



Full wwPDB X-ray Structure Validation Report ⓘ

May 20, 2021 – 03:47 pm BST

PDB ID : 6ZE6
Title : FAD-dependent oxidoreductase from Chaetomium thermophilum in complex with fragment 4-nitrocatechol
Authors : Svecova, L.; Skalova, T.; Kolenko, P.; Koval, T.; Oestergaard, L.H.; Dohnalek, J.
Deposited on : 2020-06-16
Resolution : 1.26 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	:	2.18
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)	:	2.18

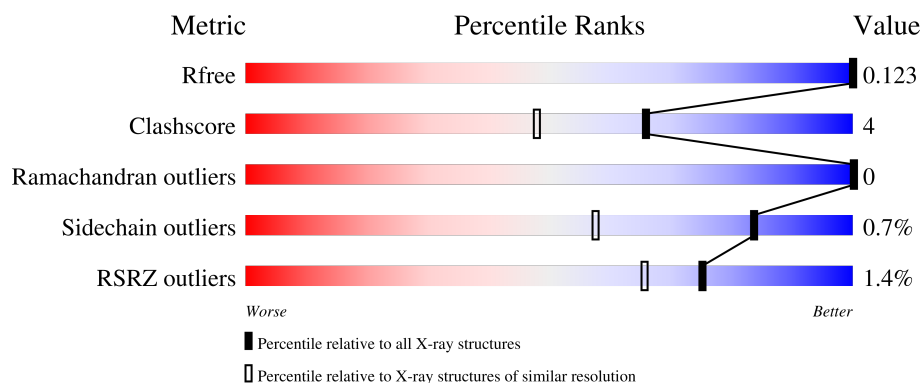
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.26 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	1023 (1.28-1.24)
Clashscore	141614	1060 (1.28-1.24)
Ramachandran outliers	138981	1029 (1.28-1.24)
Sidechain outliers	138945	1028 (1.28-1.24)
RSRZ outliers	127900	1004 (1.28-1.24)

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	595	<div> <div style="width: 100%; height: 10px; background-color: red;"></div> <div style="display: flex; justify-content: space-between; align-items: center;"> % 92% 6% .. </div> </div>
1	B	595	<div> <div style="width: 100%; height: 10px; background-color: red;"></div> <div style="display: flex; justify-content: space-between; align-items: center;"> % 93% 5% . </div> </div>
2	C	2	<div style="display: flex; justify-content: space-between; align-items: center;"> 50% 50% </div>
2	D	2	<div style="display: flex; justify-content: space-between; align-items: center;"> 100% </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
5	4NC	A	708	-	-	X	-
7	MG	A	711	-	-	-	X

2 Entry composition [i](#)

There are 10 unique types of molecules in this entry. The entry contains 11641 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.

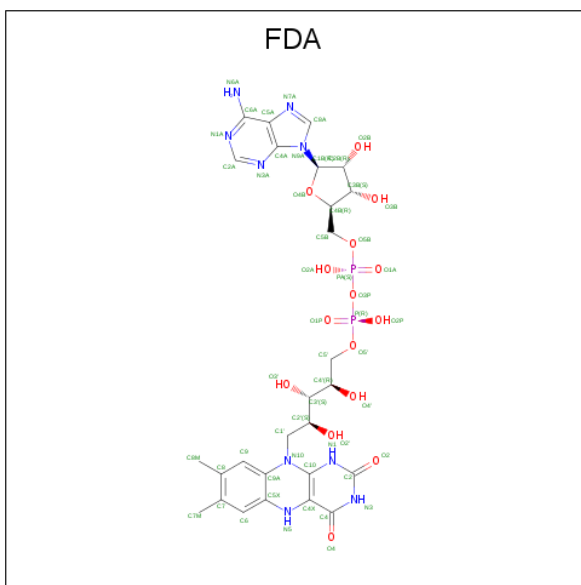
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	585	Total	C	N	O	S	0	45	0
			4685	2990	809	869	17			
1	B	584	Total	C	N	O	S	0	37	0
			4661	2965	815	864	17			

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



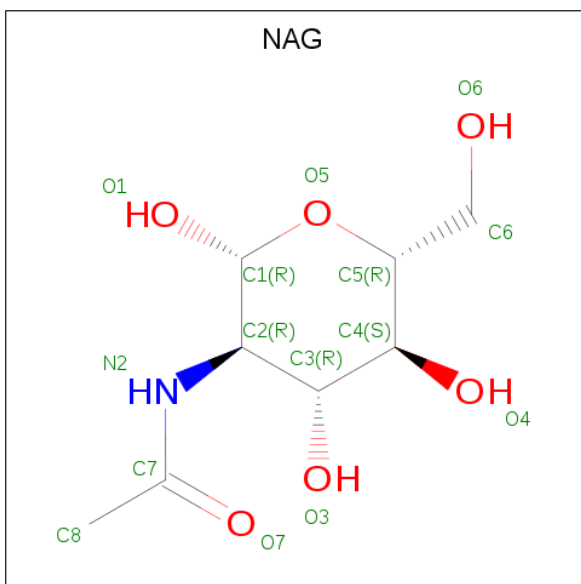
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	D	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 3 is DIHYDROFLAVINE-ADENINE DINUCLEOTIDE (three-letter code: FDA) (formula: C₂₇H₃₅N₉O₁₅P₂) (labeled as "Ligand of Interest" by depositor).



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: $\text{C}_8\text{H}_{15}\text{NO}_6$).



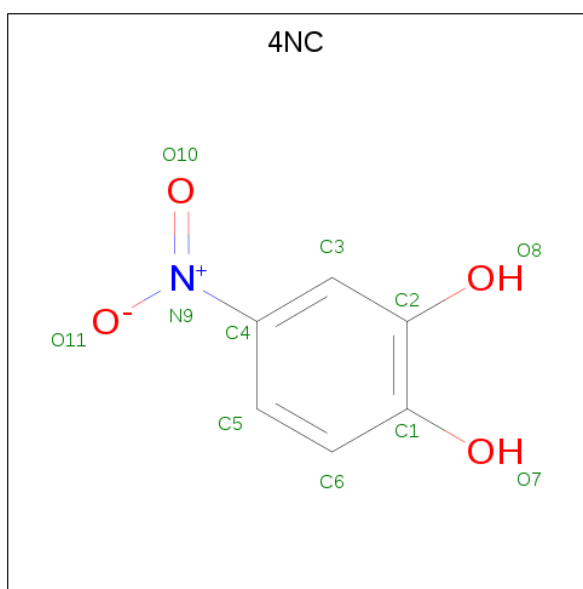
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			14	8	1	5		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	1
			28	16	2	10		
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	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	1
			16	9	1	6		
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 4-NITROCATECHOL (three-letter code: 4NC) (formula: C₆H₅NO₄) (labeled as "Ligand of Interest" by depositor).



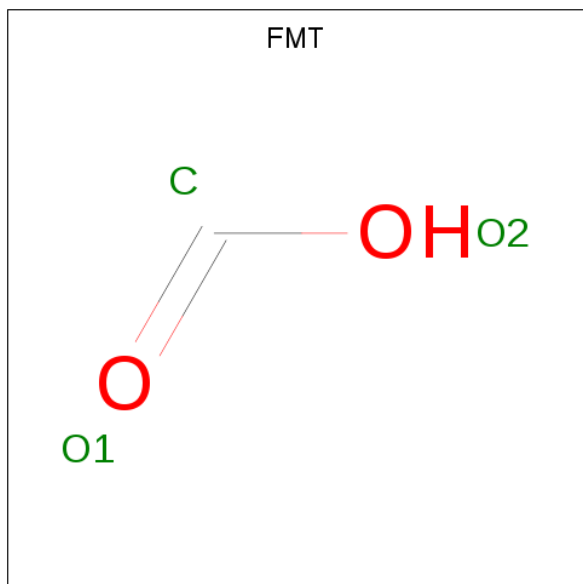
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			11	6	1	4		
5	A	1	Total	C	N	O	0	0
			11	6	1	4		
5	B	1	Total	C	N	O	0	0
			11	6	1	4		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	B	1	Total	C	N	O	0	0
			11	6	1	4		

- Molecule 6 is FORMIC ACID (three-letter code: FMT) (formula: CH₂O₂).



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

- Molecule 7 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	2	Total	Mg	0	0
			2	2		
7	B	1	Total	Mg	0	0
			1	1		

- Molecule 8 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	1	Total Cl 1 1	0	0

- Molecule 9 is SODIUM ION (three-letter code: NA) (formula: Na).

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

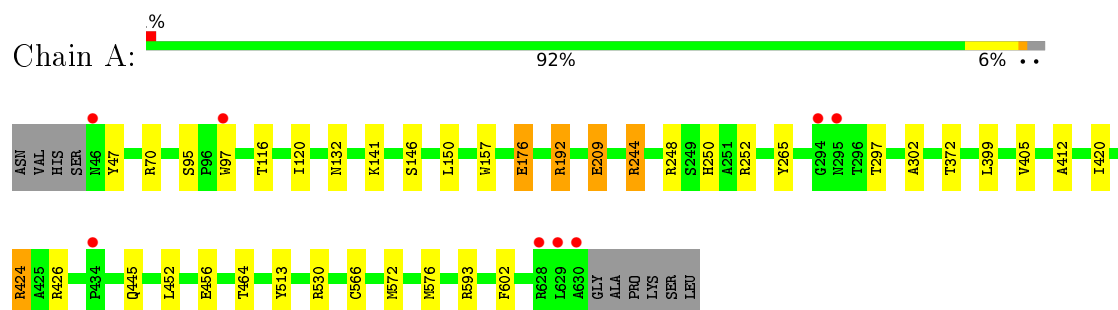
- Molecule 10 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	A	963	Total O 985 985	0	22
10	B	921	Total O 945 945	0	24

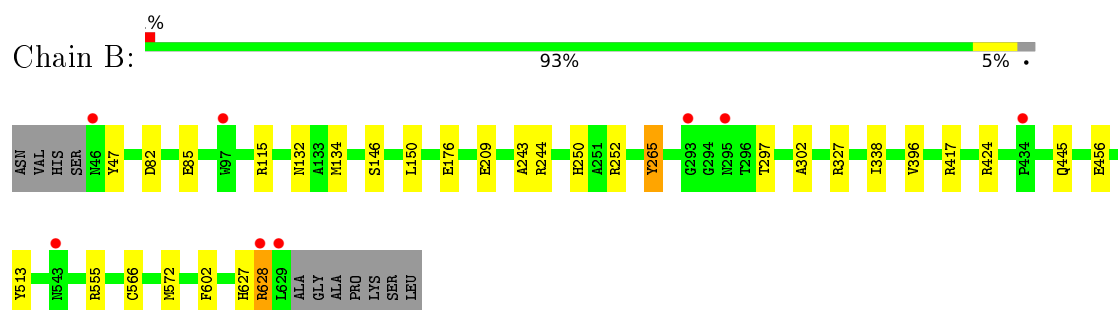
3 Residue-property plots [i](#)

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



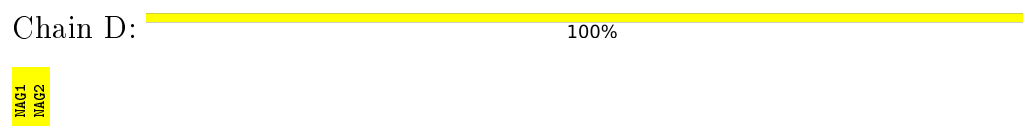
- Molecule 1: FAD-dependent oxidoreductase



- 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, α , β , γ	93.56Å 109.75Å 116.07Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.06 – 1.26 29.05 – 1.26	Depositor EDS
% Data completeness (in resolution range)	98.2 (29.06-1.26) 98.2 (29.05-1.26)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.05 (at 1.26Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.113 , 0.147 0.115 , 0.123	Depositor DCC
R_{free} test set	6192 reflections (1.97%)	wwPDB-VP
Wilson B-factor (Å ²)	11.4	Xtriage
Anisotropy	0.310	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 44.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.98	EDS
Total number of atoms	11641	wwPDB-VP
Average B, all atoms (Å ²)	16.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 79.60 % 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 5.3857e-07. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: FMT, 4NC, NA, NAG, MG, CL, FDA

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	0.71	2/4937 (0.0%)	0.90	8/6733 (0.1%)
1	B	0.74	4/4881 (0.1%)	0.88	2/6653 (0.0%)
All	All	0.72	6/9818 (0.1%)	0.89	10/13386 (0.1%)

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 (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	176	GLU	CD-OE1	9.31	1.35	1.25
1	B	85[A]	GLU	CD-OE2	7.44	1.33	1.25
1	B	85[B]	GLU	CD-OE2	7.44	1.33	1.25
1	A	176	GLU	CD-OE1	6.24	1.32	1.25
1	A	209	GLU	CD-OE1	5.32	1.31	1.25
1	B	209	GLU	CD-OE2	-5.10	1.20	1.25

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	593	ARG	NE-CZ-NH2	-6.78	116.91	120.30
1	A	424[A]	ARG	NE-CZ-NH2	-6.33	117.14	120.30
1	A	424[B]	ARG	NE-CZ-NH2	-6.33	117.14	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	248	ARG	NE-CZ-NH1	-6.24	117.18	120.30
1	B	265	TYR	CB-CG-CD1	5.71	124.43	121.00
1	B	244	ARG	NE-CZ-NH2	-5.66	117.47	120.30
1	A	192[A]	ARG	NE-CZ-NH2	-5.37	117.61	120.30
1	A	192[B]	ARG	NE-CZ-NH2	-5.37	117.61	120.30
1	A	593	ARG	NE-CZ-NH1	5.12	122.86	120.30
1	A	530	ARG	NE-CZ-NH1	-5.10	117.75	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 ⓘ

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	4685	0	4769	44	0
1	B	4661	0	4715	29	0
2	C	28	0	25	1	0
2	D	28	0	25	0	0
3	A	53	0	33	3	0
3	B	53	0	33	4	0
4	A	84	0	77	3	0
4	B	58	0	47	0	0
5	A	22	0	7	4	0
5	B	22	0	8	0	0
6	A	6	0	2	2	0
6	B	6	0	2	1	0
7	A	2	0	0	0	0
7	B	1	0	0	0	0
8	A	1	0	0	0	0
9	A	1	0	0	0	0
10	A	985	0	0	26	0
10	B	945	0	0	14	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	11641	0	9743	77	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 4.

All (77) 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:576[A]:MET:HE1	10:A:835:HOH:O	1.13	1.28
1:A:244[B]:ARG:CZ	10:A:809:HOH:O	1.81	1.21
1:A:576[A]:MET:CE	10:A:835:HOH:O	1.64	1.19
5:A:708:4NC:O10	10:A:808:HOH:O	1.60	1.19
1:A:576[A]:MET:SD	10:A:835:HOH:O	1.97	1.05
1:A:244[B]:ARG:NE	10:A:809:HOH:O	1.83	1.03
1:A:372[A]:THR:HG23	10:A:1301:HOH:O	1.61	0.99
1:A:445[B]:GLN:NE2	10:A:807:HOH:O	1.58	0.98
1:A:244[B]:ARG:NH1	10:A:809:HOH:O	1.81	0.97
5:A:708:4NC:H3	10:A:808:HOH:O	1.70	0.91
1:A:372[A]:THR:CG2	10:A:1301:HOH:O	2.15	0.90
1:A:297[B]:THR:HG22	10:A:952:HOH:O	1.75	0.86
1:A:445[B]:GLN:OE1	10:A:810:HOH:O	1.95	0.83
1:A:244[B]:ARG:HG3	2:C:1:NAG:H83	1.59	0.82
1:A:116[A]:THR:HG21	10:A:1243:HOH:O	1.85	0.76
1:A:192[B]:ARG:NH1	10:A:812:HOH:O	2.20	0.74
1:A:399[B]:LEU:CD2	10:A:1355:HOH:O	2.41	0.69
1:B:417[A]:ARG:NH2	10:B:808:HOH:O	2.26	0.68
1:A:244[B]:ARG:NH1	10:A:816:HOH:O	2.31	0.64
5:A:708:4NC:C3	10:A:808:HOH:O	2.37	0.63
1:B:132:ASN:HB2	3:B:701:FDA:C5X	2.31	0.61
1:B:132:ASN:HB2	3:B:701:FDA:N5	2.16	0.58
1:A:132:ASN:HB2	3:A:701:FDA:N5	2.18	0.57
1:A:399[B]:LEU:HD23	10:A:1355:HOH:O	2.03	0.56
1:A:209:GLU:CG	4:A:703[B]:NAG:O3	2.54	0.55
1:B:424[B]:ARG:HH11	1:B:456[B]:GLU:CD	2.09	0.55
1:B:628[B]:ARG:CG	10:B:1519:HOH:O	2.55	0.55
1:B:297[B]:THR:HG22	10:B:927:HOH:O	2.05	0.55
1:A:209:GLU:HG3	4:A:703[B]:NAG:O3	2.07	0.54
1:B:555[B]:ARG:NH2	10:B:810:HOH:O	2.34	0.54
1:A:132:ASN:HB2	3:A:701:FDA:C4X	2.38	0.53
1:B:628[B]:ARG:HG3	10:B:1519:HOH:O	2.08	0.53
1:A:424[B]:ARG:HG3	1:A:424[B]:ARG:NH2	2.24	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:132:ASN:HB2	3:A:701:FDA:C5X	2.39	0.52
1:B:132:ASN:HB2	3:B:701:FDA:C4X	2.39	0.52
1:A:150:LEU:HD13	1:A:572[B]:MET:SD	2.49	0.52
1:B:134[B]:MET:CE	1:B:396:VAL:HG22	2.40	0.52
6:A:709:FMT:C	10:A:825:HOH:O	2.58	0.51
1:B:628[A]:ARG:HG3	10:B:1519:HOH:O	2.10	0.51
1:A:146[B]:SER:HG	1:A:602:PHE:HZ	1.58	0.51
1:B:445[B]:GLN:OE1	10:B:806:HOH:O	2.19	0.50
1:B:338:ILE:HD11	10:B:875:HOH:O	2.12	0.48
1:A:209:GLU:OE2	4:A:703[B]:NAG:O3	2.25	0.48
1:B:627:HIS:O	1:B:628[A]:ARG:HG2	2.14	0.47
1:A:399[B]:LEU:HD22	10:A:1355:HOH:O	2.08	0.47
1:B:146[B]:SER:HG	1:B:602:PHE:HZ	1.61	0.47
1:B:327[B]:ARG:HD3	10:B:896:HOH:O	2.15	0.47
1:A:297[B]:THR:CG2	10:A:952:HOH:O	2.49	0.46
1:A:420:ILE:HD13	1:A:456[B]:GLU:CG	2.46	0.46
1:B:115[B]:ARG:HD2	10:B:1352:HOH:O	2.16	0.46
6:B:708:FMT:C	10:B:814:HOH:O	2.64	0.46
1:A:70:ARG:NE	10:A:823:HOH:O	2.48	0.45
1:B:134[B]:MET:CE	1:B:396:VAL:CG2	2.94	0.45
1:B:297[B]:THR:HG21	10:B:958:HOH:O	2.16	0.45
1:A:176:GLU:HB3	1:B:243:ALA:O	2.17	0.44
1:A:95[B]:SER:HB2	1:A:97:TRP:CZ2	2.53	0.44
1:A:116[A]:THR:HG23	10:A:915:HOH:O	2.17	0.44
1:A:405:VAL:HG22	1:A:464[B]:THR:HG22	2.00	0.44
1:A:95[B]:SER:HB2	1:A:97:TRP:CE2	2.53	0.43
1:A:250:HIS:CD2	1:A:252[A]:ARG:HB3	2.53	0.43
1:B:134[B]:MET:HE2	1:B:396:VAL:HG22	2.00	0.43
1:A:120:ILE:HG13	5:A:708:4NC:C3	2.48	0.43
1:B:150:LEU:HD13	1:B:572[B]:MET:SD	2.58	0.43
1:B:338:ILE:HD11	10:B:1694:HOH:O	2.18	0.43
1:A:424[B]:ARG:HG2	1:A:452:LEU:HD13	2.01	0.42
1:B:250:HIS:CD2	1:B:252[A]:ARG:HB3	2.54	0.42
1:A:420:ILE:HD13	1:A:456[B]:GLU:HG2	2.01	0.42
1:B:297[B]:THR:CG2	10:B:958:HOH:O	2.68	0.42
1:B:47:TYR:O	1:B:302:ALA:HA	2.21	0.41
1:B:132:ASN:HA	3:B:701:FDA:C6	2.50	0.41
1:A:47:TYR:O	1:A:302:ALA:HA	2.20	0.41
1:B:134[B]:MET:HE2	1:B:396:VAL:CG2	2.50	0.41
1:A:372[A]:THR:HG22	10:A:1301:HOH:O	2.04	0.40
1:A:426:ARG:HG3	10:A:972:HOH:O	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:412:ALA:CA	6:A:710:FMT:H	2.52	0.40
1:A:141[B]:LYS:HG2	1:A:157:TRP:CD2	2.57	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	628/595 (106%)	604 (96%)	24 (4%)	0	100	100
1	B	618/595 (104%)	595 (96%)	23 (4%)	0	100	100
All	All	1246/1190 (105%)	1199 (96%)	47 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	522/485 (108%)	518 (99%)	4 (1%)	81	53
1	B	514/485 (106%)	509 (99%)	5 (1%)	76	42
All	All	1036/970 (107%)	1027 (99%)	9 (1%)	84	47

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	244[A]	ARG
1	A	244[B]	ARG
1	A	265	TYR
1	A	513	TYR
1	B	82	ASP
1	B	265	TYR
1	B	513	TYR
1	B	628[A]	ARG
1	B	628[B]	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	331	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	2,1	14,14,15	1.84	3 (21%)	17,19,21	2.29	5 (29%)
2	NAG	C	2	2	14,14,15	1.85	4 (28%)	17,19,21	1.73	4 (23%)
2	NAG	D	1	2,1	14,14,15	1.11	3 (21%)	17,19,21	1.44	1 (5%)
2	NAG	D	2	2	14,14,15	1.50	3 (21%)	17,19,21	1.15	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	-	1/6/23/26	0/1/1/1
2	NAG	D	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	D	2	2	-	2/6/23/26	0/1/1/1

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1	NAG	O5-C1	4.86	1.51	1.43
2	D	2	NAG	O5-C1	-4.28	1.36	1.43
2	C	2	NAG	O7-C7	4.23	1.32	1.23
2	C	2	NAG	O5-C1	-3.05	1.38	1.43
2	C	1	NAG	C1-C2	2.46	1.56	1.52
2	D	1	NAG	C8-C7	-2.32	1.45	1.50
2	C	1	NAG	C8-C7	-2.26	1.45	1.50
2	C	2	NAG	C8-C7	2.21	1.55	1.50
2	D	1	NAG	O5-C1	2.16	1.47	1.43
2	D	2	NAG	O7-C7	2.06	1.27	1.23
2	D	2	NAG	O5-C5	2.05	1.47	1.43
2	D	1	NAG	O4-C4	2.04	1.47	1.43
2	C	2	NAG	C1-C2	-2.01	1.49	1.52

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1	NAG	O5-C1-C2	-7.28	99.79	111.29
2	D	1	NAG	O5-C1-C2	-4.90	103.55	111.29
2	C	2	NAG	O5-C1-C2	3.98	117.58	111.29
2	C	1	NAG	C1-O5-C5	3.15	116.46	112.19
2	C	2	NAG	O4-C4-C5	-3.06	101.70	109.30
2	C	2	NAG	C1-O5-C5	-2.89	108.27	112.19
2	C	1	NAG	O3-C3-C4	-2.43	104.73	110.35
2	C	1	NAG	O4-C4-C5	-2.25	103.70	109.30
2	C	2	NAG	C4-C3-C2	-2.25	107.72	111.02
2	C	1	NAG	O4-C4-C3	2.10	115.21	110.35
2	D	2	NAG	O7-C7-N2	2.02	125.67	121.95

There are no chirality outliers.

All (3) torsion outliers are listed below:

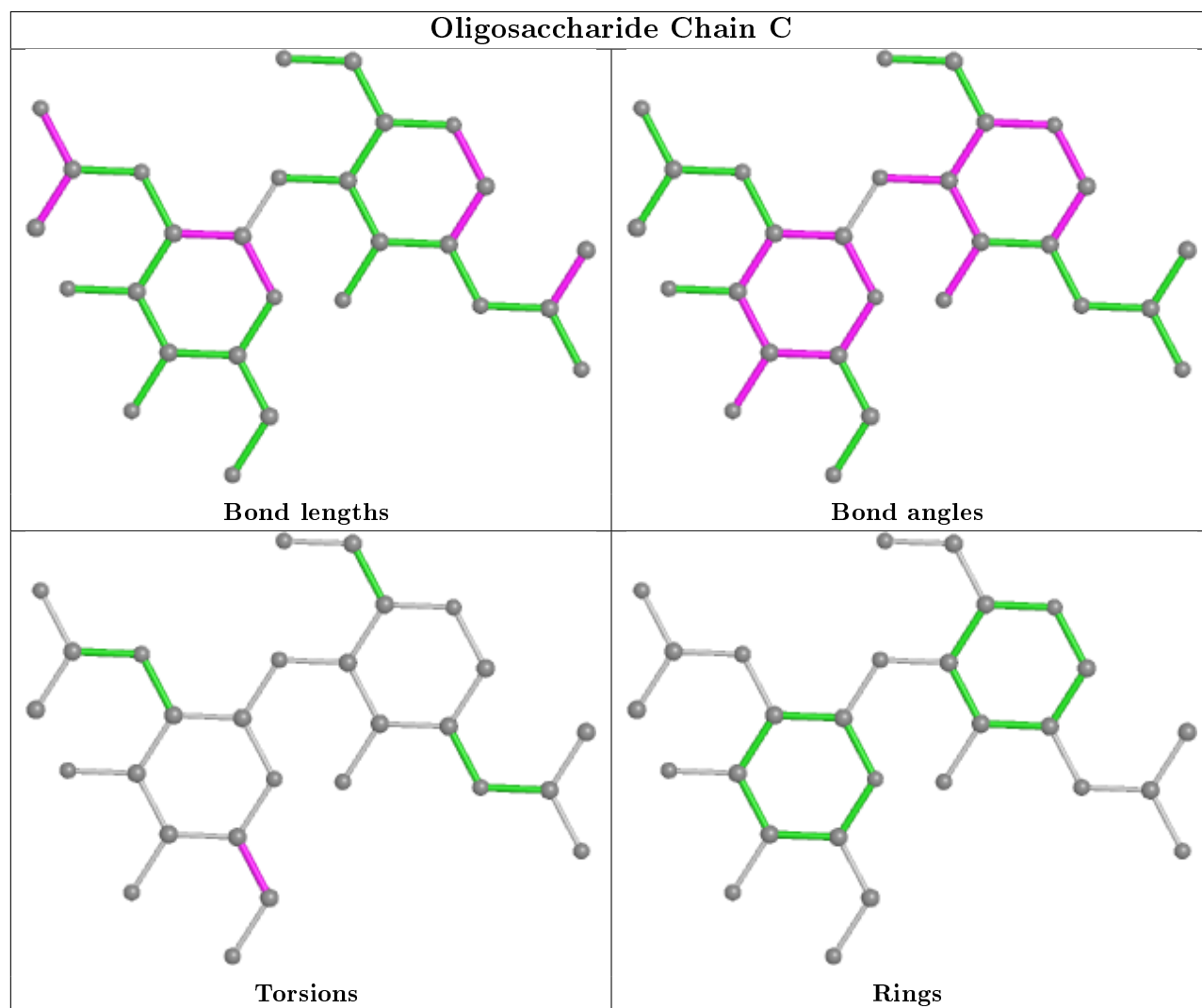
Mol	Chain	Res	Type	Atoms
2	D	2	NAG	C4-C5-C6-O6
2	D	2	NAG	O5-C5-C6-O6
2	C	2	NAG	C4-C5-C6-O6

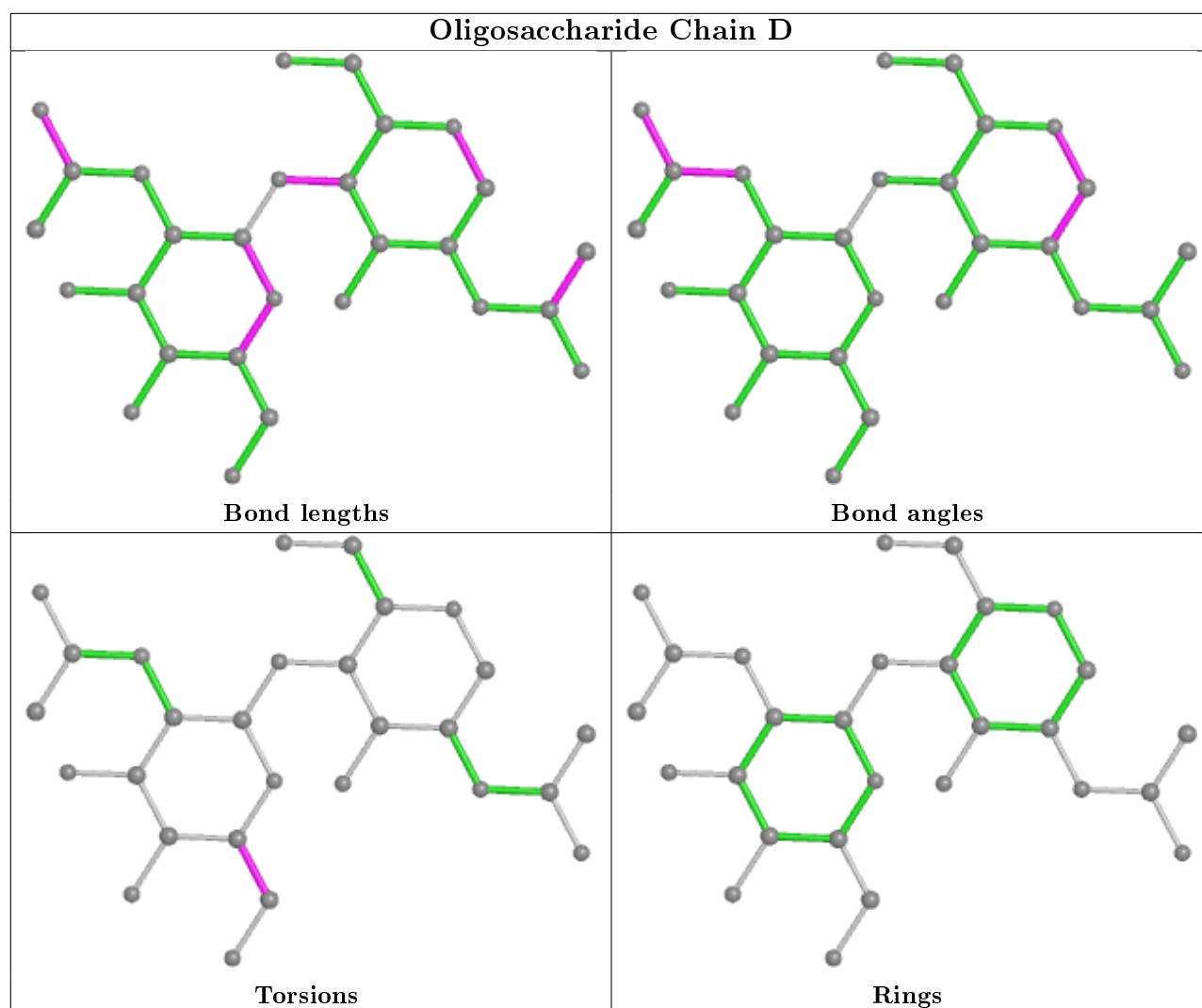
There are no ring outliers.

1 monomer is involved in 1 short contact:

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

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





5.6 Ligand geometry [i](#)

Of 26 ligands modelled in this entry, 5 are monoatomic - leaving 21 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	A	703[A]	1	14,14,15	0.58	0	17,19,21	1.36	2 (11%)
4	NAG	B	703[B]	-	14,14,15	0.77	0	17,19,21	0.93	1 (5%)
5	4NC	A	708	-	10,11,11	1.20	1 (10%)	13,15,15	0.74	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	A	706	1	14,14,15	0.74	0	17,19,21	1.56	2 (11%)
6	FMT	B	708	-	0,2,2	0.00	-	0,1,1	0.00	-
4	NAG	B	703[A]	-	14,14,15	0.78	0	17,19,21	1.07	2 (11%)
5	4NC	B	706	-	10,11,11	0.87	1 (10%)	13,15,15	1.85	3 (23%)
3	FDA	A	701	-	51,58,58	1.08	3 (5%)	60,89,89	2.09	6 (10%)
3	FDA	B	701	-	51,58,58	1.24	5 (9%)	60,89,89	2.17	11 (18%)
6	FMT	B	709	-	0,2,2	0.00	-	0,1,1	0.00	-
4	NAG	B	705	1	14,14,15	0.46	0	17,19,21	0.92	0
6	FMT	A	709	-	0,2,2	0.00	-	0,1,1	0.00	-
4	NAG	A	703[B]	1	14,14,15	1.05	1 (7%)	17,19,21	1.45	4 (23%)
4	NAG	B	702	1	14,14,15	0.43	0	17,19,21	0.67	0
4	NAG	A	702	1	14,14,15	0.45	0	17,19,21	0.85	0
4	NAG	B	704	1	14,14,15	0.80	0	17,19,21	0.96	1 (5%)
4	NAG	A	705	1	14,14,15	0.78	0	17,19,21	1.08	2 (11%)
5	4NC	B	707	-	10,11,11	0.70	0	13,15,15	0.89	0
6	FMT	A	710	-	0,2,2	0.00	-	0,1,1	0.00	-
5	4NC	A	707	-	10,11,11	0.41	0	13,15,15	1.39	1 (7%)
4	NAG	A	704	1	14,14,15	0.45	0	17,19,21	0.95	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
5	4NC	A	708	-	-	1/2/4/4	0/1/1/1
5	4NC	B	706	-	-	0/2/4/4	0/1/1/1
4	NAG	A	706	1	-	0/6/23/26	0/1/1/1
4	NAG	A	703[B]	1	-	0/6/23/26	0/1/1/1
3	FDA	A	701	-	-	4/30/50/50	0/6/6/6
3	FDA	B	701	-	-	4/30/50/50	0/6/6/6
4	NAG	B	702	1	-	0/6/23/26	0/1/1/1
5	4NC	A	707	-	-	0/2/4/4	0/1/1/1
4	NAG	A	703[A]	1	-	0/6/23/26	0/1/1/1
4	NAG	A	702	1	-	0/6/23/26	0/1/1/1
4	NAG	B	704	1	-	0/6/23/26	0/1/1/1
4	NAG	A	705	1	-	0/6/23/26	0/1/1/1
5	4NC	B	707	-	-	0/2/4/4	0/1/1/1
4	NAG	B	703[B]	-	-	0/6/23/26	0/1/1/1
4	NAG	A	704	1	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	B	705	1	-	0/6/23/26	0/1/1/1
4	NAG	B	703[A]	-	-	0/6/23/26	0/1/1/1

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	701	FDA	C9A-N10	3.73	1.43	1.38
3	A	701	FDA	C4-N3	3.73	1.39	1.33
5	A	708	4NC	C4-N9	3.65	1.53	1.45
3	B	701	FDA	C4-N3	3.55	1.39	1.33
3	B	701	FDA	C4X-C10	3.08	1.41	1.38
3	B	701	FDA	C10-N1	3.00	1.37	1.33
3	A	701	FDA	C10-N1	2.74	1.36	1.33
3	B	701	FDA	C4X-N5	2.60	1.37	1.33
3	A	701	FDA	C4X-N5	2.36	1.36	1.33
5	B	706	4NC	O10-N9	2.15	1.26	1.22
4	A	703[B]	NAG	O5-C1	-2.06	1.40	1.43

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	701	FDA	C4-N3-C2	12.41	125.62	115.14
3	A	701	FDA	C4-N3-C2	11.70	125.02	115.14
3	A	701	FDA	C4X-C4-N3	-6.89	114.00	123.43
3	B	701	FDA	C4X-C4-N3	-5.98	115.25	123.43
3	A	701	FDA	C4X-N5-C5X	4.91	121.67	116.77
4	A	706	NAG	O5-C1-C2	-4.00	104.98	111.29
4	A	703[A]	NAG	O5-C5-C6	3.77	113.12	107.20
3	B	701	FDA	C4X-N5-C5X	3.34	120.11	116.77
3	A	701	FDA	C10-C4X-N5	-3.31	118.97	121.26
5	B	706	4NC	O8-C2-C3	3.31	128.32	119.46
3	B	701	FDA	C1'-N10-C9A	3.29	120.88	118.29
5	B	706	4NC	C3-C2-C1	-3.06	117.16	119.86
3	B	701	FDA	C5A-C6A-N6A	2.95	124.83	120.35
3	B	701	FDA	C9A-N10-C10	-2.86	118.17	121.91
5	A	707	4NC	O8-C2-C3	2.74	126.81	119.46
4	A	703[B]	NAG	O5-C5-C4	-2.70	104.27	110.83
5	B	706	4NC	C6-C1-C2	2.69	122.62	119.67
4	A	706	NAG	C1-C2-N2	-2.69	105.89	110.49
4	A	703[B]	NAG	C1-C2-N2	2.64	114.99	110.49
4	A	705	NAG	C6-C5-C4	2.57	119.03	113.00
3	A	701	FDA	C9A-C5X-N5	-2.56	118.36	122.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	701	FDA	C5X-C9A-N10	2.52	119.54	117.72
4	B	703[A]	NAG	O5-C1-C2	-2.46	107.41	111.29
4	B	703[B]	NAG	O5-C1-C2	-2.46	107.41	111.29
3	B	701	FDA	C1'-N10-C10	2.44	120.59	118.41
4	A	703[A]	NAG	O5-C1-C2	-2.38	107.53	111.29
4	B	703[A]	NAG	C6-C5-C4	2.31	118.41	113.00
4	A	703[B]	NAG	O6-C6-C5	2.25	119.00	111.29
3	B	701	FDA	C9A-C5X-N5	-2.18	118.95	122.36
3	B	701	FDA	C4-C4X-N5	2.14	121.04	118.60
3	B	701	FDA	O2P-P-O1P	2.12	122.74	112.24
3	A	701	FDA	C5A-C6A-N6A	2.11	123.56	120.35
4	A	703[B]	NAG	C6-C5-C4	2.10	117.92	113.00
4	B	704	NAG	O5-C5-C6	2.05	110.41	107.20
4	A	705	NAG	C2-N2-C7	-2.00	120.05	122.90

There are no chirality outliers.

All (9) torsion outliers are listed below:

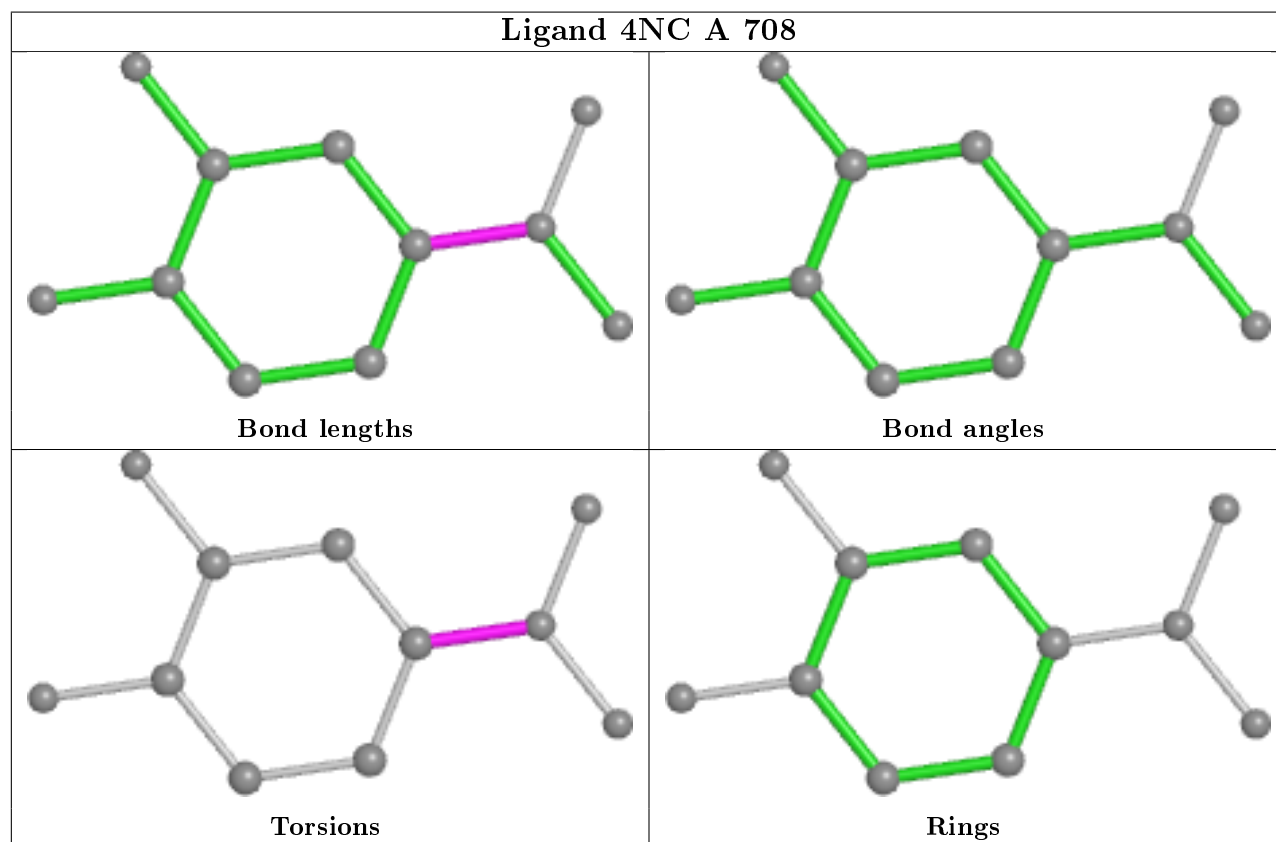
Mol	Chain	Res	Type	Atoms
3	A	701	FDA	PA-O3P-P-O5'
3	A	701	FDA	P-O3P-PA-O1A
3	B	701	FDA	P-O3P-PA-O1A
3	B	701	FDA	PA-O3P-P-O5'
3	A	701	FDA	P-O3P-PA-O2A
3	B	701	FDA	P-O3P-PA-O2A
5	A	708	4NC	C5-C4-N9-O10
3	A	701	FDA	O4B-C4B-C5B-O5B
3	B	701	FDA	O4B-C4B-C5B-O5B

There are no ring outliers.

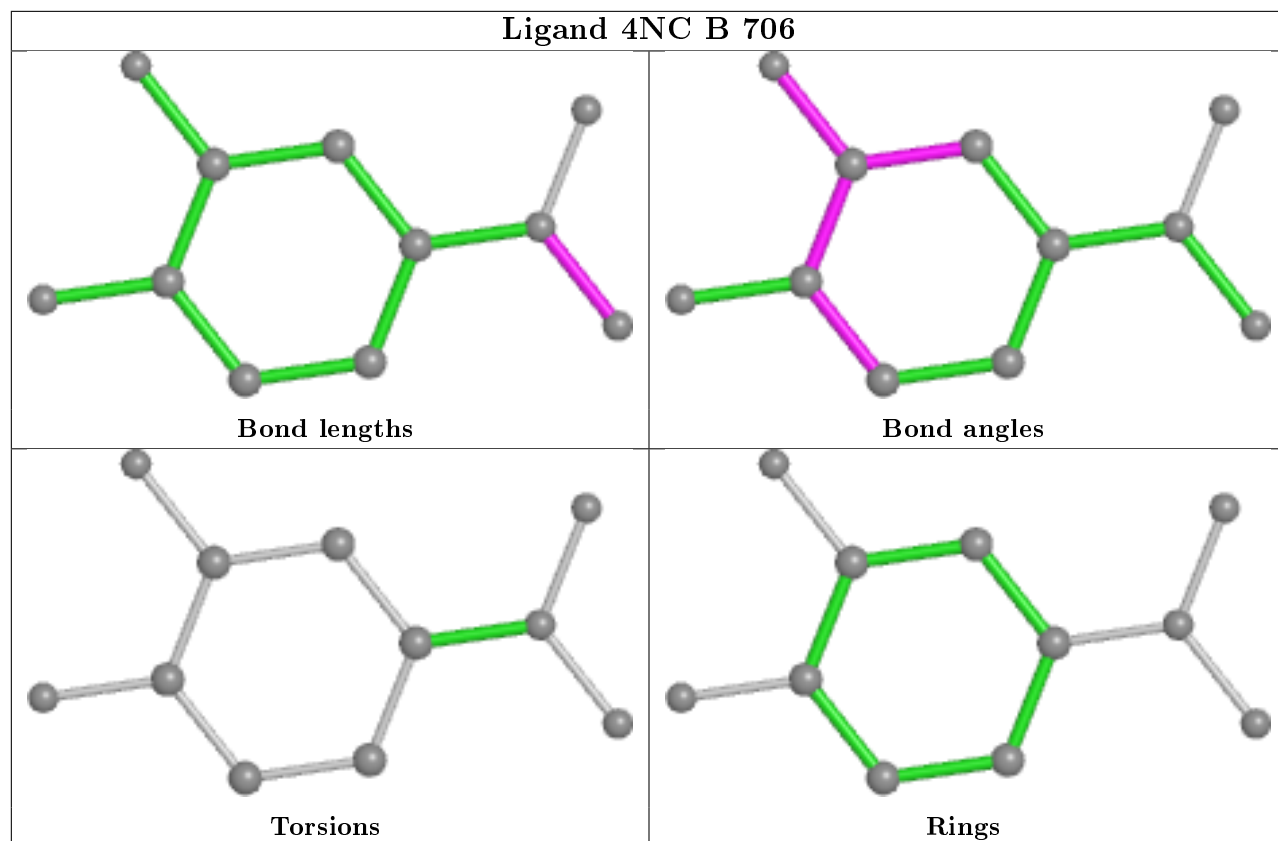
7 monomers are involved in 17 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	708	4NC	4	0
6	B	708	FMT	1	0
3	A	701	FDA	3	0
3	B	701	FDA	4	0
6	A	709	FMT	1	0
4	A	703[B]	NAG	3	0
6	A	710	FMT	1	0

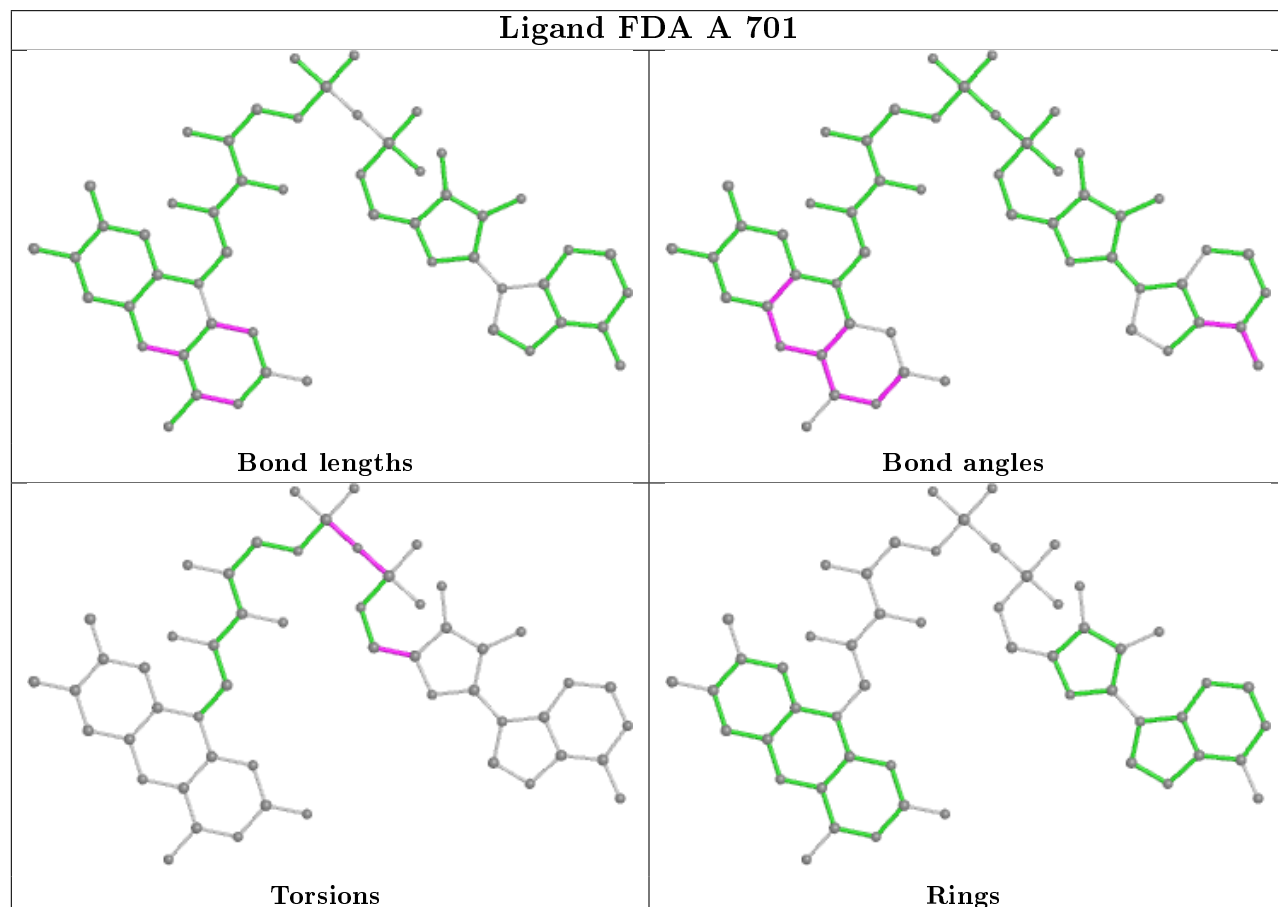
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.



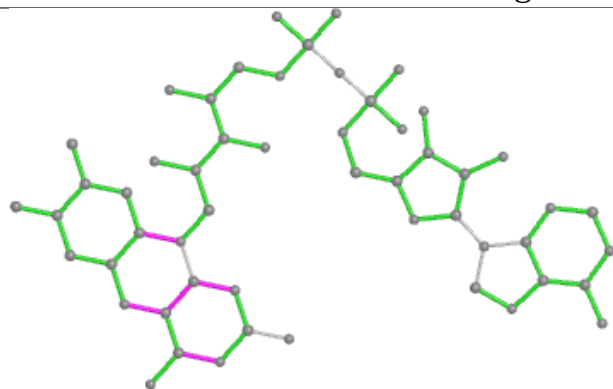
Ligand 4NC B 706



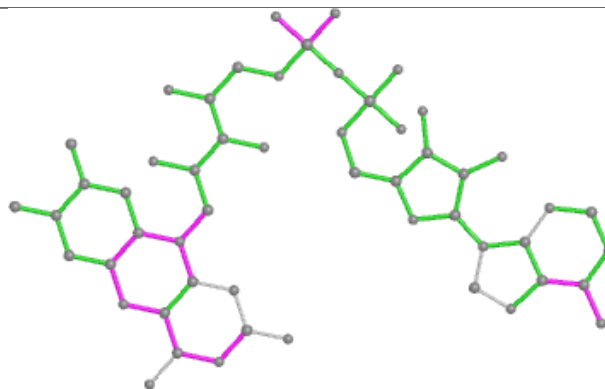
Ligand FDA A 701



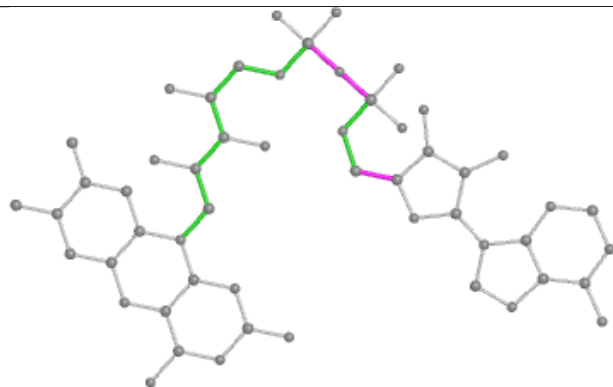
Ligand FDA B 701



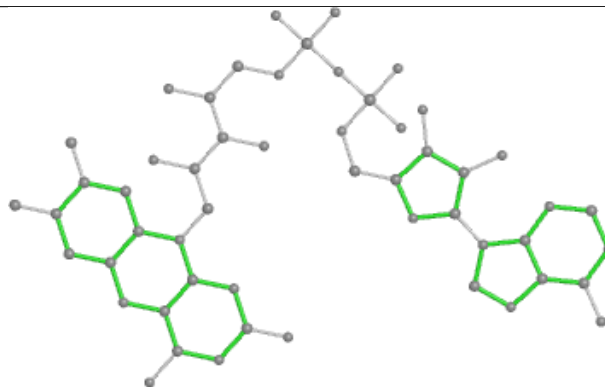
Bond lengths



Bond angles

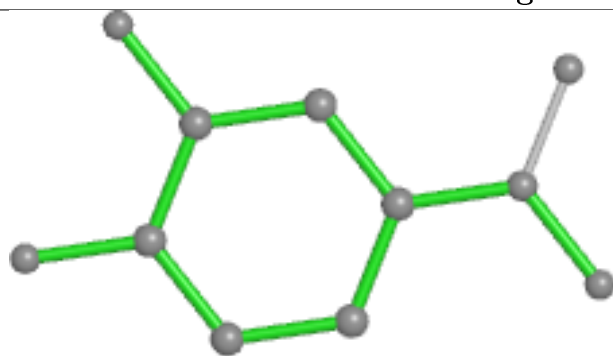


Torsions

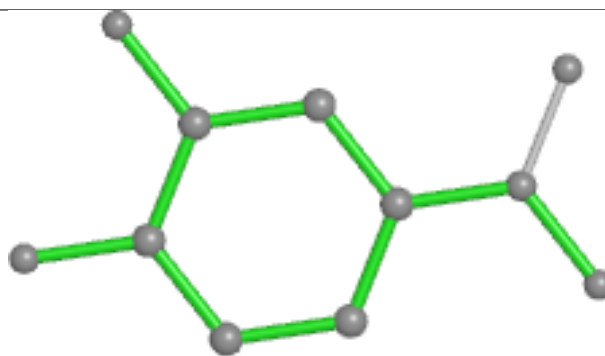


Rings

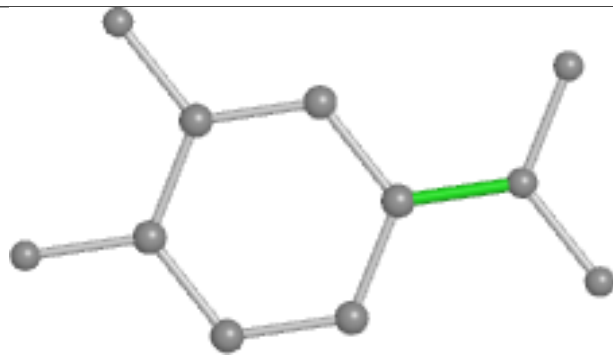
Ligand 4NC B 707



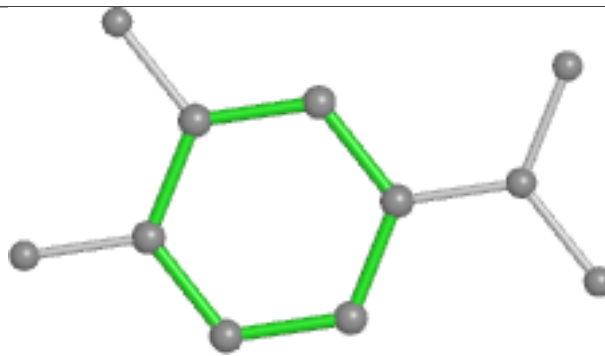
Bond lengths



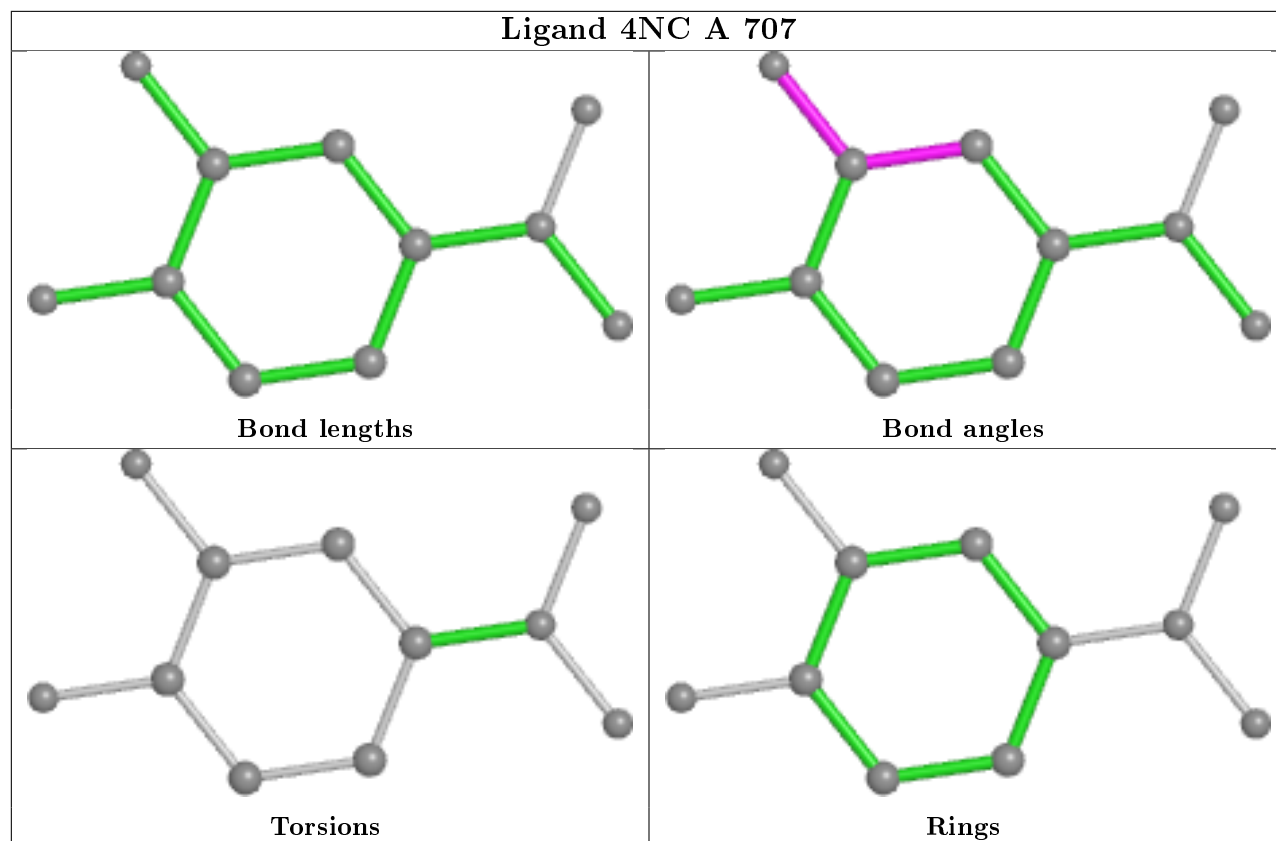
Bond angles



Torsions



Rings



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	585/595 (98%)	-0.56	8 (1%) 75 66	8, 12, 22, 46	3 (0%)
1	B	584/595 (98%)	-0.52	8 (1%) 75 66	8, 12, 22, 37	3 (0%)
All	All	1169/1190 (98%)	-0.54	16 (1%) 75 66	8, 12, 22, 46	6 (0%)

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	629	LEU	5.1
1	A	630	ALA	5.0
1	B	628[A]	ARG	4.2
1	A	46	ASN	3.8
1	B	295	ASN	3.3
1	B	97	TRP	3.0
1	A	295	ASN	3.0
1	B	46[A]	ASN	2.9
1	A	434	PRO	2.7
1	A	629	LEU	2.6
1	B	434	PRO	2.4
1	A	97	TRP	2.4
1	B	543	ASN	2.2
1	A	628	ARG	2.2
1	A	294	GLY	2.1
1	B	293	GLY	2.0

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

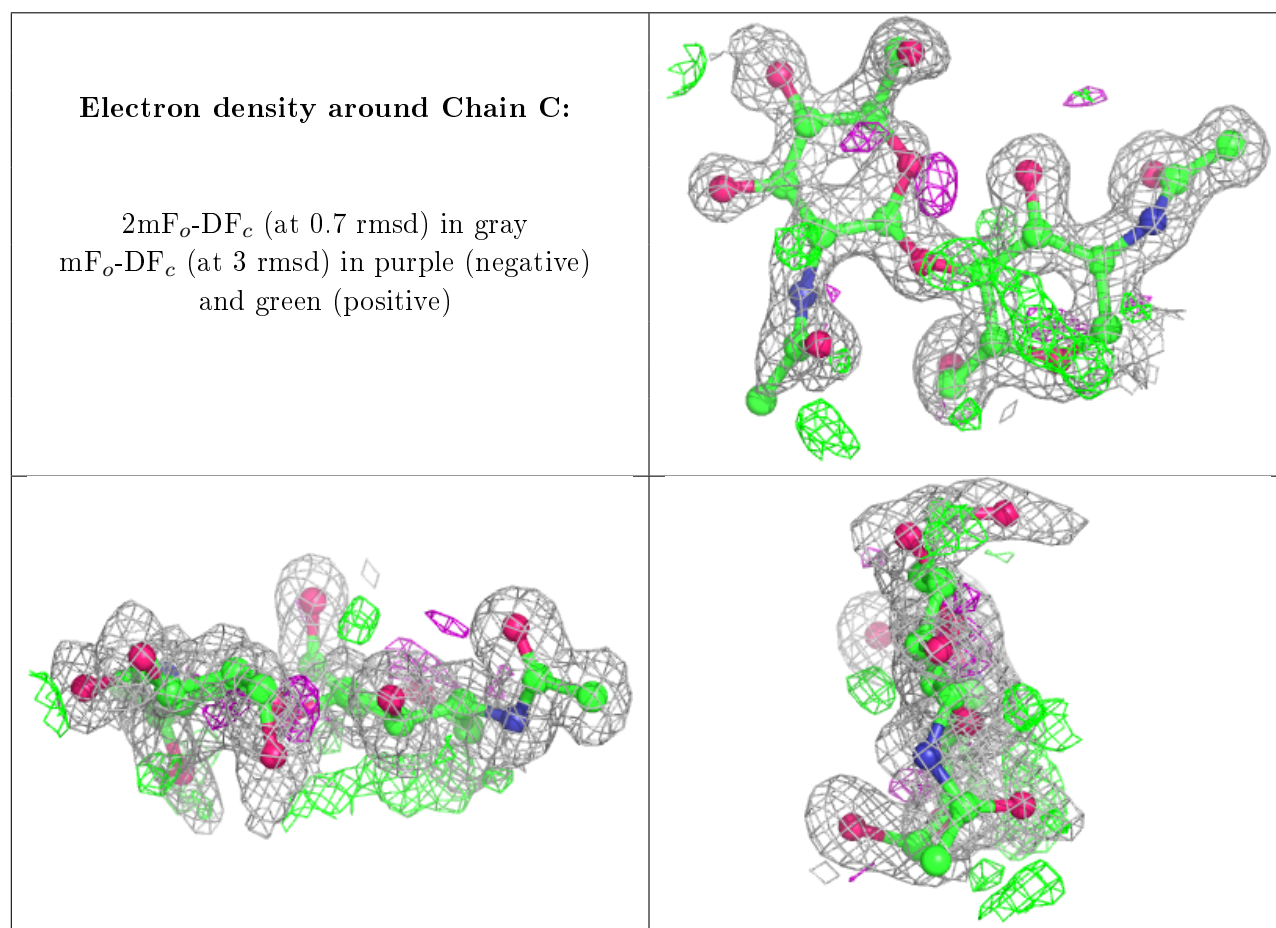
There are no non-standard protein/DNA/RNA residues in this entry.

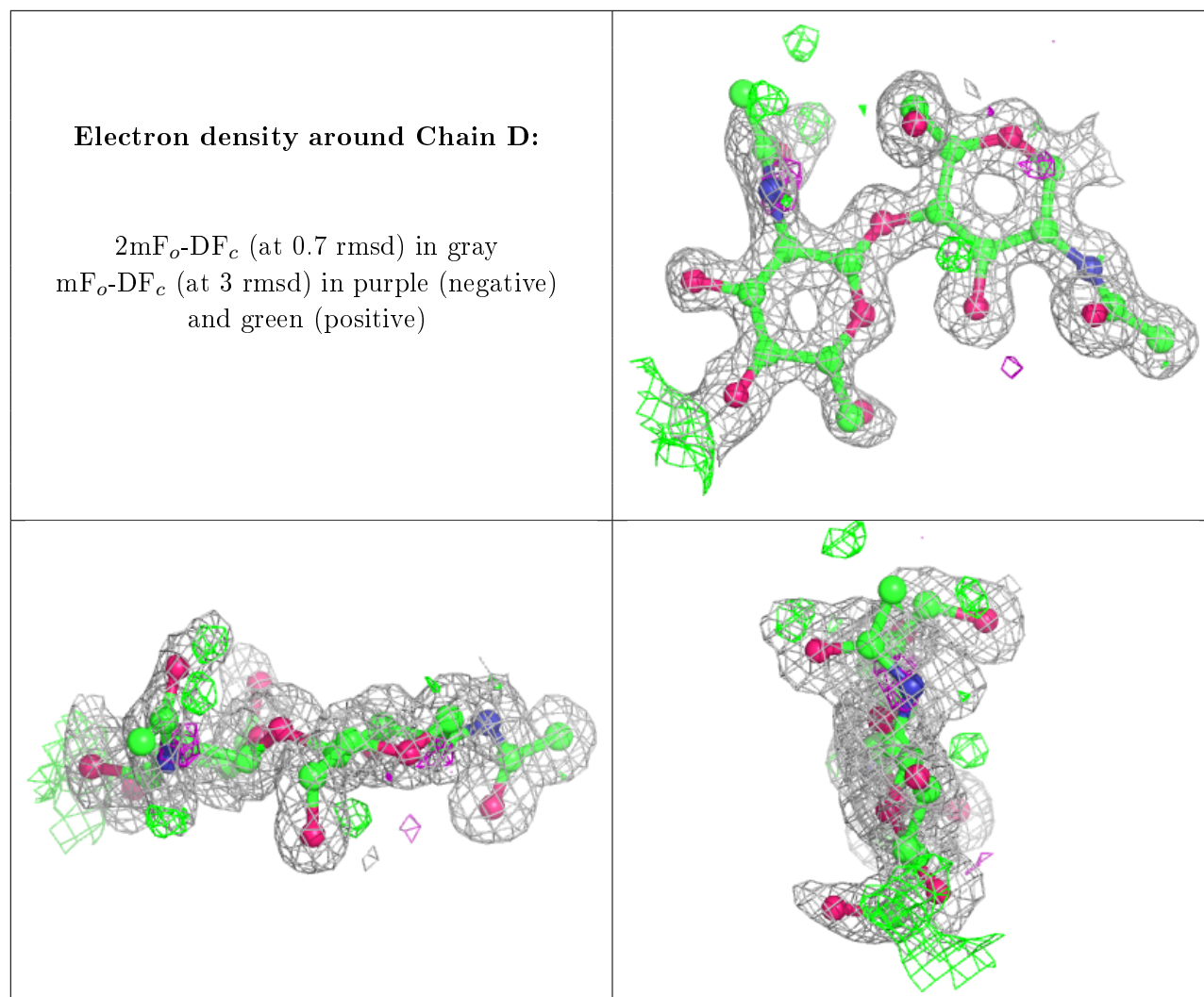
6.3 Carbohydrates ⓘ

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(\AA^2)	Q<0.9
2	NAG	C	2	14/15	0.69	0.28	33,46,61,74	0
2	NAG	D	2	14/15	0.86	0.24	23,37,63,75	0
2	NAG	C	1	14/15	0.94	0.11	11,16,19,23	0
2	NAG	D	1	14/15	0.96	0.09	12,14,16,19	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	706	14/15	0.74	0.14	19,24,38,40	14
7	MG	A	711	1/1	0.75	0.42	53,53,53,53	0
5	4NC	B	707	11/11	0.78	0.16	24,31,40,41	11
4	NAG	B	704	14/15	0.81	0.27	22,29,38,40	14
4	NAG	A	704	14/15	0.83	0.24	25,35,50,53	14
5	4NC	A	708	11/11	0.83	0.15	20,25,28,33	11
4	NAG	B	702	14/15	0.87	0.30	37,50,58,62	0
7	MG	B	710	1/1	0.88	0.30	29,29,29,29	1
4	NAG	A	702	14/15	0.89	0.26	33,42,50,54	0

Continued on next page...

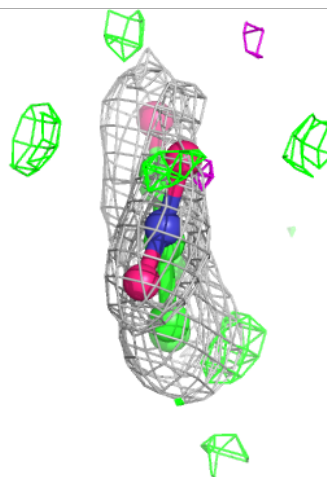
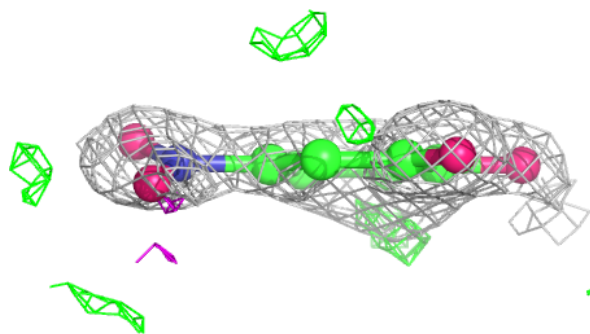
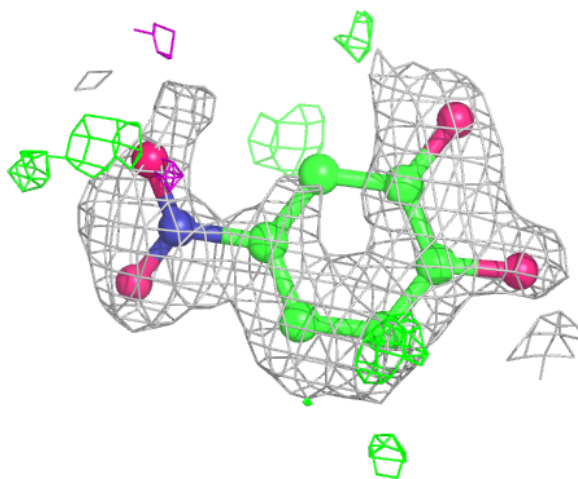
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
5	4NC	B	706	11/11	0.91	0.10	15,16,19,19	11
5	4NC	A	707	11/11	0.94	0.08	13,14,16,17	11
6	FMT	B	708	3/3	0.94	0.12	21,21,27,28	0
6	FMT	A	710	3/3	0.95	0.08	19,19,24,25	0
4	NAG	B	705	14/15	0.97	0.05	14,16,26,30	0
6	FMT	B	709	3/3	0.97	0.12	17,17,25,30	0
6	FMT	A	709	3/3	0.97	0.08	19,19,28,29	0
4	NAG	A	705	14/15	0.97	0.07	12,15,33,37	0
3	FDA	B	701	53/53	0.98	0.05	9,10,12,13	0
3	FDA	A	701	53/53	0.98	0.04	8,10,12,13	0
4	NAG	A	703[A]	14/15	0.98	0.05	8,10,12,19	14
4	NAG	A	703[B]	14/15	0.98	0.05	12,14,19,23	14
4	NAG	B	703[A]	14/15	0.98	0.04	9,10,15,21	2
4	NAG	B	703[B]	14/15	0.98	0.04	9,10,12,15	2
9	NA	A	714	1/1	0.98	0.05	21,21,21,21	0
8	CL	A	713	1/1	1.00	0.04	22,22,22,22	1
7	MG	A	712	1/1	1.00	0.05	13,13,13,13	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.

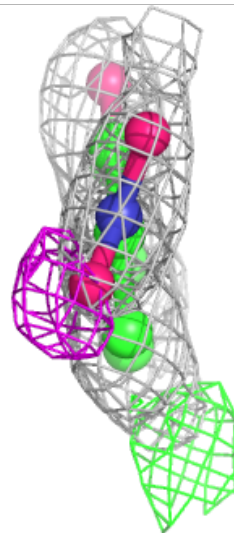
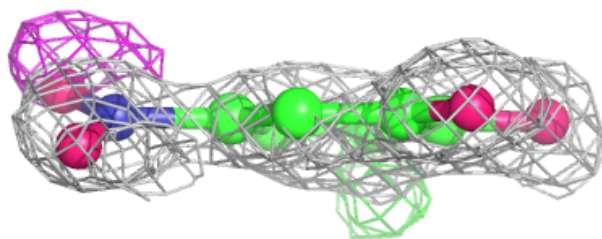
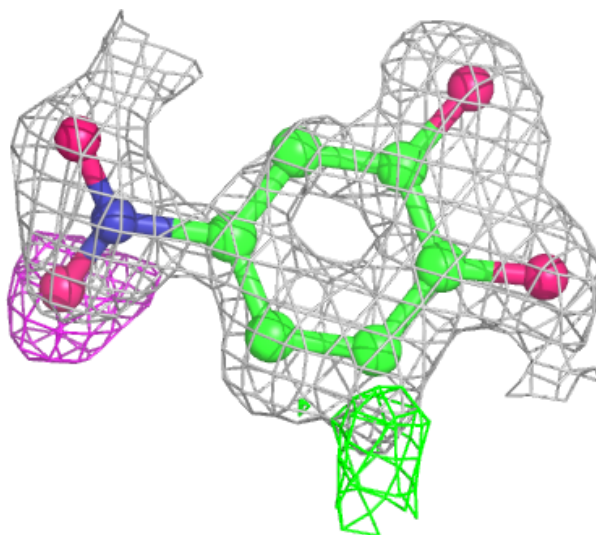
Electron density around 4NC B 707:

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



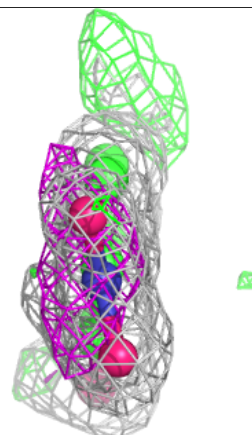
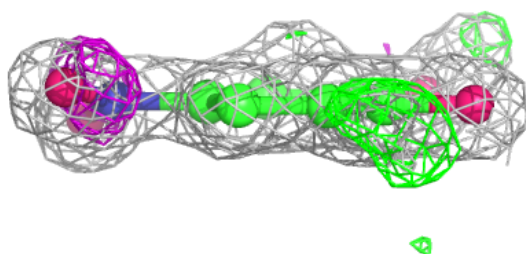
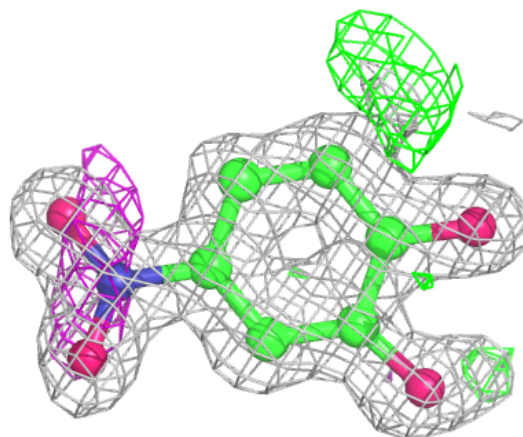
Electron density around 4NC A 708:

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

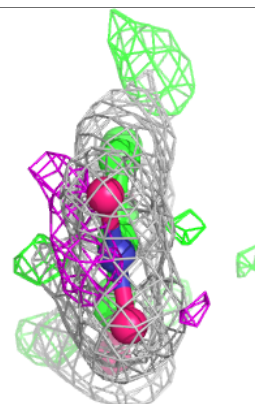
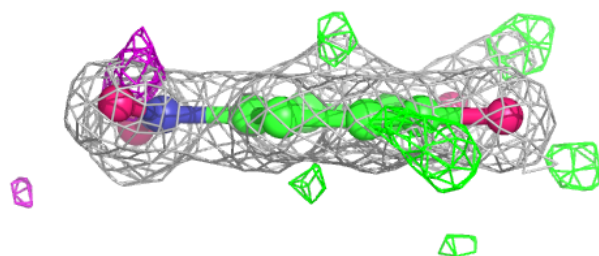
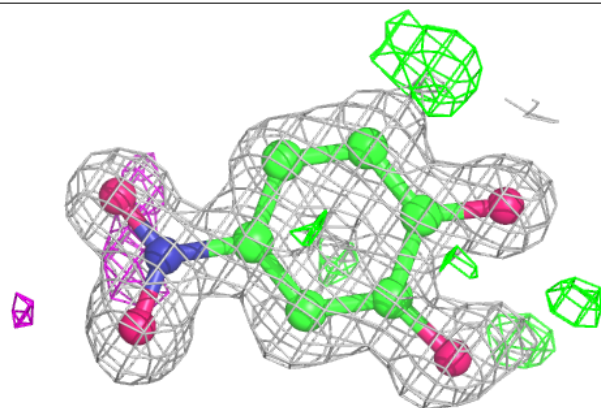


Electron density around 4NC B 706:

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

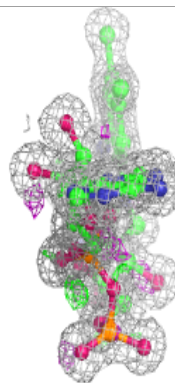
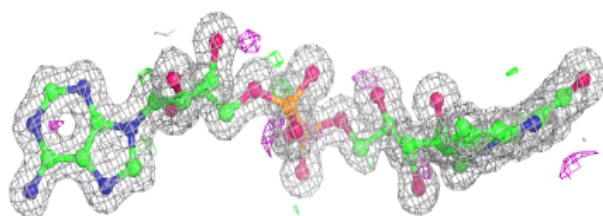
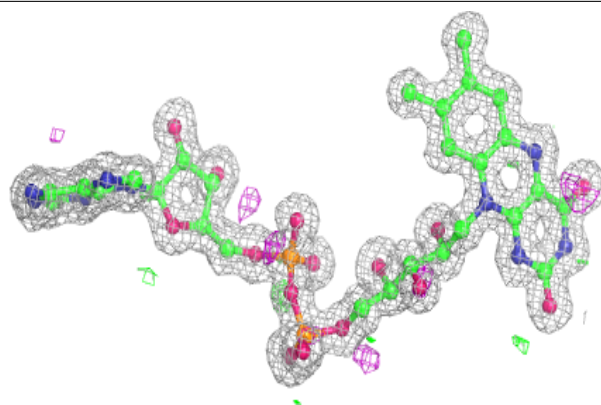
**Electron density around 4NC A 707:**

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

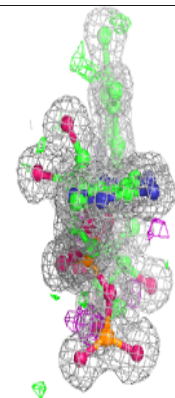
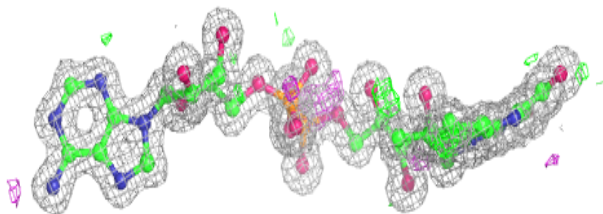
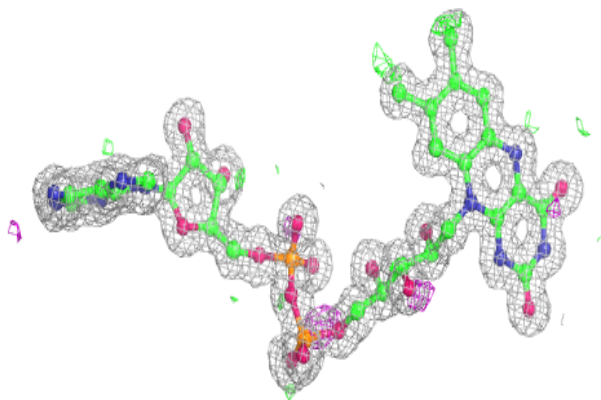


Electron density around FDA B 701:

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

**Electron density around FDA A 701:**

$2mF_o-DF_c$ (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.