



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 06:44 PM UTC

PDB ID : 9I5P / pdb_00009i5p
Title : Recombinant human butyrylcholinesterase in complex with 1-(isobutylmethyl)-5-(2,4-difluorobenzyl)-N-(2-(dimethylamino)ethyl)-1H-indazole-6-carboxamide
Authors : Brazzolotto, X.; Ferjancic Benetik, S.; Knez, D.; Proj, M.; Gobec, S.; Nachon, F.
Deposited on : 2025-01-28
Resolution : 2.75 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](#) ①) were used in the production of this report:

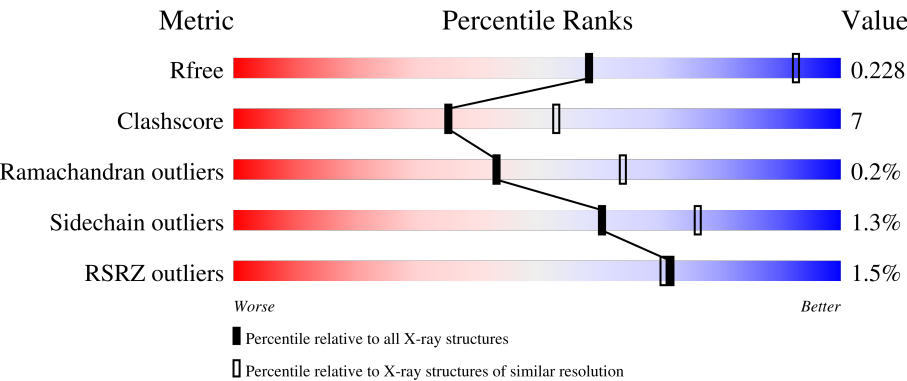
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal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

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.75 Å.

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




Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1009 (2.76-2.76)
Clashscore	190562	1044 (2.76-2.76)
Ramachandran outliers	187476	1024 (2.76-2.76)
Sidechain outliers	187428	1024 (2.76-2.76)
RSRZ outliers	180081	1009 (2.76-2.76)

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

Mol	Chain	Length	Quality of chain
1	A	529	<div><div>2%</div><div><div></div><div>81%</div><div>17%</div><div>..</div></div></div>
2	B	2	<div><div>100%</div></div>
2	C	2	<div><div>50%</div><div>50%</div></div>
2	D	2	<div><div>100%</div></div>
3	E	4	<div><div>75%</div><div>25%</div></div>

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Mol	Chain	Length	Quality of chain
4	F	2	 50%50%

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 4554 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	526	Total	C	N	O	S	0	6	0
			4237	2736	712	773	16			

There are 4 discrepancies between the modelled and reference sequences:

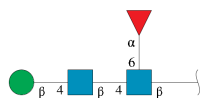
Chain	Residue	Modelled	Actual	Comment	Reference
A	17	GLN	ASN	engineered mutation	UNP P06276
A	455	GLN	ASN	engineered mutation	UNP P06276
A	481	GLN	ASN	engineered mutation	UNP P06276
A	486	GLN	ASN	engineered mutation	UNP P06276

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



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

- Molecule 3 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.



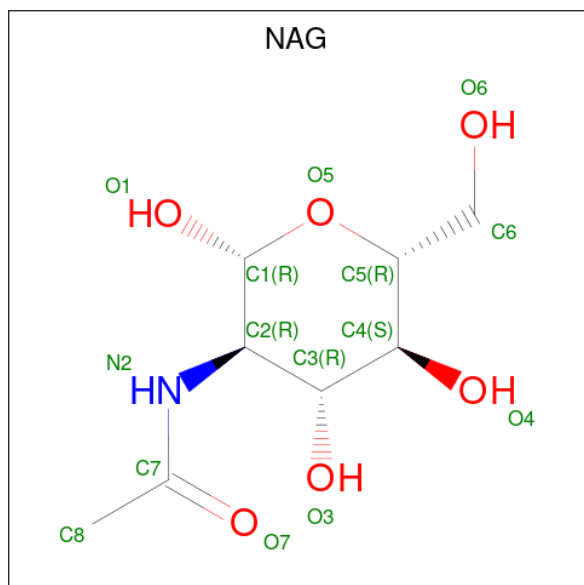
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	E	4	Total	C	N	O	0	0	0
			49	28	2	19			

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



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

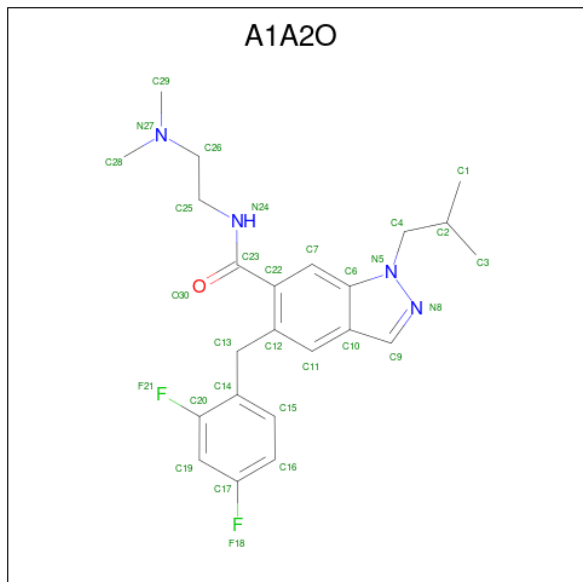
- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



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

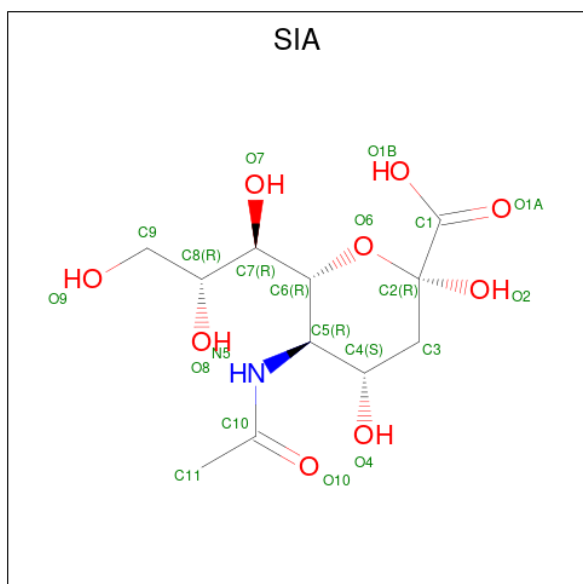
- Molecule 6 is 5-[(2,4-difluorophenyl)methyl]-N-[2-(dimethylamino)ethyl]-1-(2-methylpro

pyl)-1H-indazole-6-carboxamide (CCD ID: A1A2O) (formula: $C_{23}H_{28}F_2N_4O$) (labeled as "Ligand of Interest" by depositor).



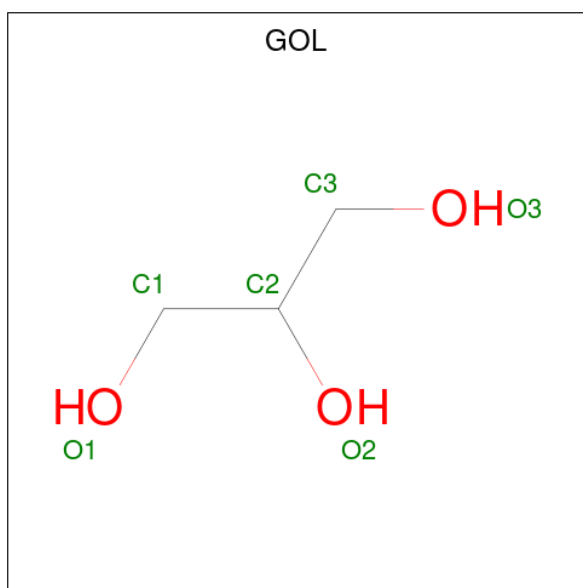
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	A	1	Total	C	F	N	O	0	0
			30	23	2	4	1		

- Molecule 7 is N-acetyl-alpha-neuraminic acid (CCD ID: SIA) (formula: $C_{11}H_{19}NO_9$).



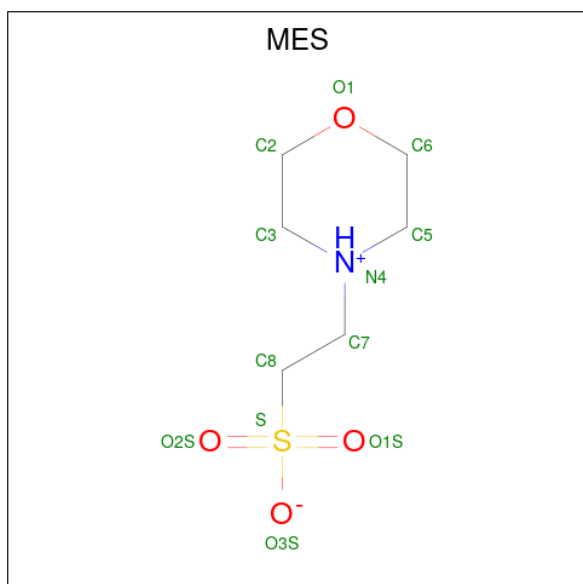
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	A	1	Total	C	N	O	0	0
			21	11	1	9		

- Molecule 8 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



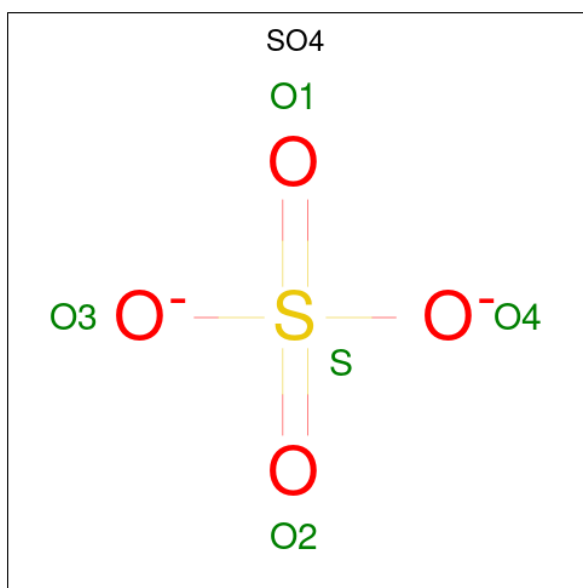
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	C	O	0	0
			6	3	3		

- Molecule 9 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (CCD ID: MES) (formula: $C_6H_{13}NO_4S$).



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

- Molecule 10 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

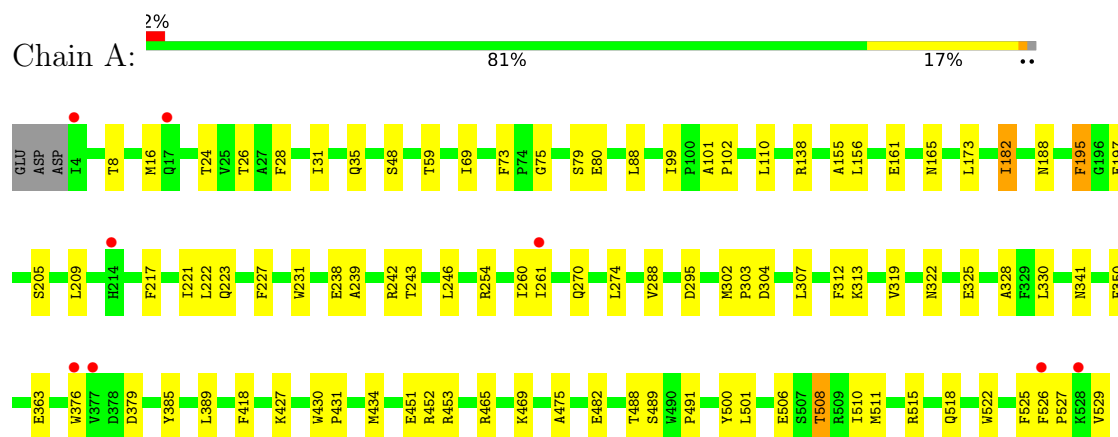
- Molecule 11 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	A	70	Total	O	0	0
			70	70		

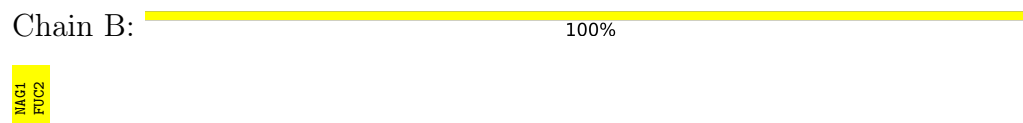
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Cholinesterase



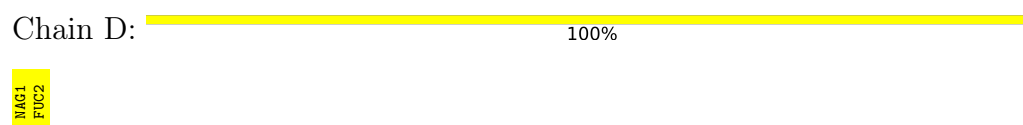
- Molecule 2: alpha-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose



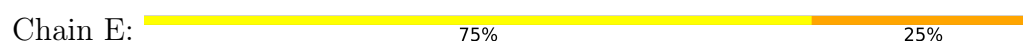
- Molecule 2: alpha-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose



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



- Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose





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

Chain F:  50% 50%



4 Data and refinement statistics

Property	Value	Source
Space group	I 4 2 2	Depositor
Cell constants a, b, c, α , β , γ	154.08Å 154.08Å 127.25Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.63 – 2.75 47.63 – 2.75	Depositor EDS
% Data completeness (in resolution range)	99.5 (47.63-2.75) 99.5 (47.63-2.75)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.59 (at 2.77Å)	Xtriage
Refinement program	PHENIX 1.21.2_5419	Depositor
R, R_{free}	0.185 , 0.229 0.185 , 0.228	Depositor DCC
R_{free} test set	1034 reflections (5.11%)	wwPDB-VP
Wilson B-factor (Å ²)	60.4	Xtriage
Anisotropy	0.405	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 45.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	4554	wwPDB-VP
Average B, all atoms (Å ²)	68.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.58% 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: A1A2O, GOL, NAG, MES, BMA, FUC, SO4, SIA

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	0.36	0/4367	0.52	0/5927

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	4237	0	4139	65	0
2	B	24	0	22	0	0
2	C	24	0	22	1	0
2	D	24	0	22	0	0
3	E	49	0	43	1	0
4	F	28	0	25	2	0
5	A	14	0	13	0	0
6	A	30	0	0	0	0
7	A	21	0	18	0	0
8	A	6	0	8	2	0
9	A	12	0	13	2	0
10	A	15	0	0	1	0
11	A	70	0	0	0	0
All	All	4554	0	4325	65	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 7.

All (65) 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:328:ALA:HA	1:A:434:MET:HE2	1.65	0.77
1:A:35:GLN:NE2	1:A:48:SER:O	2.22	0.72
1:A:161:GLU:HB3	1:A:261:ILE:HG21	1.70	0.72
1:A:452:ARG:NH2	4:F:2:NAG:O4	2.22	0.71
1:A:515:ARG:HG2	9:A:605:MES:H51	1.83	0.61
1:A:222:LEU:HB2	1:A:319:VAL:HG22	1.82	0.60
1:A:254:ARG:HB2	1:A:260:ILE:HG13	1.84	0.57
1:A:341:ASN:HD22	3:E:1:NAG:H83	1.68	0.57
1:A:227:PHE:CE2	1:A:303:PRO:HB2	2.39	0.57
1:A:319:VAL:O	1:A:418:PHE:HA	2.05	0.56
1:A:500:TYR:CZ	1:A:511[B]:MET:HB2	2.41	0.55
1:A:69:ILE:HD11	1:A:88:LEU:HD11	1.89	0.55
1:A:26:THR:HB	1:A:99:ILE:HG12	1.89	0.55
1:A:350:PHE:HB2	1:A:385:TYR:HB3	1.89	0.54
1:A:227:PHE:HZ	1:A:307:LEU:HB2	1.74	0.53
1:A:525:PHE:C	1:A:525:PHE:CD1	2.86	0.53
1:A:518:GLN:HE22	9:A:605:MES:H62	1.75	0.52
1:A:155:ALA:HB3	1:A:239:ALA:HB1	1.92	0.51
1:A:469:LYS:HG2	1:A:482:GLU:HG2	1.92	0.51
1:A:430:TRP:HB3	1:A:431:PRO:HD2	1.92	0.51
1:A:288:VAL:H	8:A:604:GOL:H2	1.75	0.51
1:A:500:TYR:CZ	1:A:511[A]:MET:HB2	2.46	0.51
1:A:227:PHE:CD2	1:A:303:PRO:HB2	2.47	0.50
1:A:156:LEU:HG	1:A:243:THR:HG21	1.94	0.49
1:A:488:THR:N	10:A:606:SO4:O4	2.38	0.49
1:A:28:PHE:HB3	1:A:31:ILE:HD11	1.96	0.48
1:A:110[B]:LEU:HD11	1:A:475:ALA:CB	2.42	0.48
1:A:363:GLU:H	1:A:363:GLU:CD	2.21	0.48
1:A:73:PHE:HB2	1:A:79:SER:OG	2.13	0.48
1:A:231:TRP:HA	8:A:604:GOL:H11	1.96	0.48
1:A:376:TRP:CD1	1:A:379:ASP:HA	2.48	0.48
1:A:227:PHE:CD2	1:A:227:PHE:C	2.93	0.47
1:A:330:LEU:HD22	1:A:389:LEU:HD23	1.95	0.47
1:A:452:ARG:HH22	4:F:2:NAG:HO4	1.57	0.47
1:A:102:PRO:HD2	1:A:138:ARG:HH12	1.80	0.47
1:A:188:ASN:ND2	2:C:2:FUC:H3	2.29	0.47
1:A:217:PHE:O	1:A:313:LYS:HE2	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:526:PHE:O	1:A:529:VAL:HG22	2.16	0.46
1:A:173:LEU:HA	1:A:173:LEU:HD12	1.65	0.46
1:A:304:ASP:OD1	1:A:304:ASP:N	2.45	0.45
1:A:491:PRO:HD3	1:A:510:ILE:HD12	1.99	0.44
1:A:16:MET:HE1	1:A:59:THR:O	2.17	0.44
1:A:209:LEU:HD12	1:A:312:PHE:HB3	1.99	0.44
1:A:75:GLY:H	1:A:80:GLU:CD	2.26	0.44
1:A:101:ALA:HA	1:A:102:PRO:C	2.43	0.43
1:A:16:MET:HE3	1:A:59:THR:HA	2.00	0.43
1:A:525:PHE:C	1:A:525:PHE:HD1	2.26	0.43
1:A:319:VAL:HG12	1:A:418:PHE:CE2	2.53	0.43
1:A:238:GLU:O	1:A:242:ARG:HG3	2.18	0.43
1:A:195:PHE:CB	1:A:221:ILE:HB	2.49	0.43
1:A:270:GLN:O	1:A:274:LEU:HD13	2.19	0.43
1:A:205:SER:HB3	1:A:222:LEU:HD21	2.01	0.42
1:A:195:PHE:HB3	1:A:221:ILE:HB	2.01	0.42
1:A:522:TRP:O	1:A:527:PRO:HD3	2.19	0.42
1:A:197:GLU:HA	1:A:223:GLN:O	2.20	0.42
1:A:165:ASN:HD22	1:A:295:ASP:CG	2.27	0.42
1:A:322:ASN:O	1:A:325:GLU:HG2	2.19	0.42
1:A:451:GLU:HG3	1:A:453:ARG:H	1.86	0.41
1:A:302:MET:HB2	1:A:302:MET:HE2	1.86	0.41
1:A:465:ARG:HA	1:A:465:ARG:HD2	1.96	0.41
1:A:501:LEU:HD11	1:A:508:THR:HG23	2.03	0.41
1:A:221:ILE:C	1:A:222:LEU:HD12	2.46	0.41
1:A:246:LEU:HD12	1:A:246:LEU:HA	1.88	0.40
1:A:24:THR:O	1:A:101:ALA:HB3	2.22	0.40
1:A:182:ILE:HD12	1:A:182:ILE:HA	1.86	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	530/529 (100%)	501 (94%)	28 (5%)	1 (0%)	43 64

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	506	GLU

5.3.2 Protein sidechains ⓘ

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%)	451 (99%)	6 (1%)	61 76

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	THR
1	A	182	ILE
1	A	195	PHE
1	A	427	LYS
1	A	489	SER
1	A	508	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	17	GLN
1	A	188	ASN
1	A	245	ASN
1	A	289	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

12 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	2,1	14,14,15	0.64	0	17,19,21	1.33	1 (5%)
2	FUC	B	2	2	10,10,11	0.76	0	14,14,16	1.20	1 (7%)
2	NAG	C	1	2,1	14,14,15	0.93	1 (7%)	17,19,21	1.55	3 (17%)
2	FUC	C	2	2	10,10,11	1.01	0	14,14,16	1.94	5 (35%)
2	NAG	D	1	2,1	14,14,15	0.75	0	17,19,21	1.46	2 (11%)
2	FUC	D	2	2	10,10,11	0.83	0	14,14,16	2.09	5 (35%)
3	NAG	E	1	3,1	14,14,15	0.90	0	17,19,21	1.28	3 (17%)
3	NAG	E	2	3	14,14,15	0.76	0	17,19,21	1.13	2 (11%)
3	BMA	E	3	3	11,11,12	0.84	0	15,15,17	2.26	4 (26%)
3	FUC	E	4	3	10,10,11	0.73	0	14,14,16	1.06	1 (7%)
4	NAG	F	1	1,4	14,14,15	0.73	0	17,19,21	1.56	2 (11%)
4	NAG	F	2	4	14,14,15	0.93	1 (7%)	17,19,21	1.29	2 (11%)

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	2,1	-	2/6/23/26	0/1/1/1
2	FUC	B	2	2	-	-	0/1/1/1
2	NAG	C	1	2,1	-	2/6/23/26	0/1/1/1
2	FUC	C	2	2	-	-	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	D	1	2,1	-	2/6/23/26	0/1/1/1
2	FUC	D	2	2	-	-	0/1/1/1
3	NAG	E	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	E	2	3	-	1/6/23/26	0/1/1/1
3	BMA	E	3	3	-	1/2/19/22	0/1/1/1
3	FUC	E	4	3	-	-	0/1/1/1
4	NAG	F	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	F	2	4	-	0/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	F	2	NAG	C1-C2	2.89	1.56	1.52
2	C	1	NAG	C1-C2	2.35	1.55	1.52

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	3	BMA	C1-O5-C5	6.38	120.74	112.19
2	B	1	NAG	C1-O5-C5	4.23	117.85	112.19
2	D	2	FUC	O5-C5-C4	4.10	116.93	109.55
2	D	1	NAG	C1-O5-C5	4.01	117.56	112.19
4	F	1	NAG	C2-N2-C7	3.80	128.00	122.90
2	C	2	FUC	C1-C2-C3	3.52	114.77	109.64
2	C	1	NAG	O5-C1-C2	-3.32	106.16	111.29
4	F	1	NAG	C1-O5-C5	3.26	116.56	112.19
3	E	1	NAG	C1-C2-N2	-3.22	105.36	110.43
4	F	2	NAG	C1-O5-C5	3.13	116.38	112.19
2	C	2	FUC	O5-C5-C4	3.10	115.14	109.55
2	C	1	NAG	C2-N2-C7	3.02	126.95	122.90
2	D	2	FUC	C1-O5-C5	2.88	119.75	112.97
2	C	2	FUC	C2-C3-C4	2.70	115.61	110.86
2	B	2	FUC	C1-O5-C5	2.68	119.29	112.97
2	C	2	FUC	C1-O5-C5	2.61	119.12	112.97
3	E	3	BMA	C3-C4-C5	2.46	114.70	110.23
2	D	2	FUC	O2-C2-C3	2.42	115.16	110.15
3	E	2	NAG	C2-N2-C7	2.41	126.13	122.90
2	D	2	FUC	C1-C2-C3	-2.41	106.14	109.64
2	C	2	FUC	O4-C4-C5	2.38	114.99	109.74
3	E	1	NAG	C2-N2-C7	2.32	126.00	122.90
3	E	3	BMA	O3-C3-C2	-2.28	105.40	110.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	4	FUC	C1-O5-C5	2.27	118.32	112.97
2	D	2	FUC	C2-C3-C4	-2.24	106.92	110.86
4	F	2	NAG	C1-C2-N2	2.22	113.94	110.43
3	E	3	BMA	C2-C3-C4	2.20	114.74	110.86
2	D	1	NAG	C4-C3-C2	-2.20	107.80	111.02
3	E	1	NAG	O5-C1-C2	-2.17	107.93	111.29
2	C	1	NAG	O4-C4-C5	2.12	114.56	109.32
3	E	2	NAG	O4-C4-C3	-2.11	105.40	110.38

There are no chirality outliers.

All (12) torsion outliers are listed below:

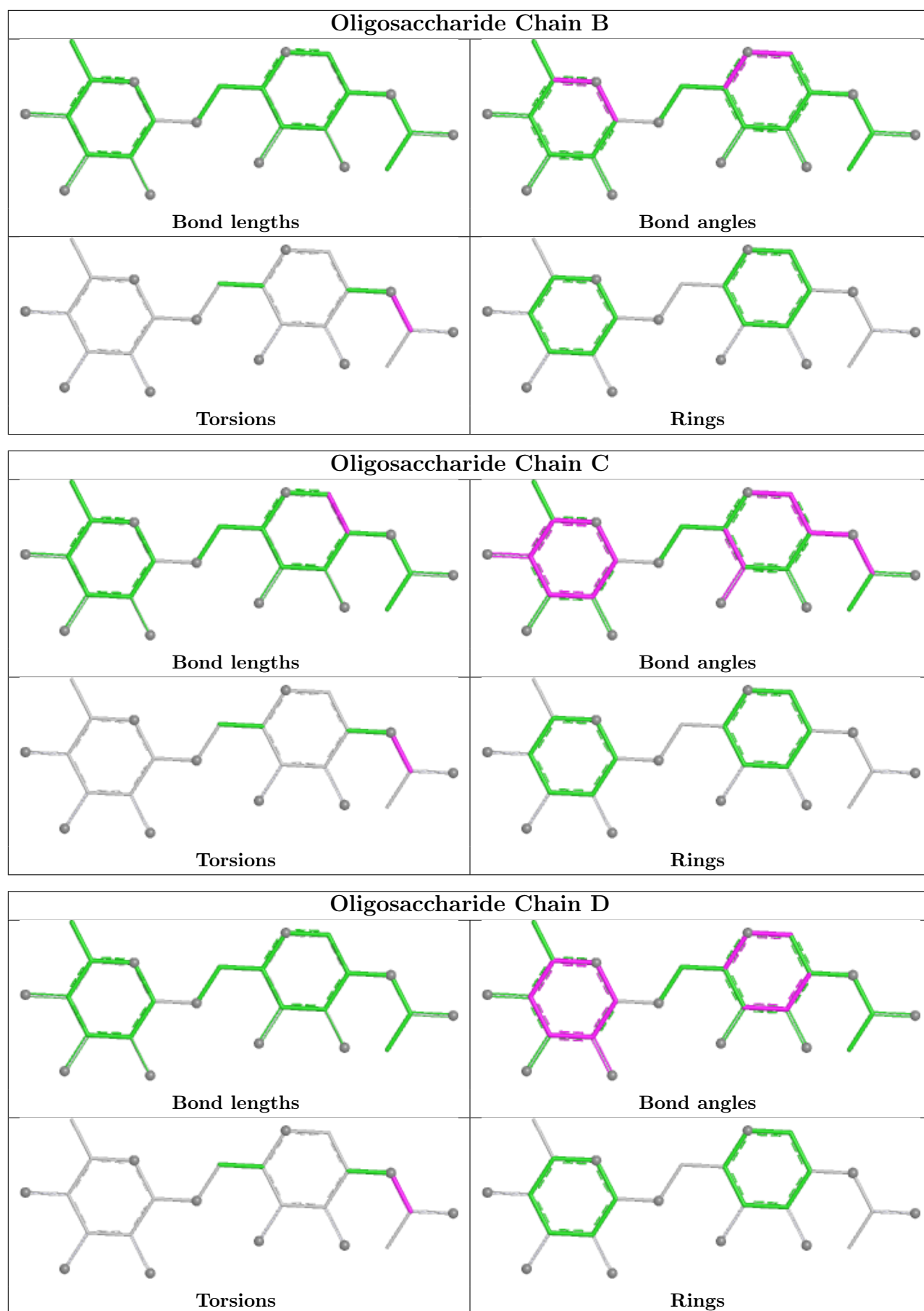
Mol	Chain	Res	Type	Atoms
3	E	3	BMA	O5-C5-C6-O6
2	B	1	NAG	C8-C7-N2-C2
2	B	1	NAG	O7-C7-N2-C2
2	C	1	NAG	C8-C7-N2-C2
2	C	1	NAG	O7-C7-N2-C2
2	D	1	NAG	C8-C7-N2-C2
2	D	1	NAG	O7-C7-N2-C2
3	E	1	NAG	C8-C7-N2-C2
3	E	1	NAG	O7-C7-N2-C2
4	F	1	NAG	C8-C7-N2-C2
4	F	1	NAG	O7-C7-N2-C2
3	E	2	NAG	O5-C5-C6-O6

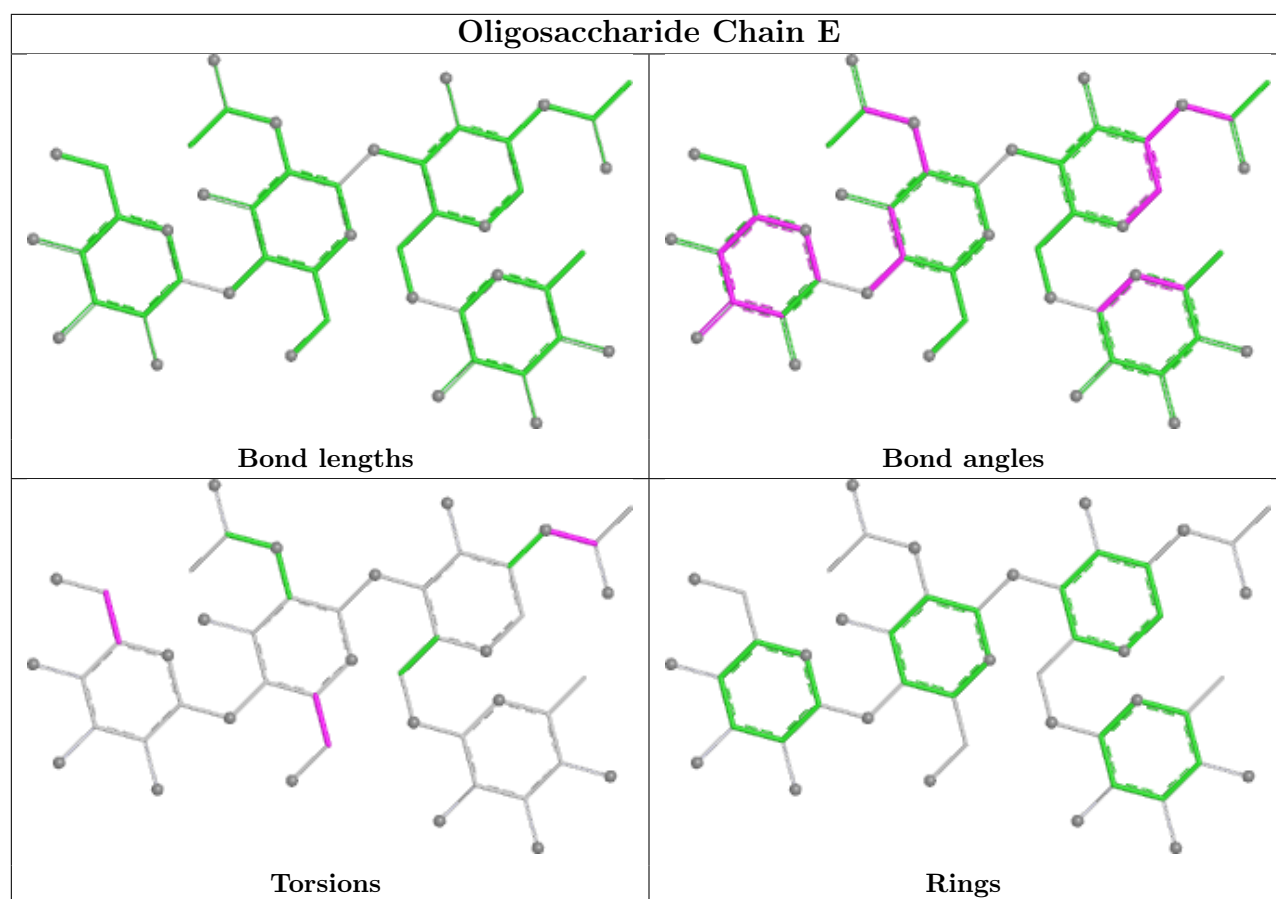
There are no ring outliers.

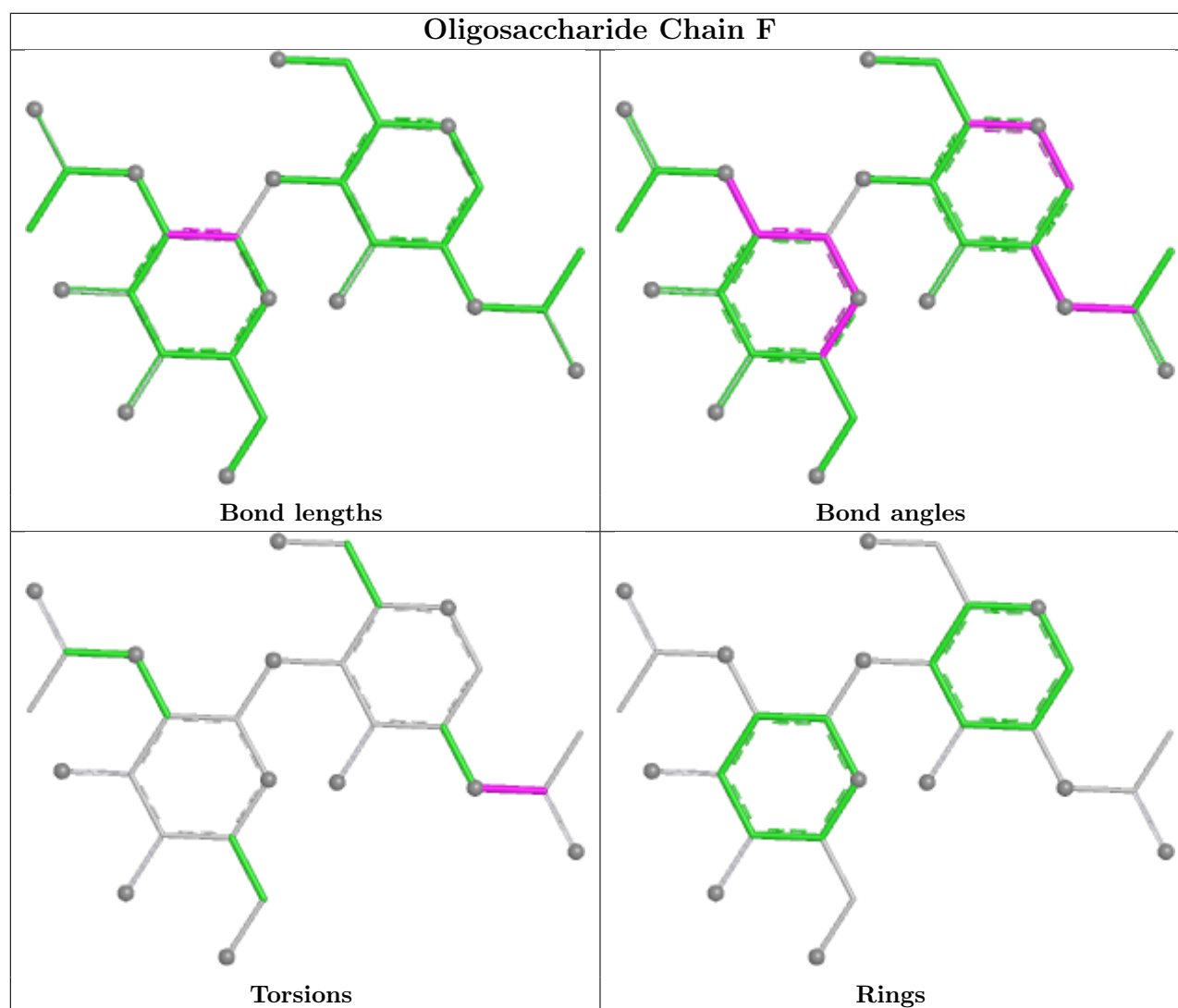
3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	2	FUC	1	0
4	F	2	NAG	2	0
3	E	1	NAG	1	0

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







5.6 Ligand geometry [i](#)

8 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
8	GOL	A	604	-	5,5,5	0.21	0	5,5,5	0.50	0
7	SIA	A	603	-	21,21,21	1.80	5 (23%)	24,31,31	1.58	5 (20%)
5	NAG	A	601	1	14,14,15	0.60	0	17,19,21	1.31	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
10	SO4	A	606	-	4,4,4	0.82	0	6,6,6	0.37	0
10	SO4	A	607	-	4,4,4	0.74	0	6,6,6	0.19	0
6	A1A2O	A	602	-	32,32,32	3.07	15 (46%)	45,45,45	2.19	16 (35%)
9	MES	A	605	-	12,12,12	1.40	1 (8%)	15,16,16	1.61	5 (33%)
10	SO4	A	608	-	4,4,4	0.77	0	6,6,6	0.16	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
8	GOL	A	604	-	-	2/4/4/4	-
7	SIA	A	603	-	-	6/20/38/38	0/1/1/1
5	NAG	A	601	1	-	2/6/23/26	0/1/1/1
6	A1A2O	A	602	-	-	6/18/18/18	0/3/3/3
9	MES	A	605	-	-	1/6/14/14	0/1/1/1

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	602	A1A2O	C4-N5	9.56	1.53	1.45
6	A	602	A1A2O	C10-C9	5.59	1.48	1.42
6	A	602	A1A2O	N5-N8	5.31	1.41	1.37
7	A	603	SIA	O6-C2	4.86	1.48	1.43
6	A	602	A1A2O	C6-N5	4.53	1.42	1.36
6	A	602	A1A2O	C22-C12	4.21	1.46	1.40
6	A	602	A1A2O	C23-N24	4.17	1.43	1.33
6	A	602	A1A2O	C9-N8	3.84	1.36	1.32
9	A	605	MES	C8-S	3.64	1.82	1.77
6	A	602	A1A2O	C22-C23	3.49	1.57	1.50
6	A	602	A1A2O	F18-C17	-3.32	1.28	1.36
7	A	603	SIA	C2-C1	3.15	1.58	1.53
6	A	602	A1A2O	C16-C17	2.85	1.42	1.37
7	A	603	SIA	C7-C6	2.63	1.56	1.52
6	A	602	A1A2O	C25-N24	2.63	1.52	1.46
6	A	602	A1A2O	F21-C20	-2.61	1.28	1.35
7	A	603	SIA	C8-C7	2.42	1.57	1.53
6	A	602	A1A2O	C14-C20	2.35	1.42	1.38
7	A	603	SIA	C3-C2	2.31	1.54	1.51
6	A	602	A1A2O	C19-C20	2.21	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	602	A1A2O	C28-N27	2.01	1.52	1.46

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	602	A1A2O	C9-N8-N5	5.60	108.85	106.06
6	A	602	A1A2O	C4-N5-C6	-4.53	126.95	130.01
6	A	602	A1A2O	C6-N5-N8	-4.13	109.39	111.26
7	A	603	SIA	O1A-C1-C2	-4.09	117.03	123.85
6	A	602	A1A2O	C16-C17-C19	-4.04	117.89	123.23
6	A	602	A1A2O	C20-C19-C17	3.82	120.74	116.67
6	A	602	A1A2O	C22-C23-N24	3.81	124.73	117.32
6	A	602	A1A2O	C10-C9-N8	-3.71	109.25	112.05
5	A	601	NAG	C2-N2-C7	3.35	127.40	122.90
6	A	602	A1A2O	O30-C23-N24	-3.07	116.62	122.59
9	A	605	MES	O1-C6-C5	2.98	118.18	111.77
7	A	603	SIA	C4-C5-N5	2.97	116.28	110.44
6	A	602	A1A2O	C7-C6-C10	-2.73	120.03	122.29
6	A	602	A1A2O	C11-C10-C6	-2.73	116.79	119.56
9	A	605	MES	C6-C5-N4	2.63	114.11	110.12
5	A	601	NAG	C1-O5-C5	2.53	115.58	112.19
6	A	602	A1A2O	C26-C25-N24	2.53	116.43	111.56
9	A	605	MES	C6-O1-C2	2.49	117.92	109.88
7	A	603	SIA	O7-C7-C8	2.29	114.14	108.93
6	A	602	A1A2O	C15-C16-C17	2.29	120.73	118.38
9	A	605	MES	O1S-S-C8	-2.27	103.29	106.73
6	A	602	A1A2O	C13-C14-C15	2.26	124.11	120.46
6	A	602	A1A2O	C4-N5-N8	2.23	123.65	119.10
9	A	605	MES	C2-C3-N4	-2.11	106.91	110.12
7	A	603	SIA	O1B-C1-O1A	2.11	130.60	123.86
6	A	602	A1A2O	C14-C13-C12	2.03	118.09	112.64
6	A	602	A1A2O	C25-N24-C23	2.02	126.67	122.11
7	A	603	SIA	O2-C2-C3	2.00	112.48	109.44

There are no chirality outliers.

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	602	A1A2O	C3-C2-C4-N5
7	A	603	SIA	O1A-C1-C2-O2
7	A	603	SIA	O1B-C1-C2-O2
7	A	603	SIA	O1B-C1-C2-O6

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Mol	Chain	Res	Type	Atoms
9	A	605	MES	C8-C7-N4-C5
6	A	602	A1A2O	C26-C25-N24-C23
6	A	602	A1A2O	C25-C26-N27-C28
6	A	602	A1A2O	N24-C25-C26-N27
5	A	601	NAG	C8-C7-N2-C2
5	A	601	NAG	O7-C7-N2-C2
8	A	604	GOL	O1-C1-C2-C3
8	A	604	GOL	O1-C1-C2-O2
7	A	603	SIA	O1B-C1-C2-C3
7	A	603	SIA	O1A-C1-C2-O6
6	A	602	A1A2O	C12-C13-C14-C15
6	A	602	A1A2O	C2-C4-N5-C6
7	A	603	SIA	O1A-C1-C2-C3

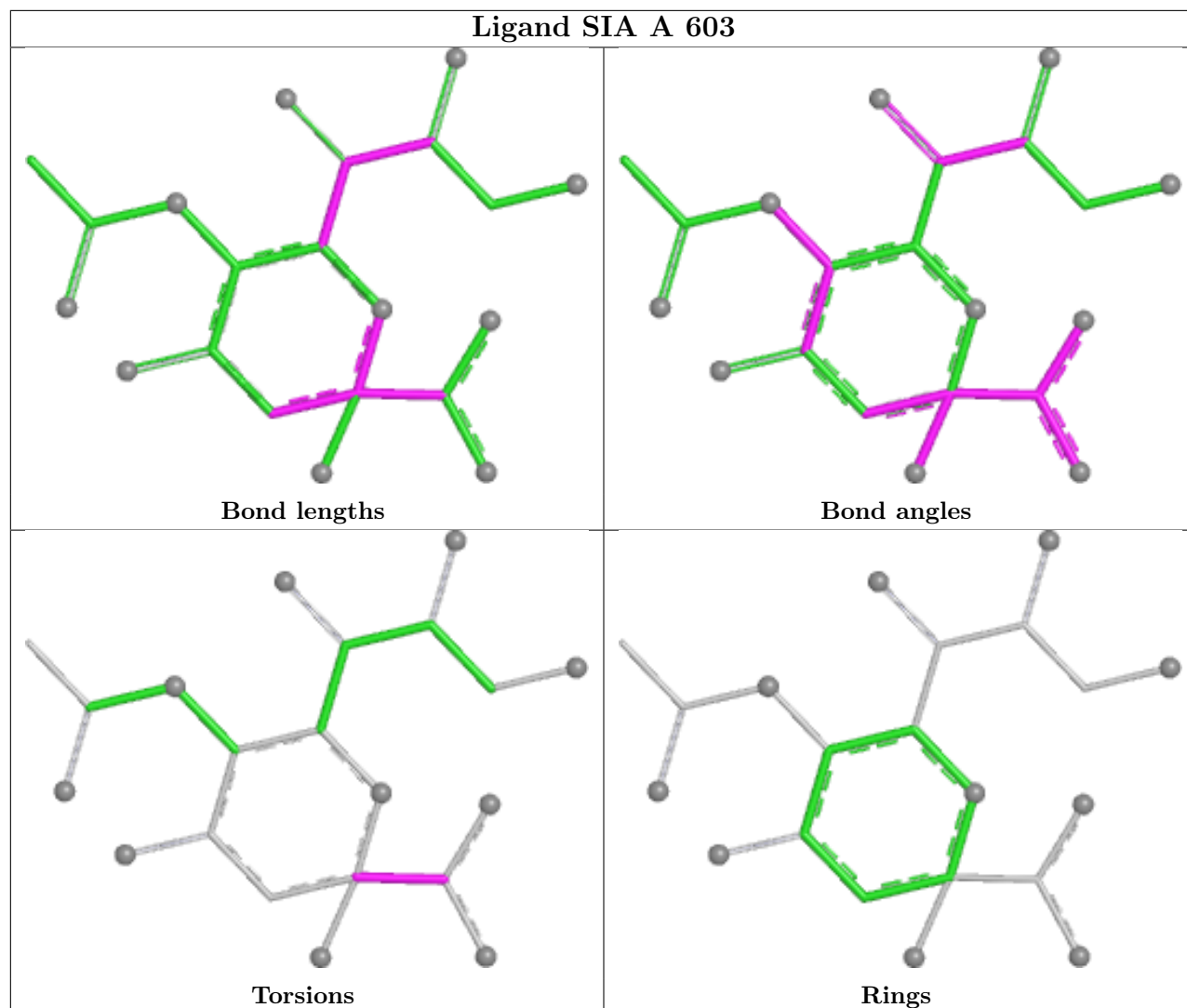
There are no ring outliers.

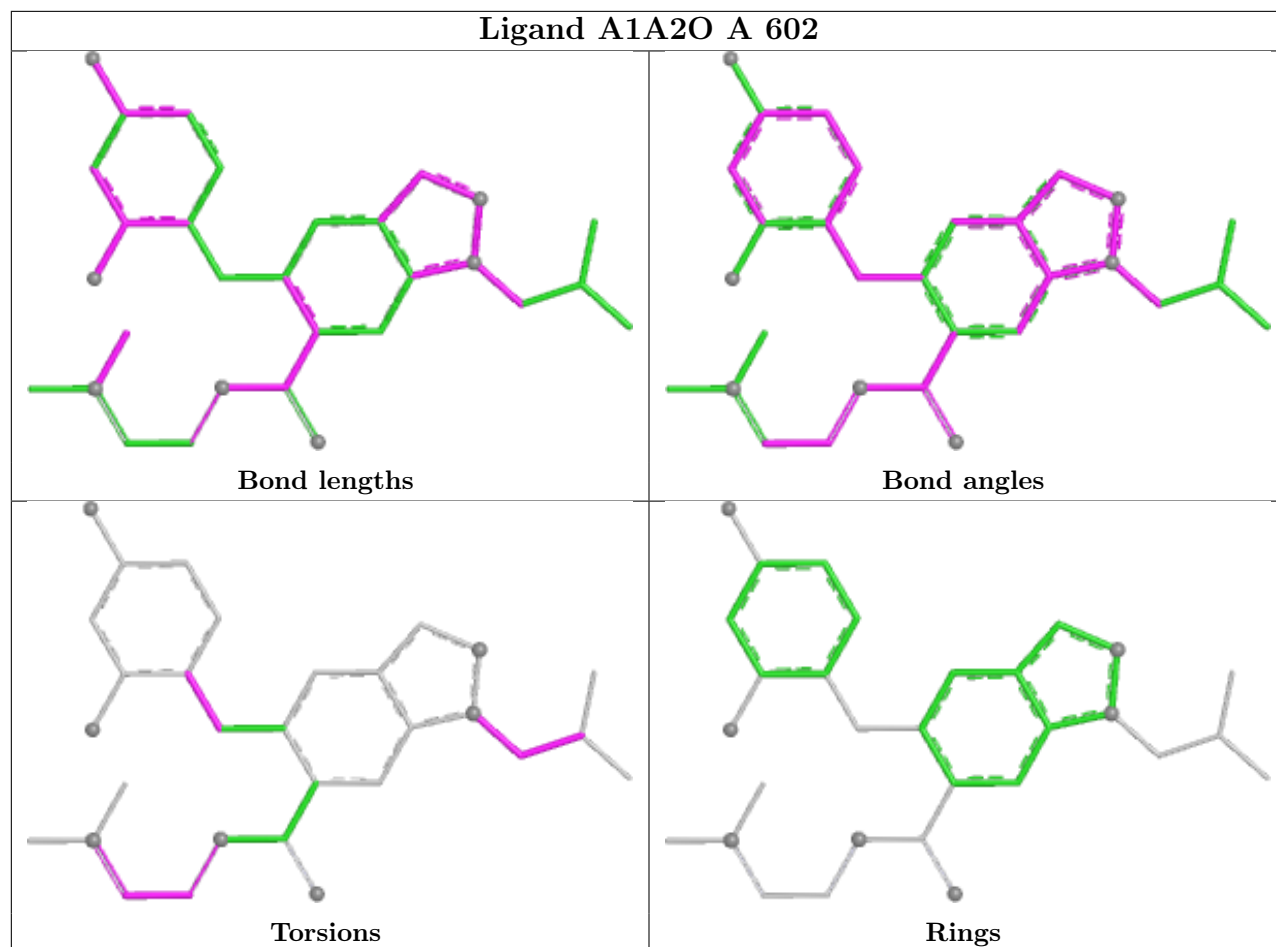
3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	A	604	GOL	2	0
10	A	606	SO4	1	0
9	A	605	MES	2	0

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

Ligand SIA A 603





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	526/529 (99%)	-0.06	8 (1%) 72 71	26, 61, 100, 146	6 (1%)

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	377	VAL	4.6
1	A	4	ILE	2.8
1	A	261	ILE	2.8
1	A	526	PHE	2.4
1	A	17	GLN	2.3
1	A	528	LYS	2.2
1	A	376	TRP	2.1
1	A	214[A]	HIS	2.1

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.

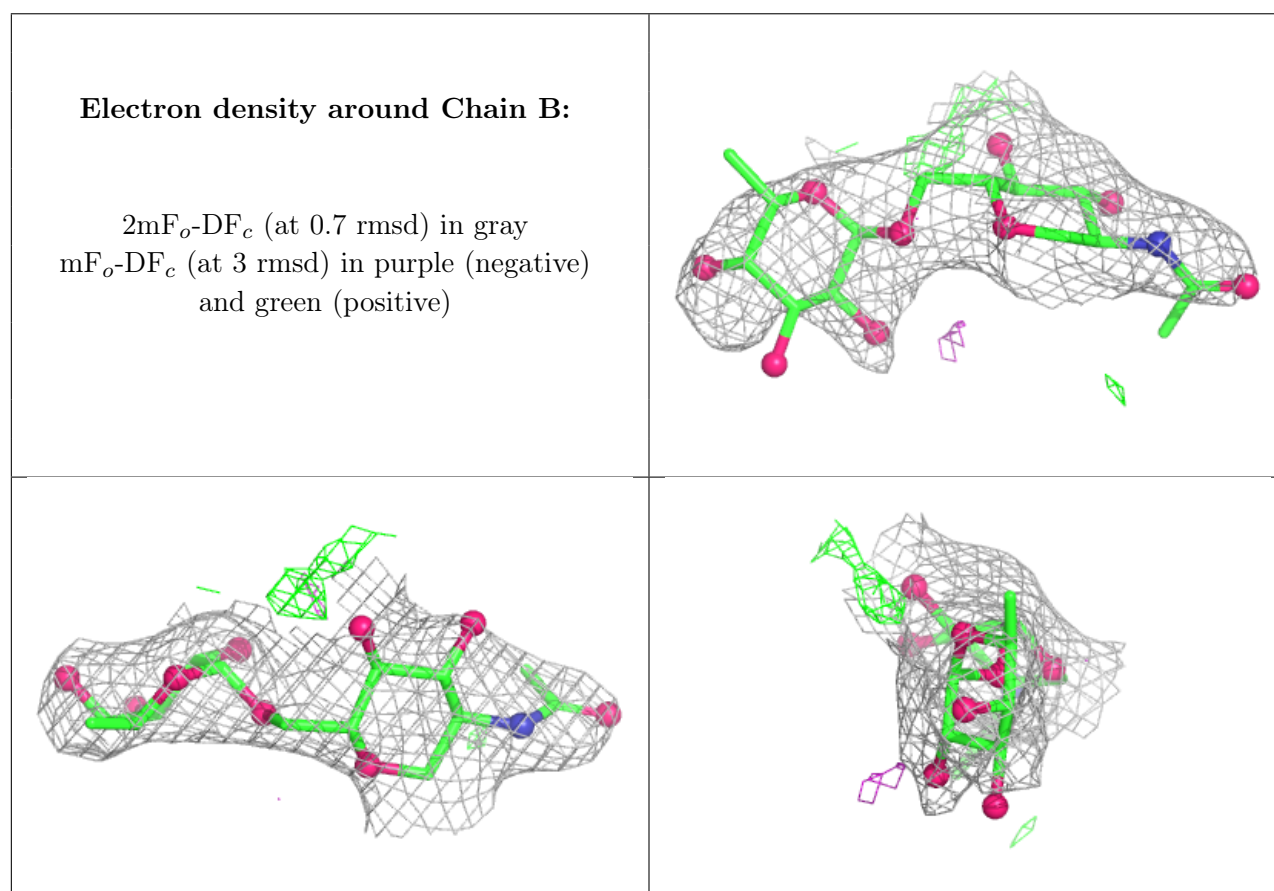
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	BMA	E	3	11/12	0.25	0.12	125,131,140,142	0
4	NAG	F	2	14/15	0.43	0.15	124,137,140,142	0
2	FUC	D	2	10/11	0.49	0.17	105,112,125,129	0
2	NAG	D	1	14/15	0.57	0.13	114,117,123,130	0

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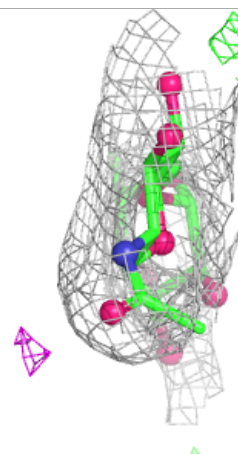
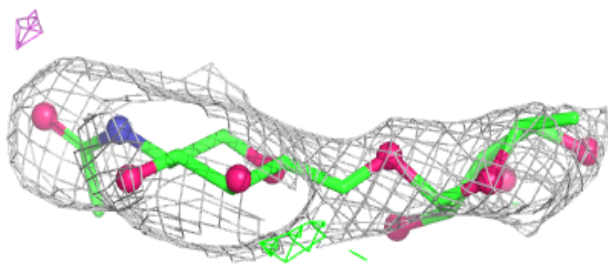
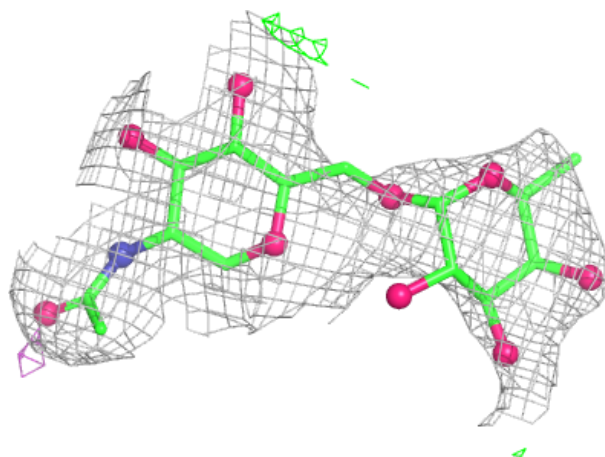
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	NAG	B	1	14/15	0.62	0.13	101,113,118,121	0
4	NAG	F	1	14/15	0.70	0.16	75,110,127,131	0
2	FUC	B	2	10/11	0.70	0.11	118,130,134,136	0
2	NAG	C	1	14/15	0.73	0.13	75,94,102,107	0
3	NAG	E	2	14/15	0.74	0.12	91,106,120,129	0
2	FUC	C	2	10/11	0.81	0.14	93,100,112,112	0
3	FUC	E	4	10/11	0.83	0.14	84,101,103,104	0
3	NAG	E	1	14/15	0.90	0.10	72,79,90,98	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.



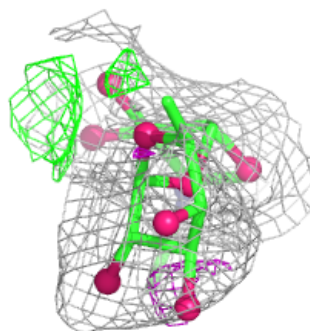
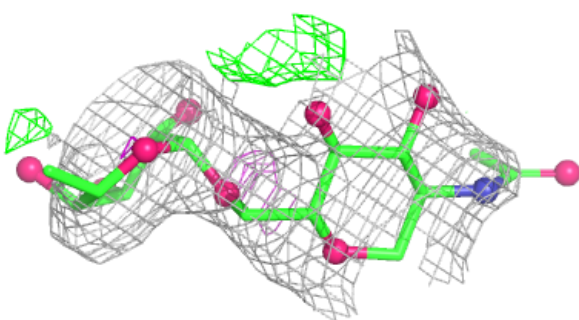
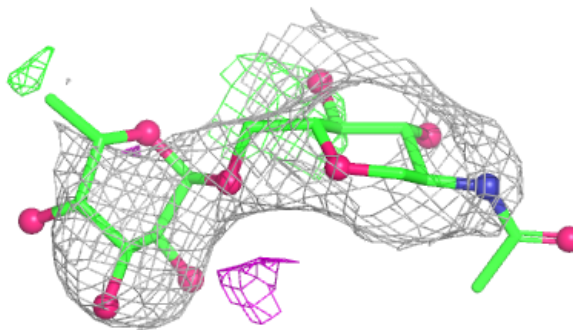
Electron density around Chain C:

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



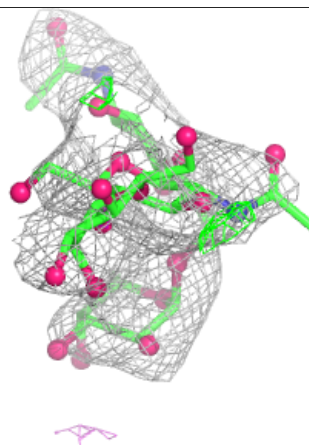
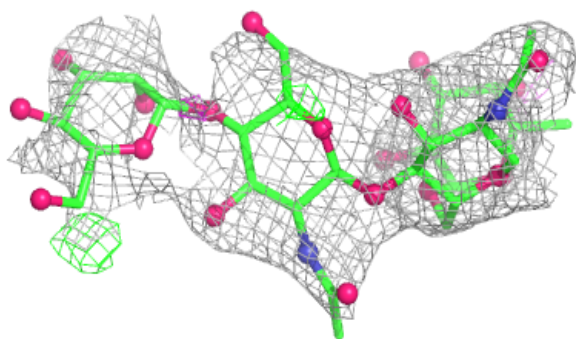
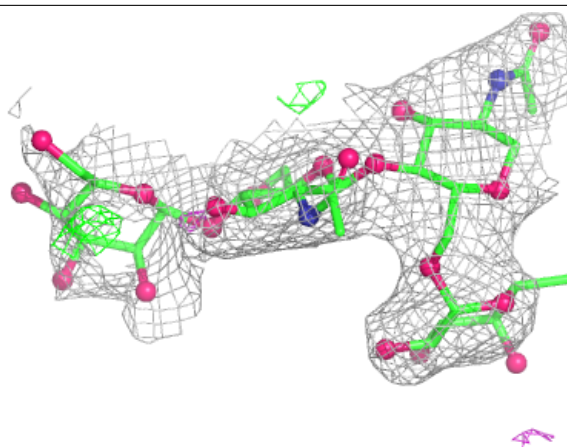
Electron density around Chain D:

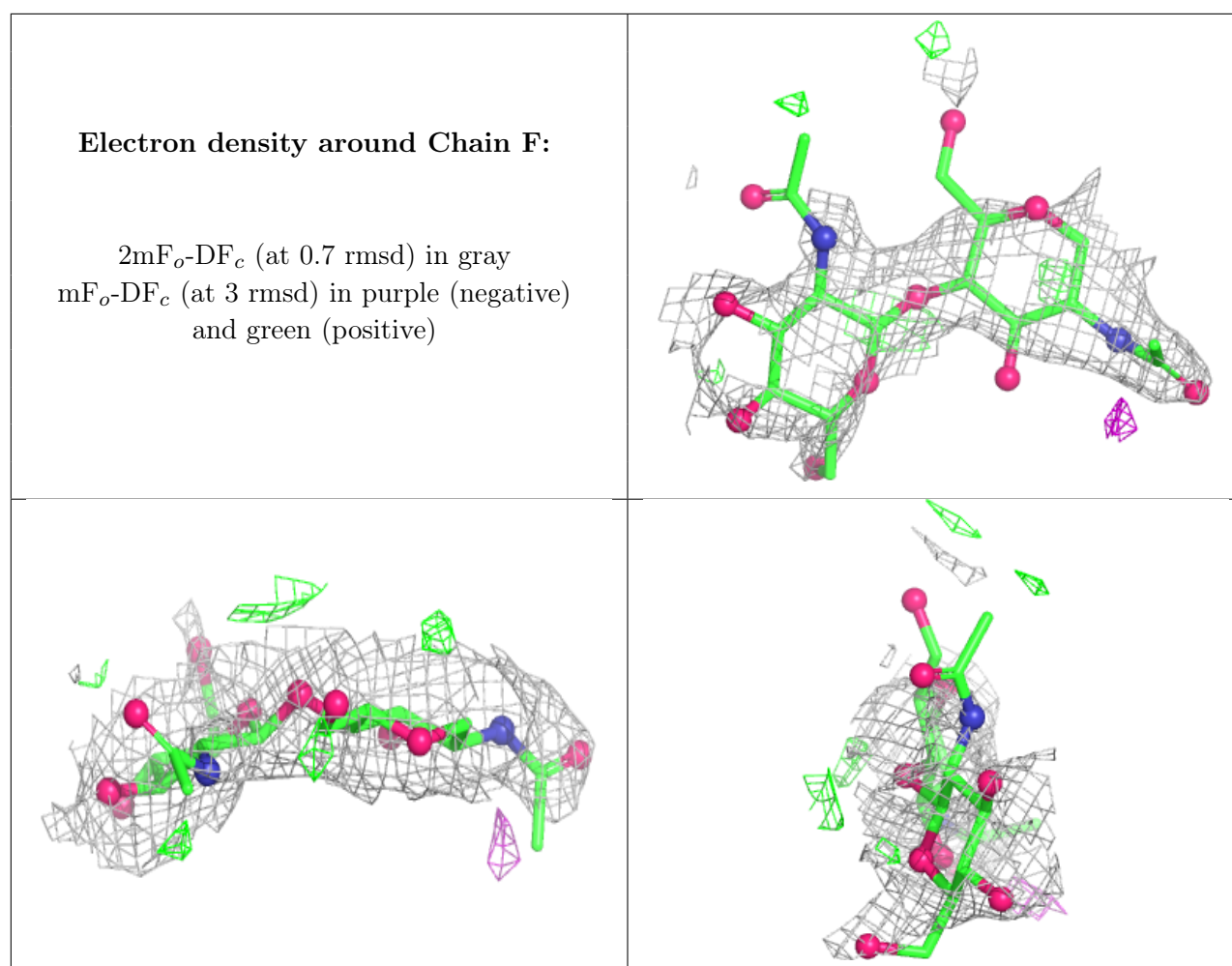
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around Chain E:

$2mF_o-DF_c$ (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.

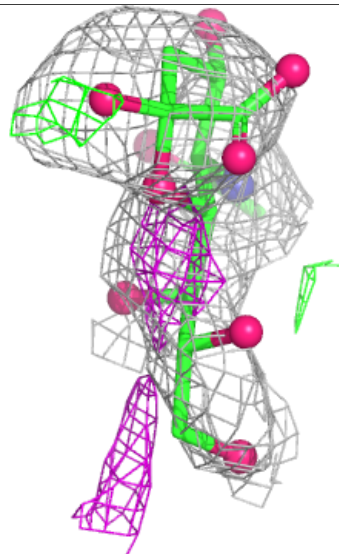
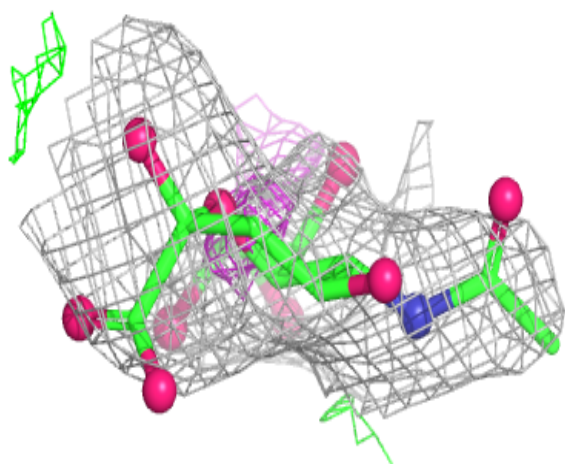
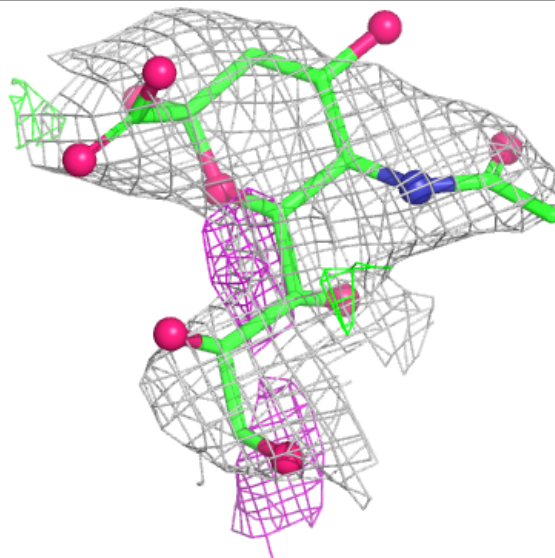
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
5	NAG	A	601	14/15	0.57	0.11	102,112,116,118	0
7	SIA	A	603	21/21	0.68	0.12	59,84,98,105	0
9	MES	A	605	12/12	0.69	0.14	73,92,108,110	0
10	SO4	A	606	5/5	0.78	0.15	81,84,97,98	0
10	SO4	A	607	5/5	0.78	0.07	106,109,124,131	0
10	SO4	A	608	5/5	0.84	0.22	66,77,91,92	0
8	GOL	A	604	6/6	0.86	0.14	76,81,82,85	0
6	A1A2O	A	602	30/30	0.90	0.13	50,61,74,80	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.

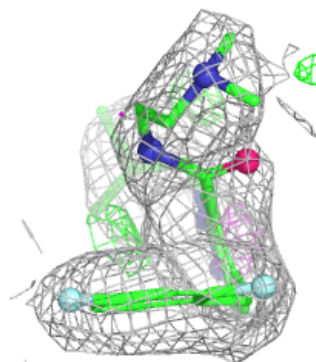
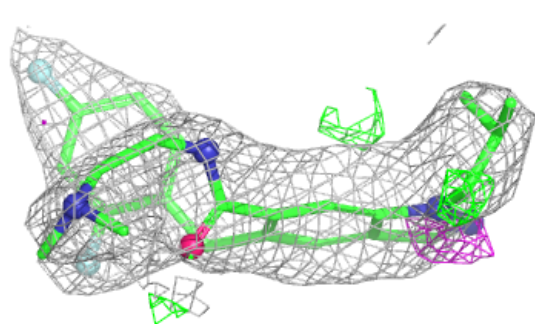
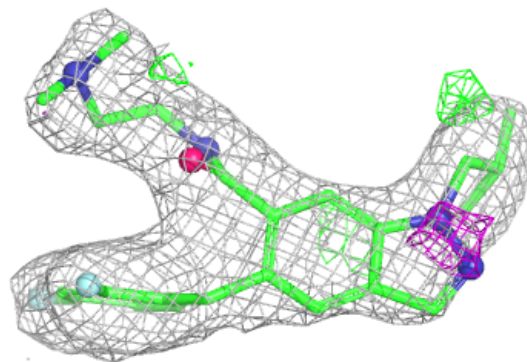
Electron density around SIA A 603:

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



Electron density around A1A2O A 602:

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



6.5 Other polymers ⓘ

There are no such residues in this entry.