



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 13, 2024 – 11:57 pm GMT

PDB ID : 6ZE7  
Title : Chaetomium thermophilum FAD-dependent oxidoreductase in complex with 4-nitrophenol  
Authors : Svecova, L.; Skalova, T.; Kolenko, P.; Koval, T.; Oestergaard, L.H.; Dohnalek, J.  
Deposited on : 2020-06-16  
Resolution : 1.50 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](mailto: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>.

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

MolProbity : 4.02b-467  
Mogul : 1.8.4, CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.36  
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) : 2.36

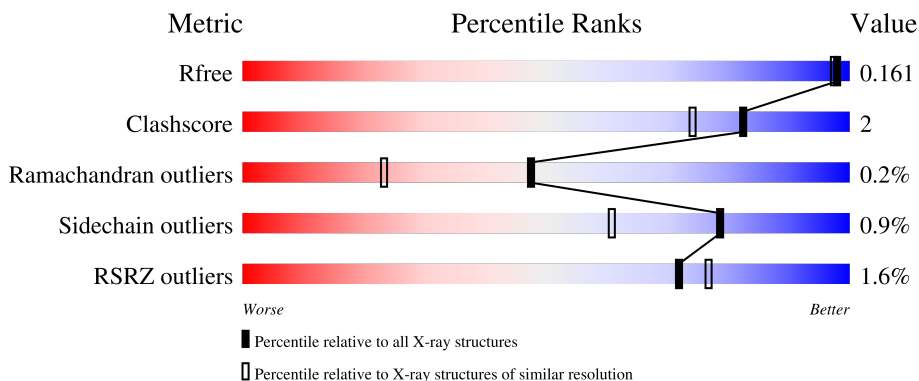
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

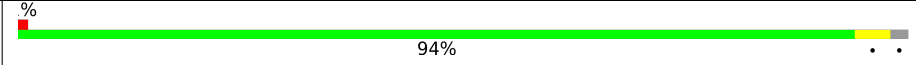
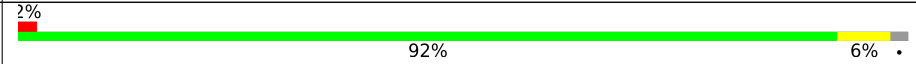

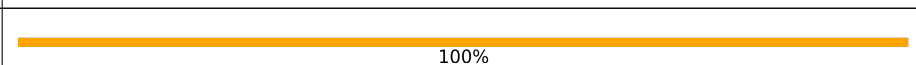
The reported resolution of this entry is 1.50 Å.

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	2936 (1.50-1.50)
Clashscore	141614	3144 (1.50-1.50)
Ramachandran outliers	138981	3066 (1.50-1.50)
Sidechain outliers	138945	3064 (1.50-1.50)
RSRZ outliers	127900	2884 (1.50-1.50)

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  $\geq 3$ , 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	595	 94%
1	B	595	 92% 6%
2	C	2	 50% 50%
2	D	2	 100%

## 2 Entry composition [i](#)

There are 12 unique types of molecules in this entry. The entry contains 11203 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-dependent oxidoreductase.

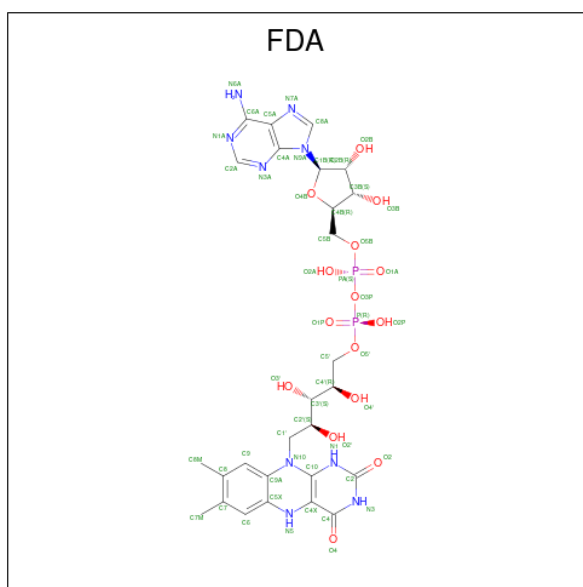
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	584	4665	2969	810	870	16	0	38	0
1	B	586	4661	2965	807	874	15	0	36	0

- 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	28	16	2	10	0	0	0
2	D	2	28	16	2	10	0	0	0

- Molecule 3 is DIHYDROFLAVINE-ADENINE DINUCLEOTIDE (three-letter code: FDA) (formula: C<sub>27</sub>H<sub>35</sub>N<sub>9</sub>O<sub>15</sub>P<sub>2</sub>) (labeled as "Ligand of Interest" by depositor).



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

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



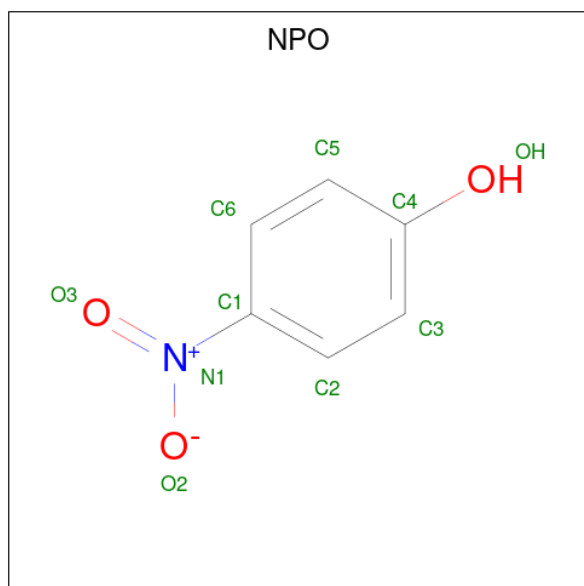
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
4	A	1	14	8	1	5	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	1
			16	9	1	6		
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 P-NITROPHENOL (three-letter code: NPO) (formula:  $C_6H_5NO_3$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	1
			10	6	1	3		
5	A	1	Total	C	N	O	0	0
			10	6	1	3		
5	B	1	Total	C	N	O	0	1
			10	6	1	3		

- Molecule 6 is FORMIC ACID (three-letter code: FMT) (formula:  $CH_2O_2$ ).



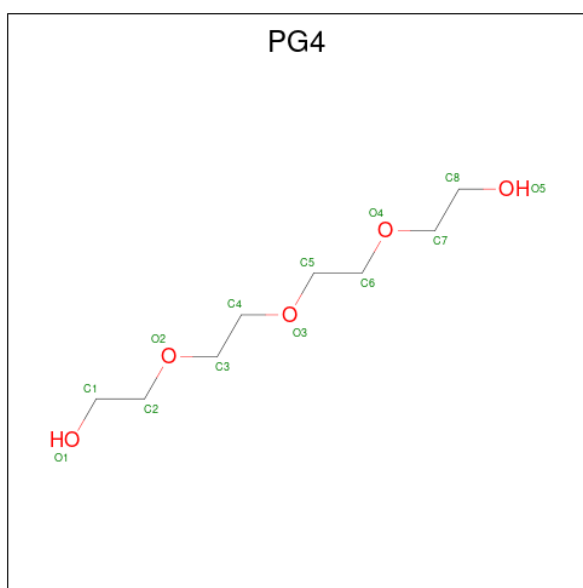
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C O 3 1 2	0	0
6	A	1	Total C O 3 1 2	0	0
6	A	1	Total C O 3 1 2	0	0
6	B	1	Total C O 3 1 2	0	0
6	B	1	Total C O 3 1 2	0	0
6	B	1	Total C O 3 1 2	0	0
6	B	1	Total C O 3 1 2	0	0
6	B	1	Total C O 3 1 2	0	0

- Molecule 7 is ACETATE ION (three-letter code: ACT) (formula: C<sub>2</sub>H<sub>3</sub>O<sub>2</sub>).



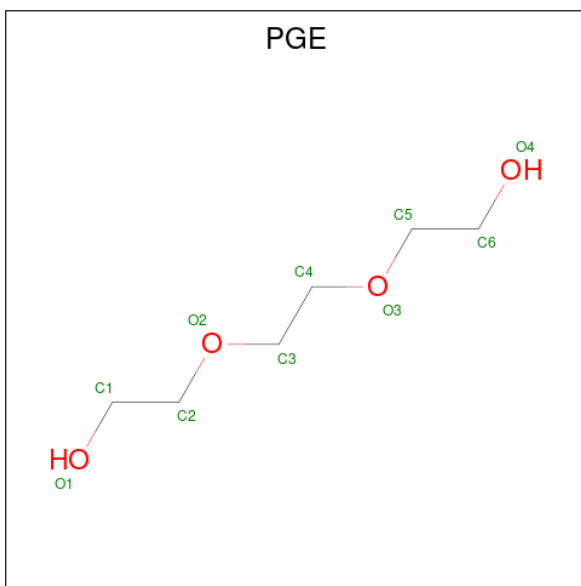
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			4	2	2		
7	B	1	Total	C	O	0	0
			4	2	2		

- Molecule 8 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: C<sub>8</sub>H<sub>18</sub>O<sub>5</sub>).



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

- Molecule 9 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: C<sub>6</sub>H<sub>14</sub>O<sub>4</sub>).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf		
9	A	1	Total	C	O	0	0
			10	6	4		
9	B	1	Total	C	O	0	0
			10	6	4		

- Molecule 10 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	
10	A	3	Total	Mg	0	0
			3	3		
10	B	2	Total	Mg	0	0
			2	2		

- Molecule 11 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	
11	A	1	Total	Na	0	0
			1	1		

- Molecule 12 is water.

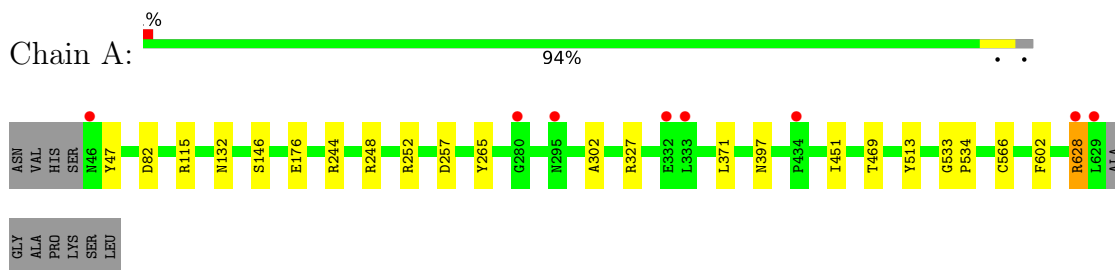
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	
12	A	735	Total	O	0	20
			752	752		
12	B	754	Total	O	0	15
			763	763		



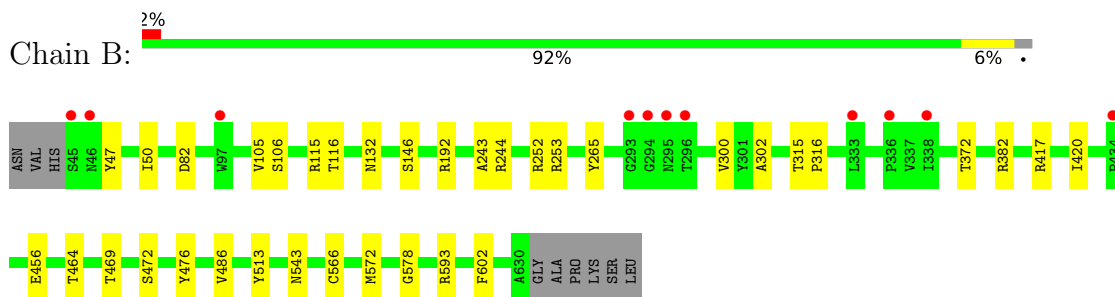
### 3 Residue-property plots [i](#)

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-dependent oxidoreductase



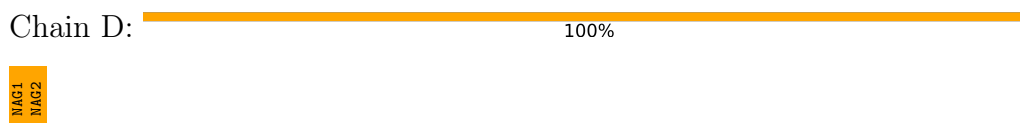
- Molecule 1: FAD-dependent oxidoreductase



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



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



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	92.61Å 109.67Å 115.63Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.23 – 1.50 47.19 – 1.50	Depositor EDS
% Data completeness (in resolution range)	99.3 (47.23-1.50) 99.3 (47.19-1.50)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.05 (at 1.50Å)	Xtrriage
Refinement program	REFMAC 5.8.0258	Depositor
R, $R_{free}$	0.155 , 0.182 0.156 , 0.161	Depositor DCC
$R_{free}$ test set	9455 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	14.3	Xtrriage
Anisotropy	0.249	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 43.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	11203	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	17.0	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 70.87 % 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 2.8998e-06. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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, NA, FDA, MG, FMT, PG4, NPO, PGE, ACT

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	0.77	0/4887	0.91	4/6664 (0.1%)
1	B	0.79	1/4876 (0.0%)	0.90	2/6649 (0.0%)
All	All	0.78	1/9763 (0.0%)	0.90	6/13313 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
All	All	0	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	472	SER	CA-CB	-5.45	1.44	1.52

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	115	ARG	NE-CZ-NH2	-8.96	115.82	120.30
1	B	115	ARG	NE-CZ-NH2	-8.83	115.89	120.30
1	B	593	ARG	NE-CZ-NH1	5.79	123.19	120.30
1	A	257	ASP	CB-CG-OD2	-5.49	113.36	118.30
1	A	115	ARG	NE-CZ-NH1	5.42	123.01	120.30
1	A	248	ARG	NE-CZ-NH2	5.14	122.87	120.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	566	CYS	Peptide
1	B	566	CYS	Peptide

## 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4665	0	4702	20	0
1	B	4661	0	4691	24	0
2	C	28	0	25	1	0
2	D	28	0	25	5	0
3	A	53	0	33	4	0
3	B	53	0	33	4	0
4	A	44	0	34	0	0
4	B	42	0	39	0	0
5	A	20	0	9	0	0
5	B	10	0	4	0	0
6	A	9	0	3	0	0
6	B	15	0	5	0	0
7	A	4	0	3	0	0
7	B	4	0	3	1	0
8	A	13	0	18	2	0
8	B	13	0	18	0	0
9	A	10	0	14	0	0
9	B	10	0	14	1	0
10	A	3	0	0	0	0
10	B	2	0	0	0	0
11	A	1	0	0	0	0
12	A	752	0	0	4	0
12	B	763	0	0	11	0
All	All	11203	0	9673	48	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 (48) 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:628[B]:ARG:NH2	12:A:802:HOH:O	1.75	1.17
12:B:1331[B]:HOH:O	2:D:2:NAG:H81	1.68	0.92
12:B:1331[B]:HOH:O	2:D:2:NAG:O7	1.93	0.86
1:A:628[B]:ARG:HG2	12:A:1397:HOH:O	1.85	0.77
1:A:244[A]:ARG:HG3	2:C:1:NAG:H83	1.68	0.75
12:B:1331[B]:HOH:O	2:D:2:NAG:C8	2.36	0.66
12:B:1331[B]:HOH:O	2:D:2:NAG:C7	2.42	0.62
1:A:146[B]:SER:HG	1:A:602:PHE:HZ	1.47	0.61
1:B:50:ILE:HD13	1:B:300[A]:VAL:HG13	1.83	0.61
1:B:132:ASN:HB2	3:B:701:FDA:C5X	2.33	0.59
1:A:132:ASN:HB2	3:A:701:FDA:C5X	2.33	0.57
1:B:417[A]:ARG:HG2	1:B:417[A]:ARG:HH11	1.68	0.57
1:B:543:ASN:ND2	12:B:806:HOH:O	2.37	0.56
1:A:327[B]:ARG:NH1	12:A:809:HOH:O	2.38	0.55
1:B:244[A]:ARG:HG3	2:D:1:NAG:H83	1.87	0.55
1:A:132:ASN:HB2	3:A:701:FDA:N5	2.22	0.55
1:B:132:ASN:HB2	3:B:701:FDA:N5	2.22	0.55
1:B:372:THR:HA	9:B:713:PGE:H62	1.88	0.55
1:A:132:ASN:HB2	3:A:701:FDA:C4X	2.38	0.54
7:B:711:ACT:H1	12:B:1324:HOH:O	2.09	0.52
1:A:132:ASN:HA	3:A:701:FDA:C6	2.41	0.51
1:B:132:ASN:HB2	3:B:701:FDA:C4X	2.42	0.50
1:B:146[B]:SER:HG	1:B:602:PHE:HZ	1.58	0.49
1:B:464[B]:THR:OG1	1:B:476[B]:TYR:HB2	2.11	0.49
1:B:253[B]:ARG:HD2	12:B:1211:HOH:O	2.13	0.47
1:A:397[B]:ASN:HD21	8:A:711:PG4:H81	1.79	0.46
1:A:47:TYR:O	1:A:302:ALA:HA	2.16	0.45
1:B:106:SER:O	1:B:116[B]:THR:HG23	2.17	0.44
1:B:486[B]:VAL:HG12	12:B:1180:HOH:O	2.17	0.44
1:A:146[B]:SER:OG	1:A:602:PHE:HZ	2.01	0.44
1:B:253[B]:ARG:HD3	12:B:1076:HOH:O	2.17	0.44
1:A:628[A]:ARG:HH21	1:A:628[A]:ARG:HG2	1.83	0.43
1:B:105[B]:VAL:HG22	12:B:1208:HOH:O	2.18	0.43
1:B:420:ILE:HD13	1:B:456[A]:GLU:CG	2.48	0.43
1:A:397[B]:ASN:HD21	8:A:711:PG4:C8	2.31	0.43
1:A:371:LEU:HD13	12:A:876[B]:HOH:O	2.18	0.43
1:B:192:ARG:NE	12:B:816:HOH:O	2.47	0.42
1:B:132:ASN:HA	3:B:701:FDA:C6	2.49	0.42
1:B:420:ILE:HD13	1:B:456[A]:GLU:HG2	2.01	0.42
1:B:382:ARG:HA	1:B:382:ARG:HD2	1.84	0.41
1:B:315:THR:N	1:B:316[B]:PRO:HD2	2.35	0.41
1:B:572:MET:O	1:B:578:GLY:HA3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:176:GLU:HB3	1:B:243:ALA:O	2.21	0.41
1:A:533:GLY:N	1:A:534:PRO:HD3	2.35	0.41
1:A:451[B]:ILE:HD11	1:A:602:PHE:CD1	2.56	0.40
1:B:47:TYR:O	1:B:302:ALA:HA	2.21	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	620/595 (104%)	598 (96%)	21 (3%)	1 (0%)	47 23
1	B	620/595 (104%)	593 (96%)	26 (4%)	1 (0%)	47 23
All	All	1240/1190 (104%)	1191 (96%)	47 (4%)	2 (0%)	47 23

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	469	THR
1	B	469	THR

### 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.

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	515/485 (106%)	508 (99%)	7 (1%)	67	42
1	B	514/485 (106%)	509 (99%)	5 (1%)	76	57
All	All	1029/970 (106%)	1017 (99%)	12 (1%)	78	48

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	82	ASP
1	A	252[A]	ARG
1	A	252[B]	ARG
1	A	265	TYR
1	A	513	TYR
1	A	628[A]	ARG
1	A	628[B]	ARG
1	B	82	ASP
1	B	252[A]	ARG
1	B	252[B]	ARG
1	B	265	TYR
1	B	513	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	331	ASN
1	B	46	ASN
1	B	331	ASN
1	B	409	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

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	1.76	2 (14%)	17,19,21	2.40	4 (23%)
2	NAG	C	2	2	14,14,15	0.48	0	17,19,21	1.02	1 (5%)
2	NAG	D	1	2,1	14,14,15	1.82	4 (28%)	17,19,21	3.25	4 (23%)
2	NAG	D	2	2	14,14,15	0.61	0	17,19,21	1.50	1 (5%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

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

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1	NAG	O5-C1	4.44	1.50	1.43
2	D	1	NAG	O4-C4	3.76	1.51	1.43
2	C	1	NAG	O4-C4	3.41	1.51	1.43
2	D	1	NAG	O5-C5	2.96	1.49	1.43
2	D	1	NAG	C1-C2	-2.77	1.48	1.52
2	D	1	NAG	C6-C5	2.46	1.60	1.51

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	1	NAG	C1-O5-C5	8.57	123.81	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1	NAG	O5-C1-C2	-7.84	98.91	111.29
2	D	1	NAG	O5-C5-C6	6.26	117.01	107.20
2	D	1	NAG	O5-C1-C2	-5.47	102.65	111.29
2	D	2	NAG	C1-O5-C5	5.21	119.25	112.19
2	D	1	NAG	O3-C3-C4	-4.95	98.92	110.35
2	C	1	NAG	C1-C2-N2	3.11	115.81	110.49
2	C	1	NAG	C1-O5-C5	2.65	115.78	112.19
2	C	1	NAG	O3-C3-C4	-2.63	104.26	110.35
2	C	2	NAG	C3-C4-C5	-2.15	106.41	110.24

There are no chirality outliers.

All (3) torsion outliers are listed below:

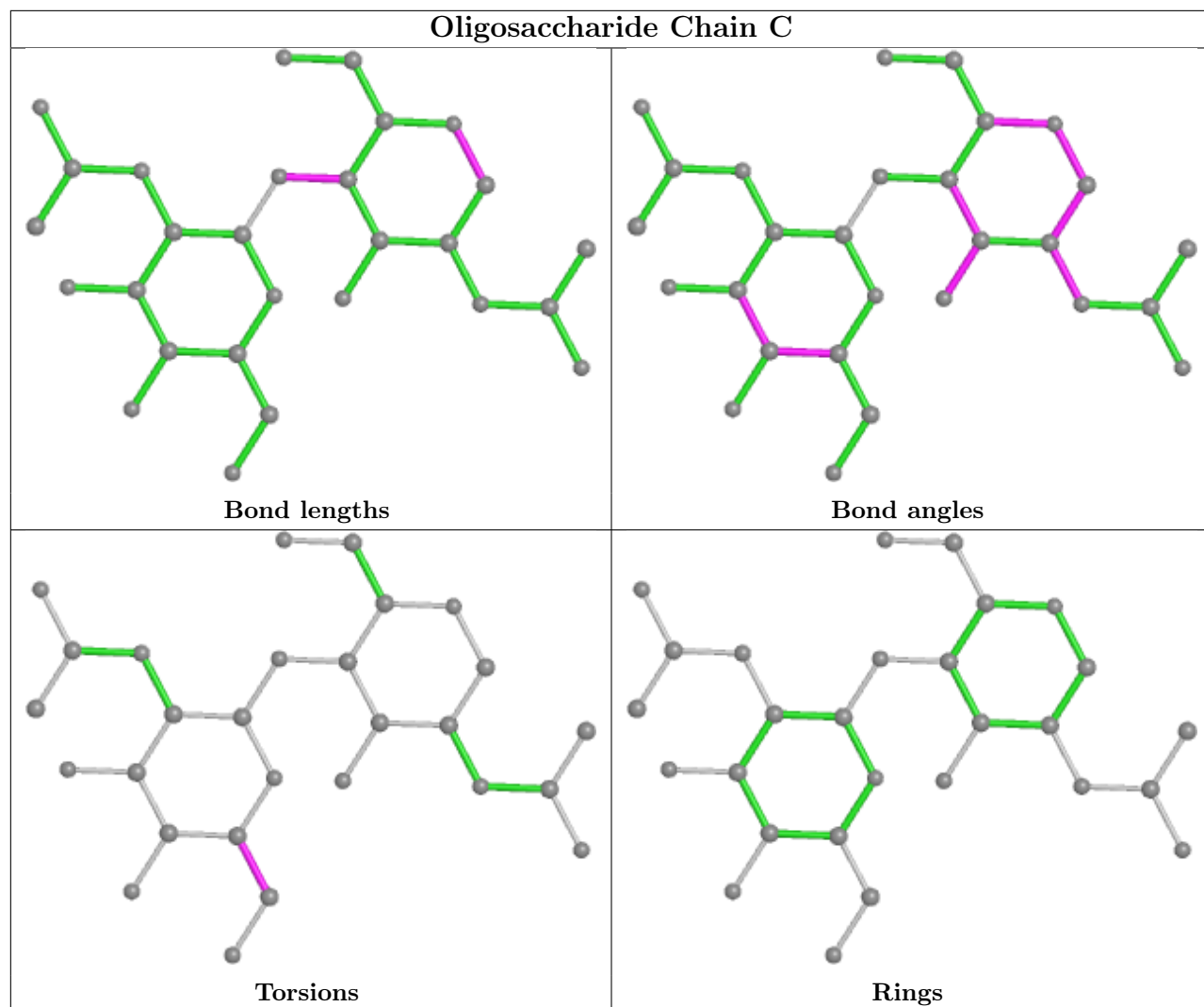
Mol	Chain	Res	Type	Atoms
2	C	2	NAG	O5-C5-C6-O6
2	C	2	NAG	C4-C5-C6-O6
2	D	1	NAG	O5-C5-C6-O6

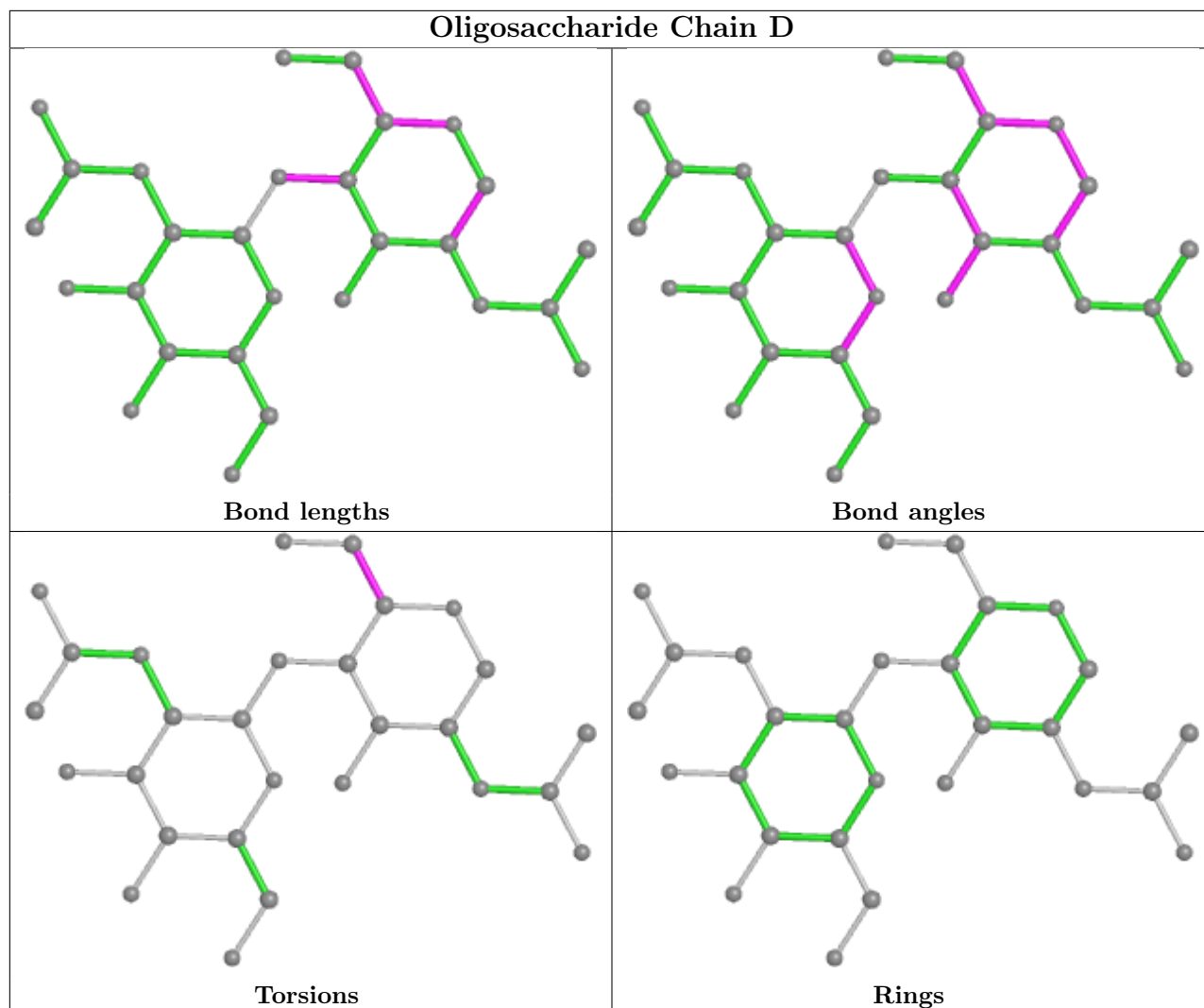
There are no ring outliers.

3 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	1	NAG	1	0
2	D	2	NAG	4	0
2	D	1	NAG	1	0

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





## 5.6 Ligand geometry [i](#)

Of 32 ligands modelled in this entry, 6 are monoatomic - leaving 26 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	$\# Z  > 2$
6	FMT	B	709	-	2,2,2	0.45	0	1,1,1	0.14	0
4	NAG	A	703[A]	-	14,14,15	0.89	0	17,19,21	1.17	2 (11%)
7	ACT	B	711	-	3,3,3	0.90	0	3,3,3	0.82	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
6	FMT	A	708	-	2,2,2	0.26	0	1,1,1	0.03	0
6	FMT	B	707	-	2,2,2	0.33	0	1,1,1	0.03	0
3	FDA	B	701	-	52,58,58	0.88	1 (1%)	60,89,89	0.89	3 (5%)
6	FMT	A	709	-	2,2,2	0.50	0	1,1,1	0.11	0
9	PGE	A	712	-	9,9,9	0.23	0	8,8,8	0.49	0
8	PG4	A	711	-	12,12,12	0.30	0	11,11,11	0.22	0
6	FMT	B	710	-	2,2,2	0.48	0	1,1,1	0.20	0
5	NPO	B	705[A]	-	9,10,10	0.84	0	11,13,13	0.89	0
6	FMT	A	707	-	2,2,2	0.39	0	1,1,1	0.39	0
4	NAG	B	703	1	14,14,15	1.42	2 (14%)	17,19,21	0.84	1 (5%)
9	PGE	B	713	-	9,9,9	0.28	0	8,8,8	0.32	0
4	NAG	A	704	1	14,14,15	0.92	0	17,19,21	1.29	1 (5%)
6	FMT	B	706	-	2,2,2	0.30	0	1,1,1	0.32	0
3	FDA	A	701	-	52,58,58	0.78	0	60,89,89	0.87	3 (5%)
8	PG4	B	712	-	12,12,12	0.21	0	11,11,11	0.19	0
4	NAG	A	702	1	14,14,15	0.36	0	17,19,21	1.11	1 (5%)
5	NPO	A	706	-	9,10,10	0.33	0	11,13,13	0.83	0
6	FMT	B	708	-	2,2,2	0.43	0	1,1,1	0.09	0
4	NAG	B	704	1	14,14,15	0.73	0	17,19,21	1.21	1 (5%)
5	NPO	A	705[A]	-	9,10,10	0.41	0	11,13,13	0.75	0
4	NAG	A	703[B]	-	14,14,15	0.89	0	17,19,21	1.26	2 (11%)
7	ACT	A	710	-	3,3,3	0.92	0	3,3,3	0.86	0
4	NAG	B	702	1	14,14,15	0.41	0	17,19,21	1.28	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
3	FDA	A	701	-	-	5/30/50/50	0/6/6/6
3	FDA	B	701	-	-	5/30/50/50	0/6/6/6
4	NAG	B	703	1	-	0/6/23/26	0/1/1/1
9	PGE	A	712	-	-	3/7/7/7	-
5	NPO	B	705[A]	-	-	0/2/4/4	0/1/1/1
4	NAG	A	703[A]	-	-	0/6/23/26	0/1/1/1
8	PG4	A	711	-	-	1/10/10/10	-
8	PG4	B	712	-	-	0/10/10/10	-
4	NAG	A	702	1	-	2/6/23/26	0/1/1/1
5	NPO	A	706	-	-	0/2/4/4	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	A	704	1	-	0/6/23/26	0/1/1/1
4	NAG	B	704	1	-	0/6/23/26	0/1/1/1
5	NPO	A	705[A]	-	-	0/2/4/4	0/1/1/1
4	NAG	A	703[B]	-	-	0/6/23/26	0/1/1/1
9	PGE	B	713	-	-	4/7/7/7	-
4	NAG	B	702	1	-	2/6/23/26	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	703	NAG	O4-C4	3.13	1.50	1.43
4	B	703	NAG	O5-C1	-2.84	1.39	1.43
3	B	701	FDA	O2'-C2'	-2.57	1.37	1.43

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	704	NAG	C6-C5-C4	3.23	120.57	113.00
4	B	702	NAG	C4-C3-C2	-3.12	106.45	111.02
3	A	701	FDA	C5A-C6A-N6A	2.91	124.77	120.35
4	A	703[A]	NAG	O5-C1-C2	-2.86	106.77	111.29
4	A	703[B]	NAG	O5-C1-C2	-2.86	106.77	111.29
4	B	702	NAG	C8-C7-N2	2.68	120.63	116.10
3	B	701	FDA	O2P-P-O1P	2.65	125.34	112.24
4	A	703[A]	NAG	C2-N2-C7	2.37	126.28	122.90
4	A	703[B]	NAG	C2-N2-C7	2.37	126.28	122.90
3	B	701	FDA	C4-C4X-N5	2.23	122.71	116.63
4	A	702	NAG	O5-C5-C6	2.17	110.61	107.20
3	A	701	FDA	O2P-P-O1P	2.15	122.86	112.24
3	B	701	FDA	O4B-C1B-C2B	-2.13	103.81	106.93
4	A	704	NAG	O7-C7-C8	2.11	125.98	122.06
4	B	703	NAG	C2-N2-C7	2.11	125.90	122.90
3	A	701	FDA	C4-C4X-N5	2.03	122.17	116.63

There are no chirality outliers.

All (22) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	701	FDA	PA-O3P-P-O5'
3	B	701	FDA	PA-O3P-P-O5'
9	A	712	PGE	C3-C4-O3-C5

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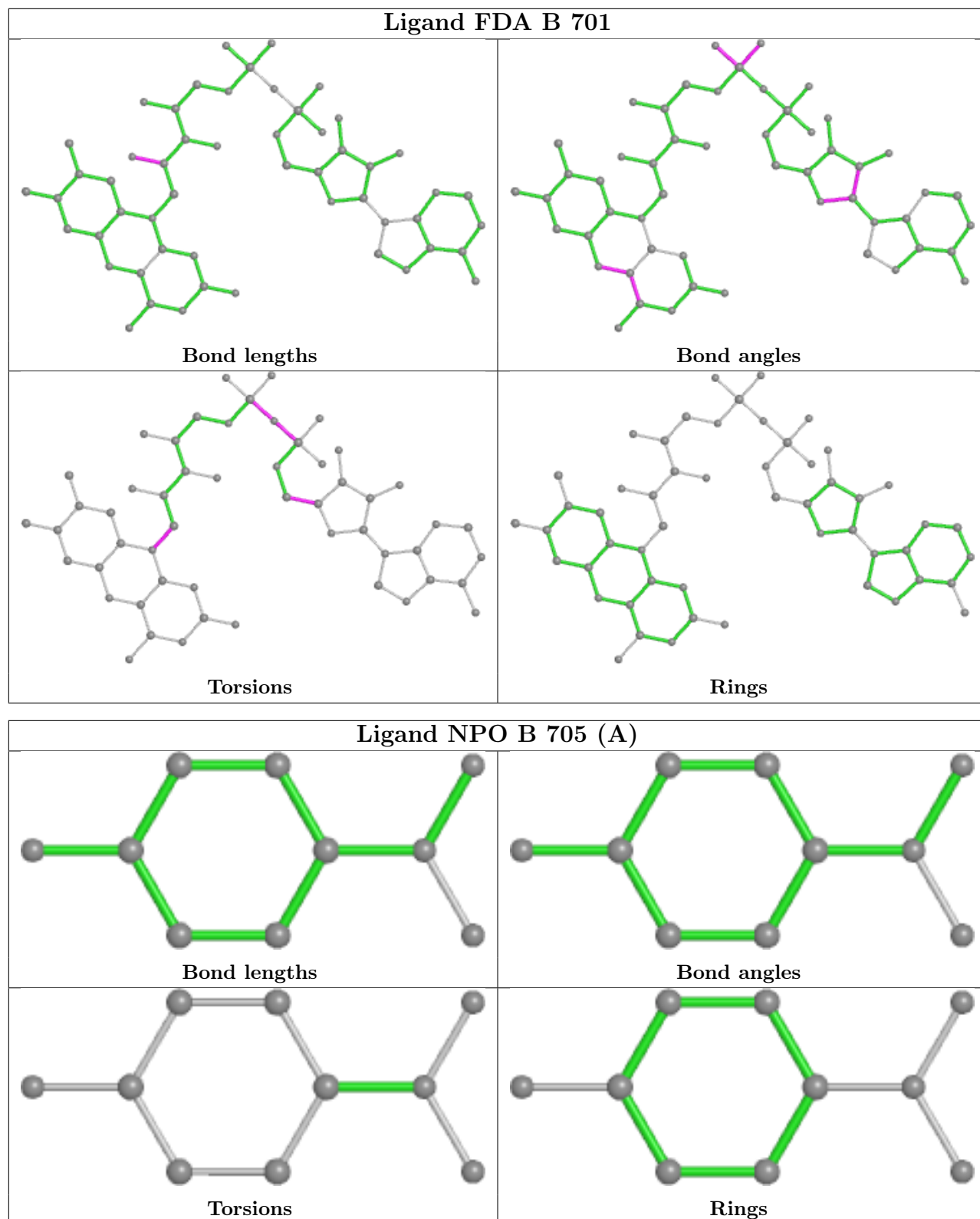
Mol	Chain	Res	Type	Atoms
9	B	713	PGE	O2-C3-C4-O3
4	A	702	NAG	O5-C5-C6-O6
9	A	712	PGE	O1-C1-C2-O2
4	B	702	NAG	C8-C7-N2-C2
4	B	702	NAG	O7-C7-N2-C2
4	A	702	NAG	C4-C5-C6-O6
9	A	712	PGE	O3-C5-C6-O4
3	A	701	FDA	P-O3P-PA-O1A
3	B	701	FDA	P-O3P-PA-O1A
9	B	713	PGE	C3-C4-O3-C5
9	B	713	PGE	C6-C5-O3-C4
8	A	711	PG4	O1-C1-C2-O2
9	B	713	PGE	C1-C2-O2-C3
3	A	701	FDA	P-O3P-PA-O2A
3	A	701	FDA	O4B-C4B-C5B-O5B
3	A	701	FDA	C2'-C1'-N10-C10
3	B	701	FDA	C2'-C1'-N10-C10
3	B	701	FDA	O4B-C4B-C5B-O5B
3	B	701	FDA	P-O3P-PA-O2A

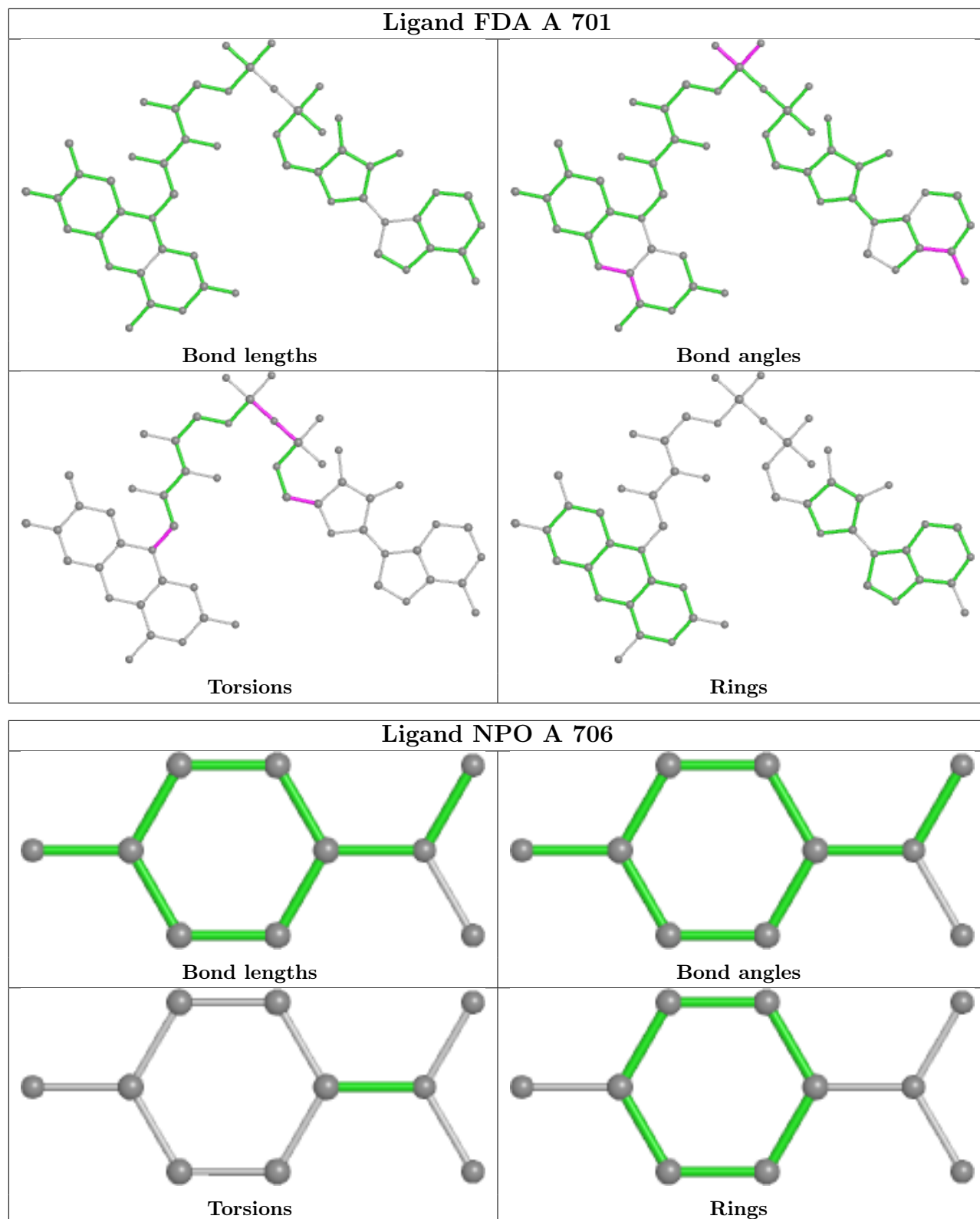
There are no ring outliers.

5 monomers are involved in 12 short contacts:

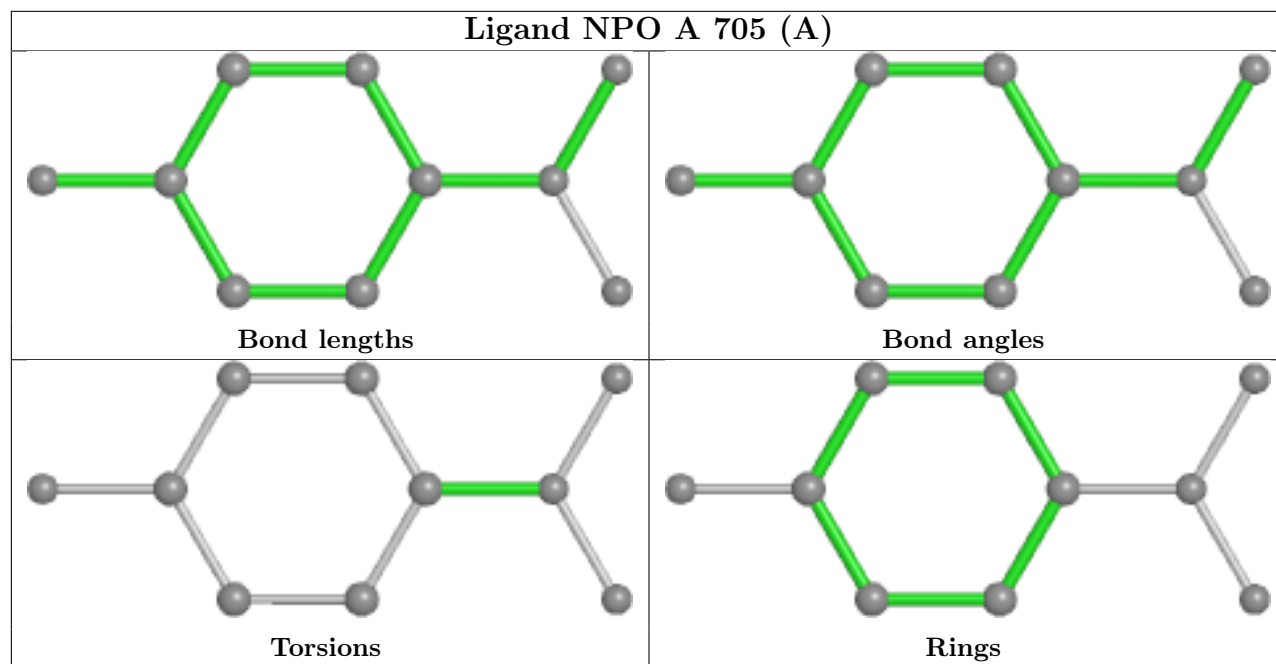
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	B	711	ACT	1	0
3	B	701	FDA	4	0
8	A	711	PG4	2	0
9	B	713	PGE	1	0
3	A	701	FDA	4	0

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	584/595 (98%)	-0.12	8 (1%) 75 79	8, 14, 27, 64	4 (0%)
1	B	586/595 (98%)	-0.09	11 (1%) 66 71	8, 14, 26, 53	5 (0%)
All	All	1170/1190 (98%)	-0.11	19 (1%) 72 77	8, 14, 27, 64	9 (0%)

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	295	ASN	5.0
1	B	296	THR	3.9
1	A	434	PRO	3.9
1	A	629	LEU	3.9
1	B	45	SER	3.7
1	B	295	ASN	3.7
1	A	628[A]	ARG	3.6
1	A	280	GLY	3.4
1	B	338	ILE	3.0
1	B	293	GLY	2.7
1	B	336	PRO	2.6
1	B	434	PRO	2.6
1	B	46	ASN	2.5
1	A	46	ASN	2.4
1	A	332	GLU	2.4
1	B	333	LEU	2.3
1	B	97	TRP	2.2
1	A	333	LEU	2.1
1	B	294	GLY	2.1

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

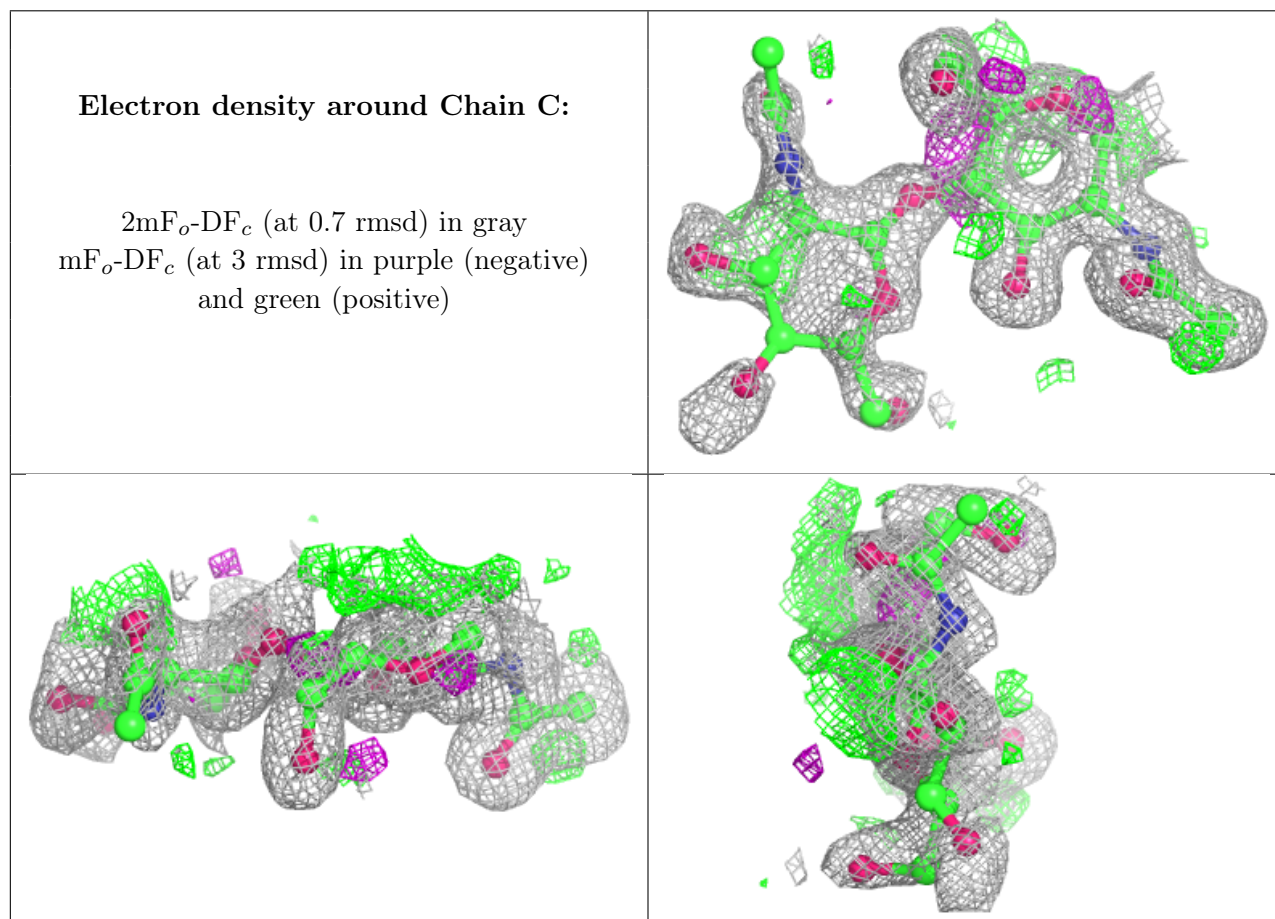
There are no non-standard protein/DNA/RNA residues in this entry.

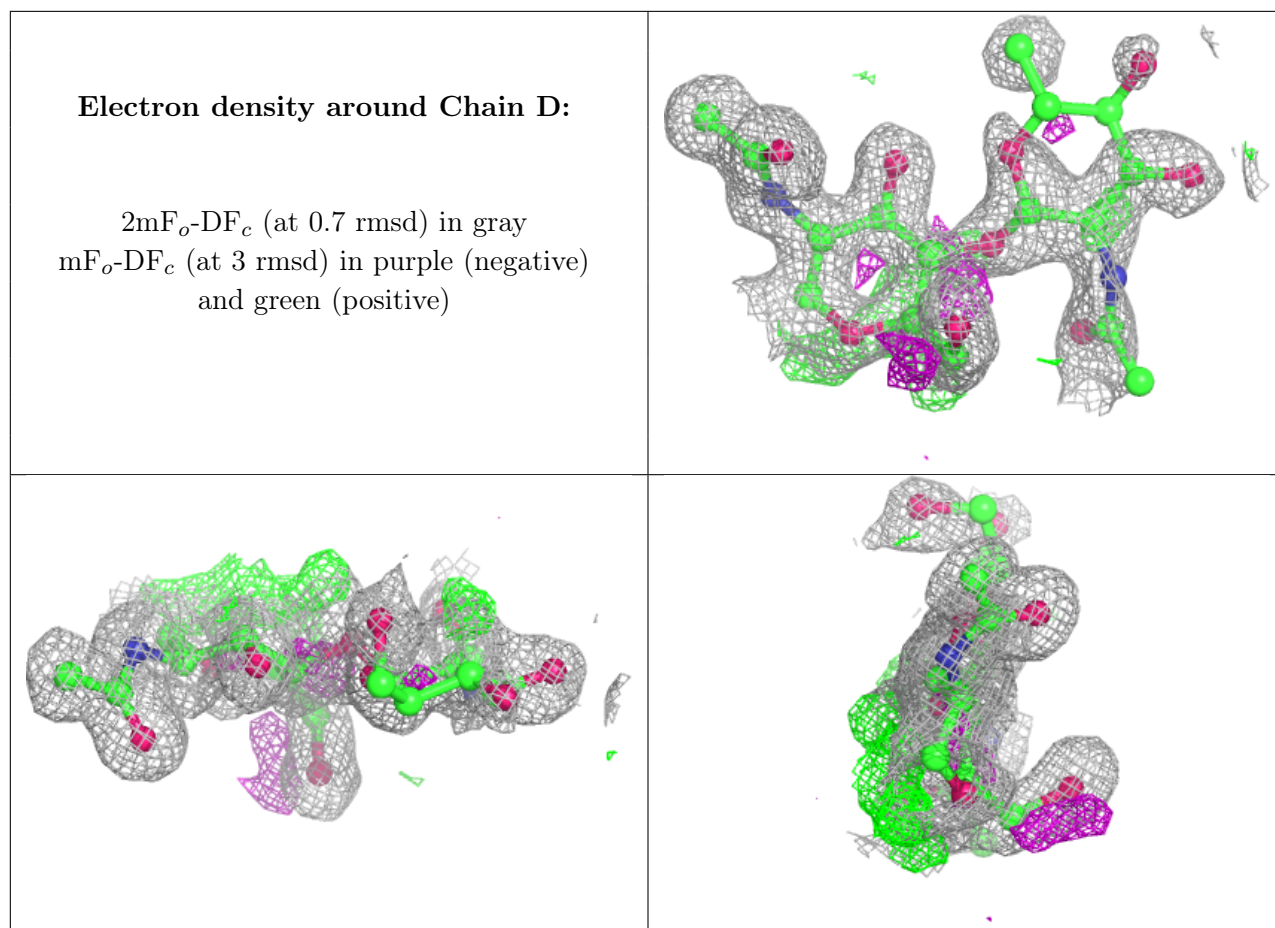
### 6.3 Carbohydrates [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
2	NAG	D	2	14/15	0.64	0.19	40,47,50,51	14
2	NAG	C	2	14/15	0.67	0.22	34,45,50,51	14
2	NAG	C	1	14/15	0.85	0.14	15,19,25,30	0
2	NAG	D	1	14/15	0.87	0.14	15,20,28,36	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 [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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
5	NPO	A	706	10/10	0.72	0.20	33,35,39,39	10
7	ACT	B	711	4/4	0.76	0.15	43,43,44,47	0
4	NAG	B	702	14/15	0.77	0.28	43,55,60,64	0
9	PGE	B	713	10/10	0.78	0.15	41,43,47,49	0
6	FMT	B	708	3/3	0.79	0.11	45,45,49,51	0
9	PGE	A	712	10/10	0.81	0.12	36,39,43,43	0
8	PG4	B	712	13/13	0.81	0.21	31,33,38,39	13
6	FMT	A	709	3/3	0.82	0.27	31,31,36,37	0
4	NAG	A	702	14/15	0.82	0.28	44,50,57,62	0
7	ACT	A	710	4/4	0.85	0.12	54,58,58,60	0
6	FMT	B	709	3/3	0.88	0.17	36,36,42,44	0
5	NPO	B	705[A]	10/10	0.89	0.14	17,19,20,20	10

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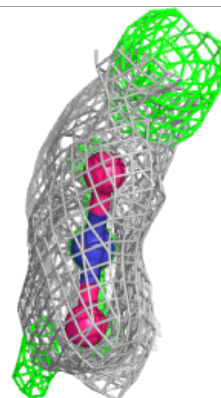
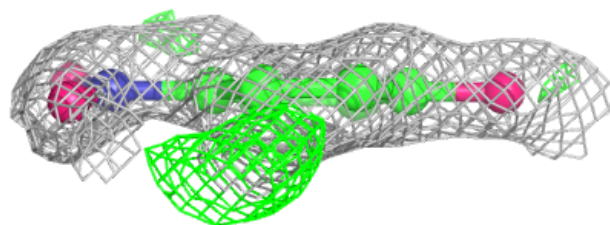
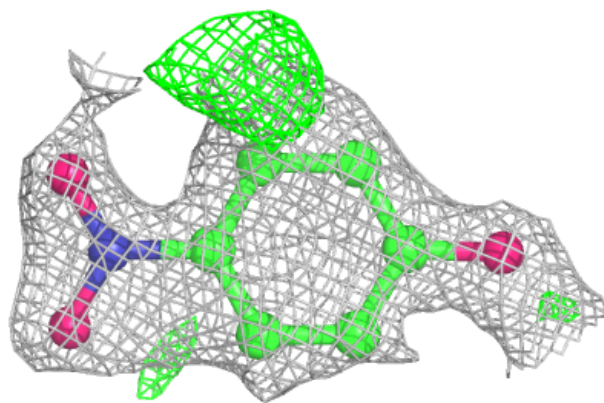
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
8	PG4	A	711	13/13	0.90	0.10	23,24,36,36	0
10	MG	A	713	1/1	0.91	0.27	23,23,23,23	1
6	FMT	A	707	3/3	0.92	0.12	26,26,29,31	0
6	FMT	B	710	3/3	0.93	0.13	27,27,34,34	0
5	NPO	A	705[A]	10/10	0.94	0.11	17,19,21,22	10
10	MG	B	714	1/1	0.94	0.27	44,44,44,44	0
4	NAG	A	704	14/15	0.95	0.07	16,18,28,33	0
4	NAG	B	704	14/15	0.95	0.07	15,17,27,36	0
6	FMT	A	708	3/3	0.96	0.15	16,16,27,30	0
3	FDA	A	701	53/53	0.96	0.07	10,13,15,16	0
6	FMT	B	706	3/3	0.96	0.07	28,28,31,32	0
6	FMT	B	707	3/3	0.96	0.11	15,15,22,29	0
3	FDA	B	701	53/53	0.96	0.08	10,12,14,15	0
10	MG	B	715	1/1	0.96	0.28	37,37,37,37	0
4	NAG	A	703[A]	14/15	0.97	0.07	10,12,15,18	2
10	MG	A	714	1/1	0.97	0.30	34,34,34,34	0
4	NAG	A	703[B]	14/15	0.97	0.07	10,12,14,14	2
4	NAG	B	703	14/15	0.97	0.07	13,15,17,22	0
10	MG	A	715	1/1	0.99	0.06	12,12,12,12	0
11	NA	A	716	1/1	0.99	0.05	18,18,18,18	0

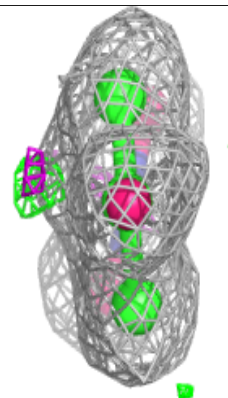
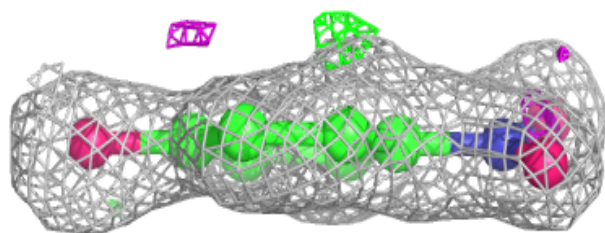
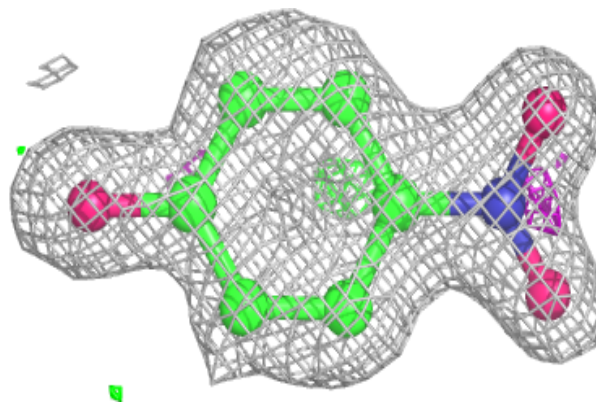
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around NPO A 706:**

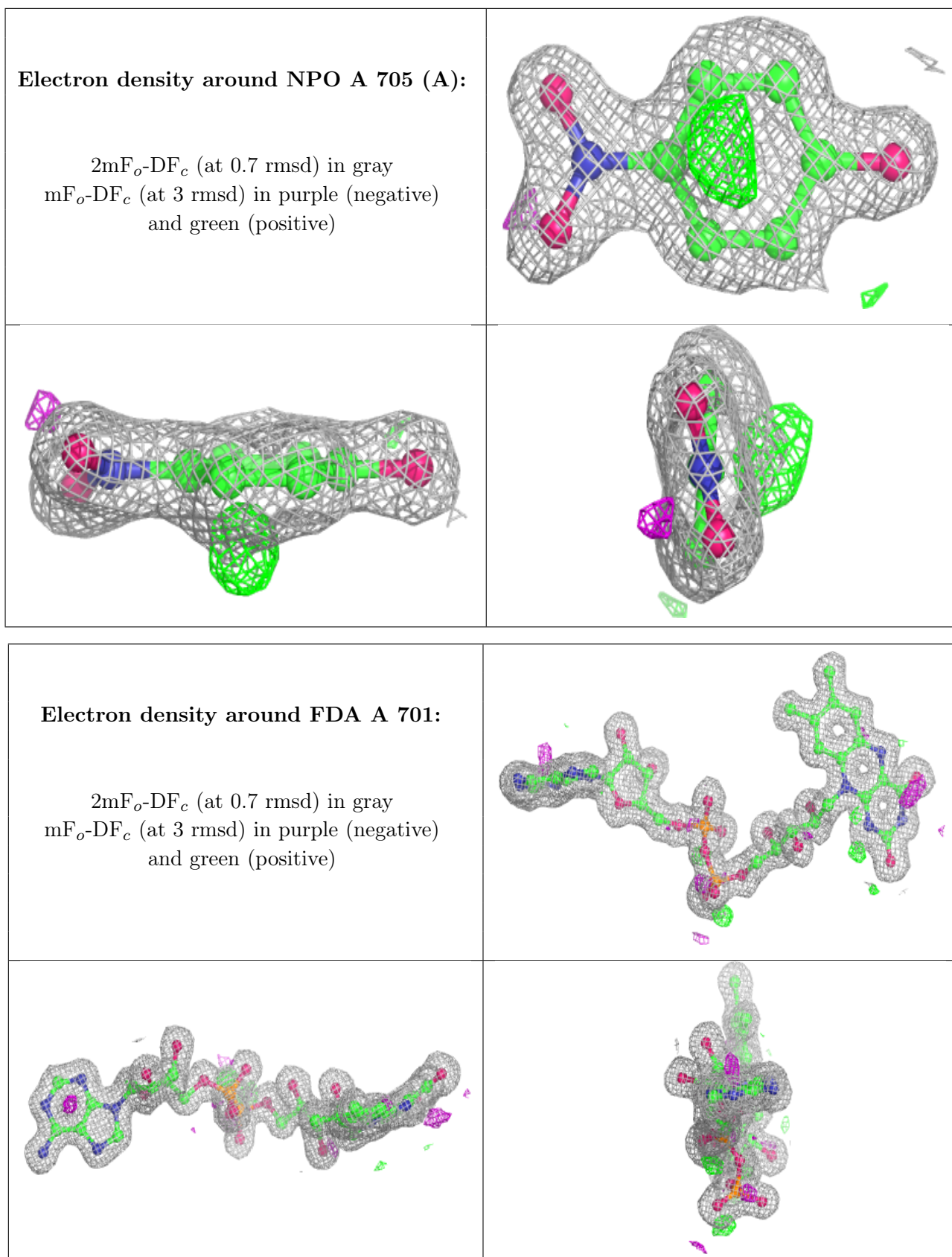
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

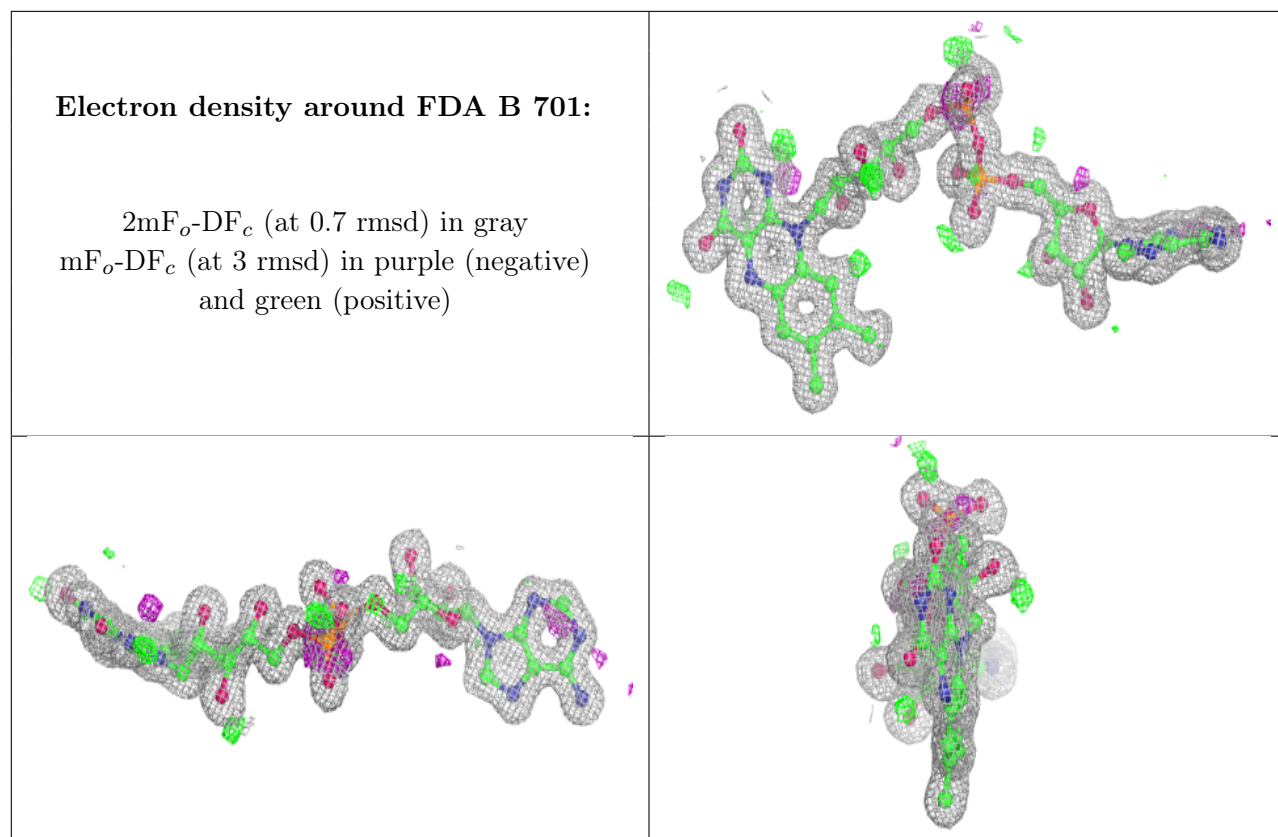
**Electron density around NPO B 705 (A):**

$2mF_o-DF_c$  (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.