



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 9, 2020 – 05:54 PM BST

PDB ID : 5NN0
Title : Crystal structure of huBChE with N-((1-(2,3-dihydro-1H-inden-2-yl)piperidin-3-yl)methyl)-N-(2-(dimethylamino)ethyl)-2-naphthamide.
Authors : Coquelle, N.; Brus, B.; Colletier, J.P.
Deposited on : 2017-04-07
Resolution : 2.10 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.13.1
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) : 2.13.1

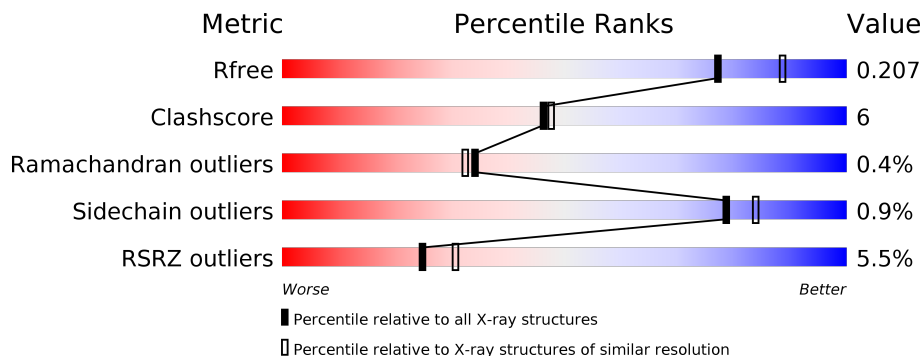
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

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 on 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	529	 5% 86% 13%
2	B	3	 67% 33%
2	D	3	 67% 33%
3	C	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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	FUC	C	2	X	-	-	-
4	NAG	A	608	X	-	-	-

2 Entry composition i

There are 12 unique types of molecules in this entry. The entry contains 4858 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.

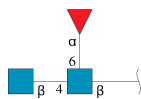
- Molecule 1 is a protein called Cholinesterase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	527	4236	2743	701	777	15	0	14	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	17	GLN	ASN	engineered mutation	UNP P06276
A	455	GLN	ASN	engineered mutation	UNP P06276
A	481	GLN	ASN	engineered mutation	UNP P06276

- 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.



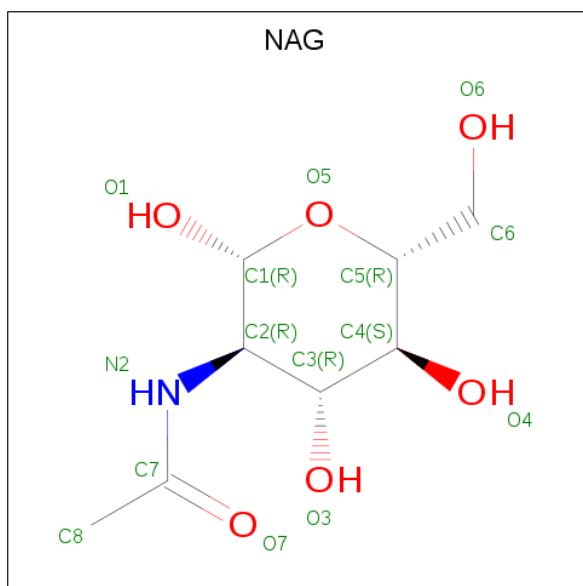
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	B	3	38	22	2	14	0	0	0
2	D	3	38	22	2	14	0	0	0

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



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

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



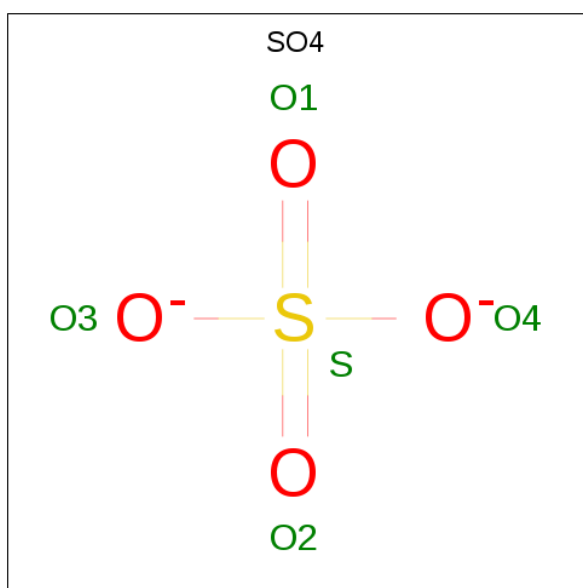
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
4	A	1	14	8	1	5	0	0
4	A	1	14	8	1	5	0	0
4	A	1	14	8	1	5	0	0

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 6 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	O	S	0	0
			5	4	1		
6	A	1	Total	O	S	0	0
			5	4	1		

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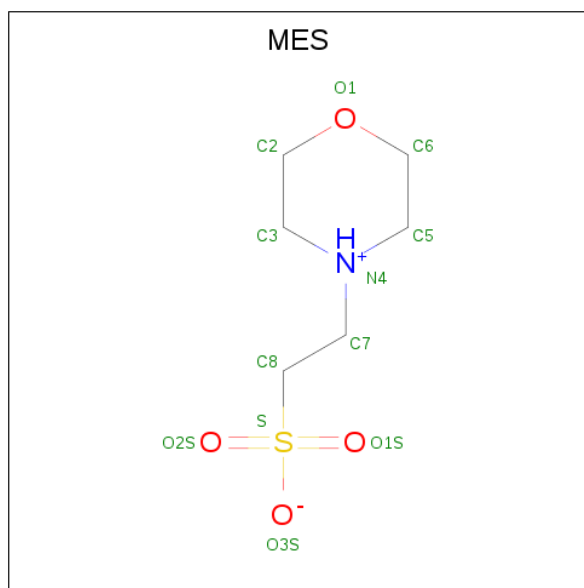
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	O	S	0	0
			5	4	1		
6	A	1	Total	O	S	0	0
			5	4	1		
6	A	1	Total	O	S	0	0
			5	4	1		
6	A	1	Total	O	S	0	0
			5	4	1		

- Molecule 7 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

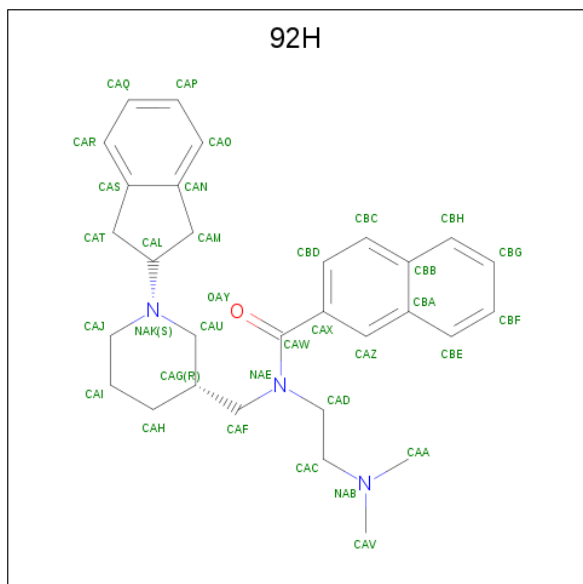
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	3	Total	Cl	0	0
			3	3		

- Molecule 8 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: C₆H₁₃NO₄S).



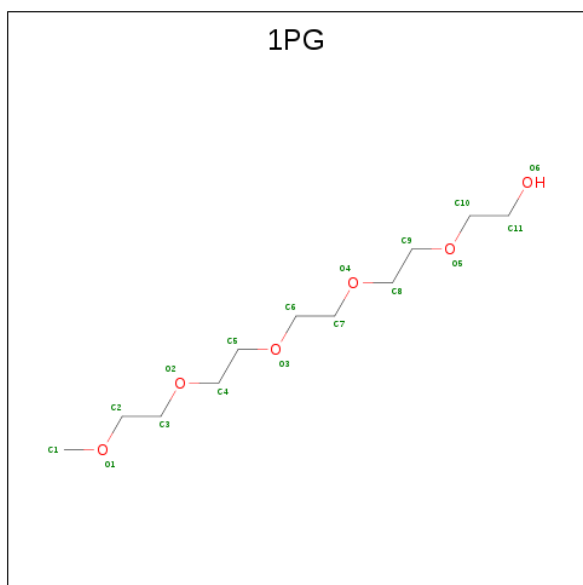
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
8	A	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
8	A	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

- Molecule 9 is {N}-[[[(3 {R})-1-(2,3-dihydro-1 {H}-inden-2-yl)piperidin-3-yl)methyl]- {N}]-[2-(dimethylamino)ethyl]naphthalene-2-carboxamide (three-letter code: 92H) (formula: C₃₀H₃₇N₃O).



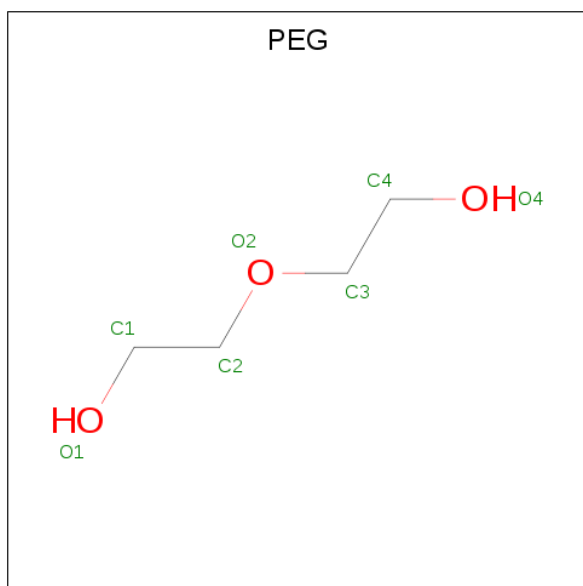
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
9	A	1	34	30	3	1	0	0
9	A	1	34	30	3	1	0	0

- Molecule 10 is 2-(2-{2-[2-(2-METHOXY-ETHOXY)-ETHOXY]-ETHOXY}-ETHOXY)-ETHANOL (three-letter code: 1PG) (formula: C₁₁H₂₄O₆).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	A	1	Total	C	O	0	0
			17	11	6		

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



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

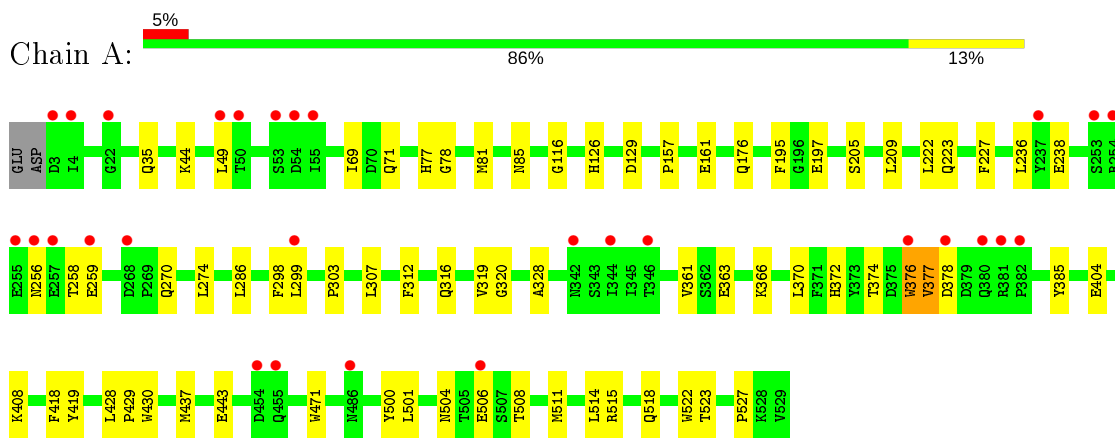
- Molecule 12 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	A	314	Total	O	0	0
			314	314		

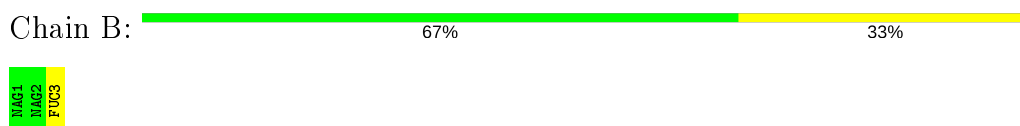
3 Residue-property plots [i](#)

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.

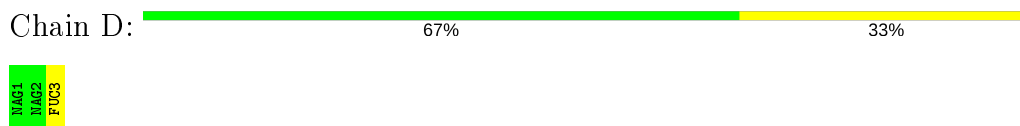
- Molecule 1: Cholinesterase



- 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



- Molecule 3: alpha-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose



4 Data and refinement statistics

Property	Value	Source
Space group	I 4 2 2	Depositor
Cell constants a, b, c, α , β , γ	154.97Å 154.97Å 126.68Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.83 – 2.10 47.83 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.2 (47.83-2.10) 99.3 (47.83-2.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.92 (at 2.10Å)	Xtrriage
Refinement program	PHENIX (1.11.1_2575: ???)	Depositor
R, R_{free}	0.169 , 0.206 0.170 , 0.207	Depositor DCC
R_{free} test set	2237 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	36.0	Xtrriage
Anisotropy	0.319	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 63.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	4858	wwPDB-VP
Average B, all atoms (Å ²)	42.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.43% 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: 92H, GOL, NAG, CL, 1PG, FUC, MES, PEG, SO4

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	0.38	0/4393	0.53	0/5970

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4236	0	4141	55	0
2	B	38	0	34	0	0
2	D	38	0	34	0	0
3	C	24	0	22	0	0
4	A	42	0	39	0	0
5	A	12	0	16	4	0
6	A	35	0	0	1	0
7	A	3	0	0	0	0
8	A	24	0	24	7	0
9	A	68	0	0	1	0
10	A	17	0	24	8	0
11	A	7	0	10	2	0
12	A	314	0	0	5	0
All	All	4858	0	4344	56	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

All (56) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:77:HIS:HE2	10:A:628:1PG:H42	1.52	0.74
1:A:85:ASN:ND2	5:A:613:GOL:H11	2.05	0.72
1:A:372:HIS:NE2	6:A:620:SO4:O4	2.19	0.70
1:A:514:LEU:HD12	8:A:625:MES:H52	1.74	0.69
1:A:316:GLN:HE22	11:A:629:PEG:H22	1.59	0.66
1:A:504[B]:ASN:OD1	12:A:701:HOH:O	2.12	0.66
1:A:85:ASN:HD22	5:A:613:GOL:H11	1.62	0.63
1:A:500:TYR:CZ	1:A:511:MET:HB2	2.35	0.62
1:A:157:PRO:HG2	1:A:236:LEU:HD12	1.83	0.60
1:A:377:VAL:HG23	1:A:378:ASP:H	1.67	0.60
1:A:515:ARG:NH2	8:A:625:MES:H71	2.18	0.59
1:A:81:MET:HE3	10:A:628:1PG:H21	1.85	0.57
1:A:69[B]:ILE:HG23	1:A:71[B]:GLN:HG2	1.87	0.57
1:A:116:GLY:HA2	9:A:627:92H:OAY	2.05	0.56
1:A:361:VAL:O	1:A:366:LYS:NZ	2.38	0.56
1:A:515:ARG:HD3	8:A:625:MES:H32	1.87	0.56
1:A:522:TRP:O	1:A:527:PRO:HD3	2.06	0.54
1:A:176[A]:GLN:NE2	12:A:714:HOH:O	2.40	0.54
1:A:508:THR:OG1	12:A:702:HOH:O	2.18	0.54
1:A:77:HIS:NE2	10:A:628:1PG:H42	2.20	0.53
1:A:319:VAL:O	1:A:418:PHE:HA	2.08	0.53
1:A:443:GLU:OE2	10:A:628:1PG:H13	2.10	0.52
1:A:316:GLN:NE2	11:A:629:PEG:H22	2.25	0.51
1:A:428:LEU:HD23	1:A:430:TRP:H	1.76	0.51
1:A:77:HIS:HE2	10:A:628:1PG:H32	1.76	0.50
1:A:126:HIS:HB2	5:A:613:GOL:H12	1.92	0.50
1:A:81:MET:HE3	10:A:628:1PG:H51	1.93	0.50
1:A:515:ARG:HH22	8:A:625:MES:H71	1.77	0.49
1:A:209:LEU:HD23	1:A:312:PHE:HB3	1.94	0.48
1:A:518:GLN:HG3	8:A:624:MES:H62	1.96	0.47
1:A:77:HIS:HE1	10:A:628:1PG:H72	1.78	0.47
1:A:81:MET:CE	10:A:628:1PG:H21	2.45	0.46
1:A:129:ASP:OD1	5:A:612:GOL:H31	2.14	0.46
1:A:270:GLN:O	1:A:274:LEU:HG	2.15	0.46
1:A:238:GLU:OE1	12:A:703:HOH:O	2.19	0.46
1:A:197:GLU:HA	1:A:223:GLN:O	2.16	0.46
1:A:320:GLY:HA3	1:A:419:TYR:CE2	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:328:ALA:HB2	1:A:437:MET:HE3	1.99	0.45
1:A:256:ASN:OD1	1:A:259:GLU:HG2	2.17	0.45
1:A:227:PHE:HZ	1:A:307:LEU:HB2	1.82	0.45
1:A:363[A]:GLU:CD	1:A:363[A]:GLU:H	2.20	0.44
1:A:404[B]:GLU:OE2	1:A:408:LYS:HE2	2.16	0.44
1:A:370:LEU:O	1:A:374:THR:OG1	2.30	0.44
1:A:518:GLN:HA	8:A:624:MES:H62	2.01	0.43
1:A:35:GLN:HA	1:A:49:LEU:HD13	2.01	0.43
1:A:501:LEU:HD11	1:A:508:THR:CG2	2.48	0.43
1:A:370:LEU:HD12	1:A:374:THR:HG21	2.01	0.43
1:A:205:SER:HB3	1:A:222[A]:LEU:HD21	2.02	0.42
1:A:298:PHE:HD2	1:A:299[B]:LEU:HG	1.84	0.42
8:A:625:MES:H82	8:A:625:MES:H31	1.85	0.41
1:A:376:TRP:HH2	1:A:385:TYR:CE1	2.37	0.41
1:A:523:THR:HG22	12:A:974:HOH:O	2.20	0.41
1:A:78:GLY:HA2	1:A:429:PRO:HG2	2.01	0.41
1:A:44[B]:LYS:NZ	1:A:161:GLU:OE1	2.51	0.41
1:A:161:GLU:HG3	1:A:258:THR:HG23	2.03	0.40
1:A:227:PHE:CE1	1:A:303:PRO:HB2	2.56	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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	539/529 (102%)	519 (96%)	18 (3%)	2 (0%)	34 32

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	377	VAL
1	A	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	457/454 (101%)	453 (99%)	4 (1%)	78 84

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	195	PHE
1	A	286	LEU
1	A	376	TRP
1	A	471	TRP

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

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

8 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	B	1	1,2	14,14,15	0.59	0	17,19,21	0.50	0
2	NAG	B	2	2	14,14,15	0.35	0	17,19,21	0.33	0
2	FUC	B	3	2	10,10,11	1.63	1 (10%)	14,14,16	1.40	2 (14%)
3	NAG	C	1	1,3	14,14,15	0.34	0	17,19,21	0.39	0
3	FUC	C	2	3	10,10,11	1.91	3 (30%)	14,14,16	1.09	2 (14%)
2	NAG	D	1	1,2	14,14,15	0.34	0	17,19,21	0.59	0
2	NAG	D	2	2	14,14,15	0.29	0	17,19,21	0.49	0
2	FUC	D	3	2	10,10,11	1.83	2 (20%)	14,14,16	1.17	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
2	NAG	B	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	B	2	2	-	2/6/23/26	0/1/1/1
2	FUC	B	3	2	-	-	0/1/1/1
3	NAG	C	1	1,3	-	2/6/23/26	0/1/1/1
3	FUC	C	2	3	1/1/4/5	-	0/1/1/1
2	NAG	D	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	D	2	2	-	2/6/23/26	0/1/1/1
2	FUC	D	3	2	-	-	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	2	FUC	O5-C1	4.72	1.51	1.43
2	D	3	FUC	O5-C1	4.50	1.50	1.43
2	B	3	FUC	O5-C1	4.04	1.50	1.43
2	D	3	FUC	C2-C3	-2.50	1.48	1.52
3	C	2	FUC	C2-C3	-2.40	1.49	1.52
3	C	2	FUC	O5-C5	2.15	1.48	1.43

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	3	FUC	C1-C2-C3	3.74	114.27	109.67
3	C	2	FUC	C6-C5-C4	-2.58	108.31	113.07
2	B	3	FUC	C2-C3-C4	2.26	114.80	110.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	2	FUC	O5-C5-C4	2.21	113.49	109.52
2	D	3	FUC	C6-C5-C4	-2.04	109.30	113.07
2	D	3	FUC	O5-C5-C4	2.01	113.12	109.52

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	C	2	FUC	C1

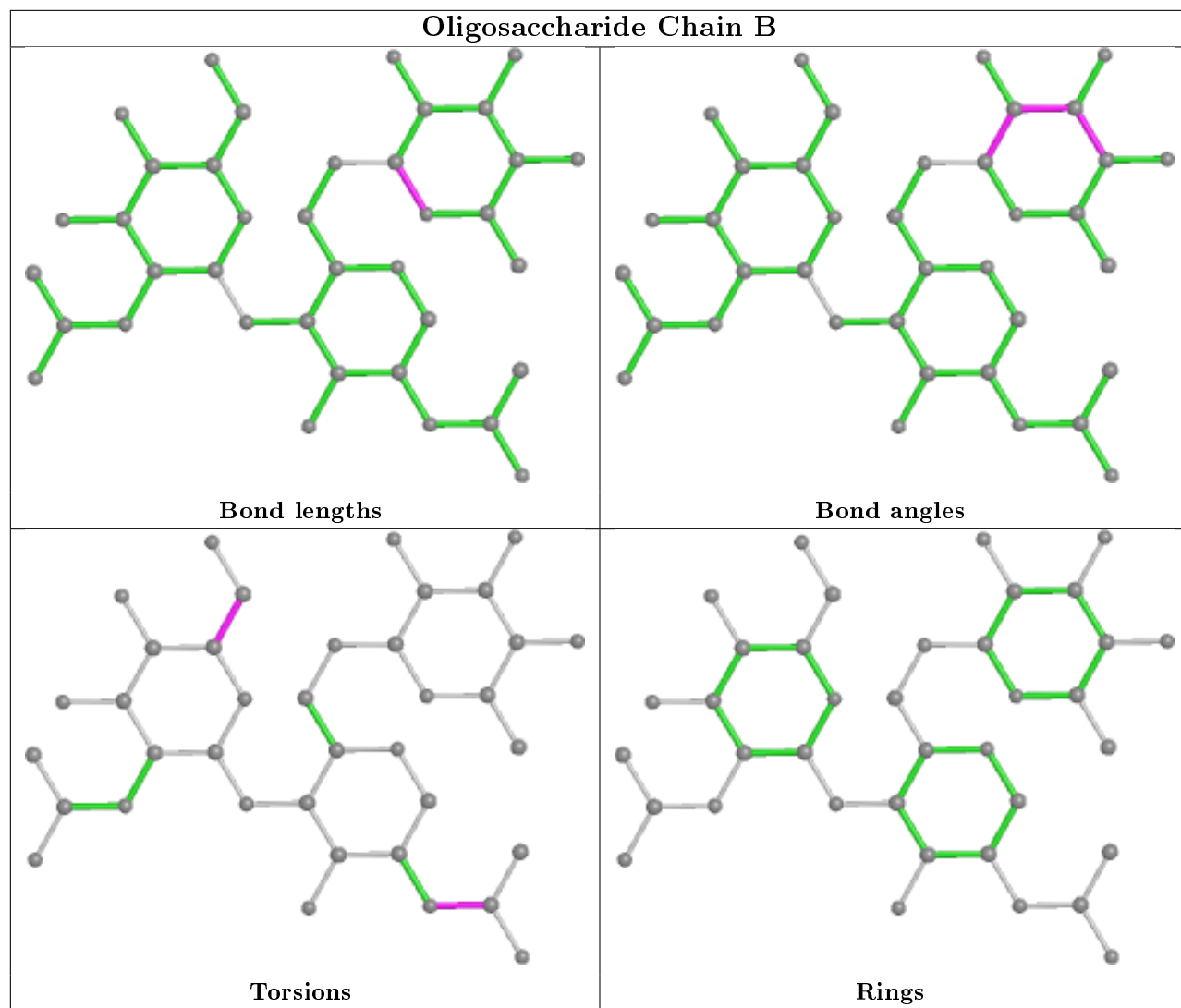
All (8) torsion outliers are listed below:

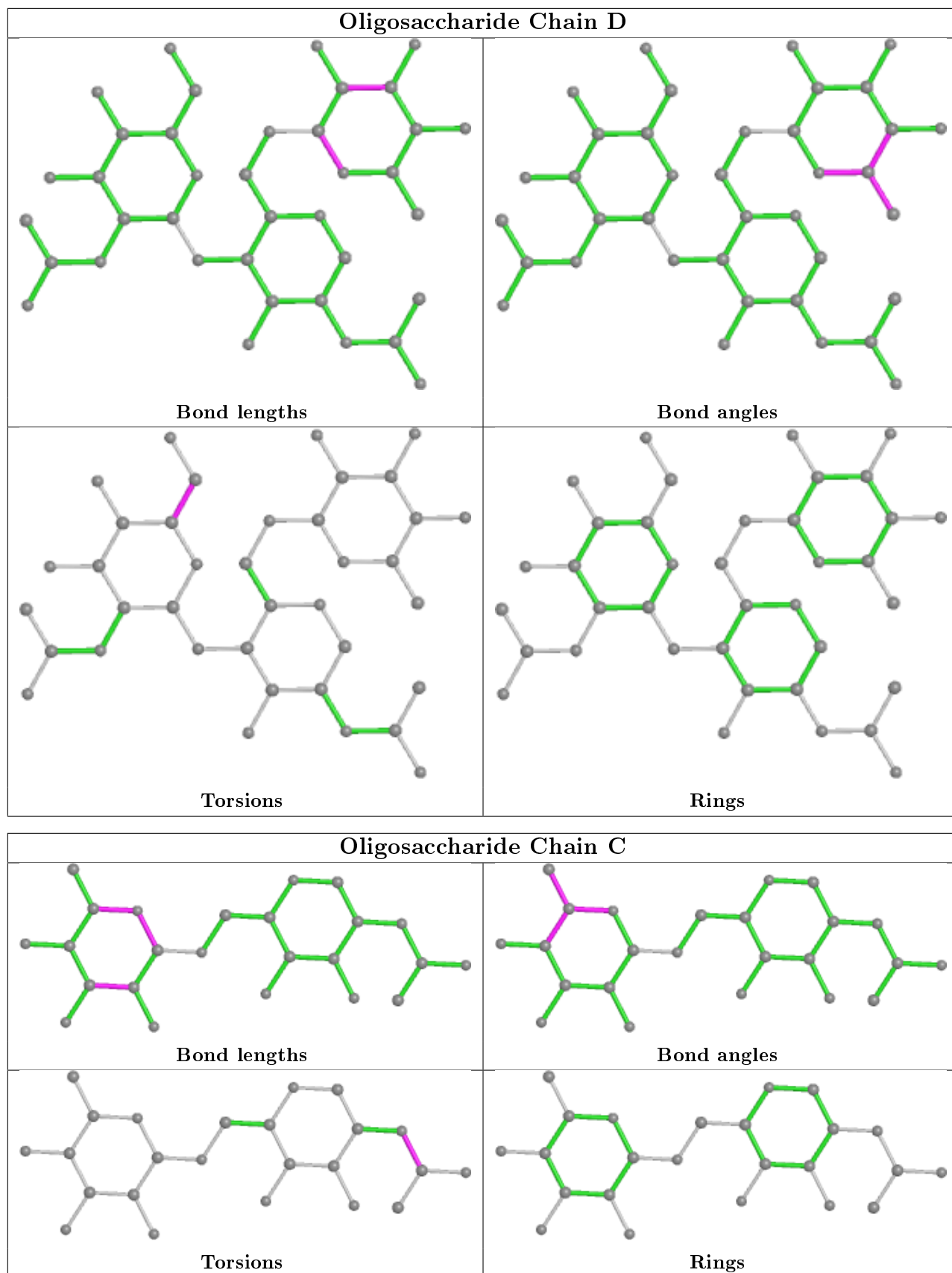
Mol	Chain	Res	Type	Atoms
2	D	2	NAG	O5-C5-C6-O6
2	B	2	NAG	O5-C5-C6-O6
2	D	2	NAG	C4-C5-C6-O6
3	C	1	NAG	C8-C7-N2-C2
3	C	1	NAG	O7-C7-N2-C2
2	B	1	NAG	C8-C7-N2-C2
2	B	1	NAG	O7-C7-N2-C2
2	B	2	NAG	C4-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

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





5.6 Ligand geometry

Of 21 ligands modelled in this entry, 3 are monoatomic - leaving 18 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
6	SO4	A	619	-	4,4,4	0.14	0	6,6,6	0.06	0
10	1PG	A	628	-	16,16,16	0.53	0	15,15,15	0.37	0
6	SO4	A	616	-	4,4,4	0.19	0	6,6,6	0.16	0
6	SO4	A	618	9	4,4,4	0.35	0	6,6,6	0.28	0
4	NAG	A	607	1	14,14,15	0.31	0	17,19,21	0.43	0
6	SO4	A	617	9	4,4,4	0.12	0	6,6,6	0.24	0
8	MES	A	624	-	12,12,12	2.32	1 (8%)	14,16,16	1.93	2 (14%)
11	PEG	A	629	-	6,6,6	0.49	0	5,5,5	0.20	0
6	SO4	A	620	-	4,4,4	0.17	0	6,6,6	0.19	0
4	NAG	A	606	1	14,14,15	0.29	0	17,19,21	0.87	1 (5%)
6	SO4	A	614	-	4,4,4	0.13	0	6,6,6	0.16	0
5	GOL	A	612	-	5,5,5	0.50	0	5,5,5	0.49	0
8	MES	A	625	-	12,12,12	2.11	1 (8%)	14,16,16	2.03	5 (35%)
9	92H	A	627	-	38,38,38	2.05	7 (18%)	49,53,53	1.20	3 (6%)
4	NAG	A	608	1	14,14,15	0.43	0	17,19,21	0.48	0
9	92H	A	626	6	38,38,38	2.08	7 (18%)	49,53,53	1.39	6 (12%)
6	SO4	A	615	-	4,4,4	0.16	0	6,6,6	0.12	0
5	GOL	A	613	-	5,5,5	0.39	0	5,5,5	0.67	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
9	92H	A	627	-	-	2/21/39/39	0/5/5/5
4	NAG	A	607	1	-	1/6/23/26	0/1/1/1
4	NAG	A	606	1	-	4/6/23/26	0/1/1/1
8	MES	A	624	-	-	0/6/14/14	0/1/1/1
11	PEG	A	629	-	-	2/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	1PG	A	628	-	-	11/14/14/14	-
5	GOL	A	612	-	-	2/4/4/4	-
8	MES	A	625	-	-	3/6/14/14	0/1/1/1
4	NAG	A	608	1	1/1/5/7	0/6/23/26	0/1/1/1
9	92H	A	626	6	-	7/21/39/39	1/5/5/5
5	GOL	A	613	-	-	2/4/4/4	-

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	A	624	MES	C8-S	-7.75	1.66	1.77
9	A	626	92H	CAT-CAS	-7.24	1.38	1.50
8	A	625	MES	C8-S	-7.01	1.67	1.77
9	A	626	92H	CAX-CAW	-6.40	1.39	1.50
9	A	627	92H	CAM-CAN	-6.22	1.40	1.50
9	A	627	92H	CAT-CAS	-6.05	1.40	1.50
9	A	627	92H	CAX-CAW	-5.31	1.41	1.50
9	A	626	92H	CAM-CAN	-4.40	1.43	1.50
9	A	627	92H	CAO-CAN	-3.46	1.33	1.39
9	A	627	92H	CAR-CAS	-3.29	1.34	1.39
9	A	626	92H	CAO-CAN	-3.25	1.34	1.39
9	A	626	92H	CAR-CAS	-3.19	1.34	1.39
9	A	626	92H	CAT-CAL	-2.54	1.50	1.54
9	A	626	92H	CAS-CAN	-2.21	1.35	1.39
9	A	627	92H	CAM-CAL	-2.12	1.50	1.54
9	A	627	92H	CAS-CAN	-2.10	1.35	1.39

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	624	MES	C5-N4-C3	5.88	122.06	108.83
9	A	626	92H	CAN-CAM-CAL	-5.31	97.72	103.39
9	A	627	92H	CAJ-NAK-CAU	4.51	112.63	108.19
8	A	625	MES	C5-N4-C3	3.80	117.39	108.83
9	A	626	92H	CAH-CAI-CAJ	-3.65	105.74	110.85
8	A	625	MES	O2S-S-C8	3.21	110.78	106.92
9	A	627	92H	CAX-CAW-NAE	3.14	122.71	118.72
4	A	606	NAG	C1-O5-C5	2.73	115.89	112.19
9	A	627	92H	CAG-CAU-NAK	2.67	115.67	110.45
8	A	625	MES	O3S-S-C8	2.65	110.06	105.77
8	A	625	MES	C7-N4-C3	2.63	117.97	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	A	626	92H	CAZ-CAX-CAW	-2.48	115.66	120.52
8	A	624	MES	O3S-S-C8	2.31	109.51	105.77
8	A	625	MES	C7-N4-C5	2.28	117.07	111.23
9	A	626	92H	CAT-CAS-CAN	-2.13	109.09	110.56
9	A	626	92H	CAS-CAT-CAL	-2.01	101.25	103.39
9	A	626	92H	CAJ-NAK-CAU	2.00	110.16	108.19

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	A	608	NAG	C1

All (34) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	A	627	92H	NAE-CAF-CAG-CAH
5	A	612	GOL	O1-C1-C2-C3
8	A	625	MES	C7-C8-S-O1S
8	A	625	MES	C7-C8-S-O3S
9	A	626	92H	NAE-CAF-CAG-CAH
9	A	626	92H	NAE-CAF-CAG-CAU
9	A	626	92H	CAM-CAL-NAK-CAJ
9	A	626	92H	CAM-CAL-NAK-CAU
9	A	626	92H	CAT-CAL-NAK-CAJ
9	A	626	92H	CAT-CAL-NAK-CAU
5	A	613	GOL	O1-C1-C2-C3
4	A	606	NAG	O5-C5-C6-O6
4	A	606	NAG	C8-C7-N2-C2
4	A	606	NAG	O7-C7-N2-C2
10	A	628	1PG	C4-C5-O3-C6
11	A	629	PEG	O2-C3-C4-O4
4	A	606	NAG	C4-C5-C6-O6
9	A	626	92H	CAD-CAC-NAB-CAV
10	A	628	1PG	O5-C10-C11-O6
5	A	612	GOL	O1-C1-C2-O2
5	A	613	GOL	O1-C1-C2-O2
10	A	628	1PG	C3-C2-O1-C1
9	A	627	92H	NAE-CAF-CAG-CAU
10	A	628	1PG	C2-C3-O2-C4
10	A	628	1PG	C5-C4-O2-C3
10	A	628	1PG	C8-C9-O5-C10
8	A	625	MES	C7-C8-S-O2S

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Mol	Chain	Res	Type	Atoms
11	A	629	PEG	C4-C3-O2-C2
10	A	628	1PG	O4-C8-C9-O5
10	A	628	1PG	C9-C8-O4-C7
10	A	628	1PG	O1-C2-C3-O2
10	A	628	1PG	C7-C6-O3-C5
10	A	628	1PG	O2-C4-C5-O3
4	A	607	NAG	C4-C5-C6-O6

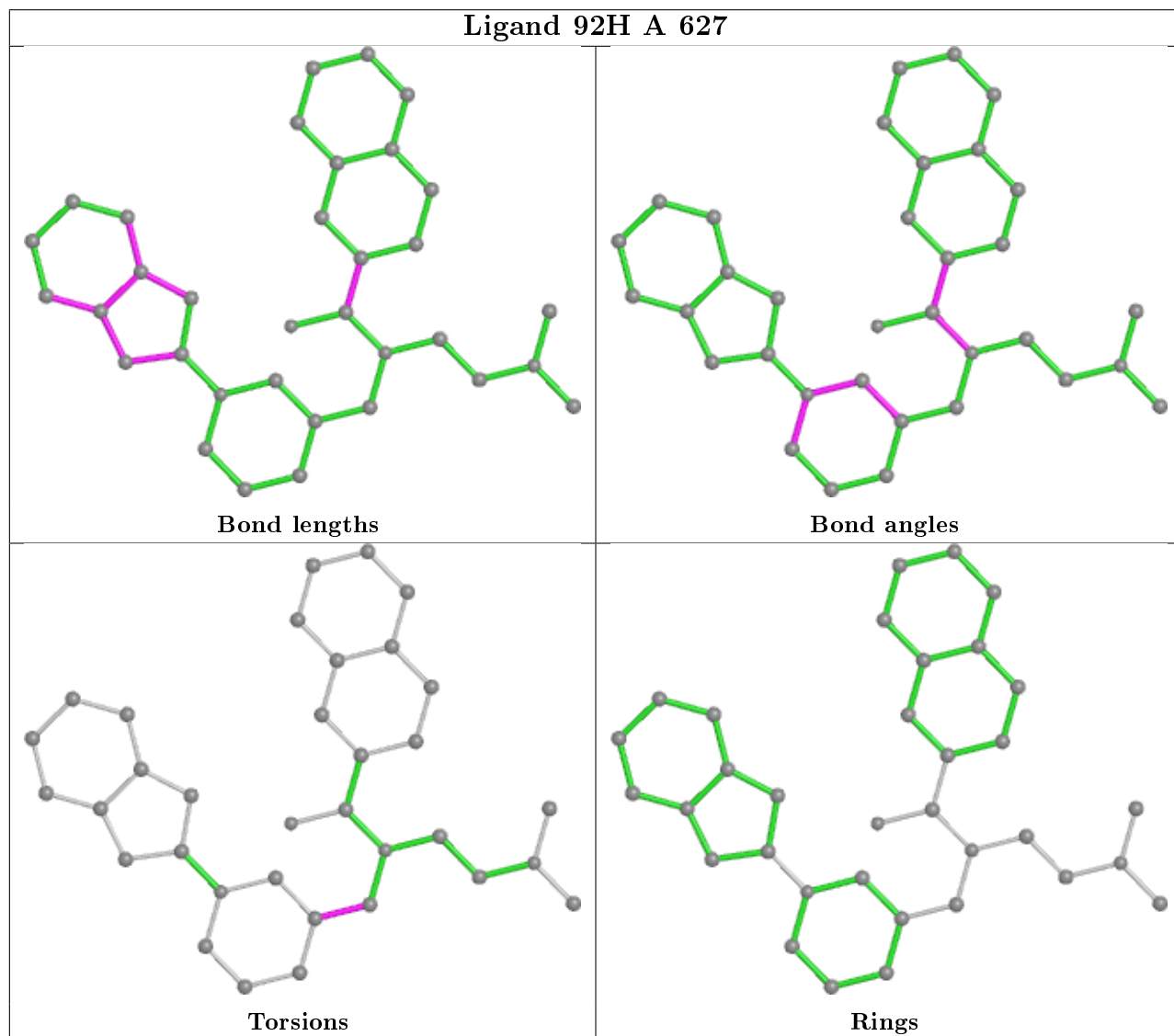
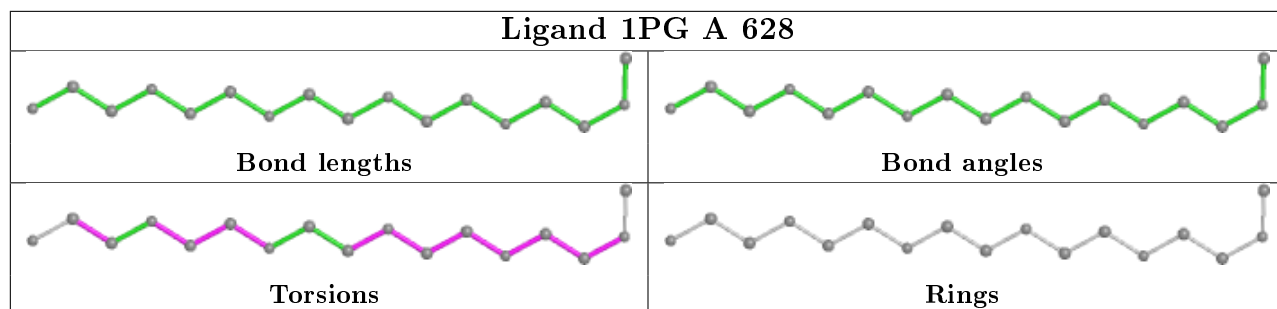
All (1) ring outliers are listed below:

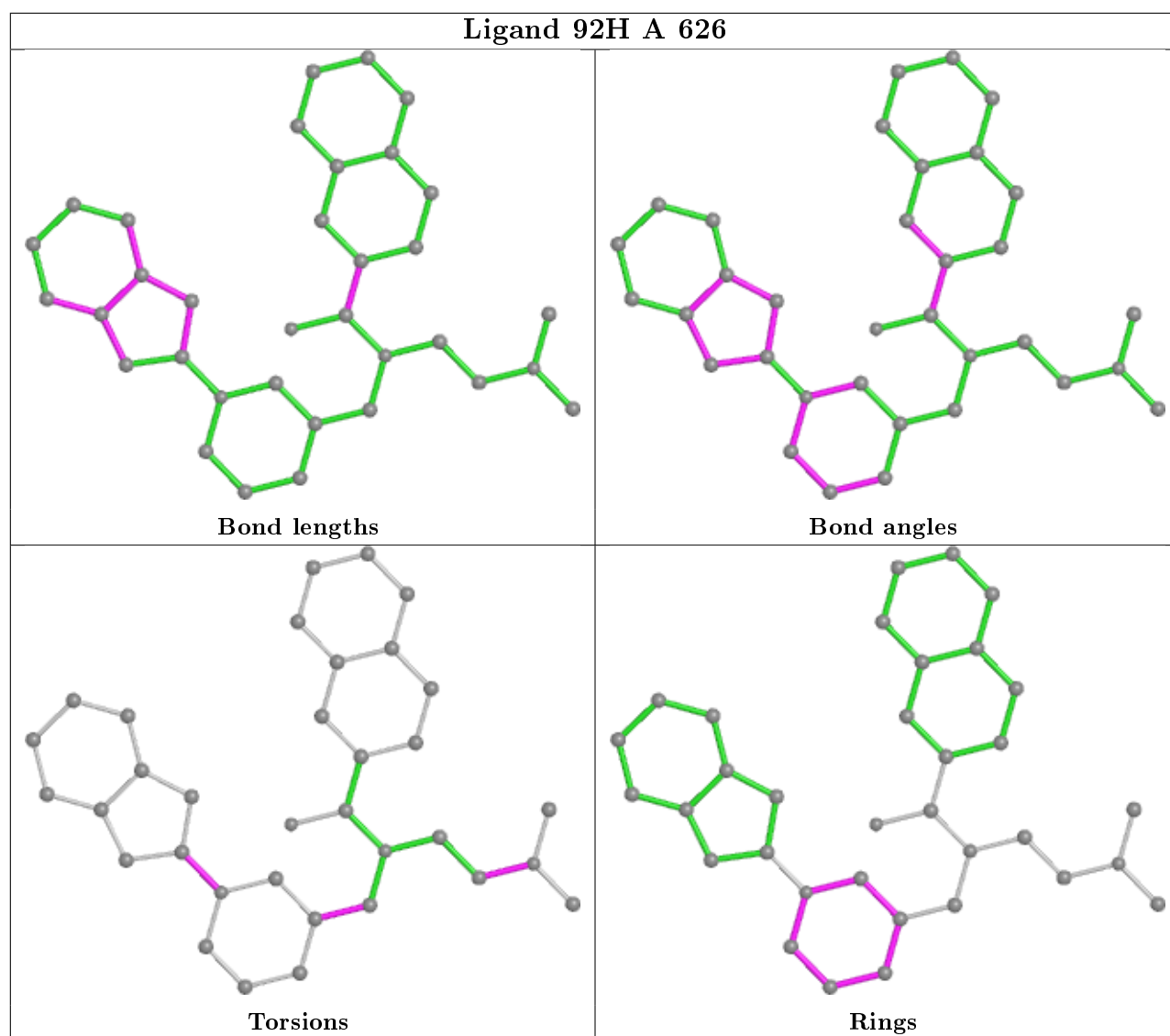
Mol	Chain	Res	Type	Atoms
9	A	626	92H	CAG-CAH-CAI-CAJ-CAU-NAK

8 monomers are involved in 23 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	A	628	1PG	8	0
8	A	624	MES	2	0
11	A	629	PEG	2	0
6	A	620	SO4	1	0
5	A	612	GOL	1	0
8	A	625	MES	5	0
9	A	627	92H	1	0
5	A	613	GOL	3	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.





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, 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	527/529 (99%)	0.10	29 (5%) 25 31	24, 37, 63, 90	6 (1%)

All (29) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	3	ASP	6.1
1	A	53	SER	5.9
1	A	255	GLU	4.5
1	A	380	GLN	4.5
1	A	378	ASP	4.0
1	A	259	GLU	3.8
1	A	454	ASP	3.2
1	A	4	ILE	3.2
1	A	455	GLN	3.2
1	A	376	TRP	3.2
1	A	253	SER	3.1
1	A	54	ASP	3.1
1	A	256	ASN	3.1
1	A	344	ILE	2.9
1	A	254	ARG	2.7
1	A	381	ARG	2.5
1	A	50	THR	2.4
1	A	382	PRO	2.4
1	A	299[A]	LEU	2.3
1	A	49	LEU	2.3
1	A	22	GLY	2.3
1	A	268	ASP	2.3
1	A	506	GLU	2.2
1	A	486	ASN	2.2
1	A	342	ASN	2.2
1	A	257[A]	GLU	2.2
1	A	346	THR	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	237	TYR	2.1
1	A	55	ILE	2.0

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

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

6.3 Carbohydrates [i](#)

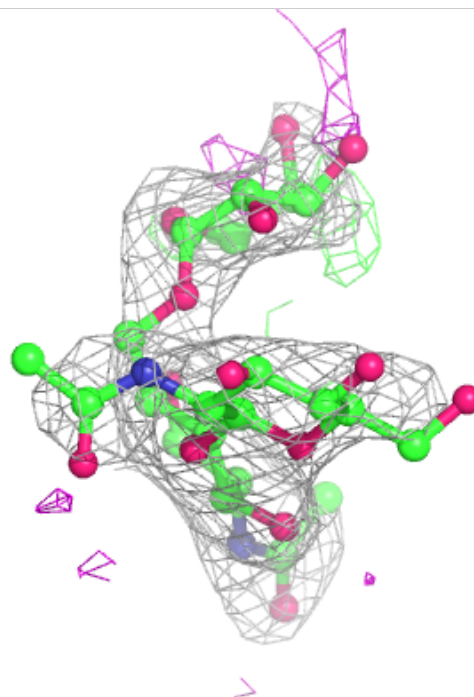
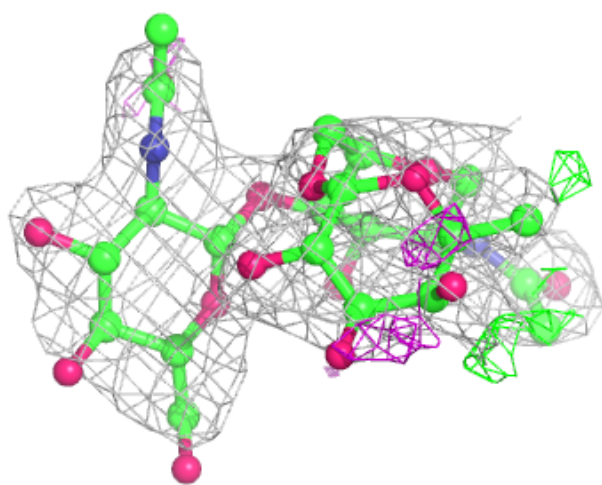
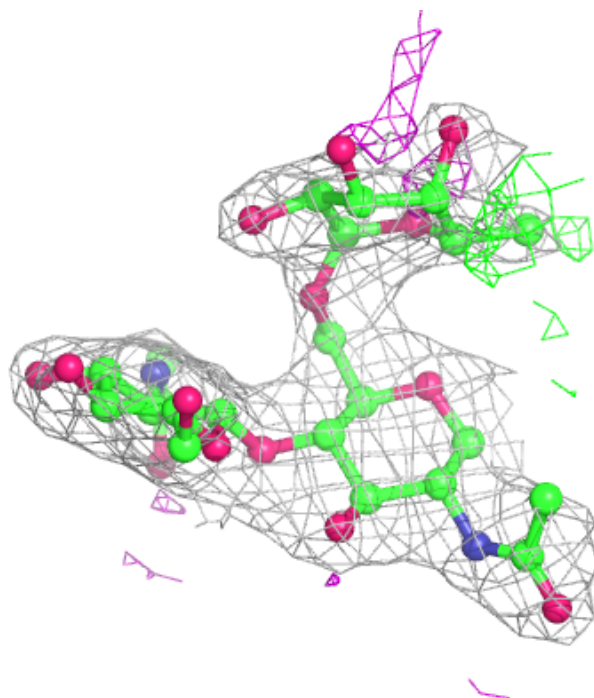
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	NAG	D	2	14/15	0.75	0.38	72,85,93,94	0
3	FUC	C	2	10/11	0.76	0.24	50,57,65,72	10
2	FUC	B	3	10/11	0.81	0.34	58,65,74,77	0
2	NAG	B	2	14/15	0.91	0.31	70,75,90,91	0
3	NAG	C	1	14/15	0.91	0.19	63,67,73,74	0
2	NAG	D	1	14/15	0.91	0.27	68,74,78,79	0
2	FUC	D	3	10/11	0.91	0.26	60,65,72,81	0
2	NAG	B	1	14/15	0.96	0.20	43,55,66,71	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.

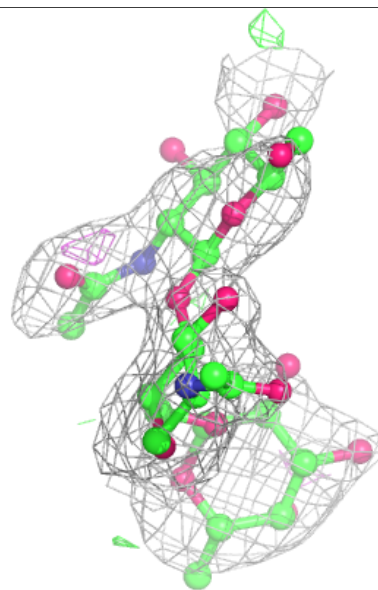
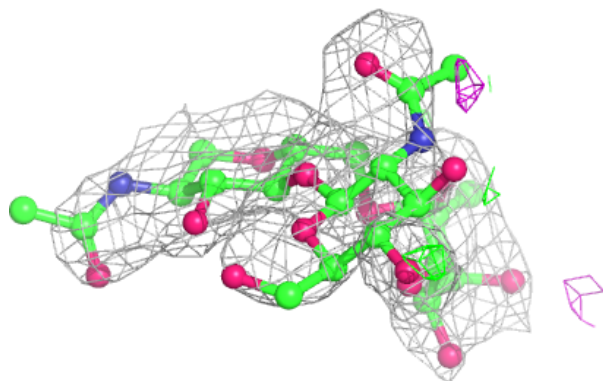
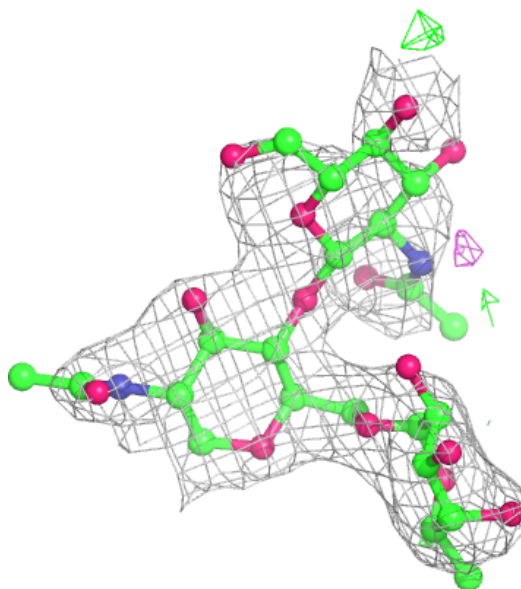
Electron density around Chain B:

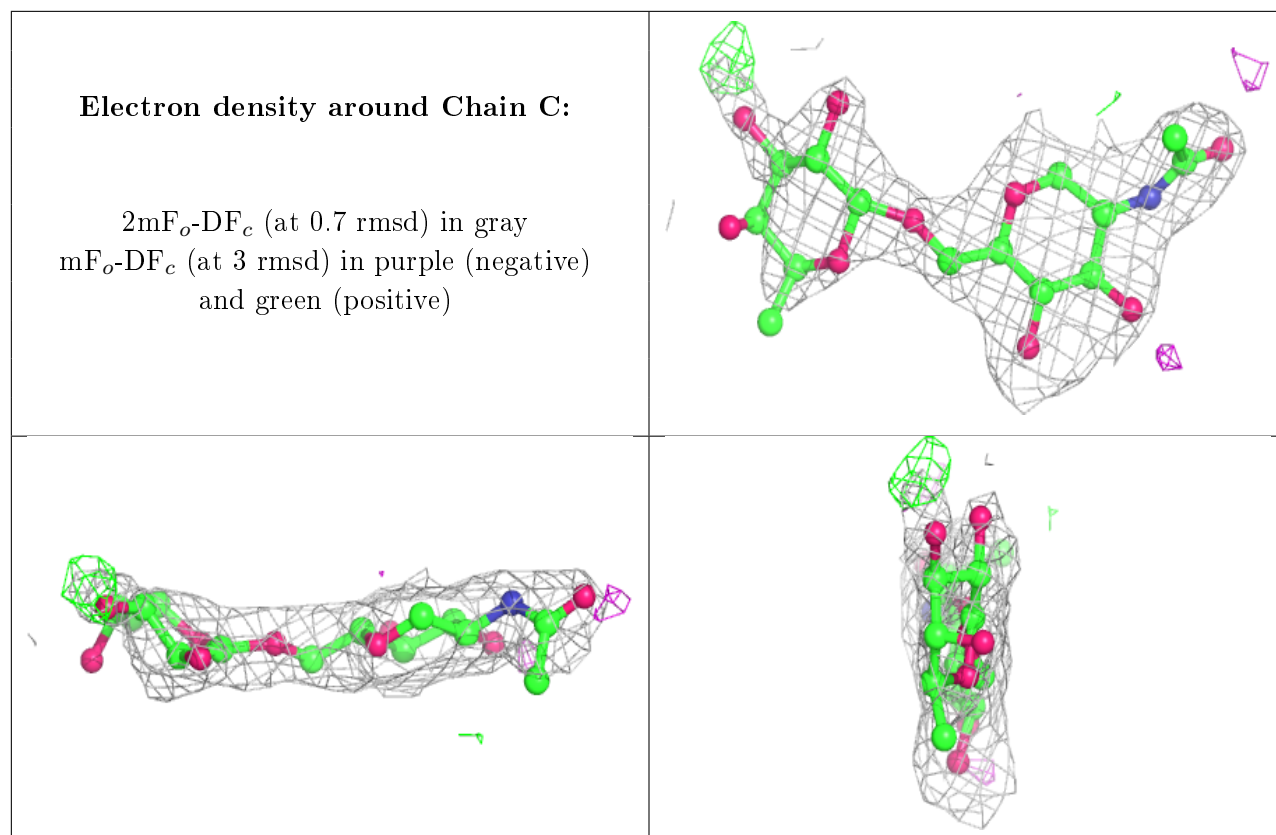
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



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)





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, 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.

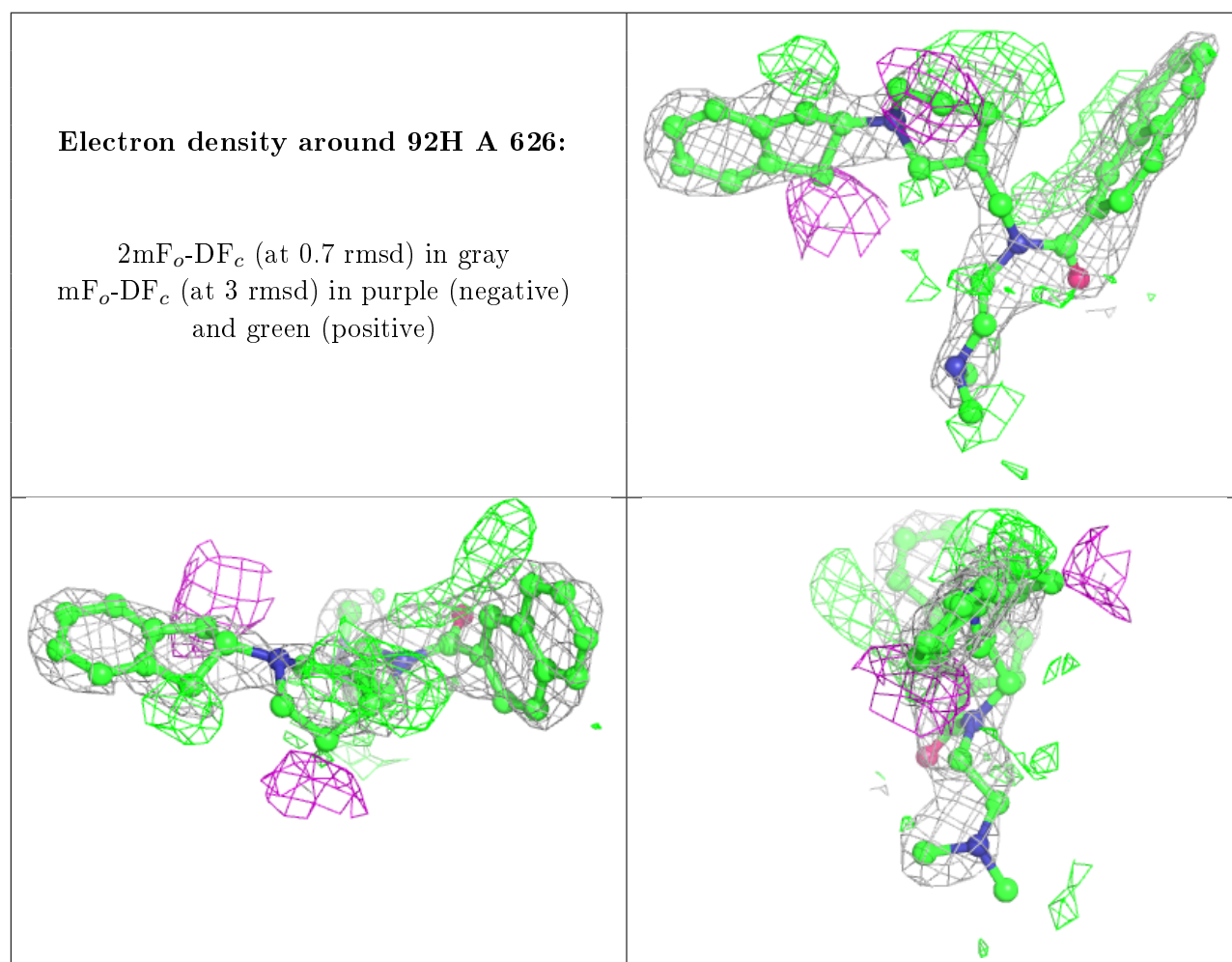
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	GOL	A	613	6/6	0.62	0.24	49,64,65,71	0
9	92H	A	626	34/34	0.67	0.28	37,51,67,71	34
8	MES	A	624	12/12	0.72	0.22	38,51,84,97	12
4	NAG	A	606	14/15	0.75	0.35	87,93,99,103	0
4	NAG	A	607	14/15	0.78	0.23	43,74,88,90	0
6	SO4	A	617	5/5	0.80	0.35	80,85,93,100	0
8	MES	A	625	12/12	0.81	0.21	45,58,61,68	12
6	SO4	A	620	5/5	0.81	0.40	81,84,89,118	5
10	1PG	A	628	17/17	0.81	0.17	41,55,67,71	0
11	PEG	A	629	7/7	0.82	0.21	45,52,62,63	7
6	SO4	A	618	5/5	0.82	0.23	66,66,75,79	0
7	CL	A	623	1/1	0.85	0.06	85,85,85,85	0
7	CL	A	622	1/1	0.86	0.04	79,79,79,79	0
4	NAG	A	608	14/15	0.86	0.37	81,85,90,91	0

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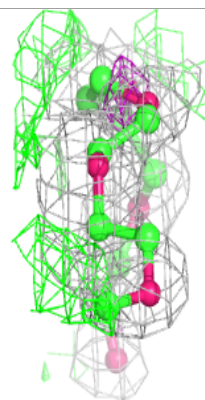
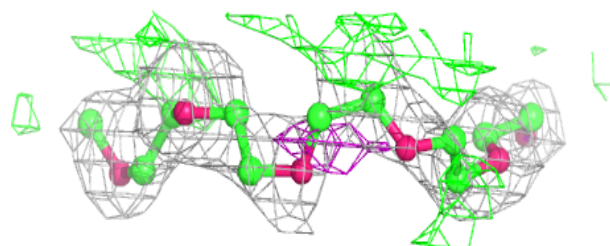
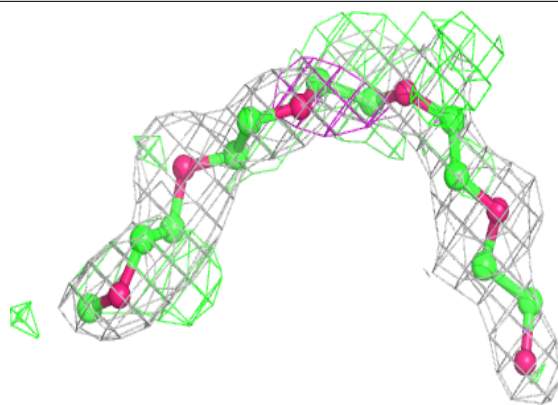
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
6	SO4	A	614	5/5	0.88	0.20	30,49,51,60	5
5	GOL	A	612	6/6	0.92	0.11	41,45,46,50	0
9	92H	A	627	34/34	0.92	0.16	28,34,46,47	0
6	SO4	A	616	5/5	0.93	0.18	36,42,54,57	5
6	SO4	A	619	5/5	0.96	0.11	54,56,59,67	5
7	CL	A	621	1/1	0.96	0.07	70,70,70,70	0
6	SO4	A	615	5/5	0.98	0.11	27,42,43,44	5

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.



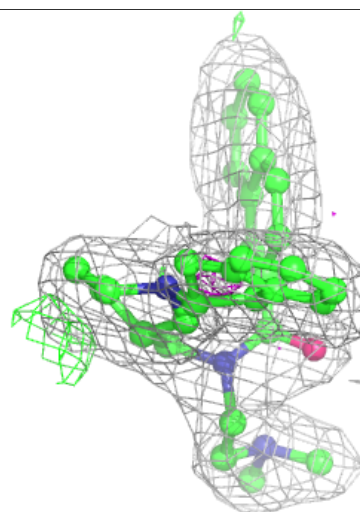
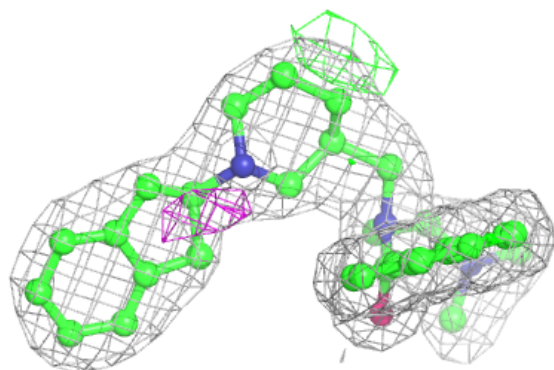
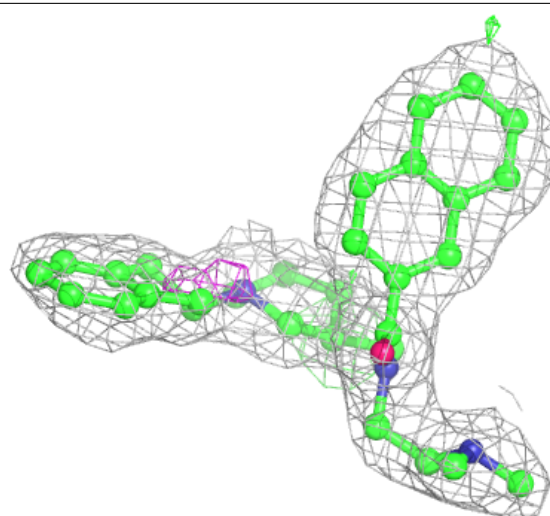
Electron density around 1PG A 628:

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



Electron density around 92H A 627:

$2mF_o-DF_c$ (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.