



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 25, 2024 – 08:23 PM EDT

PDB ID : 6YJI
Title : Structure of FgCelDH7C
Authors : Haddad Momeni, M.; Fredslund, F.; Berrin, J.G.; Abou Hachem, M.; Welner, D.H.
Deposited on : 2020-04-03
Resolution : 1.64 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 : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.37.1
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) : 2.37.1

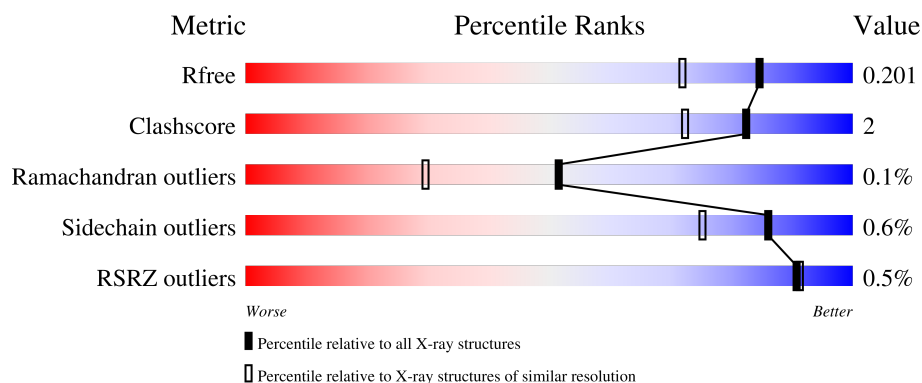
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.64 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	3122 (1.66-1.62)
Clashscore	141614	3268 (1.66-1.62)
Ramachandran outliers	138981	3215 (1.66-1.62)
Sidechain outliers	138945	3215 (1.66-1.62)
RSRZ outliers	127900	3079 (1.66-1.62)

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	488	<div> <div></div> <div>94%</div> </div>
1	B	488	<div> <div></div> <div>93%</div> </div>
2	C	2	<div> <div>50%</div> <div>50%</div> </div>
2	D	2	<div> <div>100%</div> </div>

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
9	PEG	B	609	-	-	X	-

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 16021 atoms, of which 7316 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 PCMH-type domain-containing protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	477	Total	C	H	N	O	S	0	18	0
			7439	2389	3680	640	716	14			
1	B	475	Total	C	H	N	O	S	0	15	0
			7346	2360	3636	630	706	14			

There are 18 discrepancies between the modelled and reference sequences:

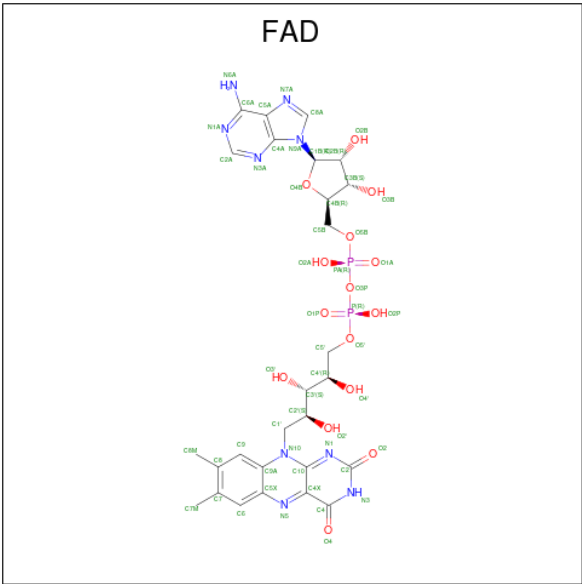
Chain	Residue	Modelled	Actual	Comment	Reference
A	500	ALA	-	expression tag	UNP I1RWY4
A	501	ALA	-	expression tag	UNP I1RWY4
A	502	ALA	-	expression tag	UNP I1RWY4
A	503	HIS	-	expression tag	UNP I1RWY4
A	504	HIS	-	expression tag	UNP I1RWY4
A	505	HIS	-	expression tag	UNP I1RWY4
A	506	HIS	-	expression tag	UNP I1RWY4
A	507	HIS	-	expression tag	UNP I1RWY4
A	508	HIS	-	expression tag	UNP I1RWY4
B	500	ALA	-	expression tag	UNP I1RWY4
B	501	ALA	-	expression tag	UNP I1RWY4
B	502	ALA	-	expression tag	UNP I1RWY4
B	503	HIS	-	expression tag	UNP I1RWY4
B	504	HIS	-	expression tag	UNP I1RWY4
B	505	HIS	-	expression tag	UNP I1RWY4
B	506	HIS	-	expression tag	UNP I1RWY4
B	507	HIS	-	expression tag	UNP I1RWY4
B	508	HIS	-	expression tag	UNP I1RWY4

- 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			

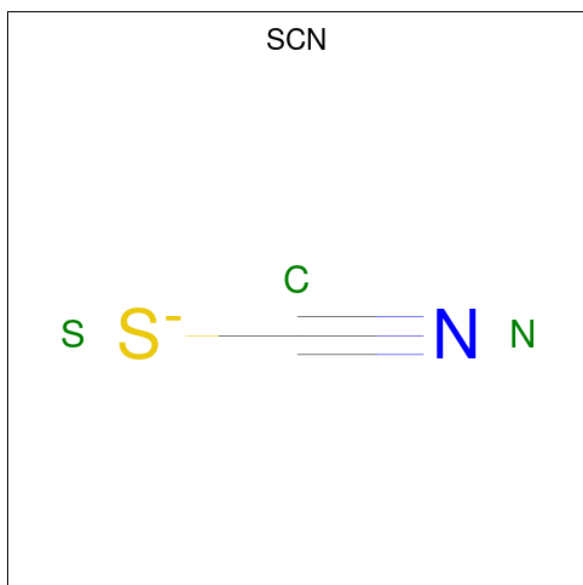
- Molecule 3 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: C₂₇H₃₃N₉O₁₅P₂) (labeled as "Ligand of Interest" by depositor).





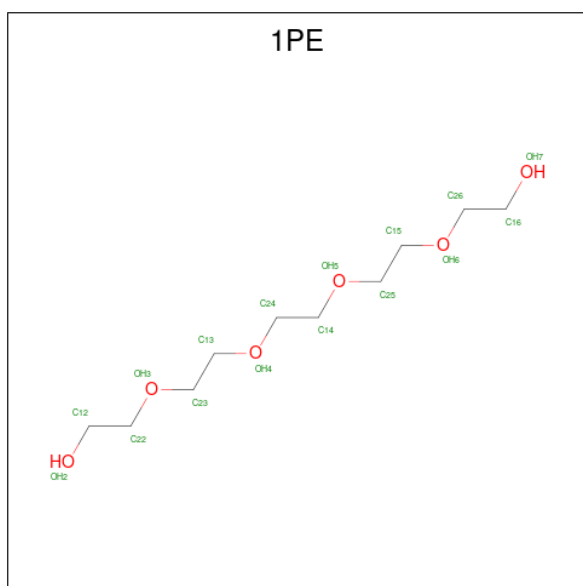
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	B	1	Total	C	N	O	0	0
			14	8	1	5		
4	B	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 5 is THIOCYANATE ION (three-letter code: SCN) (formula: CNS).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	S	0	0
			3	1	1	1		
5	A	1	Total	C	N	S	0	0
			3	1	1	1		
5	A	1	Total	C	N	S	0	0
			3	1	1	1		
5	A	1	Total	C	N	S	0	0
			3	1	1	1		
5	A	1	Total	C	N	S	0	0
			3	1	1	1		
5	B	1	Total	C	N	S	0	0
			3	1	1	1		
5	B	1	Total	C	N	S	0	0
			3	1	1	1		

- Molecule 6 is PENTAETHYLENE GLYCOL (three-letter code: 1PE) (formula: $C_{10}H_{22}O_6$).

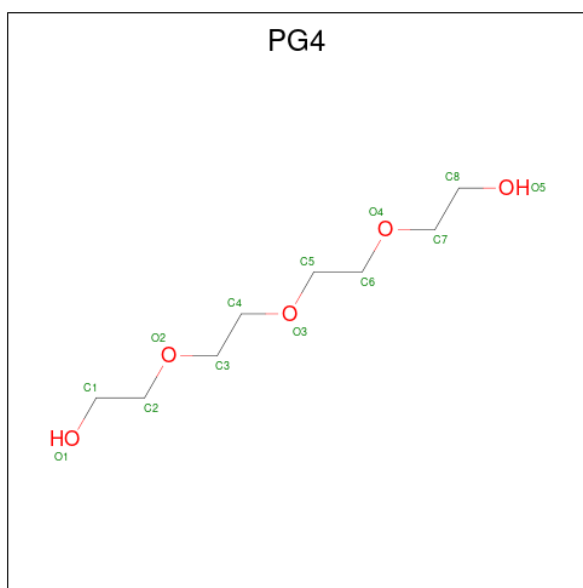


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			16	10	6		

- Molecule 7 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

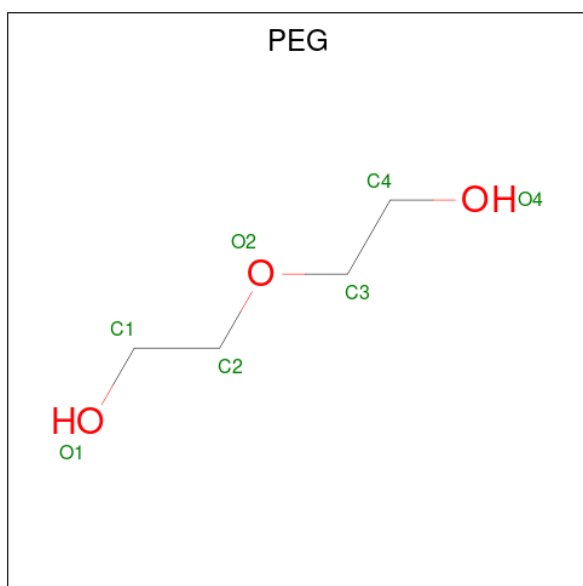
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	1	Total	Cl	0	0
			1	1		
7	B	1	Total	Cl	0	0
			1	1		

- Molecule 8 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: $C_8H_{18}O_5$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	B	1	Total	C	O	0	0
			13	8	5		
8	B	1	Total	C	O	0	0
			13	8	5		

- Molecule 9 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



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

- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	468	Total 468	O 468	0	0
10	B	478	Total 478	O 478	0	0

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.

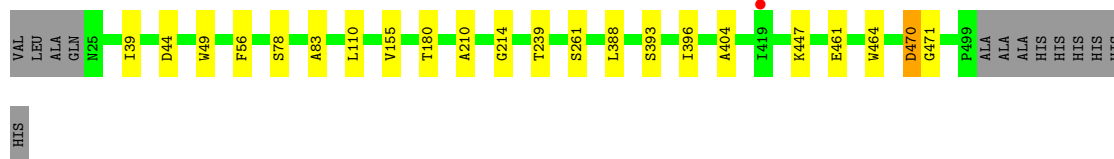
- Molecule 1: FAD-binding PCMH-type domain-containing protein

Chain A: 



- Molecule 1: FAD-binding PCMH-type domain-containing protein

Chain B: 



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

Chain C: 



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

Chain D: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	96.54Å 187.82Å 55.45Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	53.18 – 1.64 53.18 – 1.64	Depositor EDS
% Data completeness (in resolution range)	95.4 (53.18-1.64) 95.6 (53.18-1.64)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.45 (at 1.64Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.164 , 0.201 0.163 , 0.201	Depositor DCC
R_{free} test set	5929 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	21.6	Xtriage
Anisotropy	0.806	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 48.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	16021	wwPDB-VP
Average B, all atoms (Å ²)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.73% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: PG4, SCN, CL, 1PE, FAD, NAG, PEG

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	0.49	0/3904	0.63	0/5294
1	B	0.47	0/3860	0.61	0/5233
All	All	0.48	0/7764	0.62	0/10527

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 [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	3759	3680	3606	12	0
1	B	3710	3636	3571	18	0
2	C	28	0	25	1	0
2	D	28	0	25	2	0
3	A	53	0	30	0	0
3	B	53	0	30	6	0
4	A	28	0	26	0	0
4	B	28	0	26	0	0
5	A	15	0	0	0	0
5	B	6	0	0	1	0
6	A	16	0	22	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	A	1	0	0	1	0
7	B	1	0	0	0	0
8	B	26	0	36	3	0
9	B	7	0	10	5	0
10	A	468	0	0	4	0
10	B	478	0	0	4	0
All	All	8705	7316	7407	38	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 2.

All (38) 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:470:ASP:OD1	1:A:471:GLY:N	2.07	0.86
1:B:470:ASP:OD2	1:B:471:GLY:N	2.21	0.70
3:B:601:FAD:C5X	9:B:609:PEG:H41	2.26	0.66
1:B:470:ASP:CG	1:B:471:GLY:H	1.97	0.66
1:A:233[B]:ASP:OD1	7:A:612:CL:CL	2.52	0.65
1:A:39:ILE:HD11	1:A:78:SER:HB2	1.80	0.62
1:A:470:ASP:HB3	10:A:920:HOH:O	1.99	0.62
1:B:39:ILE:HD11	1:B:78:SER:HB2	1.85	0.57
1:B:470:ASP:HB3	10:B:976:HOH:O	2.08	0.53
1:B:261:SER:HB2	1:B:388:LEU:HD21	1.89	0.53
1:B:470:ASP:CG	1:B:471:GLY:N	2.61	0.52
3:B:601:FAD:C6	9:B:609:PEG:H41	2.40	0.52
1:B:180:THR:HG21	5:B:607:SCN:C	2.41	0.51
1:A:239:THR:HG23	2:C:1:NAG:H81	1.94	0.49
1:B:404:ALA:CB	1:B:470:ASP:OD1	2.62	0.48
1:B:470:ASP:HB2	10:B:986:HOH:O	2.14	0.47
1:B:83:ALA:HB2	1:B:110:LEU:HD23	1.96	0.46
1:B:44:ASP:HA	1:B:49:TRP:CD2	2.51	0.46
8:B:606:PG4:H42	8:B:606:PG4:H62	1.45	0.46
1:B:239:THR:HG23	2:D:1:NAG:H81	1.98	0.46
1:A:303:LYS:NZ	10:A:711:HOH:O	2.47	0.45
8:B:606:PG4:H62	10:B:734:HOH:O	2.17	0.45
1:B:155:VAL:HB	3:B:601:FAD:C4	2.47	0.44
3:B:601:FAD:N5	9:B:609:PEG:H41	2.33	0.43
1:B:393:SER:HA	1:B:396:ILE:HD12	2.00	0.43
1:A:404:ALA:CB	1:A:470:ASP:OD2	2.67	0.43
1:A:44:ASP:HA	1:A:49:TRP:CD2	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:95:PRO:O	1:A:96:ALA:HB3	2.19	0.42
1:B:44:ASP:HA	1:B:49:TRP:CG	2.54	0.42
3:B:601:FAD:HM72	8:B:606:PG4:H61	2.01	0.42
1:B:210:ALA:HA	1:B:214:GLY:HA2	2.03	0.41
1:A:121:SER:O	1:A:129[B]:LEU:HD22	2.20	0.41
1:A:124[B]:LYS:NZ	10:A:721:HOH:O	2.53	0.41
1:A:447:LYS:HD3	10:A:790:HOH:O	2.19	0.41
1:B:461:GLU:HA	1:B:464:TRP:NE1	2.36	0.41
3:B:601:FAD:N5	9:B:609:PEG:C4	2.84	0.41
1:B:56:PHE:CZ	9:B:609:PEG:H11	2.56	0.40
10:B:1133:HOH:O	2:D:2:NAG:C8	2.70	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	493/488 (101%)	477 (97%)	15 (3%)	1 (0%)	47	26
1	B	488/488 (100%)	469 (96%)	19 (4%)	0	100	100
All	All	981/976 (100%)	946 (96%)	34 (4%)	1 (0%)	51	29

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	470	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	402/394 (102%)	398 (99%)	4 (1%)	76	59
1	B	399/394 (101%)	397 (100%)	2 (0%)	88	80
All	All	801/788 (102%)	795 (99%)	6 (1%)	86	71

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	26	LYS
1	A	110	LEU
1	A	231[A]	GLN
1	A	231[B]	GLN
1	B	447	LYS
1	B	470	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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	2,1	14,14,15	0.43	0	17,19,21	0.70	0
2	NAG	C	2	2	14,14,15	0.18	0	17,19,21	0.54	0
2	NAG	D	1	2,1	14,14,15	0.43	0	17,19,21	0.64	0
2	NAG	D	2	2	14,14,15	0.34	0	17,19,21	0.51	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	-	2/6/23/26	0/1/1/1
2	NAG	C	2	2	-	1/6/23/26	0/1/1/1
2	NAG	D	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	D	2	2	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (7) torsion outliers are listed below:

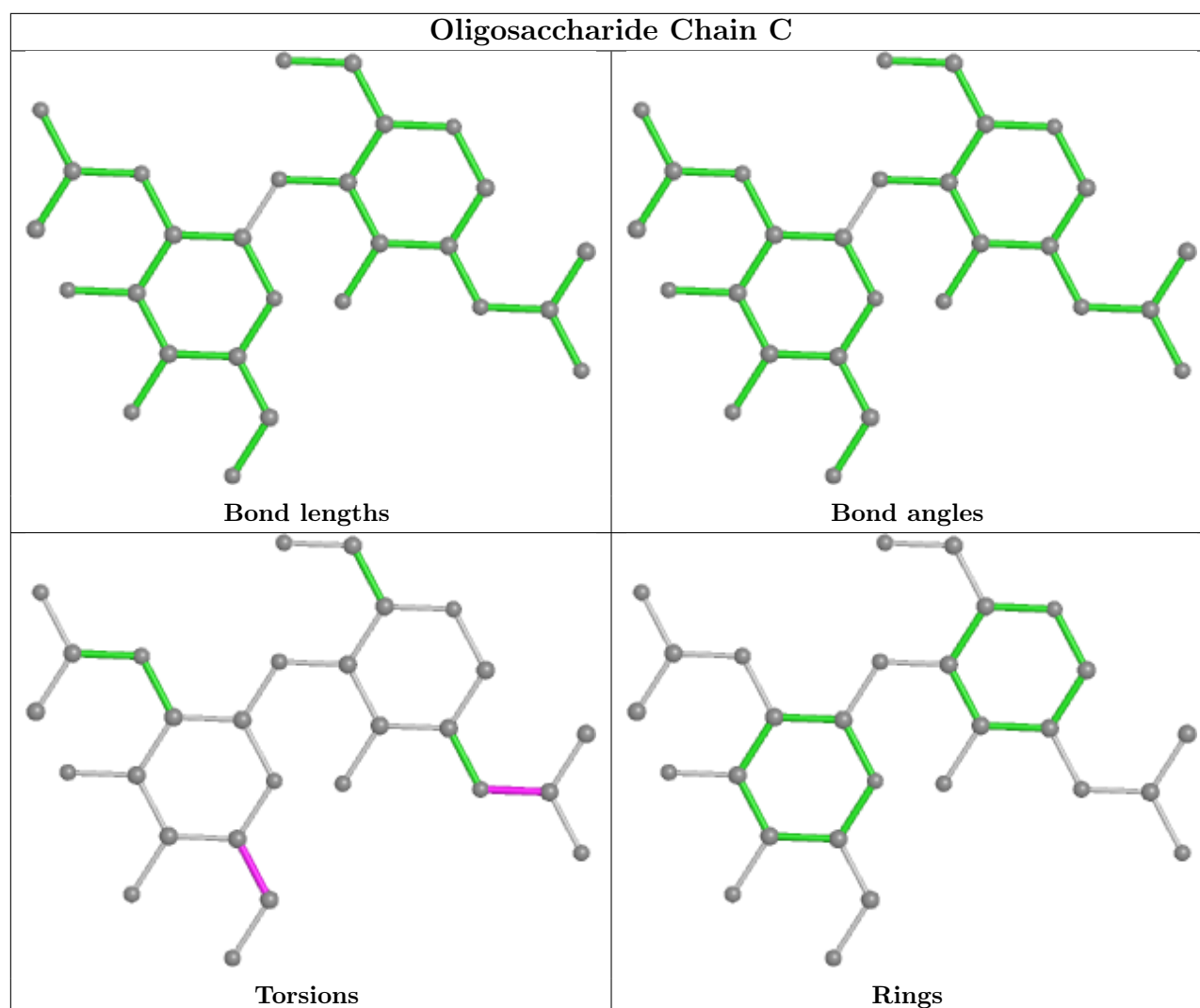
Mol	Chain	Res	Type	Atoms
2	C	1	NAG	C8-C7-N2-C2
2	C	1	NAG	O7-C7-N2-C2
2	D	1	NAG	C8-C7-N2-C2
2	D	1	NAG	O7-C7-N2-C2
2	D	2	NAG	O5-C5-C6-O6
2	D	2	NAG	C4-C5-C6-O6
2	C	2	NAG	O5-C5-C6-O6

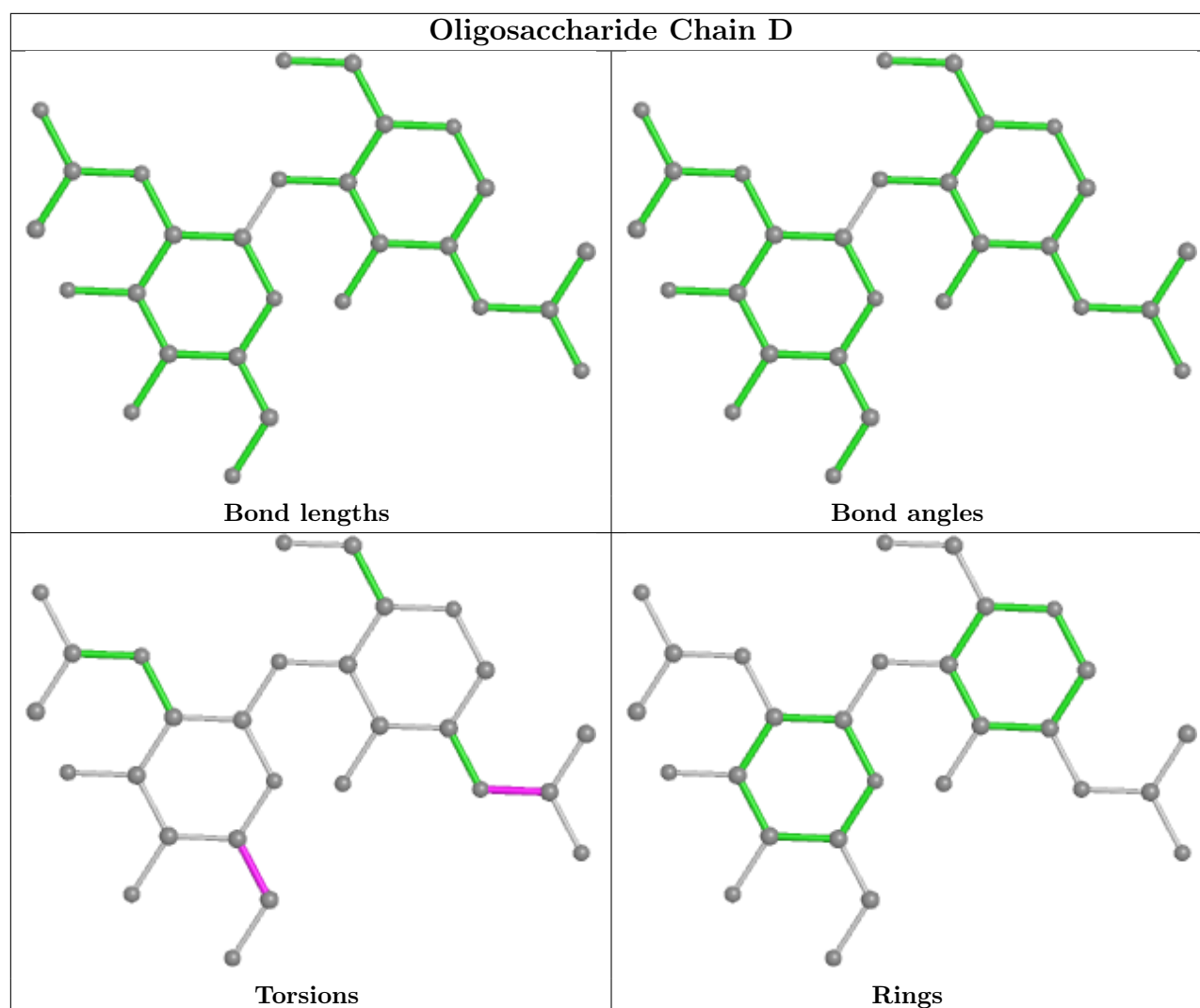
There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	1	NAG	1	0
2	C	1	NAG	1	0
2	D	2	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](#)

Of 19 ligands modelled in this entry, 2 are monoatomic - leaving 17 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	$\# Z > 2$
4	NAG	B	604	1	14,14,15	0.45	0	17,19,21	0.68	0
4	NAG	B	610	1	14,14,15	0.13	0	17,19,21	0.77	1 (5%)
8	PG4	B	606	-	12,12,12	0.52	0	11,11,11	0.19	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	1PE	A	609	-	15,15,15	0.50	0	14,14,14	0.46	0
4	NAG	A	610	1	14,14,15	0.24	0	17,19,21	0.58	0
5	SCN	A	605	-	1,2,2	0.66	0	0,1,1	-	-
5	SCN	B	607	-	1,2,2	0.38	0	0,1,1	-	-
5	SCN	A	608	-	1,2,2	0.84	0	0,1,1	-	-
5	SCN	A	606	-	1,2,2	0.74	0	0,1,1	-	-
3	FAD	B	601	1	53,58,58	0.56	0	68,89,89	0.61	1 (1%)
5	SCN	A	611	-	1,2,2	0.57	0	0,1,1	-	-
5	SCN	B	605	-	1,2,2	0.18	0	0,1,1	-	-
4	NAG	A	604	1	14,14,15	0.44	0	17,19,21	0.53	0
3	FAD	A	601	1	53,58,58	0.56	0	68,89,89	0.67	2 (2%)
5	SCN	A	607	-	1,2,2	0.91	0	0,1,1	-	-
9	PEG	B	609	-	6,6,6	0.45	0	5,5,5	0.21	0
8	PG4	B	608	-	12,12,12	0.54	0	11,11,11	0.21	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
4	NAG	B	604	1	-	0/6/23/26	0/1/1/1
4	NAG	B	610	1	-	0/6/23/26	0/1/1/1
8	PG4	B	606	-	-	6/10/10/10	-
6	1PE	A	609	-	-	1/13/13/13	-
4	NAG	A	610	1	-	2/6/23/26	0/1/1/1
3	FAD	B	601	1	-	1/30/50/50	0/6/6/6
4	NAG	A	604	1	-	2/6/23/26	0/1/1/1
3	FAD	A	601	1	-	1/30/50/50	0/6/6/6
8	PG4	B	608	-	-	0/10/10/10	-
9	PEG	B	609	-	-	2/4/4/4	-

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	610	NAG	C1-O5-C5	2.78	115.95	112.19
3	A	601	FAD	C5A-C6A-N6A	2.69	124.44	120.35
3	B	601	FAD	C5A-C6A-N6A	2.43	124.05	120.35
3	A	601	FAD	P-O3P-PA	2.39	141.02	132.83

There are no chirality outliers.

All (15) torsion outliers are listed below:

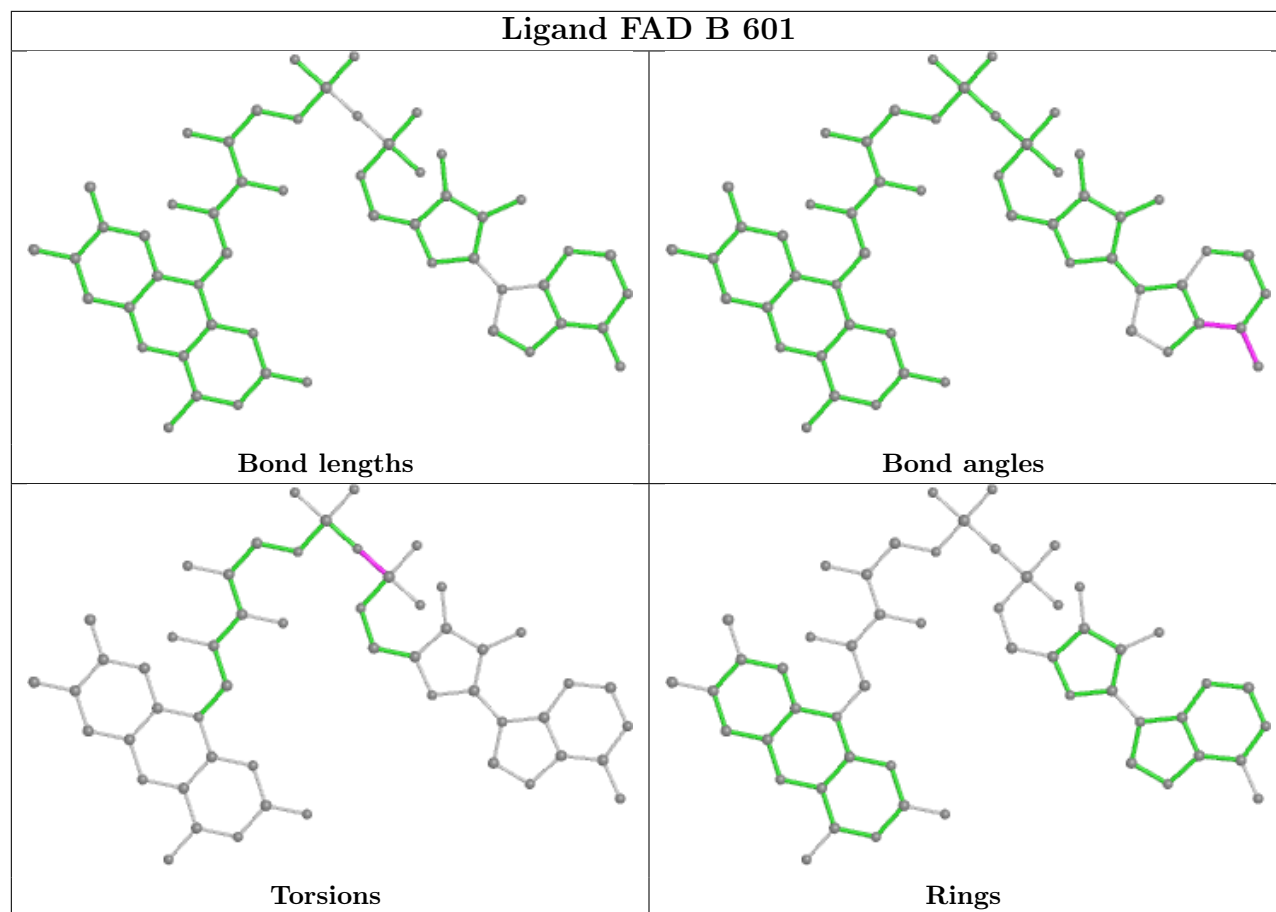
Mol	Chain	Res	Type	Atoms
3	B	601	FAD	P-O3P-PA-O5B
8	B	606	PG4	C6-C5-O3-C4
4	A	604	NAG	C4-C5-C6-O6
8	B	606	PG4	O2-C3-C4-O3
4	A	604	NAG	O5-C5-C6-O6
4	A	610	NAG	C4-C5-C6-O6
6	A	609	1PE	OH7-C16-C26-OH6
8	B	606	PG4	O3-C5-C6-O4
8	B	606	PG4	O1-C1-C2-O2
4	A	610	NAG	O5-C5-C6-O6
3	A	601	FAD	P-O3P-PA-O5B
9	B	609	PEG	C1-C2-O2-C3
8	B	606	PG4	C1-C2-O2-C3
9	B	609	PEG	O1-C1-C2-O2
8	B	606	PG4	C3-C4-O3-C5

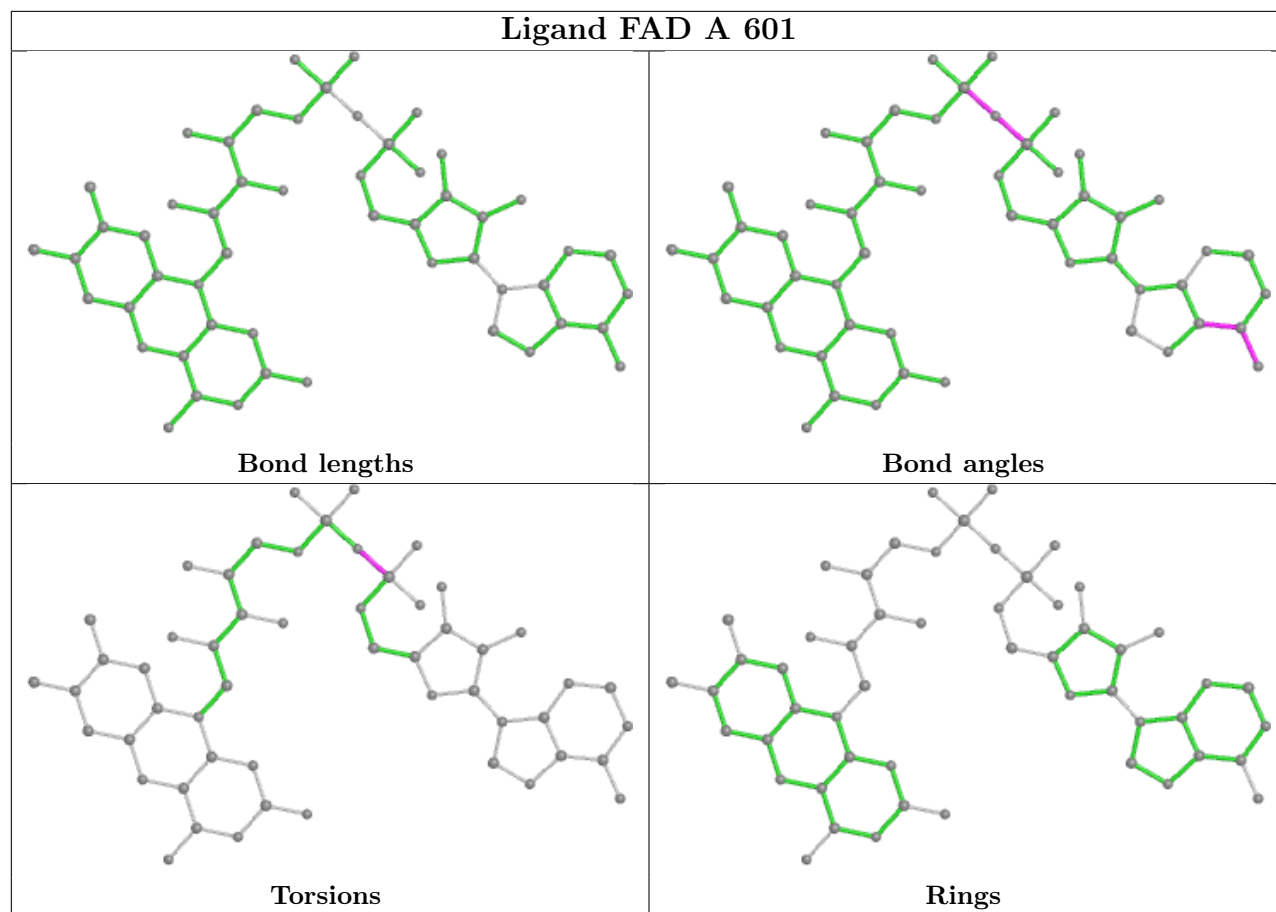
There are no ring outliers.

4 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	B	606	PG4	3	0
5	B	607	SCN	1	0
3	B	601	FAD	6	0
9	B	609	PEG	5	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	477/488 (97%)	-0.14	4 (0%) 86 87	18, 27, 54, 99	0
1	B	475/488 (97%)	-0.14	1 (0%) 95 94	21, 28, 53, 119	0
All	All	952/976 (97%)	-0.14	5 (0%) 91 91	18, 28, 54, 119	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	419	ILE	3.6
1	A	24	GLN	3.5
1	B	419	ILE	2.7
1	A	23	ALA	2.2
1	A	25	ASN	2.2

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

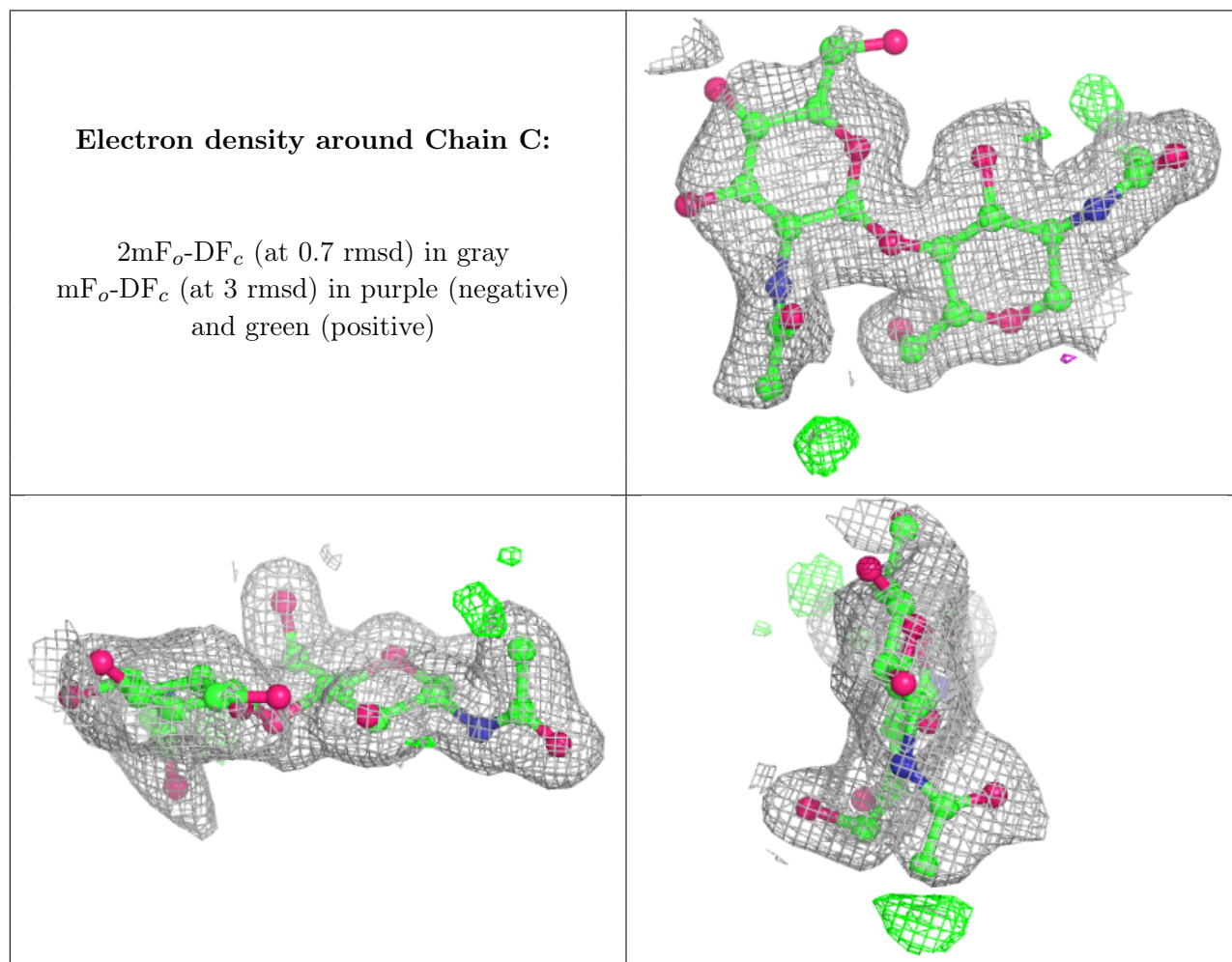
There are no non-standard protein/DNA/RNA residues in this entry.

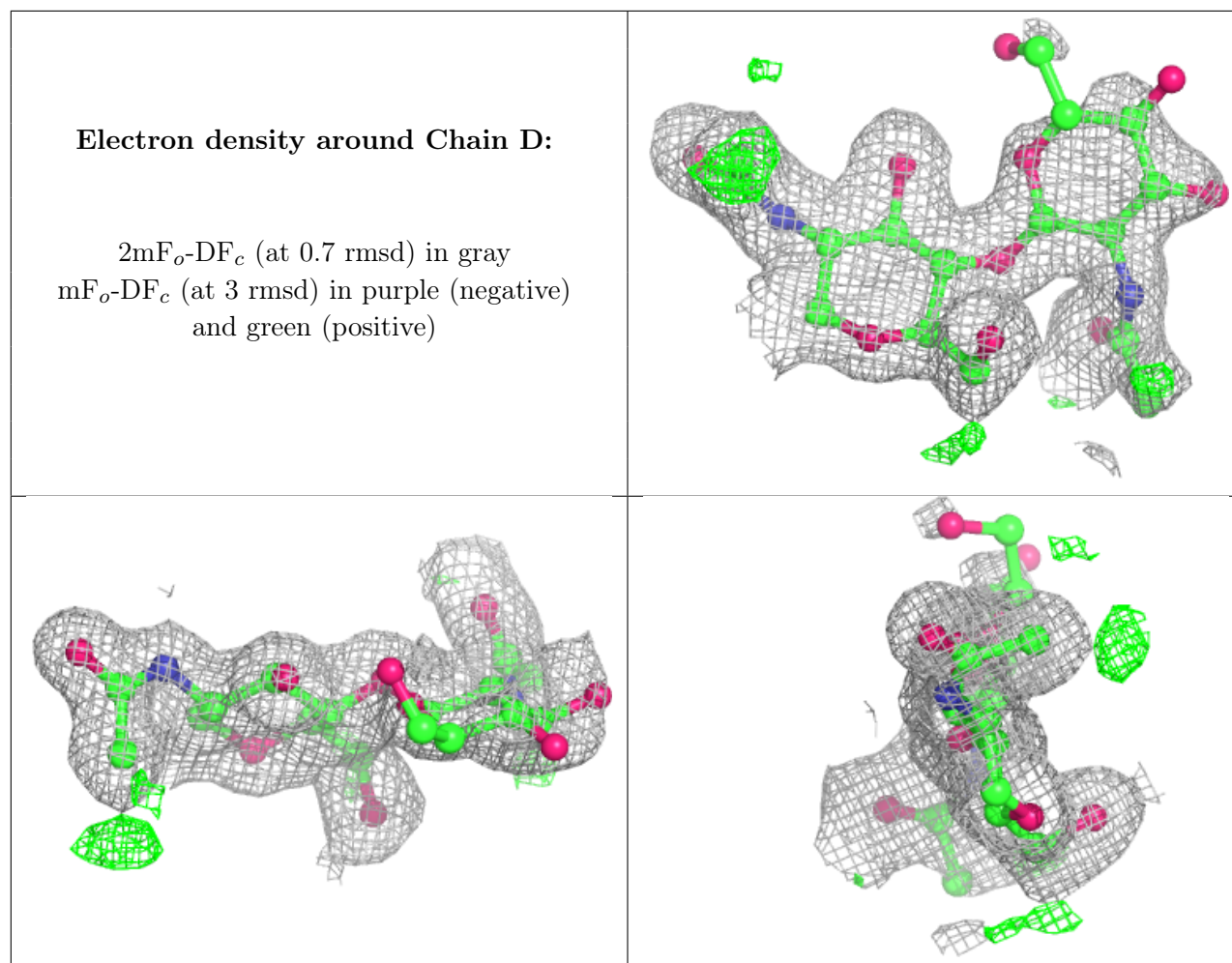
6.3 Carbohydrates [i](#)

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	0.85	0.17	55,68,87,93	0
2	NAG	D	2	14/15	0.86	0.21	59,81,118,121	0
2	NAG	D	1	14/15	0.94	0.07	19,29,35,41	0
2	NAG	C	1	14/15	0.95	0.08	21,29,42,44	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(\AA^2)	Q<0.9
4	NAG	A	610	14/15	0.65	0.24	62,78,93,95	0
4	NAG	B	610	14/15	0.67	0.29	65,108,128,129	0
8	PG4	B	608	13/13	0.77	0.17	73,75,83,86	0
8	PG4	B	606	13/13	0.78	0.20	62,70,78,79	0
9	PEG	B	609	7/7	0.81	0.21	47,53,65,66	0
6	1PE	A	609	16/16	0.88	0.14	38,53,72,77	0
4	NAG	A	604	14/15	0.90	0.13	38,51,67,74	0
4	NAG	B	604	14/15	0.92	0.11	31,38,45,53	0
3	FAD	A	601	53/53	0.94	0.09	17,21,25,26	0
7	CL	B	611	1/1	0.95	0.12	40,40,40,40	0

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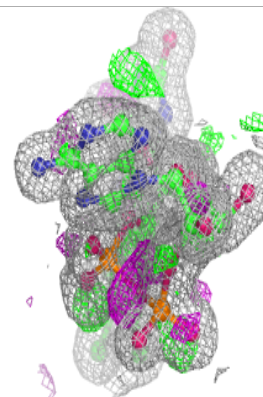
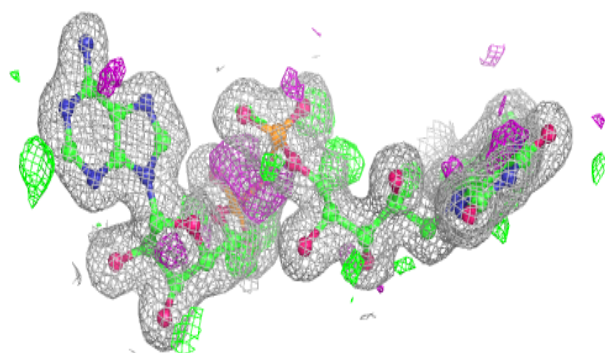
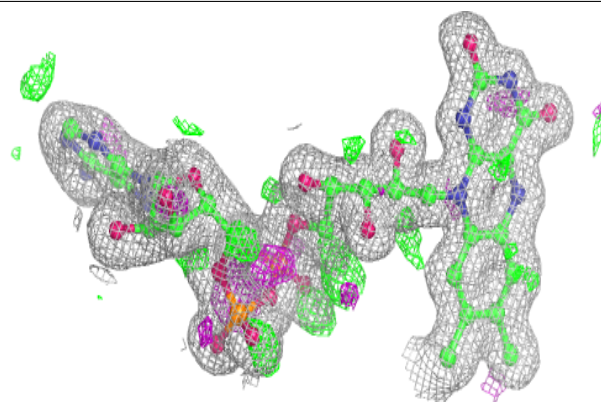
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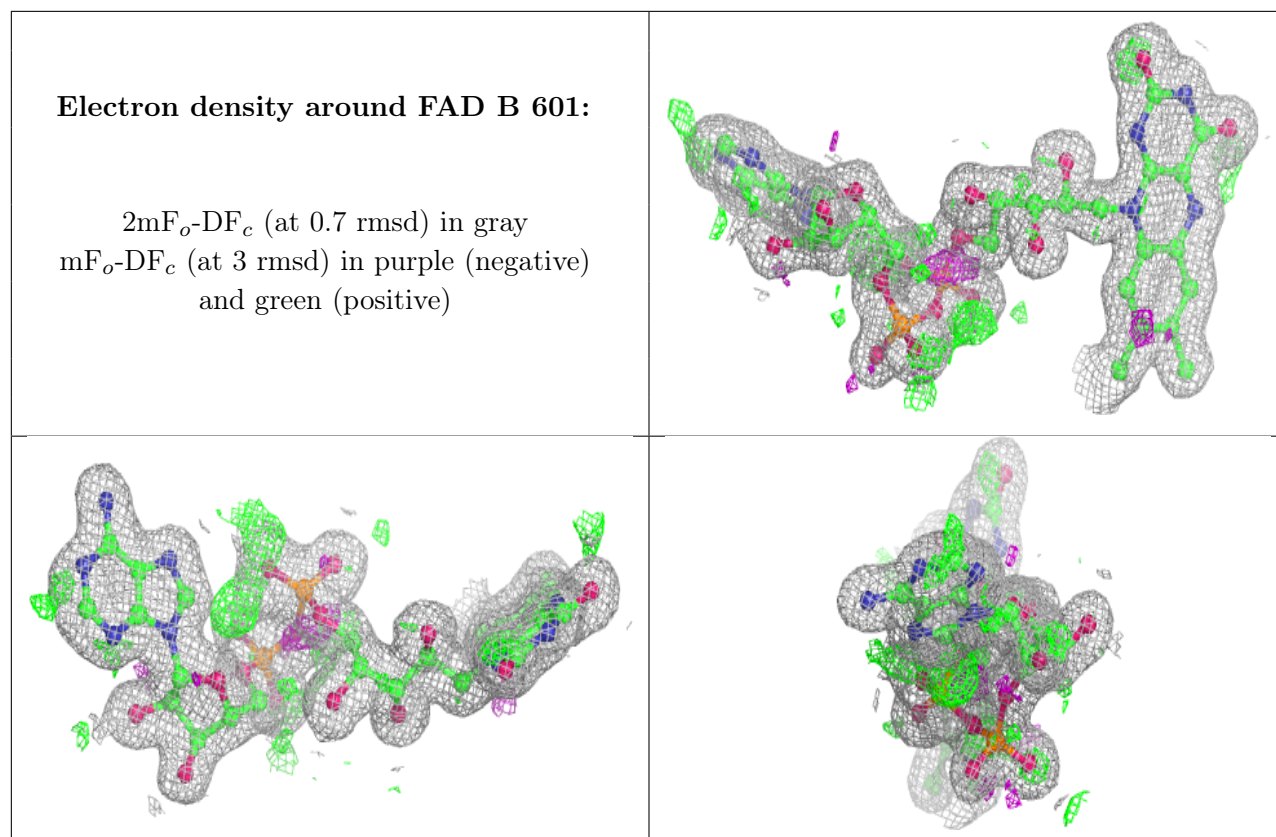
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	FAD	B	601	53/53	0.96	0.09	15,21,26,27	0
5	SCN	A	611	3/3	0.97	0.09	35,35,44,52	0
5	SCN	A	606	3/3	0.97	0.10	30,30,33,34	0
5	SCN	A	608	3/3	0.97	0.09	39,39,46,47	0
5	SCN	B	605	3/3	0.98	0.07	30,30,31,36	0
5	SCN	A	607	3/3	0.98	0.06	36,36,48,56	0
5	SCN	A	605	3/3	0.99	0.10	17,17,23,25	0
7	CL	A	612	1/1	0.99	0.07	38,38,38,38	0
5	SCN	B	607	3/3	0.99	0.06	26,26,27,28	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 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 ⓘ

There are no such residues in this entry.