



wwPDB X-ray Structure Validation Summary Report ⓘ

Apr 9, 2026 – 10:08 PM UTC

PDB ID : 9SYA / pdb_00009sya
Title : Crystal structure of HERV-K envelope glycoprotein surface subunit with
cholates and sulfates bound
Authors : Nikolopoulos, N.; Modis, Y.
Deposited on : 2025-10-10
Resolution : 2.25 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

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

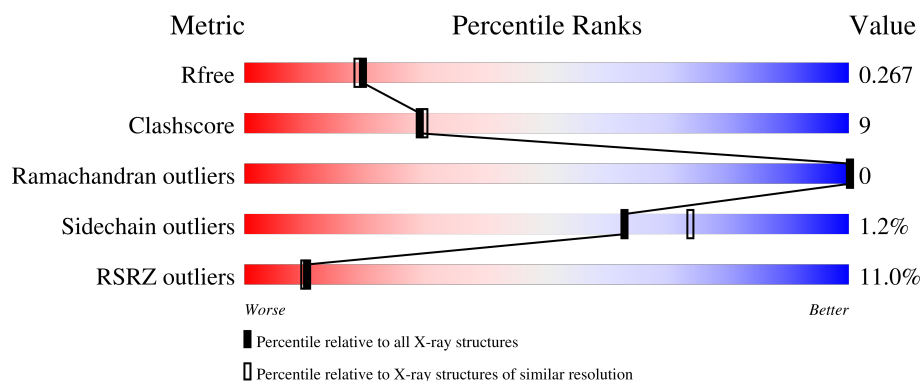
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.25 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.




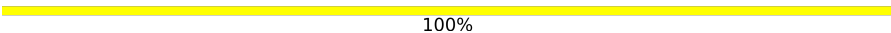
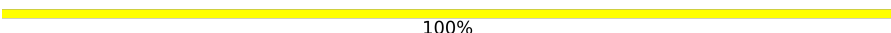

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1898 (2.26-2.26)
Clashscore	190562	2005 (2.26-2.26)
Ramachandran outliers	187476	1965 (2.26-2.26)
Sidechain outliers	187428	1966 (2.26-2.26)
RSRZ outliers	180081	1898 (2.26-2.26)

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	343	<div> <div>10%</div> <div>75%</div> <div>20%</div> <div>6%</div> </div>
1	B	343	<div> <div>11%</div> <div>77%</div> <div>17%</div> <div>6%</div> </div>
2	C	2	<div> <div>100%</div> </div>
2	H	2	<div> <div>100%</div> </div>
2	I	2	<div> <div>50%</div> <div>50%</div> </div>

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Mol	Chain	Length	Quality of chain
3	D	3	 33%67%
4	E	6	 100%
4	F	6	 100%
4	G	6	 50%50%

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 5923 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 Surface protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	324	Total	C	N	O	S	0	1	0
			2576	1643	446	470	17			
1	B	323	Total	C	N	O	S	0	1	0
			2569	1641	445	466	17			

There are 52 discrepancies between the modelled and reference sequences:

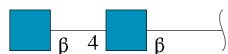
Chain	Residue	Modelled	Actual	Comment	Reference
A	96	ALA	-	expression tag	UNP P61570
A	97	PRO	-	expression tag	UNP P61570
A	98	PHE	-	expression tag	UNP P61570
A	99	ASP	-	expression tag	UNP P61570
A	100	ASP	-	expression tag	UNP P61570
A	101	ASP	-	expression tag	UNP P61570
A	102	ASP	-	expression tag	UNP P61570
A	103	LYS	-	expression tag	UNP P61570
A	104	LEU	-	expression tag	UNP P61570
A	105	GLU	-	expression tag	UNP P61570
A	106	VAL	-	expression tag	UNP P61570
A	107	LEU	-	expression tag	UNP P61570
A	108	PHE	-	expression tag	UNP P61570
A	109	GLN	-	expression tag	UNP P61570
A	110	GLY	-	expression tag	UNP P61570
A	141	ALA	CYS	conflict	UNP P61570
A	167	ARG	THR	conflict	UNP P61570
A	185	THR	ILE	conflict	UNP P61570
A	431	PRO	-	expression tag	UNP P61570
A	432	GLY	-	expression tag	UNP P61570
A	433	HIS	-	expression tag	UNP P61570
A	434	HIS	-	expression tag	UNP P61570
A	435	HIS	-	expression tag	UNP P61570
A	436	HIS	-	expression tag	UNP P61570
A	437	HIS	-	expression tag	UNP P61570

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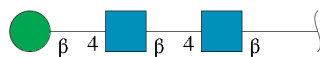
Chain	Residue	Modelled	Actual	Comment	Reference
A	438	HIS	-	expression tag	UNP P61570
B	96	ALA	-	expression tag	UNP P61570
B	97	PRO	-	expression tag	UNP P61570
B	98	PHE	-	expression tag	UNP P61570
B	99	ASP	-	expression tag	UNP P61570
B	100	ASP	-	expression tag	UNP P61570
B	101	ASP	-	expression tag	UNP P61570
B	102	ASP	-	expression tag	UNP P61570
B	103	LYS	-	expression tag	UNP P61570
B	104	LEU	-	expression tag	UNP P61570
B	105	GLU	-	expression tag	UNP P61570
B	106	VAL	-	expression tag	UNP P61570
B	107	LEU	-	expression tag	UNP P61570
B	108	PHE	-	expression tag	UNP P61570
B	109	GLN	-	expression tag	UNP P61570
B	110	GLY	-	expression tag	UNP P61570
B	141	ALA	CYS	conflict	UNP P61570
B	167	ARG	THR	conflict	UNP P61570
B	185	THR	ILE	conflict	UNP P61570
B	431	PRO	-	expression tag	UNP P61570
B	432	GLY	-	expression tag	UNP P61570
B	433	HIS	-	expression tag	UNP P61570
B	434	HIS	-	expression tag	UNP P61570
B	435	HIS	-	expression tag	UNP P61570
B	436	HIS	-	expression tag	UNP P61570
B	437	HIS	-	expression tag	UNP P61570
B	438	HIS	-	expression tag	UNP P61570

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



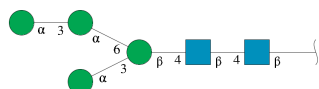
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	H	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	I	2	Total	C	N	O	0	0	0
			28	16	2	10			

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



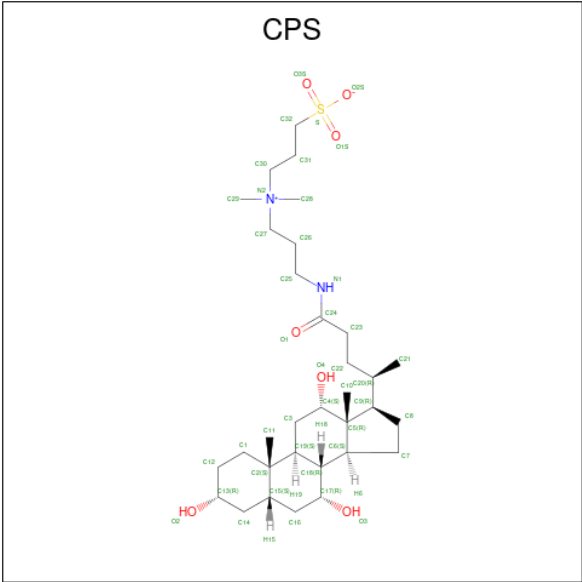
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	D	3	Total	C	N	O	0	0	0
			39	22	2	15			

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



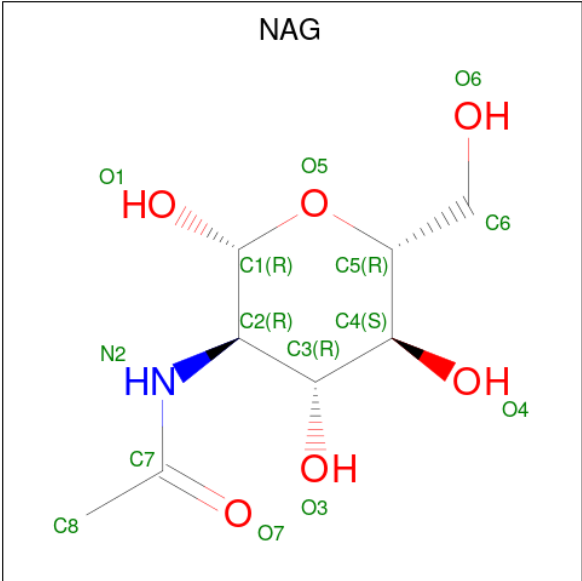
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	E	6	Total	C	N	O	0	0	0
			72	40	2	30			
4	F	6	Total	C	N	O	0	0	0
			72	40	2	30			
4	G	6	Total	C	N	O	0	0	0
			72	40	2	30			

- Molecule 5 is 3-[(3-CHOLAMIDOPROPYL)DIMETHYLAMMONIO]-1-PROPANESULFONATE (CCD ID: CPS) (formula: C₃₂H₅₈N₂O₇S).



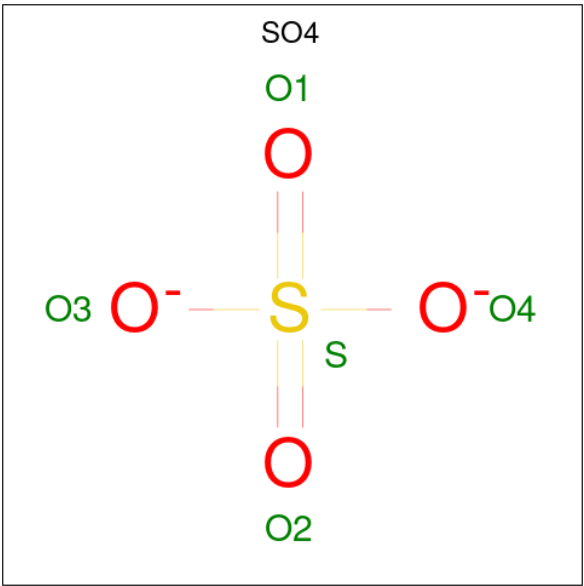
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	S	0	0
			42	32	2	7	1		
5	B	1	Total	C	N	O	S	0	0
			42	32	2	7	1		

- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



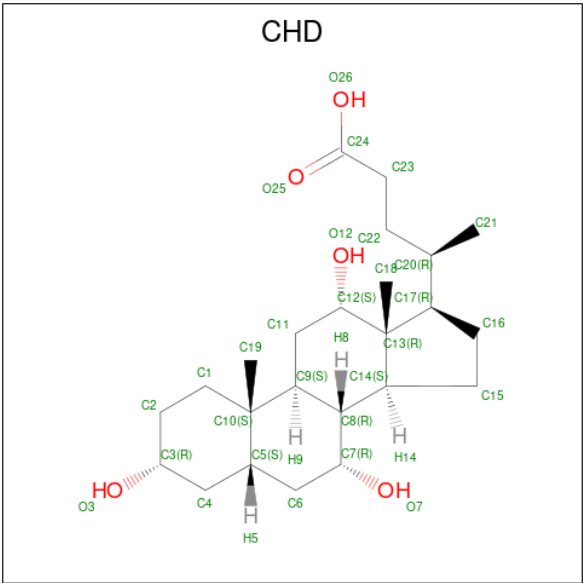
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 7 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

- Molecule 8 is CHOLIC ACID (CCD ID: CHD) (formula: C₂₄H₄₀O₅).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	B	1	Total	C	O	0	0
			29	24	5		

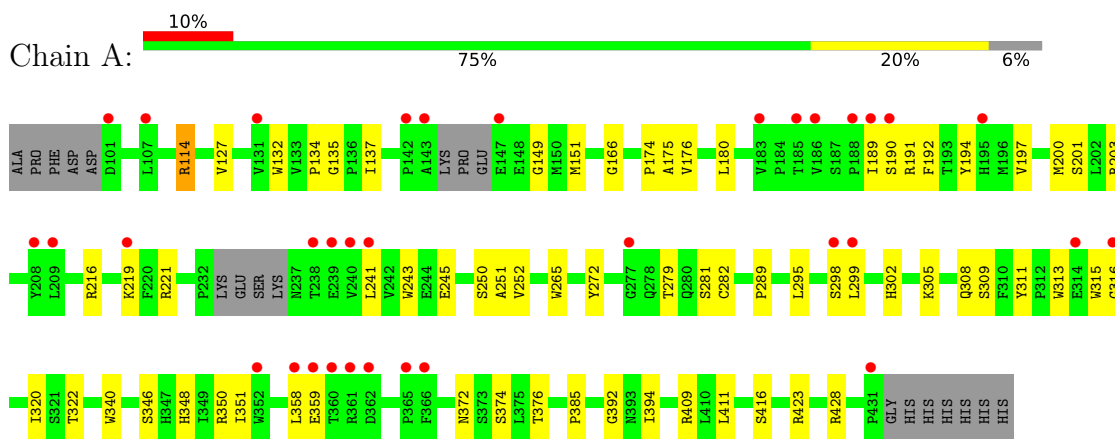
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	149	Total	O	0	0
			149	149		
9	B	143	Total	O	0	0
			143	143		

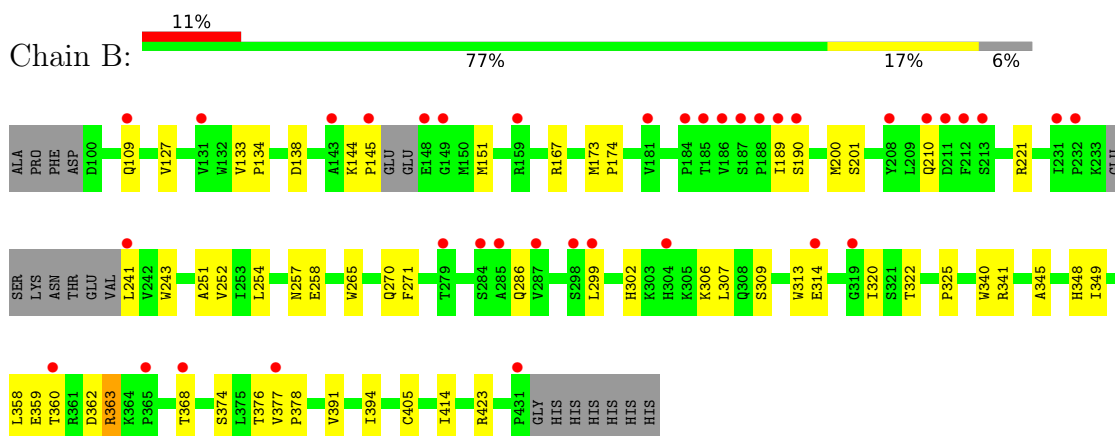
3 Residue-property plots

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.

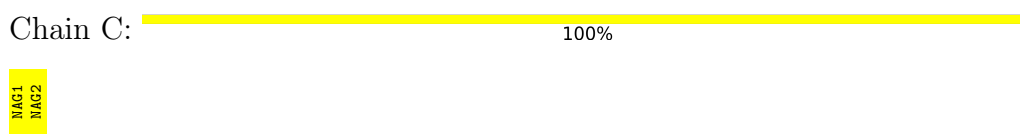
- Molecule 1: Surface protein



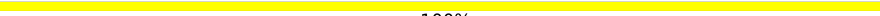
- Molecule 1: Surface protein



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



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

Chain H:  100%

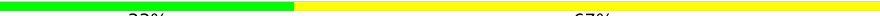
NAG1
NAG2

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

Chain I:  50% 50%

NAG1
NAG2

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

Chain D:  33% 67%

NAG1
NAG2
BMA3

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

Chain E:  100%

NAG1
NAG2
BMA3
MAN4
MAN5
MAN6

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

Chain F:  100%

NAG1
NAG2
BMA3
MAN4
MAN5
MAN6

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

Chain G:  50% 50%

NAG1
NAG2
BMA3
MAN4
MAN5
MAN6

4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	60.04Å 63.52Å 70.68Å 101.94° 101.83° 104.06°	Depositor
Resolution (Å)	59.32 – 2.25 59.32 – 2.25	Depositor EDS
% Data completeness (in resolution range)	98.3 (59.32-2.25) 98.3 (59.32-2.25)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.18 (at 2.25Å)	Xtriage
Refinement program	PHENIX 2.0_5936	Depositor
R, R_{free}	0.213 , 0.267 0.214 , 0.267	Depositor DCC
R_{free} test set	2024 reflections (4.49%)	wwPDB-VP
Wilson B-factor (Å ²)	47.2	Xtriage
Anisotropy	0.373	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 50.4	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	5923	wwPDB-VP
Average B, all atoms (Å ²)	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.59% 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: BMA, MAN, CHD, CPS, SO4, NAG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.37	0/2651	0.60	0/3625
1	B	0.37	0/2645	0.59	2/3615 (0.1%)
All	All	0.37	0/5296	0.60	2/7240 (0.0%)

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.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	B	363	ARG	CA-C-N	-5.19	113.28	123.56
1	B	363	ARG	C-N-CA	-5.19	113.28	123.56

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	315	TRP	Peptide

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2576	0	2507	47	0
1	B	2569	0	2508	38	0
2	C	28	0	25	0	0
2	H	28	0	25	0	0
2	I	28	0	25	0	0
3	D	39	0	34	0	0
4	E	72	0	61	0	0
4	F	72	0	61	0	0
4	G	72	0	61	3	0
5	A	42	0	58	2	0
5	B	42	0	58	7	0
6	A	14	0	13	0	0
7	A	10	0	0	0	0
7	B	10	0	0	0	0
8	B	29	0	39	3	0
9	A	149	0	0	4	0
9	B	143	0	0	2	0
All	All	5923	0	5475	97	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 9.

The worst 5 of 97 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)
5:B:602:CPS:H262	5:B:602:CPS:H23A	1.64	0.79
8:B:601:CHD:H151	5:B:602:CPS:H7	1.69	0.74
1:B:322:THR:HG21	1:B:340:TRP:CZ2	2.33	0.64
1:B:302:HIS:HD2	1:B:374:SER:HB3	1.67	0.60
1:B:167:ARG:HG2	1:B:173:MET:HG2	1.86	0.56

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	319/343 (93%)	305 (96%)	14 (4%)	0	100	100
1	B	318/343 (93%)	308 (97%)	10 (3%)	0	100	100
All	All	637/686 (93%)	613 (96%)	24 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	292/313 (93%)	288 (99%)	4 (1%)	59	70
1	B	291/313 (93%)	287 (99%)	4 (1%)	59	70
All	All	583/626 (93%)	575 (99%)	8 (1%)	63	70

5 of 8 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	360	THR
1	B	252	VAL
1	B	109[A]	GLN
1	A	372	ASN
1	B	109[B]	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 6 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	372	ASN
1	B	302	HIS
1	B	380	GLN
1	A	270	GLN

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Mol	Chain	Res	Type
1	A	195	HIS

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 ⓘ

27 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	0.81	0	17,19,21	1.43	3 (17%)
2	NAG	C	2	2	14,14,15	0.81	1 (7%)	17,19,21	1.20	1 (5%)
3	NAG	D	1	3,1	14,14,15	1.05	1 (7%)	17,19,21	1.56	3 (17%)
3	NAG	D	2	3	14,14,15	0.75	0	17,19,21	1.04	0
3	BMA	D	3	3	11,11,12	0.97	1 (9%)	15,15,17	2.44	5 (33%)
4	NAG	E	1	4,1	14,14,15	0.84	0	17,19,21	1.30	2 (11%)
4	NAG	E	2	4	14,14,15	0.85	1 (7%)	17,19,21	1.19	1 (5%)
4	BMA	E	3	4	11,11,12	0.85	0	15,15,17	2.47	6 (40%)
4	MAN	E	4	4	11,11,12	0.68	0	15,15,17	1.58	2 (13%)
4	MAN	E	5	4	11,11,12	0.72	0	15,15,17	0.96	1 (6%)
4	MAN	E	6	4	11,11,12	0.63	0	15,15,17	1.55	1 (6%)
4	NAG	F	1	4,1	14,14,15	0.78	1 (7%)	17,19,21	1.28	2 (11%)
4	NAG	F	2	4	14,14,15	0.73	0	17,19,21	1.73	3 (17%)
4	BMA	F	3	4	11,11,12	1.01	1 (9%)	15,15,17	2.29	6 (40%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	MAN	F	4	4	11,11,12	0.76	0	15,15,17	1.04	1 (6%)
4	MAN	F	5	4	11,11,12	0.59	0	15,15,17	1.62	1 (6%)
4	MAN	F	6	4	11,11,12	0.61	0	15,15,17	1.46	1 (6%)
4	NAG	G	1	4,1	14,14,15	0.98	0	17,19,21	1.96	5 (29%)
4	NAG	G	2	4	14,14,15	0.74	0	17,19,21	2.28	6 (35%)
4	BMA	G	3	4	11,11,12	1.05	1 (9%)	15,15,17	2.15	7 (46%)
4	MAN	G	4	4	11,11,12	0.75	0	15,15,17	3.62	6 (40%)
4	MAN	G	5	4	11,11,12	0.68	0	15,15,17	2.55	2 (13%)
4	MAN	G	6	4	11,11,12	0.62	0	15,15,17	2.07	2 (13%)
2	NAG	H	1	2,1	14,14,15	0.70	0	17,19,21	1.10	1 (5%)
2	NAG	H	2	2	14,14,15	0.82	1 (7%)	17,19,21	1.72	5 (29%)
2	NAG	I	1	2,1	14,14,15	0.85	1 (7%)	17,19,21	1.90	4 (23%)
2	NAG	I	2	2	14,14,15	0.71	0	17,19,21	0.93	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
2	NAG	C	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	C	2	2	-	0/6/23/26	0/1/1/1
3	NAG	D	1	3,1	-	1/6/23/26	0/1/1/1
3	NAG	D	2	3	-	2/6/23/26	0/1/1/1
3	BMA	D	3	3	-	0/2/19/22	0/1/1/1
4	NAG	E	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	E	2	4	-	0/6/23/26	0/1/1/1
4	BMA	E	3	4	-	2/2/19/22	0/1/1/1
4	MAN	E	4	4	-	0/2/19/22	0/1/1/1
4	MAN	E	5	4	-	0/2/19/22	0/1/1/1
4	MAN	E	6	4	-	0/2/19/22	0/1/1/1
4	NAG	F	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	F	2	4	-	0/6/23/26	0/1/1/1
4	BMA	F	3	4	-	0/2/19/22	0/1/1/1
4	MAN	F	4	4	-	0/2/19/22	0/1/1/1
4	MAN	F	5	4	-	0/2/19/22	0/1/1/1
4	MAN	F	6	4	-	1/2/19/22	0/1/1/1
4	NAG	G	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	G	2	4	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	BMA	G	3	4	-	0/2/19/22	0/1/1/1
4	MAN	G	4	4	-	1/2/19/22	0/1/1/1
4	MAN	G	5	4	-	0/2/19/22	0/1/1/1
4	MAN	G	6	4	-	0/2/19/22	0/1/1/1
2	NAG	H	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	H	2	2	-	2/6/23/26	0/1/1/1
2	NAG	I	1	2,1	-	4/6/23/26	0/1/1/1
2	NAG	I	2	2	-	0/6/23/26	0/1/1/1

The worst 5 of 9 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	1	NAG	O5-C1	-2.43	1.39	1.43
4	G	3	BMA	C2-C3	2.40	1.56	1.52
4	F	3	BMA	C2-C3	2.23	1.55	1.52
2	C	2	NAG	C1-C2	2.22	1.55	1.52
2	I	1	NAG	O5-C1	-2.17	1.40	1.43

The worst 5 of 77 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	G	4	MAN	C1-O5-C5	11.71	127.88	112.19
4	G	5	MAN	C1-O5-C5	8.18	123.15	112.19
4	G	6	MAN	C1-O5-C5	6.86	121.38	112.19
4	E	3	BMA	C1-O5-C5	6.37	120.72	112.19
3	D	3	BMA	C1-O5-C5	5.60	119.69	112.19

There are no chirality outliers.

5 of 17 torsion outliers are listed below:

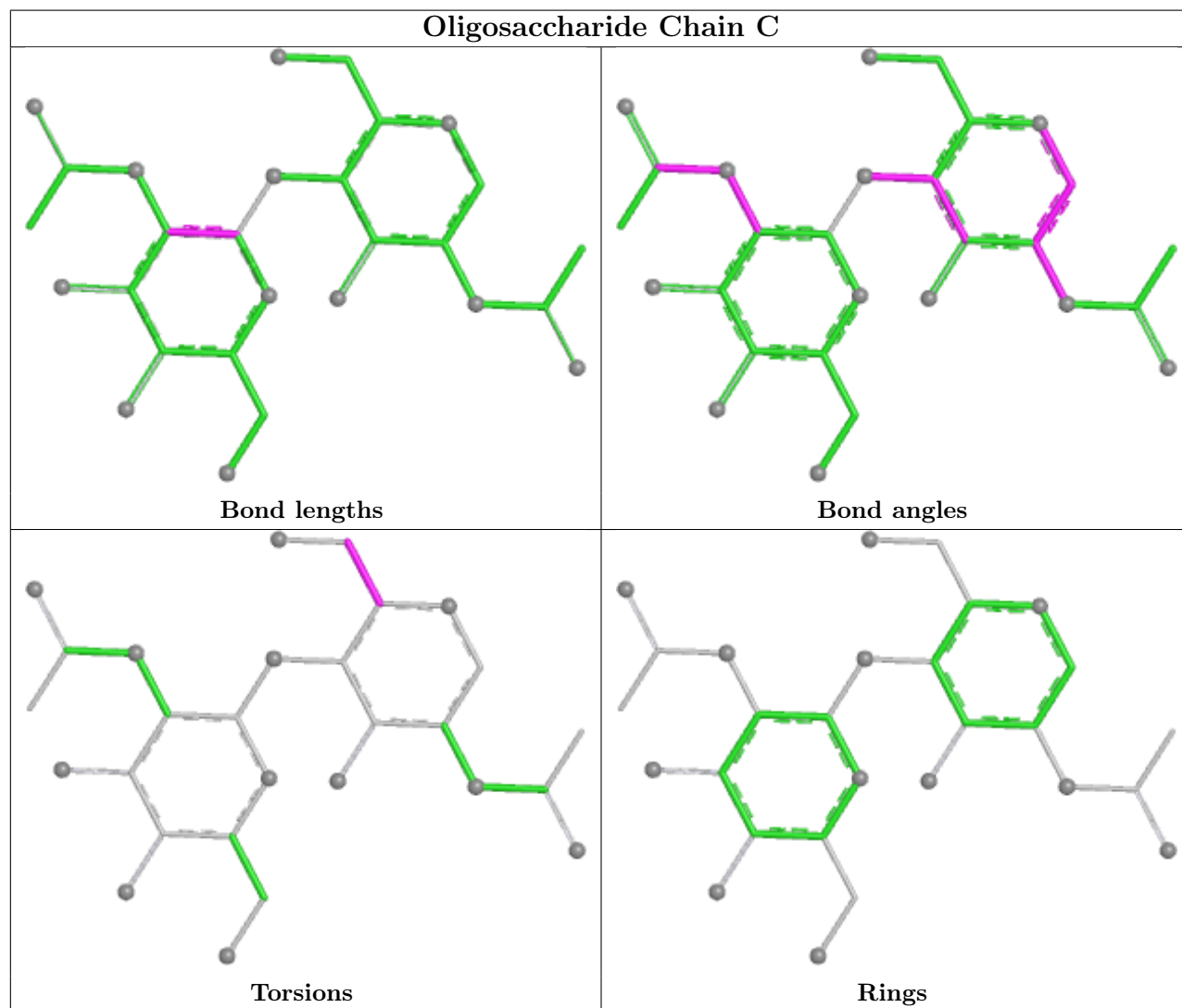
Mol	Chain	Res	Type	Atoms
4	G	2	NAG	C1-C2-N2-C7
2	I	1	NAG	O5-C5-C6-O6
3	D	2	NAG	O5-C5-C6-O6
2	C	1	NAG	O5-C5-C6-O6
2	I	1	NAG	C4-C5-C6-O6

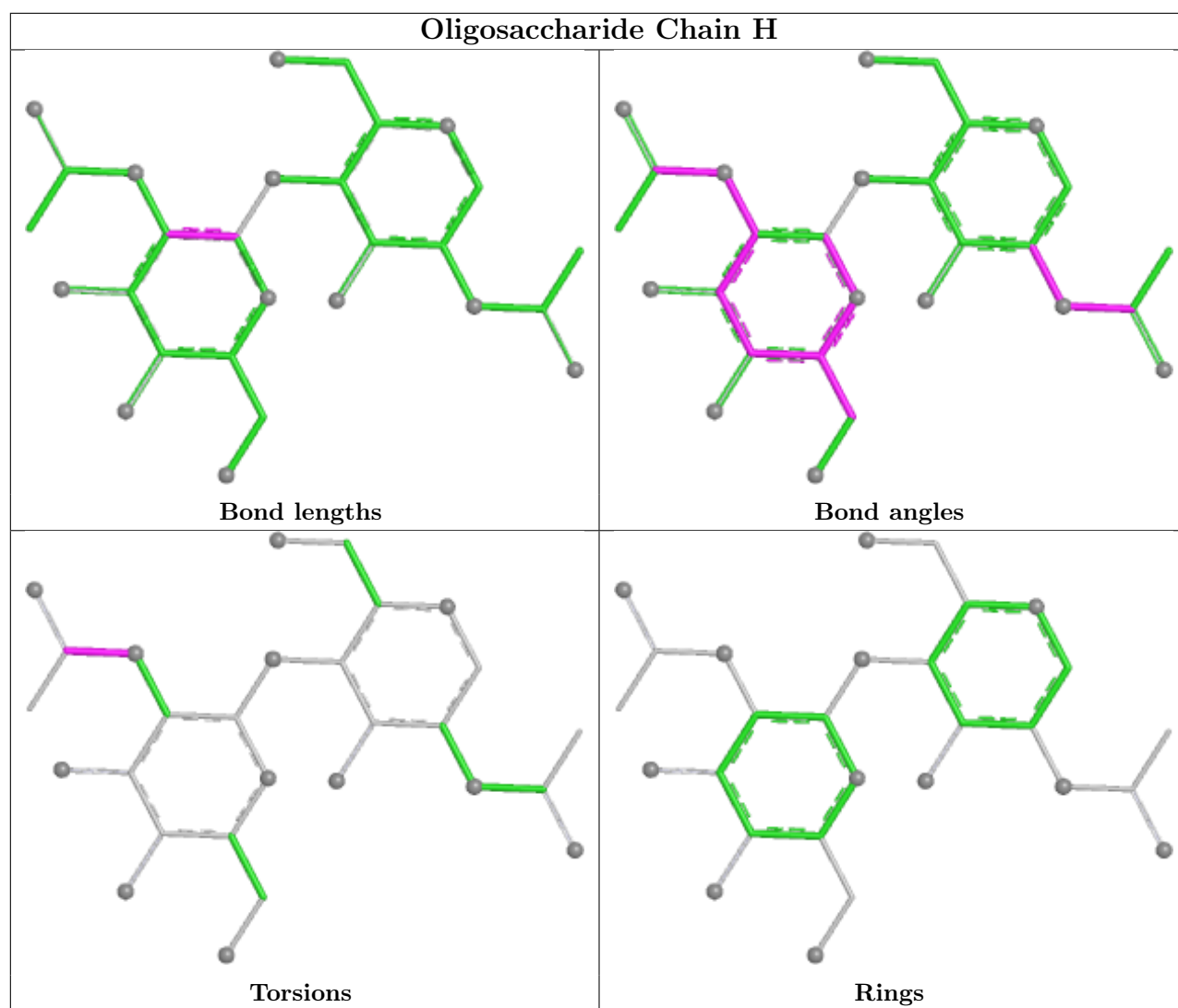
There are no ring outliers.

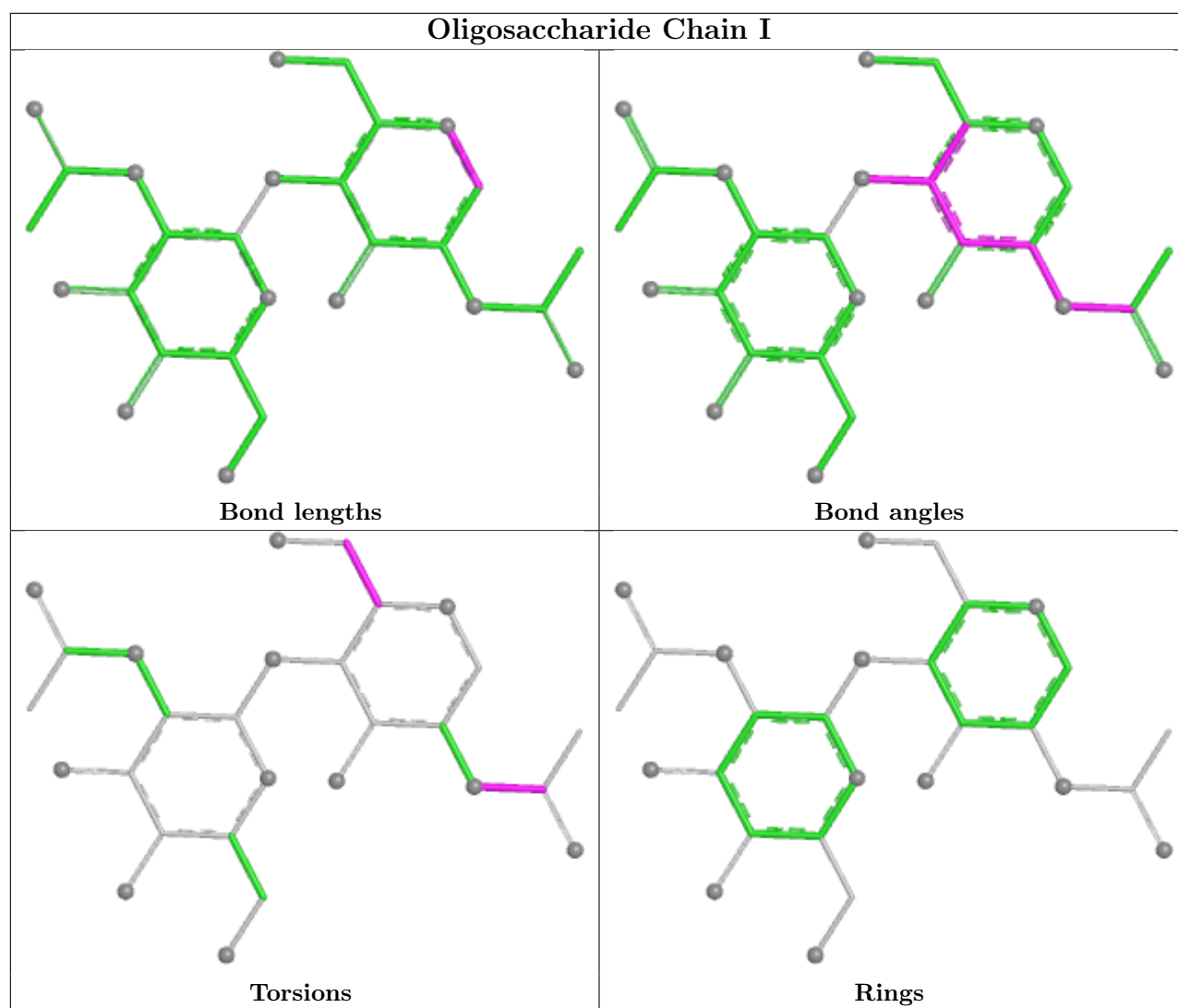
3 monomers are involved in 3 short contacts:

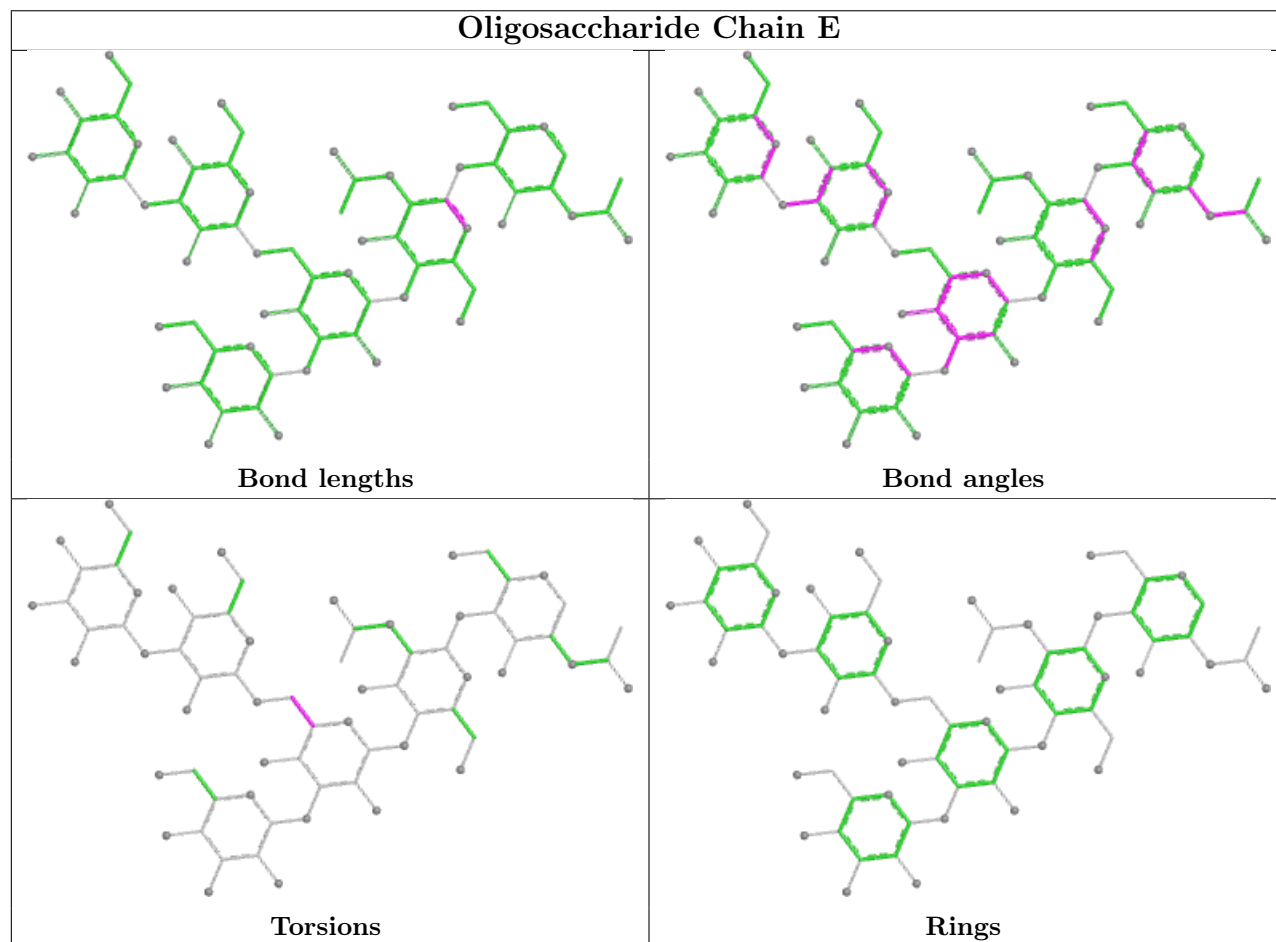
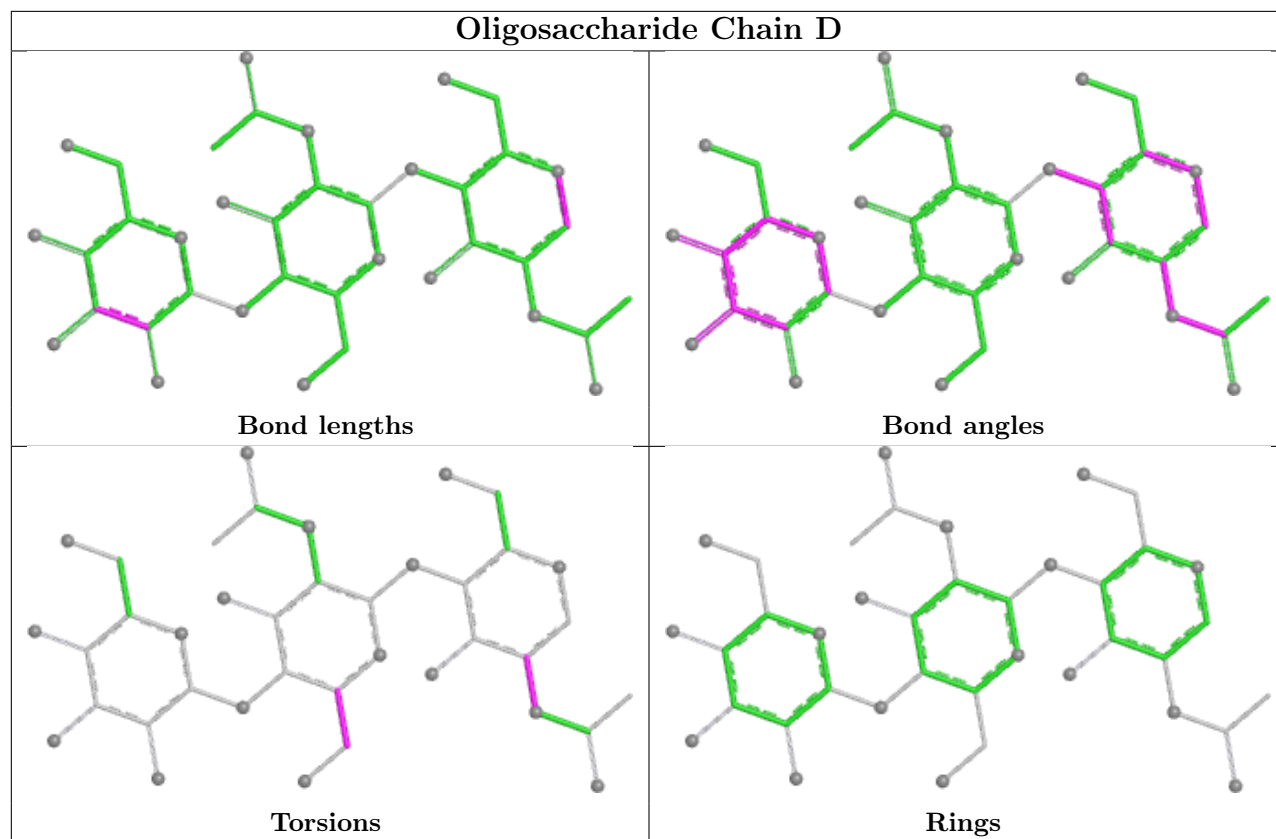
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	G	4	MAN	2	0
4	G	3	BMA	2	0
4	G	2	NAG	1	0

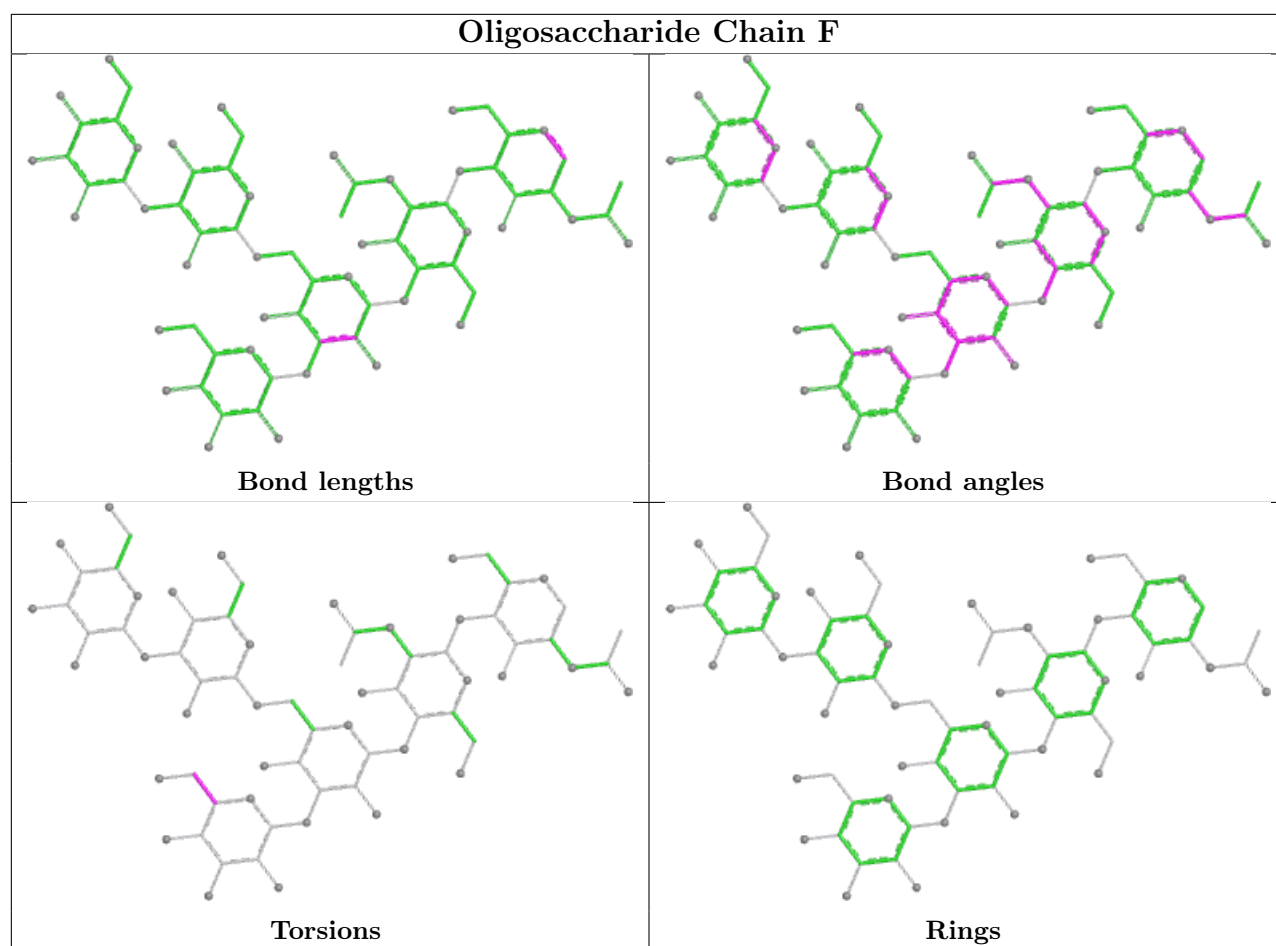
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

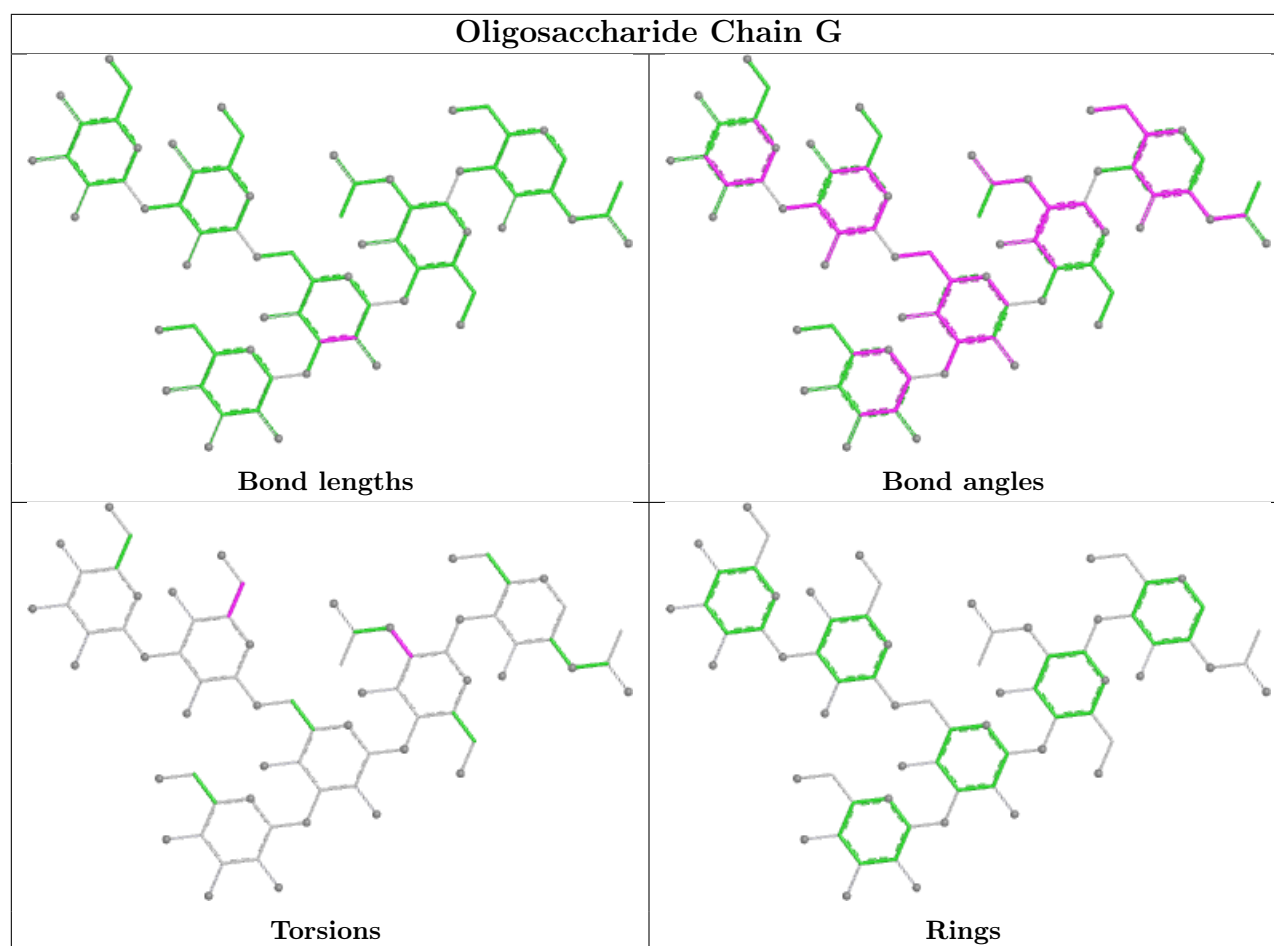












5.6 Ligand geometry [i](#)

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
5	CPS	A	501	-	45,45,45	0.64	1 (2%)	70,70,70	0.85	1 (1%)
7	SO4	B	604	-	4,4,4	0.79	0	6,6,6	0.27	0
7	SO4	A	503	-	4,4,4	0.64	0	6,6,6	0.21	0
7	SO4	B	603	-	4,4,4	0.66	0	6,6,6	0.19	0
6	NAG	A	502	1	14,14,15	0.62	0	17,19,21	1.16	1 (5%)
8	CHD	B	601	-	32,32,32	0.68	0	51,51,51	1.52	7 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	SO4	A	504	-	4,4,4	0.76	0	6,6,6	0.44	0
5	CPS	B	602	-	45,45,45	0.80	1 (2%)	70,70,70	1.87	19 (27%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	CPS	A	501	-	-	8/25/90/90	0/4/4/4
6	NAG	A	502	1	-	0/6/23/26	0/1/1/1
8	CHD	B	601	-	-	9/9/74/74	0/4/4/4
5	CPS	B	602	-	-	18/25/90/90	0/4/4/4

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	602	CPS	C32-S	3.15	1.82	1.77
5	A	501	CPS	C32-S	2.74	1.81	1.77

The worst 5 of 28 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	602	CPS	C25-N1-C24	5.54	133.14	122.82
8	B	601	CHD	C13-C17-C20	5.34	125.96	119.48
5	B	602	CPS	C5-C6-C18	-4.82	108.61	114.72
5	B	602	CPS	C23-C22-C20	-4.26	106.51	114.46
5	B	602	CPS	C14-C15-C2	4.19	117.12	112.66

There are no chirality outliers.

5 of 35 torsion outliers are listed below:

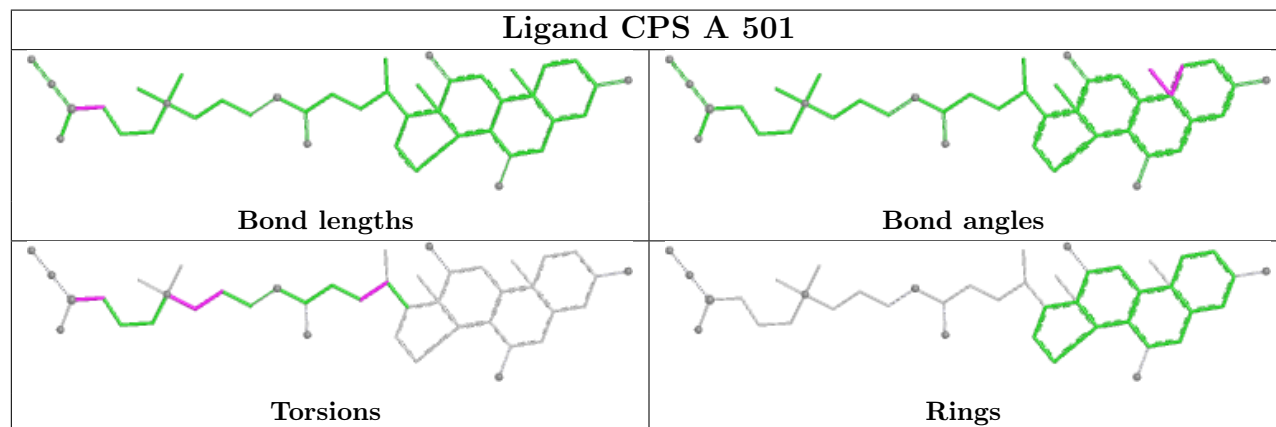
Mol	Chain	Res	Type	Atoms
5	A	501	CPS	C31-C32-S-O3S
5	B	602	CPS	N2-C30-C31-C32
5	B	602	CPS	C31-C30-N2-C27
5	B	602	CPS	C31-C30-N2-C29
8	B	601	CHD	C16-C17-C20-C22

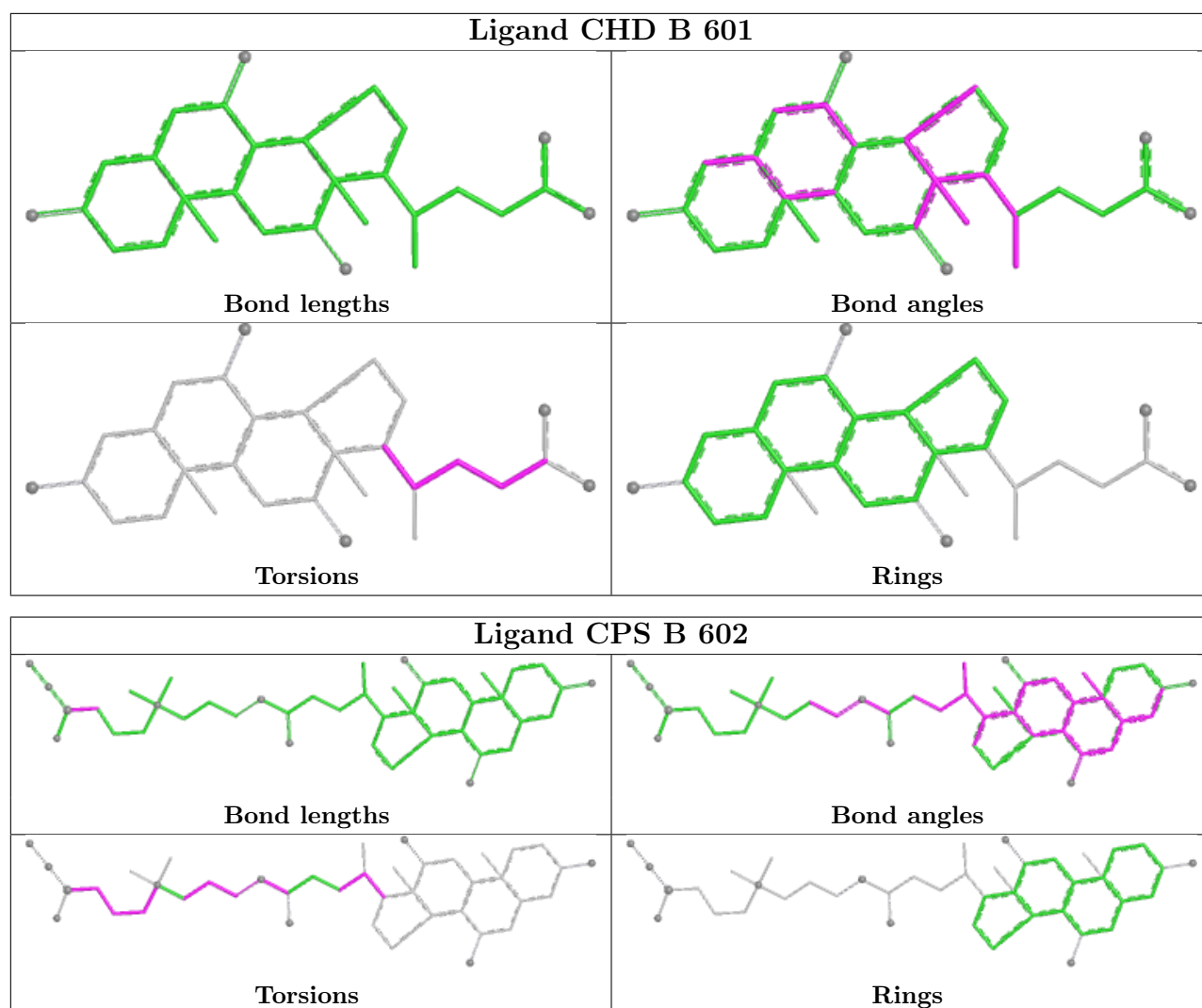
There are no ring outliers.

3 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	501	CPS	2	0
8	B	601	CHD	3	0
5	B	602	CPS	7	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 [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	324/343 (94%)	0.74	34 (10%) 11 11	37, 52, 108, 154	1 (0%)
1	B	323/343 (94%)	0.74	37 (11%) 9 9	30, 52, 98, 137	1 (0%)
All	All	647/686 (94%)	0.74	71 (10%) 10 10	30, 52, 103, 154	2 (0%)

The worst 5 of 71 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	316	GLY	7.1
1	B	189	ILE	5.2
1	A	240	VAL	5.1
1	A	209	LEU	4.7
1	B	431	PRO	4.3

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
4	MAN	G	5	11/12	0.25	0.15	119,135,136,137	0
4	MAN	G	6	11/12	0.32	0.21	132,138,141,141	0
2	NAG	C	2	14/15	0.34	0.16	113,122,126,127	0
3	BMA	D	3	11/12	0.34	0.15	124,130,136,138	0
2	NAG	H	2	14/15	0.35	0.17	101,112,116,119	0

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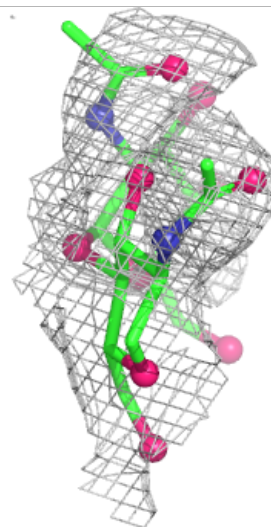
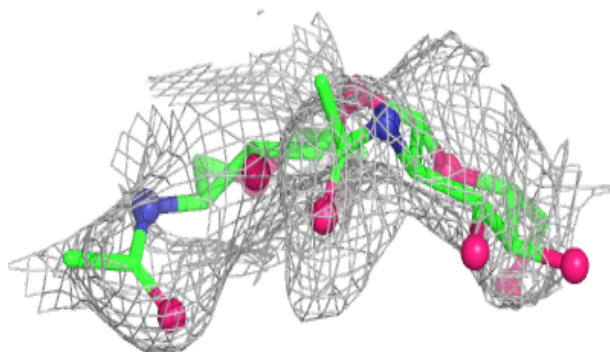
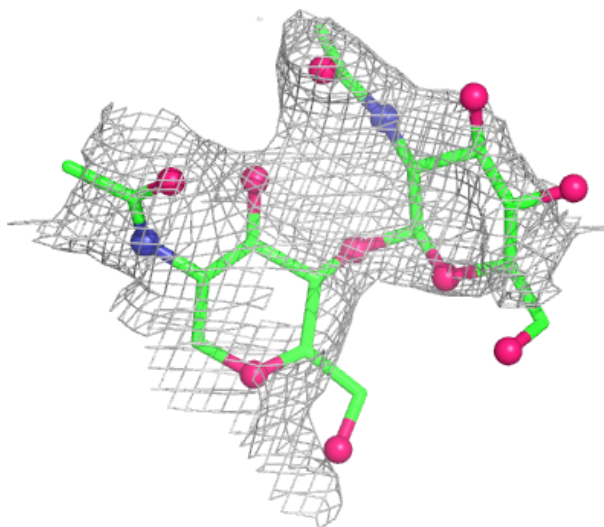
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	NAG	I	2	14/15	0.36	0.18	113,131,137,138	0
4	MAN	E	5	11/12	0.37	0.15	123,134,140,142	0
4	MAN	F	6	11/12	0.38	0.15	97,103,108,109	0
4	MAN	F	4	11/12	0.41	0.15	109,112,114,116	0
4	MAN	E	6	11/12	0.44	0.14	137,144,148,150	0
4	MAN	E	4	11/12	0.46	0.13	123,128,131,135	0
4	BMA	G	3	11/12	0.47	0.14	126,129,133,134	0
4	MAN	F	5	11/12	0.49	0.14	102,115,118,118	0
2	NAG	C	1	14/15	0.53	0.14	98,103,114,119	0
4	MAN	G	4	11/12	0.59	0.14	113,122,127,129	0
4	NAG	G	2	14/15	0.62	0.15	93,103,117,124	0
2	NAG	H	1	14/15	0.63	0.15	86,97,105,111	0
2	NAG	I	1	14/15	0.70	0.18	86,94,108,120	0
4	BMA	E	3	11/12	0.71	0.12	99,114,122,131	0
4	BMA	F	3	11/12	0.75	0.12	88,98,102,107	0
3	NAG	D	2	14/15	0.79	0.12	79,96,111,115	0
4	NAG	G	1	14/15	0.90	0.11	60,72,82,90	0
4	NAG	F	2	14/15	0.90	0.10	49,63,73,82	0
3	NAG	D	1	14/15	0.91	0.10	56,67,78,82	0
4	NAG	E	2	14/15	0.92	0.10	57,67,80,92	0
4	NAG	E	1	14/15	0.93	0.11	45,49,58,62	0
4	NAG	F	1	14/15	0.94	0.09	46,49,57,60	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.

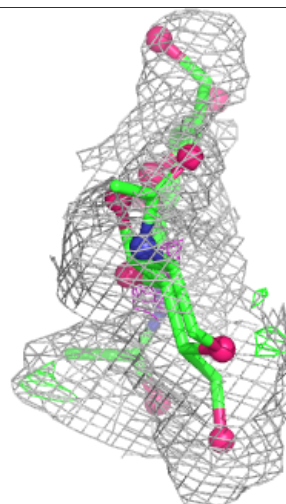
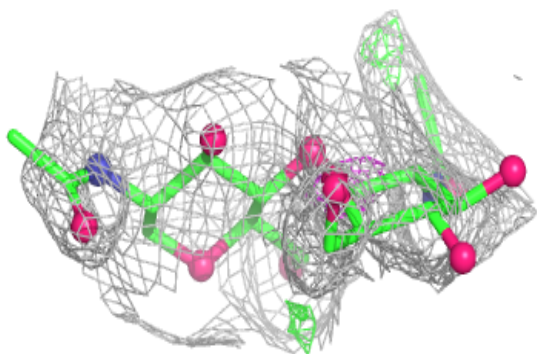
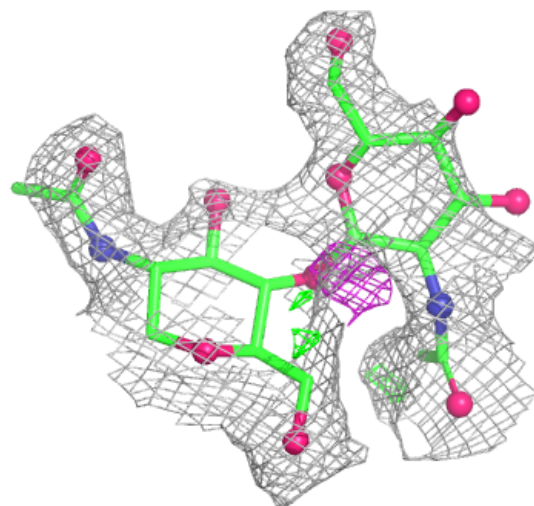
Electron density around Chain C:

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



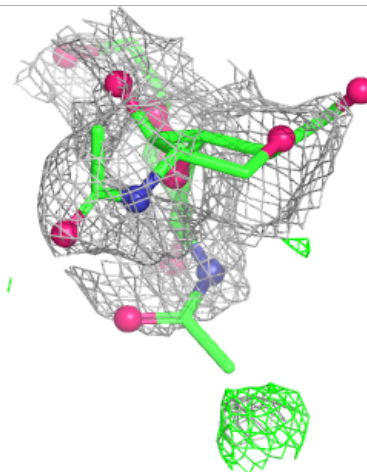
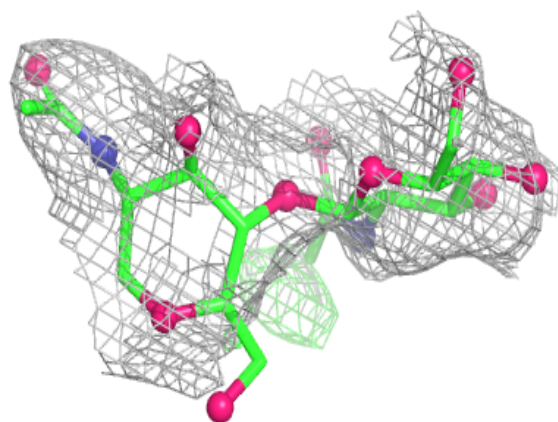
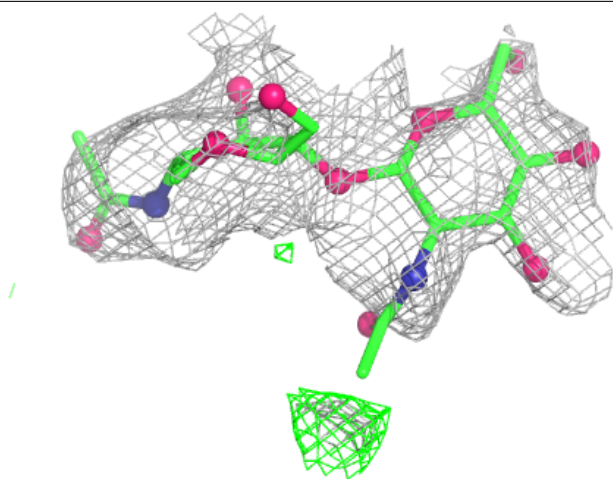
Electron density around Chain H:

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



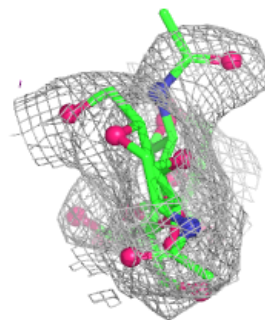
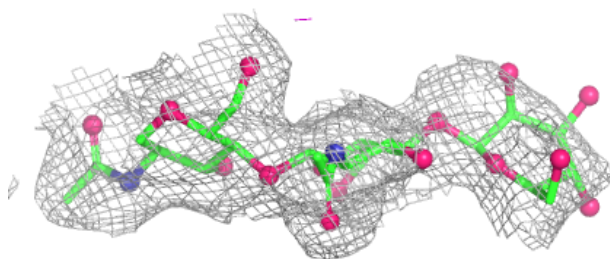
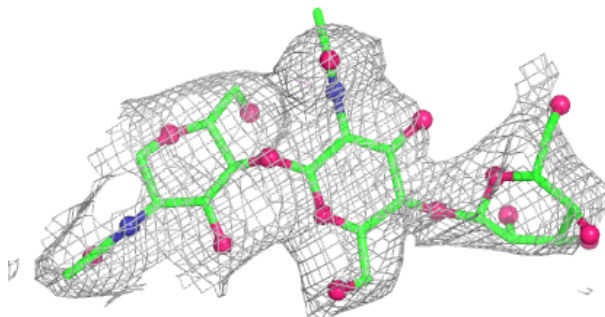
Electron density around Chain I:

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

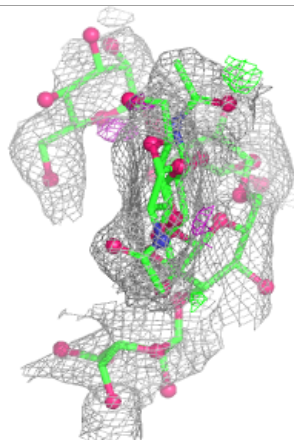
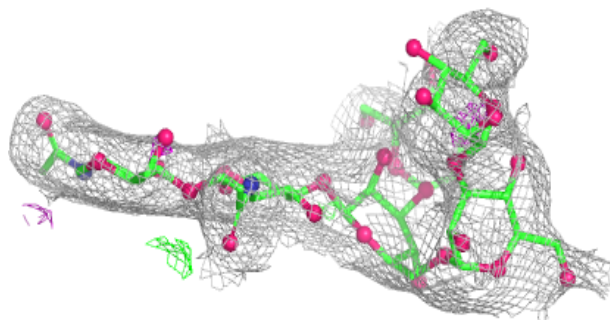
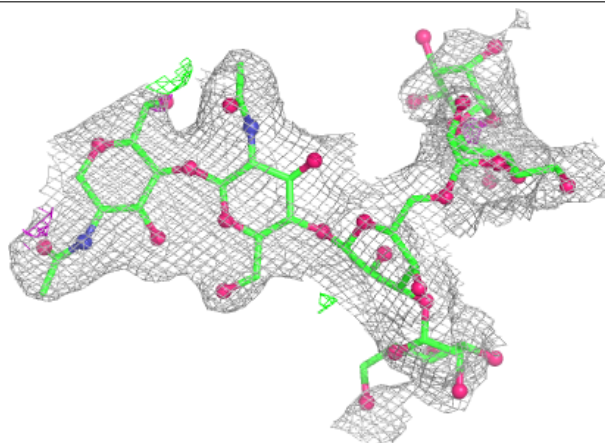


Electron density around Chain D:

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

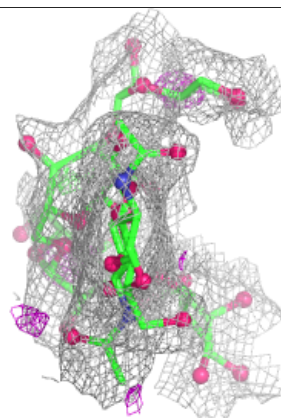
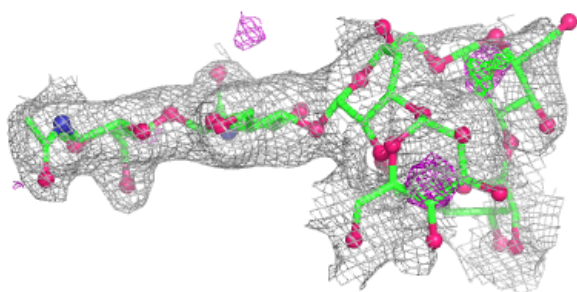
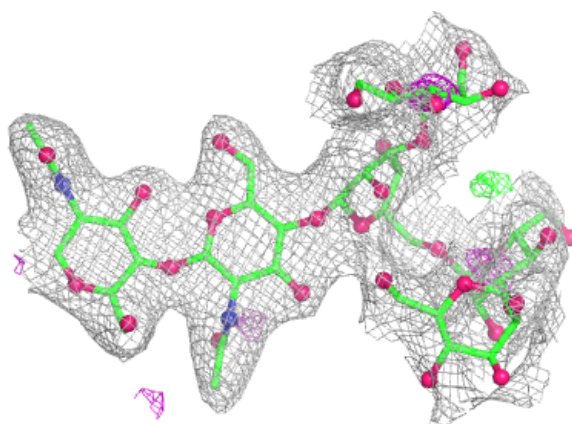
**Electron density around Chain E:**

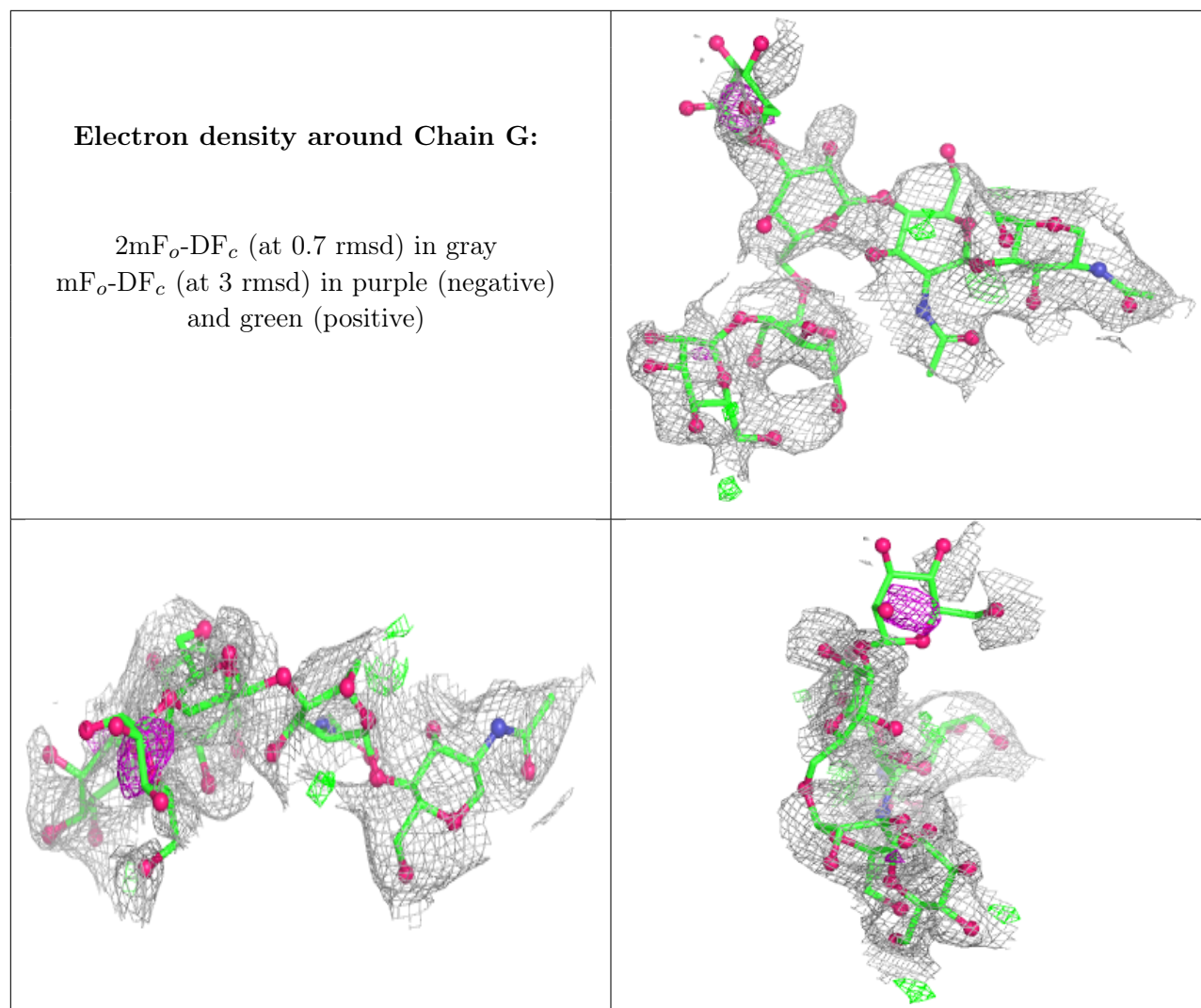
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



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)





6.4 Ligands [i](#)

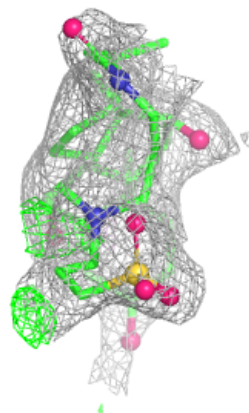
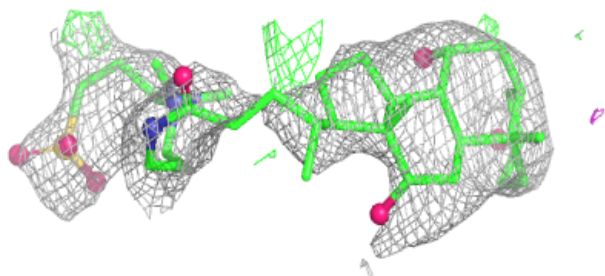
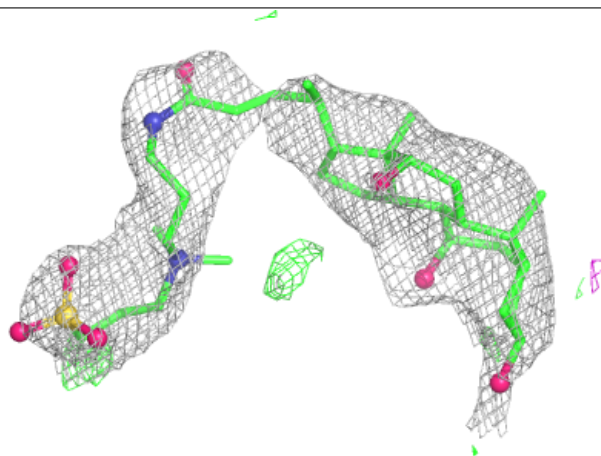
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	CPS	B	602	42/42	0.71	0.20	84,96,134,163	0
6	NAG	A	502	14/15	0.71	0.16	71,77,84,84	0
8	CHD	B	601	29/29	0.78	0.18	80,89,111,113	0
5	CPS	A	501	42/42	0.83	0.14	47,59,120,127	0
7	SO4	B	604	5/5	0.86	0.19	51,59,61,74	5
7	SO4	A	503	5/5	0.87	0.15	52,58,65,69	5
7	SO4	B	603	5/5	0.90	0.13	60,60,63,64	5
7	SO4	A	504	5/5	0.91	0.15	43,45,46,63	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.

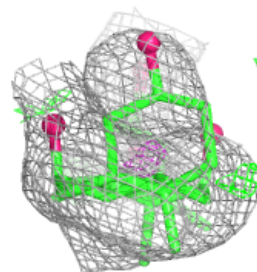
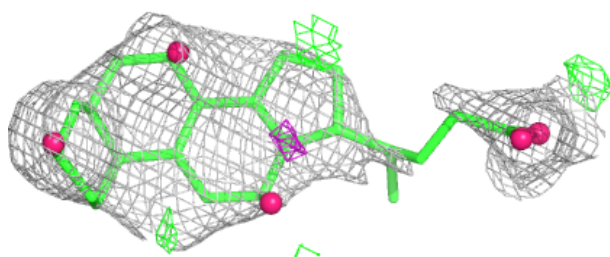
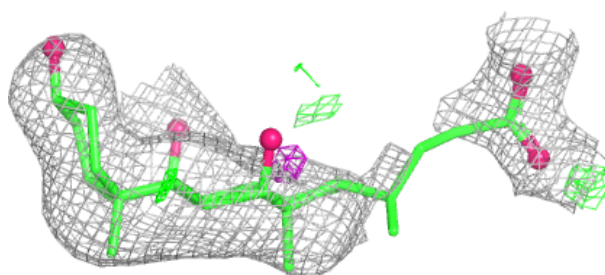
Electron density around CPS B 602:

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

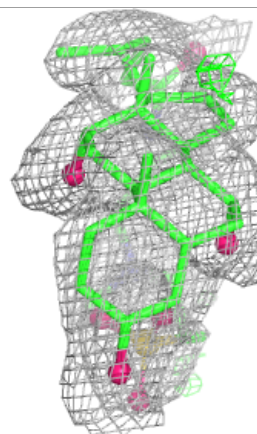
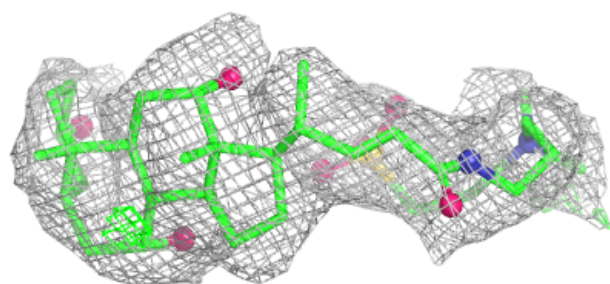
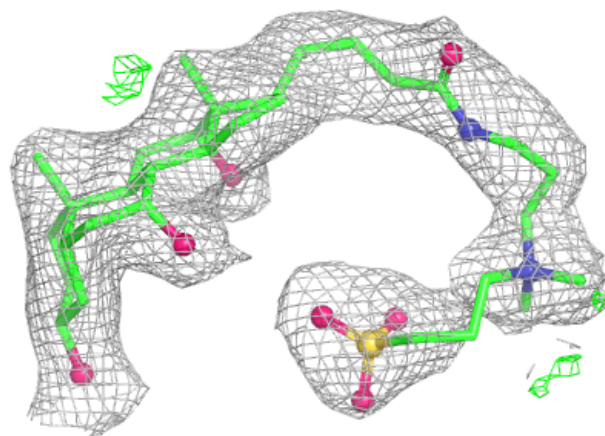


Electron density around CHD B 601:

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

**Electron density around CPS A 501:**

$2mF_o-DF_c$ (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.