



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 9, 2020 – 12:36 PM BST

PDB ID : 1INY  
Title : A SIALIC ACID DERIVED PHOSPHONATE ANALOG INHIBITS DIFFERENT STRAINS OF INFLUENZA VIRUS NEURAMINIDASE WITH DIFFERENT EFFICIENCIES  
Authors : White, C.L.; Janakiraman, M.N.; Laver, W.G.; Philippon, C.; Vasella, A.; Air, G.M.; Luo, M.  
Deposited on : 1994-09-26  
Resolution : 2.40 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.

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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 : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.13.1  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.13.1

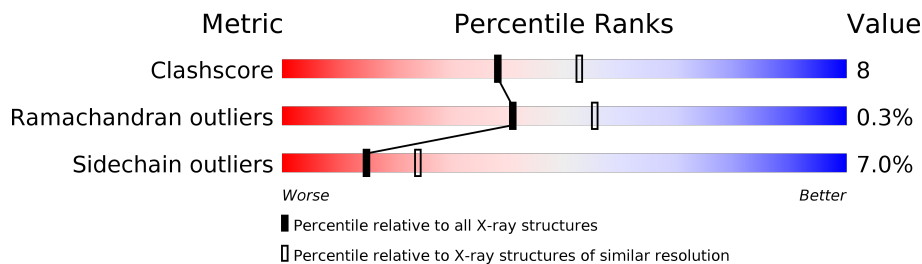
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*


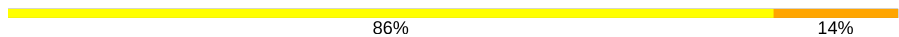
The reported resolution of this entry is 2.40 Å.

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))
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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  $\leq 5\%$ .

Mol	Chain	Length	Quality of chain
1	A	388	 80% 18% .
2	B	7	 86% 14%

## 2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 4202 atoms, of which 945 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.

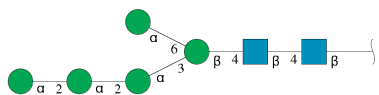
- Molecule 1 is a protein called INFLUENZA A SUBTYPE N9 NEURAMINIDASE.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	A	388	3780	1917	711	538	591	23	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	370	LEU	SER	conflict	UNP P03472

- Molecule 2 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-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	H	N	O			
2	B	7	160	46	77	2	35	0	0	0

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).

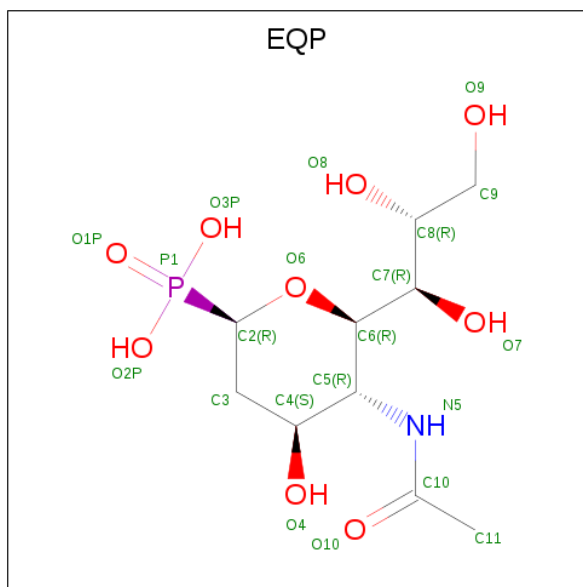


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
			Total	C	H	N			O
3	A	1	28	8	14	1	5	0	0
3	A	1	28	8	14	1	5	0	0

- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Ca		
4	A	1	1	1	0	0

- Molecule 5 is (1R)-4-acetamido-1,5-anhydro-2,4-dideoxy-1-phosphono-D-glycero-D-galacto-octitol (three-letter code: EQP) (formula: C<sub>10</sub>H<sub>20</sub>NO<sub>9</sub>P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
			Total	C	H	N	O			P
5	A	1	40	10	19	1	9	1	0	0

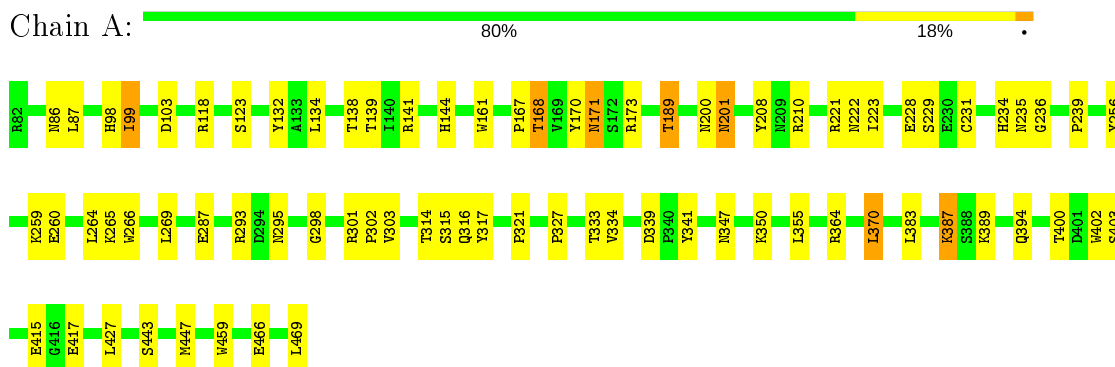
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	H O		
6	A	55	165	110 55	0	0

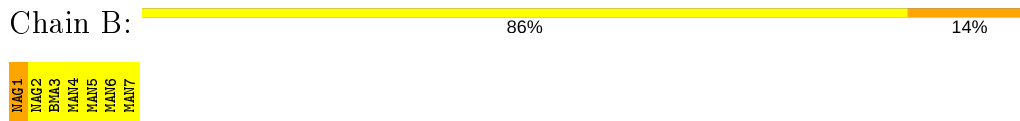
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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. 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: INFLUENZA A SUBTYPE N9 NEURAMINIDASE



- Molecule 2: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-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	I 4 3 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	184.86Å 184.86Å 184.86Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	8.00 – 2.40 28.52 – 2.39	Depositor EDS
% Data completeness (in resolution range)	(Not available) (8.00-2.40) 81.1 (28.52-2.39)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.04 (at 2.39Å)	Xtrriage
Refinement program	X-PLOR	Depositor
R, $R_{free}$	0.187 , (Not available) 0.394 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	20.8	Xtrriage
Anisotropy	0.000	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.24 , 12.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.69	EDS
Total number of atoms	4202	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	8.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.63% of the height of the origin peak. No significant pseudotranslation is detected.*

<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: EQP, CA, BMA, NAG, MAN

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	0.70	0/3152	0.84	0/4293

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	3069	711	2900	46	2
2	B	83	77	70	3	0
3	A	28	28	26	0	0
4	A	1	0	0	0	0
5	A	21	19	17	0	0
6	A	55	110	0	1	0
All	All	3257	945	3013	46	2

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 8.

All (46) 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:200:ASN:HD21	2:B:1:NAG:C1	1.08	1.57
1:A:173:ARG:HD3	1:A:210:ARG:HH22	1.45	0.79
1:A:87:LEU:H	1:A:234:HIS:HD2	1.31	0.78
1:A:334:VAL:HG12	1:A:387:LYS:HD3	1.66	0.77
1:A:173:ARG:HD3	1:A:210:ARG:NH2	2.02	0.74
1:A:200:ASN:HD22	2:B:1:NAG:C1	1.97	0.73
1:A:189:THR:HG22	1:A:208:TYR:CZ	2.26	0.71
1:A:201:ASN:HB3	1:A:221:ARG:NH1	2.07	0.69
1:A:327:PRO:HD2	1:A:347:ASN:HB3	1.75	0.69
1:A:168:THR:HG22	1:A:171:ASN:H	1.61	0.65
1:A:370:LEU:HD13	1:A:402:TRP:HZ3	1.62	0.64
1:A:293:ARG:HH21	1:A:295:ASN:ND2	1.98	0.62
1:A:87:LEU:H	1:A:234:HIS:CD2	2.17	0.60
1:A:98:HIS:HD2	1:A:99:ILE:O	1.85	0.59
1:A:86:ASN:OD1	1:A:235:ASN:HB2	2.03	0.59
1:A:355:LEU:HD13	1:A:383:LEU:HD13	1.88	0.56
1:A:259:LYS:HB2	1:A:264:LEU:HD11	1.87	0.55
1:A:236:GLY:HA3	1:A:259:LYS:HE3	1.89	0.54
1:A:99:ILE:HG12	1:A:459:TRP:CZ2	2.42	0.54
1:A:201:ASN:OD1	2:B:1:NAG:O5	2.26	0.53
1:A:321:PRO:HG2	1:A:389:LYS:HE2	1.91	0.53
1:A:201:ASN:N	1:A:201:ASN:HD22	2.07	0.53
1:A:161:TRP:CZ2	1:A:167:PRO:HG3	2.45	0.51
1:A:427:LEU:HB2	1:A:443:SER:HB3	1.95	0.48
1:A:123:SER:HB3	1:A:132:TYR:CE1	2.48	0.48
1:A:201:ASN:HB3	1:A:221:ARG:HH12	1.79	0.47
1:A:394:GLN:NE2	6:A:515:HOH:O	2.49	0.45
1:A:168:THR:CG2	1:A:170:TYR:H	2.30	0.45
1:A:168:THR:HG23	1:A:170:TYR:H	1.81	0.45
1:A:403:SER:HA	1:A:427:LEU:HD23	1.99	0.45
1:A:229:SER:HB3	1:A:350:LYS:HE2	1.98	0.44
1:A:168:THR:HG22	1:A:171:ASN:N	2.32	0.44
1:A:316:GLN:HG3	1:A:317:TYR:N	2.33	0.43
1:A:301:ARG:HA	1:A:302:PRO:HD3	1.93	0.43
1:A:138:THR:HG22	1:A:139:THR:N	2.33	0.43
1:A:138:THR:HG23	1:A:144:HIS:HB2	2.00	0.43
1:A:239:PRO:HA	1:A:256:TYR:O	2.19	0.43
1:A:466:GLU:HA	1:A:469:LEU:HG	2.01	0.42
1:A:265:LYS:HG2	1:A:266:TRP:N	2.35	0.42
1:A:138:THR:CG2	1:A:144:HIS:HB2	2.50	0.42
1:A:370:LEU:HD13	1:A:402:TRP:CZ3	2.50	0.42
1:A:264:LEU:HD23	1:A:264:LEU:HA	1.89	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:236:GLY:O	1:A:259:LYS:HD2	2.20	0.41
1:A:173:ARG:CD	1:A:210:ARG:HH22	2.23	0.41
1:A:303:VAL:O	1:A:315:SER:HA	2.21	0.41
1:A:298:GLY:HA2	1:A:341:TYR:O	2.20	0.41

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:333:THR:H	1:A:341:TYR:HH[48_555]	0.79	0.81
1:A:333:THR:N	1:A:341:TYR:HH[48_555]	1.50	0.10

## 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	386/388 (100%)	354 (92%)	31 (8%)	1 (0%)	41 55

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	223	ILE

### 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	341/341 (100%)	317 (93%)	24 (7%)	15 24

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	99	ILE
1	A	103	ASP
1	A	118	ARG
1	A	134	LEU
1	A	141	ARG
1	A	168	THR
1	A	171	ASN
1	A	189	THR
1	A	201	ASN
1	A	222	ASN
1	A	228	GLU
1	A	231	CYS
1	A	260	GLU
1	A	269	LEU
1	A	287	GLU
1	A	314	THR
1	A	339	ASP
1	A	364	ARG
1	A	370	LEU
1	A	387	LYS
1	A	400	THR
1	A	415	GLU
1	A	417	GLU
1	A	447	MET

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

Mol	Chain	Res	Type
1	A	95	ASN
1	A	98	HIS
1	A	171	ASN
1	A	200	ASN
1	A	201	ASN
1	A	222	ASN
1	A	234	HIS
1	A	295	ASN
1	A	346	ASN

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Mol	Chain	Res	Type
1	A	394	GLN
1	A	399	ASN

### 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](#)

7 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	B	1	1,2	14,14,15	5.43	7 (50%)	17,19,21	4.31	10 (58%)
2	NAG	B	2	2	14,14,15	3.06	5 (35%)	17,19,21	2.33	2 (11%)
2	BMA	B	3	2	11,11,12	1.56	1 (9%)	15,15,17	2.12	4 (26%)
2	MAN	B	4	2	11,11,12	2.34	3 (27%)	15,15,17	2.12	6 (40%)
2	MAN	B	5	2	11,11,12	1.46	1 (9%)	15,15,17	1.77	4 (26%)
2	MAN	B	6	2	11,11,12	1.78	3 (27%)	15,15,17	3.27	8 (53%)
2	MAN	B	7	2	11,11,12	0.89	0	15,15,17	1.43	2 (13%)

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	B	1	1,2	-	3/6/23/26	0/1/1/1
2	NAG	B	2	2	-	2/6/23/26	0/1/1/1
2	BMA	B	3	2	-	0/2/19/22	0/1/1/1
2	MAN	B	4	2	-	0/2/19/22	0/1/1/1
2	MAN	B	5	2	-	1/2/19/22	0/1/1/1
2	MAN	B	6	2	-	2/2/19/22	0/1/1/1
2	MAN	B	7	2	-	1/2/19/22	0/1/1/1

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1	NAG	O5-C1	10.51	1.60	1.43
2	B	1	NAG	C3-C2	9.46	1.72	1.52
2	B	1	NAG	O4-C4	8.22	1.62	1.43
2	B	2	NAG	C1-C2	7.23	1.63	1.52
2	B	1	NAG	C4-C5	6.83	1.67	1.53
2	B	1	NAG	O5-C5	6.83	1.57	1.43
2	B	2	NAG	C3-C2	6.59	1.66	1.52
2	B	1	NAG	C1-C2	6.24	1.61	1.52
2	B	4	MAN	C2-C3	6.22	1.61	1.52
2	B	6	MAN	C4-C5	4.06	1.61	1.53
2	B	2	NAG	O5-C5	4.04	1.51	1.43
2	B	3	BMA	O5-C5	3.56	1.50	1.43
2	B	5	MAN	O5-C1	3.52	1.49	1.43
2	B	4	MAN	O5-C5	3.19	1.49	1.43
2	B	4	MAN	C4-C5	2.82	1.59	1.53
2	B	2	NAG	C4-C5	2.64	1.58	1.53
2	B	2	NAG	O4-C4	2.49	1.48	1.43
2	B	1	NAG	C4-C3	2.44	1.58	1.52
2	B	6	MAN	C4-C3	2.39	1.58	1.52
2	B	6	MAN	O5-C5	2.37	1.48	1.43

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	6	MAN	C1-O5-C5	8.98	124.35	112.19
2	B	1	NAG	O5-C1-C2	-7.83	98.93	111.29
2	B	1	NAG	C3-C4-C5	-7.48	96.89	110.24
2	B	1	NAG	C1-O5-C5	7.45	122.29	112.19
2	B	1	NAG	C4-C3-C2	6.32	120.27	111.02
2	B	2	NAG	O5-C1-C2	-6.21	101.49	111.29
2	B	2	NAG	O3-C3-C2	6.04	121.97	109.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	3	BMA	C1-O5-C5	5.52	119.67	112.19
2	B	1	NAG	O3-C3-C4	-5.34	97.99	110.35
2	B	1	NAG	O4-C4-C5	5.23	122.28	109.30
2	B	7	MAN	C1-O5-C5	4.28	118.00	112.19
2	B	6	MAN	C3-C4-C5	-4.21	102.72	110.24
2	B	3	BMA	O5-C5-C6	4.02	113.51	107.20
2	B	1	NAG	C1-C2-N2	-3.93	103.78	110.49
2	B	4	MAN	C3-C4-C5	-3.73	103.58	110.24
2	B	4	MAN	C1-O5-C5	3.65	117.14	112.19
2	B	6	MAN	O5-C5-C6	-3.61	101.54	107.20
2	B	6	MAN	O4-C4-C5	3.50	118.00	109.30
2	B	4	MAN	O3-C3-C2	3.47	116.64	109.99
2	B	5	MAN	C1-C2-C3	3.36	113.80	109.67
2	B	1	NAG	O5-C5-C6	3.32	112.41	107.20
2	B	5	MAN	O2-C2-C3	-3.30	103.52	110.14
2	B	6	MAN	O3-C3-C2	-3.24	103.79	109.99
2	B	5	MAN	C1-O5-C5	3.13	116.43	112.19
2	B	6	MAN	C2-C3-C4	3.13	116.30	110.89
2	B	4	MAN	C1-C2-C3	2.90	113.23	109.67
2	B	3	BMA	C6-C5-C4	2.82	119.60	113.00
2	B	4	MAN	O4-C4-C5	2.79	116.22	109.30
2	B	3	BMA	O5-C5-C4	-2.59	104.53	110.83
2	B	7	MAN	O5-C1-C2	-2.44	107.00	110.77
2	B	1	NAG	O3-C3-C2	2.38	114.40	109.47
2	B	1	NAG	O6-C6-C5	2.27	119.10	111.29
2	B	4	MAN	O5-C1-C2	-2.26	107.28	110.77
2	B	6	MAN	O2-C2-C1	2.22	113.70	109.15
2	B	5	MAN	O5-C5-C6	2.21	110.67	107.20
2	B	6	MAN	C6-C5-C4	2.04	117.78	113.00

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	1	NAG	C4-C5-C6-O6
2	B	1	NAG	O5-C5-C6-O6
2	B	2	NAG	C1-C2-N2-C7
2	B	6	MAN	C4-C5-C6-O6
2	B	6	MAN	O5-C5-C6-O6
2	B	1	NAG	C3-C2-N2-C7
2	B	7	MAN	C4-C5-C6-O6
2	B	2	NAG	C3-C2-N2-C7

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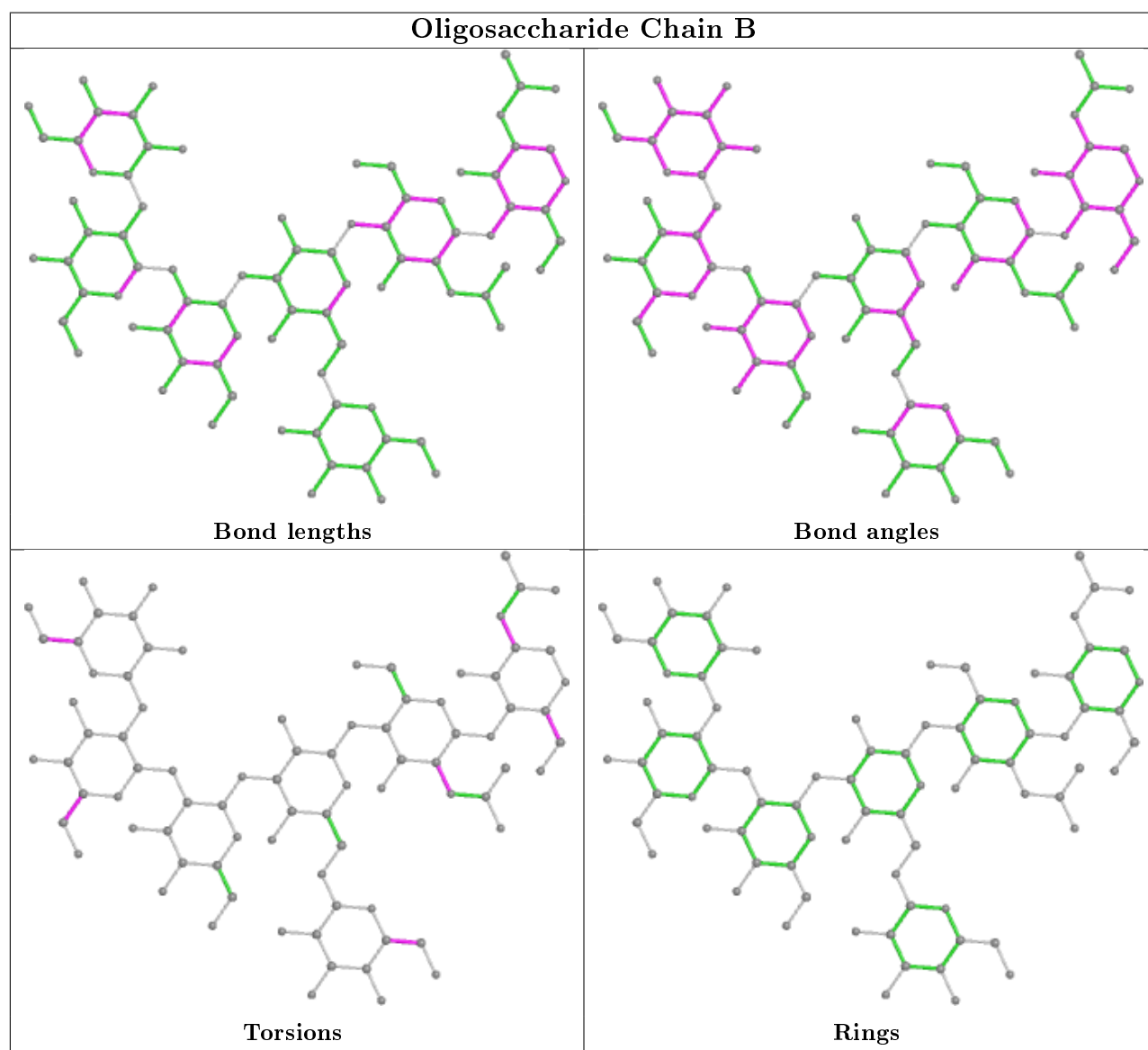
Mol	Chain	Res	Type	Atoms
2	B	5	MAN	C4-C5-C6-O6

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1	NAG	3	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

Of 4 ligands modelled in this entry, 1 is monoatomic - leaving 3 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	NAG	A	471(A)	1	14,14,15	1.46	3 (21%)	17,19,21	1.45	3 (17%)
5	EQP	A	500	-	18,21,21	2.48	6 (33%)	22,31,31	2.54	8 (36%)
3	NAG	A	470(A)	1	14,14,15	1.38	2 (14%)	17,19,21	1.48	4 (23%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	A	471(A)	1	-	0/6/23/26	0/1/1/1
5	EQP	A	500	-	-	1/14/36/36	0/1/1/1
3	NAG	A	470(A)	1	-	3/6/23/26	0/1/1/1

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	500	EQP	P1-O2P	-5.55	1.46	1.54
5	A	500	EQP	O6-C6	4.22	1.50	1.44
5	A	500	EQP	C6-C5	3.99	1.59	1.53
3	A	470(A)	NAG	C4-C5	3.86	1.61	1.53
3	A	471(A)	NAG	C3-C2	3.69	1.60	1.52
5	A	500	EQP	P1-O3P	-3.42	1.49	1.54
5	A	500	EQP	O4-C4	-3.36	1.36	1.43
5	A	500	EQP	P1-O1P	-2.53	1.45	1.49
3	A	470(A)	NAG	C1-C2	2.15	1.55	1.52
3	A	471(A)	NAG	C4-C5	2.10	1.57	1.53
3	A	471(A)	NAG	C4-C3	2.09	1.57	1.52

All (15) bond angle outliers are listed below:



Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	500	EQP	O3P-P1-O1P	-7.85	93.73	113.45
5	A	500	EQP	O6-C2-C3	-4.31	104.67	110.59
5	A	500	EQP	C8-C7-C6	-4.11	105.23	113.03
3	A	471(A)	NAG	O3-C3-C2	3.33	116.35	109.47
5	A	500	EQP	O1P-P1-C2	-3.15	106.20	113.34
3	A	470(A)	NAG	C1-O5-C5	3.02	116.28	112.19
5	A	500	EQP	C3-C4-C5	-2.64	108.27	111.46
3	A	470(A)	NAG	O5-C5-C6	-2.54	103.22	107.20
5	A	500	EQP	C9-C8-C7	-2.49	107.01	112.41
5	A	500	EQP	C4-C5-N5	-2.45	105.52	110.38
3	A	470(A)	NAG	O4-C4-C3	-2.38	104.86	110.35
3	A	470(A)	NAG	O3-C3-C2	2.35	114.33	109.47
3	A	471(A)	NAG	C6-C5-C4	2.26	118.30	113.00
3	A	471(A)	NAG	C2-N2-C7	-2.10	119.91	122.90
5	A	500	EQP	O7-C7-C8	2.00	113.65	108.81

There are no chirality outliers.

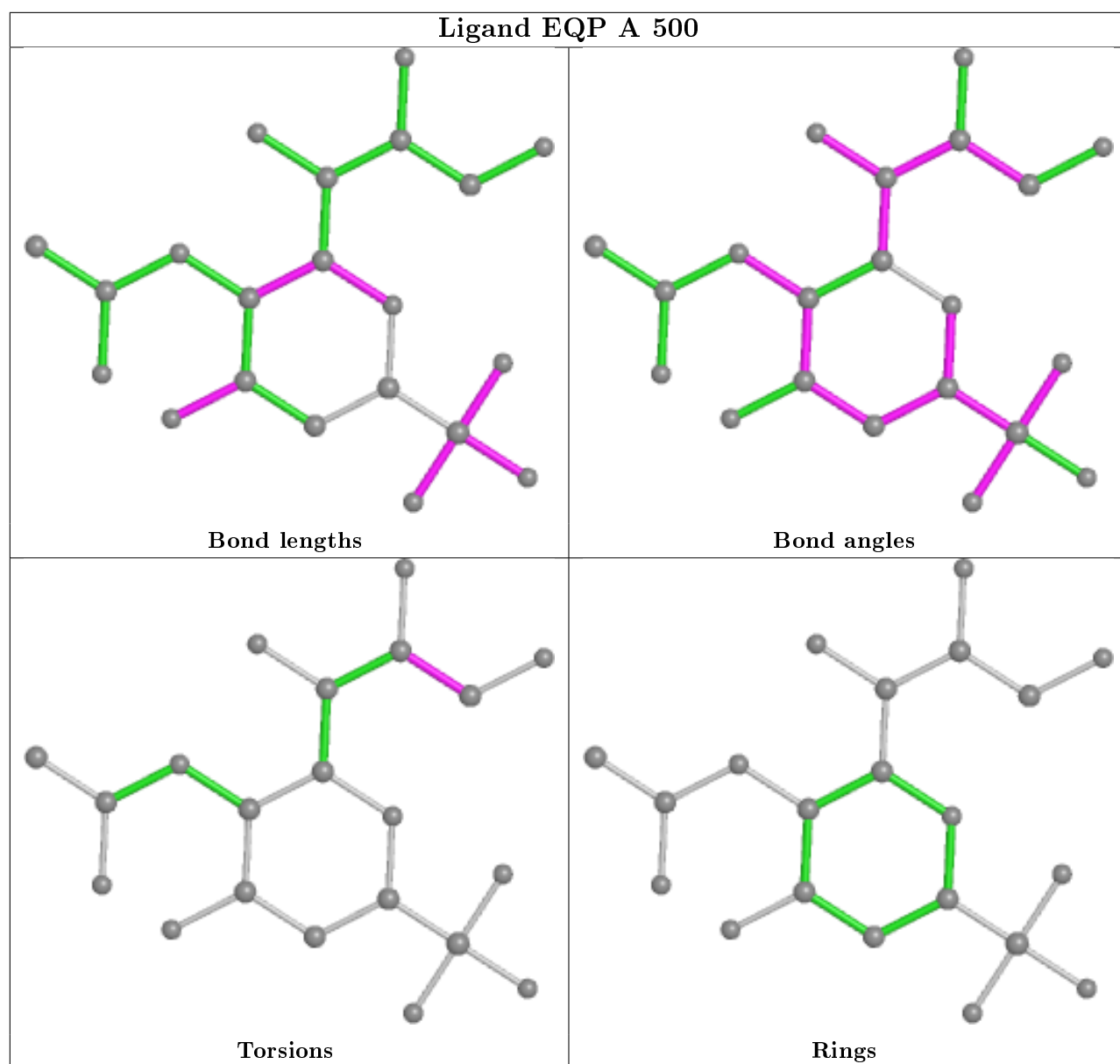
All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	470(A)	NAG	O5-C5-C6-O6
3	A	470(A)	NAG	C1-C2-N2-C7
5	A	500	EQP	O8-C8-C9-O9
3	A	470(A)	NAG	C4-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for 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](#)

Unable to reproduce the depositors R factor - this section is therefore empty.

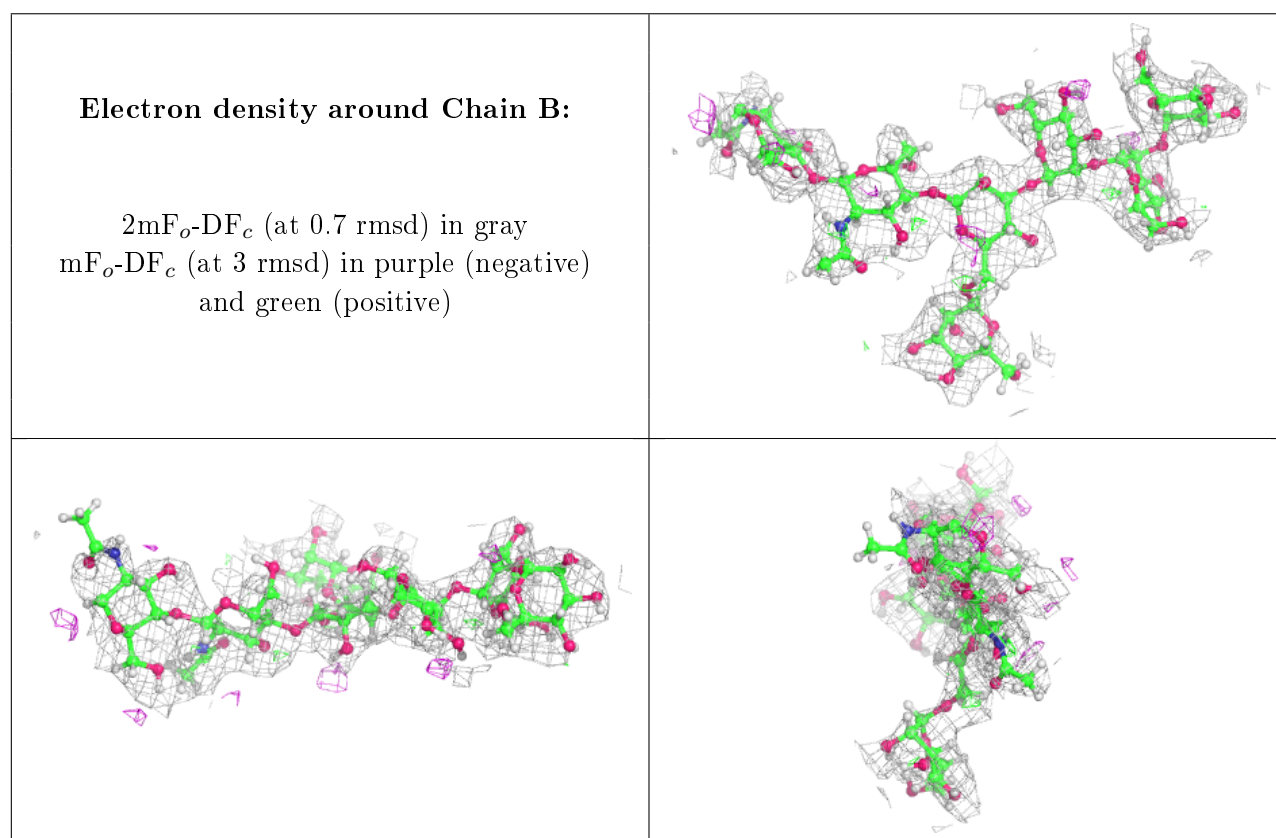
### 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

Unable to reproduce the depositors R factor - this section is therefore empty.

### 6.3 Carbohydrates [i](#)

Unable to reproduce the depositors R factor - this section is therefore empty.

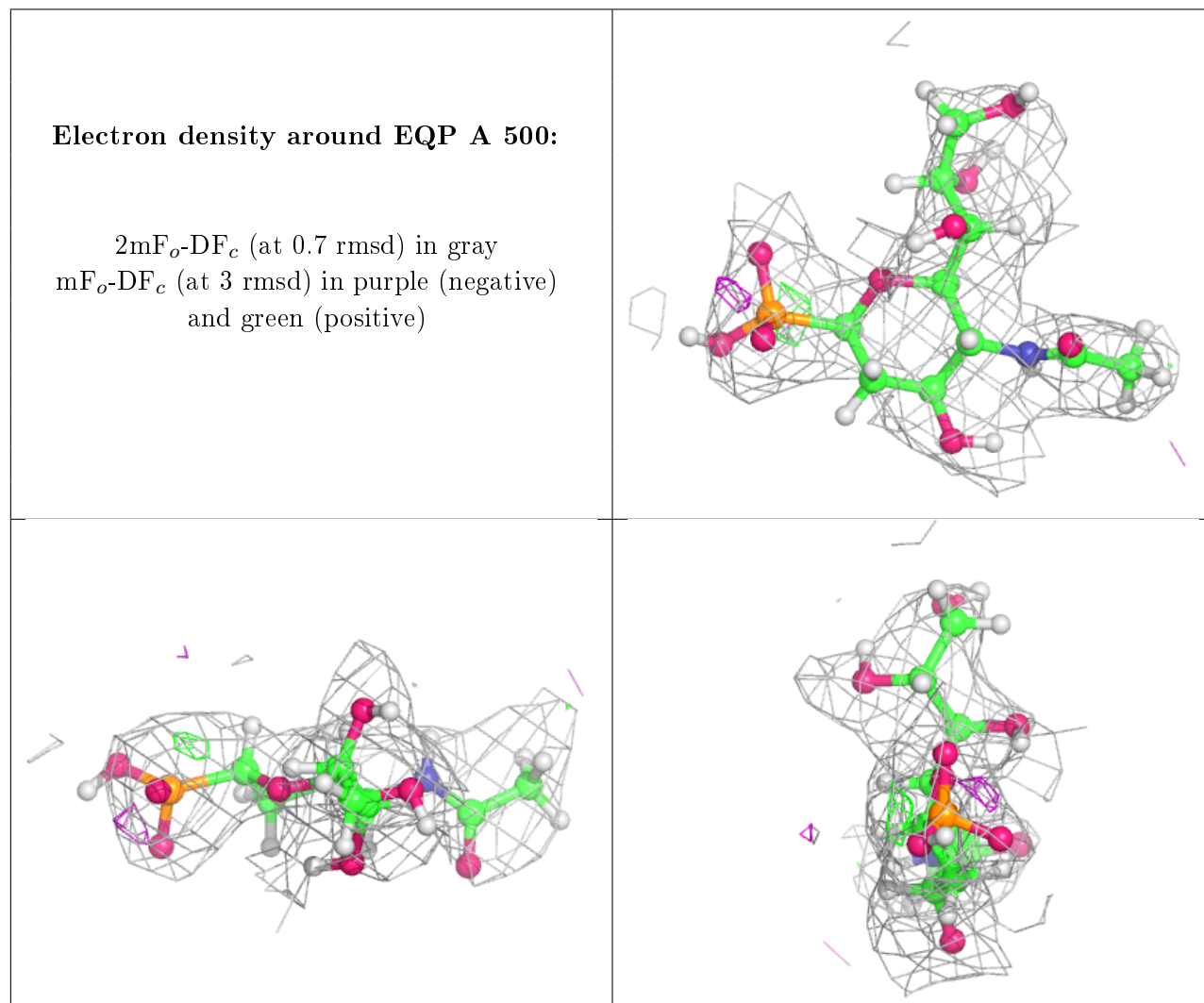
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.



### 6.4 Ligands [i](#)

Unable to reproduce the depositors R factor - this section is therefore empty.

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



## 6.5 Other polymers [\(i\)](#)

Unable to reproduce the depositor's R factor - this section is therefore empty.