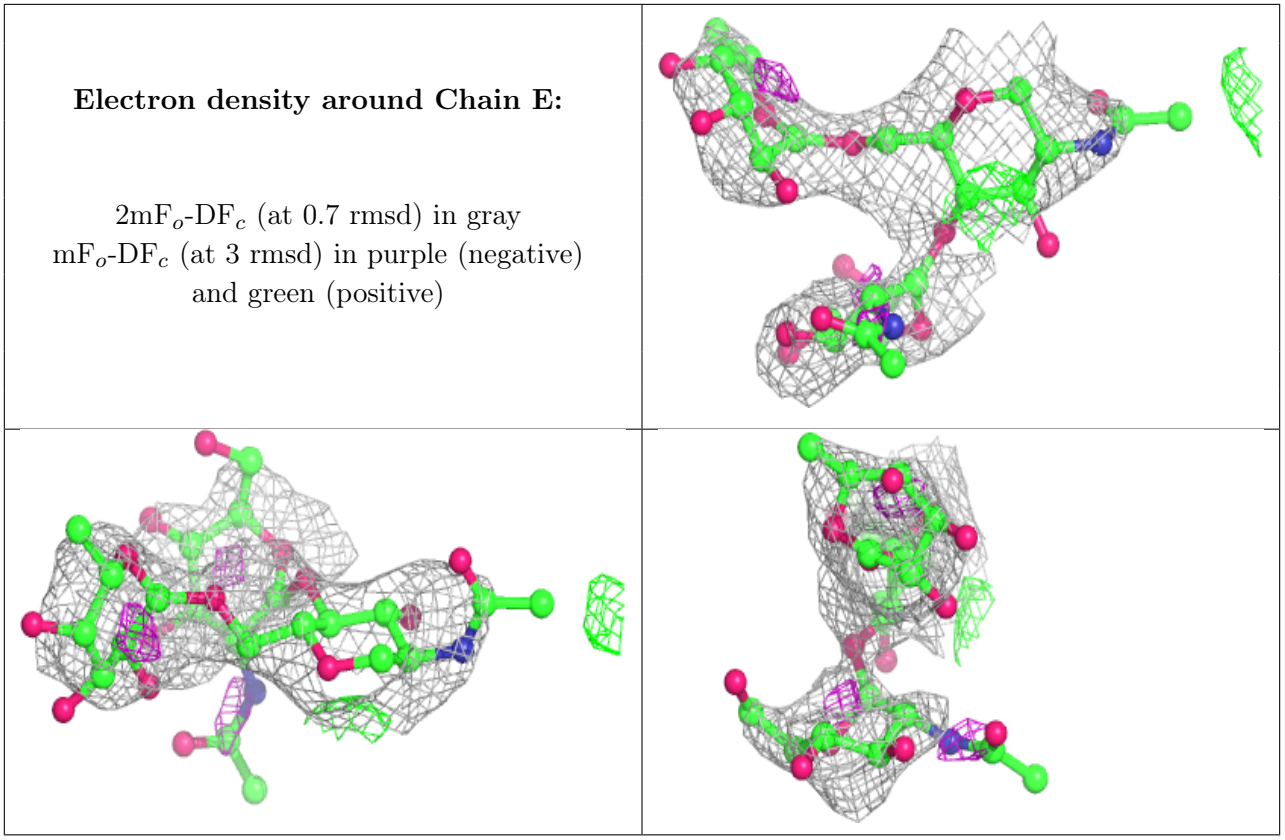






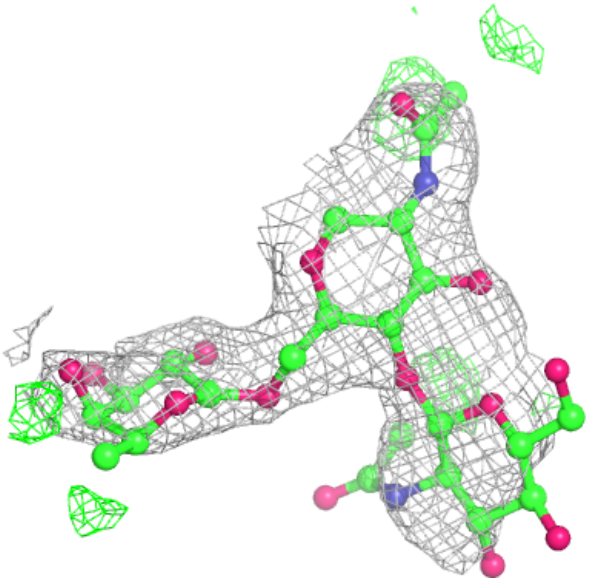
Electron density around Chain E:

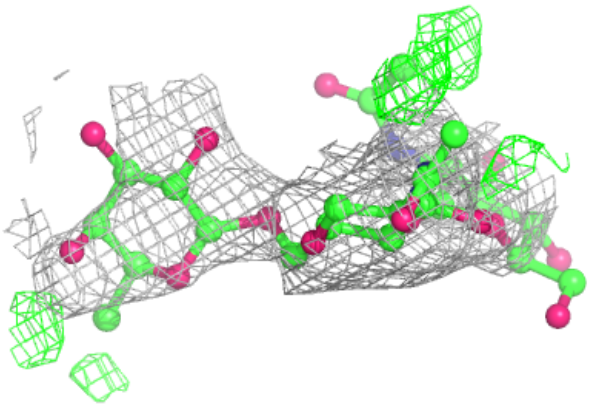
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

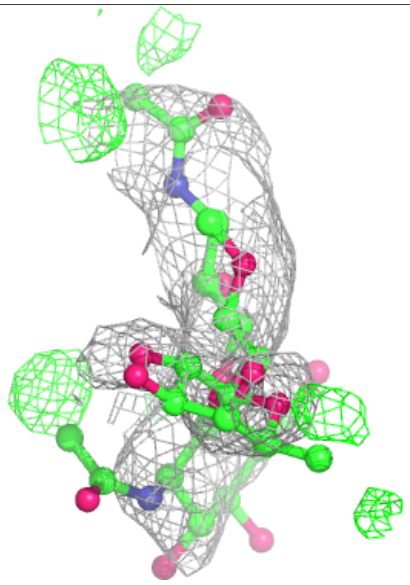


Electron density around Chain G:

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

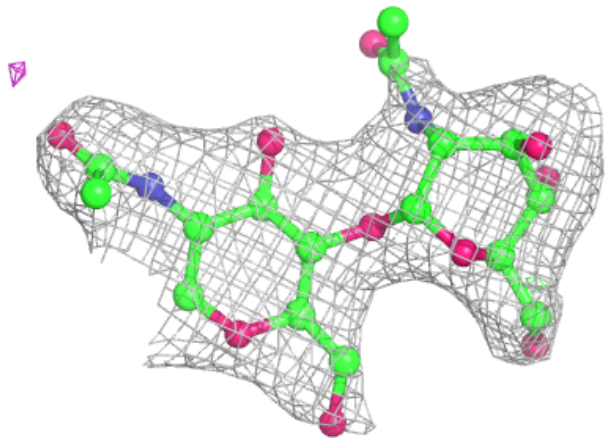


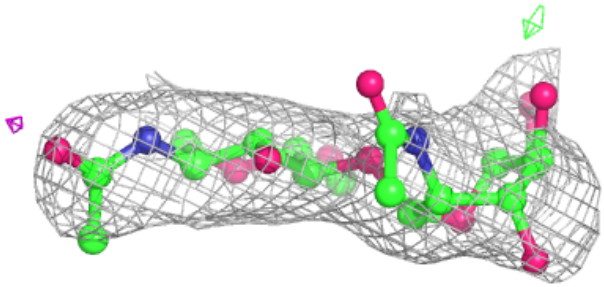


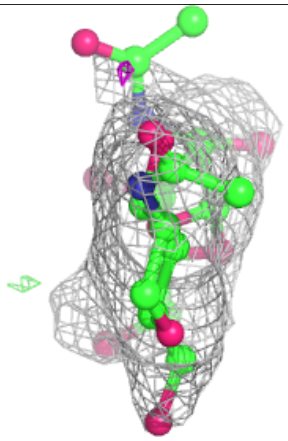


Electron density around Chain D:

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

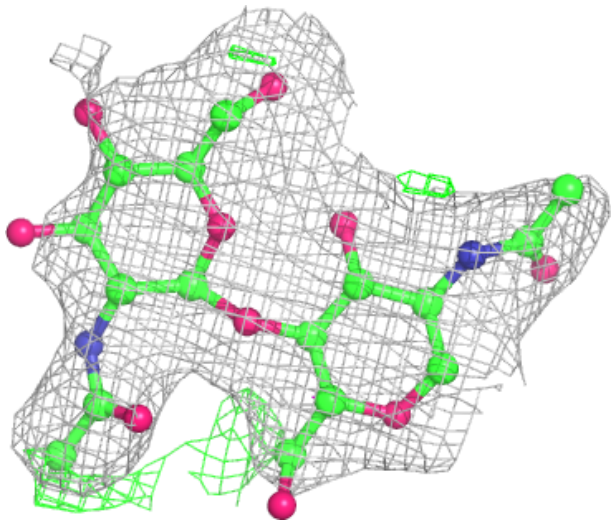


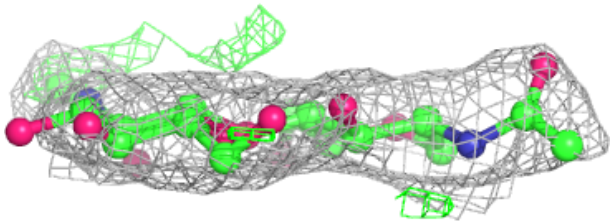


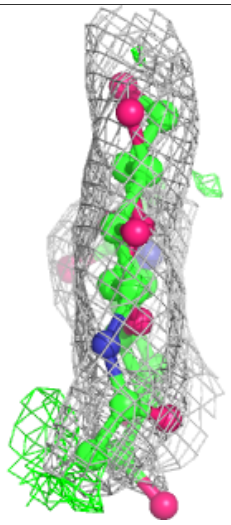


Electron density around Chain F:

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

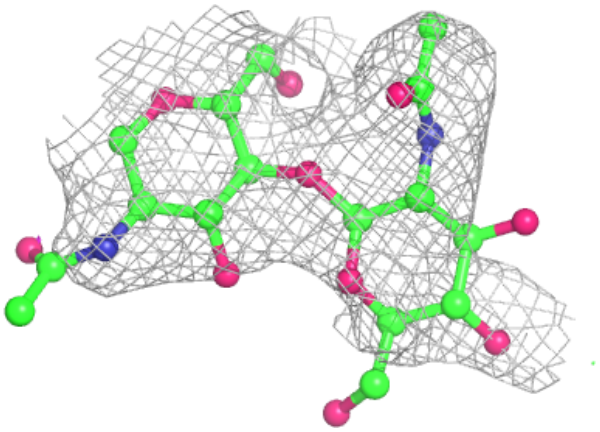


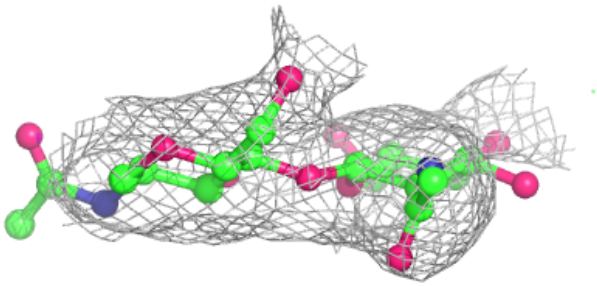


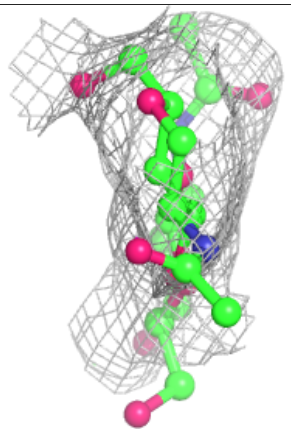


Electron density around Chain H:

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

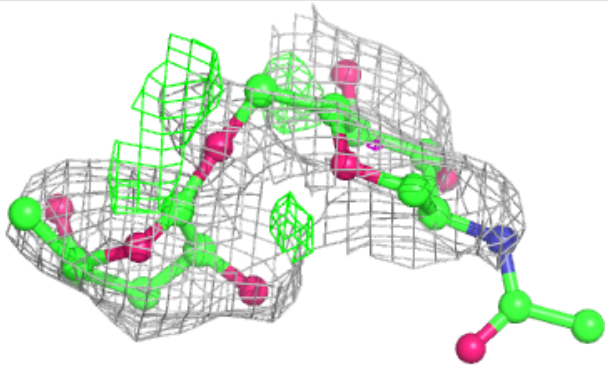


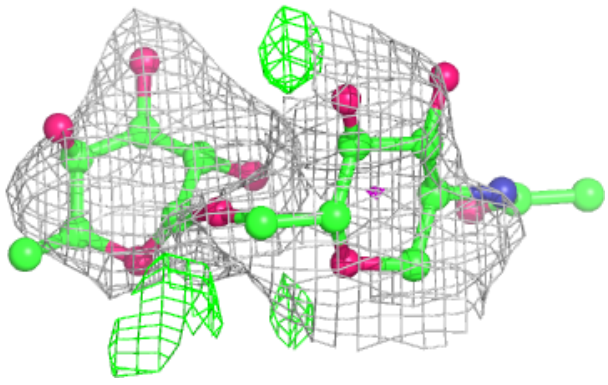


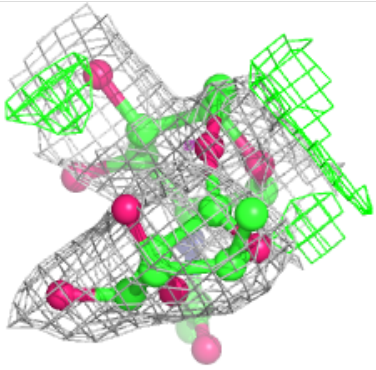


Electron density around Chain I:

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







6.4 Ligands (i)

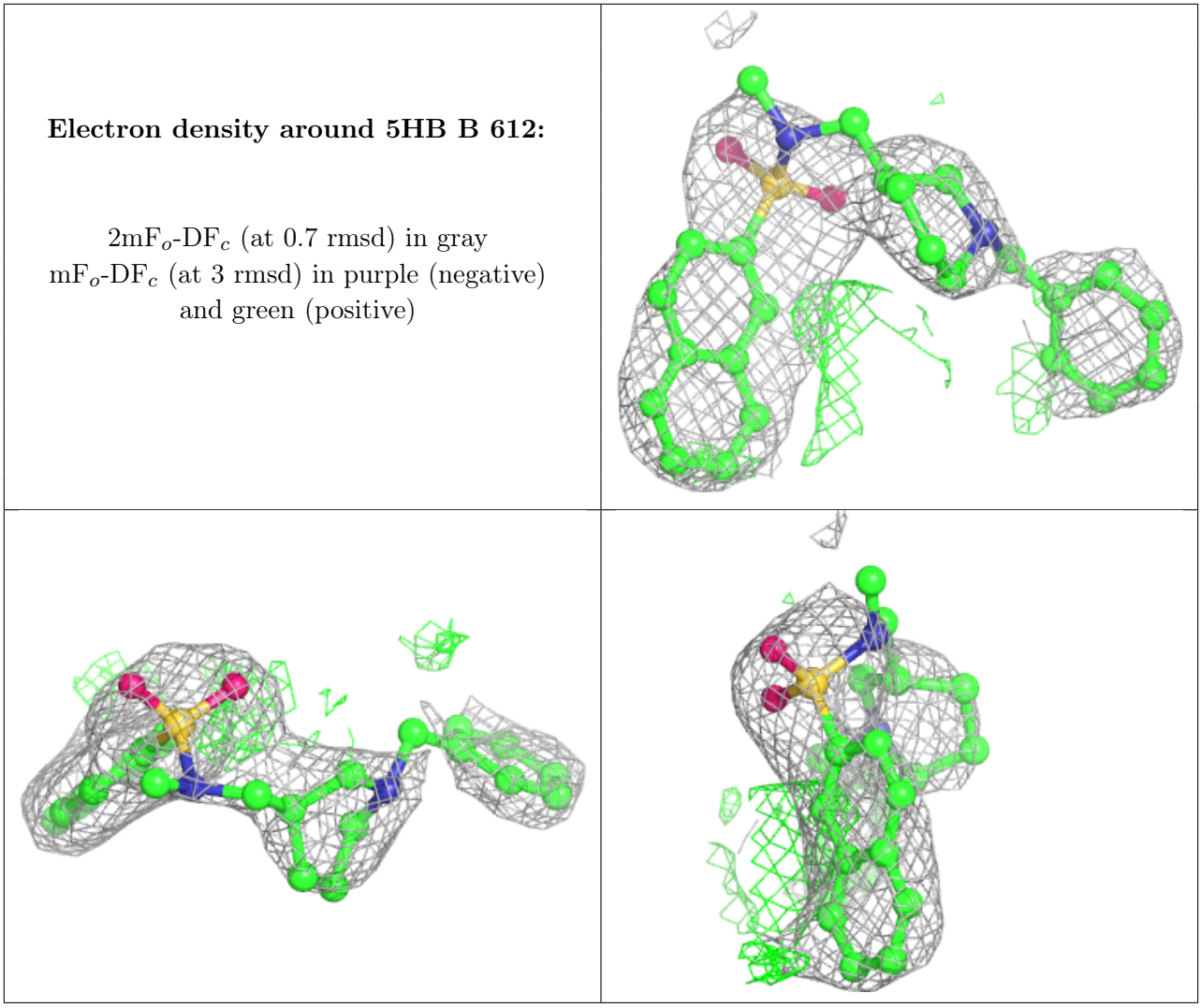
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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	0.65	0.30	105,114,121,122	0
5	NAG	B	602	14/15	0.67	0.24	96,113,122,123	0
5	NAG	A	601	14/15	0.74	0.31	76,91,96,99	0
8	EDO	B	615	4/4	0.76	0.20	67,71,75,76	0
5	NAG	B	607	14/15	0.78	0.17	103,108,112,113	0
7	GOL	B	614	6/6	0.79	0.35	78,83,87,93	0
5	NAG	B	611	14/15	0.81	0.28	96,111,115,117	0
5	NAG	B	603	14/15	0.82	0.35	97,100,109,110	0
11	PEG	B	621	7/7	0.82	0.21	75,83,87,87	0
5	NAG	A	610	14/15	0.83	0.21	74,79,84,84	0
10	FUL	B	606	10/11	0.85	0.36	96,103,105,105	0
8	EDO	B	616	4/4	0.85	0.34	82,83,84,87	0
7	GOL	A	618	6/6	0.86	0.30	64,73,77,78	0
8	EDO	A	620	4/4	0.87	0.14	75,77,78,78	0
7	GOL	A	617	6/6	0.88	0.23	76,79,81,82	0
6	5HB	B	612	29/29	0.89	0.25	60,82,89,89	0
7	GOL	A	619	6/6	0.89	0.28	78,83,87,91	0
6	5HB	A	616	29/29	0.90	0.24	55,90,95,95	0
5	NAG	B	608	14/15	0.91	0.28	67,74,82,83	0
7	GOL	B	613	6/6	0.93	0.19	60,65,74,77	0
8	EDO	B	617	4/4	0.93	0.11	80,81,83,84	0
9	UNX	B	620	1/1	0.96	0.61	64,64,64,64	0
9	UNX	A	621	1/1	0.96	0.48	82,82,82,82	0
9	UNX	B	618	1/1	0.96	0.69	62,62,62,62	0
9	UNX	A	623	1/1	0.97	0.52	66,66,66,66	0
9	UNX	B	619	1/1	0.98	1.09	73,73,73,73	0
9	UNX	A	622	1/1	0.98	0.71	65,65,65,65	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.

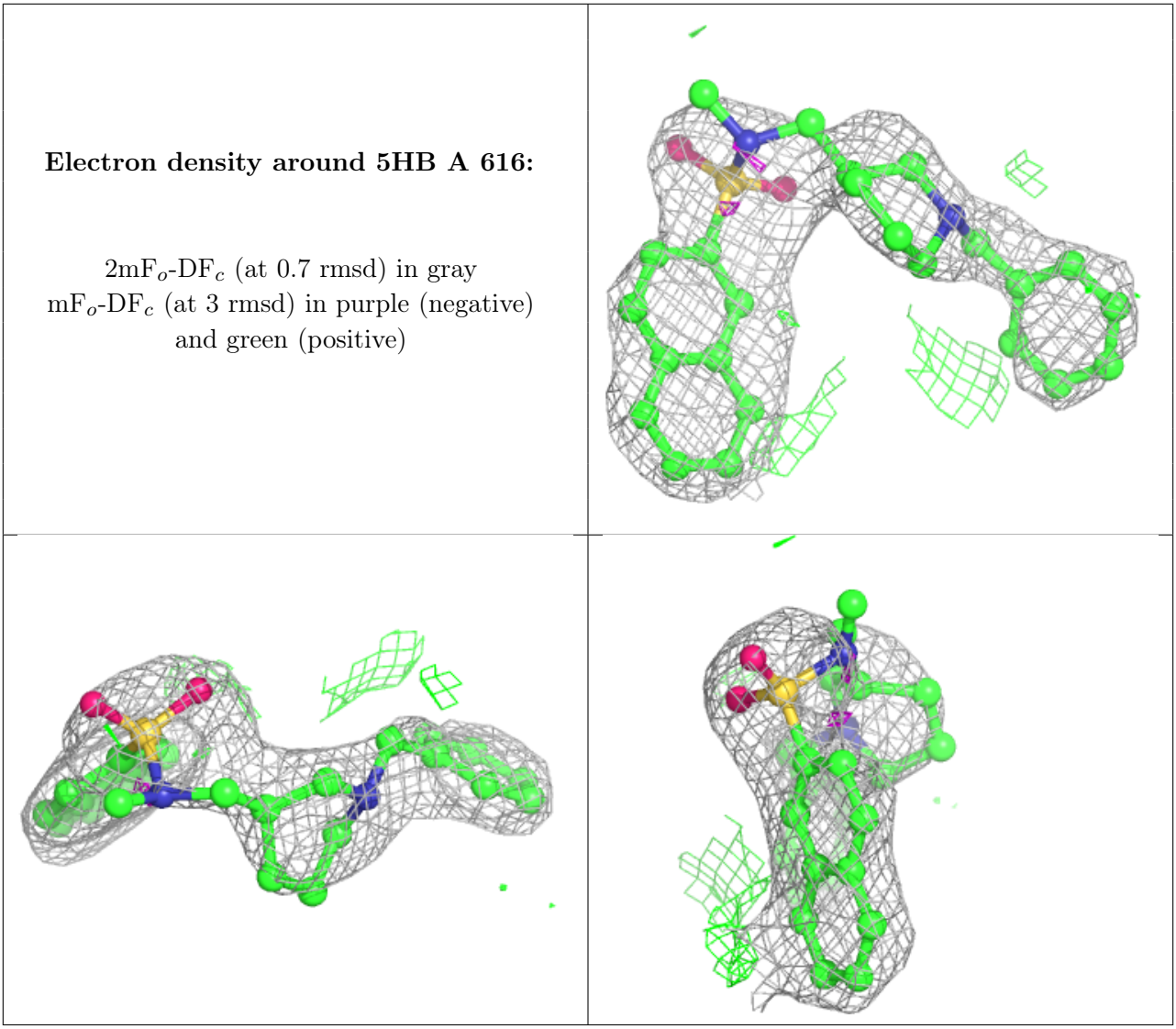
Electron density around 5HB B 612:

$2mF_o$-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 616:

$2mF_o$-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.