WORLDWIDE PDB PROTEIN DATA BANK

wwPDB X-ray Structure Validation Summary Report (i)

Aug 26, 2023 – 11:09 PM EDT

PDB ID	:	3GDN
Title	:	Almond hydroxynitrile lyase in complex with benzaldehyde
Authors	:	Dreveny, I.; Gruber, K.; Kratky, C.
Deposited on	:	2009-02-24
Resolution	:	1.67 Å(reported)

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

|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

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 1.67 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.
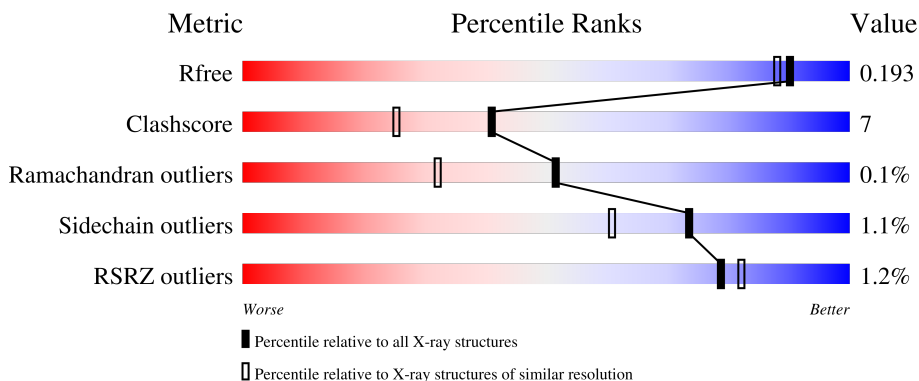
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	6780 (1.70-1.66)
Clashscore	141614	7310 (1.70-1.66)
Ramachandran outliers	138981	7173 (1.70-1.66)
Sidechain outliers	138945	7172 (1.70-1.66)
RSRZ outliers	127900	6661 (1.70-1.66)

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 <=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	521	%: 85% / 15%
1	B	521	%: 85% / 14%
2	C	3	67% / 33%
3	D	3	67% / 33%
4	E	5	20% / 80%

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Mol	Chain	Length	Quality of chain
5	F	4	75% 25%

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
5	MAN	F	4	-	-	-	X

2 Entry composition ⓘ

There are 10 unique types of molecules in this entry. The entry contains 9681 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 R-oxynitrile lyase isoenzyme 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	521	Total	C	N	O	S	0	8	0
			4016	2552	668	788	8			
1	B	521	Total	C	N	O	S	0	9	0
			4019	2553	669	789	8			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	346	SER	ALA	SEE REMARK 999	UNP Q945K2
B	346	SER	ALA	SEE REMARK 999	UNP Q945K2

- Molecule 2 is an oligosaccharide called alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.
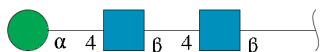
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	3	Total	C	N	O	0	0	0
			39	22	2	15			

- Molecule 3 is an oligosaccharide called alpha-L-fucopyranose-(1-3)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)]2-acetamido-2-deoxy-beta-D-glucopyranose.
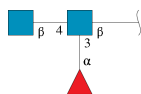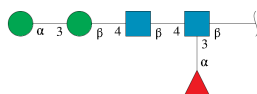
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	D	3	Total	C	N	O	0	0	0
			38	22	2	14			

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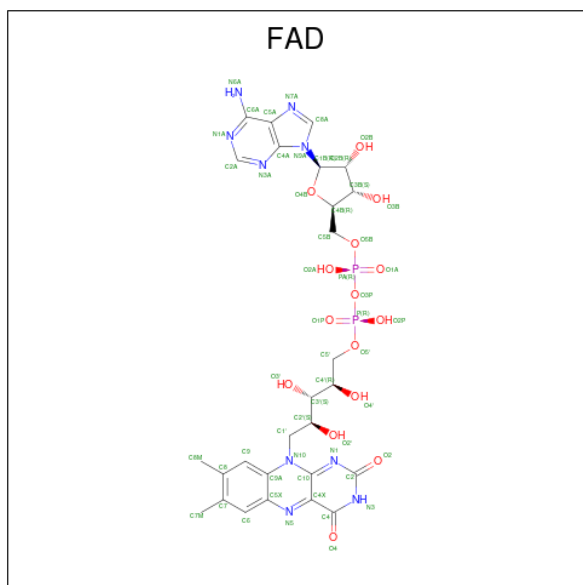

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	E	5	Total	C	N	O	0	0	0
			60	34	2	24			

- Molecule 5 is an oligosaccharide called alpha-D-mannopyranose-(1-6)-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
5	F	4	Total	C	N	O	0	0	0
			50	28	2	20			

- Molecule 6 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).

FAD

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
6	B	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

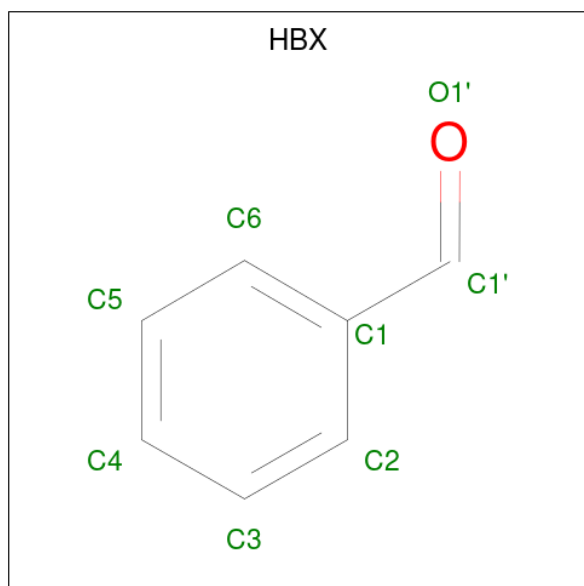- Molecule 7 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).
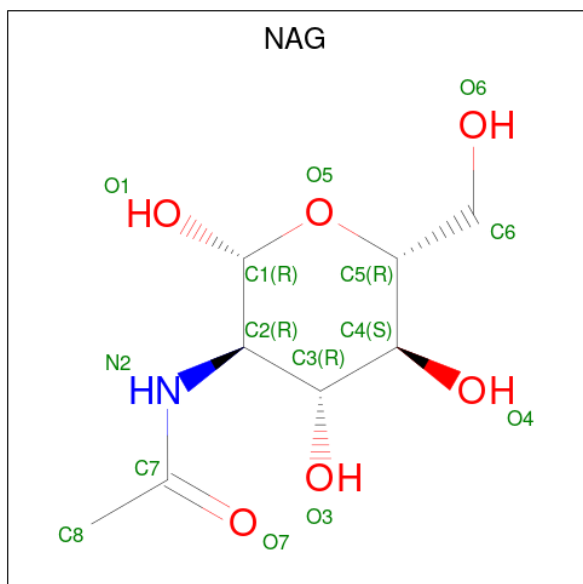
NAG

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

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

- Molecule 8 is benzaldehyde (three-letter code: HBX) (formula: C_7H_6O).

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total 8	C 7	O 1	0	0
8	B	1	Total 8	C 7	O 1	0	0

- Molecule 9 is (2R)-hydroxy(phenyl)ethanenitrile (three-letter code: MXN) (formula: C_8H_7NO).

MXN

O10

OH

C6

C5 C1 C8

C7(R)

N N9

C4 C2

C3
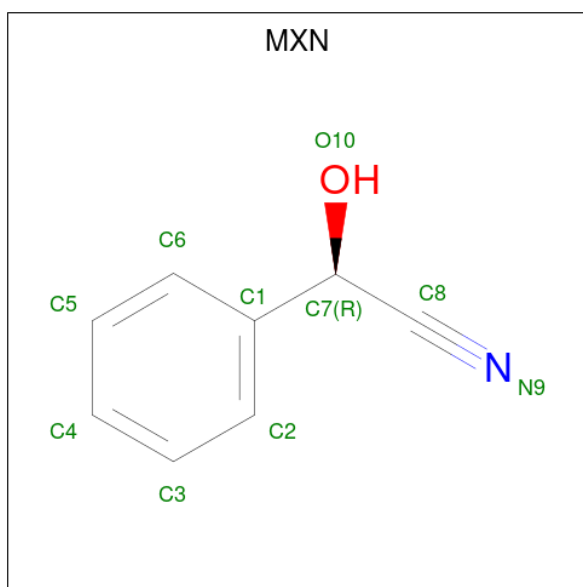
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	A	1	Total 10	C 8	N 1	O 1	0	0
9	A	1	Total 10	C 8	N 1	O 1	0	0
9	B	1	Total 10	C 8	N 1	O 1	0	0
9	B	1	Total 10	C 8	N 1	O 1	0	0

- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	643	Total 643	O 643	0	0
10	B	626	Total 626	O 626	0	0

W O R L D W I D E
PDB
PROTEIN DATA BANK

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.
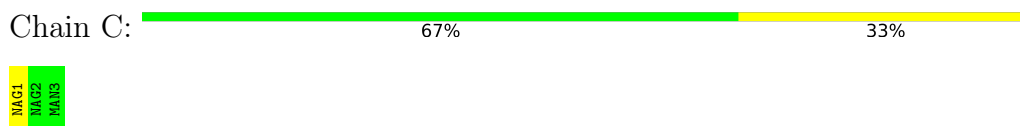
• Molecule 1: R-oxynitrile lyase isoenzyme 1
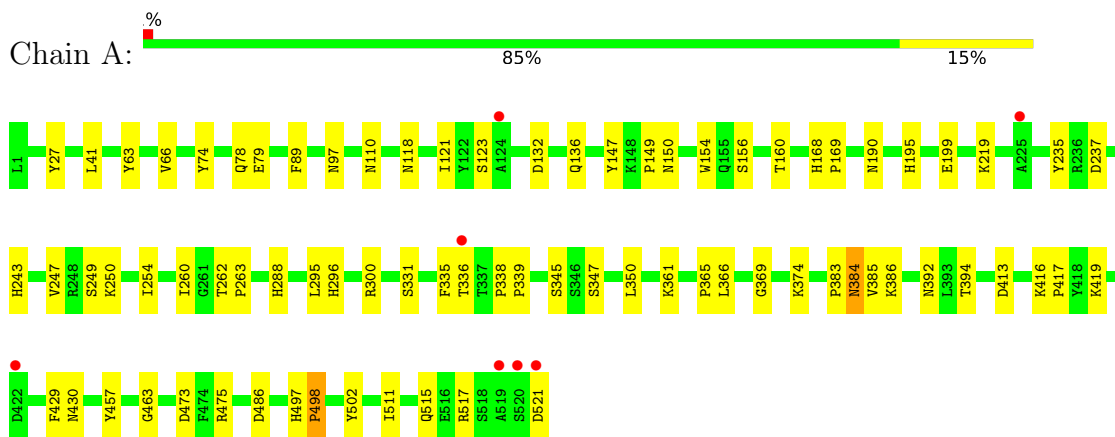
• Molecule 1: R-oxynitrile lyase isoenzyme 1
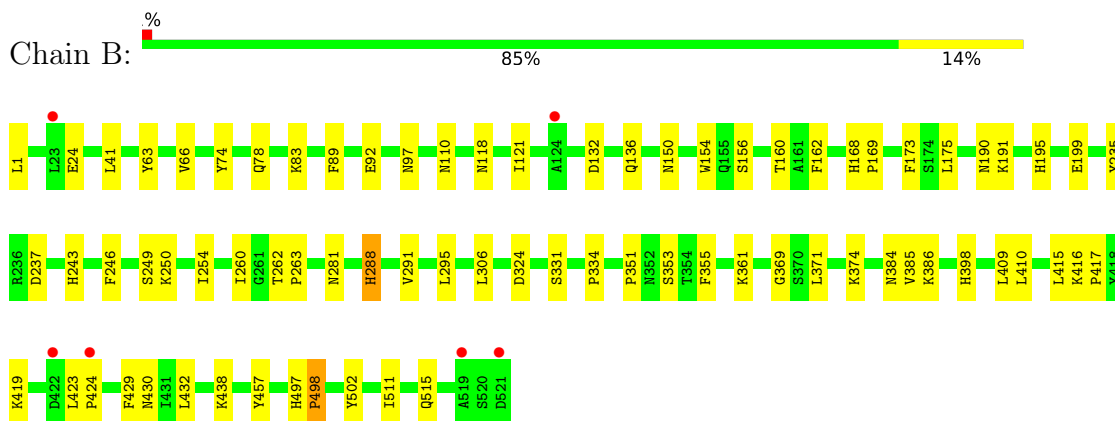
• Molecule 2: alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

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

Chain D:

67%   33%

NAG1 FUC2 NAG3

• Molecule 4: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-b eta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-3)]2-acetamido-2-deoxy-beta-D-glucopyranos e

Chain E:

20%   80%

NAG1 NAG2 BMA3 MAN4 FUC5

• Molecule 5: alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-b eta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain F:

75%   25%

NAG1 NAG2 BMA3 MAN4

4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	68.98Å 93.79Å 86.90Å 90.00° 106.47° 90.00°	Depositor
Resolution (Å)	19.97 – 1.67 19.96 – 1.67	Depositor EDS
% Data completeness (in resolution range)	86.3 (19.97-1.67) 86.3 (19.96-1.67)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.05	Depositor
$< I/\sigma(I) >$ [1]	8.30 (at 1.67Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.174 , 0.197 0.169 , 0.193	Depositor DCC
R_{free} test set	10799 reflections (10.01%)	wwPDB-VP
Wilson B-factor (Å^2)	13.5	Xtriage
Anisotropy	0.444	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 43.9	EDS
L-test for twinning[2]	$< |L| > = 0.51$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	9681	wwPDB-VP
Average B, all atoms (Å^2)	16.0	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 47.14 % 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 1.0353e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: MXN, FAD, NAG, MAN, BMA, FUC, HBX

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	0.35	2/4162 (0.0%)	0.63	0/5677
1	B	0.30	0/4170	0.63	0/5688
All	All	0.32	2/8332 (0.0%)	0.63	0/11365

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	384[A]	ASN	CB-CG	-8.21	1.32	1.51
1	A	384[B]	ASN	CB-CG	-8.21	1.32	1.51

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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	4016	0	3882	58	0
1	B	4019	0	3884	55	0
2	C	39	0	34	0	0
3	D	38	0	34	2	0
4	E	60	0	52	3	0
5	F	50	0	43	0	0
6	A	53	0	31	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	53	0	31	3	0
7	A	14	0	13	0	0
7	B	14	0	13	0	0
8	A	8	0	6	0	0
8	B	8	0	6	0	0
9	A	20	0	14	1	0
9	B	20	0	14	1	0
10	A	643	0	0	5	0
10	B	626	0	0	6	0
All	All	9681	0	8057	117	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

The worst 5 of 117 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:150:ASN:ND2	1:A:190:ASN:HD22	1.60	0.99
1:B:295:LEU:HD23	1:B:385[A]:VAL:HG13	1.53	0.91
1:B:92[A]:GLU:CD	1:B:384[A]:ASN:HD21	1.78	0.85
1:B:295:LEU:CD2	1:B:385[A]:VAL:HG13	2.10	0.81
1:A:374:LYS:HE2	1:A:384[B]:ASN:OD1	1.86	0.75

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	527/521 (101%)	512 (97%)	14 (3%)	1 (0%)	47	29
1	B	528/521 (101%)	512 (97%)	16 (3%)	0	100	100
All	All	1055/1042 (101%)	1024 (97%)	30 (3%)	1 (0%)	51	32

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	486	ASP

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	451/443 (102%)	443 (98%)	8 (2%)	59	40
1	B	452/443 (102%)	449 (99%)	3 (1%)	84	76
All	All	903/886 (102%)	892 (99%)	11 (1%)	73	57

5 of 11 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	498	PRO
1	B	288	HIS
1	B	498	PRO
1	B	430	ASN
1	A	345[A]	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 11 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	190	ASN
1	B	243	HIS
1	B	430	ASN
1	B	281	ASN
1	A	430	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 ⓘ

15 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	0.63	0	17,19,21	0.85	1 (5%)
2	NAG	C	2	2	14,14,15	0.66	0	17,19,21	0.70	0
2	MAN	C	3	2	11,11,12	0.57	0	15,15,17	0.45	0
3	NAG	D	1	1,3	14,14,15	0.52	0	17,19,21	0.75	1 (5%)
3	FUC	D	2	3	10,10,11	0.49	0	14,14,16	0.35	0
3	NAG	D	3	3	14,14,15	0.51	0	17,19,21	0.65	0
4	NAG	E	1	1,4	14,14,15	0.51	0	17,19,21	0.72	1 (5%)
4	NAG	E	2	4	14,14,15	0.51	0	17,19,21	0.61	0
4	BMA	E	3	4	11,11,12	0.48	0	15,15,17	0.27	0
4	MAN	E	4	4	11,11,12	0.47	0	15,15,17	0.54	0
4	FUC	E	5	4	10,10,11	0.48	0	14,14,16	0.34	0
5	NAG	F	1	1,5	14,14,15	0.57	0	17,19,21	1.19	2 (11%)
5	NAG	F	2	5	14,14,15	0.55	0	17,19,21	0.61	0
5	BMA	F	3	5	11,11,12	0.47	0	15,15,17	0.44	0
5	MAN	F	4	5	11,11,12	0.49	0	15,15,17	0.52	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	-	0/6/23/26	0/1/1/1
2	NAG	C	2	2	-	0/6/23/26	0/1/1/1
2	MAN	C	3	2	-	1/2/19/22	0/1/1/1
3	NAG	D	1	1,3	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	FUC	D	2	3	-	-	0/1/1/1
3	NAG	D	3	3	-	4/6/23/26	0/1/1/1
4	NAG	E	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	E	2	4	-	2/6/23/26	0/1/1/1
4	BMA	E	3	4	-	0/2/19/22	0/1/1/1
4	MAN	E	4	4	-	2/2/19/22	0/1/1/1
4	FUC	E	5	4	-	-	0/1/1/1
5	NAG	F	1	1,5	-	0/6/23/26	0/1/1/1
5	NAG	F	2	5	-	0/6/23/26	0/1/1/1
5	BMA	F	3	5	-	1/2/19/22	0/1/1/1
5	MAN	F	4	5	-	0/2/19/22	0/1/1/1

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	F	1	NAG	C4-C3-C2	-3.05	106.56	111.02
4	E	1	NAG	C2-N2-C7	-2.26	119.69	122.90
5	F	1	NAG	C2-N2-C7	-2.23	119.72	122.90
3	D	1	NAG	C2-N2-C7	-2.22	119.75	122.90
2	C	1	NAG	C2-N2-C7	-2.06	119.96	122.90

There are no chirality outliers.

5 of 14 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	E	1	NAG	C8-C7-N2-C2
4	E	1	NAG	O7-C7-N2-C2
4	E	4	MAN	O5-C5-C6-O6
3	D	3	NAG	C8-C7-N2-C2
4	E	4	MAN	C4-C5-C6-O6

There are no ring outliers.

6 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	E	4	MAN	2	0
3	D	3	NAG	1	0
3	D	2	FUC	1	0
4	E	2	NAG	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	E	5	FUC	1	0
3	D	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.

Oligosaccharide Chain C

Bond lengths

Bond angles

Torsions

Rings

Oligosaccharide Chain D

Bond lengths

Bond angles

Torsions

Rings

Oligosaccharide Chain E

Bond lengths

Bond angles

Torsions

Rings

Oligosaccharide Chain F

Bond lengths

Bond angles

Torsions

Rings
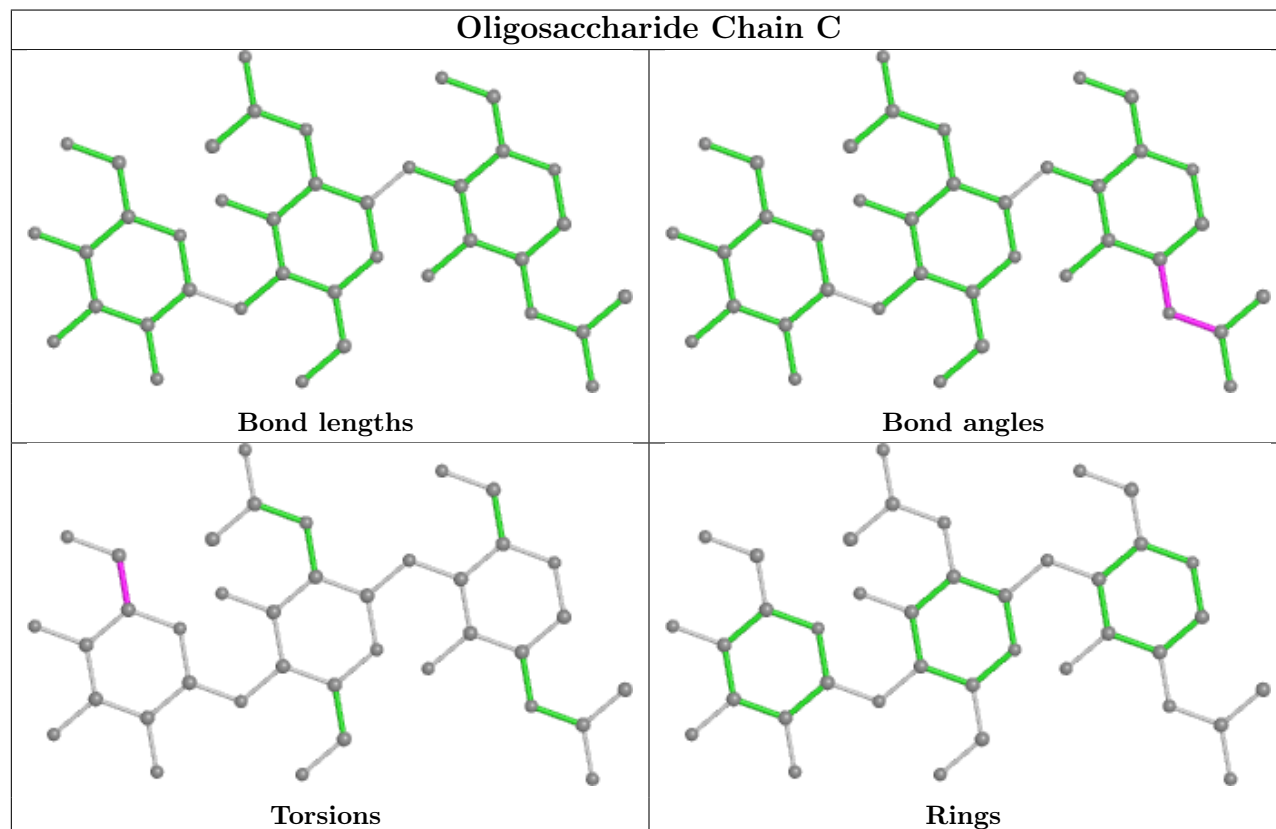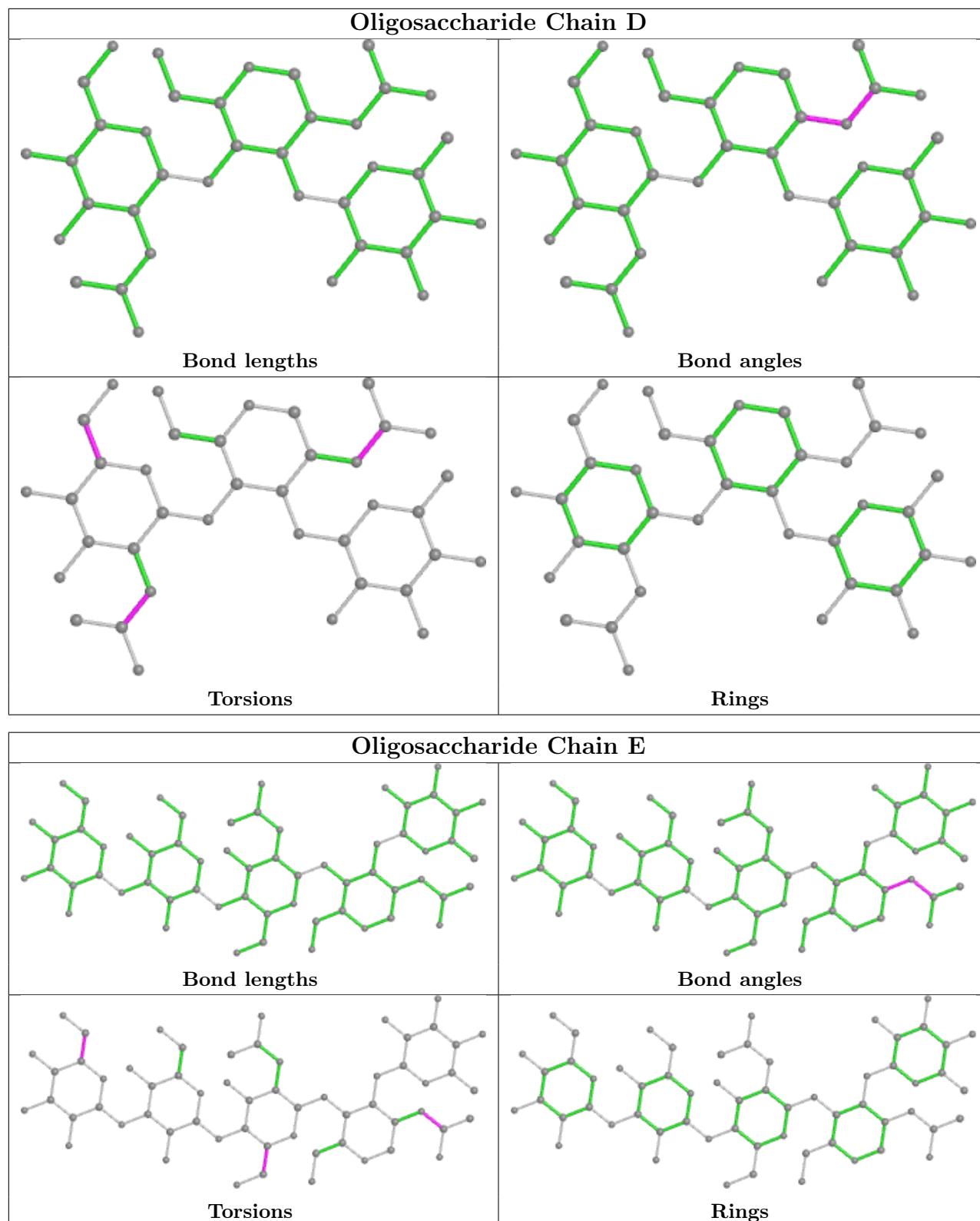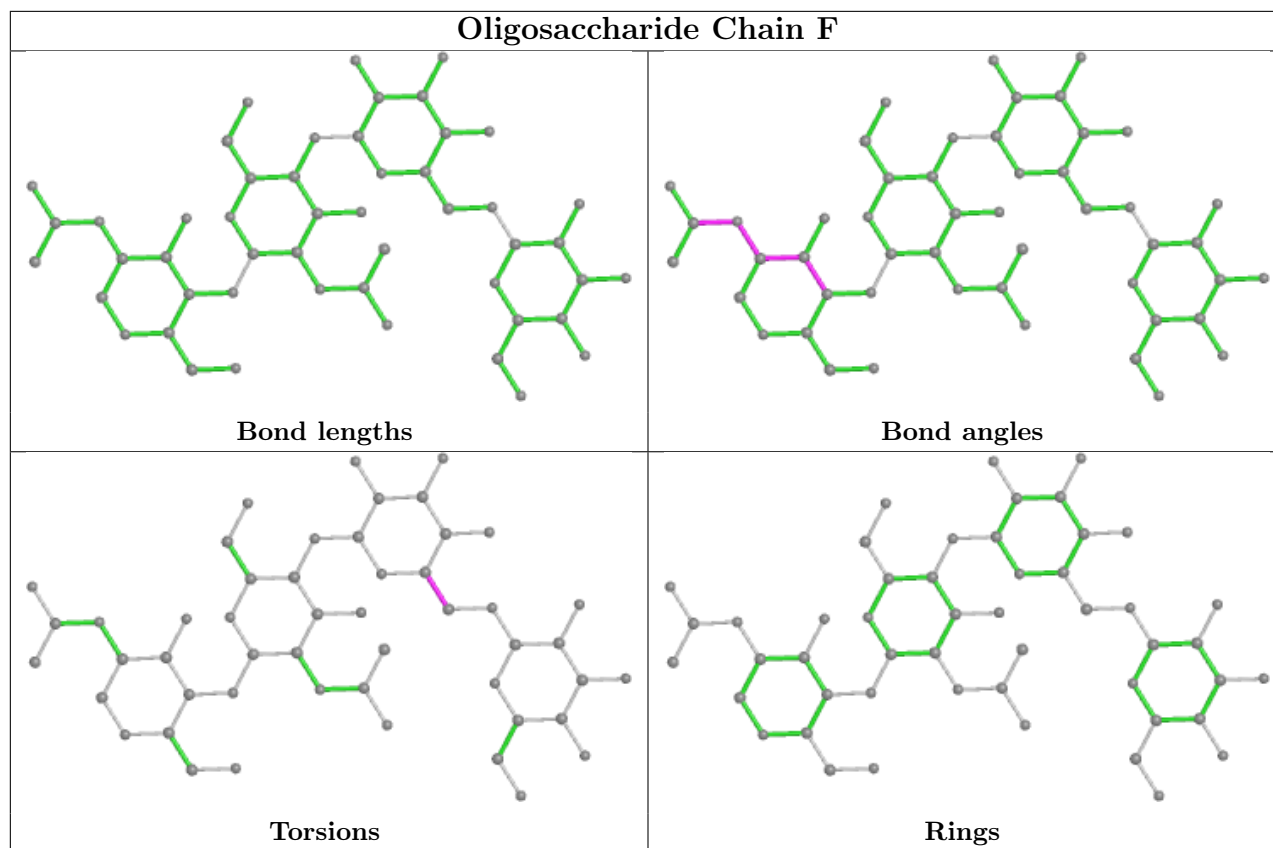
5.6 Ligand geometry ⓘ

10 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	#$|Z| > 2$
7	NAG	A	523	1	14,14,15	0.48	0	17,19,21	0.60	0
7	NAG	B	532	1	14,14,15	0.51	0	17,19,21	0.57	0
9	MXN	B	535	-	10,10,10	1.83	3 (30%)	11,12,12	0.62	0
8	HBX	A	530	-	8,8,8	1.72	1 (12%)	9,9,9	0.72	0
9	MXN	B	534	-	10,10,10	2.68	4 (40%)	11,12,12	0.61	0
9	MXN	A	531	-	10,10,10	2.16	4 (40%)	11,12,12	0.58	0
8	HBX	B	533	-	8,8,8	1.70	0	9,9,9	0.71	0
6	FAD	A	522	-	53,58,58	1.90	19 (35%)	68,89,89	1.14	7 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
9	MXN	A	532	-	10,10,10	1.79	2 (20%)	11,12,12	0.65	0
6	FAD	B	522	-	53,58,58	1.91	19 (35%)	68,89,89	1.14	5 (7%)

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
7	NAG	A	523	1	-	0/6/23/26	0/1/1/1
7	NAG	B	532	1	-	0/6/23/26	0/1/1/1
9	MXN	B	535	-	-	0/4/6/6	0/1/1/1
8	HBX	A	530	-	-	0/2/2/2	0/1/1/1
9	MXN	B	534	-	-	0/4/6/6	0/1/1/1
9	MXN	A	531	-	-	0/4/6/6	0/1/1/1
8	HBX	B	533	-	-	0/2/2/2	0/1/1/1
6	FAD	A	522	-	-	2/30/50/50	0/6/6/6
9	MXN	A	532	-	-	0/4/6/6	0/1/1/1
6	FAD	B	522	-	-	2/30/50/50	0/6/6/6

The worst 5 of 52 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	B	534	MXN	C7-C8	6.17	1.64	1.48
6	A	522	FAD	O4B-C1B	4.53	1.47	1.41
6	B	522	FAD	O4B-C1B	4.23	1.47	1.41
6	B	522	FAD	PA-O2A	-3.86	1.37	1.55
6	A	522	FAD	PA-O2A	-3.79	1.37	1.55

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	B	522	FAD	O5B-PA-O1A	-2.65	98.70	109.07
6	A	522	FAD	O5B-PA-O1A	-2.55	99.10	109.07
6	A	522	FAD	C5'-C4'-C3'	-2.36	107.64	112.20
6	B	522	FAD	C5'-C4'-C3'	-2.36	107.64	112.20
6	A	522	FAD	C2A-N1A-C6A	2.33	122.75	118.75

There are no chirality outliers.
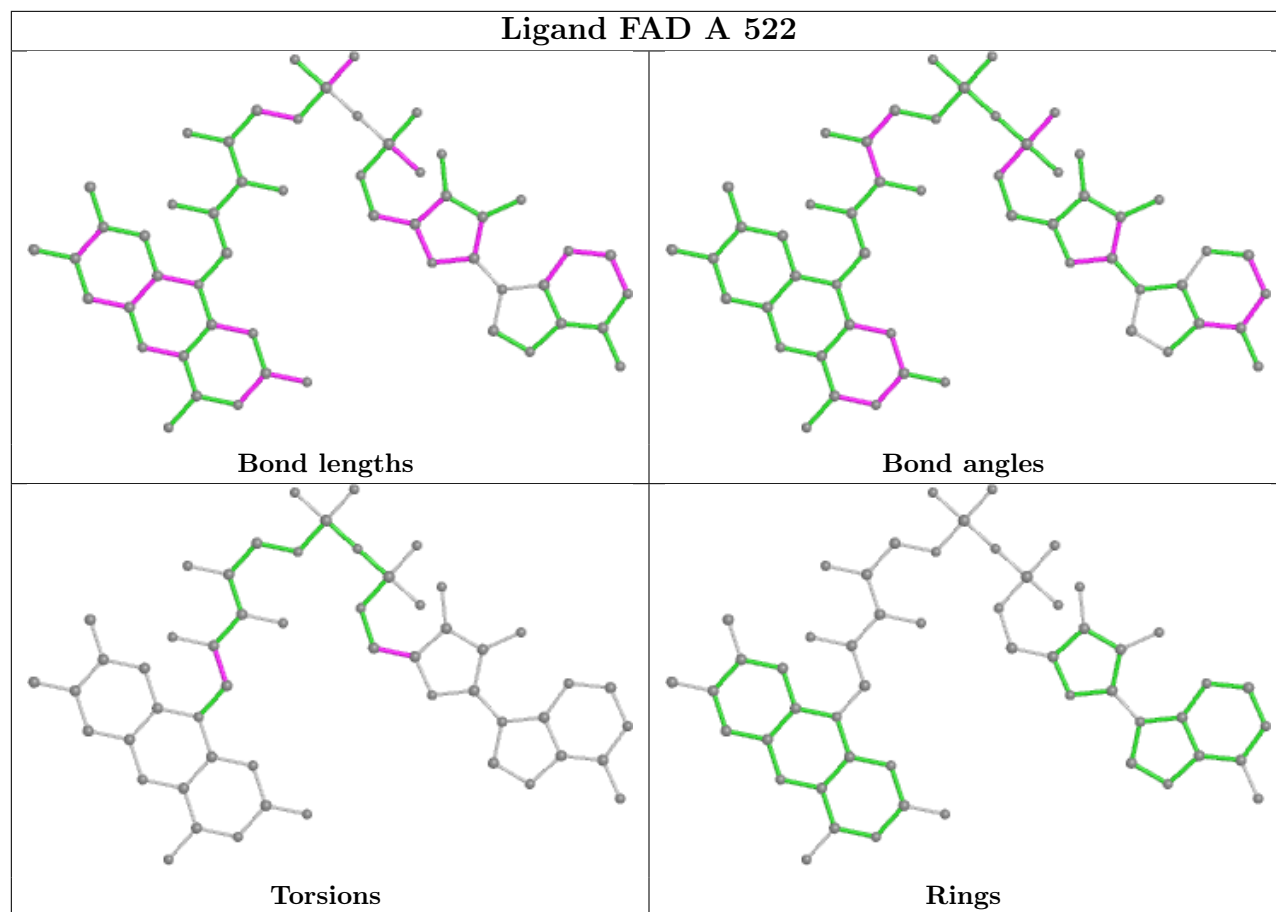
All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	522	FAD	N10-C1'-C2'-O2'
6	A	522	FAD	O4B-C4B-C5B-O5B
6	B	522	FAD	O4B-C4B-C5B-O5B
6	B	522	FAD	N10-C1'-C2'-O2'

There are no ring outliers.

4 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	B	535	MXN	1	0
6	A	522	FAD	3	0
9	A	532	MXN	1	0
6	B	522	FAD	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 then 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 FAD A 522

Bond lengths

Bond angles

Torsions

Rings

Ligand FAD B 522

Bond lengths

Bond angles

Torsions

Rings
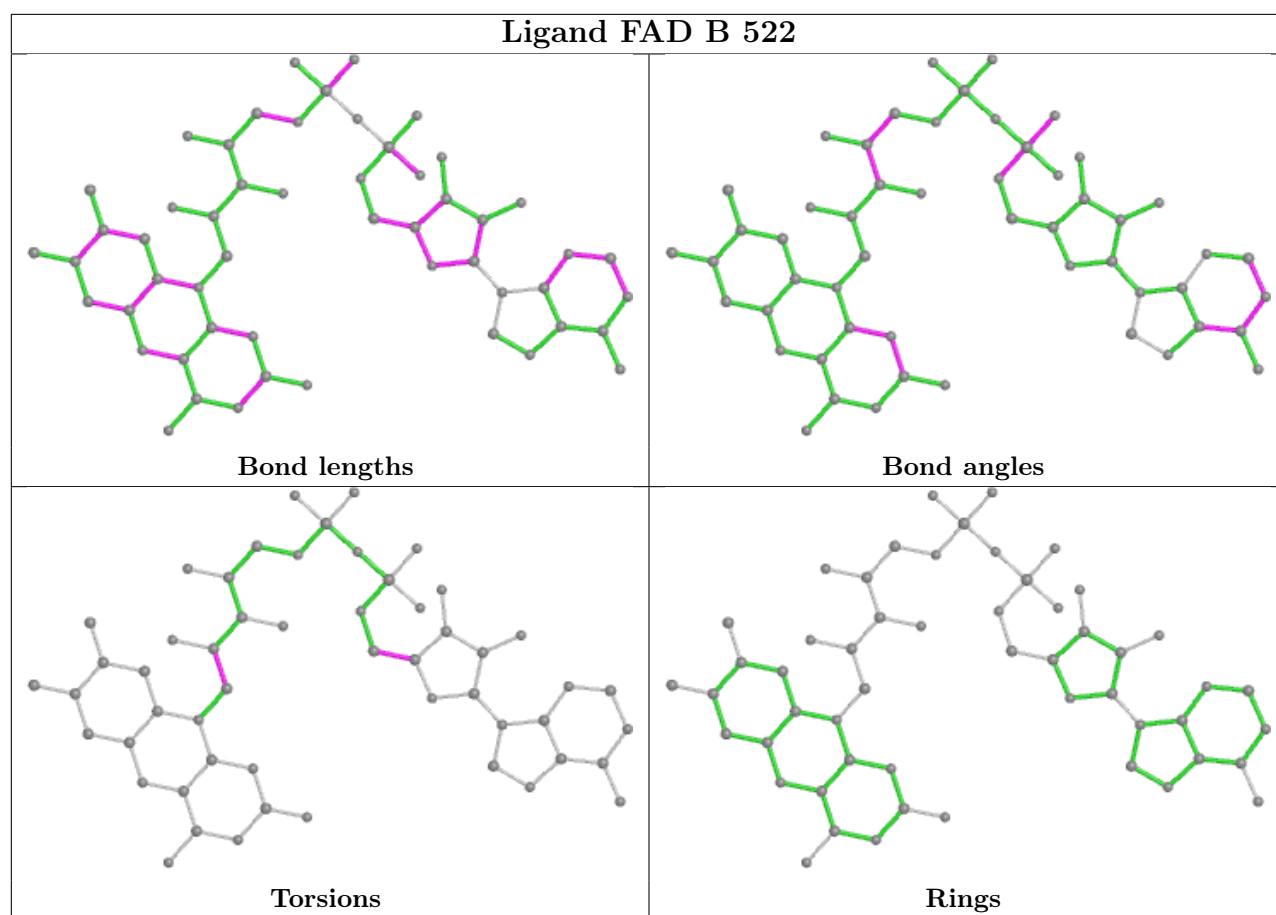
5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	521/521 (100%)	-0.40	7 (1%)	77	80	7, 12, 24, 48	0
1	B	521/521 (100%)	-0.36	6 (1%)	79	82	7, 13, 26, 42	0
All	All	1042/1042 (100%)	-0.38	13 (1%)	79	82	7, 13, 26, 48	0

The worst 5 of 13 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	225	ALA	4.2
1	A	336	THR	3.9
1	A	521	ASP	3.8
1	A	422	ASP	3.0
1	A	520	SER	3.0

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

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

6.3 Carbohydrates ⓘ

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.
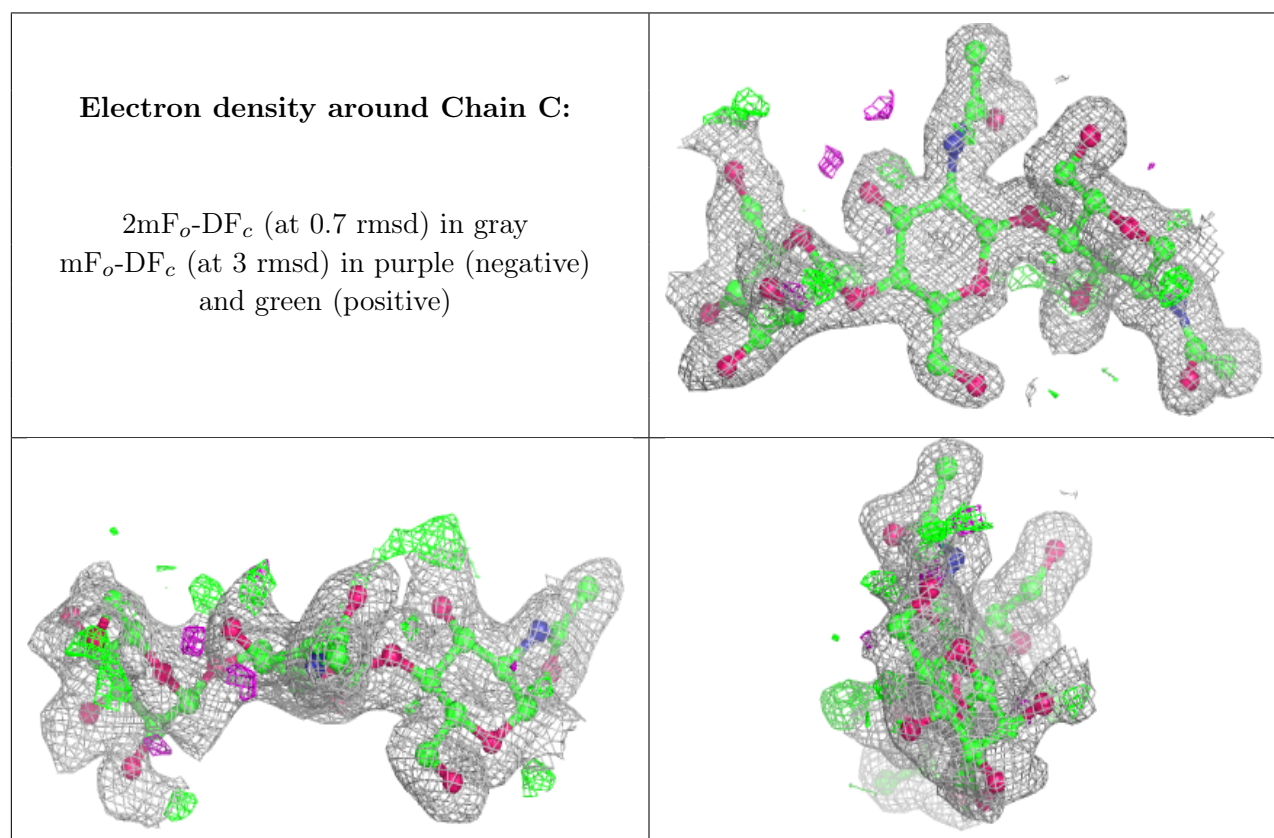
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	MAN	F	4	11/12	0.36	0.42	54,55,56,56	0
2	MAN	C	3	11/12	0.58	0.28	46,49,50,51	0
5	BMA	F	3	11/12	0.62	0.29	45,47,50,53	0
4	MAN	E	4	11/12	0.63	0.25	48,50,50,50	0
4	BMA	E	3	11/12	0.66	0.29	42,44,46,47	0

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W O R L D W I D E
wwPDB
PROTEIN DATA BANK

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	FUC	D	2	10/11	0.74	0.34	44,46,47,47	0
2	NAG	C	2	14/15	0.75	0.19	27,30,38,42	0
5	NAG	F	2	14/15	0.76	0.20	30,32,40,41	0
3	NAG	D	3	14/15	0.78	0.34	45,48,49,49	0
5	NAG	F	1	14/15	0.82	0.12	16,21,25,25	0
3	NAG	D	1	14/15	0.82	0.16	27,33,40,41	0
4	FUC	E	5	10/11	0.87	0.29	33,35,36,37	0
4	NAG	E	2	14/15	0.88	0.22	31,32,38,38	0
4	NAG	E	1	14/15	0.88	0.14	21,26,29,30	0
2	NAG	C	1	14/15	0.90	0.10	13,19,22,23	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.
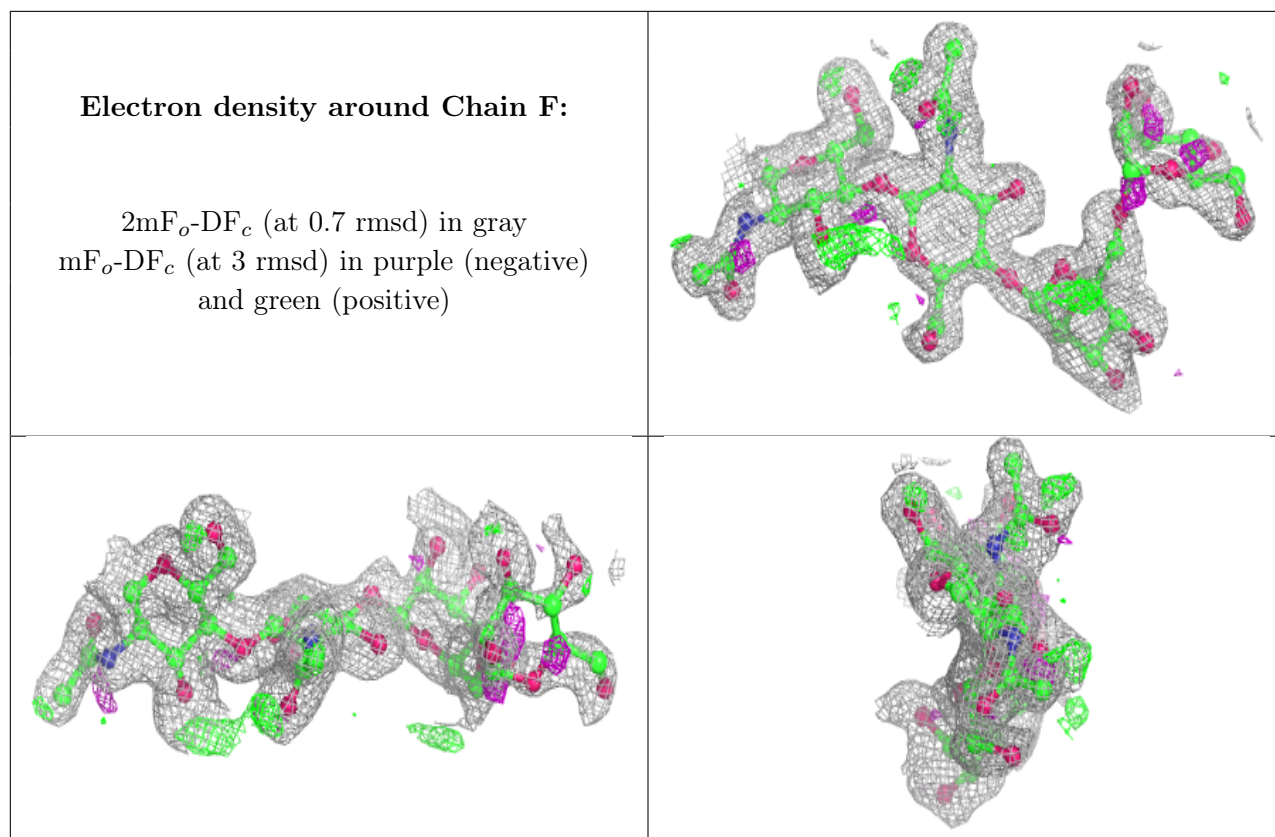

Electron density around Chain C:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (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)
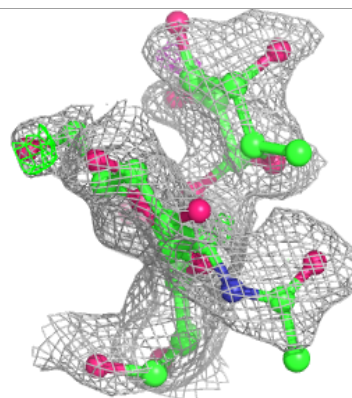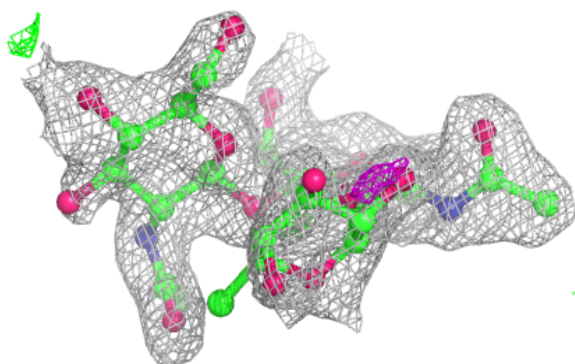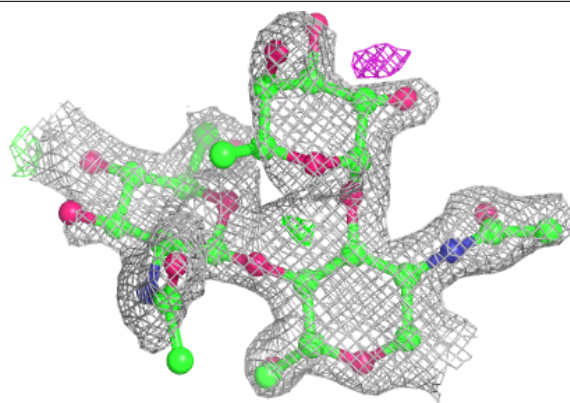
Electron density around Chain E:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
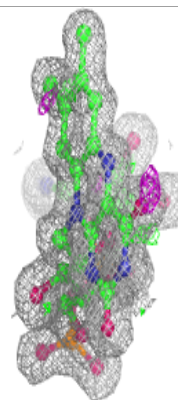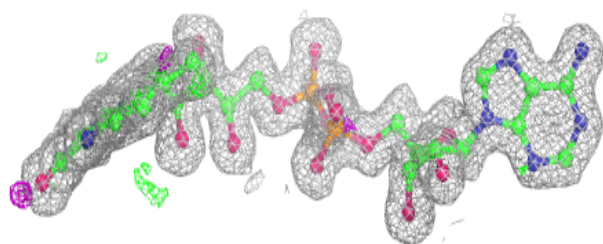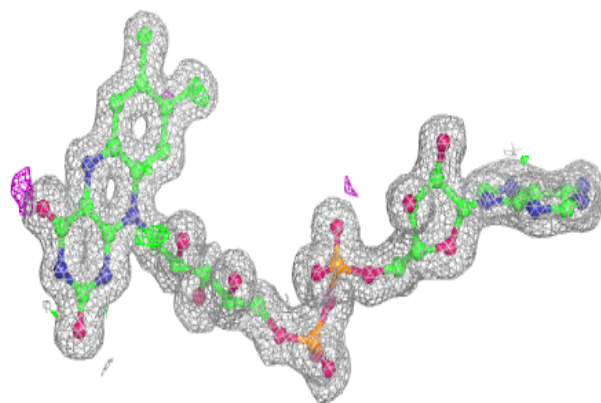mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
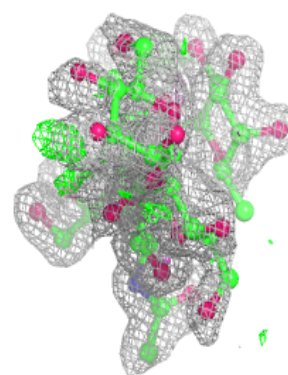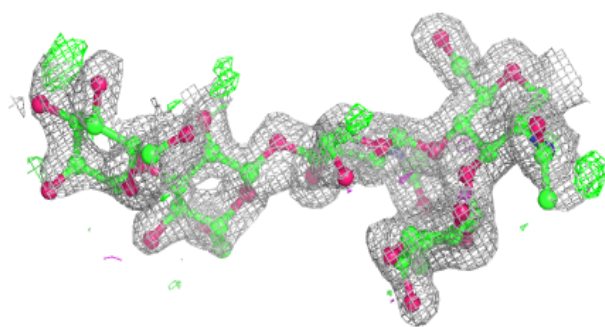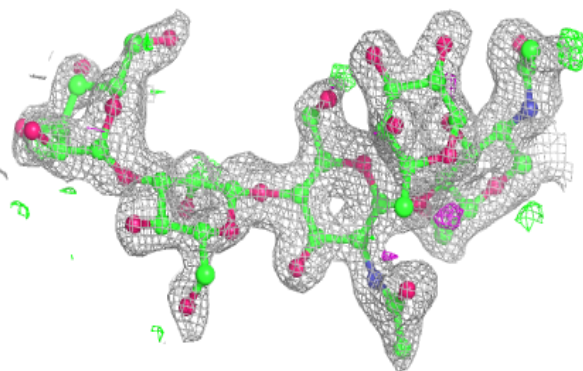
Electron density around Chain F:

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

6.4 Ligands ⓘ

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
9	MXN	A	532	10/10	0.75	0.21	36,38,38,40	0
9	MXN	B	535	10/10	0.85	0.24	40,41,42,43	0
9	MXN	B	534	10/10	0.91	0.09	14,17,18,23	0
9	MXN	A	531	10/10	0.91	0.10	14,15,17,23	0
7	NAG	A	523	14/15	0.93	0.08	14,17,20,21	0
7	NAG	B	532	14/15	0.94	0.07	14,16,21,21	0
8	HBX	A	530	8/8	0.95	0.08	21,21,22,22	0
8	HBX	B	533	8/8	0.95	0.08	20,23,23,23	0
6	FAD	A	522	53/53	0.98	0.06	5,8,9,10	0
6	FAD	B	522	53/53	0.98	0.06	6,8,10,11	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 FAD A 522:

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

Electron density around FAD B 522:

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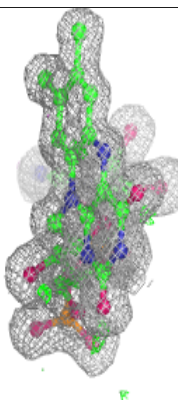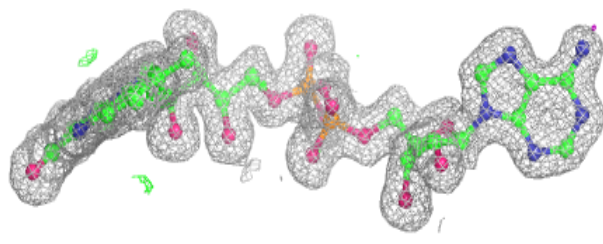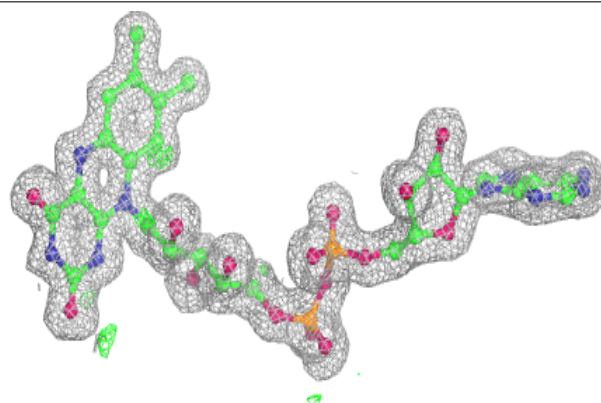
6.5 Other polymers (i)

There are no such residues in this entry.