



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 8, 2026 – 08:30 AM UTC

PDB ID : 9NTH / pdb_00009nth
Title : Helix pomatia AMP deaminase (HPAMPD) in complex with Pentostatin
monophosphate (PMP)
Authors : Kaur, G.; Horton, J.R.; Cheng, X.
Deposited on : 2025-03-18
Resolution : 1.61 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

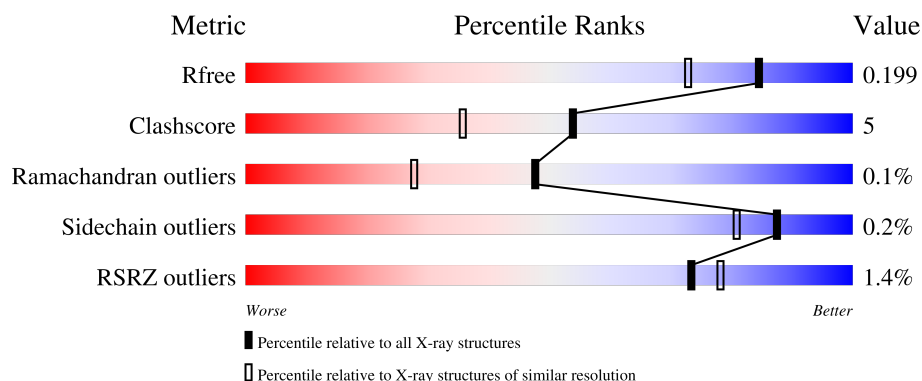
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.61 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	6728 (1.64-1.60)
Clashscore	190562	7023 (1.64-1.60)
Ramachandran outliers	187476	6898 (1.64-1.60)
Sidechain outliers	187428	6896 (1.64-1.60)
RSRZ outliers	180081	6727 (1.64-1.60)

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	541	% 86% 6% 8%
1	B	541	2% 85% 8% 7%
1	C	541	% 85% 6% 8%
1	D	541	% 85% 6% 8%
2	E	2	 100%

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

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	EDO	A	626	-	-	X	-
3	EDO	B	618	-	-	X	-
3	EDO	B	623	-	-	X	-
3	EDO	C	620	-	-	X	-
6	GOL	A	629	-	-	X	-
6	GOL	B	626	-	-	X	-
6	GOL	C	623	-	-	X	-

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 19325 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 AMP Deaminase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	497	Total	C	N	O	S	0	7	0
			4032	2582	684	754	12			
1	B	505	Total	C	N	O	S	0	8	0
			4099	2622	700	765	12			
1	C	496	Total	C	N	O	S	0	7	0
			4024	2577	683	752	12			
1	D	497	Total	C	N	O	S	0	5	0
			4016	2571	681	752	12			

- 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 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



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

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

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

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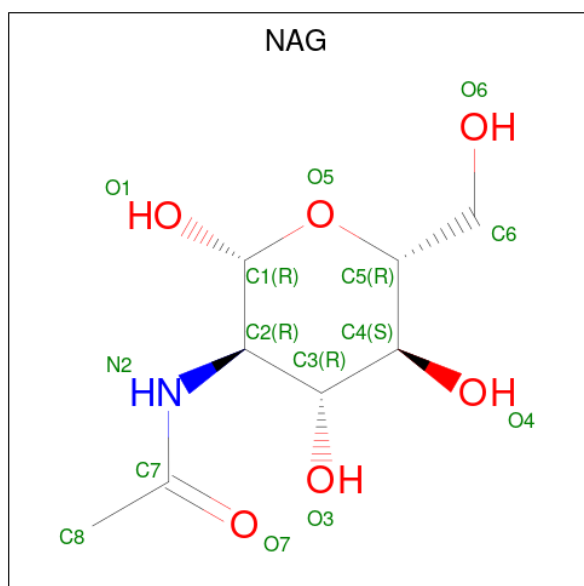
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	C	1	Total 4	C 2	O 2	0	0
3	C	1	Total 4	C 2	O 2	0	0
3	C	1	Total 4	C 2	O 2	0	0
3	C	1	Total 4	C 2	O 2	0	0
3	C	1	Total 4	C 2	O 2	0	0
3	C	1	Total 4	C 2	O 2	0	0
3	C	1	Total 4	C 2	O 2	0	0
3	D	1	Total 4	C 2	O 2	0	0
3	D	1	Total 4	C 2	O 2	0	0
3	D	1	Total 4	C 2	O 2	0	0
3	D	1	Total 4	C 2	O 2	0	0
3	D	1	Total 4	C 2	O 2	0	0
3	D	1	Total 4	C 2	O 2	0	0
3	D	1	Total 4	C 2	O 2	0	0
3	D	1	Total 4	C 2	O 2	0	0
3	D	1	Total 4	C 2	O 2	0	0
3	D	1	Total 4	C 2	O 2	0	0
3	D	1	Total 4	C 2	O 2	0	0
3	D	1	Total 4	C 2	O 2	0	0
3	D	1	Total 4	C 2	O 2	0	0
3	D	1	Total 4	C 2	O 2	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	D	1	Total	C	O	0	0
			4	2	2		
3	D	1	Total	C	O	0	0
			4	2	2		
3	D	1	Total	C	O	0	0
			4	2	2		

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



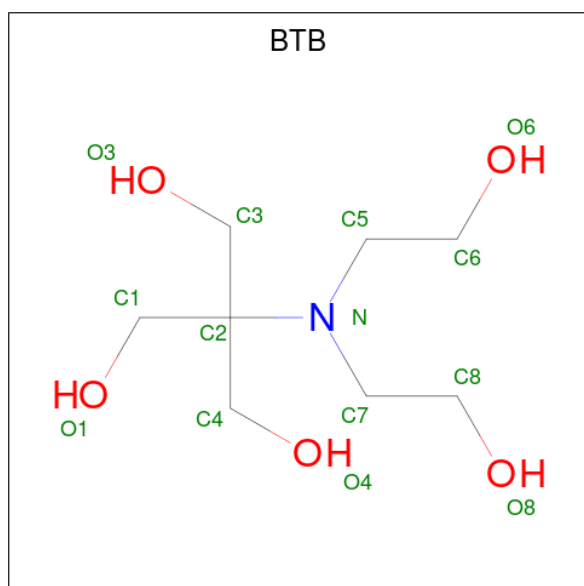
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	B	1	Total	C	N	O	0	0
			14	8	1	5		
4	B	1	Total	C	N	O	0	0
			14	8	1	5		
4	B	1	Total	C	N	O	0	0
			14	8	1	5		
4	C	1	Total	C	N	O	0	0
			14	8	1	5		
4	C	1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

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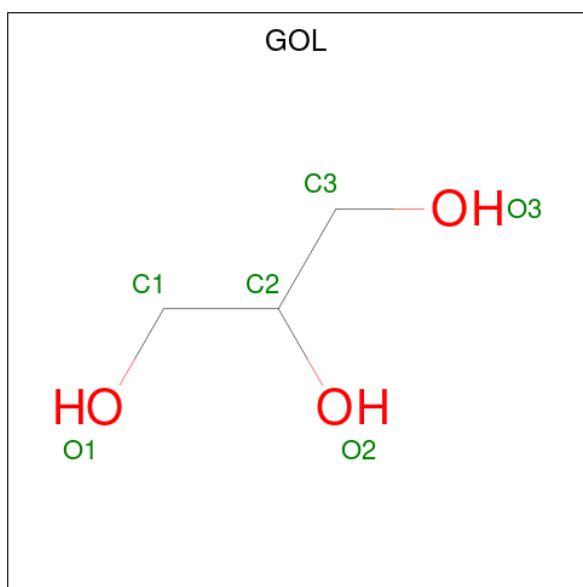
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	D	1	Total	C	N	O	0	0
			14	8	1	5		
4	D	1	Total	C	N	O	0	0
			14	8	1	5		
4	D	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 5 is 2-[BIS-(2-HYDROXY-ETHYL)-AMINO]-2-HYDROXYMETHYL-PROPAN E-1,3-DIOL (CCD ID: BTB) (formula: $C_8H_{19}NO_5$).



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

- Molecule 6 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).

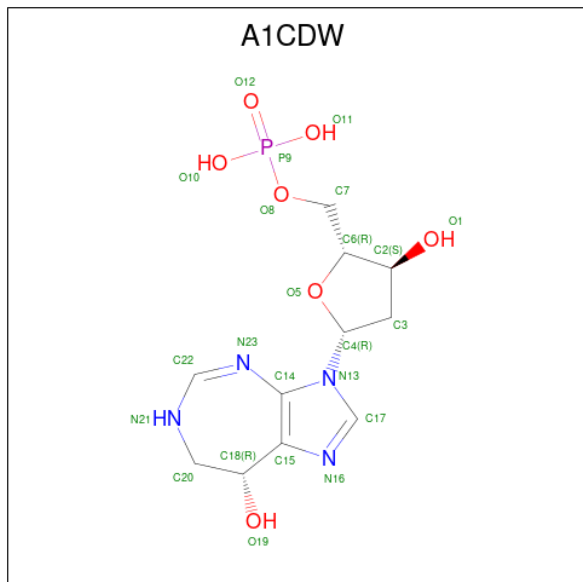


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			6	3	3		
6	A	1	Total	C	O	0	0
			6	3	3		
6	B	1	Total	C	O	0	0
			6	3	3		
6	C	1	Total	C	O	0	0
			6	3	3		
6	C	1	Total	C	O	0	0
			6	3	3		
6	C	1	Total	C	O	0	0
			6	3	3		
6	D	1	Total	C	O	0	0
			6	3	3		
6	D	1	Total	C	O	0	0
			6	3	3		

- Molecule 7 is ZINC ION (CCD ID: ZN) (formula: Zn).

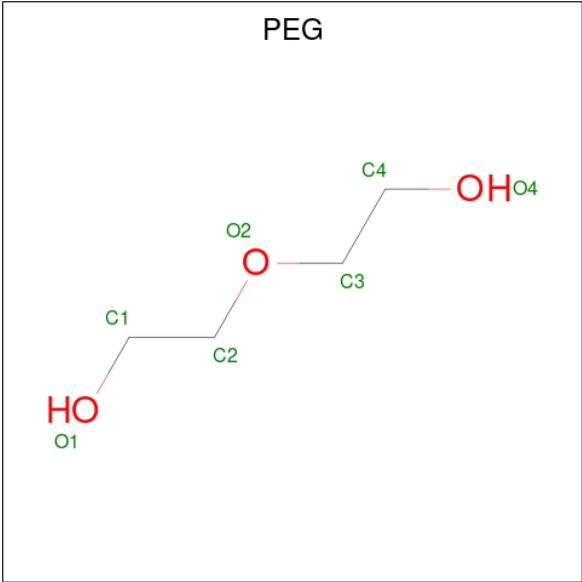
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	1	Total	Zn	0	0
			1	1		
7	B	1	Total	Zn	0	0
			1	1		
7	C	1	Total	Zn	0	0
			1	1		
7	D	1	Total	Zn	0	0
			1	1		

- Molecule 8 is pentostatin 5'-phosphate (CCD ID: A1CDW) (formula: $C_{11}H_{17}N_4O_7P$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
8	A	1	Total	C	N	O	P	0	0
			23	11	4	7	1		
8	B	1	Total	C	N	O	P	0	0
			23	11	4	7	1		
8	C	1	Total	C	N	O	P	0	0
			23	11	4	7	1		
8	D	1	Total	C	N	O	P	0	0
			23	11	4	7	1		

- Molecule 9 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: $C_4H_{10}O_3$).



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

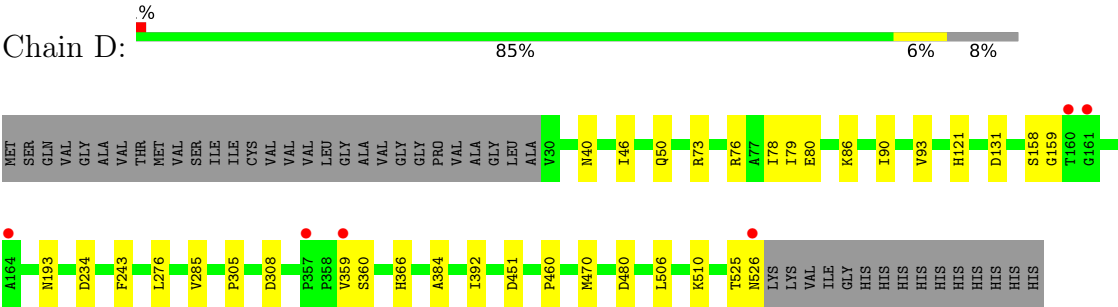
- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	549	Total	O	0	0
			549	549		
10	B	599	Total	O	0	0
			599	599		
10	C	617	Total	O	0	0
			617	617		
10	D	540	Total	O	0	0
			540	540		

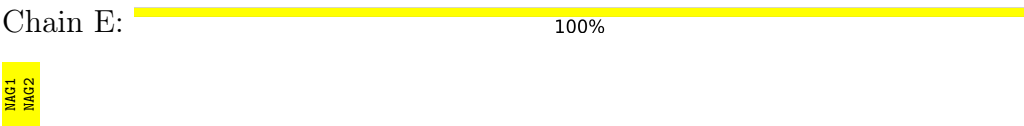
- Molecule 1: AMP Deaminase



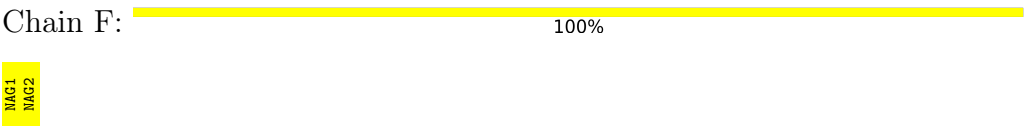
• Molecule 1: AMP Deaminase



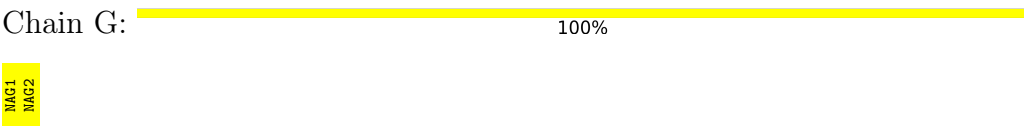
• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



• 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 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	75.99Å 81.94Å 212.19Å 90.00° 92.13° 90.00°	Depositor
Resolution (Å)	42.73 – 1.61 42.73 – 1.61	Depositor EDS
% Data completeness (in resolution range)	98.9 (42.73-1.61) 98.9 (42.73-1.61)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.21 (at 1.61Å)	Xtriage
Refinement program	PHENIX 1.21.2_5419	Depositor
R, R_{free}	0.167 , 0.199 0.167 , 0.199	Depositor DCC
R_{free} test set	16271 reflections (4.85%)	wwPDB-VP
Wilson B-factor (Å ²)	19.1	Xtriage
Anisotropy	0.463	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 47.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.010 for h,-k,-l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	19325	wwPDB-VP
Average B, all atoms (Å ²)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.89% 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: NAG, EDO, PEG, A1CDW, GOL, ZN, BTB

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	0.66	0/4147	0.74	0/5632
1	B	0.70	0/4224	0.75	0/5736
1	C	0.71	0/4136	0.75	0/5618
1	D	0.64	0/4128	0.71	0/5609
All	All	0.68	0/16635	0.74	0/22595

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	C	0	2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	214	ARG	Sidechain
1	C	365	PHE	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	4032	0	4002	35	0
1	B	4099	0	4058	49	0
1	C	4024	0	3992	36	0
1	D	4016	0	3977	27	0
2	E	28	0	25	0	0
2	F	28	0	25	0	0
2	G	28	0	25	0	0
2	H	28	0	25	0	0
3	A	92	0	138	15	0
3	B	116	0	174	25	0
3	C	128	0	191	25	0
3	D	68	0	102	14	0
4	A	42	0	39	0	0
4	B	42	0	39	1	0
4	C	28	0	26	0	0
4	D	42	0	39	0	0
5	A	14	0	19	0	0
5	B	14	0	19	1	0
6	A	12	0	16	5	0
6	B	6	0	8	4	0
6	C	18	0	24	6	0
6	D	12	0	16	2	0
7	A	1	0	0	0	0
7	B	1	0	0	0	0
7	C	1	0	0	0	0
7	D	1	0	0	0	0
8	A	23	0	0	0	0
8	B	23	0	0	0	0
8	C	23	0	0	0	0
8	D	23	0	0	0	0
9	C	7	0	10	2	0
10	A	549	0	0	5	0
10	B	599	0	0	7	0
10	C	617	0	0	14	0
10	D	540	0	0	10	0
All	All	19325	0	16989	166	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 5.

The worst 5 of 166 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:73:ARG:HH21	3:B:629:EDO:H12	1.27	0.98
1:B:306:ASN:HD22	3:B:623:EDO:H12	1.32	0.92
1:C:87:THR:HA	3:C:635:EDO:H21	1.57	0.87
1:B:360:SER:HB3	3:B:614:EDO:H21	1.59	0.84
1:B:306:ASN:HD22	3:B:623:EDO:C1	1.93	0.81

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	502/541 (93%)	487 (97%)	15 (3%)	0	100	100
1	B	511/541 (94%)	494 (97%)	17 (3%)	0	100	100
1	C	501/541 (93%)	482 (96%)	19 (4%)	0	100	100
1	D	500/541 (92%)	484 (97%)	15 (3%)	1 (0%)	43	25
All	All	2014/2164 (93%)	1947 (97%)	66 (3%)	1 (0%)	48	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	451	ASP

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	447/474 (94%)	446 (100%)	1 (0%)	87	81
1	B	455/474 (96%)	454 (100%)	1 (0%)	87	81
1	C	446/474 (94%)	446 (100%)	0	100	100
1	D	445/474 (94%)	444 (100%)	1 (0%)	87	81
All	All	1793/1896 (95%)	1790 (100%)	3 (0%)	87	81

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	193	ASN
1	B	193	ASN
1	D	193	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 24 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	484	GLN
1	D	69	GLN
1	C	512	ASN
1	D	249	GLN
1	B	306	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 ⓘ

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	1,2	14,14,15	0.60	0	17,19,21	1.38	3 (17%)
2	NAG	E	2	2	14,14,15	0.83	0	17,19,21	1.49	3 (17%)
2	NAG	F	1	1,2	14,14,15	0.69	0	17,19,21	1.56	3 (17%)
2	NAG	F	2	2	14,14,15	0.94	1 (7%)	17,19,21	1.67	3 (17%)
2	NAG	G	1	1,2	14,14,15	0.74	0	17,19,21	0.94	1 (5%)
2	NAG	G	2	2	14,14,15	0.96	2 (14%)	17,19,21	1.24	1 (5%)
2	NAG	H	1	1,2	14,14,15	0.96	1 (7%)	17,19,21	1.20	2 (11%)
2	NAG	H	2	2	14,14,15	0.83	0	17,19,21	1.00	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	E	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	E	2	2	-	2/6/23/26	0/1/1/1
2	NAG	F	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	F	2	2	-	0/6/23/26	0/1/1/1
2	NAG	G	1	1,2	-	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	1,2	-	0/6/23/26	0/1/1/1
2	NAG	H	2	2	-	2/6/23/26	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	2	NAG	C2-N2	-2.58	1.42	1.46
2	H	1	NAG	C1-C2	2.28	1.55	1.52
2	G	2	NAG	C1-C2	2.22	1.55	1.52
2	G	2	NAG	O5-C1	-2.01	1.40	1.43

The worst 5 of 16 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	2	NAG	C1-C2-N2	-3.86	104.35	110.43
2	F	1	NAG	C1-O5-C5	3.79	117.27	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	2	NAG	C1-O5-C5	3.54	116.93	112.19
2	E	1	NAG	C1-O5-C5	3.34	116.66	112.19
2	F	1	NAG	C3-C4-C5	-3.14	104.54	110.23

There are no chirality outliers.

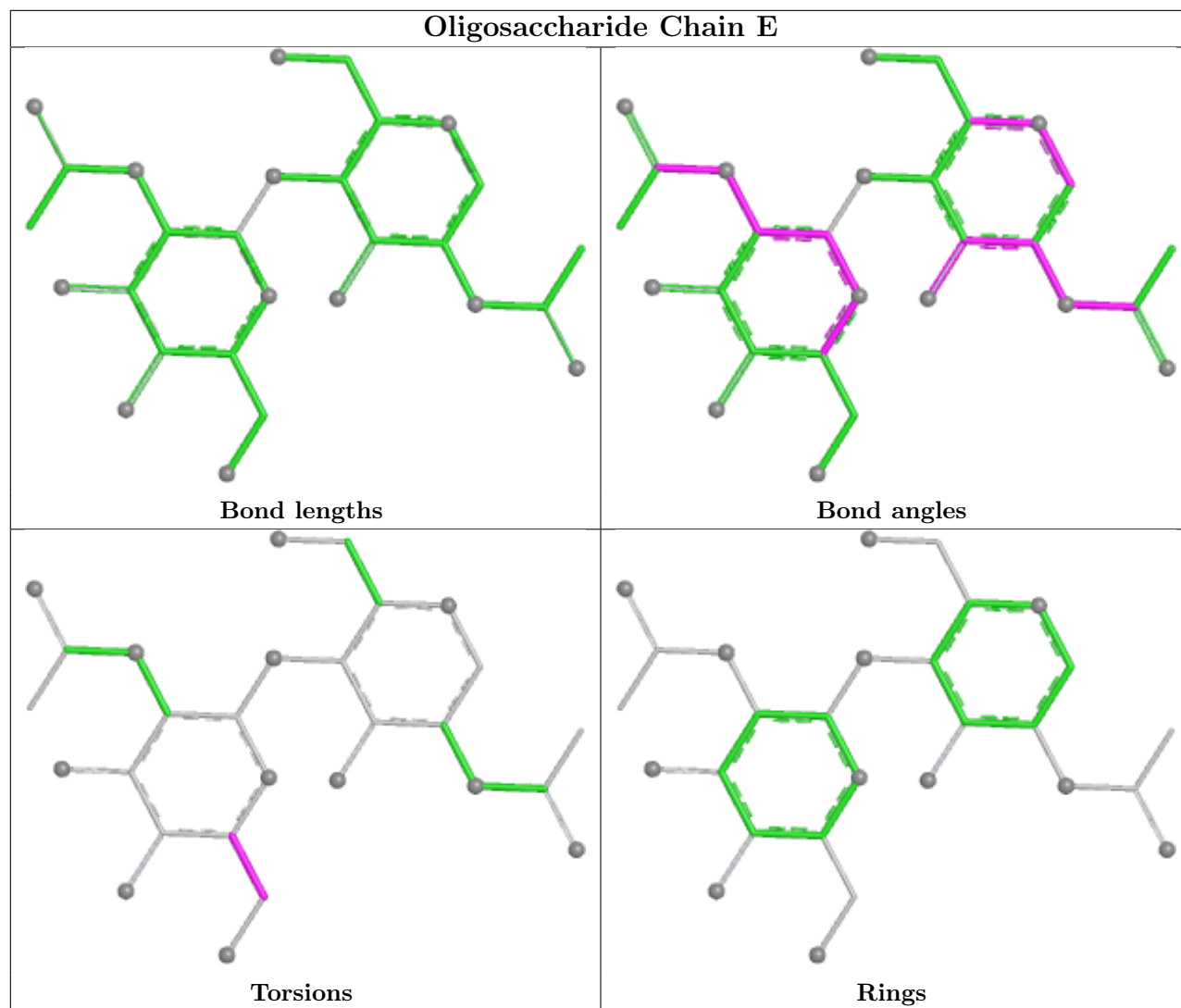
5 of 6 torsion outliers are listed below:

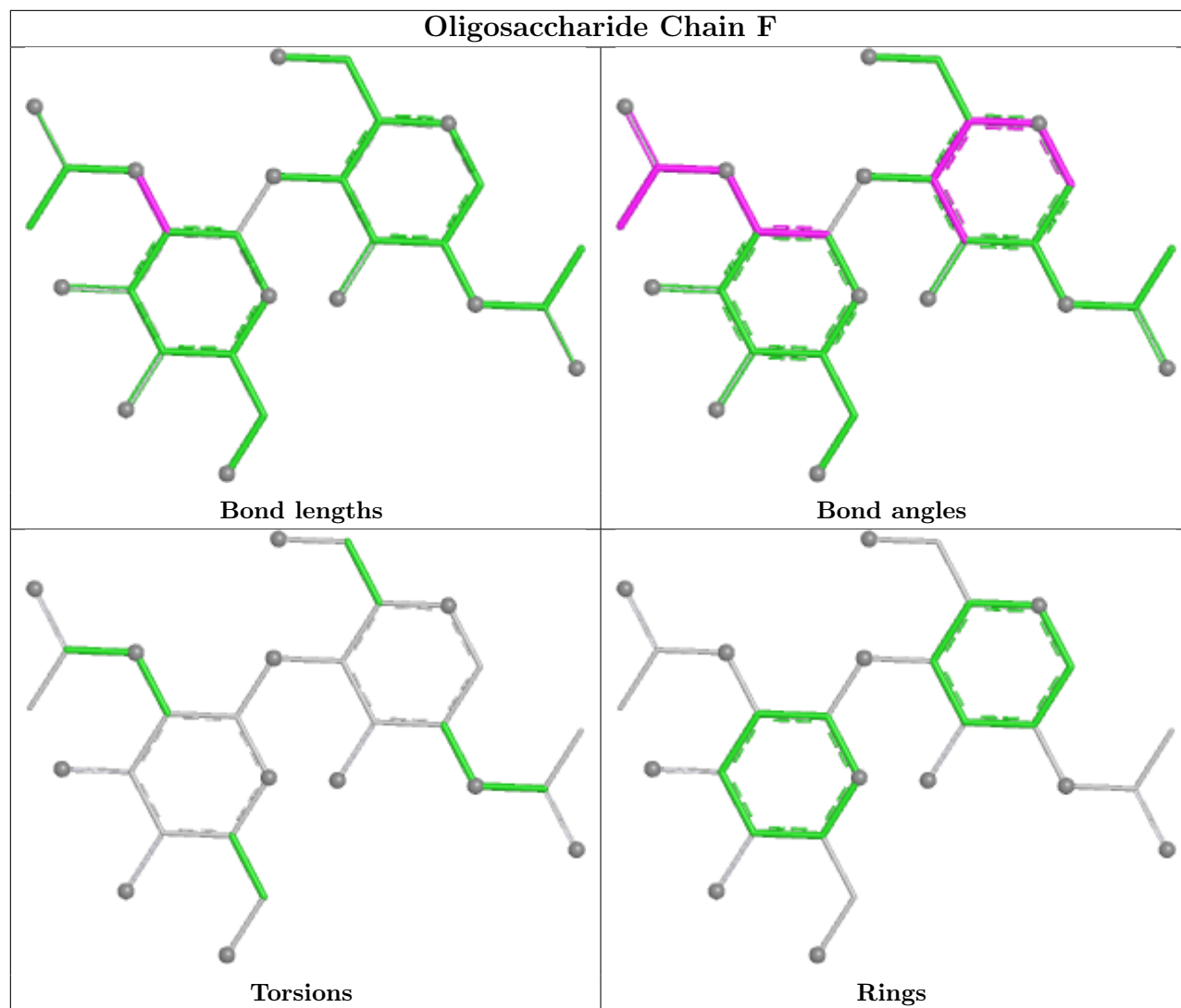
Mol	Chain	Res	Type	Atoms
2	H	2	NAG	O5-C5-C6-O6
2	G	2	NAG	C4-C5-C6-O6
2	G	2	NAG	O5-C5-C6-O6
2	H	2	NAG	C4-C5-C6-O6
2	E	2	NAG	O5-C5-C6-O6

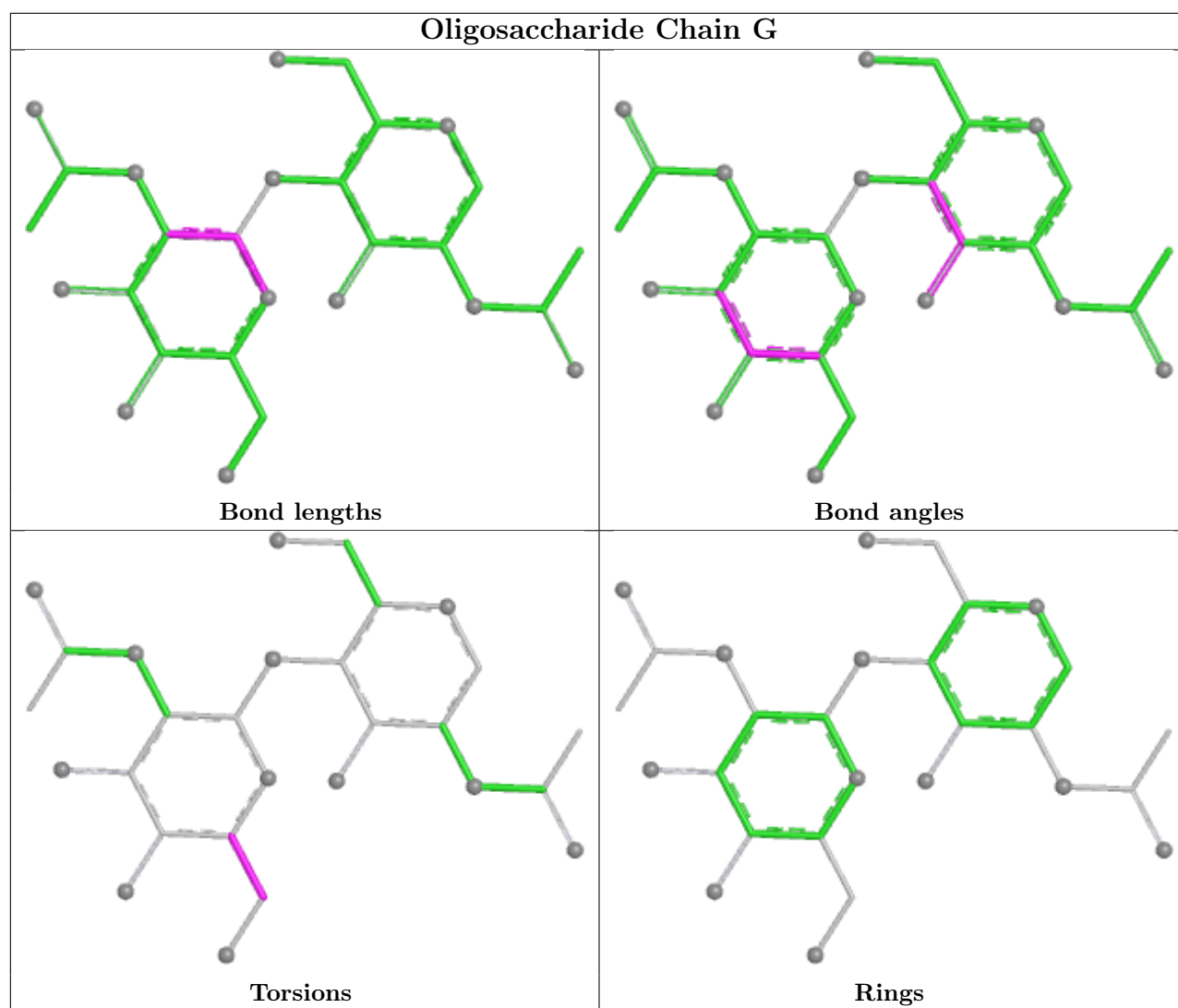
There are no ring outliers.

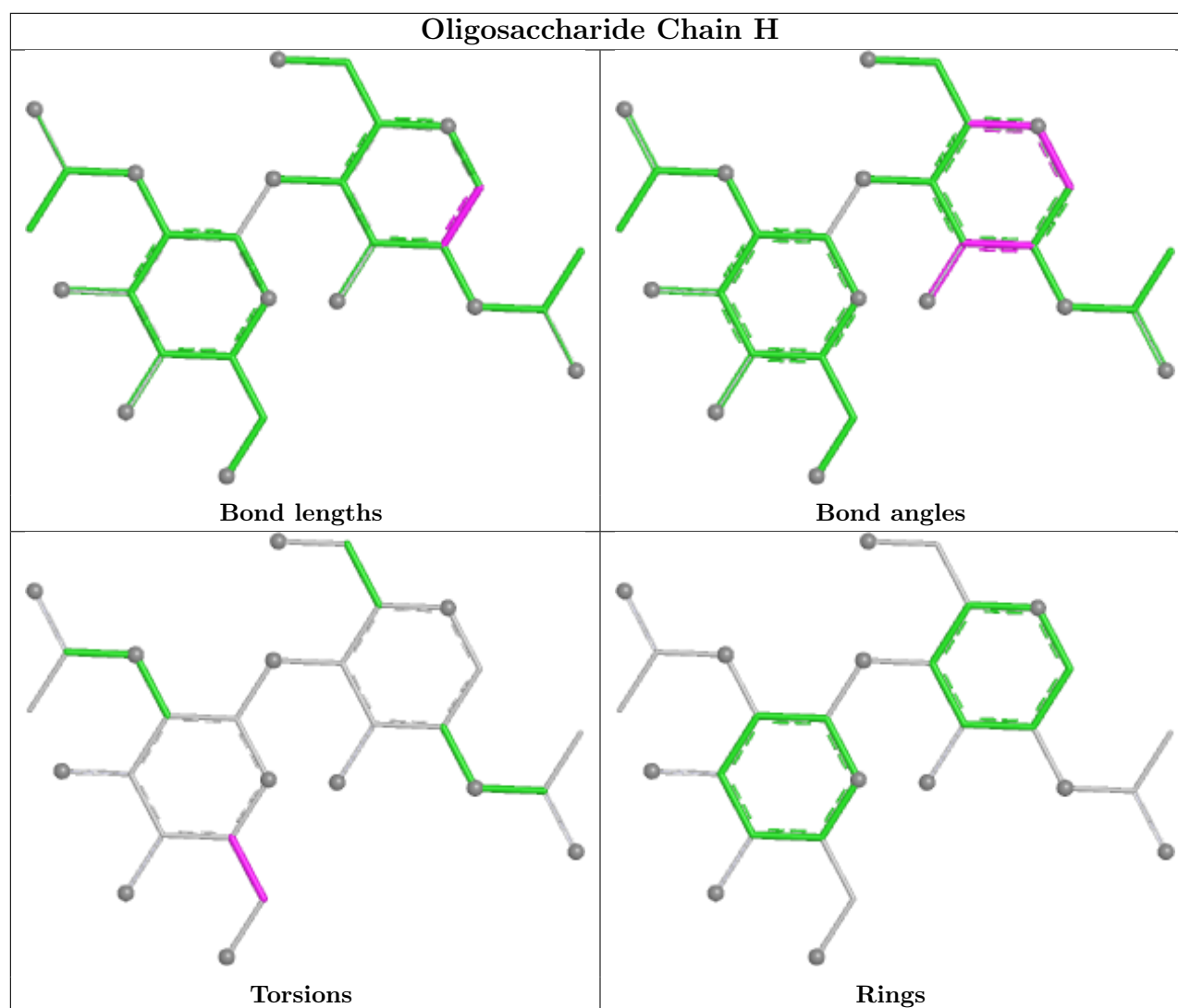
No monomer is involved in short contacts.

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









5.6 Ligand geometry [i](#)

Of 131 ligands modelled in this entry, 4 are monoatomic - leaving 127 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	EDO	A	628	-	3,3,3	0.27	0	2,2,2	0.48	0
6	GOL	A	629	-	5,5,5	0.48	0	5,5,5	1.14	0
3	EDO	A	601	-	3,3,3	0.43	0	2,2,2	0.09	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	EDO	C	615	-	3,3,3	0.25	0	2,2,2	0.48	0
3	EDO	B	631	-	3,3,3	0.28	0	2,2,2	0.33	0
3	EDO	D	610	-	3,3,3	0.26	0	2,2,2	0.22	0
8	A1CDW	D	624	7	20,25,25	0.57	0	25,37,37	0.65	0
3	EDO	D	609	-	3,3,3	0.22	0	2,2,2	0.48	0
3	EDO	A	608	-	3,3,3	0.25	0	2,2,2	0.81	0
3	EDO	C	614	-	3,3,3	0.27	0	2,2,2	0.44	0
3	EDO	C	638	-	3,3,3	0.23	0	2,2,2	0.24	0
3	EDO	A	623	-	3,3,3	0.43	0	2,2,2	0.70	0
3	EDO	A	606	-	3,3,3	0.30	0	2,2,2	0.46	0
3	EDO	B	611	-	3,3,3	0.35	0	2,2,2	0.14	0
3	EDO	A	617	-	3,3,3	0.29	0	2,2,2	0.65	0
5	BTB	B	610	-	13,13,13	1.02	1 (7%)	7,16,16	0.73	0
3	EDO	B	606	-	3,3,3	0.33	0	2,2,2	0.39	0
3	EDO	B	616	-	3,3,3	0.21	0	2,2,2	0.51	0
3	EDO	D	616	-	3,3,3	0.20	0	2,2,2	0.78	0
3	EDO	D	617	-	3,3,3	0.29	0	2,2,2	0.43	0
3	EDO	C	634	-	3,3,3	0.28	0	2,2,2	0.45	0
3	EDO	A	615	-	3,3,3	0.33	0	2,2,2	0.29	0
3	EDO	D	618	-	3,3,3	0.28	0	2,2,2	0.17	0
3	EDO	B	615	-	3,3,3	0.23	0	2,2,2	0.10	0
3	EDO	C	626	-	3,3,3	0.28	0	2,2,2	0.40	0
4	NAG	A	602	1	14,14,15	0.89	1 (7%)	17,19,21	1.77	3 (17%)
4	NAG	D	603	1	14,14,15	0.73	0	17,19,21	1.02	1 (5%)
3	EDO	D	620	-	3,3,3	0.24	0	2,2,2	0.27	0
3	EDO	A	605	-	3,3,3	0.28	0	2,2,2	0.29	0
3	EDO	B	608	-	3,3,3	0.32	0	2,2,2	0.20	0
3	EDO	C	636	-	3,3,3	0.24	0	2,2,2	0.63	0
3	EDO	A	610	-	3,3,3	0.17	0	2,2,2	0.77	0
3	EDO	B	627	-	3,3,3	0.28	0	2,2,2	0.52	0
3	EDO	B	617	-	3,3,3	0.31	0	2,2,2	0.35	0
3	EDO	B	625	-	3,3,3	0.17	0	2,2,2	0.56	0
3	EDO	C	605	-	3,3,3	0.35	0	2,2,2	0.18	0
3	EDO	B	618	-	3,3,3	0.17	0	2,2,2	0.42	0
4	NAG	A	603	1	14,14,15	0.78	0	17,19,21	1.55	2 (11%)
3	EDO	C	635	-	3,3,3	0.36	0	2,2,2	0.64	0
6	GOL	A	624	-	5,5,5	0.36	0	5,5,5	0.71	0
3	EDO	D	607	-	3,3,3	0.32	0	2,2,2	0.50	0
3	EDO	C	631	-	3,3,3	0.23	0	2,2,2	0.40	0
3	EDO	C	606	-	3,3,3	0.46	0	2,2,2	0.64	0
3	EDO	C	630	-	3,3,3	0.22	0	2,2,2	0.59	0
3	EDO	C	627	-	3,3,3	0.26	0	2,2,2	0.50	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	EDO	A	611	-	3,3,3	0.37	0	2,2,2	0.28	0
3	EDO	A	621	-	3,3,3	0.22	0	2,2,2	0.52	0
3	EDO	A	622	-	3,3,3	0.26	0	2,2,2	0.35	0
3	EDO	B	629	-	3,3,3	0.34	0	2,2,2	0.62	0
8	A1CDW	A	631	7	20,25,25	0.69	1 (5%)	25,37,37	0.46	0
3	EDO	B	621	-	3,3,3	0.31	0	2,2,2	0.24	0
3	EDO	B	622	-	3,3,3	0.28	0	2,2,2	0.31	0
3	EDO	D	611	-	3,3,3	0.26	0	2,2,2	0.56	0
4	NAG	D	601	1	14,14,15	0.80	1 (7%)	17,19,21	1.41	3 (17%)
4	NAG	B	603	1	14,14,15	0.86	1 (7%)	17,19,21	1.20	2 (11%)
3	EDO	C	629	-	3,3,3	0.26	0	2,2,2	0.52	0
6	GOL	D	615	-	5,5,5	0.42	0	5,5,5	1.47	1 (20%)
3	EDO	C	632	-	3,3,3	0.30	0	2,2,2	0.34	0
3	EDO	C	616	-	3,3,3	0.57	0	2,2,2	1.11	0
3	EDO	B	623	-	3,3,3	0.19	0	2,2,2	0.58	0
3	EDO	B	609	-	3,3,3	0.28	0	2,2,2	0.39	0
4	NAG	A	604	1	14,14,15	0.81	0	17,19,21	1.43	2 (11%)
3	EDO	B	613	-	3,3,3	0.27	0	2,2,2	0.73	0
6	GOL	B	626	-	5,5,5	0.64	0	5,5,5	1.16	0
3	EDO	C	633	-	3,3,3	0.21	0	2,2,2	0.42	0
4	NAG	D	602	1	14,14,15	0.91	0	17,19,21	1.31	3 (17%)
4	NAG	B	604	1	14,14,15	0.81	0	17,19,21	1.32	2 (11%)
3	EDO	B	632	-	3,3,3	0.26	0	2,2,2	0.52	0
3	EDO	B	614	-	3,3,3	0.34	0	2,2,2	0.02	0
3	EDO	A	620	-	3,3,3	0.20	0	2,2,2	0.55	0
3	EDO	C	608	-	3,3,3	0.25	0	2,2,2	0.32	0
3	EDO	B	630	-	3,3,3	0.45	0	2,2,2	1.25	0
4	NAG	C	603	1	14,14,15	0.73	0	17,19,21	0.90	0
6	GOL	C	602	-	5,5,5	0.26	0	5,5,5	0.66	0
3	EDO	C	607	-	3,3,3	0.29	0	2,2,2	0.37	0
3	EDO	B	620	-	3,3,3	0.29	0	2,2,2	0.33	0
6	GOL	C	624	-	5,5,5	0.32	0	5,5,5	1.36	1 (20%)
3	EDO	C	628	-	3,3,3	0.24	0	2,2,2	0.59	0
3	EDO	D	613	-	3,3,3	0.29	0	2,2,2	0.34	0
3	EDO	C	611	-	3,3,3	0.47	0	2,2,2	0.68	0
3	EDO	C	610	-	3,3,3	0.23	0	2,2,2	0.37	0
3	EDO	A	614	-	3,3,3	0.24	0	2,2,2	0.63	0
3	EDO	A	626	-	3,3,3	0.31	0	2,2,2	0.35	0
3	EDO	B	633	-	3,3,3	0.34	0	2,2,2	0.45	0
3	EDO	B	601	-	3,3,3	0.21	0	2,2,2	1.16	0
3	EDO	D	608	-	3,3,3	0.42	0	2,2,2	0.33	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	EDO	C	625	-	3,3,3	0.30	0	2,2,2	0.77	0
3	EDO	C	617	-	3,3,3	0.89	0	2,2,2	1.18	0
3	EDO	B	612	-	3,3,3	0.32	0	2,2,2	1.16	0
3	EDO	C	618	-	3,3,3	0.36	0	2,2,2	0.31	0
3	EDO	C	621	-	3,3,3	0.29	0	2,2,2	0.13	0
3	EDO	B	634	-	3,3,3	0.26	0	2,2,2	0.33	0
3	EDO	C	609	-	3,3,3	0.23	0	2,2,2	0.42	0
3	EDO	C	613	-	3,3,3	0.44	0	2,2,2	0.15	0
3	EDO	A	612	-	3,3,3	0.28	0	2,2,2	0.36	0
3	EDO	B	605	-	3,3,3	0.48	0	2,2,2	0.82	0
4	NAG	C	604	1	14,14,15	0.80	0	17,19,21	1.15	1 (5%)
3	EDO	D	605	-	3,3,3	0.30	0	2,2,2	0.17	0
3	EDO	B	607	-	3,3,3	0.23	0	2,2,2	0.46	0
3	EDO	B	619	-	3,3,3	0.27	0	2,2,2	0.26	0
3	EDO	C	601	-	3,3,3	0.30	0	2,2,2	0.27	0
3	EDO	A	609	-	3,3,3	0.25	0	2,2,2	0.32	0
3	EDO	B	628	-	3,3,3	0.28	0	2,2,2	0.55	0
3	EDO	D	612	-	3,3,3	0.28	0	2,2,2	0.04	0
3	EDO	C	612	-	3,3,3	0.31	0	2,2,2	0.64	0
3	EDO	C	620	-	3,3,3	0.94	0	2,2,2	1.12	0
8	A1CDW	B	636	7	20,25,25	0.59	0	25,37,37	0.52	0
3	EDO	A	616	-	3,3,3	0.30	0	2,2,2	0.35	0
9	PEG	C	637	-	6,6,6	0.33	0	5,5,5	0.50	0
3	EDO	D	604	-	3,3,3	0.29	0	2,2,2	0.51	0
3	EDO	D	622	-	3,3,3	0.32	0	2,2,2	0.08	0
8	A1CDW	C	640	7	20,25,25	0.53	0	25,37,37	0.60	0
6	GOL	C	623	-	5,5,5	0.55	0	5,5,5	1.68	1 (20%)
5	BTB	A	607	-	13,13,13	1.33	2 (15%)	7,16,16	0.83	0
3	EDO	C	619	-	3,3,3	0.19	0	2,2,2	0.27	0
3	EDO	D	606	-	3,3,3	0.25	0	2,2,2	0.28	0
4	NAG	B	602	1	14,14,15	0.91	0	17,19,21	3.00	6 (35%)
3	EDO	A	613	-	3,3,3	0.25	0	2,2,2	0.31	0
3	EDO	A	627	-	3,3,3	0.27	0	2,2,2	0.08	0
3	EDO	C	622	-	3,3,3	0.31	0	2,2,2	0.72	0
3	EDO	A	618	-	3,3,3	0.27	0	2,2,2	0.20	0
3	EDO	A	619	-	3,3,3	0.27	0	2,2,2	0.38	0
3	EDO	D	614	-	3,3,3	0.30	0	2,2,2	0.18	0
3	EDO	A	625	-	3,3,3	0.37	0	2,2,2	0.48	0
6	GOL	D	621	-	5,5,5	0.32	0	5,5,5	1.03	0
3	EDO	B	624	-	3,3,3	0.26	0	2,2,2	0.32	0
3	EDO	D	619	-	3,3,3	0.37	0	2,2,2	1.13	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
3	EDO	A	628	-	-	1/1/1/1	-
6	GOL	A	629	-	-	4/4/4/4	-
3	EDO	A	601	-	-	0/1/1/1	-
3	EDO	C	615	-	-	1/1/1/1	-
3	EDO	B	631	-	-	0/1/1/1	-
3	EDO	D	610	-	-	1/1/1/1	-
8	A1CDW	D	624	7	-	5/10/33/33	0/2/3/3
3	EDO	D	609	-	-	1/1/1/1	-
3	EDO	A	608	-	-	0/1/1/1	-
3	EDO	C	614	-	-	0/1/1/1	-
3	EDO	C	638	-	-	1/1/1/1	-
3	EDO	A	623	-	-	0/1/1/1	-
3	EDO	A	606	-	-	0/1/1/1	-
3	EDO	B	611	-	-	0/1/1/1	-
3	EDO	A	617	-	-	0/1/1/1	-
5	BTB	B	610	-	-	1/21/21/21	-
3	EDO	B	606	-	-	0/1/1/1	-
3	EDO	B	616	-	-	0/1/1/1	-
3	EDO	D	616	-	-	1/1/1/1	-
3	EDO	D	617	-	-	1/1/1/1	-
3	EDO	C	634	-	-	0/1/1/1	-
3	EDO	A	615	-	-	0/1/1/1	-
3	EDO	D	618	-	-	0/1/1/1	-
3	EDO	B	615	-	-	0/1/1/1	-
3	EDO	C	626	-	-	1/1/1/1	-
4	NAG	A	602	1	-	2/6/23/26	0/1/1/1
4	NAG	D	603	1	-	0/6/23/26	0/1/1/1
3	EDO	D	620	-	-	1/1/1/1	-
3	EDO	A	605	-	-	0/1/1/1	-
3	EDO	B	608	-	-	0/1/1/1	-
3	EDO	C	636	-	-	1/1/1/1	-
3	EDO	A	610	-	-	0/1/1/1	-
3	EDO	B	627	-	-	0/1/1/1	-
3	EDO	B	617	-	-	0/1/1/1	-
3	EDO	B	625	-	-	0/1/1/1	-
3	EDO	C	605	-	-	0/1/1/1	-
3	EDO	B	618	-	-	1/1/1/1	-
4	NAG	A	603	1	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	EDO	C	635	-	-	1/1/1/1	-
6	GOL	A	624	-	-	0/4/4/4	-
3	EDO	D	607	-	-	0/1/1/1	-
3	EDO	C	631	-	-	1/1/1/1	-
3	EDO	C	606	-	-	0/1/1/1	-
3	EDO	C	630	-	-	1/1/1/1	-
3	EDO	C	627	-	-	1/1/1/1	-
3	EDO	A	611	-	-	1/1/1/1	-
3	EDO	A	621	-	-	0/1/1/1	-
3	EDO	A	622	-	-	0/1/1/1	-
3	EDO	B	629	-	-	1/1/1/1	-
8	A1CDW	A	631	7	-	5/10/33/33	0/2/3/3
3	EDO	B	621	-	-	1/1/1/1	-
3	EDO	B	622	-	-	1/1/1/1	-
3	EDO	D	611	-	-	1/1/1/1	-
4	NAG	D	601	1	-	0/6/23/26	0/1/1/1
4	NAG	B	603	1	-	2/6/23/26	0/1/1/1
3	EDO	C	629	-	-	0/1/1/1	-
6	GOL	D	615	-	-	2/4/4/4	-
3	EDO	C	632	-	-	1/1/1/1	-
3	EDO	C	616	-	-	1/1/1/1	-
3	EDO	B	623	-	-	1/1/1/1	-
3	EDO	B	609	-	-	1/1/1/1	-
4	NAG	A	604	1	-	0/6/23/26	0/1/1/1
3	EDO	B	613	-	-	0/1/1/1	-
6	GOL	B	626	-	-	2/4/4/4	-
3	EDO	C	633	-	-	1/1/1/1	-
4	NAG	D	602	1	-	0/6/23/26	0/1/1/1
4	NAG	B	604	1	-	0/6/23/26	0/1/1/1
3	EDO	B	632	-	-	0/1/1/1	-
3	EDO	B	614	-	-	1/1/1/1	-
3	EDO	A	620	-	-	1/1/1/1	-
3	EDO	C	608	-	-	1/1/1/1	-
3	EDO	B	630	-	-	1/1/1/1	-
4	NAG	C	603	1	-	0/6/23/26	0/1/1/1
6	GOL	C	602	-	-	0/4/4/4	-
3	EDO	C	607	-	-	0/1/1/1	-
3	EDO	B	620	-	-	0/1/1/1	-
6	GOL	C	624	-	-	2/4/4/4	-
3	EDO	C	628	-	-	0/1/1/1	-
3	EDO	D	613	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	EDO	C	611	-	-	1/1/1/1	-
3	EDO	C	610	-	-	0/1/1/1	-
3	EDO	A	614	-	-	1/1/1/1	-
3	EDO	A	626	-	-	1/1/1/1	-
3	EDO	B	633	-	-	1/1/1/1	-
3	EDO	B	601	-	-	1/1/1/1	-
3	EDO	D	608	-	-	0/1/1/1	-
3	EDO	C	625	-	-	1/1/1/1	-
3	EDO	C	617	-	-	1/1/1/1	-
3	EDO	B	612	-	-	1/1/1/1	-
3	EDO	C	618	-	-	1/1/1/1	-
3	EDO	C	621	-	-	0/1/1/1	-
3	EDO	B	634	-	-	1/1/1/1	-
3	EDO	C	609	-	-	1/1/1/1	-
3	EDO	C	613	-	-	1/1/1/1	-
3	EDO	A	612	-	-	1/1/1/1	-
3	EDO	B	605	-	-	0/1/1/1	-
4	NAG	C	604	1	-	2/6/23/26	0/1/1/1
3	EDO	D	605	-	-	1/1/1/1	-
3	EDO	B	607	-	-	1/1/1/1	-
3	EDO	B	619	-	-	0/1/1/1	-
3	EDO	C	601	-	-	0/1/1/1	-
3	EDO	A	609	-	-	1/1/1/1	-
3	EDO	B	628	-	-	0/1/1/1	-
3	EDO	D	612	-	-	1/1/1/1	-
3	EDO	C	612	-	-	1/1/1/1	-
3	EDO	C	620	-	-	1/1/1/1	-
8	A1CDW	B	636	7	-	5/10/33/33	0/2/3/3
3	EDO	A	616	-	-	1/1/1/1	-
9	PEG	C	637	-	-	1/4/4/4	-
3	EDO	D	604	-	-	0/1/1/1	-
3	EDO	D	622	-	-	1/1/1/1	-
8	A1CDW	C	640	7	-	4/10/33/33	0/2/3/3
6	GOL	C	623	-	-	4/4/4/4	-
5	BTB	A	607	-	-	2/21/21/21	-
3	EDO	C	619	-	-	1/1/1/1	-
3	EDO	D	606	-	-	1/1/1/1	-
4	NAG	B	602	1	-	2/6/23/26	0/1/1/1
3	EDO	A	613	-	-	0/1/1/1	-
3	EDO	A	627	-	-	0/1/1/1	-
3	EDO	C	622	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	EDO	A	618	-	-	1/1/1/1	-
3	EDO	A	619	-	-	1/1/1/1	-
3	EDO	D	614	-	-	1/1/1/1	-
3	EDO	A	625	-	-	0/1/1/1	-
6	GOL	D	621	-	-	2/4/4/4	-
3	EDO	B	624	-	-	0/1/1/1	-
3	EDO	D	619	-	-	0/1/1/1	-

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	607	BTB	C3-C2	3.67	1.57	1.53
5	A	607	BTB	C4-C2	2.60	1.56	1.53
4	A	602	NAG	C1-C2	2.51	1.55	1.52
8	A	631	A1CDW	O19-C18	2.43	1.48	1.42
4	B	603	NAG	C2-N2	-2.31	1.42	1.46

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	602	NAG	C1-C2-N2	-7.98	97.86	110.43
4	B	602	NAG	C2-N2-C7	-5.72	115.23	122.90
4	A	602	NAG	O4-C4-C3	-4.63	99.46	110.38
4	A	603	NAG	C1-O5-C5	4.04	117.59	112.19
4	B	602	NAG	O7-C7-C8	3.99	129.16	122.05

There are no chirality outliers.

5 of 106 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	610	BTB	O1-C1-C2-N
6	A	629	GOL	O1-C1-C2-C3
6	B	626	GOL	O1-C1-C2-C3
6	C	623	GOL	O1-C1-C2-C3
6	C	624	GOL	C1-C2-C3-O3

There are no ring outliers.

56 monomers are involved in 99 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	629	GOL	4	0

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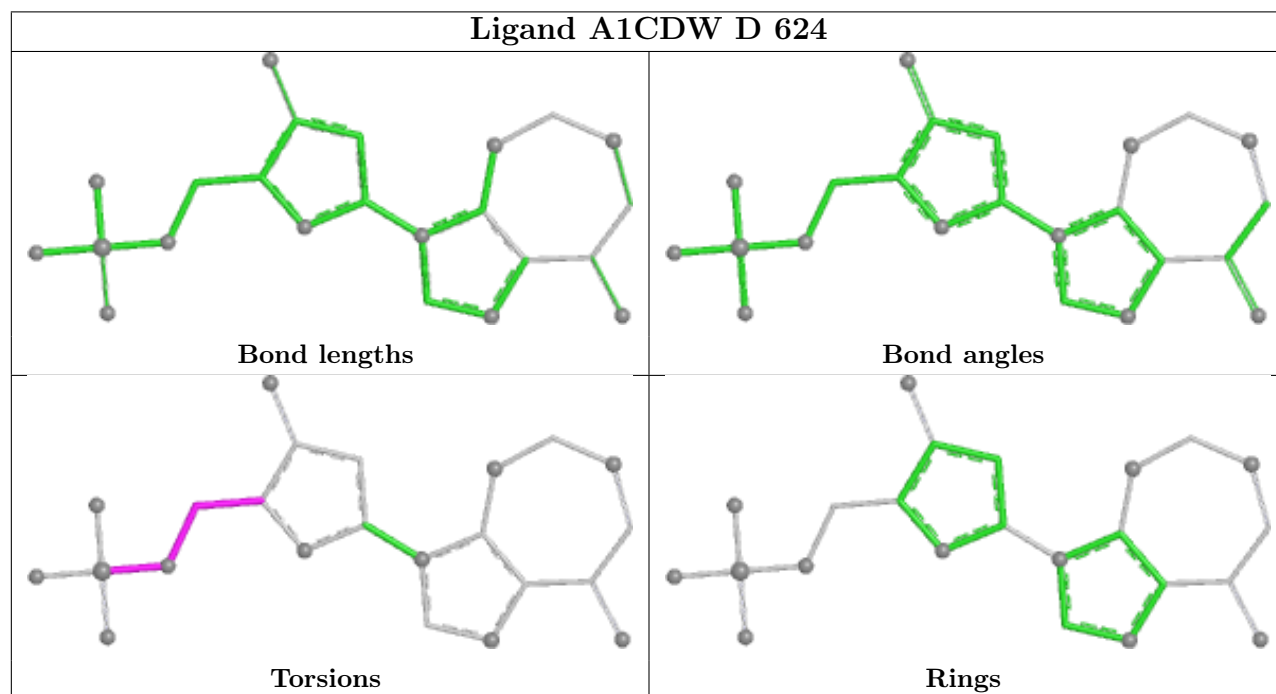
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	610	EDO	2	0
3	D	609	EDO	1	0
3	C	638	EDO	1	0
5	B	610	BTB	1	0
3	D	616	EDO	2	0
3	D	617	EDO	1	0
3	A	615	EDO	1	0
3	D	620	EDO	1	0
3	B	608	EDO	1	0
3	C	636	EDO	1	0
3	A	610	EDO	1	0
3	B	625	EDO	2	0
3	B	618	EDO	4	0
3	C	635	EDO	1	0
6	A	624	GOL	1	0
3	C	627	EDO	1	0
3	A	611	EDO	1	0
3	B	629	EDO	2	0
3	D	611	EDO	1	0
3	C	629	EDO	1	0
6	D	615	GOL	2	0
3	C	616	EDO	2	0
3	B	623	EDO	5	0
3	B	613	EDO	2	0
6	B	626	GOL	4	0
3	C	633	EDO	1	0
4	B	604	NAG	1	0
3	B	614	EDO	2	0
3	B	630	EDO	2	0
6	C	602	GOL	1	0
6	C	624	GOL	1	0
3	C	628	EDO	1	0
3	D	613	EDO	1	0
3	A	626	EDO	7	0
3	B	633	EDO	1	0
3	B	601	EDO	1	0
3	C	625	EDO	2	0
3	C	617	EDO	2	0
3	C	618	EDO	1	0
3	C	621	EDO	1	0
3	B	634	EDO	2	0
3	C	609	EDO	1	0

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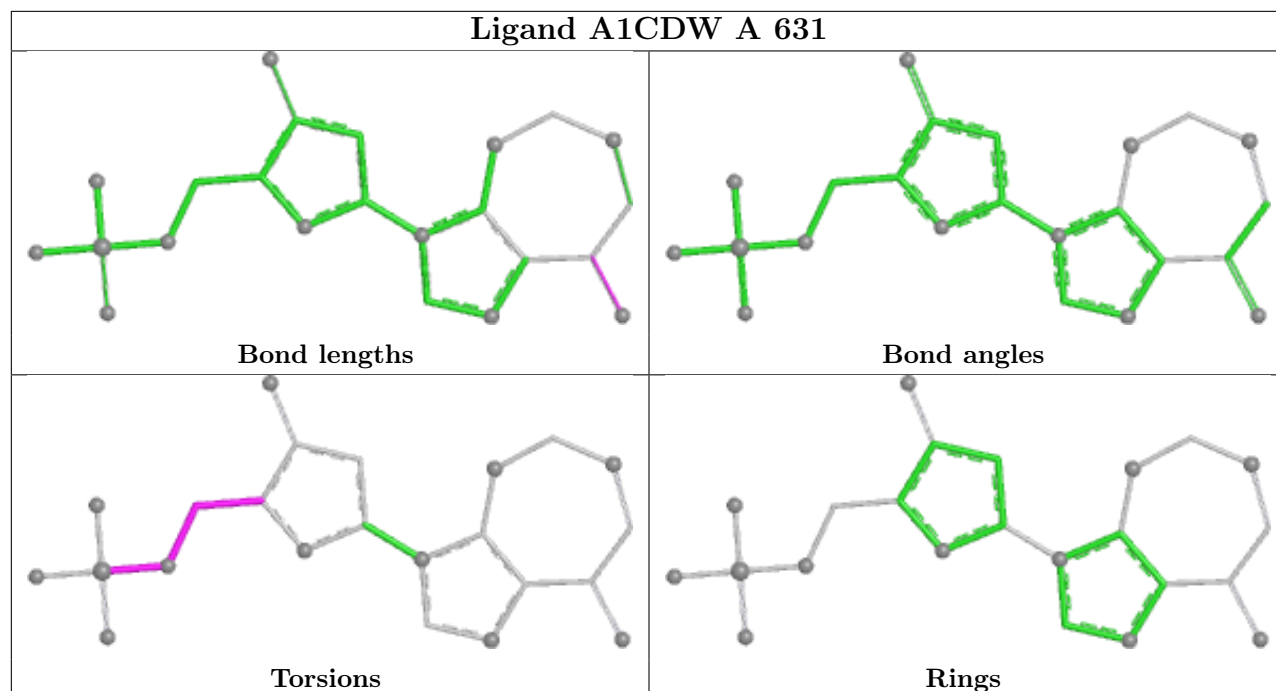
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	613	EDO	1	0
3	A	612	EDO	2	0
3	D	605	EDO	1	0
3	B	607	EDO	1	0
3	C	601	EDO	1	0
3	A	609	EDO	2	0
3	C	620	EDO	7	0
9	C	637	PEG	2	0
3	D	622	EDO	1	0
6	C	623	GOL	4	0
3	C	622	EDO	1	0
3	A	619	EDO	1	0
3	D	619	EDO	3	0

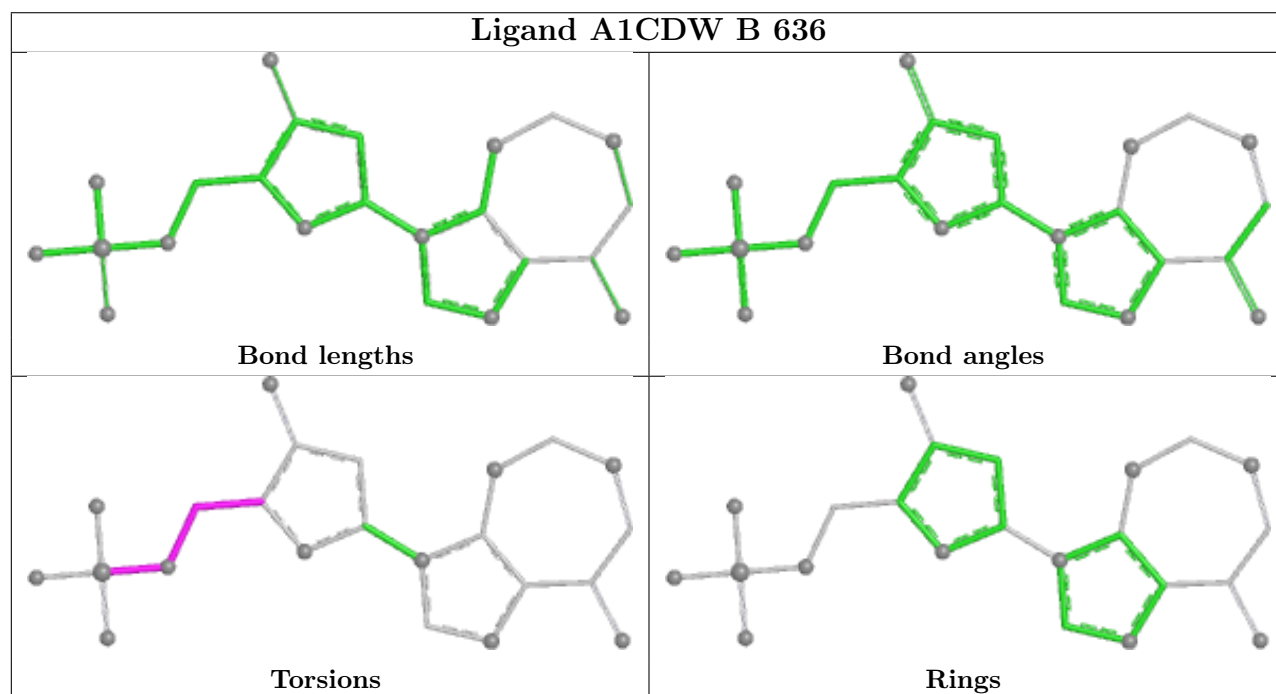
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

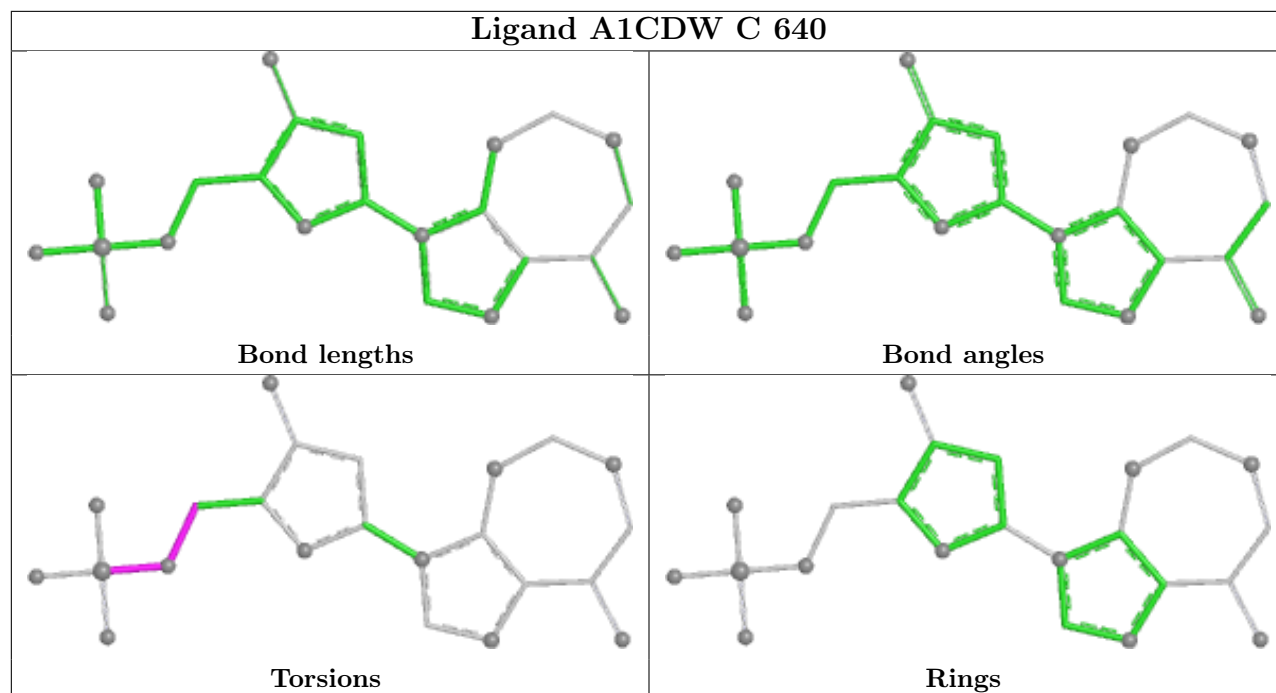


Ligand A1CDW A 631



Ligand A1CDW B 636





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	497/541 (91%)	-0.38	4 (0%) 82 86	13, 22, 41, 65	7 (1%)
1	B	505/541 (93%)	-0.45	9 (1%) 67 72	12, 20, 37, 55	8 (1%)
1	C	496/541 (91%)	-0.46	8 (1%) 70 75	9, 20, 35, 58	7 (1%)
1	D	497/541 (91%)	-0.27	6 (1%) 76 81	14, 24, 41, 72	5 (1%)
All	All	1995/2164 (92%)	-0.39	27 (1%) 73 78	9, 22, 38, 72	27 (1%)

The worst 5 of 27 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	165	ASN	3.9
1	C	164	ALA	3.4
1	C	30	VAL	3.3
1	D	161	GLY	3.2
1	B	160	THR	3.1

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.

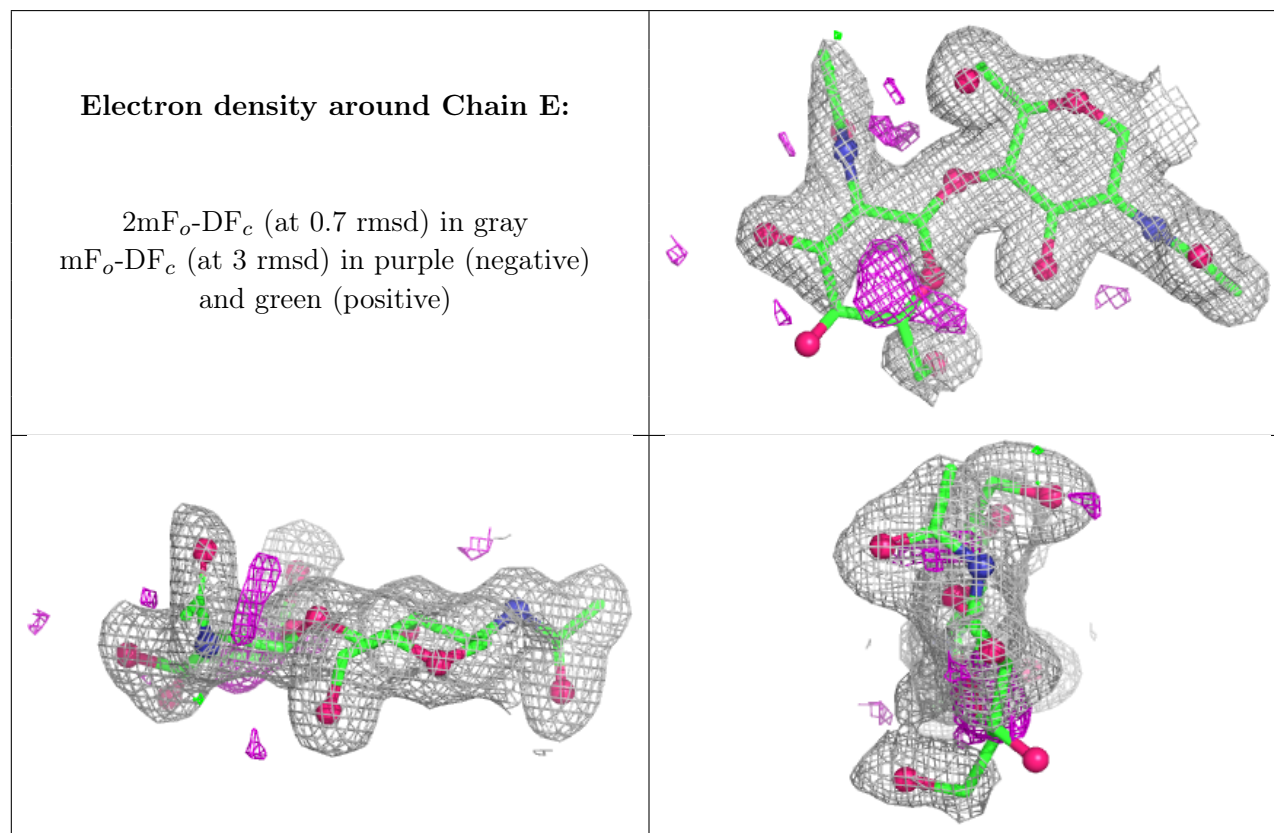
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	NAG	H	2	14/15	0.66	0.16	42,62,76,82	0
2	NAG	F	2	14/15	0.73	0.16	41,54,73,88	0

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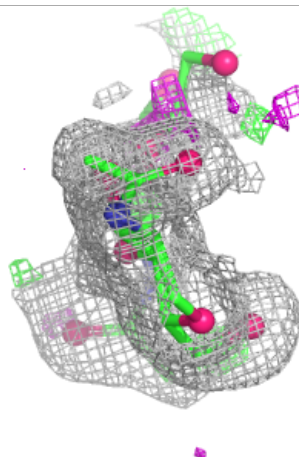
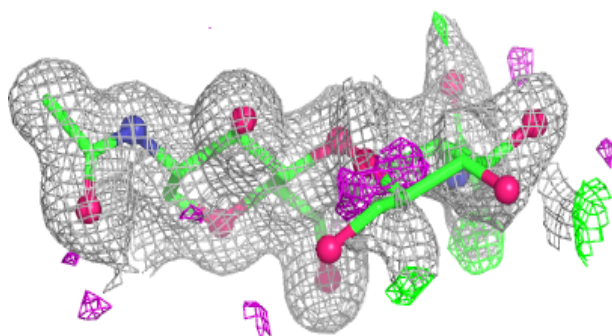
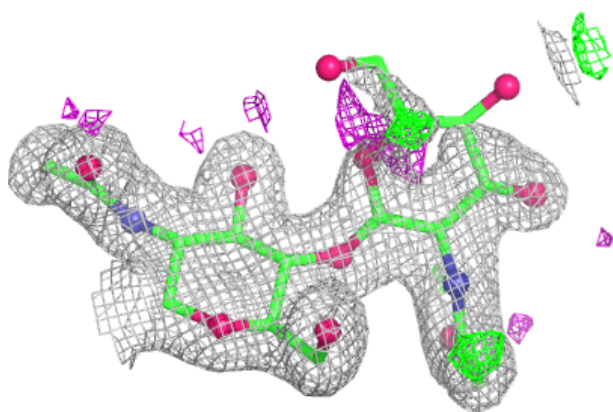
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	NAG	E	2	14/15	0.73	0.16	46,54,71,81	0
2	NAG	G	2	14/15	0.80	0.14	39,52,64,74	0
2	NAG	H	1	14/15	0.93	0.08	22,30,38,46	0
2	NAG	G	1	14/15	0.95	0.07	20,27,30,31	0
2	NAG	F	1	14/15	0.97	0.05	18,25,29,30	0
2	NAG	E	1	14/15	0.97	0.06	20,23,30,31	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.



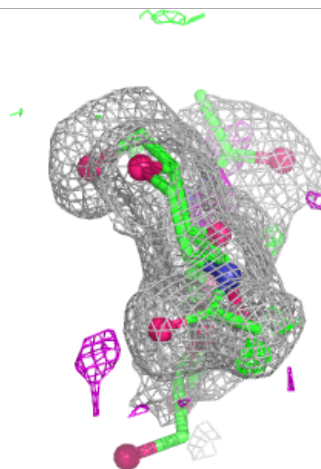
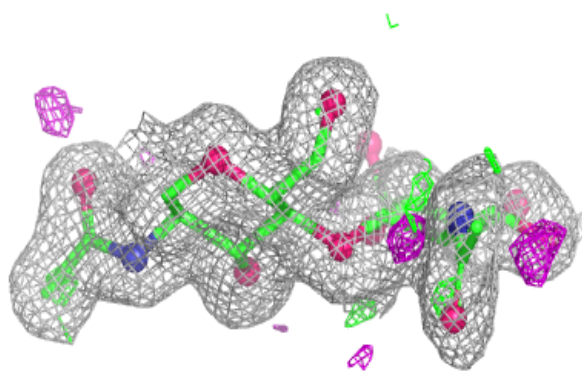
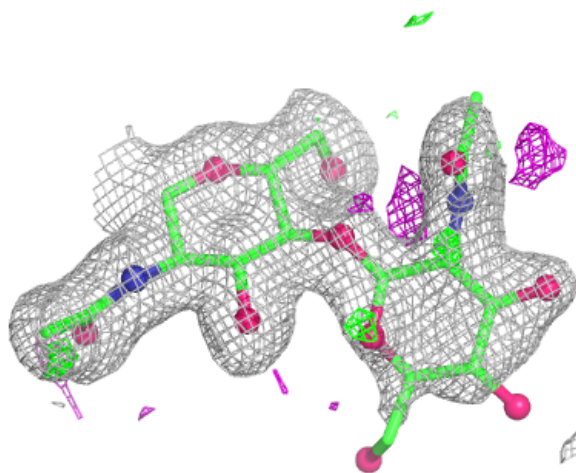
Electron density around Chain F:

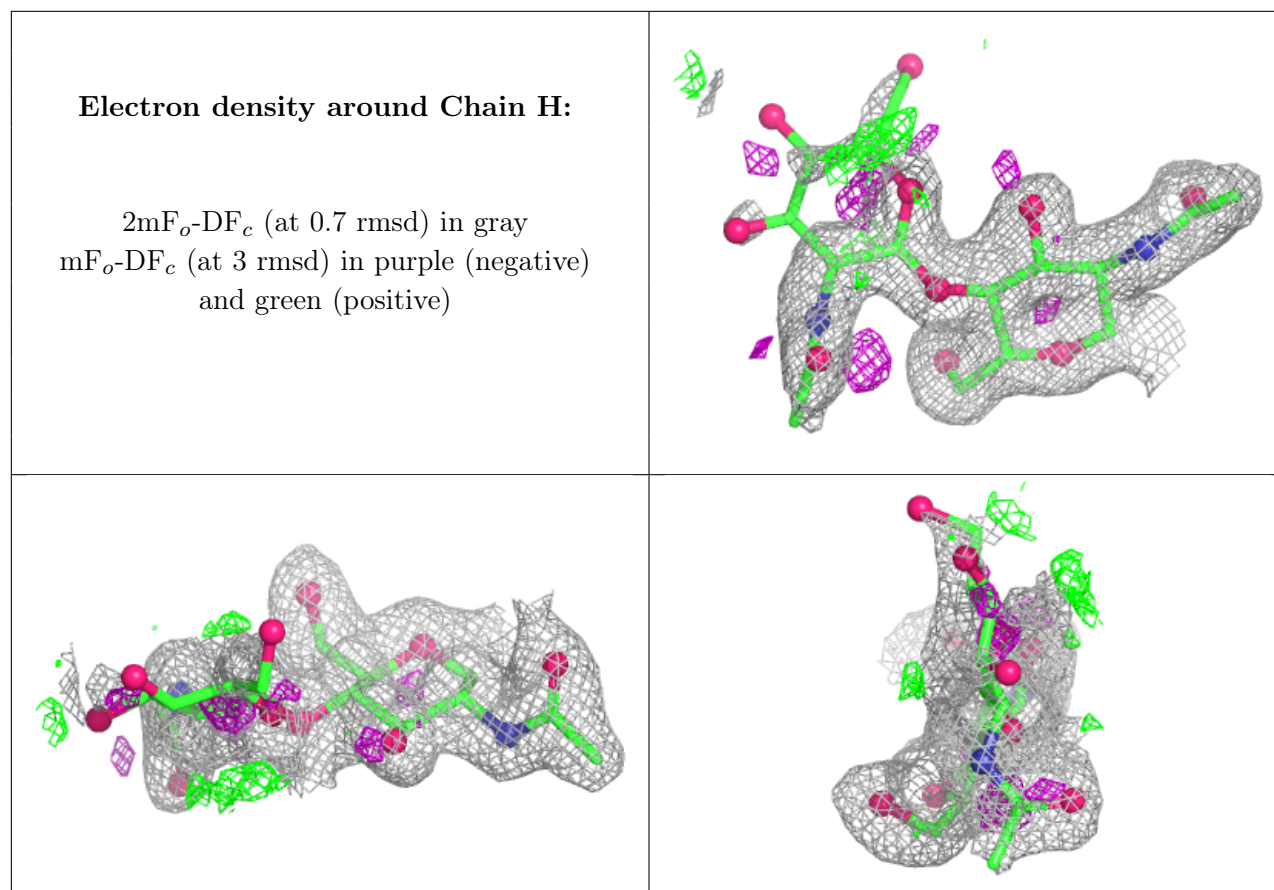
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



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 ⓘ

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($\text{\AA}^2$)	Q<0.9
3	EDO	A	626	4/4	0.59	0.21	37,49,50,62	0
3	EDO	D	614	4/4	0.62	0.18	57,61,61,67	0
3	EDO	B	623	4/4	0.68	0.19	42,48,49,50	0
9	PEG	C	637	7/7	0.68	0.20	45,50,55,56	0
3	EDO	A	619	4/4	0.69	0.20	49,52,59,61	0
3	EDO	D	617	4/4	0.71	0.15	37,41,47,60	0
3	EDO	B	617	4/4	0.72	0.21	45,45,48,55	0
3	EDO	A	617	4/4	0.72	0.17	37,44,46,60	0
3	EDO	B	634	4/4	0.72	0.17	53,54,56,60	0
3	EDO	D	610	4/4	0.73	0.18	45,46,49,55	0
6	GOL	A	624	6/6	0.75	0.16	42,50,59,66	0
3	EDO	C	615	4/4	0.75	0.17	43,44,45,55	0
3	EDO	C	633	4/4	0.76	0.16	36,49,51,74	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	EDO	A	621	4/4	0.77	0.18	41,48,48,51	0
3	EDO	A	616	4/4	0.77	0.17	39,46,52,57	0
3	EDO	A	610	4/4	0.78	0.17	36,42,44,48	0
3	EDO	C	625	4/4	0.79	0.15	35,40,48,55	0
3	EDO	D	611	4/4	0.79	0.18	33,46,50,50	0
3	EDO	A	618	4/4	0.79	0.15	47,52,56,60	0
3	EDO	C	622	4/4	0.80	0.14	33,37,42,44	0
3	EDO	B	620	4/4	0.80	0.14	39,43,45,61	0
3	EDO	C	632	4/4	0.80	0.11	41,44,48,48	0
3	EDO	C	610	4/4	0.80	0.14	42,44,51,63	0
3	EDO	B	629	4/4	0.80	0.15	34,45,46,49	0
3	EDO	B	631	4/4	0.81	0.13	37,46,50,55	0
4	NAG	B	604	14/15	0.81	0.12	34,53,63,69	0
3	EDO	C	613	4/4	0.81	0.13	27,32,41,56	0
6	GOL	C	602	6/6	0.81	0.12	61,63,67,67	0
3	EDO	D	616	4/4	0.81	0.16	38,47,53,53	0
3	EDO	D	620	4/4	0.82	0.13	42,44,45,58	0
4	NAG	A	604	14/15	0.82	0.12	35,49,60,67	0
4	NAG	B	602	14/15	0.82	0.14	28,45,56,57	0
3	EDO	C	628	4/4	0.82	0.13	44,46,47,48	0
3	EDO	C	609	4/4	0.82	0.15	40,40,42,51	0
3	EDO	B	618	4/4	0.82	0.15	35,42,54,54	0
3	EDO	A	614	4/4	0.82	0.14	31,39,39,70	0
3	EDO	C	618	4/4	0.83	0.15	37,38,42,48	0
3	EDO	D	619	4/4	0.83	0.17	24,40,45,51	0
3	EDO	B	632	4/4	0.83	0.13	40,44,49,56	0
4	NAG	A	603	14/15	0.83	0.12	31,50,63,65	0
3	EDO	C	629	4/4	0.83	0.14	44,50,53,59	0
3	EDO	B	601	4/4	0.84	0.15	29,32,45,45	0
3	EDO	B	622	4/4	0.84	0.13	34,40,41,47	0
3	EDO	B	614	4/4	0.84	0.15	44,44,45,49	0
3	EDO	B	633	4/4	0.84	0.12	34,38,38,45	0
3	EDO	B	627	4/4	0.84	0.13	40,45,46,50	0
3	EDO	A	620	4/4	0.85	0.12	39,43,43,54	0
3	EDO	B	628	4/4	0.85	0.12	38,39,41,56	0
3	EDO	B	612	4/4	0.85	0.15	26,30,30,46	0
3	EDO	B	621	4/4	0.85	0.13	43,47,49,52	0
4	NAG	C	604	14/15	0.85	0.12	28,41,58,72	0
3	EDO	A	612	4/4	0.85	0.13	36,43,47,49	0
3	EDO	A	609	4/4	0.85	0.12	33,34,39,48	0
3	EDO	C	636	4/4	0.85	0.15	35,43,50,55	0
3	EDO	C	601	4/4	0.86	0.12	29,41,44,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	EDO	C	611	4/4	0.86	0.20	30,30,53,64	0
3	EDO	D	605	4/4	0.86	0.12	35,37,44,49	0
3	EDO	C	620	4/4	0.86	0.33	20,22,29,33	0
3	EDO	C	630	4/4	0.86	0.12	35,38,40,55	0
3	EDO	B	630	4/4	0.86	0.24	29,31,33,44	0
3	EDO	C	631	4/4	0.87	0.14	48,48,52,54	0
3	EDO	C	627	4/4	0.87	0.12	31,39,42,49	0
4	NAG	D	603	14/15	0.87	0.11	33,48,61,63	0
3	EDO	B	608	4/4	0.87	0.12	40,42,43,44	0
3	EDO	B	619	4/4	0.87	0.14	32,43,48,48	0
3	EDO	B	625	4/4	0.87	0.13	31,40,53,57	0
3	EDO	D	606	4/4	0.88	0.12	37,37,40,40	0
3	EDO	C	608	4/4	0.88	0.13	36,42,44,52	0
3	EDO	B	615	4/4	0.88	0.12	32,41,46,47	0
3	EDO	C	626	4/4	0.88	0.12	33,40,42,57	0
3	EDO	B	613	4/4	0.88	0.11	32,37,40,43	0
4	NAG	D	602	14/15	0.88	0.11	26,35,55,64	0
3	EDO	C	634	4/4	0.88	0.13	26,36,37,52	0
3	EDO	C	619	4/4	0.88	0.13	35,43,44,48	0
3	EDO	B	607	4/4	0.88	0.12	30,36,42,42	0
4	NAG	A	602	14/15	0.88	0.11	29,37,46,49	0
3	EDO	C	614	4/4	0.89	0.13	39,42,45,50	0
3	EDO	D	618	4/4	0.89	0.11	48,51,53,62	0
3	EDO	D	609	4/4	0.89	0.13	30,36,44,49	0
3	EDO	A	628	4/4	0.89	0.12	34,39,44,51	0
4	NAG	B	603	14/15	0.89	0.10	29,39,53,56	0
6	GOL	D	615	6/6	0.89	0.12	27,33,37,44	0
3	EDO	D	622	4/4	0.89	0.11	38,45,45,52	0
6	GOL	C	624	6/6	0.90	0.11	26,30,35,35	0
3	EDO	B	624	4/4	0.90	0.11	35,36,41,54	0
3	EDO	D	613	4/4	0.90	0.11	33,35,44,55	0
3	EDO	A	622	4/4	0.91	0.10	44,44,47,47	0
4	NAG	D	601	14/15	0.92	0.09	31,37,46,53	0
3	EDO	C	616	4/4	0.92	0.19	23,34,38,39	0
3	EDO	B	609	4/4	0.92	0.10	37,39,44,47	0
5	BTB	A	607	14/14	0.92	0.10	25,33,40,41	0
3	EDO	A	625	4/4	0.92	0.10	33,35,36,41	0
6	GOL	A	629	6/6	0.92	0.10	29,35,39,42	0
6	GOL	B	626	6/6	0.92	0.11	19,34,38,42	0
3	EDO	B	605	4/4	0.92	0.13	22,22,23,26	0
6	GOL	C	623	6/6	0.92	0.10	23,32,38,40	0
3	EDO	A	608	4/4	0.92	0.13	26,27,28,32	0

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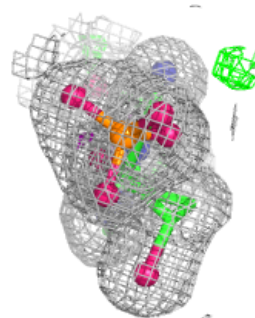
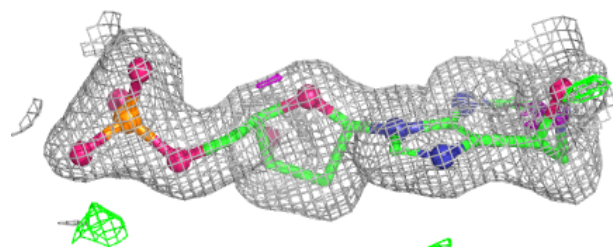
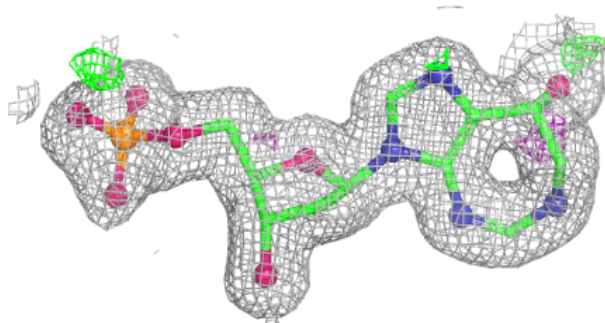
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	NAG	C	603	14/15	0.92	0.08	24,27,29,31	0
6	GOL	D	621	6/6	0.92	0.10	26,35,39,52	0
3	EDO	A	605	4/4	0.92	0.10	35,41,44,46	0
3	EDO	B	616	4/4	0.93	0.12	25,26,29,32	0
3	EDO	C	606	4/4	0.93	0.15	22,26,27,28	0
5	BTB	B	610	14/14	0.93	0.08	23,29,36,37	0
3	EDO	C	617	4/4	0.94	0.13	28,29,31,37	0
3	EDO	A	623	4/4	0.94	0.13	23,29,32,48	0
3	EDO	C	635	4/4	0.94	0.15	28,30,34,42	0
3	EDO	C	621	4/4	0.94	0.12	24,30,31,40	0
3	EDO	C	638	4/4	0.94	0.11	24,28,32,43	0
3	EDO	D	604	4/4	0.95	0.09	25,28,34,35	0
3	EDO	D	607	4/4	0.95	0.12	25,29,29,30	0
3	EDO	D	608	4/4	0.95	0.10	21,24,28,28	0
3	EDO	A	613	4/4	0.95	0.09	27,30,31,33	0
3	EDO	A	601	4/4	0.96	0.08	25,26,27,28	0
3	EDO	A	611	4/4	0.96	0.12	27,29,29,33	0
3	EDO	A	615	4/4	0.96	0.10	20,23,39,42	0
3	EDO	C	612	4/4	0.96	0.08	25,28,30,31	0
3	EDO	A	606	4/4	0.96	0.07	23,26,28,31	0
3	EDO	D	612	4/4	0.96	0.09	26,33,33,34	0
3	EDO	A	627	4/4	0.97	0.06	28,31,32,33	0
3	EDO	B	611	4/4	0.97	0.06	24,27,27,29	0
8	A1CDW	A	631	23/23	0.97	0.06	15,18,30,39	0
8	A1CDW	C	640	23/23	0.97	0.05	15,18,28,33	0
8	A1CDW	D	624	23/23	0.97	0.06	17,22,29,36	0
3	EDO	B	606	4/4	0.97	0.06	23,25,27,32	0
3	EDO	C	607	4/4	0.98	0.07	21,25,28,29	0
3	EDO	C	605	4/4	0.98	0.05	22,22,22,27	0
8	A1CDW	B	636	23/23	0.98	0.05	14,18,26,35	0
7	ZN	B	635	1/1	1.00	0.01	17,17,17,17	0
7	ZN	C	639	1/1	1.00	0.01	17,17,17,17	0
7	ZN	D	623	1/1	1.00	0.02	21,21,21,21	0
7	ZN	A	630	1/1	1.00	0.01	18,18,18,18	0

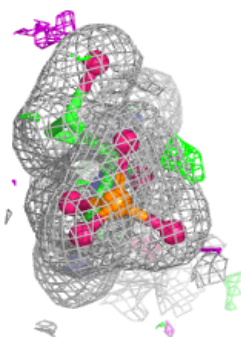
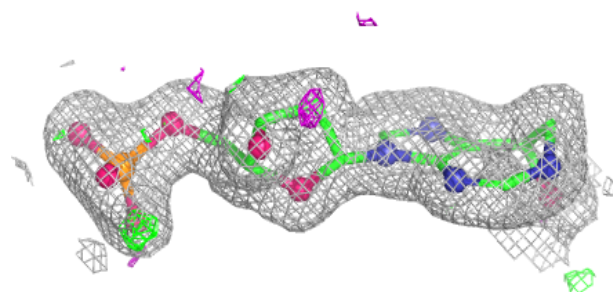
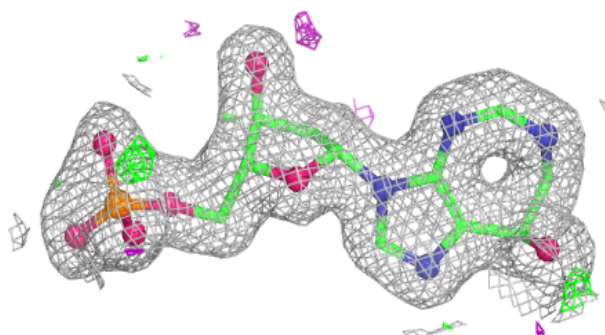
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around A1CDW A 631:

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

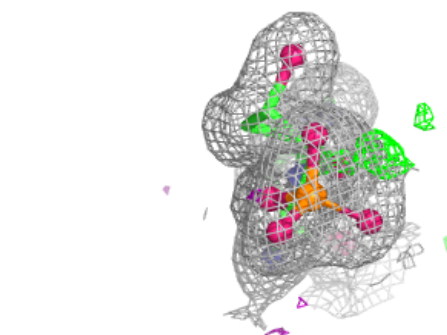
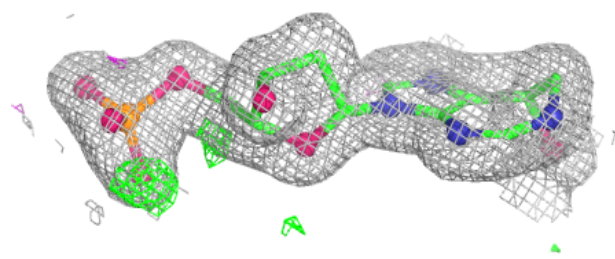
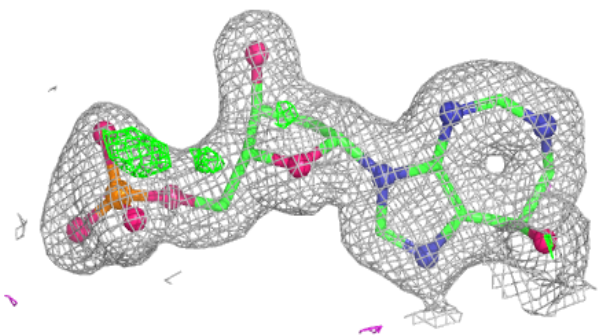
**Electron density around A1CDW C 640:**

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

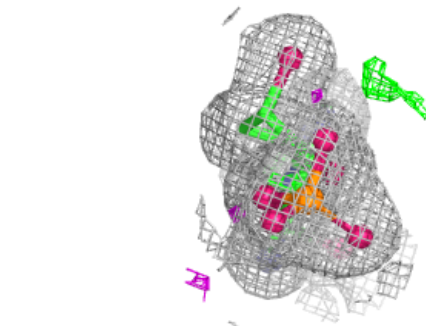
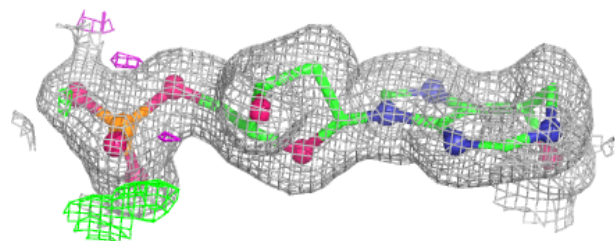
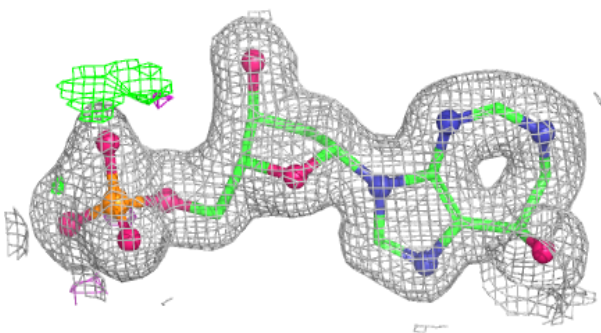


Electron density around A1CDW D 624:

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

**Electron density around A1CDW B 636:**

$2mF_o-DF_c$ (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.