



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 8, 2020 – 01:03 AM BST

PDB ID : 4UD8
Title : AtBBE15
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Deposited on : 2014-12-09
Resolution : 2.09 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 following versions of software and data (see [references ⓘ](#)) 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 : 2.13.1
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) : 2.13.1

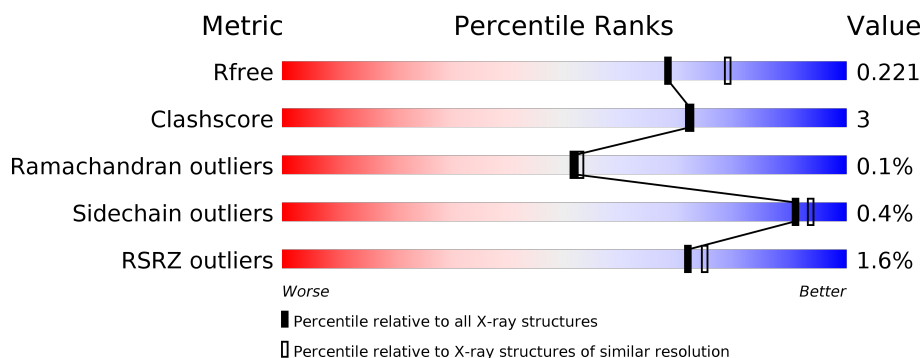
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.09 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	6189 (2.10-2.06)
Clashscore	141614	6738 (2.10-2.06)
Ramachandran outliers	138981	6663 (2.10-2.06)
Sidechain outliers	138945	6664 (2.10-2.06)
RSRZ outliers	127900	6057 (2.10-2.06)

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 on 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	<div> <div style="width: 100%; height: 10px; position: relative;"> <div style="position: absolute; top: -10px; left: 0;">%</div> <div style="position: absolute; top: 0; left: 0; width: 100%; height: 100%; background: linear-gradient(to right, red 0%, orange 1%, yellow 86%, green 94%, grey 100%);"></div> <div style="position: absolute; bottom: -10px; left: 0;">86% 8% 6%</div> </div> </div>
1	B	532	<div> <div style="width: 100%; height: 10px; position: relative;"> <div style="position: absolute; top: -10px; left: 0;">2%</div> <div style="position: absolute; top: 0; left: 0; width: 100%; height: 100%; background: linear-gradient(to right, red 0%, orange 2%, yellow 84%, green 93%, grey 100%);"></div> <div style="position: absolute; bottom: -10px; left: 0;">84% 9% 7%</div> </div> </div>
2	C	2	<div> <div style="width: 100%; height: 10px; position: relative;"> <div style="position: absolute; top: 0; left: 0; width: 100%; height: 100%; background: linear-gradient(to right, green 50%, yellow 50%, grey 100%);"></div> <div style="position: absolute; bottom: -10px; left: 0;">50% 50%</div> </div> </div>
2	D	2	<div> <div style="width: 100%; height: 10px; position: relative;"> <div style="position: absolute; top: 0; left: 0; width: 100%; height: 100%; background: linear-gradient(to right, green 100%, grey 100%);"></div> <div style="position: absolute; bottom: -10px; left: 0;">100%</div> </div> </div>

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 8808 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 FAD-BINDING AND BBE DOMAIN-CONTAINING PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	500	Total	C	N	O	S	0	1	0
			3975	2544	669	746	16			
1	B	497	Total	C	N	O	S	0	3	0
			3970	2545	670	739	16			

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



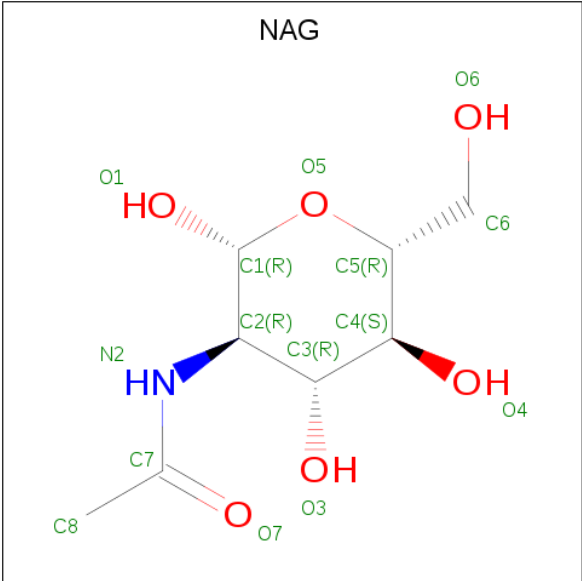
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	D	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 3 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: C₂₇H₃₃N₉O₁₅P₂).



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

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C₈H₁₅NO₆).



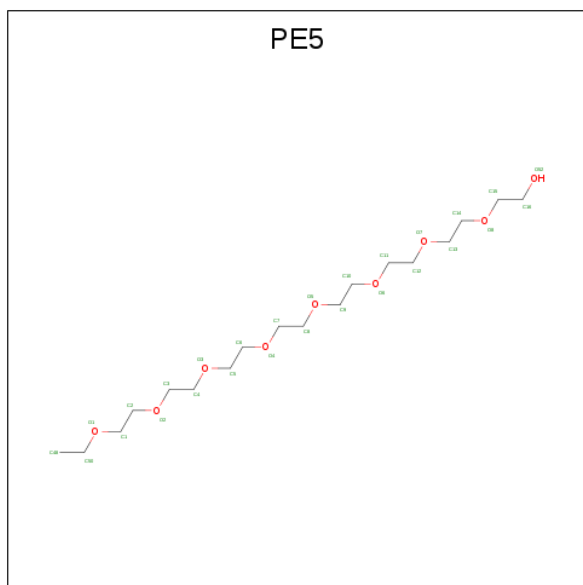
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			14	8	1	5		

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

- Molecule 5 is 3,6,9,12,15,18,21,24-OCTAOXAHEXACOSAN-1-OL (three-letter code: PE5) (formula: C₁₈H₃₈O₉).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			27	18	9		
5	B	1	Total	C	O	0	0
			27	18	9		

- Molecule 6 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	2	Total	Na	0	0
			2	2		
6	A	1	Total	Na	0	0
			1	1		

- Molecule 7 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	B	1	Total	K	0	0
			1	1		

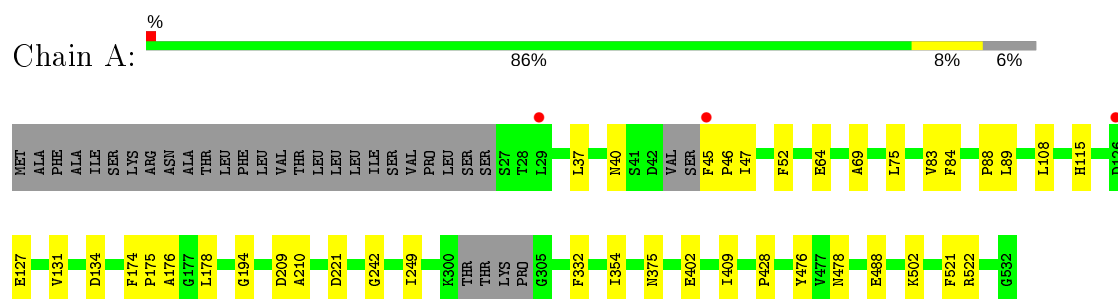
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	338	Total 338	O 338	0	0
8	B	277	Total 277	O 277	0	0

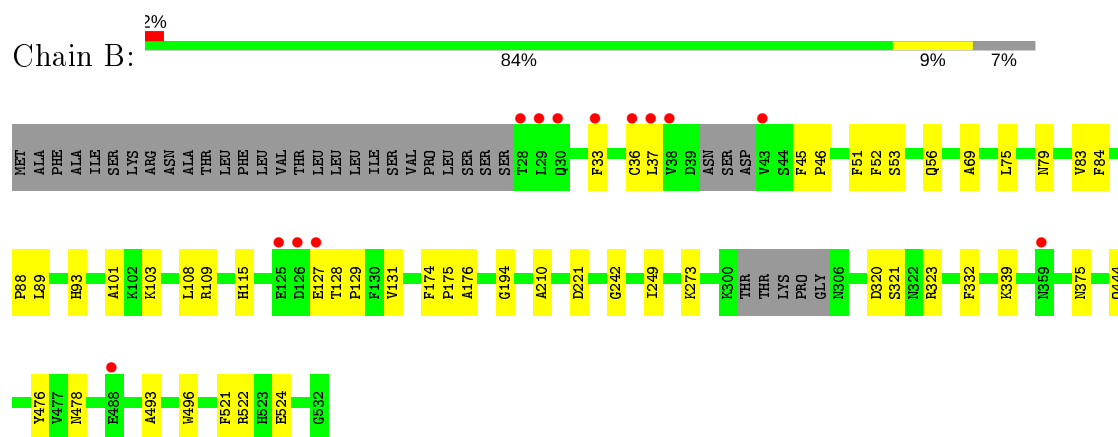
3 Residue-property plots [i](#)

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: FAD-BINDING AND BBE DOMAIN-CONTAINING PROTEIN



- Molecule 1: FAD-BINDING AND BBE DOMAIN-CONTAINING PROTEIN



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



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



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4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	63.60 Å 94.74 Å 188.30 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.37 – 2.09 47.37 – 2.09	Depositor EDS
% Data completeness (in resolution range)	98.0 (47.37-2.09) 92.4 (47.37-2.09)	Depositor EDS
R_{merge}	0.19	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.03 (at 2.08 Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.183 , 0.221 0.185 , 0.221	Depositor DCC
R_{free} test set	3400 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	22.8	Xtriage
Anisotropy	0.439	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 43.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	8808	wwPDB-VP
Average B, all atoms (Å ²)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.29% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NA, K, NAG, FAD, PE5

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	0.26	0/4075	0.42	0/5511
1	B	0.26	0/4076	0.42	0/5512
All	All	0.26	0/8151	0.42	0/11023

There are no bond length outliers.

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	3975	0	3890	23	0
1	B	3970	0	3905	30	0
2	C	28	0	25	0	0
2	D	28	0	25	0	0
3	A	53	0	29	2	0
3	B	53	0	28	1	0
4	A	14	0	13	0	0
4	B	14	0	13	0	0
5	A	27	0	38	3	0
5	B	27	0	38	1	0
6	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	2	0	0	0	0
7	B	1	0	0	0	0
8	A	338	0	0	1	0
8	B	277	0	0	4	0
All	All	8808	0	8004	55	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 (55) 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:323[B]:ARG:NH2	8:B:2151:HOH:O	2.20	0.74
1:A:428:PRO:HB2	1:A:502:LYS:HD3	1.86	0.57
1:B:375:ASN:ND2	1:B:444:GLN:HE22	2.02	0.57
1:A:45:PHE:CE2	1:A:89:LEU:HD12	2.40	0.57
1:B:79:ASN:ND2	8:B:2030:HOH:O	2.35	0.56
5:B:901:PE5:H151	5:B:901:PE5:H121	1.87	0.55
1:A:209:ASP:OD1	1:A:210:ALA:N	2.38	0.55
1:B:524:GLU:N	1:B:524:GLU:OE1	2.36	0.55
1:A:108:LEU:HD12	1:A:131:VAL:HG13	1.90	0.54
1:B:88:PRO:HB3	1:B:93:HIS:HB2	1.89	0.53
1:B:174:PHE:CE1	1:B:249:ILE:HB	2.47	0.50
1:B:33:PHE:CD1	1:B:84:PHE:HZ	2.29	0.50
1:A:45:PHE:CG	1:A:46:PRO:HD2	2.47	0.49
1:A:127:GLU:OE2	1:A:522:ARG:NE	2.37	0.48
1:B:242:GLY:HA2	1:B:521:PHE:CE2	2.49	0.48
1:A:52:PHE:CD2	1:A:64:GLU:HG2	2.48	0.48
1:B:320:ASP:OD1	8:B:2144:HOH:O	2.20	0.48
1:A:409:ILE:HD11	5:A:901:PE5:H91	1.95	0.47
1:B:53:SER:OG	1:B:56:GLN:HB2	2.14	0.47
1:A:69:ALA:HB3	1:A:75:LEU:HD11	1.96	0.47
1:A:476:TYR:CZ	1:A:478:ASN:HB2	2.49	0.47
1:B:493:ALA:HA	1:B:496:TRP:NE1	2.30	0.46
1:B:69:ALA:HB3	1:B:75:LEU:HD11	1.97	0.46
1:B:128:THR:HA	1:B:129:PRO:HA	1.62	0.46
1:B:83:VAL:HG23	1:B:129:PRO:HB2	1.98	0.46
1:B:476:TYR:CZ	1:B:478:ASN:HB2	2.51	0.45
1:B:52:PHE:O	1:B:84:PHE:HB2	2.16	0.45
1:A:115:HIS:HE1	3:A:601:FAD:HM71	1.81	0.44
1:B:127:GLU:OE2	1:B:522:ARG:NE	2.46	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:174:PHE:CD1	1:A:175:PRO:HD2	2.52	0.44
1:B:45:PHE:CD1	1:B:46:PRO:HA	2.52	0.44
1:A:37:LEU:O	1:A:40:ASN:HB3	2.17	0.44
1:A:115:HIS:CE1	3:A:601:FAD:HM71	2.53	0.44
1:B:33:PHE:HE2	1:B:101:ALA:HA	1.82	0.44
1:B:210:ALA:O	1:B:221:ASP:HA	2.18	0.43
1:A:375:ASN:OD1	5:A:901:PE5:H31	2.18	0.43
1:B:37:LEU:HD12	1:B:51:PHE:HE2	1.84	0.43
1:B:115:HIS:HE1	3:B:601:FAD:HM71	1.83	0.43
1:A:176:ALA:O	1:A:194:GLY:HA3	2.19	0.42
1:A:174:PHE:CE1	1:A:249:ILE:HB	2.54	0.42
1:A:178:LEU:HD22	1:A:354:ILE:HG21	2.01	0.42
1:A:488:GLU:OE1	1:A:488:GLU:N	2.48	0.42
1:A:210:ALA:O	1:A:221:ASP:HA	2.20	0.42
1:A:242:GLY:HA2	1:A:521:PHE:CE2	2.55	0.41
1:B:273:LYS:NZ	8:B:2130:HOH:O	2.52	0.41
1:B:36:CYS:SG	1:B:103:LYS:NZ	2.90	0.41
1:A:88:PRO:HD2	1:A:134:ASP:O	2.21	0.41
1:B:174:PHE:CD1	1:B:175:PRO:HD2	2.56	0.41
1:B:321:SER:OG	1:B:339:LYS:HE3	2.20	0.41
1:A:83:VAL:HG12	1:A:84:PHE:HD2	1.85	0.41
5:A:901:PE5:H72	8:A:2338:HOH:O	2.19	0.40
1:B:108:LEU:HD12	1:B:131:VAL:HG13	2.02	0.40
1:B:176:ALA:O	1:B:194:GLY:HA3	2.20	0.40
1:B:89:LEU:HD23	1:B:89:LEU:HA	1.91	0.40
1:B:109:ARG:NH2	1:B:524:GLU:OE1	2.55	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	495/532 (93%)	475 (96%)	19 (4%)	1 (0%)	47	47
1	B	494/532 (93%)	474 (96%)	20 (4%)	0	100	100
All	All	989/1064 (93%)	949 (96%)	39 (4%)	1 (0%)	51	53

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	47	ILE

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	427/455 (94%)	425 (100%)	2 (0%)	88	92
1	B	427/455 (94%)	426 (100%)	1 (0%)	93	95
All	All	854/910 (94%)	851 (100%)	3 (0%)	91	93

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

Mol	Chain	Res	Type
1	A	332	PHE
1	A	402	GLU
1	B	332	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	444	GLN
1	B	478	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 ⓘ

4 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	0.64	0	17,19,21	1.10	2 (11%)
2	NAG	C	2	2	14,14,15	0.50	0	17,19,21	0.79	0
2	NAG	D	1	1,2	14,14,15	0.52	0	17,19,21	0.80	0
2	NAG	D	2	2	14,14,15	0.55	0	17,19,21	0.67	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	1,2	-	2/6/23/26	0/1/1/1
2	NAG	C	2	2	-	4/6/23/26	0/1/1/1
2	NAG	D	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	D	2	2	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1	NAG	C3-C4-C5	2.38	114.48	110.24
2	C	1	NAG	C4-C3-C2	2.34	114.45	111.02

There are no chirality outliers.

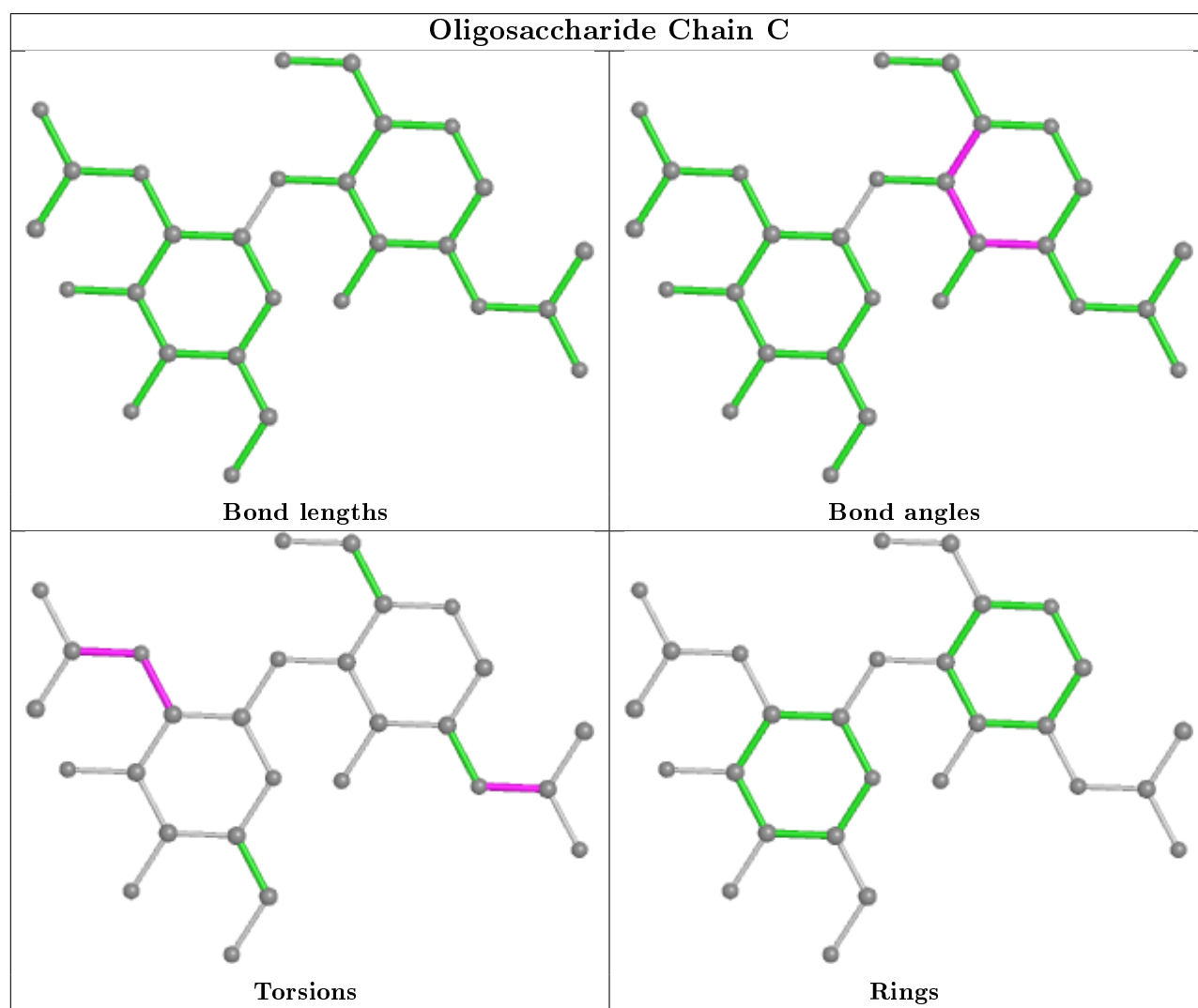
All (8) torsion outliers are listed below:

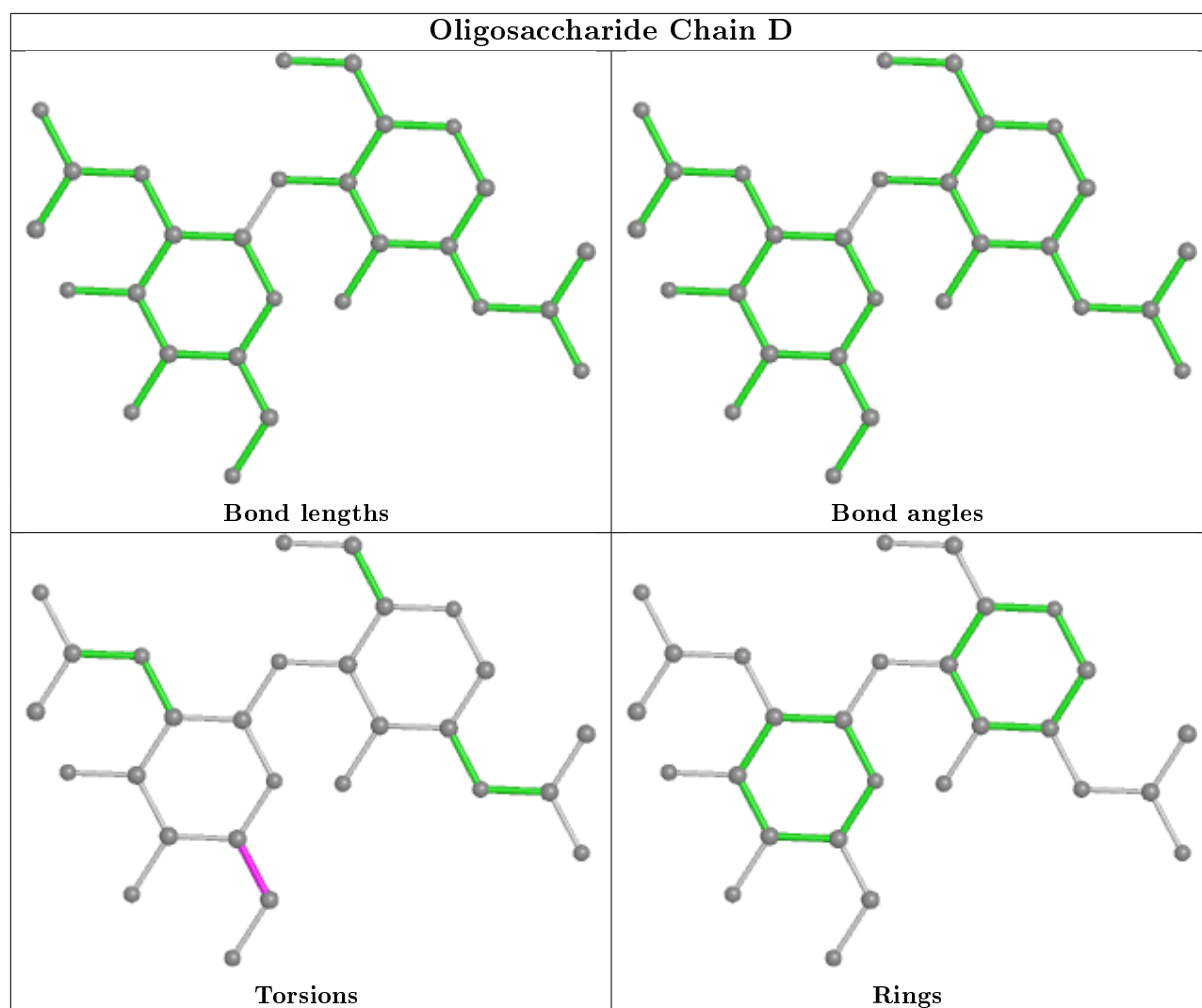
Mol	Chain	Res	Type	Atoms
2	C	2	NAG	C8-C7-N2-C2
2	C	2	NAG	O7-C7-N2-C2
2	C	1	NAG	C8-C7-N2-C2
2	C	1	NAG	O7-C7-N2-C2
2	D	2	NAG	C4-C5-C6-O6
2	D	2	NAG	O5-C5-C6-O6
2	C	2	NAG	C1-C2-N2-C7
2	C	2	NAG	C3-C2-N2-C7

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 ⓘ

Of 10 ligands modelled in this entry, 4 are monoatomic - leaving 6 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	FAD	B	601	1	51,58,58	1.87	6 (11%)	60,89,89	1.95	11 (18%)
3	FAD	A	601	1	51,58,58	1.83	6 (11%)	60,89,89	1.88	10 (16%)
5	PE5	A	901	-	26,26,26	0.46	0	25,25,25	0.97	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	B	801	1	14,14,15	0.46	0	17,19,21	0.93	1 (5%)
5	PE5	B	901	-	26,26,26	0.44	0	25,25,25	0.99	0
4	NAG	A	801	1	14,14,15	0.52	0	17,19,21	0.77	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	FAD	B	601	1	-	2/30/50/50	0/6/6/6
3	FAD	A	601	1	-	2/30/50/50	0/6/6/6
5	PE5	A	901	-	-	11/24/24/24	-
4	NAG	B	801	1	-	2/6/23/26	0/1/1/1
5	PE5	B	901	-	-	11/24/24/24	-
4	NAG	A	801	1	-	0/6/23/26	0/1/1/1

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	601	FAD	C4X-C10	9.47	1.48	1.38
3	A	601	FAD	C4X-C10	9.31	1.48	1.38
3	B	601	FAD	C4-C4X	4.28	1.48	1.41
3	A	601	FAD	C4-C4X	4.15	1.48	1.41
3	B	601	FAD	C9A-C5X	3.67	1.49	1.42
3	A	601	FAD	C8-C7	3.54	1.49	1.40
3	B	601	FAD	C8-C7	3.50	1.49	1.40
3	A	601	FAD	C9A-C5X	3.49	1.49	1.42
3	B	601	FAD	C9A-N10	2.90	1.42	1.38
3	B	601	FAD	C5A-C4A	2.45	1.47	1.40
3	A	601	FAD	C9A-N10	2.41	1.41	1.38
3	A	601	FAD	C5A-C4A	2.40	1.47	1.40

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	601	FAD	C4-N3-C2	8.01	121.90	115.14
3	A	601	FAD	C4-N3-C2	7.90	121.81	115.14
3	B	601	FAD	C4-C4X-C10	-5.36	116.40	119.95
3	A	601	FAD	C4-C4X-C10	-5.36	116.40	119.95
3	B	601	FAD	C1'-N10-C9A	4.45	121.79	118.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	601	FAD	C9A-N10-C10	-3.91	116.79	121.91
3	B	601	FAD	C4-C4X-N5	3.77	122.91	118.60
3	A	601	FAD	C9A-N10-C10	-3.76	116.98	121.91
3	A	601	FAD	C4-C4X-N5	3.73	122.86	118.60
3	B	601	FAD	C4X-C4-N3	-3.61	118.50	123.43
3	A	601	FAD	C4X-C4-N3	-3.58	118.54	123.43
3	A	601	FAD	C1'-N10-C9A	3.40	120.97	118.29
3	B	601	FAD	N3A-C2A-N1A	-3.29	123.53	128.68
3	A	601	FAD	N3A-C2A-N1A	-3.21	123.66	128.68
3	B	601	FAD	C4X-N5-C5X	3.20	119.97	116.77
3	A	601	FAD	C4X-N5-C5X	3.00	119.77	116.77
4	B	801	NAG	C1-O5-C5	2.98	116.23	112.19
3	B	601	FAD	C4A-C5A-N7A	-2.86	106.42	109.40
3	A	601	FAD	C4A-C5A-N7A	-2.64	106.65	109.40
3	B	601	FAD	P-O3P-PA	-2.41	124.55	132.83
3	A	601	FAD	P-O3P-PA	-2.16	125.43	132.83
3	B	601	FAD	C2A-N1A-C6A	2.01	122.18	118.75

There are no chirality outliers.

All (28) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	901	PE5	O1-C1-C2-O2
5	A	901	PE5	O3-C5-C6-O4
5	B	901	PE5	O2-C3-C4-O3
5	B	901	PE5	O6-C10-C9-O5
5	A	901	PE5	O4-C7-C8-O5
5	B	901	PE5	O7-C13-C14-O8
5	B	901	PE5	O4-C7-C8-O5
5	B	901	PE5	O3-C5-C6-O4
5	B	901	PE5	O6-C11-C12-O7
5	B	901	PE5	C48-C50-O1-C1
4	B	801	NAG	C4-C5-C6-O6
5	A	901	PE5	C9-C10-O6-C11
5	A	901	PE5	C7-C8-O5-C9
5	A	901	PE5	C3-C4-O3-C5
5	B	901	PE5	C11-C12-O7-C13
5	B	901	PE5	O8-C15-C16-O52
5	A	901	PE5	C5-C6-O4-C7
5	B	901	PE5	O1-C1-C2-O2
5	A	901	PE5	C14-C13-O7-C12
4	B	801	NAG	O5-C5-C6-O6

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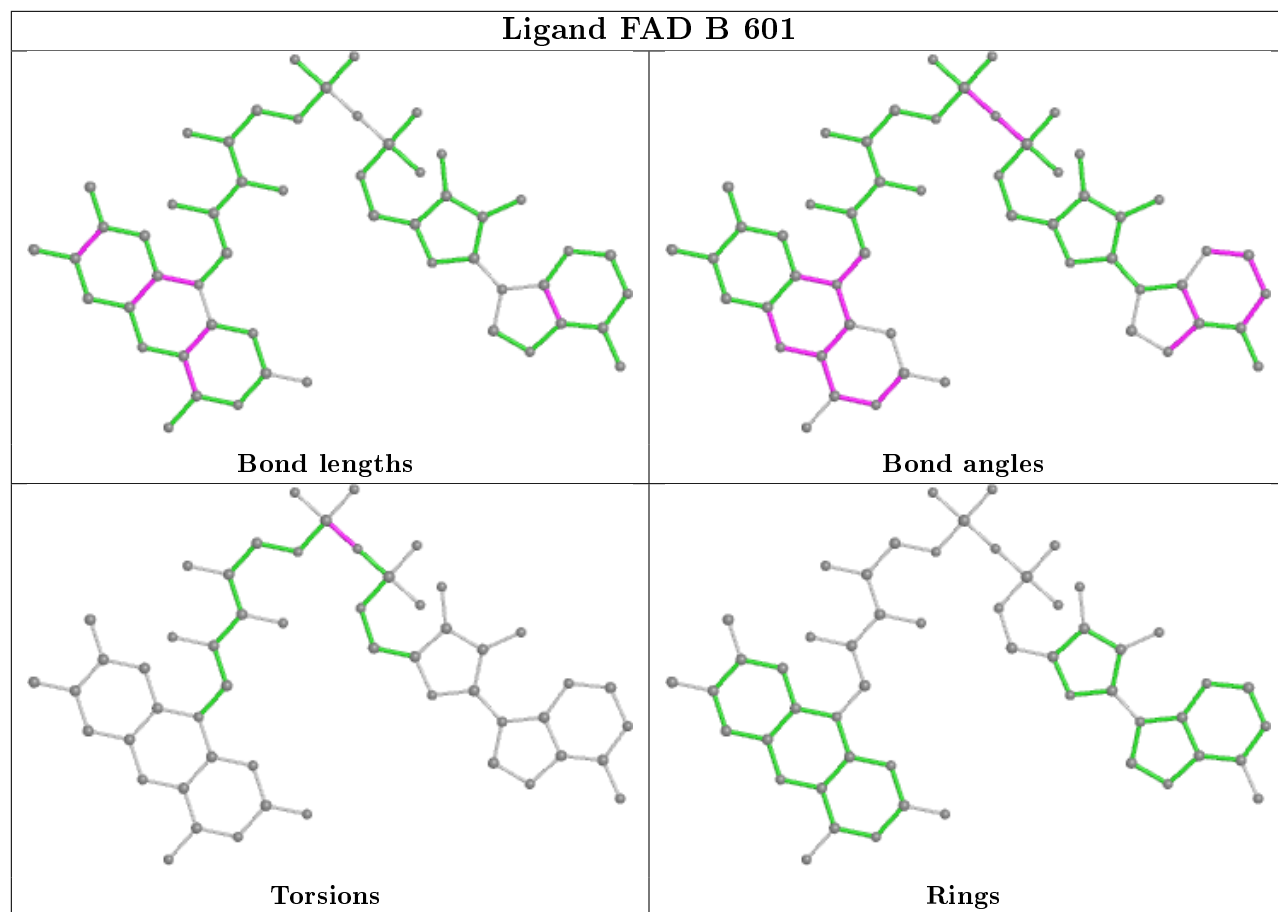
Mol	Chain	Res	Type	Atoms
5	A	901	PE5	C4-C3-O2-C2
3	B	601	FAD	PA-O3P-P-O2P
3	A	601	FAD	PA-O3P-P-O2P
5	A	901	PE5	O2-C3-C4-O3
5	B	901	PE5	C3-C4-O3-C5
3	B	601	FAD	PA-O3P-P-O1P
3	A	601	FAD	PA-O3P-P-O1P
5	A	901	PE5	O6-C10-C9-O5

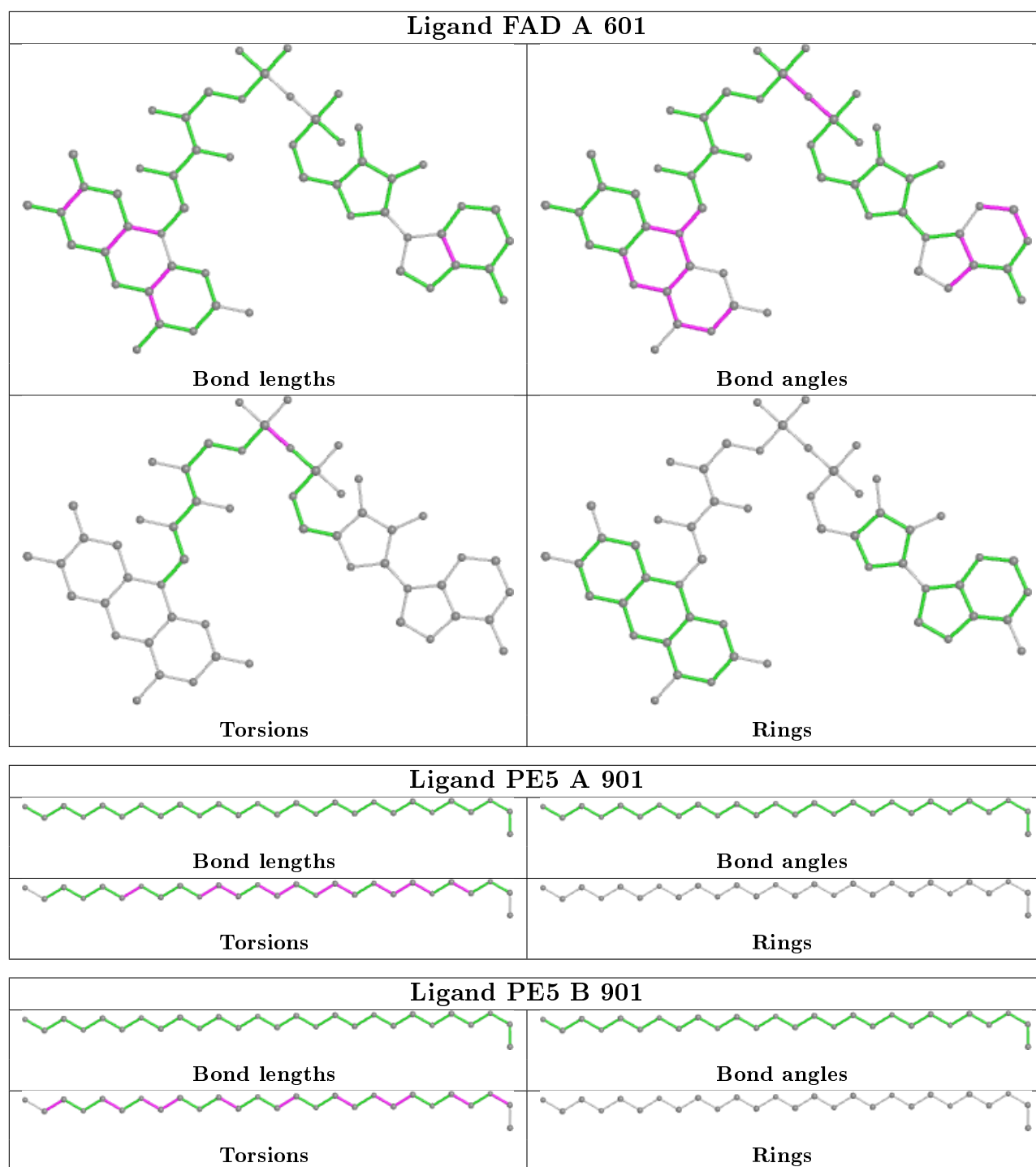
There are no ring outliers.

4 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	601	FAD	1	0
3	A	601	FAD	2	0
5	A	901	PE5	3	0
5	B	901	PE5	1	0

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





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	500/532 (93%)	-0.29	3 (0%) 89 91	17, 27, 51, 88	0
1	B	497/532 (93%)	-0.16	13 (2%) 56 60	18, 28, 56, 99	0
All	All	997/1064 (93%)	-0.23	16 (1%) 72 75	17, 28, 54, 99	0

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	126	ASP	4.9
1	A	45	PHE	4.3
1	B	29	LEU	4.2
1	B	33	PHE	3.6
1	B	36	CYS	3.5
1	A	126	ASP	3.3
1	B	359	ASN	2.6
1	B	125	GLU	2.4
1	B	28	THR	2.4
1	B	30	GLN	2.3
1	B	43	VAL	2.3
1	B	37	LEU	2.2
1	A	29	LEU	2.2
1	B	488	GLU	2.1
1	B	38	VAL	2.0
1	B	127	GLU	2.0

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

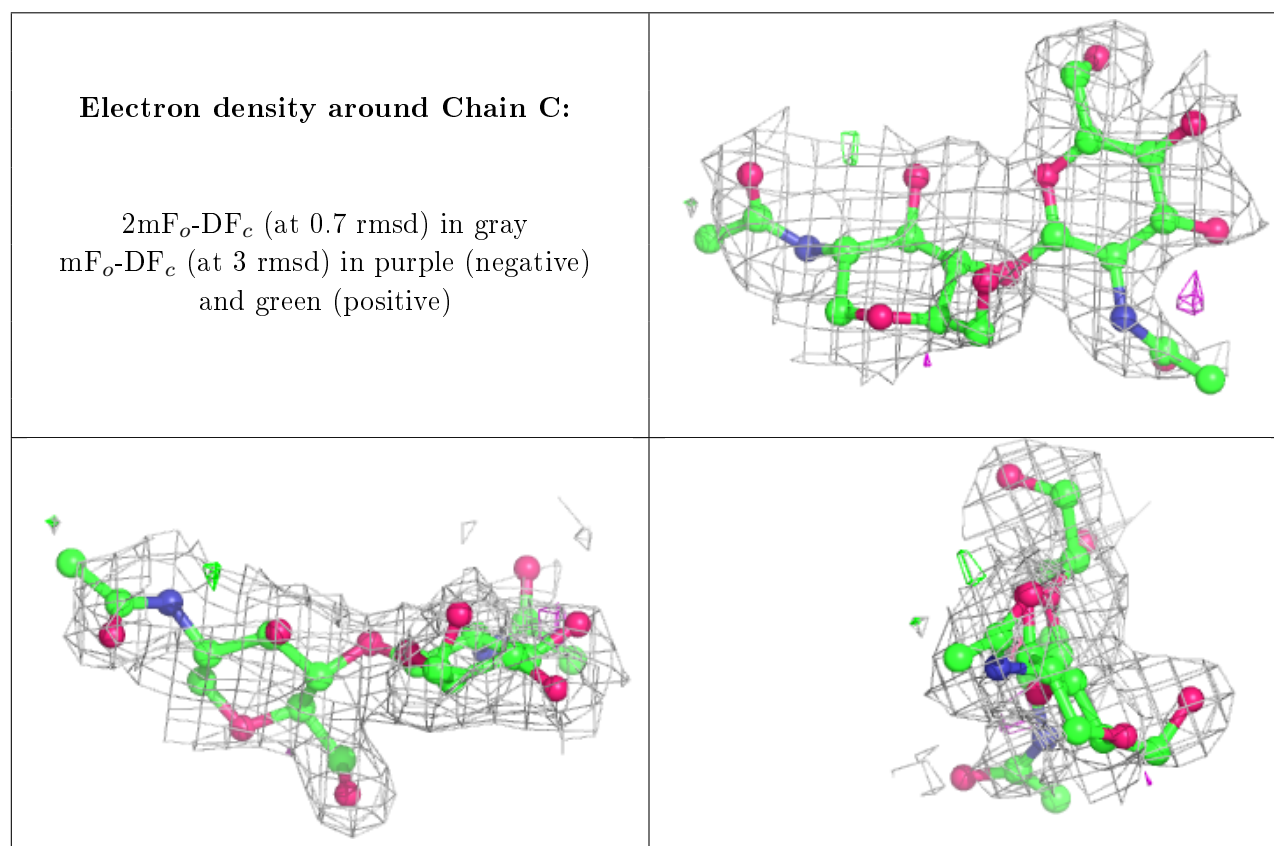
There are no non-standard protein/DNA/RNA residues in this entry.

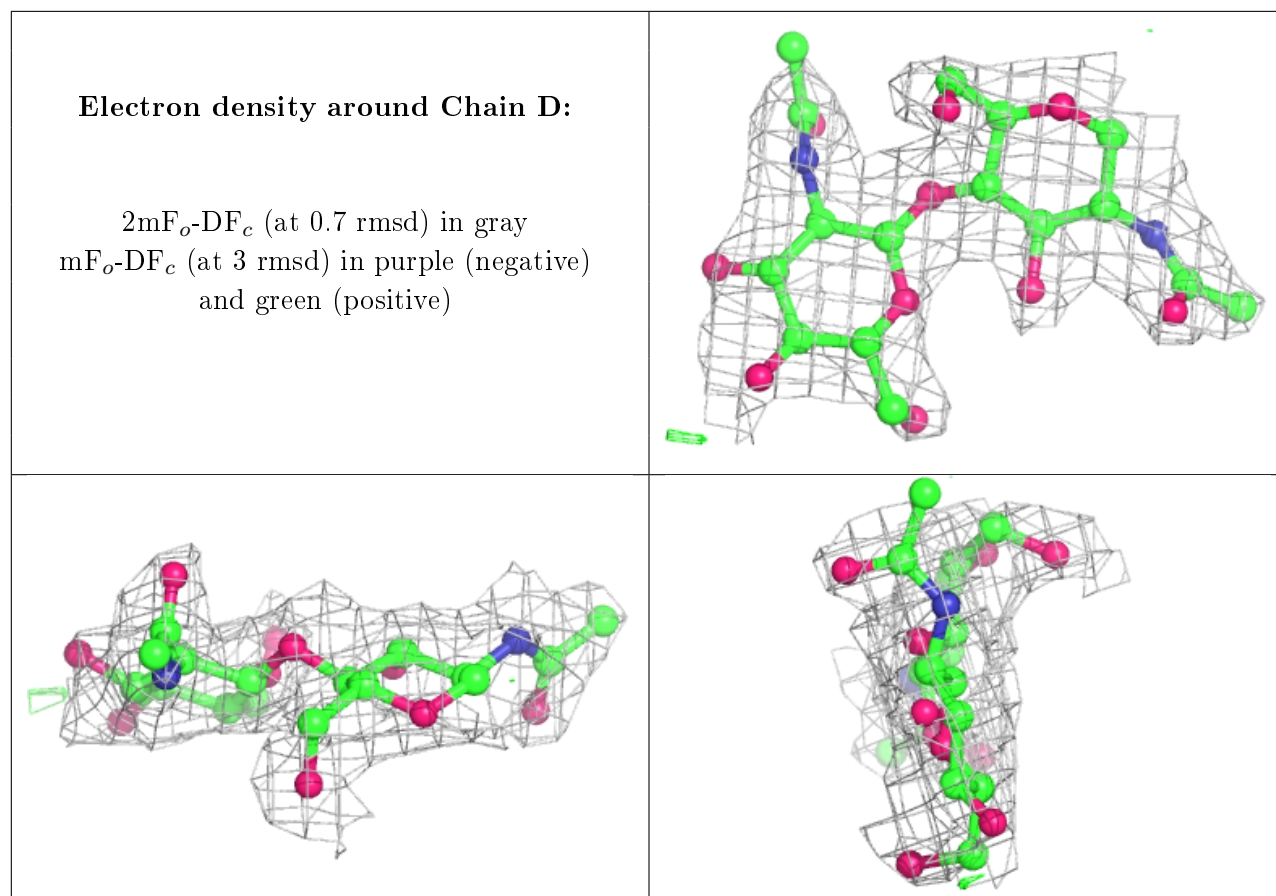
6.3 Carbohydrates ⓘ

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	0.72	0.25	70,72,76,77	0
2	NAG	C	1	14/15	0.82	0.16	52,58,62,67	0
2	NAG	D	2	14/15	0.86	0.23	65,67,69,70	0
2	NAG	D	1	14/15	0.88	0.14	49,57,59,61	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.





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.

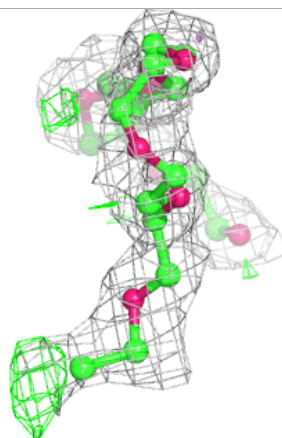
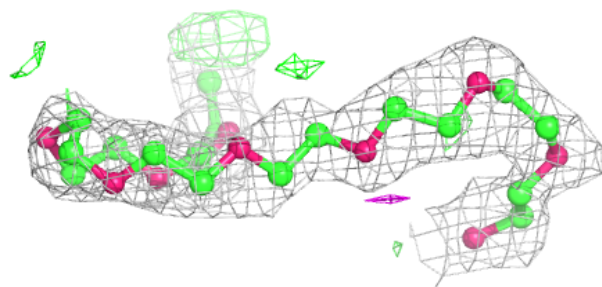
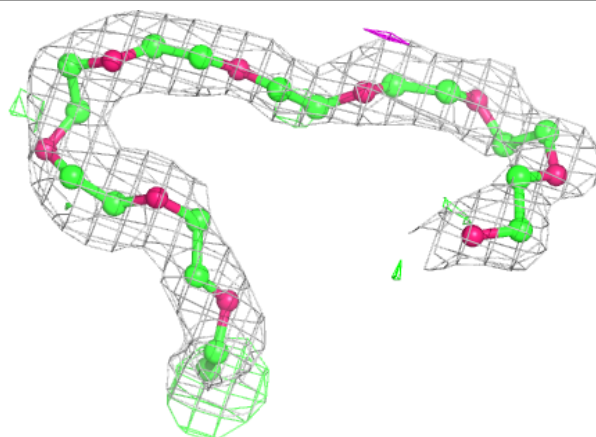
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	PE5	B	901	27/27	0.75	0.21	49,58,62,62	0
5	PE5	A	901	27/27	0.81	0.16	41,53,63,64	0
4	NAG	B	801	14/15	0.83	0.14	43,50,52,53	0
4	NAG	A	801	14/15	0.84	0.17	41,50,53,56	0
7	K	B	905	1/1	0.89	0.07	60,60,60,60	0
6	NA	A	906	1/1	0.94	0.05	26,26,26,26	0
6	NA	B	907	1/1	0.95	0.18	34,34,34,34	0
3	FAD	B	601	53/53	0.97	0.10	16,21,24,26	0
3	FAD	A	601	53/53	0.97	0.09	14,20,24,25	0
6	NA	B	906	1/1	0.98	0.07	26,26,26,26	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.

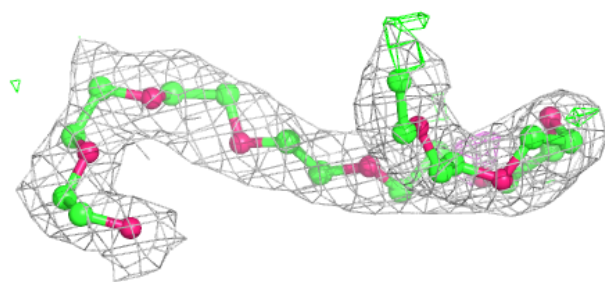
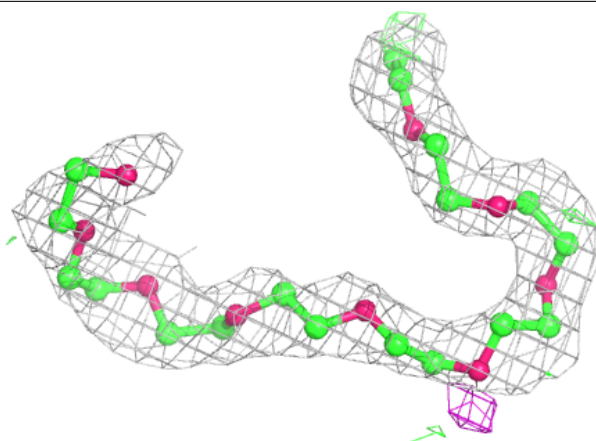
Electron density around PE5 B 901:

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

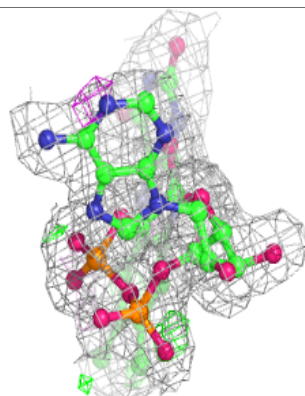
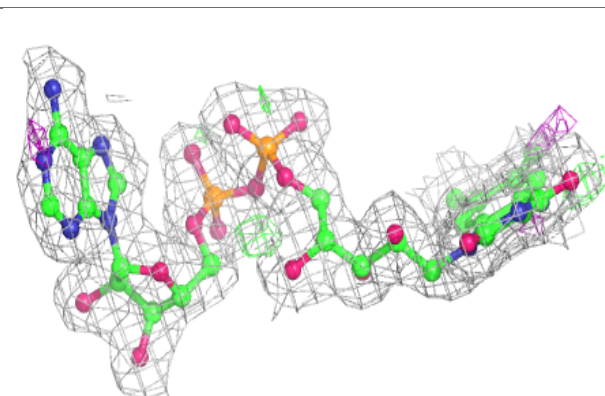
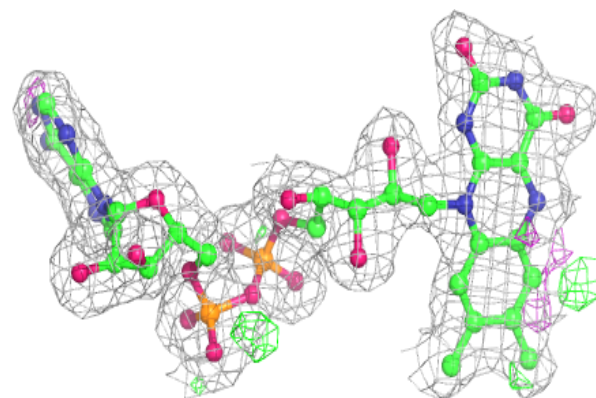


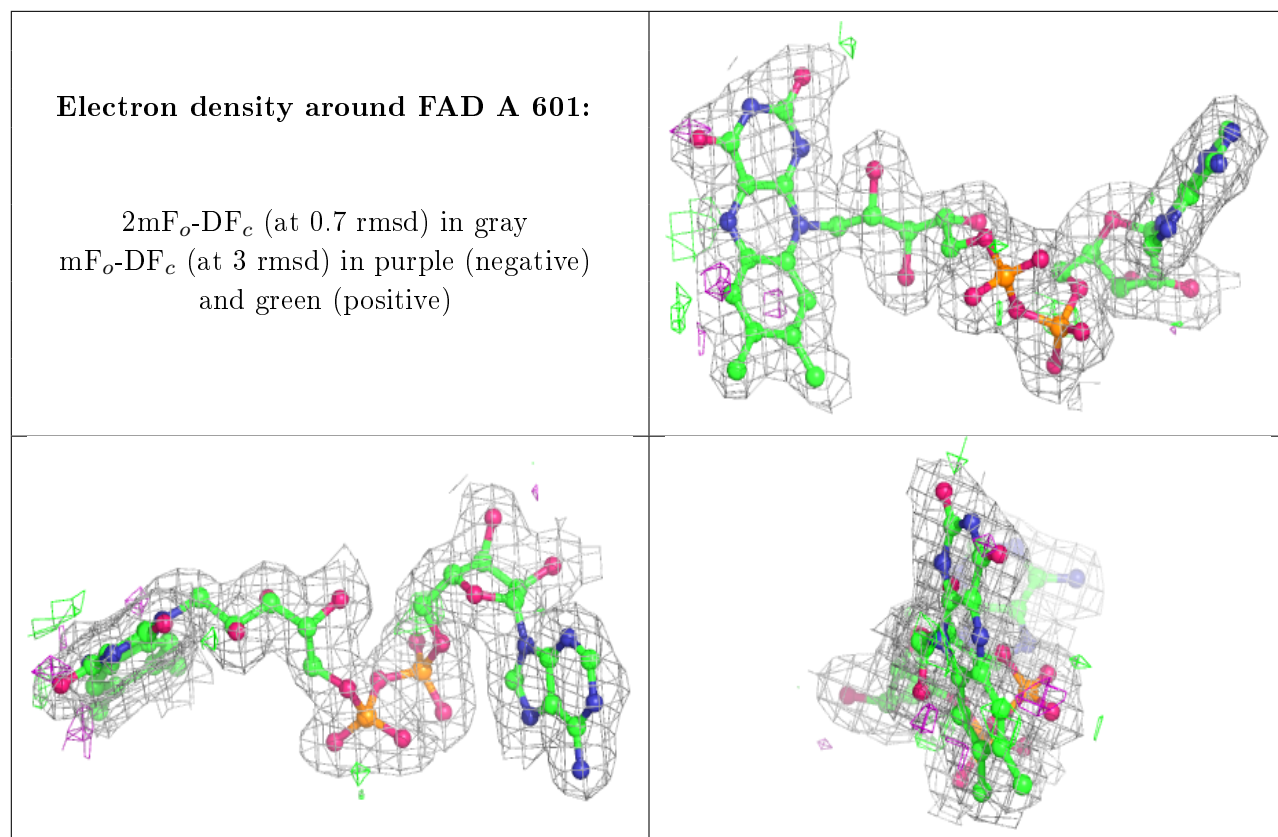
Electron density around PE5 A 901:

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

**Electron density around FAD B 601:**

$2mF_o-DF_c$ (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.