



wwPDB X-ray Structure Validation Summary Report ⓘ

Jul 27, 2026 – 04:06 AM EDT

PDB ID : 10JV / pdb_000010jv
Title : Crystal structure of human CHI3L1 in complex with the CHI-DEL small molecule
Authors : Upadhyay, S.; Zhang, L.; Teplova, M.; Gabr, M.
Deposited on : 2026-01-22
Resolution : 2.81 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 : 9.0.015 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

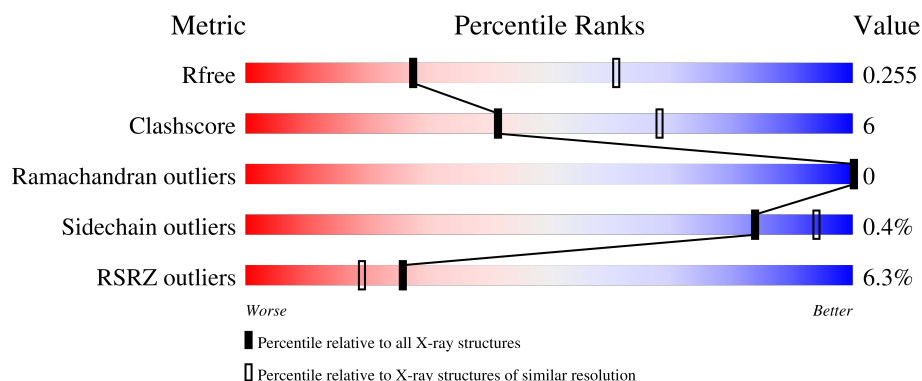
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.81 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.



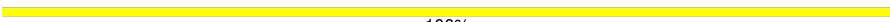
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	4591 (2.84-2.80)
Clashscore	190562	5010 (2.84-2.80)
Ramachandran outliers	187476	4916 (2.84-2.80)
Sidechain outliers	187428	4918 (2.84-2.80)
RSRZ outliers	180081	4594 (2.84-2.80)

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	401	84% 6% 10%
1	B	401	84% 6% 10%
1	C	401	5% 74% 15% 10%
1	D	401	16% 70% 18% 11%
2	E	2	50% 50%

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Mol	Chain	Length	Quality of chain
2	F	2	 50%50%
2	G	2	 100%
2	H	2	 100%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 22659 atoms, of which 10995 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 Chitinase-3-like protein 1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	362	Total	C	H	N	O	S	0	0	0
			5582	1817	2742	485	527	11			
1	B	362	Total	C	H	N	O	S	0	0	0
			5585	1817	2745	485	527	11			
1	C	362	Total	C	H	N	O	S	0	0	0
			5545	1817	2705	484	528	11			
1	D	356	Total	C	H	N	O	S	0	0	0
			5518	1795	2711	479	522	11			

There are 76 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	145	GLY	ARG	variant	UNP P36222
A	384	LEU	-	expression tag	UNP P36222
A	385	GLU	-	expression tag	UNP P36222
A	386	VAL	-	expression tag	UNP P36222
A	387	LEU	-	expression tag	UNP P36222
A	388	PHE	-	expression tag	UNP P36222
A	389	GLN	-	expression tag	UNP P36222
A	390	GLY	-	expression tag	UNP P36222
A	391	PRO	-	expression tag	UNP P36222
A	392	HIS	-	expression tag	UNP P36222
A	393	HIS	-	expression tag	UNP P36222
A	394	HIS	-	expression tag	UNP P36222
A	395	HIS	-	expression tag	UNP P36222
A	396	HIS	-	expression tag	UNP P36222
A	397	HIS	-	expression tag	UNP P36222
A	398	HIS	-	expression tag	UNP P36222
A	399	HIS	-	expression tag	UNP P36222
A	400	HIS	-	expression tag	UNP P36222
A	401	HIS	-	expression tag	UNP P36222
B	145	GLY	ARG	variant	UNP P36222
B	384	LEU	-	expression tag	UNP P36222

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Chain	Residue	Modelled	Actual	Comment	Reference
B	385	GLU	-	expression tag	UNP P36222
B	386	VAL	-	expression tag	UNP P36222
B	387	LEU	-	expression tag	UNP P36222
B	388	PHE	-	expression tag	UNP P36222
B	389	GLN	-	expression tag	UNP P36222
B	390	GLY	-	expression tag	UNP P36222
B	391	PRO	-	expression tag	UNP P36222
B	392	HIS	-	expression tag	UNP P36222
B	393	HIS	-	expression tag	UNP P36222
B	394	HIS	-	expression tag	UNP P36222
B	395	HIS	-	expression tag	UNP P36222
B	396	HIS	-	expression tag	UNP P36222
B	397	HIS	-	expression tag	UNP P36222
B	398	HIS	-	expression tag	UNP P36222
B	399	HIS	-	expression tag	UNP P36222
B	400	HIS	-	expression tag	UNP P36222
B	401	HIS	-	expression tag	UNP P36222
C	145	GLY	ARG	variant	UNP P36222
C	384	LEU	-	expression tag	UNP P36222
C	385	GLU	-	expression tag	UNP P36222
C	386	VAL	-	expression tag	UNP P36222
C	387	LEU	-	expression tag	UNP P36222
C	388	PHE	-	expression tag	UNP P36222
C	389	GLN	-	expression tag	UNP P36222
C	390	GLY	-	expression tag	UNP P36222
C	391	PRO	-	expression tag	UNP P36222
C	392	HIS	-	expression tag	UNP P36222
C	393	HIS	-	expression tag	UNP P36222
C	394	HIS	-	expression tag	UNP P36222
C	395	HIS	-	expression tag	UNP P36222
C	396	HIS	-	expression tag	UNP P36222
C	397	HIS	-	expression tag	UNP P36222
C	398	HIS	-	expression tag	UNP P36222
C	399	HIS	-	expression tag	UNP P36222
C	400	HIS	-	expression tag	UNP P36222
C	401	HIS	-	expression tag	UNP P36222
D	145	GLY	ARG	variant	UNP P36222
D	384	LEU	-	expression tag	UNP P36222
D	385	GLU	-	expression tag	UNP P36222
D	386	VAL	-	expression tag	UNP P36222
D	387	LEU	-	expression tag	UNP P36222
D	388	PHE	-	expression tag	UNP P36222

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Chain	Residue	Modelled	Actual	Comment	Reference
D	389	GLN	-	expression tag	UNP P36222
D	390	GLY	-	expression tag	UNP P36222
D	391	PRO	-	expression tag	UNP P36222
D	392	HIS	-	expression tag	UNP P36222
D	393	HIS	-	expression tag	UNP P36222
D	394	HIS	-	expression tag	UNP P36222
D	395	HIS	-	expression tag	UNP P36222
D	396	HIS	-	expression tag	UNP P36222
D	397	HIS	-	expression tag	UNP P36222
D	398	HIS	-	expression tag	UNP P36222
D	399	HIS	-	expression tag	UNP P36222
D	400	HIS	-	expression tag	UNP P36222
D	401	HIS	-	expression tag	UNP P36222

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



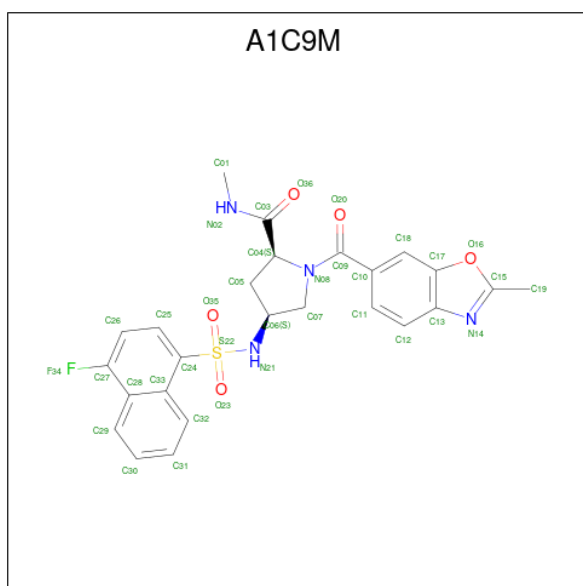
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	E	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	F	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	G	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	H	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



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

- Molecule 4 is (4S)-4-(4-fluoronaphthalene-1-sulfonamido)-N-methyl-1-(2-methyl-1,3-benzoxazole-6-carbonyl)-L-prolinamide (CCD ID: A1C9M) (formula: $C_{25}H_{23}FN_4O_5S$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms							ZeroOcc	AltConf
4	A	1	Total	C	F	H	N	O	S	0	0
			59	25	1	23	4	5	1		
4	B	1	Total	C	F	H	N	O	S	0	0
			59	25	1	23	4	5	1		

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Mol	Chain	Residues	Atoms							ZeroOcc	AltConf
4	C	1	Total	C	F	H	N	O	S	0	0
			59	25	1	23	4	5	1		
4	D	1	Total	C	F	H	N	O	S	0	0
			59	25	1	23	4	5	1		

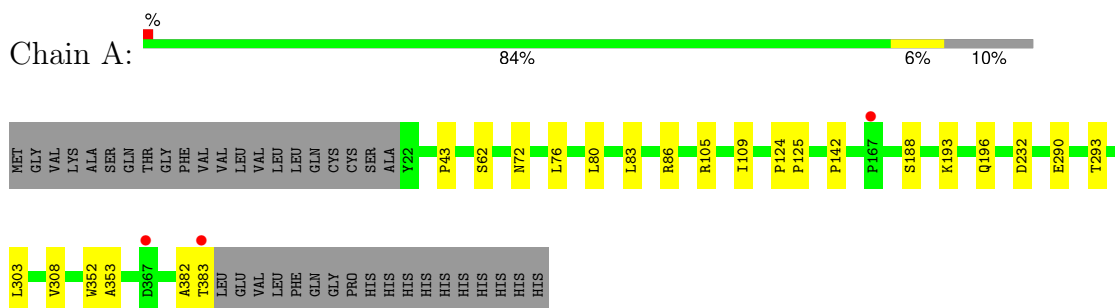
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	25	Total	O	0	0
			25	25		
5	B	30	Total	O	0	0
			30	30		
5	C	14	Total	O	0	0
			14	14		
5	D	6	Total	O	0	0
			6	6		

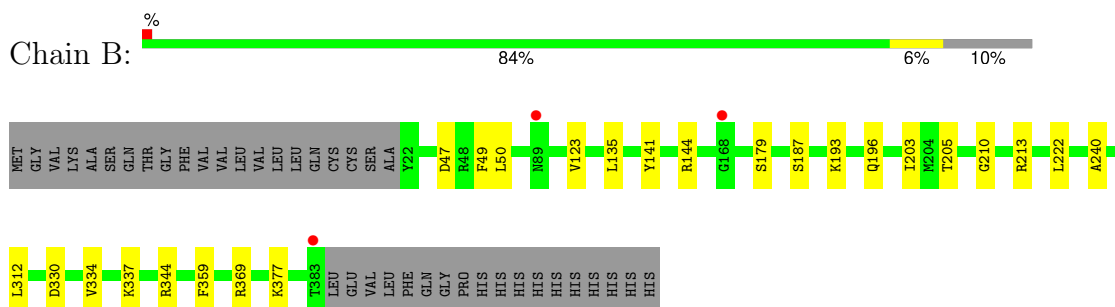
3 Residue-property plots [i](#)

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.

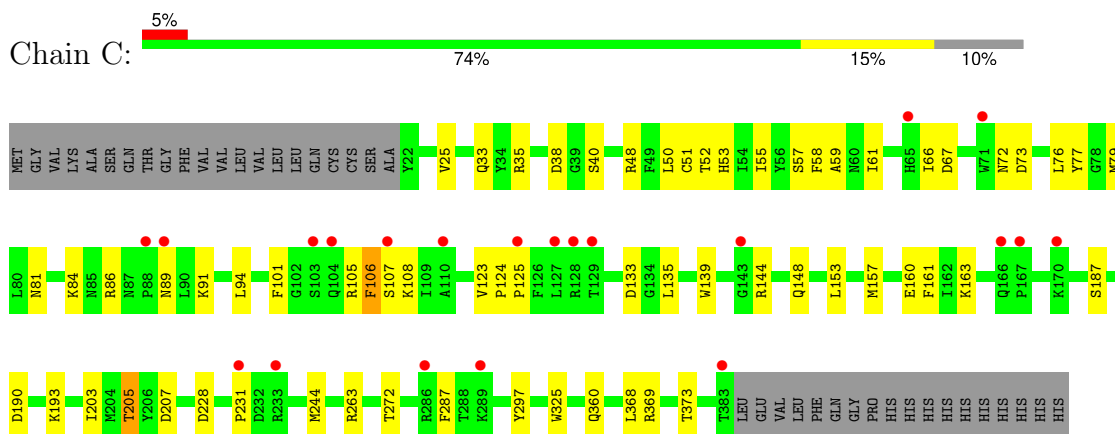
- Molecule 1: Chitinase-3-like protein 1



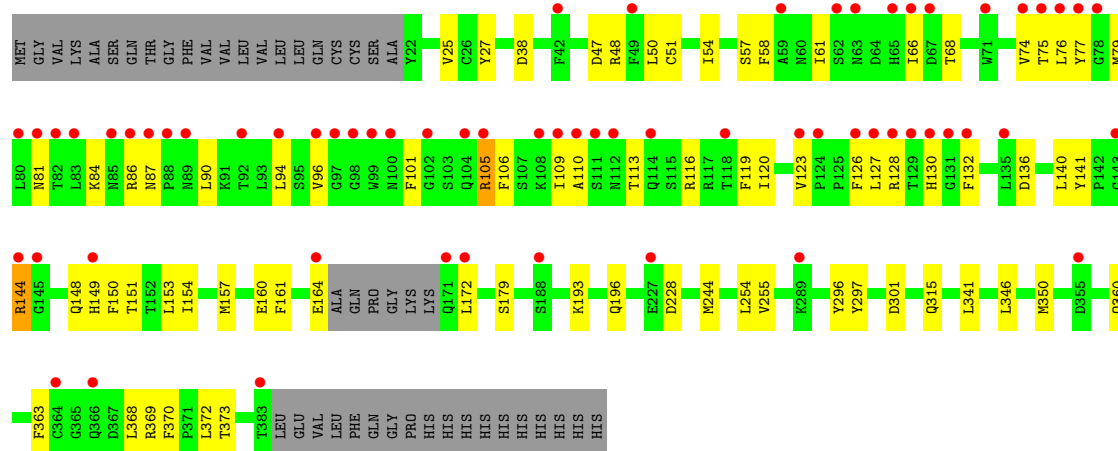
- Molecule 1: Chitinase-3-like protein 1



- Molecule 1: Chitinase-3-like protein 1



- Molecule 1: Chitinase-3-like protein 1



- 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



- 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



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	108.96Å 122.31Å 136.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	34.58 – 2.81 34.58 – 2.81	Depositor EDS
% Data completeness (in resolution range)	99.4 (34.58-2.81) 92.2 (34.58-2.81)	Depositor EDS
R_{merge}	0.26	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.17 (at 2.81Å)	Xtriage
Refinement program	PHENIX 1.21.1_5286	Depositor
R, R_{free}	0.215 , 0.253 0.217 , 0.255	Depositor DCC
R_{free} test set	2000 reflections (4.44%)	wwPDB-VP
Wilson B-factor (Å ²)	30.1	Xtriage
Anisotropy	1.161	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 41.9	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	0.92	EDS
Total number of atoms	22659	wwPDB-VP
Average B, all atoms (Å ²)	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 32.59 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 9.1683e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: A1C9M, NAG, GOL

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.16	0/2916	0.34	0/3953
1	B	0.15	0/2916	0.35	0/3953
1	C	0.15	0/2916	0.36	0/3953
1	D	0.22	0/2881	0.42	0/3904
All	All	0.17	0/11629	0.37	0/15763

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	D	0	3

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	105	ARG	Sidechain
1	D	144	ARG	Sidechain
1	D	86	ARG	Sidechain

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	2840	2742	2747	16	0
1	B	2840	2745	2750	15	0
1	C	2840	2705	2749	46	0
1	D	2807	2711	2716	70	0
2	E	28	0	25	1	0
2	F	28	0	25	0	0
2	G	28	0	25	0	0
2	H	28	0	25	0	0
3	A	6	0	8	1	0
4	A	36	23	0	0	0
4	B	36	23	0	0	0
4	C	36	23	0	0	0
4	D	36	23	0	0	0
5	A	25	0	0	0	0
5	B	30	0	0	0	0
5	C	14	0	0	0	0
5	D	6	0	0	0	0
All	All	11664	10995	11070	145	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.

The worst 5 of 145 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:D:120:ILE:HD13	1:D:157:MET:SD	2.16	0.86
1:D:61:ILE:HG21	1:D:109:ILE:HD11	1.61	0.81
1:D:101:PHE:O	1:D:105:ARG:HD2	1.81	0.80
1:D:66:ILE:HG23	1:D:126:PHE:HD2	1.45	0.80
1:D:127:LEU:HD12	1:D:172:LEU:HD13	1.71	0.73

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	360/401 (90%)	356 (99%)	4 (1%)	0	100	100
1	B	360/401 (90%)	351 (98%)	9 (2%)	0	100	100
1	C	360/401 (90%)	349 (97%)	11 (3%)	0	100	100
1	D	352/401 (88%)	342 (97%)	10 (3%)	0	100	100
All	All	1432/1604 (89%)	1398 (98%)	34 (2%)	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	297/335 (89%)	297 (100%)	0	100	100
1	B	298/335 (89%)	298 (100%)	0	100	100
1	C	298/335 (89%)	295 (99%)	3 (1%)	68	88
1	D	296/335 (88%)	294 (99%)	2 (1%)	76	91
All	All	1189/1340 (89%)	1184 (100%)	5 (0%)	84	94

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	67	ASP
1	C	106	PHE
1	C	205	THR
1	D	144	ARG
1	D	255	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 12 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	331	GLN
1	C	366	GLN
1	D	309	HIS
1	D	148	GLN
1	B	339	GLN

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 ⓘ

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	E	1	2,1	14,14,15	0.72	0	17,19,21	0.93	1 (5%)
2	NAG	E	2	2	14,14,15	0.74	0	17,19,21	1.14	2 (11%)
2	NAG	F	1	2,1	14,14,15	0.74	0	17,19,21	0.96	1 (5%)
2	NAG	F	2	2	14,14,15	0.70	0	17,19,21	0.82	0
2	NAG	G	1	2,1	14,14,15	0.65	0	17,19,21	0.97	1 (5%)
2	NAG	G	2	2	14,14,15	0.75	0	17,19,21	0.97	1 (5%)
2	NAG	H	1	2,1	14,14,15	0.70	0	17,19,21	0.92	1 (5%)
2	NAG	H	2	2	14,14,15	0.74	0	17,19,21	1.14	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	E	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	E	2	2	-	0/6/23/26	0/1/1/1
2	NAG	F	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	F	2	2	-	0/6/23/26	0/1/1/1
2	NAG	G	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	G	2	2	-	2/6/23/26	0/1/1/1
2	NAG	H	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	H	2	2	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	2	NAG	C1-O5-C5	2.84	116.00	112.19
2	F	1	NAG	O5-C1-C2	-2.65	107.19	111.29
2	E	1	NAG	O5-C1-C2	-2.59	107.29	111.29
2	H	2	NAG	C1-O5-C5	2.49	115.52	112.19
2	H	2	NAG	C2-N2-C7	2.43	126.16	122.90

There are no chirality outliers.

5 of 6 torsion outliers are listed below:

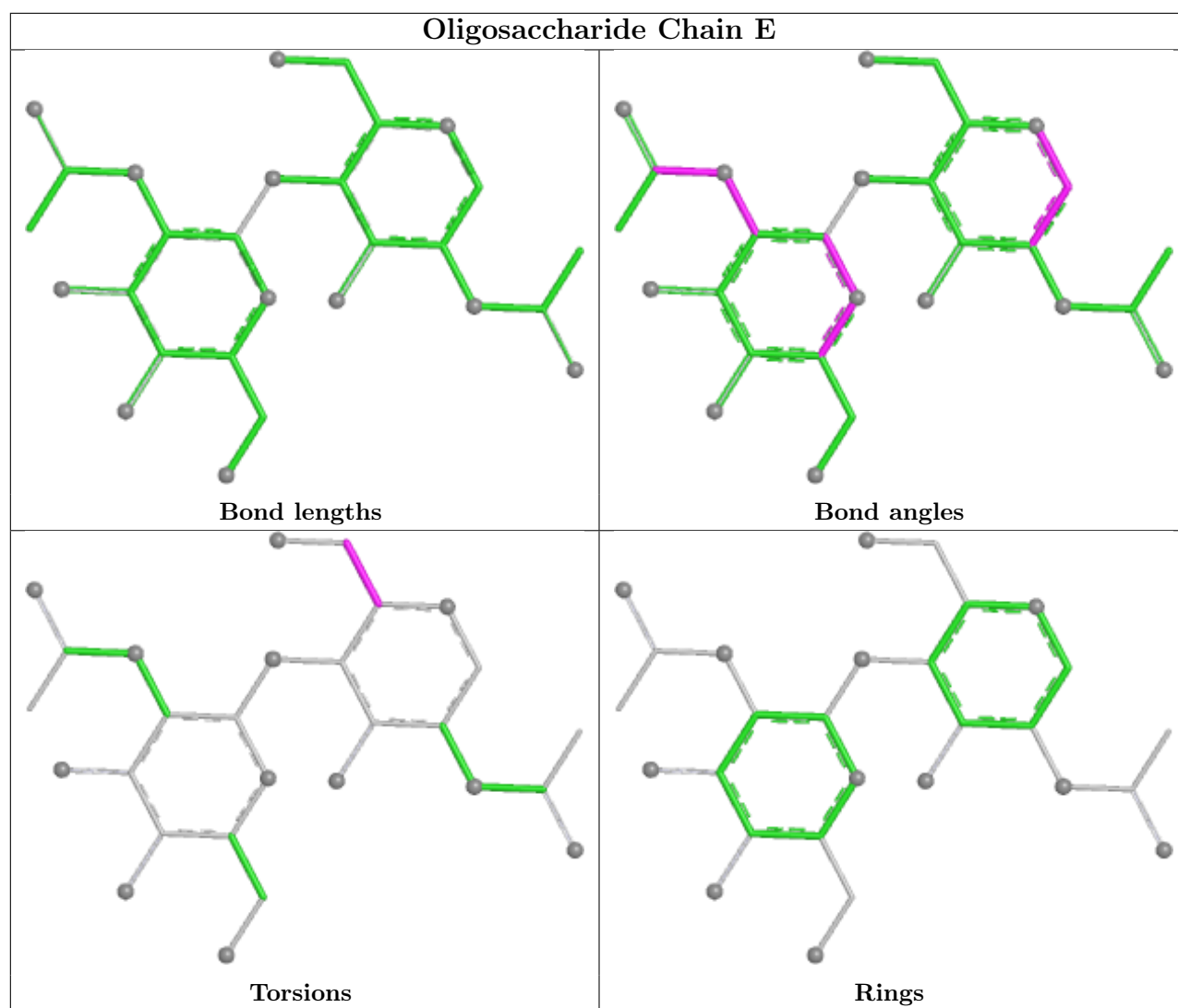
Mol	Chain	Res	Type	Atoms
2	F	1	NAG	O5-C5-C6-O6
2	F	1	NAG	C4-C5-C6-O6
2	E	1	NAG	C4-C5-C6-O6
2	G	2	NAG	O5-C5-C6-O6
2	E	1	NAG	O5-C5-C6-O6

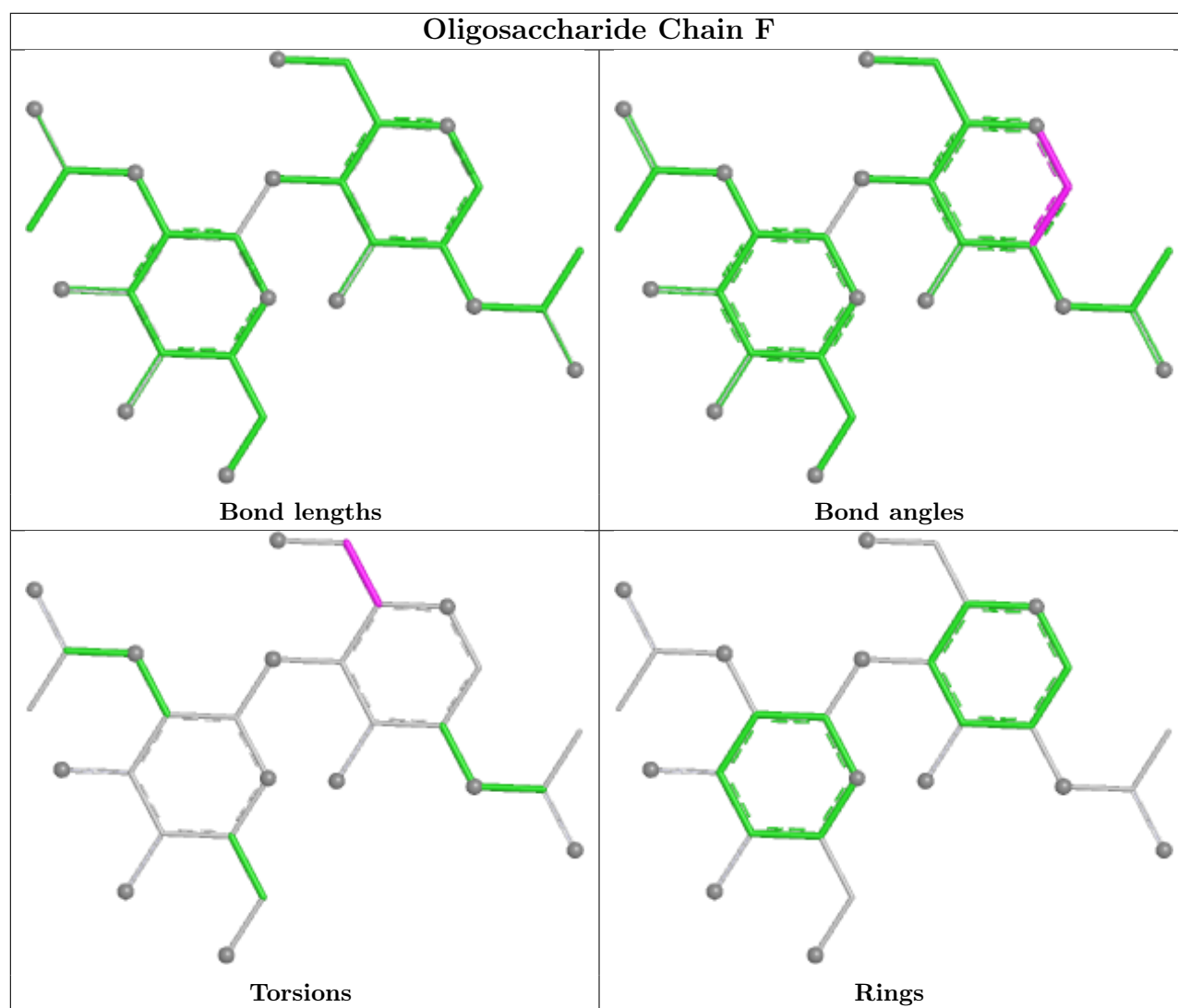
There are no ring outliers.

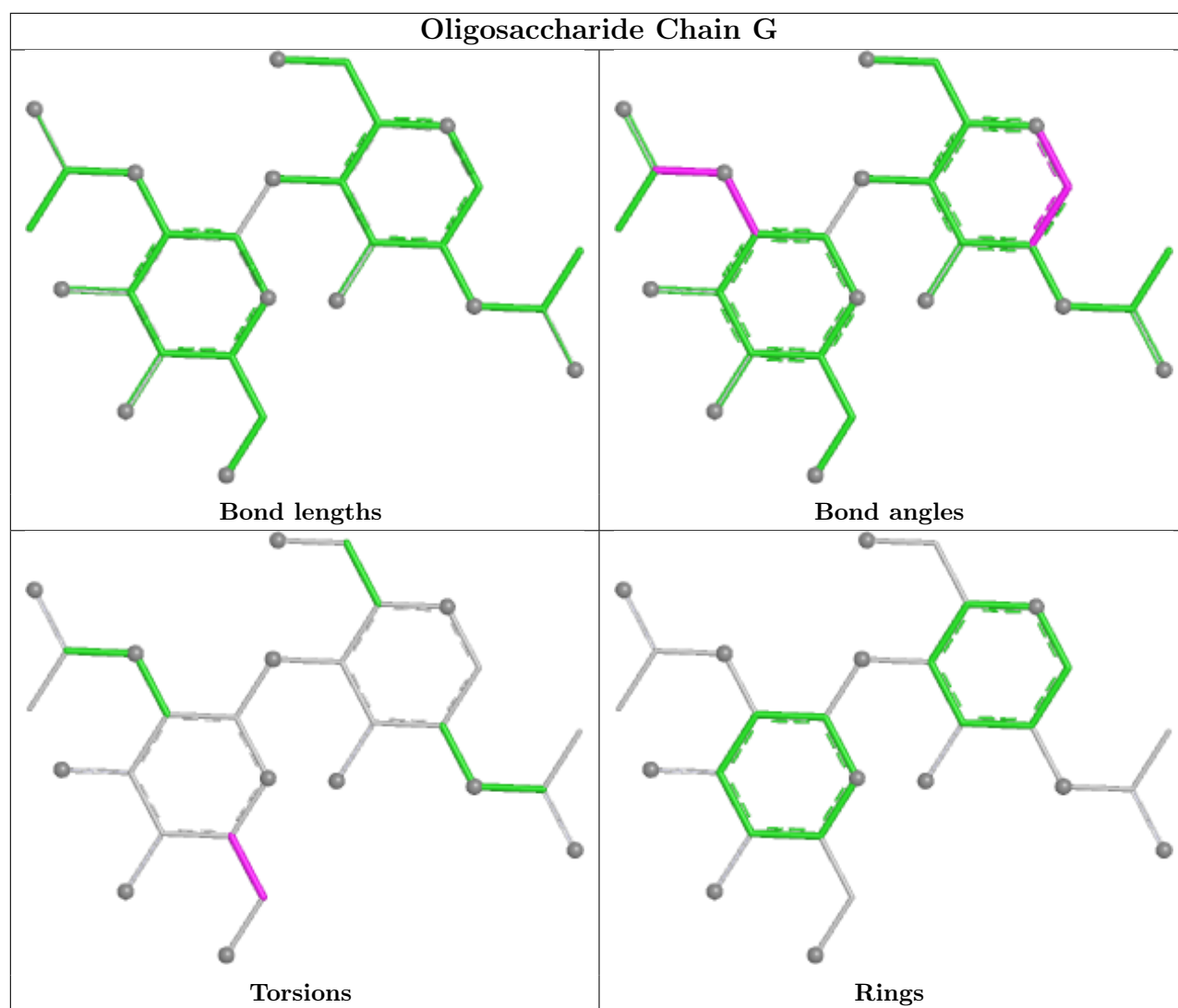
1 monomer is involved in 1 short contact:

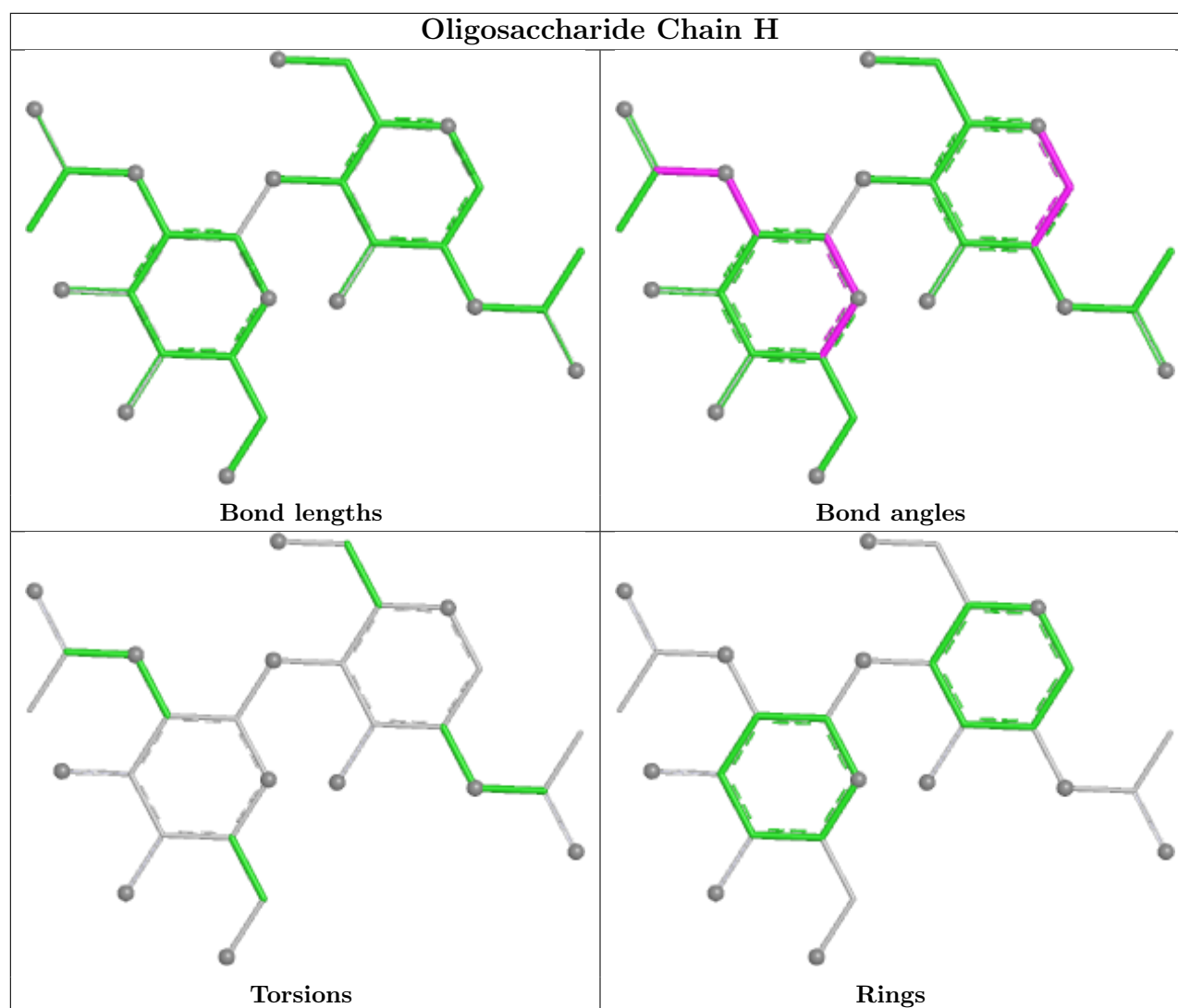
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	1	NAG	1	0

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](#)

5 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	$\# Z > 2$
4	A1C9M	D	501	-	40,40,40	4.79	25 (62%)	57,60,60	3.04	23 (40%)
4	A1C9M	B	501	-	40,40,40	4.72	25 (62%)	57,60,60	2.94	20 (35%)
3	GOL	A	501	-	5,5,5	0.30	0	5,5,5	0.46	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	A1C9M	A	502	-	40,40,40	4.70	26 (65%)	57,60,60	3.00	24 (42%)
4	A1C9M	C	501	-	40,40,40	4.77	25 (62%)	57,60,60	3.01	23 (40%)

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
4	A1C9M	D	501	-	-	1/25/37/37	0/5/5/5
4	A1C9M	B	501	-	-	1/25/37/37	0/5/5/5
3	GOL	A	501	-	-	0/4/4/4	-
4	A1C9M	A	502	-	-	0/25/37/37	0/5/5/5
4	A1C9M	C	501	-	-	0/25/37/37	0/5/5/5

The worst 5 of 101 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	502	A1C9M	C05-C04	-11.27	1.33	1.53
4	C	501	A1C9M	C05-C04	-11.21	1.33	1.53
4	D	501	A1C9M	C05-C04	-11.09	1.34	1.53
4	B	501	A1C9M	C05-C04	-11.04	1.34	1.53
4	B	501	A1C9M	C07-C06	-10.80	1.34	1.53

The worst 5 of 90 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	501	A1C9M	O35-S22-O23	-15.02	101.28	119.52
4	C	501	A1C9M	O35-S22-O23	-14.79	101.56	119.52
4	B	501	A1C9M	O35-S22-O23	-14.78	101.57	119.52
4	A	502	A1C9M	O35-S22-O23	-14.48	101.93	119.52
4	D	501	A1C9M	C17-O16-C15	7.20	109.81	103.94

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	D	501	A1C9M	C06-N21-S22-O23
4	B	501	A1C9M	C33-C24-S22-O35

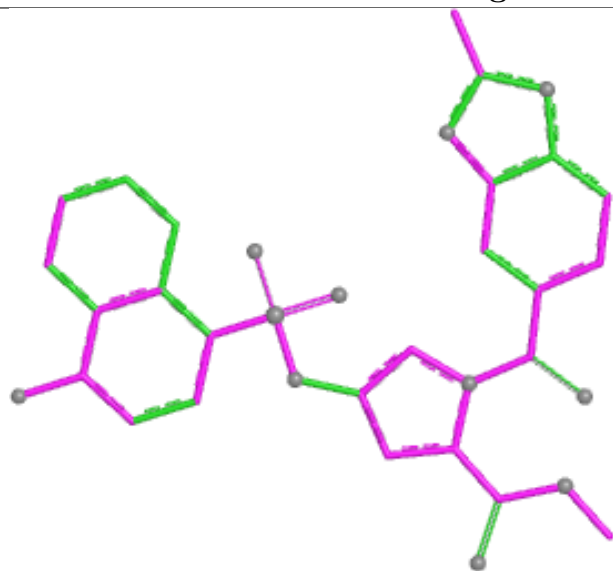
There are no ring outliers.

1 monomer is involved in 1 short contact:

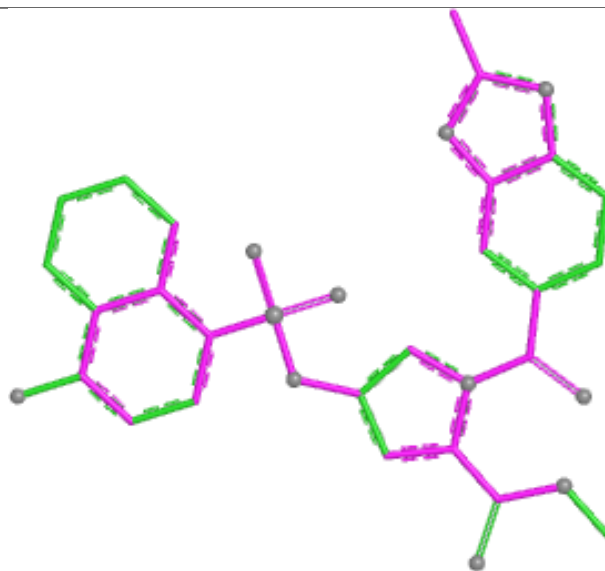
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	501	GOL	1	0

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

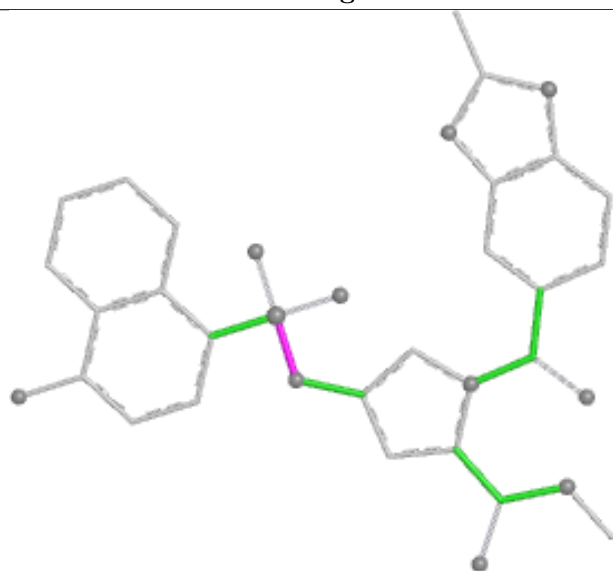
Ligand A1C9M D 501



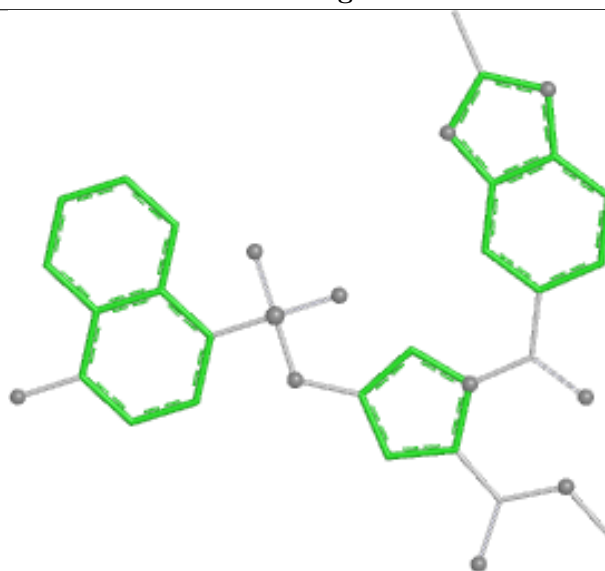
Bond lengths



Bond angles

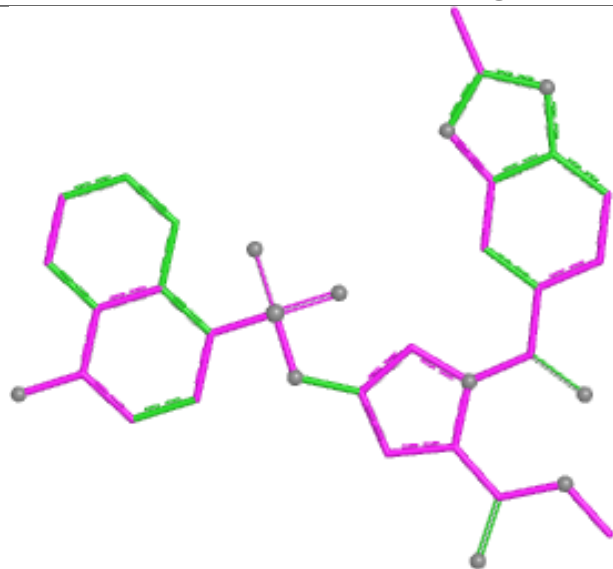


Torsions

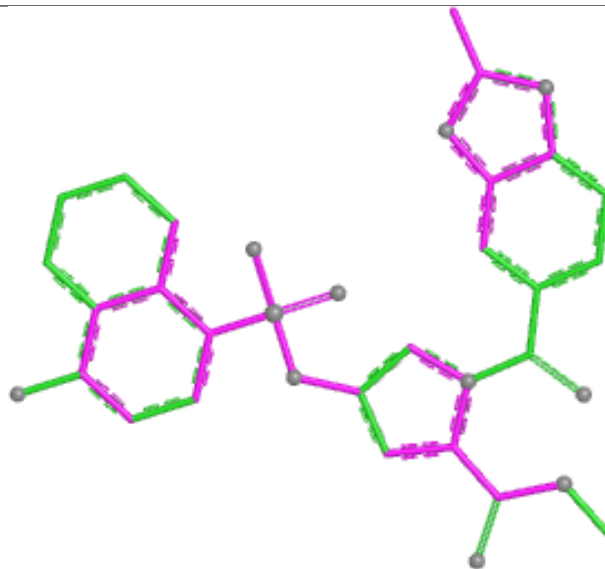


Rings

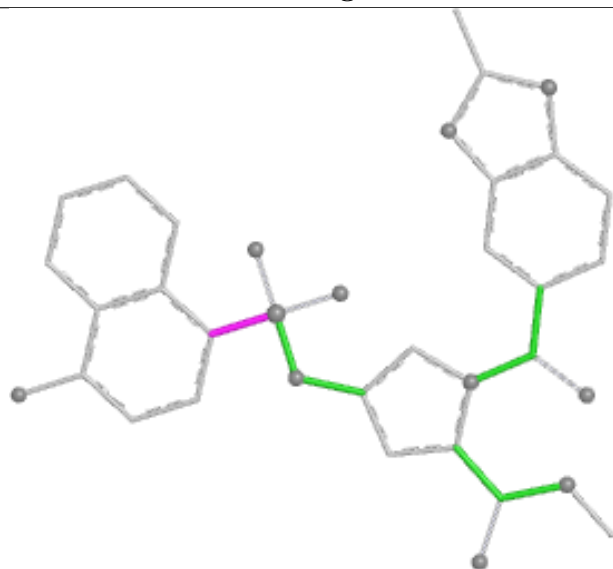
Ligand A1C9M B 501



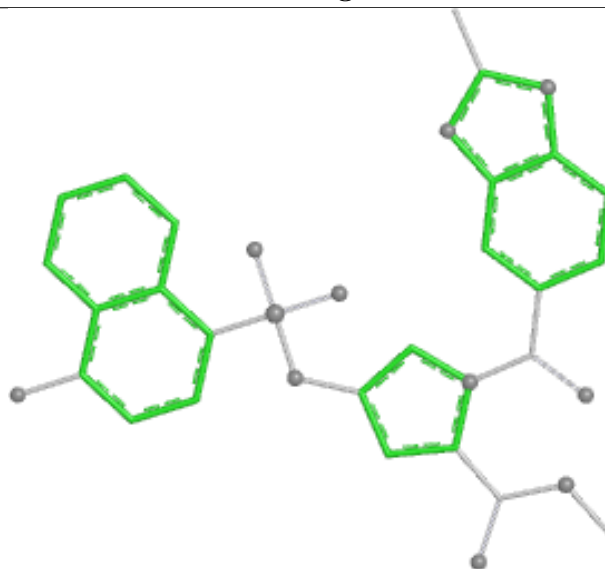
Bond lengths



Bond angles

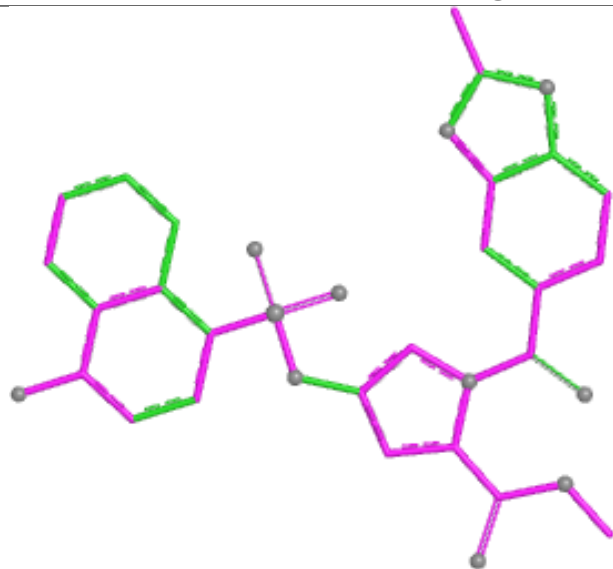


Torsions

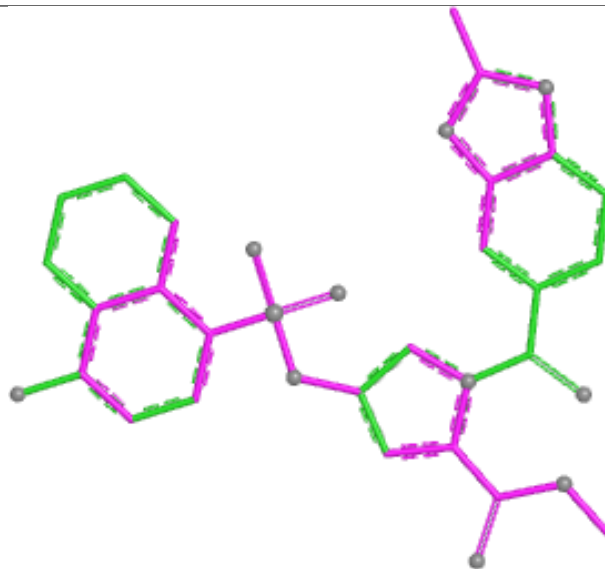


Rings

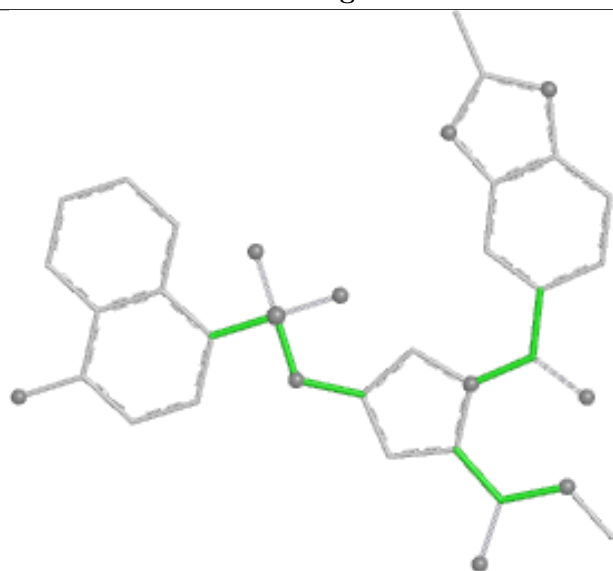
Ligand A1C9M A 502



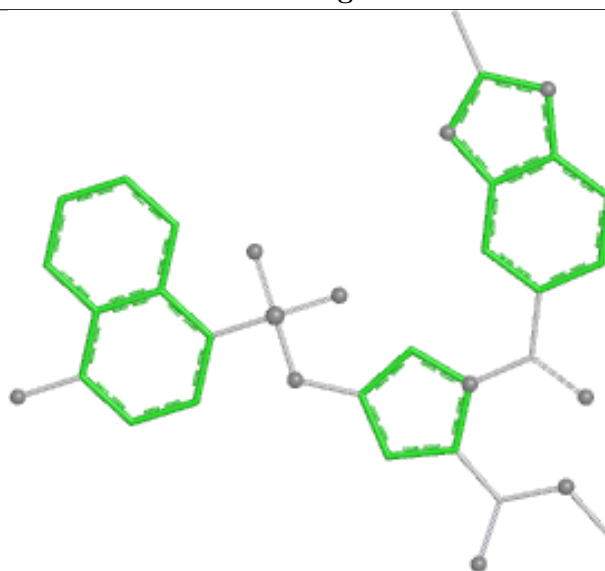
Bond lengths



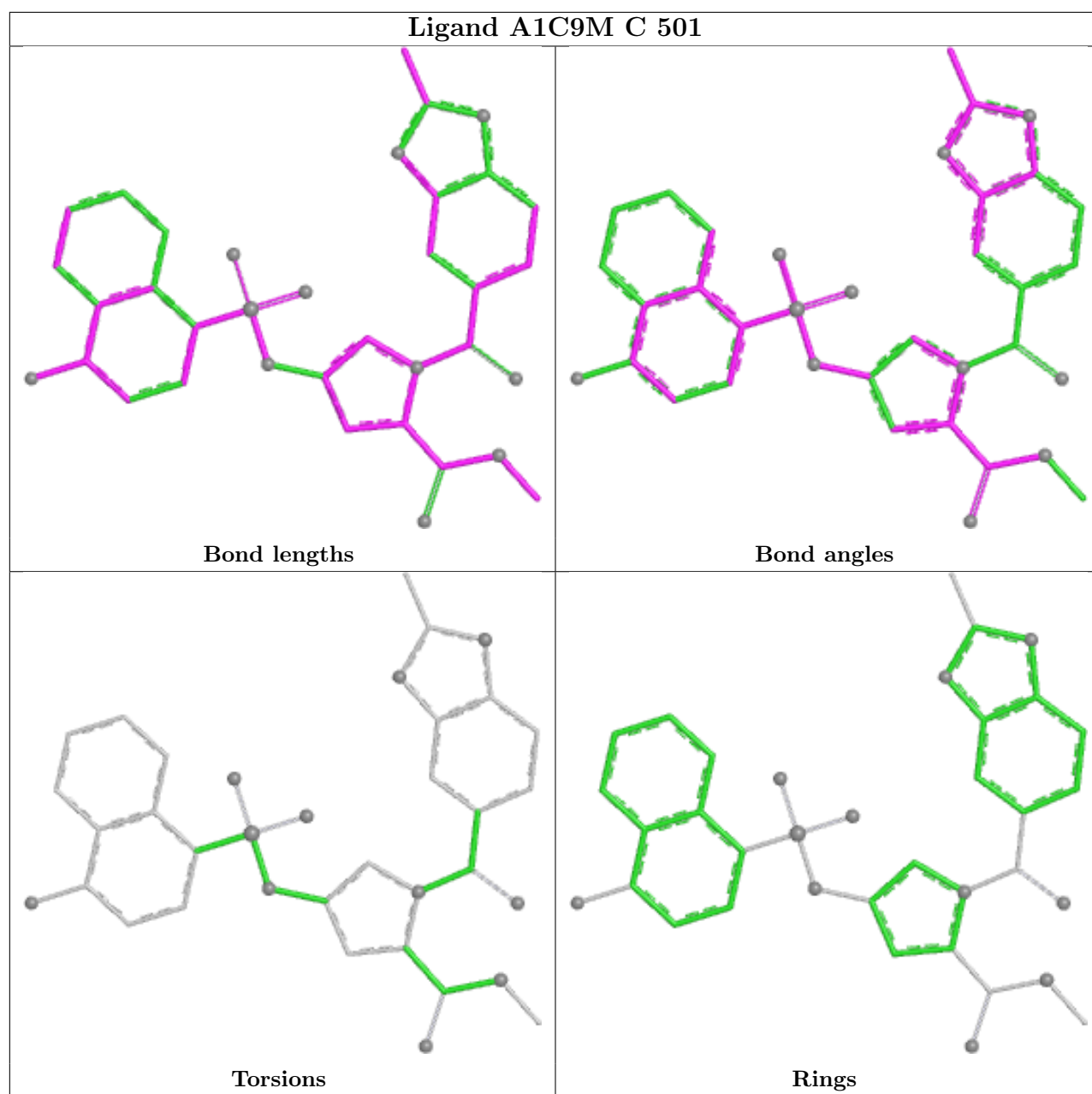
Bond angles



Torsions



Rings



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	362/401 (90%)	0.09	3 (0%) 82 75	29, 40, 67, 117	0
1	B	362/401 (90%)	0.11	3 (0%) 82 75	29, 40, 65, 123	0
1	C	362/401 (90%)	0.62	21 (5%) 29 21	35, 64, 98, 144	0
1	D	356/401 (88%)	1.13	64 (17%) 3 2	39, 74, 127, 155	0
All	All	1442/1604 (89%)	0.49	91 (6%) 26 19	29, 49, 109, 155	0

The worst 5 of 91 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	127	LEU	5.6
1	D	74	VAL	4.6
1	C	383	THR	4.6
1	B	383	THR	4.5
1	A	383	THR	4.5

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.

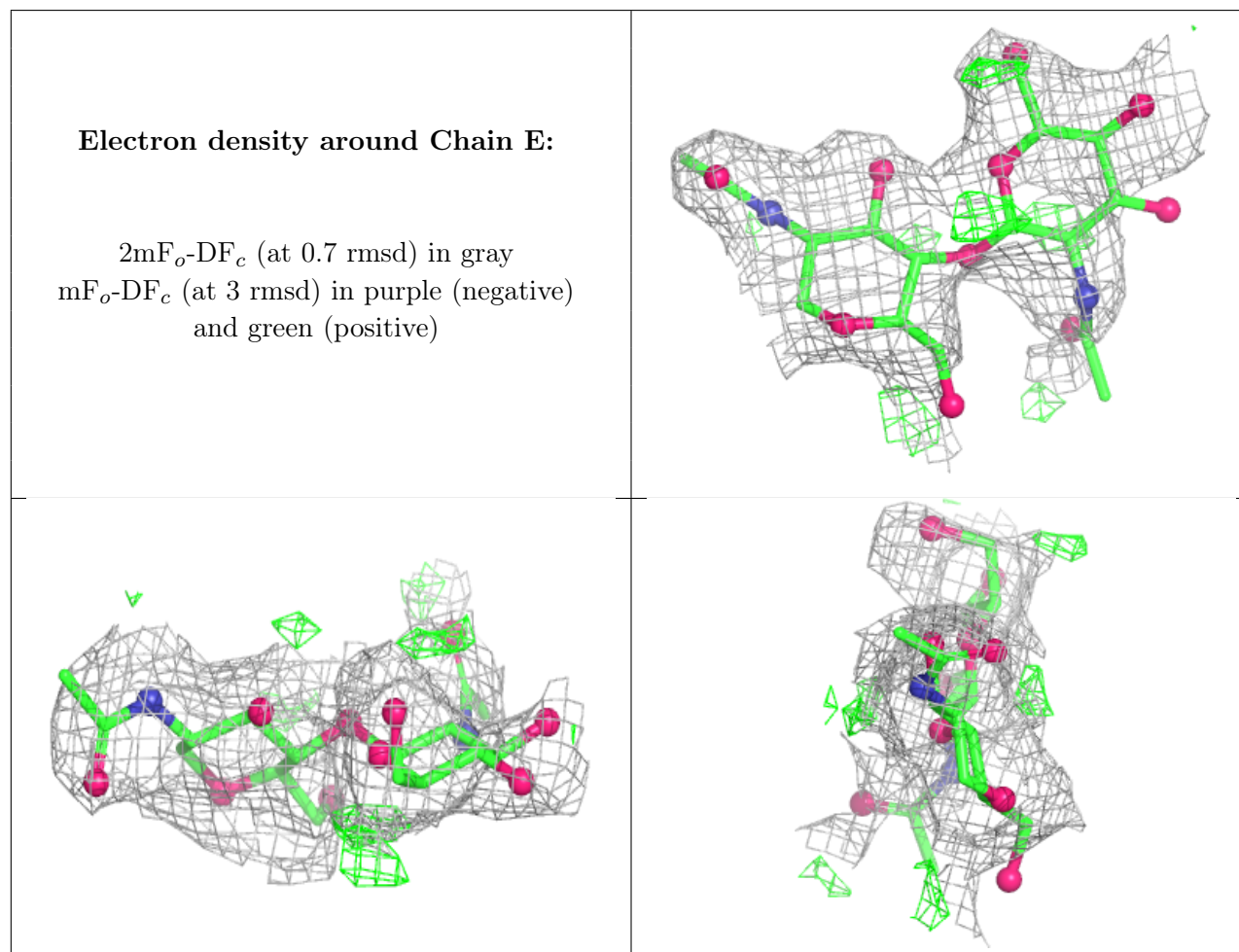
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	NAG	H	2	14/15	0.55	0.23	101,106,109,111	0
2	NAG	F	2	14/15	0.65	0.18	74,81,86,89	0

Continued on next page...

Continued from previous page...

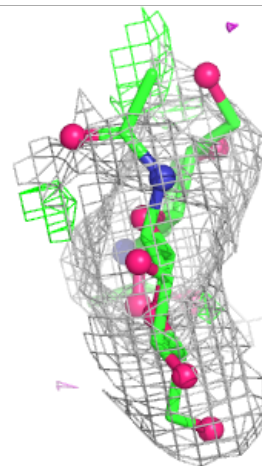
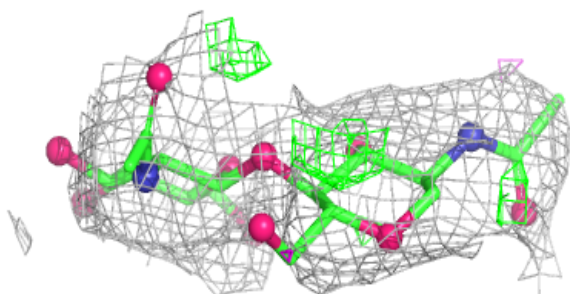
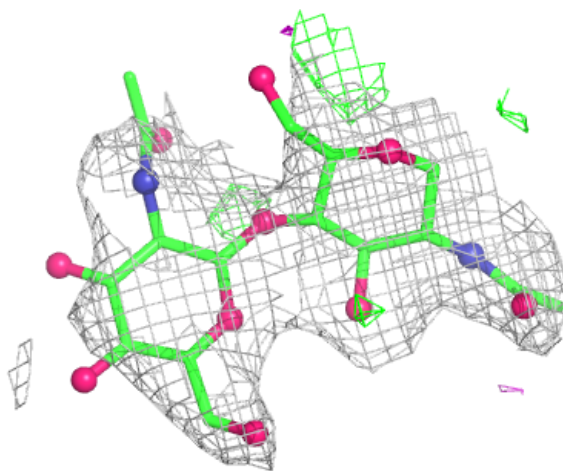
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	NAG	G	1	14/15	0.66	0.18	73,83,90,90	0
2	NAG	H	1	14/15	0.69	0.20	86,102,109,111	0
2	NAG	E	2	14/15	0.69	0.19	77,80,87,94	0
2	NAG	G	2	14/15	0.70	0.18	85,88,91,91	0
2	NAG	F	1	14/15	0.80	0.16	42,55,72,74	0
2	NAG	E	1	14/15	0.81	0.15	46,55,65,70	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.



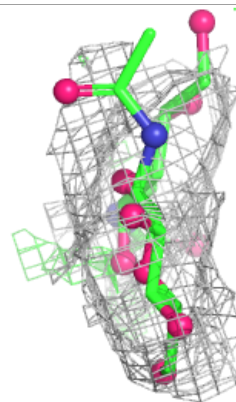
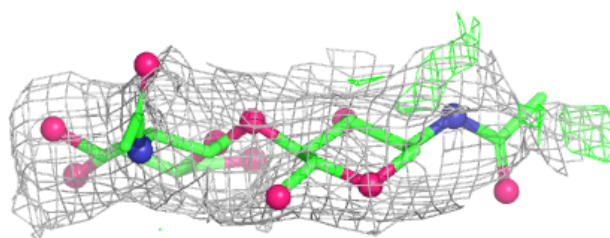
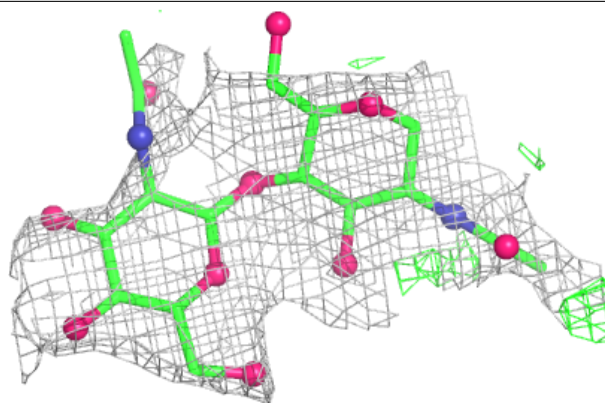
Electron density around Chain F:

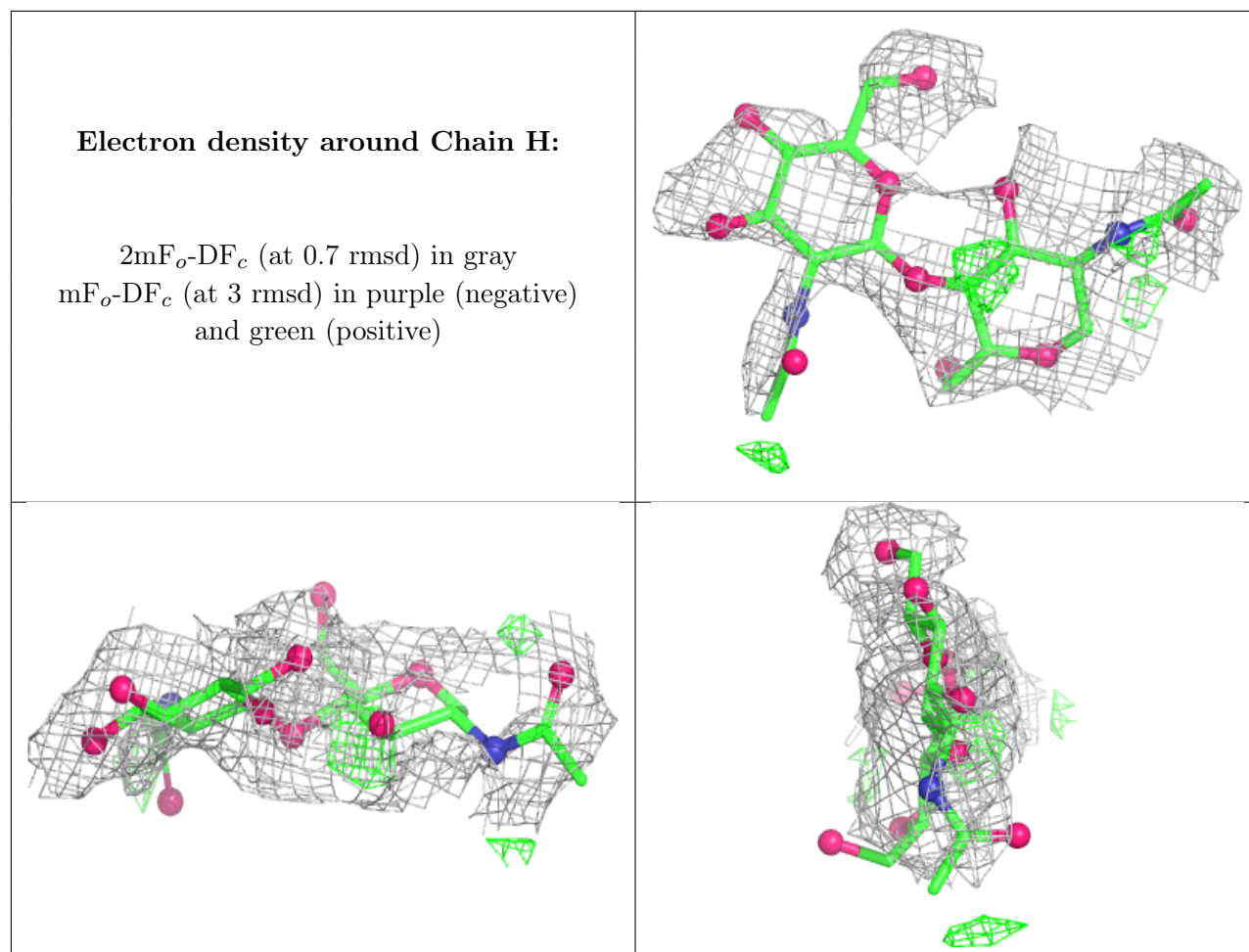
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around Chain G:

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





6.4 Ligands [i](#)

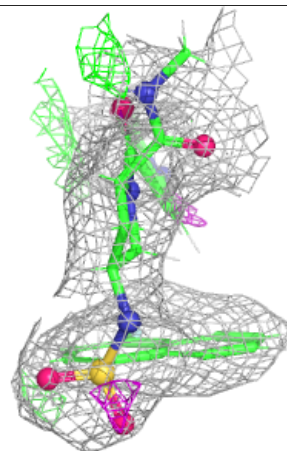
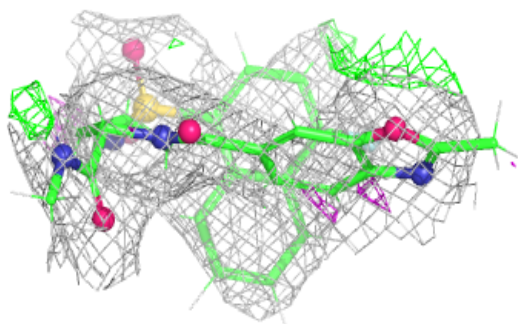
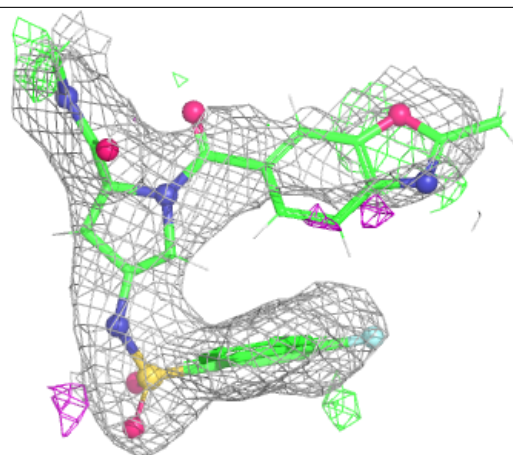
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	A1C9M	D	501	36/36	0.81	0.18	52,68,86,88	0
3	GOL	A	501	6/6	0.89	0.14	29,30,31,31	0
4	A1C9M	C	501	36/36	0.92	0.12	39,49,63,64	0
4	A1C9M	B	501	36/36	0.92	0.12	29,33,42,43	0
4	A1C9M	A	502	36/36	0.93	0.10	29,33,42,43	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.

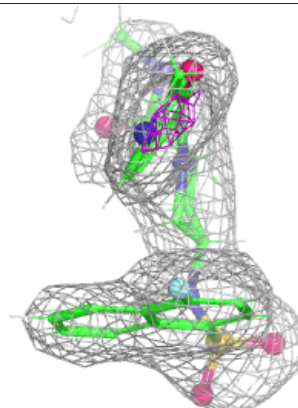
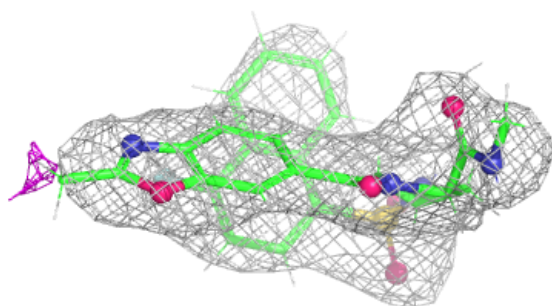
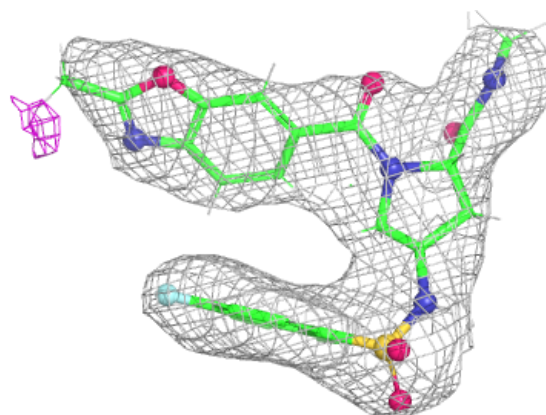
Electron density around A1C9M D 501:

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



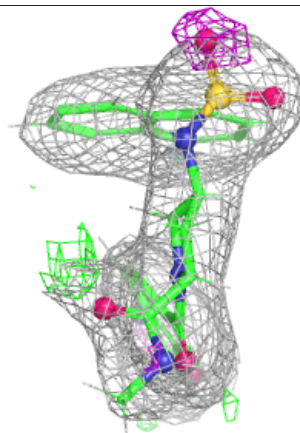
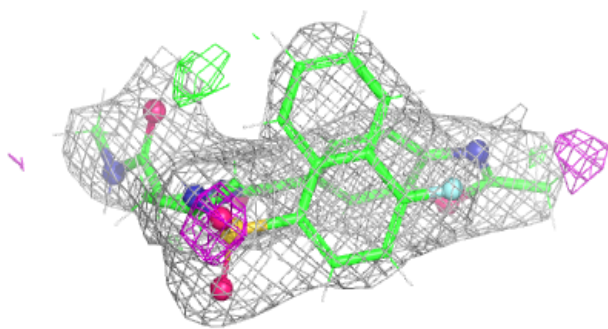
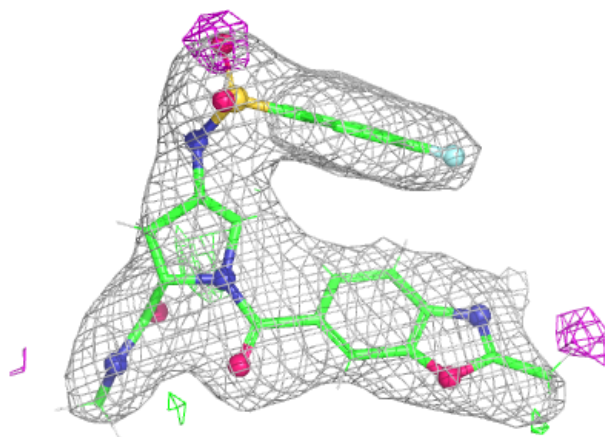
Electron density around A1C9M C 501:

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



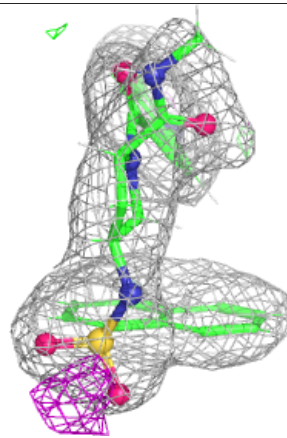
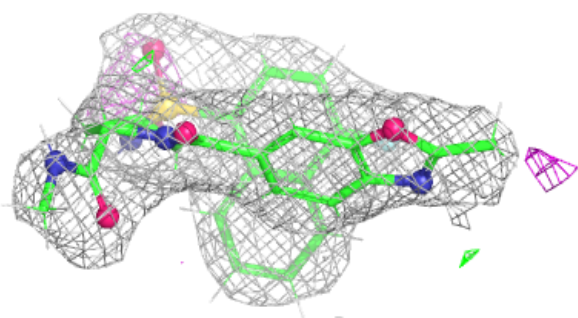
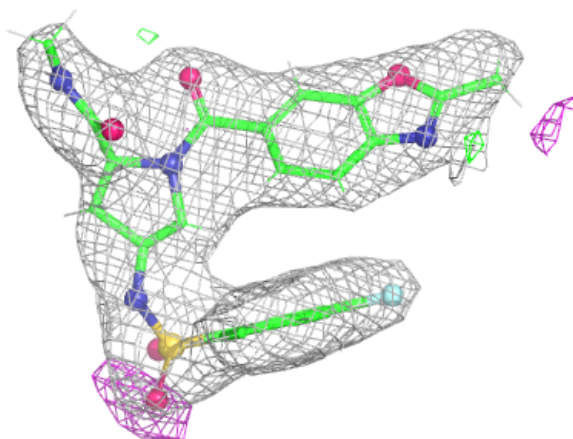
Electron density around A1C9M B 501:

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



Electron density around A1C9M A 502:

$2mF_o-DF_c$ (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.