



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 18, 2026 – 12:35 AM UTC

PDB ID : 5EB4 / pdb_00005eb4
Title : The crystal structure of almond HNL, PaHNL5 V317A, expressed in *Aspergillus niger*
Authors : Pavkov-Keller, T.; Steinkellner, G.; Gruber, K.
Deposited on : 2015-10-17
Resolution : 2.30 Å (reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

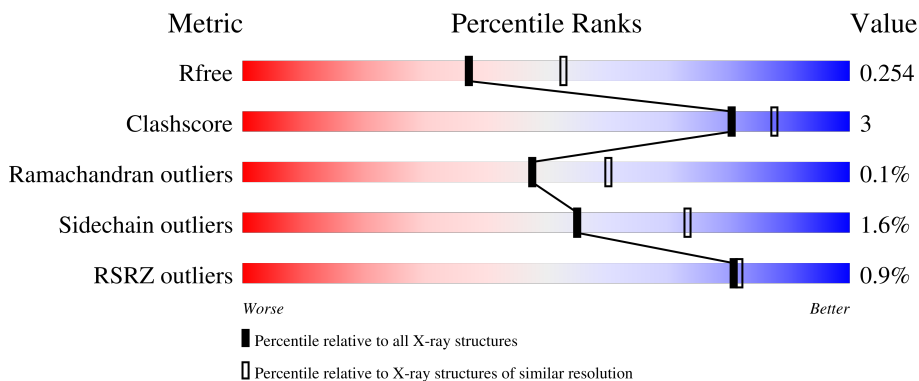
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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	532	
1	B	532	
2	C	2	
2	D	2	
2	E	2	

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	NAG	A	605	X	-	-	-
3	NAG	B	607	X	-	-	-

2 Entry composition i

There are 5 unique types of molecules in this entry. The entry contains 8673 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.

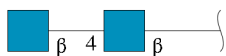
- Molecule 1 is a protein called Hnl isoenzyme 5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	515	Total	C	N	O	S	0	3	0
			3974	2520	659	789	6			
1	B	509	Total	C	N	O	S	0	0	0
			3905	2484	647	768	6			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	317	ALA	VAL	engineered mutation	UNP Q7XJE8
A	360	VAL	UNK	conflict	UNP Q7XJE8
A	496	ASN	UNK	conflict	UNP Q7XJE8
B	317	ALA	VAL	engineered mutation	UNP Q7XJE8
B	360	VAL	UNK	conflict	UNP Q7XJE8
B	496	ASN	UNK	conflict	UNP Q7XJE8

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



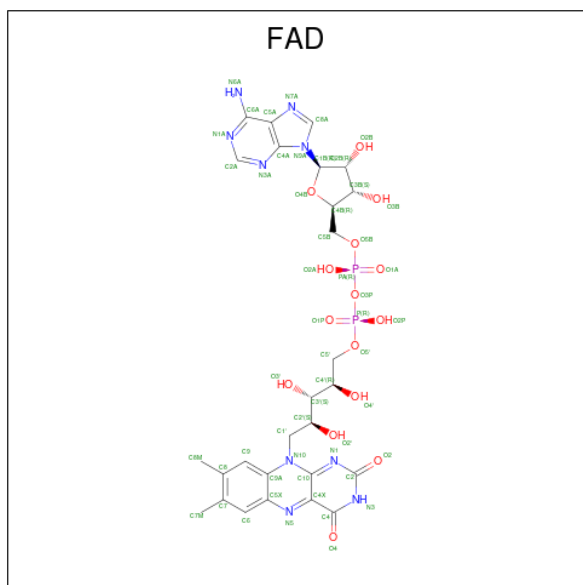
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	C	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	D	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	E	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



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

- Molecule 4 is FLAVIN-ADENINE DINUCLEOTIDE (CCD ID: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).



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

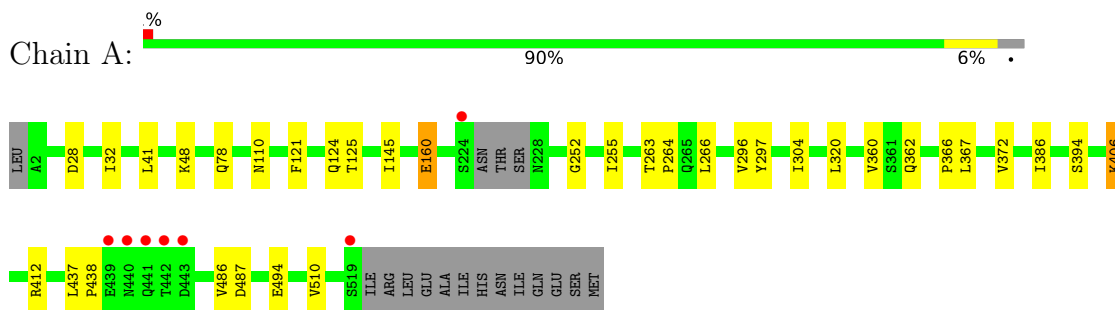
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	A	239	239	239	0	0
5	B	225	225	225	0	0

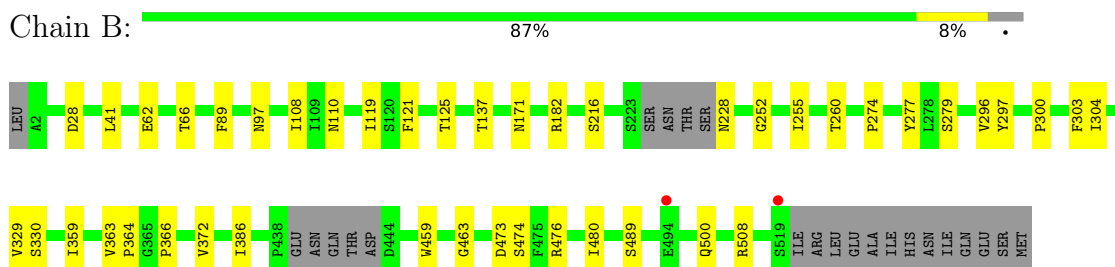
3 Residue-property plots [i](#)

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: Hnl isoenzyme 5



- Molecule 1: Hnl isoenzyme 5



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

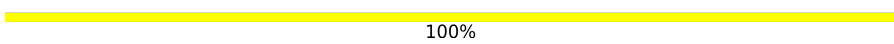


- Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



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

Chain E:



100%

MAG1
MAG2

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	68.88Å 92.30Å 97.59Å 90.00° 93.73° 90.00°	Depositor
Resolution (Å)	49.09 – 2.30 49.09 – 2.30	Depositor EDS
% Data completeness (in resolution range)	91.7 (49.09-2.30) 91.7 (49.09-2.30)	Depositor EDS
R_{merge}	0.19	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.60 (at 2.29Å)	Xtrriage
Refinement program	REFMAC 5.8.0131	Depositor
R, R_{free}	0.186 , 0.247 0.191 , 0.254	Depositor DCC
R_{free} test set	2491 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	22.8	Xtrriage
Anisotropy	0.097	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 35.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	8673	wwPDB-VP
Average B, all atoms (Å ²)	25.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 44.08 % 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 1.6075e-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: NAG, FAD

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	0.86	0/4067	1.05	2/5551 (0.0%)
1	B	0.88	0/3997	1.05	1/5454 (0.0%)
All	All	0.87	0/8064	1.05	3/11005 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	145	ILE	N-CA-C	6.65	119.59	113.20
1	B	480	ILE	N-CA-C	5.29	115.60	107.77
1	A	412	ARG	CG-CD-NE	-5.01	100.99	112.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3974	0	3828	17	0
1	B	3905	0	3778	22	0
2	C	28	0	25	1	0
2	D	28	0	25	0	0
2	E	28	0	25	0	0
3	A	70	0	65	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	70	0	65	0	0
4	A	53	0	31	1	0
4	B	53	0	31	4	0
5	A	239	0	0	3	0
5	B	225	0	0	2	0
All	All	8673	0	7873	41	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 3.

All (41) 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:279:SER:HB3	5:B:872:HOH:O	1.55	1.02
1:A:362:GLN:NE2	1:A:494:GLU:OE2	2.28	0.67
1:A:296:VAL:HG21	1:A:372:VAL:HG23	1.76	0.67
1:B:41:LEU:HD21	1:B:255:ILE:HG21	1.85	0.58
1:B:110:ASN:HB2	4:B:610:FAD:C5X	2.36	0.55
1:B:364:PRO:O	1:B:366:PRO:HA	2.07	0.54
1:B:297:TYR:HB3	1:B:366:PRO:HD2	1.89	0.54
1:A:160:GLU:HB3	5:A:938:HOH:O	2.08	0.53
1:A:297:TYR:HB3	1:A:366:PRO:HD2	1.91	0.53
1:B:137:THR:HG23	1:B:508:ARG:HD3	1.91	0.52
1:B:372:VAL:HG22	1:B:386:ILE:HD12	1.91	0.51
1:A:41:LEU:HD21	1:A:255:ILE:HG21	1.93	0.51
1:A:486:VAL:HG21	1:A:510:VAL:HG11	1.92	0.51
1:B:274:PRO:HB2	1:B:277:TYR:HB3	1.92	0.51
1:A:78:GLN:NE2	5:A:701:HOH:O	2.28	0.51
1:A:372:VAL:HG22	1:A:386:ILE:HD12	1.93	0.51
1:B:296:VAL:HG21	1:B:372:VAL:HG23	1.94	0.49
1:A:110:ASN:HB2	4:A:608:FAD:C5X	2.42	0.49
1:A:367:LEU:HD13	3:A:605:NAG:H62	1.95	0.49
1:B:459:TRP:HB3	4:B:610:FAD:HM82	1.95	0.48
1:B:66:THR:HB	1:B:108:ILE:HG23	1.97	0.47
1:B:300:PRO:HD2	1:B:363:VAL:HB	1.99	0.45
1:B:121:PHE:O	1:B:125:THR:HG23	2.17	0.45
1:B:476:ARG:NH1	5:B:704:HOH:O	2.48	0.45
4:B:610:FAD:H9	4:B:610:FAD:H1'1	1.68	0.44
1:B:89:PHE:CZ	1:B:97:ASN:HB3	2.52	0.44
1:B:329:VAL:HG22	1:B:330:SER:N	2.32	0.44
1:A:406:LYS:HE3	1:A:406:LYS:HA	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:394:SER:H	3:A:605:NAG:H82	1.84	0.43
1:A:437:LEU:O	1:A:438:PRO:C	2.61	0.42
1:A:121:PHE:O	1:A:125:THR:HG23	2.19	0.42
1:B:260:THR:HG23	1:B:463:GLY:O	2.20	0.42
1:A:28:ASP:O	1:A:252:GLY:HA3	2.20	0.42
1:B:260:THR:HA	1:B:489:SER:HB3	2.02	0.42
1:B:500:GLN:HG2	4:B:610:FAD:O2	2.20	0.41
1:A:263:THR:HB	1:A:264:PRO:HD3	2.02	0.41
1:A:32:ILE:HD13	1:A:266:LEU:HD21	2.03	0.41
1:B:303:PHE:HA	1:B:359:ILE:O	2.21	0.40
1:B:28:ASP:O	1:B:252:GLY:HA3	2.22	0.40
5:A:723:HOH:O	2:C:1:NAG:H61	2.20	0.40
1:B:171:ASN:HB2	1:B:182:ARG:HB3	2.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	514/532 (97%)	493 (96%)	20 (4%)	1 (0%)	43	55
1	B	503/532 (94%)	483 (96%)	20 (4%)	0	100	100
All	All	1017/1064 (96%)	976 (96%)	40 (4%)	1 (0%)	48	60

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	487	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	440/453 (97%)	433 (98%)	7 (2%)	55	73
1	B	431/453 (95%)	424 (98%)	7 (2%)	55	73
All	All	871/906 (96%)	857 (98%)	14 (2%)	55	73

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	48	LYS
1	A	124	GLN
1	A	160	GLU
1	A	304	ILE
1	A	320	LEU
1	A	360	VAL
1	A	406	LYS
1	B	62	GLU
1	B	119	ILE
1	B	216	SER
1	B	228	ASN
1	B	304	ILE
1	B	473	ASP
1	B	474	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	75	ASN
1	A	214	GLN
1	A	228	ASN
1	A	242	ASN
1	A	310	ASN
1	A	328	GLN
1	B	75	ASN
1	B	124	GLN

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Mol	Chain	Res	Type
1	B	228	ASN
1	B	287	GLN
1	B	513	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

6 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	1,2	14,14,15	0.49	0	17,19,21	1.37	4 (23%)
2	NAG	C	2	2	14,14,15	0.68	0	17,19,21	2.90	6 (35%)
2	NAG	D	1	1,2	14,14,15	0.81	1 (7%)	17,19,21	1.35	2 (11%)
2	NAG	D	2	2	14,14,15	0.76	0	17,19,21	1.22	2 (11%)
2	NAG	E	1	1,2	14,14,15	0.45	0	17,19,21	1.68	3 (17%)
2	NAG	E	2	2	14,14,15	0.65	0	17,19,21	1.32	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	C	1	1,2	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	C	2	2	-	2/6/23/26	0/1/1/1
2	NAG	D	1	1,2	-	1/6/23/26	0/1/1/1
2	NAG	D	2	2	-	0/6/23/26	0/1/1/1
2	NAG	E	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	E	2	2	-	0/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	1	NAG	C1-C2	2.28	1.55	1.52

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	2	NAG	C1-O5-C5	9.24	124.57	112.19
2	E	1	NAG	C1-O5-C5	4.79	118.60	112.19
2	C	2	NAG	O5-C1-C2	3.76	117.11	111.29
2	D	1	NAG	C1-O5-C5	3.49	116.87	112.19
2	C	2	NAG	C1-C2-N2	-3.33	105.18	110.43
2	E	2	NAG	C1-O5-C5	3.06	116.28	112.19
2	D	2	NAG	C1-O5-C5	3.01	116.22	112.19
2	E	2	NAG	C2-N2-C7	2.95	126.85	122.90
2	C	2	NAG	C2-N2-C7	2.87	126.75	122.90
2	E	1	NAG	C4-C3-C2	2.78	115.09	111.02
2	C	2	NAG	O3-C3-C4	-2.76	103.87	110.38
2	C	1	NAG	C1-O5-C5	2.71	115.81	112.19
2	C	1	NAG	O7-C7-C8	-2.67	117.30	122.05
2	D	1	NAG	C1-C2-N2	2.50	114.37	110.43
2	C	2	NAG	O5-C5-C4	2.38	116.61	110.83
2	C	1	NAG	C4-C3-C2	2.20	114.24	111.02
2	D	2	NAG	C1-C2-N2	2.12	113.77	110.43
2	E	1	NAG	O7-C7-C8	-2.11	118.30	122.05
2	C	1	NAG	C8-C7-N2	2.09	119.58	116.12

There are no chirality outliers.

All (3) torsion outliers are listed below:

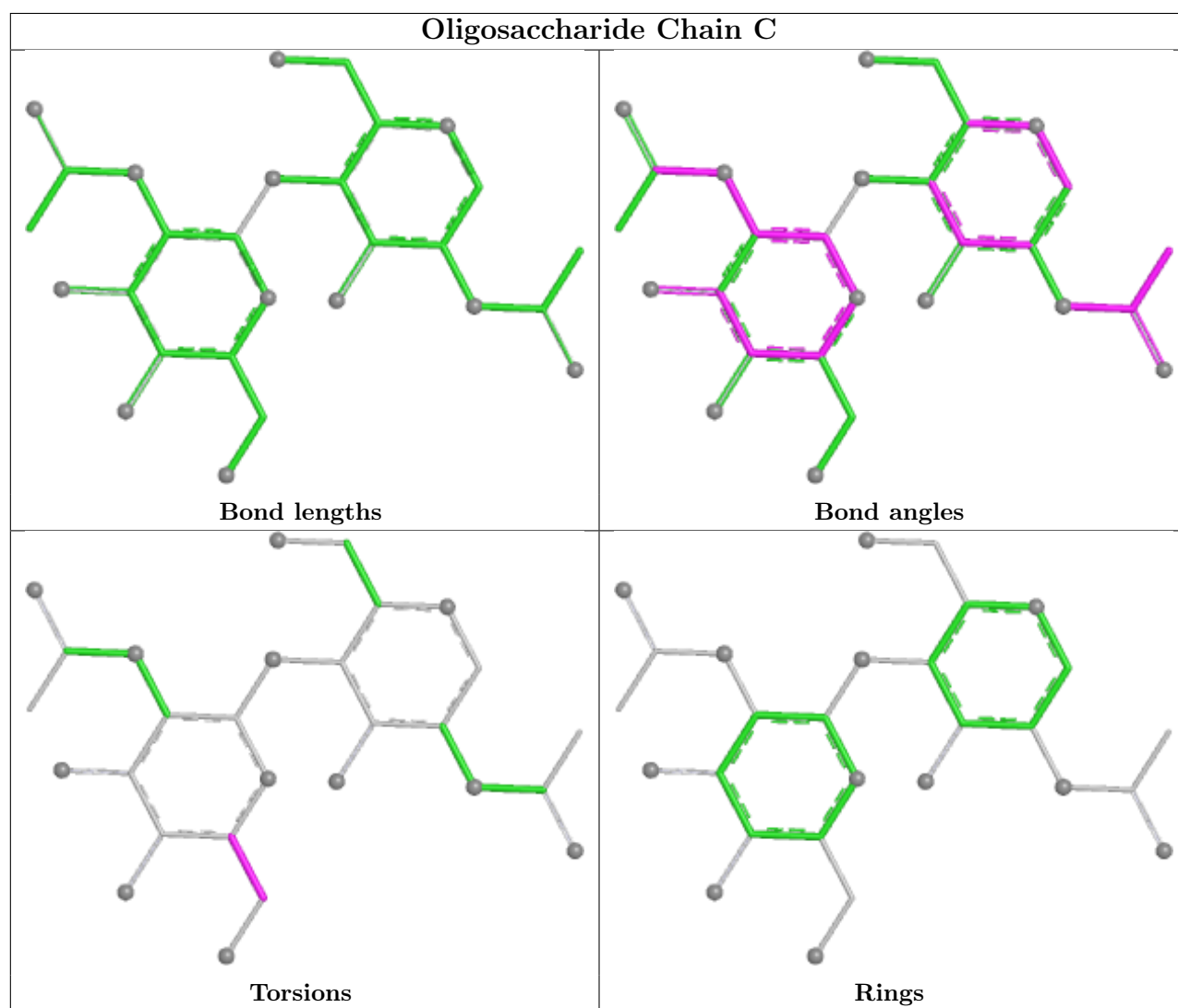
Mol	Chain	Res	Type	Atoms
2	C	2	NAG	C4-C5-C6-O6
2	C	2	NAG	O5-C5-C6-O6
2	D	1	NAG	C4-C5-C6-O6

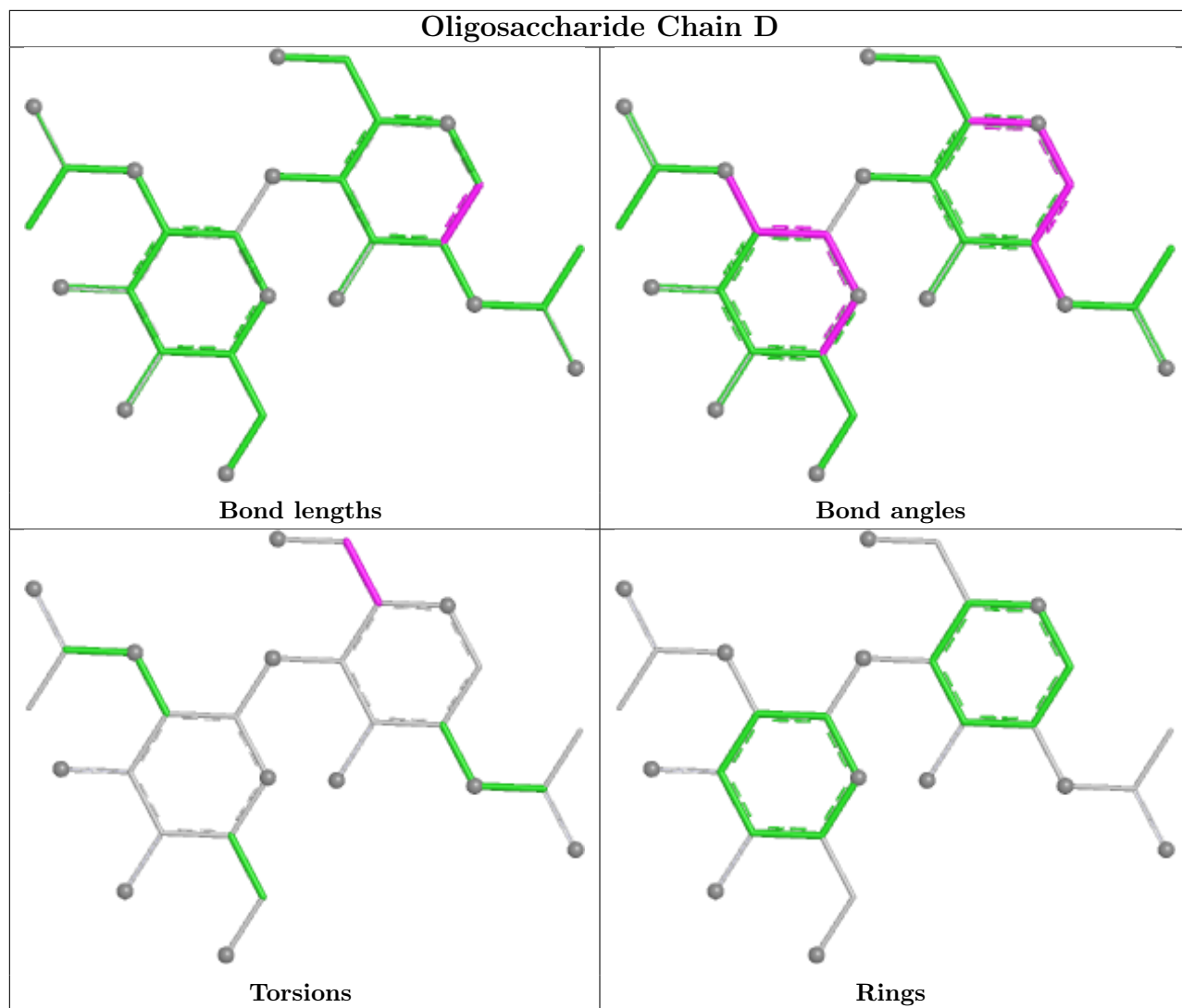
There are no ring outliers.

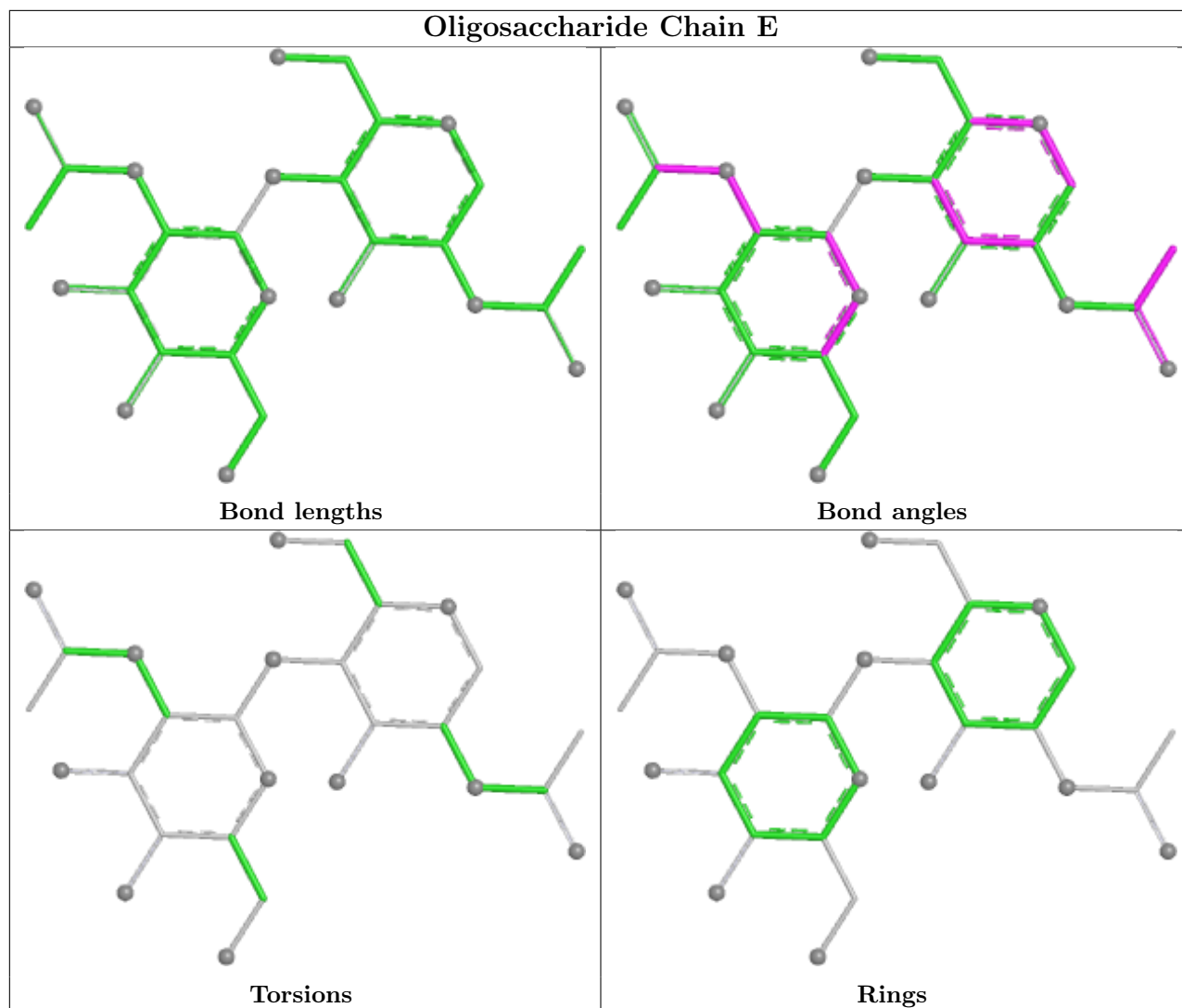
1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	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](#)

12 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	$\# Z > 2$
3	NAG	A	601	1	14,14,15	0.60	0	17,19,21	2.26	4 (23%)
3	NAG	A	606	1	14,14,15	0.64	0	17,19,21	1.53	2 (11%)
3	NAG	A	607	1	14,14,15	0.72	0	17,19,21	1.78	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAG	B	608	1	14,14,15	0.82	0	17,19,21	1.87	5 (29%)
4	FAD	A	608	-	58,58,58	1.36	5 (8%)	85,89,89	1.79	24 (28%)
3	NAG	A	604	1	14,14,15	0.86	1 (7%)	17,19,21	1.65	1 (5%)
4	FAD	B	610	-	58,58,58	1.37	6 (10%)	85,89,89	1.82	22 (25%)
3	NAG	B	606	1	14,14,15	0.73	0	17,19,21	1.59	2 (11%)
3	NAG	A	605	1	14,14,15	0.61	0	17,19,21	0.93	0
3	NAG	B	607	1	14,14,15	0.79	0	17,19,21	1.50	2 (11%)
3	NAG	B	603	1	14,14,15	0.74	0	17,19,21	1.52	2 (11%)
3	NAG	B	609	1	14,14,15	0.52	0	17,19,21	1.41	3 (17%)

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	NAG	A	601	1	-	0/6/23/26	0/1/1/1
3	NAG	A	606	1	-	0/6/23/26	0/1/1/1
3	NAG	A	607	1	-	0/6/23/26	0/1/1/1
3	NAG	B	608	1	-	2/6/23/26	0/1/1/1
4	FAD	A	608	-	-	3/34/50/50	0/6/6/6
3	NAG	A	604	1	-	1/6/23/26	0/1/1/1
4	FAD	B	610	-	-	1/34/50/50	0/6/6/6
3	NAG	B	606	1	-	2/6/23/26	0/1/1/1
3	NAG	A	605	1	1/1/5/7	2/6/23/26	0/1/1/1
3	NAG	B	607	1	1/1/5/7	2/6/23/26	0/1/1/1
3	NAG	B	603	1	-	2/6/23/26	0/1/1/1
3	NAG	B	609	1	-	1/6/23/26	0/1/1/1

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	608	FAD	C4X-N5	6.08	1.43	1.30
4	B	610	FAD	C4X-N5	5.75	1.43	1.30
4	B	610	FAD	C10-N1	3.48	1.40	1.33
4	A	608	FAD	C10-N1	2.80	1.38	1.33
4	B	610	FAD	C5A-N7A	-2.72	1.34	1.39
4	A	608	FAD	C7M-C7	2.64	1.56	1.51
4	B	610	FAD	PA-O3P	2.53	1.62	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	610	FAD	C10-N10	2.53	1.42	1.37
3	A	604	NAG	C1-C2	2.32	1.55	1.52
4	B	610	FAD	C1'-C2'	2.19	1.55	1.52
4	A	608	FAD	C4A-N9A	-2.06	1.33	1.37
4	A	608	FAD	C5A-N7A	-2.03	1.35	1.39

All (69) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	601	NAG	C1-O5-C5	7.05	121.63	112.19
3	A	604	NAG	C1-O5-C5	5.74	119.87	112.19
4	B	610	FAD	N3A-C2A-N1A	-5.57	120.15	128.58
3	A	607	NAG	C1-O5-C5	5.09	119.01	112.19
3	B	603	NAG	C1-O5-C5	4.83	118.65	112.19
4	A	608	FAD	C5A-C4A-N3A	-4.46	120.58	126.72
4	A	608	FAD	N3A-C2A-N1A	-4.36	121.98	128.58
4	B	610	FAD	N9A-C8A-N7A	-4.29	107.85	113.94
3	B	608	NAG	C3-C4-C5	-4.19	102.64	110.23
4	B	610	FAD	C5A-C4A-N3A	-4.13	121.02	126.72
3	B	607	NAG	C4-C3-C2	4.09	117.02	111.02
4	A	608	FAD	N9A-C8A-N7A	-4.02	108.23	113.94
3	A	606	NAG	C1-O5-C5	3.83	117.31	112.19
3	B	606	NAG	C3-C4-C5	-3.81	103.32	110.23
4	A	608	FAD	C4A-N9A-C8A	3.77	109.69	105.74
4	B	610	FAD	C5A-N7A-C8A	3.76	109.35	103.45
4	B	610	FAD	O4B-C1B-N9A	-3.64	101.10	108.09
4	A	608	FAD	C4X-C10-N10	3.48	121.47	116.48
4	B	610	FAD	C4A-C5A-N7A	-3.46	106.62	110.58
4	A	608	FAD	C4A-C5A-N7A	-3.39	106.71	110.58
4	A	608	FAD	C5A-N7A-C8A	3.38	108.77	103.45
4	B	610	FAD	C2A-N3A-C4A	3.36	120.03	111.83
4	A	608	FAD	N3A-C4A-N9A	3.34	132.84	127.17
4	B	610	FAD	C4A-N9A-C8A	3.30	109.20	105.74
3	A	606	NAG	C3-C4-C5	-3.29	104.26	110.23
4	A	608	FAD	C2A-N3A-C4A	3.24	119.73	111.83
4	B	610	FAD	C2A-N1A-C6A	3.13	123.87	118.73
4	A	608	FAD	C8M-C8-C9	-3.12	114.08	119.57
4	B	610	FAD	C8M-C8-C9	-3.11	114.09	119.57
3	A	601	NAG	C4-C3-C2	3.10	115.57	111.02
4	A	608	FAD	C4-N3-C2	-3.09	120.15	125.64
3	B	606	NAG	O5-C5-C6	3.00	113.50	107.66
3	B	608	NAG	O5-C5-C6	2.99	113.48	107.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	608	NAG	O4-C4-C5	2.97	116.64	109.32
4	A	608	FAD	O2-C2-N1	-2.96	116.89	121.80
4	A	608	FAD	C5X-C9A-N10	2.93	120.62	117.97
4	B	610	FAD	C5X-C9A-N10	2.92	120.61	117.97
3	B	603	NAG	O5-C1-C2	2.92	115.81	111.29
4	B	610	FAD	C8M-C8-C7	2.90	126.69	120.76
3	A	607	NAG	C2-N2-C7	-2.87	119.05	122.90
4	B	610	FAD	N3A-C4A-N9A	2.85	132.01	127.17
4	A	608	FAD	O4-C4-C4X	-2.80	119.15	126.53
3	B	609	NAG	C3-C4-C5	-2.77	105.21	110.23
3	B	607	NAG	O5-C1-C2	-2.71	107.10	111.29
3	A	601	NAG	C3-C4-C5	2.70	115.14	110.23
4	A	608	FAD	C7M-C7-C6	-2.70	114.82	119.57
4	B	610	FAD	C10-C4X-N5	-2.64	119.42	124.81
4	B	610	FAD	C4-N3-C2	-2.63	120.97	125.64
3	A	601	NAG	O5-C1-C2	2.62	115.35	111.29
4	A	608	FAD	C4X-C4-N3	2.60	119.87	113.25
4	A	608	FAD	C5B-C4B-C3B	-2.45	106.39	115.21
4	A	608	FAD	C8M-C8-C7	2.39	125.64	120.76
4	A	608	FAD	O2-C2-N3	2.36	123.11	118.58
4	B	610	FAD	C9A-C5X-N5	-2.34	119.97	122.45
4	B	610	FAD	O3B-C3B-C4B	-2.34	104.36	111.08
3	B	609	NAG	C8-C7-N2	-2.29	112.32	116.12
4	A	608	FAD	O2P-P-O3P	-2.28	101.12	107.27
4	B	610	FAD	C7M-C7-C6	-2.22	115.66	119.57
3	B	608	NAG	C8-C7-N2	-2.20	112.47	116.12
4	B	610	FAD	C4X-C10-N10	2.17	119.59	116.48
4	B	610	FAD	O2P-P-O3P	-2.16	101.42	107.27
4	B	610	FAD	C4X-C4-N3	2.16	118.75	113.25
3	B	608	NAG	O3-C3-C4	-2.15	105.31	110.38
4	A	608	FAD	C7M-C7-C8	2.13	125.11	120.76
4	A	608	FAD	O2A-PA-O1A	2.09	122.15	112.44
4	A	608	FAD	C9A-C5X-N5	-2.03	120.30	122.45
4	A	608	FAD	C9A-N10-C10	-2.03	117.66	120.75
3	B	609	NAG	O4-C4-C5	2.02	114.31	109.32
4	B	610	FAD	C7M-C7-C8	2.00	124.85	120.76

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	605	NAG	C1
3	B	607	NAG	C1

All (16) torsion outliers are listed below:

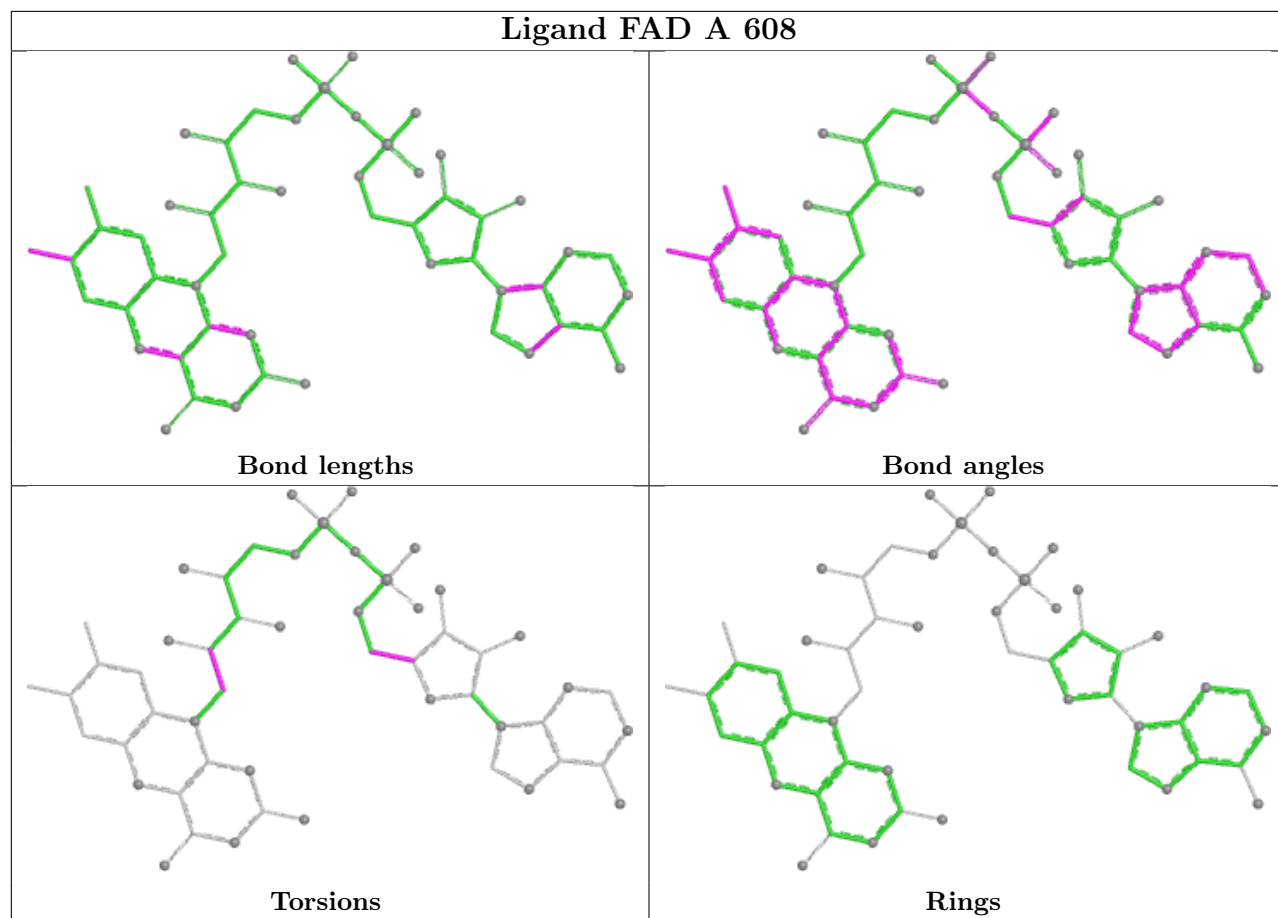
Mol	Chain	Res	Type	Atoms
4	A	608	FAD	N10-C1'-C2'-O2'
4	B	610	FAD	N10-C1'-C2'-O2'
3	B	607	NAG	O5-C5-C6-O6
3	B	607	NAG	C4-C5-C6-O6
3	B	608	NAG	C4-C5-C6-O6
4	A	608	FAD	C3B-C4B-C5B-O5B
4	A	608	FAD	O4B-C4B-C5B-O5B
3	B	606	NAG	C4-C5-C6-O6
3	A	605	NAG	O5-C5-C6-O6
3	B	603	NAG	C4-C5-C6-O6
3	B	608	NAG	O5-C5-C6-O6
3	A	605	NAG	C4-C5-C6-O6
3	B	603	NAG	O5-C5-C6-O6
3	B	606	NAG	O5-C5-C6-O6
3	B	609	NAG	C1-C2-N2-C7
3	A	604	NAG	O5-C5-C6-O6

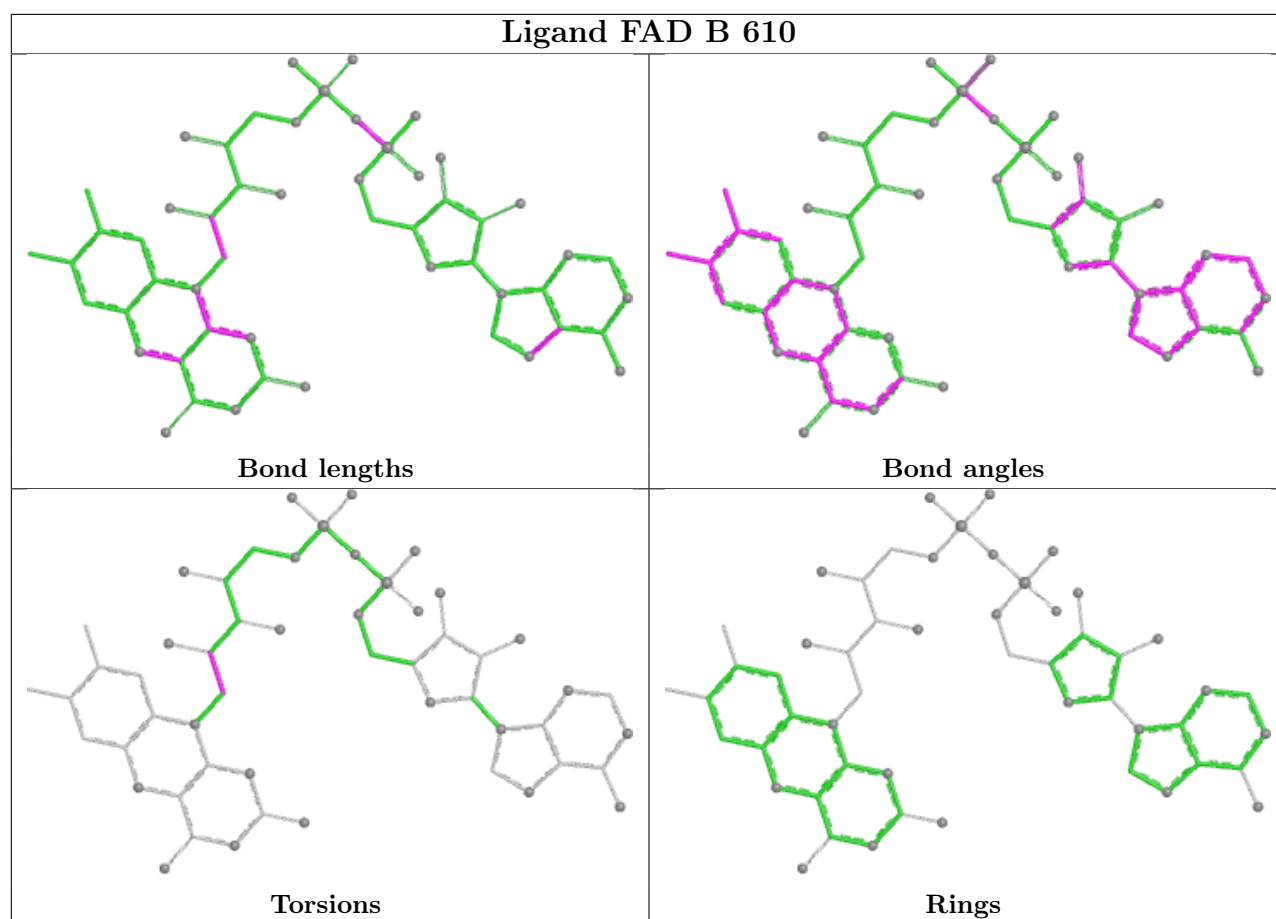
There are no ring outliers.

3 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	608	FAD	1	0
4	B	610	FAD	4	0
3	A	605	NAG	2	0

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





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	515/532 (96%)	-0.32	7 (1%) 73 75	10, 23, 40, 121	3 (0%)
1	B	509/532 (95%)	-0.36	2 (0%) 88 89	13, 23, 39, 57	0
All	All	1024/1064 (96%)	-0.34	9 (0%) 81 82	10, 23, 40, 121	3 (0%)

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	442	THR	5.1
1	A	440	ASN	4.9
1	A	519	SER	3.2
1	B	519	SER	3.0
1	A	224	SER	2.9
1	A	439	GLU	2.8
1	A	441	GLN	2.7
1	A	443	ASP	2.5
1	B	494	GLU	2.3

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

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

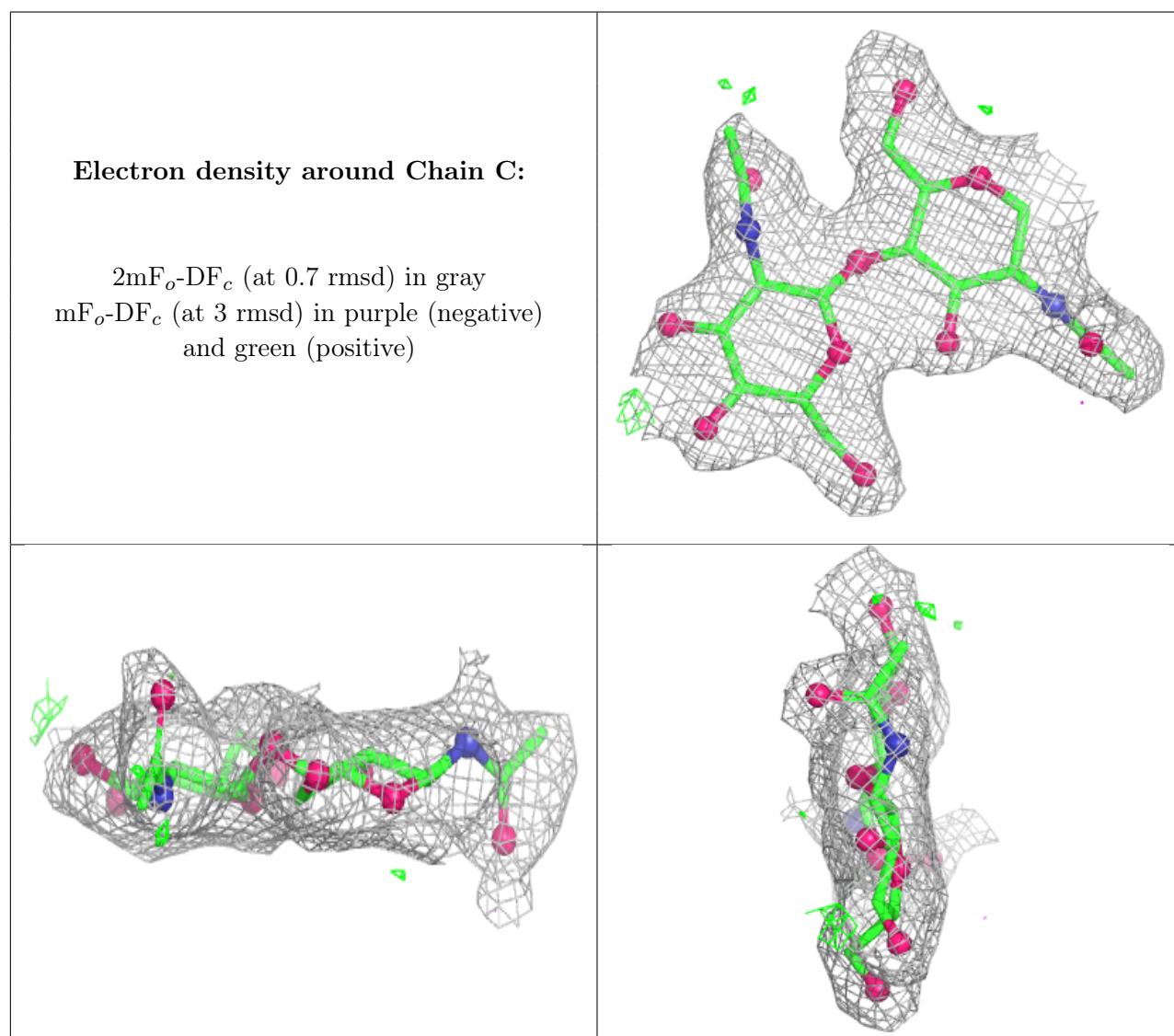
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	NAG	C	2	14/15	0.88	0.10	45,47,49,52	0

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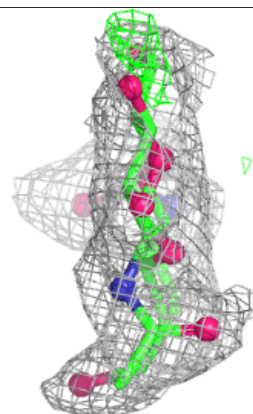
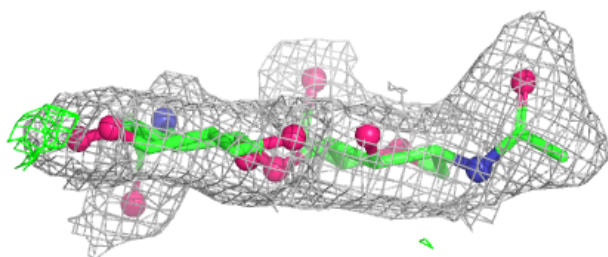
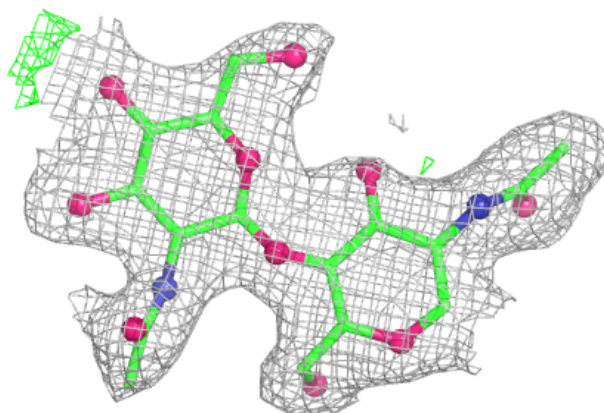
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	NAG	E	2	14/15	0.88	0.10	40,43,46,51	0
2	NAG	D	2	14/15	0.93	0.07	32,38,41,44	0
2	NAG	D	1	14/15	0.93	0.07	31,36,39,41	0
2	NAG	E	1	14/15	0.94	0.07	26,29,32,36	0
2	NAG	C	1	14/15	0.96	0.06	27,30,35,37	0

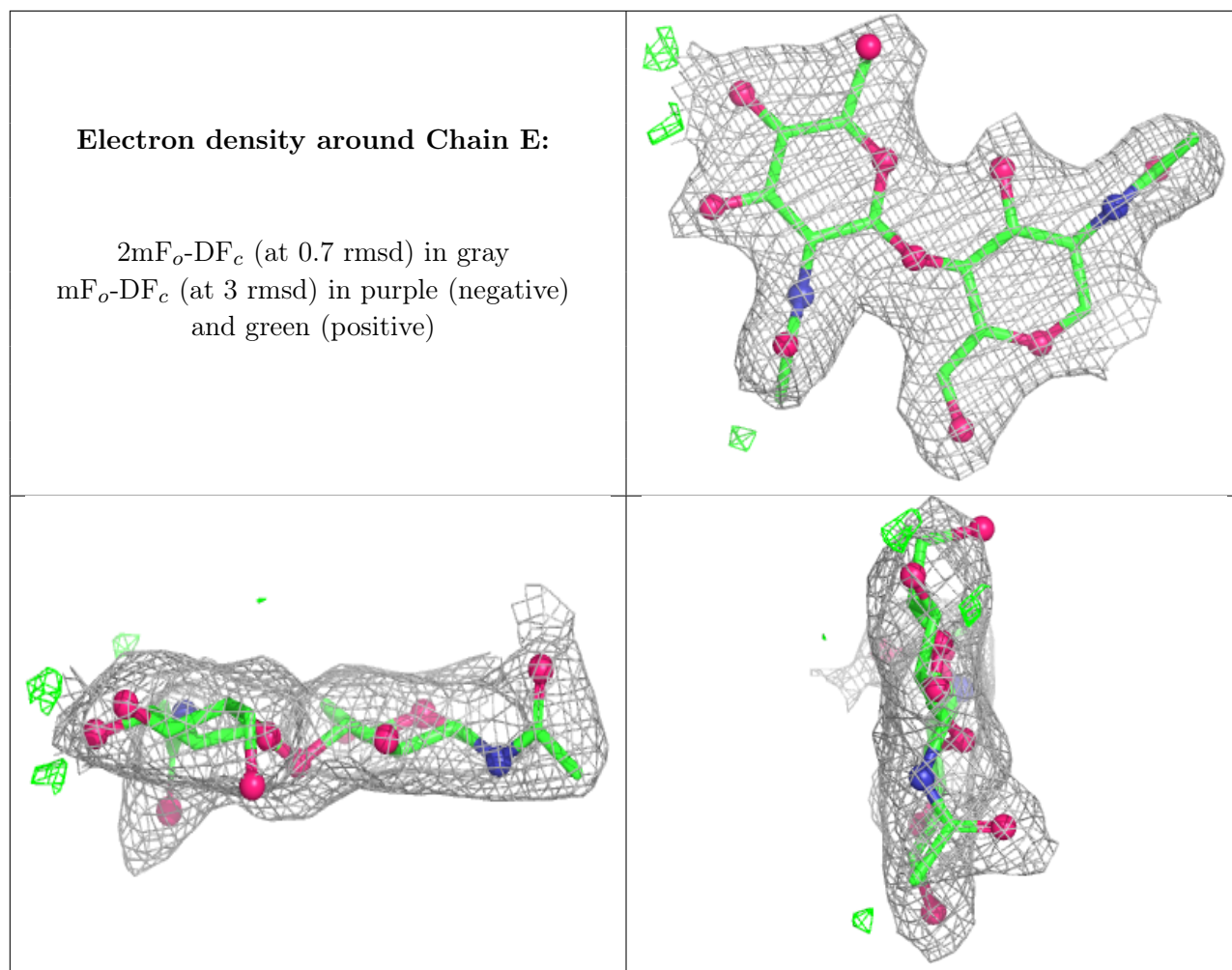
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.



Electron density around Chain D:

$2mF_o-DF_c$ (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.

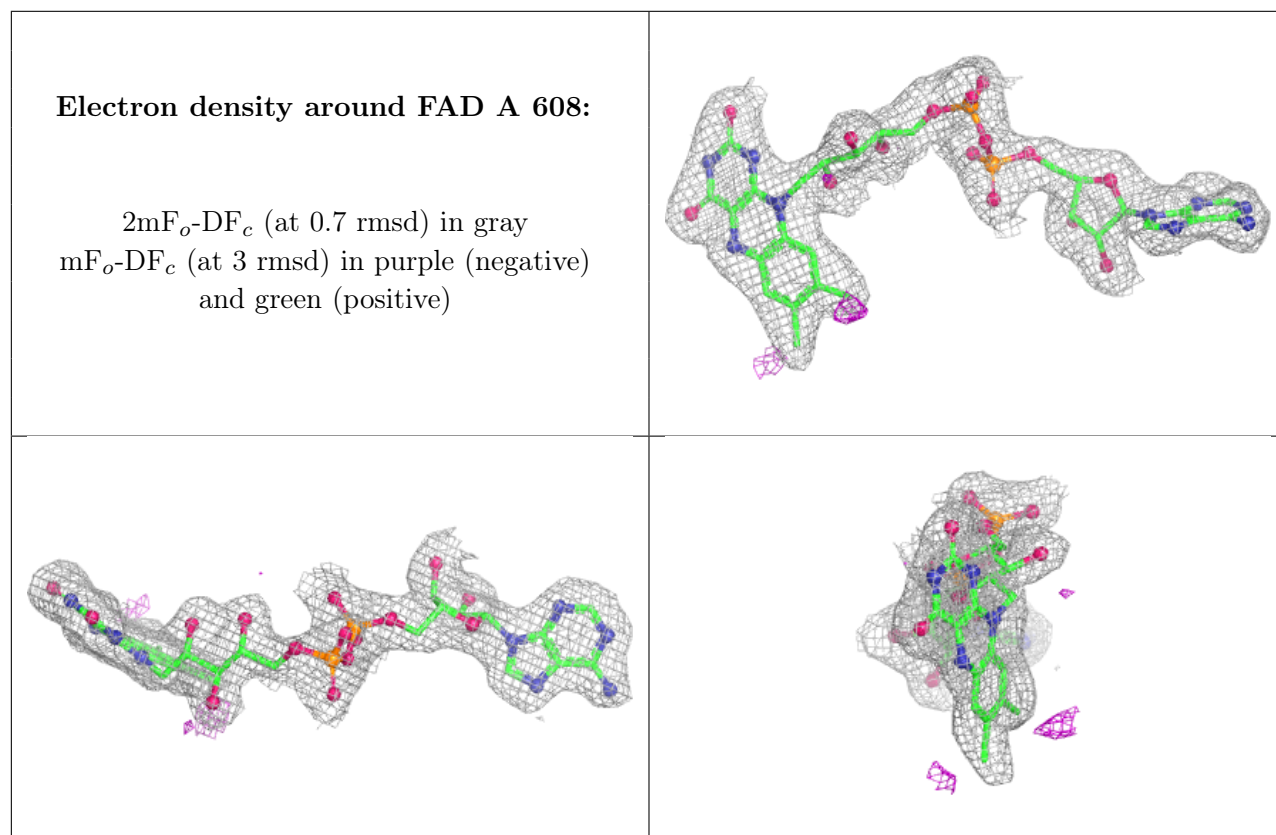
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	NAG	B	607	14/15	0.78	0.15	50,61,66,68	0
3	NAG	B	603	14/15	0.81	0.13	52,61,67,68	0
3	NAG	A	605	14/15	0.82	0.14	52,64,73,74	0
3	NAG	A	601	14/15	0.85	0.11	50,57,63,65	0
3	NAG	A	604	14/15	0.89	0.10	34,39,45,48	0
3	NAG	B	606	14/15	0.90	0.10	45,51,53,55	0
3	NAG	A	607	14/15	0.90	0.09	32,39,42,43	0
3	NAG	B	609	14/15	0.91	0.09	34,39,41,45	0
3	NAG	B	608	14/15	0.92	0.09	23,28,36,37	0
3	NAG	A	606	14/15	0.93	0.08	25,29,37,43	0

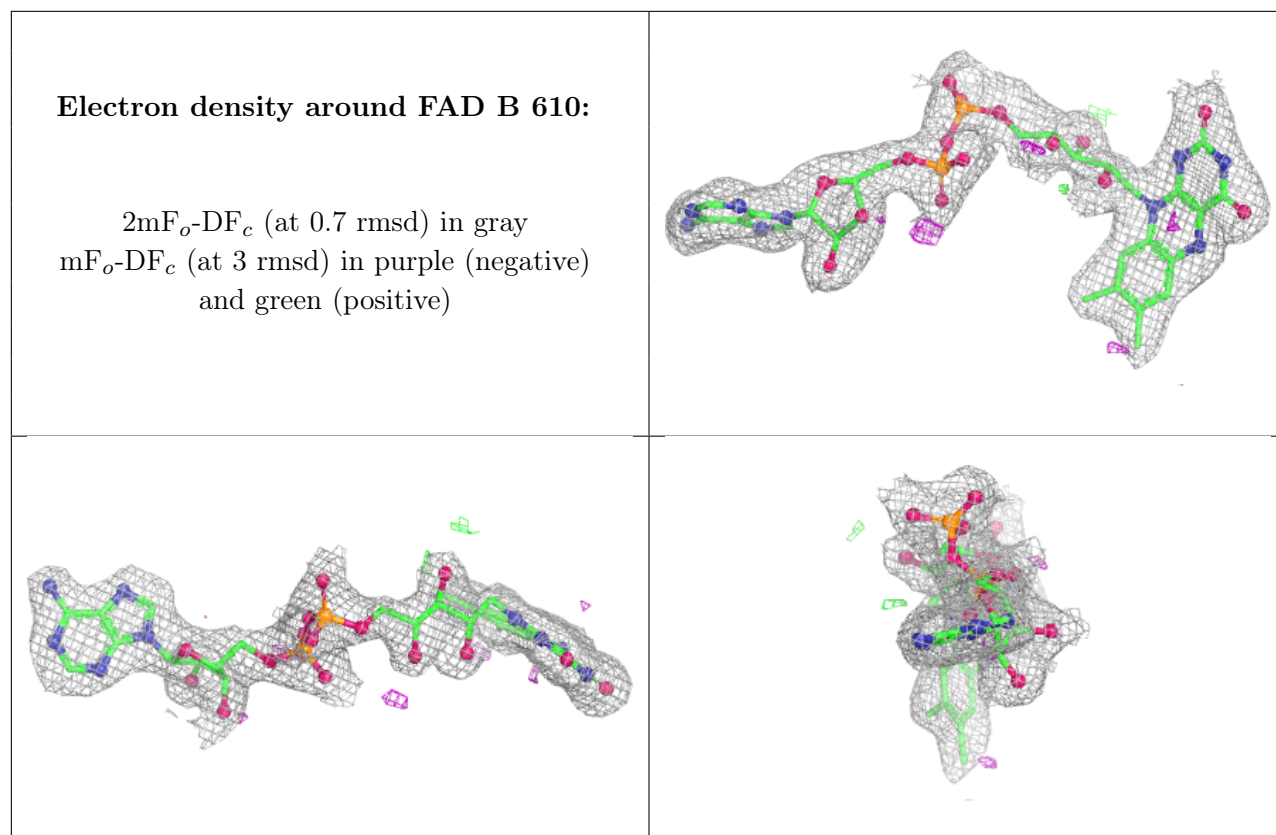
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	FAD	A	608	53/53	0.98	0.05	9,13,15,16	0
4	FAD	B	610	53/53	0.98	0.05	11,13,16,16	0

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.





6.5 Other polymers [i](#)

There are no such residues in this entry.