



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 05:15 PM UTC

PDB ID : 1INX / pdb\_00001inx  
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.

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](#) ①) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0  
Mogul : 2022.3.0, CSD as543be (2022)  
Xtrriage (Phenix) : 2.0  
EDS : 3.0  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
CCP4 : 9.0.010 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

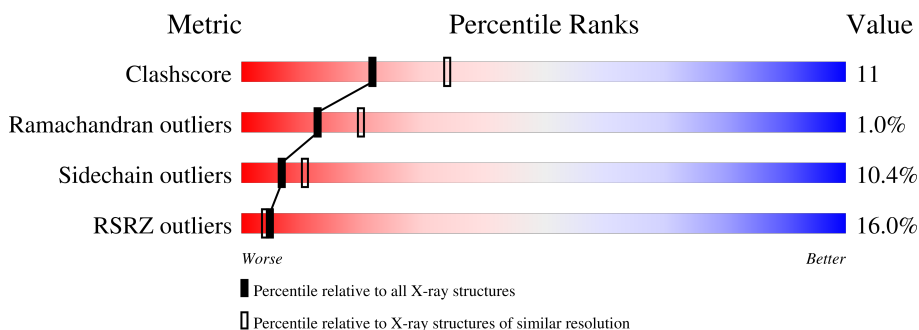
# 1 Overall quality at a glance

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	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (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 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	388	
2	B	5	

## 2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 4225 atoms, of which 999 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.

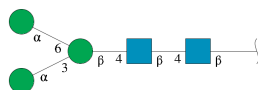
- Molecule 1 is a protein called INFLUENZA A SUBTYPE N2 NEURAMINIDASE.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	A	388	3745	1866	723	545	588	23	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	339	ASP	ASN	conflict	UNP P06820

- Molecule 2 is an oligosaccharide called 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	5	118	34	57	2	25	0	0	0

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

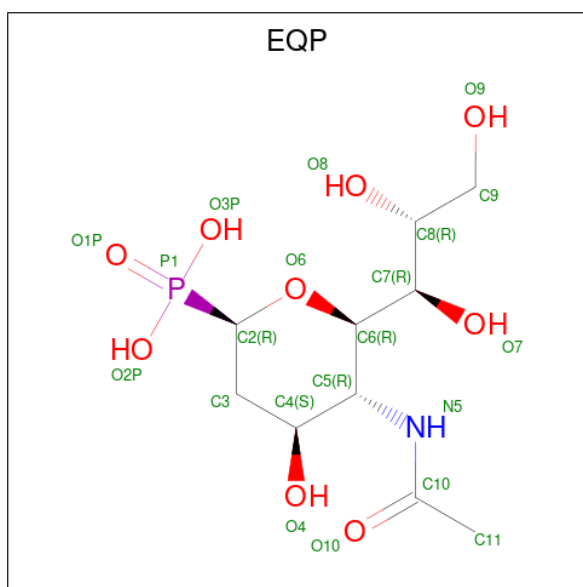


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
			Total	C	H	N			O
3	A	1	28	8	14	1	5	0	0
3	A	1	28	8	14	1	5	0	0
3	A	1	28	8	14	1	5	0	0

- Molecule 4 is CALCIUM ION (CCD ID: 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 (CCD ID: 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

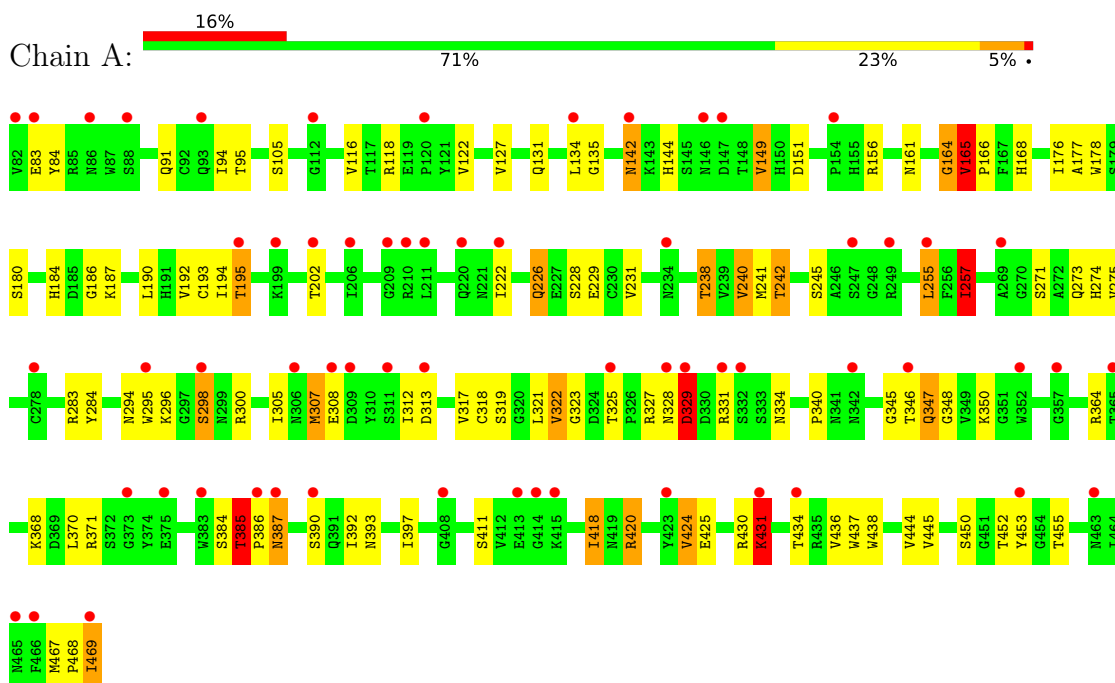
- Molecule 6 is water.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	H	O		
6	A	79	237	158	79	0	0

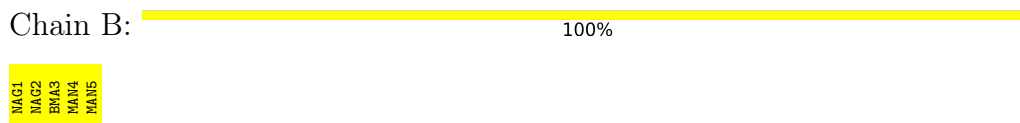
### 3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: INFLUENZA A SUBTYPE N2 NEURAMINIDASE



- Molecule 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	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	120.42Å 139.83Å 140.07Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	8.00 – 2.40 8.00 – 2.40	Depositor EDS
% Data completeness (in resolution range)	(Not available) (8.00-2.40) 67.9 (8.00-2.40)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.83 (at 2.39Å)	Xtrriage
Refinement program	X-PLOR	Depositor
R, $R_{free}$	0.179 , (Not available) 0.428 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	17.4	Xtrriage
Anisotropy	0.538	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.39 , 49.3	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	0.57	EDS
Total number of atoms	4225	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	7.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.53% 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: BMA, MAN, EQP, CA, NAG

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	0.81	3/3092 (0.1%)	1.16	26/4194 (0.6%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	307	MET	SD-CE	-5.55	1.65	1.79
1	A	424	VAL	C-O	-5.52	1.18	1.24
1	A	165	VAL	CA-CB	5.42	1.59	1.53

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	226	GLN	N-CA-C	12.56	124.97	111.28
1	A	431	LYS	N-CA-C	-8.72	92.22	110.80
1	A	298	SER	N-CA-C	-7.99	103.55	113.38
1	A	300	ARG	N-CA-C	7.22	118.75	109.72
1	A	229	GLU	N-CA-C	6.86	120.18	110.50
1	A	180	SER	N-CA-C	6.58	117.81	108.74
1	A	345	GLY	N-CA-C	6.57	120.62	112.73
1	A	271	SER	N-CA-C	6.46	120.86	112.92
1	A	444	VAL	N-CA-C	-6.35	99.97	108.35
1	A	384	SER	N-CA-C	6.17	120.98	112.90
1	A	397	ILE	N-CA-C	-6.14	105.83	111.67
1	A	385	THR	CA-C-N	5.83	126.17	119.93
1	A	385	THR	C-N-CA	5.83	126.17	119.93
1	A	164	GLY	CA-C-N	-5.72	118.47	122.59
1	A	164	GLY	C-N-CA	-5.72	118.47	122.59
1	A	105	SER	N-CA-C	5.67	117.46	111.28
1	A	450	SER	N-CA-C	-5.56	106.17	113.17
1	A	116	VAL	N-CA-C	-5.45	100.57	108.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	257	ILE	N-CA-C	5.38	115.87	108.12
1	A	329	ASP	N-CA-C	-5.37	99.36	110.80
1	A	151	ASP	N-CA-C	5.37	119.00	112.23
1	A	467	MET	N-CA-C	5.30	117.40	110.08
1	A	323	GLY	N-CA-C	5.23	124.90	115.80
1	A	319	SER	N-CA-C	5.06	117.80	110.42
1	A	308	GLU	N-CA-C	5.02	116.83	111.36
1	A	318	CYS	N-CA-C	5.00	116.73	111.28

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	3022	723	2852	66	0
2	B	61	57	52	0	0
3	A	42	42	39	0	0
4	A	1	0	0	0	0
5	A	21	19	18	0	0
6	A	79	158	0	3	0
All	All	3226	999	2961	66	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 11.

All (66) 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:431:LYS:HA	1:A:431:LYS:NZ	1.89	0.87
1:A:334:ASN:HA	1:A:387:ASN:HD21	1.41	0.85
1:A:437:TRP:H	1:A:469:ILE:HG21	1.42	0.83
1:A:226:GLN:HE21	1:A:240:VAL:H	1.26	0.80
1:A:430:ARG:O	1:A:431:LYS:HB2	1.83	0.77
1:A:418:ILE:HD11	1:A:420:ARG:NH2	2.06	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:228:SER:HB3	1:A:350:LYS:HE2	1.73	0.70
1:A:242:THR:HG21	1:A:275:VAL:O	1.92	0.68
1:A:431:LYS:HA	1:A:431:LYS:HZ2	1.56	0.68
1:A:177:ALA:HB2	1:A:193:CYS:HB3	1.76	0.68
1:A:118:ARG:HD2	1:A:425:GLU:OE2	1.98	0.64
1:A:176:ILE:HG22	1:A:195:THR:HG21	1.81	0.62
1:A:274:HIS:HD2	1:A:294:ASN:H	1.47	0.62
1:A:437:TRP:H	1:A:469:ILE:CG2	2.12	0.62
1:A:95:THR:HG22	1:A:453:TYR:HE2	1.64	0.61
1:A:184:HIS:CD2	1:A:186:GLY:H	2.19	0.60
1:A:149:VAL:HG22	6:A:508:HOH:O	2.03	0.58
1:A:245:SER:O	1:A:274:HIS:HE1	1.86	0.58
1:A:135:GLY:O	1:A:156:ARG:HD2	2.03	0.57
1:A:95:THR:HG22	1:A:453:TYR:CE2	2.40	0.56
1:A:431:LYS:HA	1:A:431:LYS:HZ3	1.70	0.56
1:A:438:TRP:HD1	1:A:469:ILE:HD12	1.70	0.55
1:A:142:ASN:HD22	1:A:144:HIS:H	1.56	0.54
1:A:238:THR:HG21	1:A:305:ILE:HG21	1.90	0.54
1:A:328:ASN:HB2	6:A:547:HOH:O	2.08	0.54
1:A:273:GLN:HG3	1:A:340:PRO:HG3	1.90	0.54
1:A:298:SER:O	1:A:322:VAL:HG13	2.08	0.53
1:A:436:VAL:HA	1:A:469:ILE:HG22	1.91	0.52
1:A:327:ARG:HH21	1:A:364:ARG:HD2	1.75	0.52
1:A:255:LEU:HD23	1:A:255:LEU:N	2.25	0.52
1:A:346:THR:O	1:A:347:GLN:HB2	2.09	0.52
1:A:437:TRP:N	1:A:469:ILE:HG21	2.19	0.52
1:A:334:ASN:HA	1:A:387:ASN:ND2	2.20	0.51
1:A:84:TYR:CE1	1:A:187:LYS:HD2	2.45	0.51
1:A:437:TRP:HD1	1:A:469:ILE:HG23	1.74	0.51
1:A:190:LEU:CD1	1:A:257:ILE:HD11	2.41	0.51
1:A:131:GLN:NE2	1:A:164:GLY:H	2.10	0.49
1:A:434:THR:O	1:A:434:THR:HG22	2.13	0.48
1:A:468:PRO:O	1:A:469:ILE:HB	2.12	0.48
1:A:283:ARG:O	1:A:284:TYR:C	2.55	0.48
1:A:131:GLN:HE21	1:A:164:GLY:H	1.62	0.48
1:A:312:ILE:HG22	1:A:313:ASP:N	2.29	0.47
1:A:194:ILE:HD11	1:A:241:MET:HE3	1.95	0.47
1:A:190:LEU:HD13	1:A:257:ILE:HD11	1.97	0.46
1:A:228:SER:HB3	1:A:350:LYS:CE	2.45	0.46
1:A:305:ILE:HG22	1:A:307:MET:HE2	1.98	0.46
1:A:328:ASN:O	1:A:329:ASP:HB2	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:91:GLN:OE1	1:A:420:ARG:HD2	2.18	0.44
1:A:325:THR:O	1:A:348:GLY:HA2	2.17	0.44
1:A:176:ILE:HG22	1:A:195:THR:CG2	2.46	0.44
1:A:411:SER:HB3	1:A:418:ILE:CD1	2.48	0.43
1:A:392:ILE:HG12	1:A:393:ASN:N	2.33	0.43
1:A:430:ARG:HD3	1:A:436:VAL:O	2.18	0.43
1:A:295:TRP:CE2	1:A:296:LYS:HD3	2.54	0.43
1:A:166:PRO:O	1:A:168:HIS:HD2	2.02	0.42
1:A:184:HIS:HD2	1:A:186:GLY:H	1.67	0.42
1:A:165:VAL:HA	1:A:166:PRO:HD2	1.94	0.42
1:A:176:ILE:CG2	1:A:195:THR:HG21	2.48	0.42
1:A:226:GLN:NE2	1:A:240:VAL:H	2.06	0.42
1:A:385:THR:HA	1:A:386:PRO:HD3	1.75	0.42
1:A:321:LEU:HD23	1:A:321:LEU:HA	1.59	0.41
1:A:168:HIS:HB2	6:A:566:HOH:O	2.19	0.41
1:A:328:ASN:O	1:A:368:LYS:HD2	2.21	0.41
1:A:437:TRP:HD1	1:A:469:ILE:CG2	2.33	0.41
1:A:238:THR:CG2	1:A:307:MET:HE1	2.51	0.41
1:A:168:HIS:CD2	1:A:168:HIS:H	2.40	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	386/388 (100%)	357 (92%)	25 (6%)	4 (1%)	<b>12</b> <b>20</b>

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	431	LYS
1	A	322	VAL

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Mol	Chain	Res	Type
1	A	329	ASP
1	A	222	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	338/338 (100%)	303 (90%)	35 (10%)	<b>7</b> <b>10</b>

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	83	GLU
1	A	94	ILE
1	A	122	VAL
1	A	127	VAL
1	A	134	LEU
1	A	142	ASN
1	A	149	VAL
1	A	161	ASN
1	A	165	VAL
1	A	178	TRP
1	A	192	VAL
1	A	195	THR
1	A	202	THR
1	A	231	VAL
1	A	238	THR
1	A	240	VAL
1	A	242	THR
1	A	255	LEU
1	A	257	ILE
1	A	317	VAL
1	A	331	ARG
1	A	347	GLN
1	A	370	LEU
1	A	371	ARG

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Mol	Chain	Res	Type
1	A	385	THR
1	A	387	ASN
1	A	390	SER
1	A	418	ILE
1	A	420	ARG
1	A	424	VAL
1	A	431	LYS
1	A	445	VAL
1	A	452	THR
1	A	455	THR
1	A	469	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	104	ASN
1	A	131	GLN
1	A	142	ASN
1	A	161	ASN
1	A	168	HIS
1	A	184	HIS
1	A	226	GLN
1	A	274	HIS
1	A	334	ASN
1	A	342	ASN
1	A	356	ASN
1	A	387	ASN
1	A	393	ASN
1	A	419	ASN
1	A	432	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

5 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	2,1	14,14,15	0.62	0	17,19,21	1.65	5 (29%)
2	NAG	B	2	2	14,14,15	0.65	0	17,19,21	1.32	2 (11%)
2	BMA	B	3	2	11,11,12	1.24	1 (9%)	15,15,17	1.21	2 (13%)
2	MAN	B	4	2	11,11,12	0.93	1 (9%)	15,15,17	1.15	1 (6%)
2	MAN	B	5	2	11,11,12	0.70	0	15,15,17	0.96	1 (6%)

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	2,1	-	0/6/23/26	0/1/1/1
2	NAG	B	2	2	-	0/6/23/26	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

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	3	BMA	C4-C5	3.53	1.60	1.53
2	B	4	MAN	C2-C3	2.59	1.56	1.52

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1	NAG	C1-O5-C5	3.93	117.45	112.19
2	B	1	NAG	O7-C7-C8	-3.22	116.31	122.05
2	B	2	NAG	C1-C2-N2	3.16	115.41	110.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	4	MAN	C1-O5-C5	2.95	116.14	112.19
2	B	1	NAG	C8-C7-N2	2.67	120.55	116.12
2	B	5	MAN	C1-O5-C5	2.33	115.30	112.19
2	B	3	BMA	C2-C3-C4	-2.14	107.10	110.86
2	B	3	BMA	C1-C2-C3	-2.11	106.57	109.64
2	B	1	NAG	C1-C2-N2	2.07	113.69	110.43
2	B	1	NAG	O5-C1-C2	-2.06	108.10	111.29
2	B	2	NAG	C3-C4-C5	2.04	113.93	110.23

There are no chirality outliers.

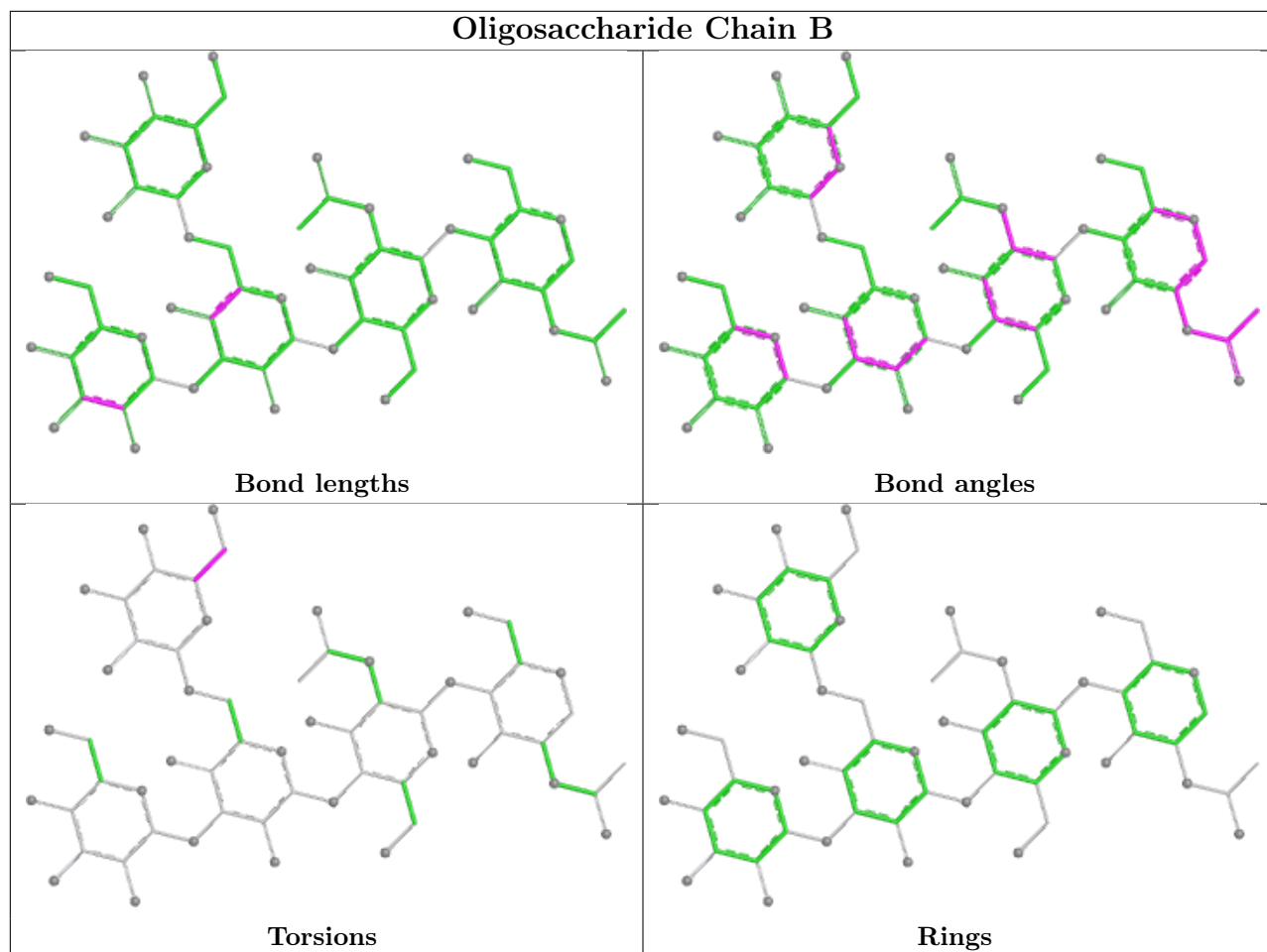
All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	5	MAN	O5-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 oligosaccharide.



## 5.6 Ligand geometry [i](#)

Of 5 ligands modelled in this entry, 1 is monoatomic - leaving 4 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	0.79	0	17,19,21	1.43	2 (11%)
3	NAG	A	477(A)	1	14,14,15	0.97	1 (7%)	17,19,21	1.40	2 (11%)
3	NAG	A	470(A)	1	14,14,15	0.65	0	17,19,21	1.31	1 (5%)
5	EQP	A	500	-	18,21,21	2.00	5 (27%)	22,31,31	2.00	4 (18%)

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	-	2/6/23/26	0/1/1/1
3	NAG	A	477(A)	1	-	0/6/23/26	0/1/1/1
3	NAG	A	470(A)	1	-	0/6/23/26	0/1/1/1
5	EQP	A	500	-	-	0/14/36/36	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	500	EQP	P1-O2P	-5.65	1.45	1.54
5	A	500	EQP	C7-C6	-3.14	1.49	1.52
5	A	500	EQP	P1-O3P	-2.67	1.50	1.54
5	A	500	EQP	O6-C6	-2.27	1.40	1.44
5	A	500	EQP	C8-C7	-2.24	1.49	1.53
3	A	477(A)	NAG	C4-C3	2.18	1.58	1.52

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	500	EQP	O2P-P1-O1P	-6.00	98.42	113.45
3	A	471(A)	NAG	C1-O5-C5	4.36	118.03	112.19
5	A	500	EQP	O1P-P1-C2	-4.27	103.68	113.34
3	A	477(A)	NAG	C1-O5-C5	3.75	117.21	112.19
5	A	500	EQP	O6-C2-C3	-3.17	106.40	110.66
3	A	470(A)	NAG	C1-C2-N2	2.65	114.61	110.43
3	A	477(A)	NAG	C4-C3-C2	-2.34	107.59	111.02
3	A	471(A)	NAG	O5-C1-C2	-2.08	108.07	111.29
5	A	500	EQP	C5-N5-C10	-2.04	118.33	123.11

There are no chirality outliers.

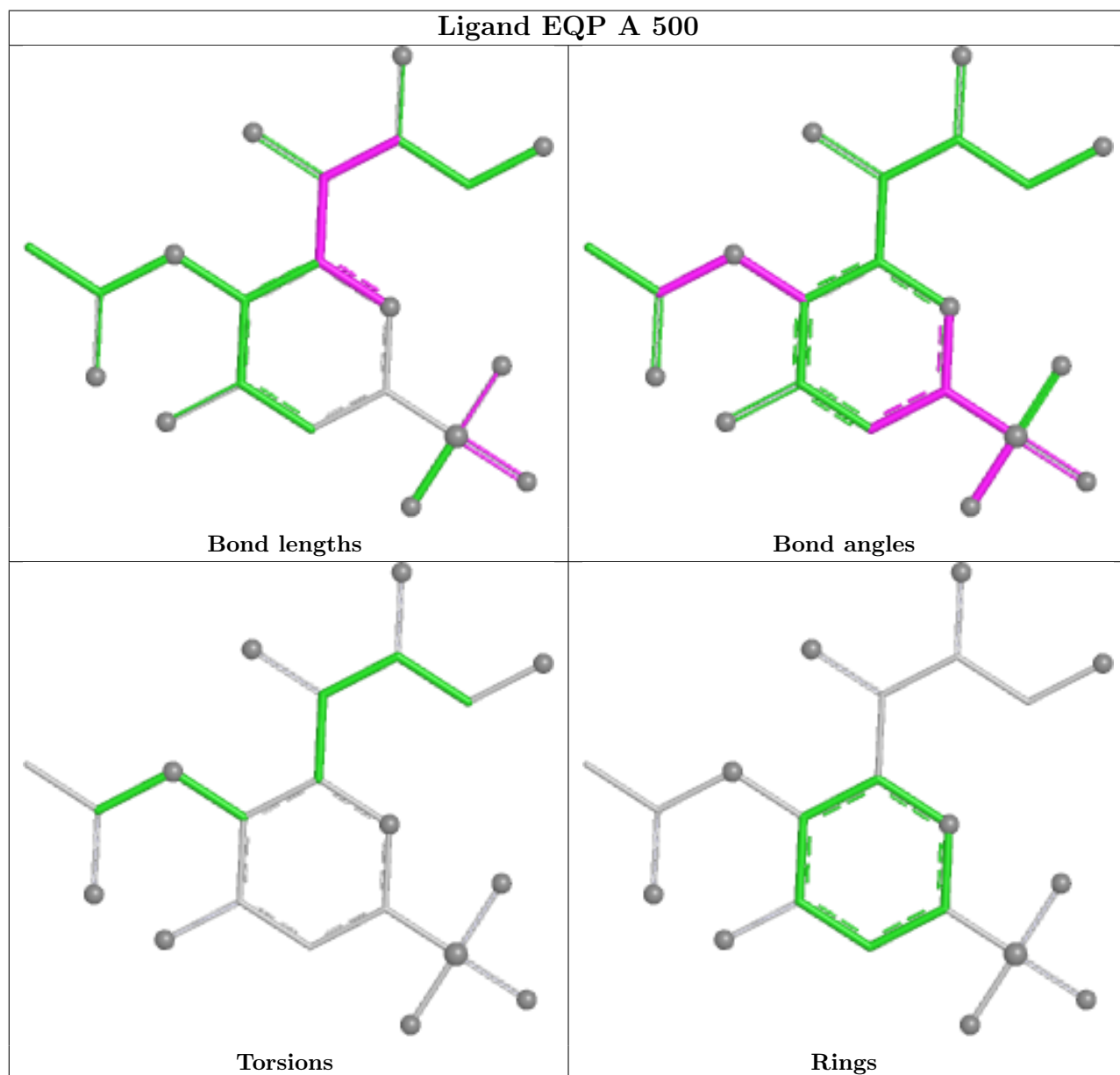
All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	471(A)	NAG	O5-C5-C6-O6
3	A	471(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

### 6.1 Protein, DNA and RNA chains

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	388/388 (100%)	1.16	62 (15%) <b>5</b> <b>4</b>	1, 6, 13, 23	90 (23%)

All (62) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	82	VAL	5.9
1	A	434	THR	4.7
1	A	331	ARG	4.4
1	A	249	ARG	4.3
1	A	342	ASN	4.1
1	A	308	GLU	4.0
1	A	311	SER	4.0
1	A	209	GLY	3.9
1	A	387	ASN	3.8
1	A	329	ASP	3.7
1	A	202	THR	3.6
1	A	247	SER	3.6
1	A	88	SER	3.4
1	A	325	THR	3.3
1	A	211	LEU	3.3
1	A	465	ASN	3.2
1	A	112	GLY	3.2
1	A	414	GLY	2.9
1	A	332	SER	2.8
1	A	415	LYS	2.8
1	A	309	ASP	2.8
1	A	357	GLY	2.7
1	A	86	ASN	2.7
1	A	142	ASN	2.7
1	A	195	THR	2.7
1	A	147	ASP	2.6
1	A	469	ILE	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	313	ASP	2.5
1	A	154	PRO	2.5
1	A	146	ASN	2.5
1	A	431	LYS	2.5
1	A	386	PRO	2.5
1	A	206	ILE	2.4
1	A	352	TRP	2.4
1	A	463	ASN	2.4
1	A	222	ILE	2.4
1	A	93	GLN	2.4
1	A	413	GLU	2.4
1	A	298	SER	2.4
1	A	255	LEU	2.4
1	A	278	CYS	2.4
1	A	120	PRO	2.3
1	A	346	THR	2.3
1	A	83	GLU	2.3
1	A	373	GLY	2.3
1	A	383	TRP	2.3
1	A	375	GLU	2.3
1	A	453	TYR	2.3
1	A	328	ASN	2.3
1	A	365	THR	2.3
1	A	390	SER	2.2
1	A	234	ASN	2.2
1	A	269	ALA	2.2
1	A	306	ASN	2.2
1	A	134	LEU	2.2
1	A	295	TRP	2.1
1	A	220	GLN	2.1
1	A	199	LYS	2.1
1	A	408	GLY	2.1
1	A	210	ARG	2.1
1	A	466	PHE	2.1
1	A	423	TYR	2.0

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

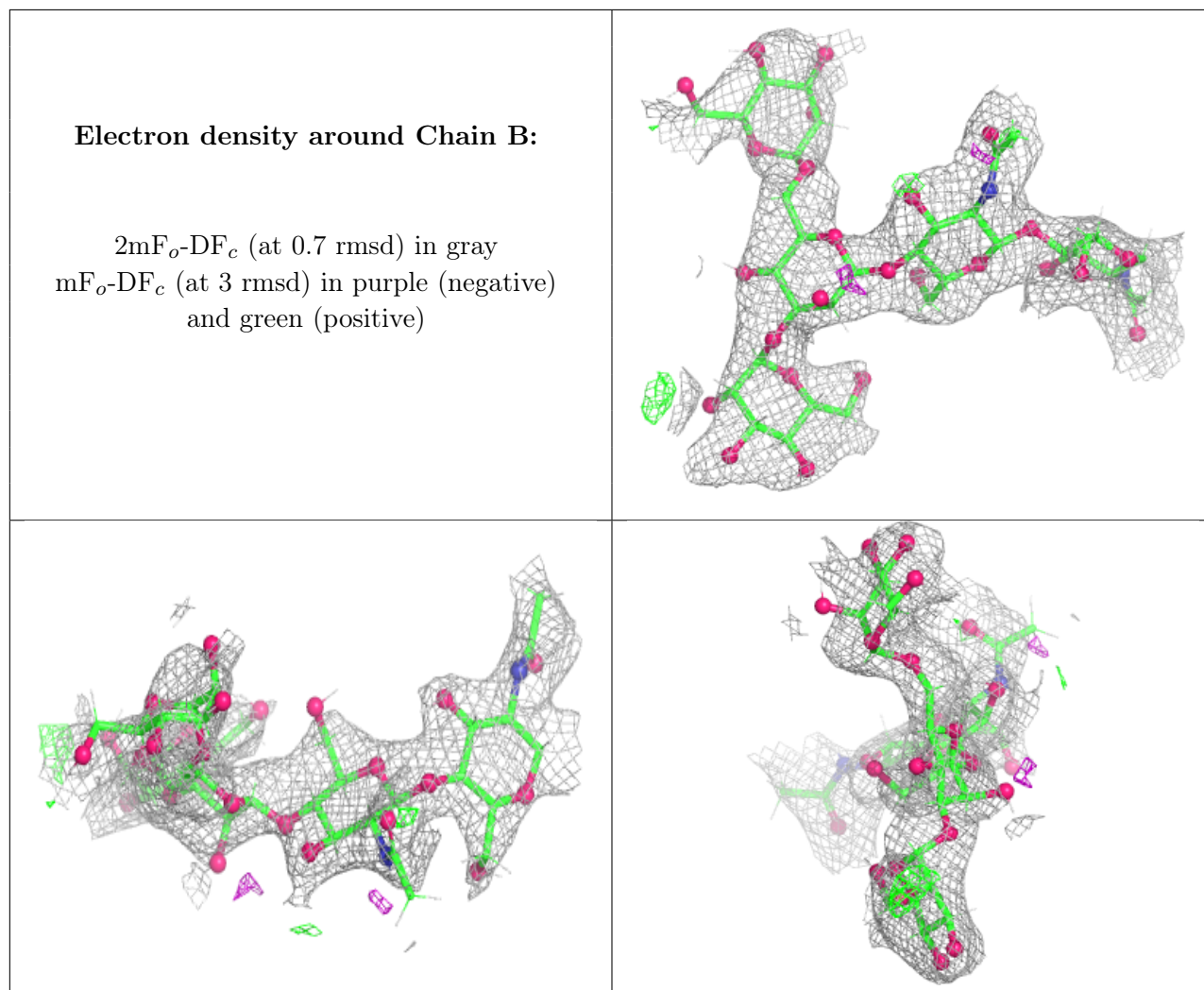
There are no non-standard protein/DNA/RNA residues in this entry.

### 6.3 Carbohydrates [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	MAN	B	5	11/12	0.50	0.40	0,0,57,58	5
2	NAG	B	2	14/15	0.70	0.20	0,0,31,36	5
2	NAG	B	1	14/15	0.71	0.19	0,0,27,38	14
2	MAN	B	4	11/12	0.73	0.24	0,0,40,43	5
2	BMA	B	3	11/12	0.73	0.20	0,9,34,34	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.

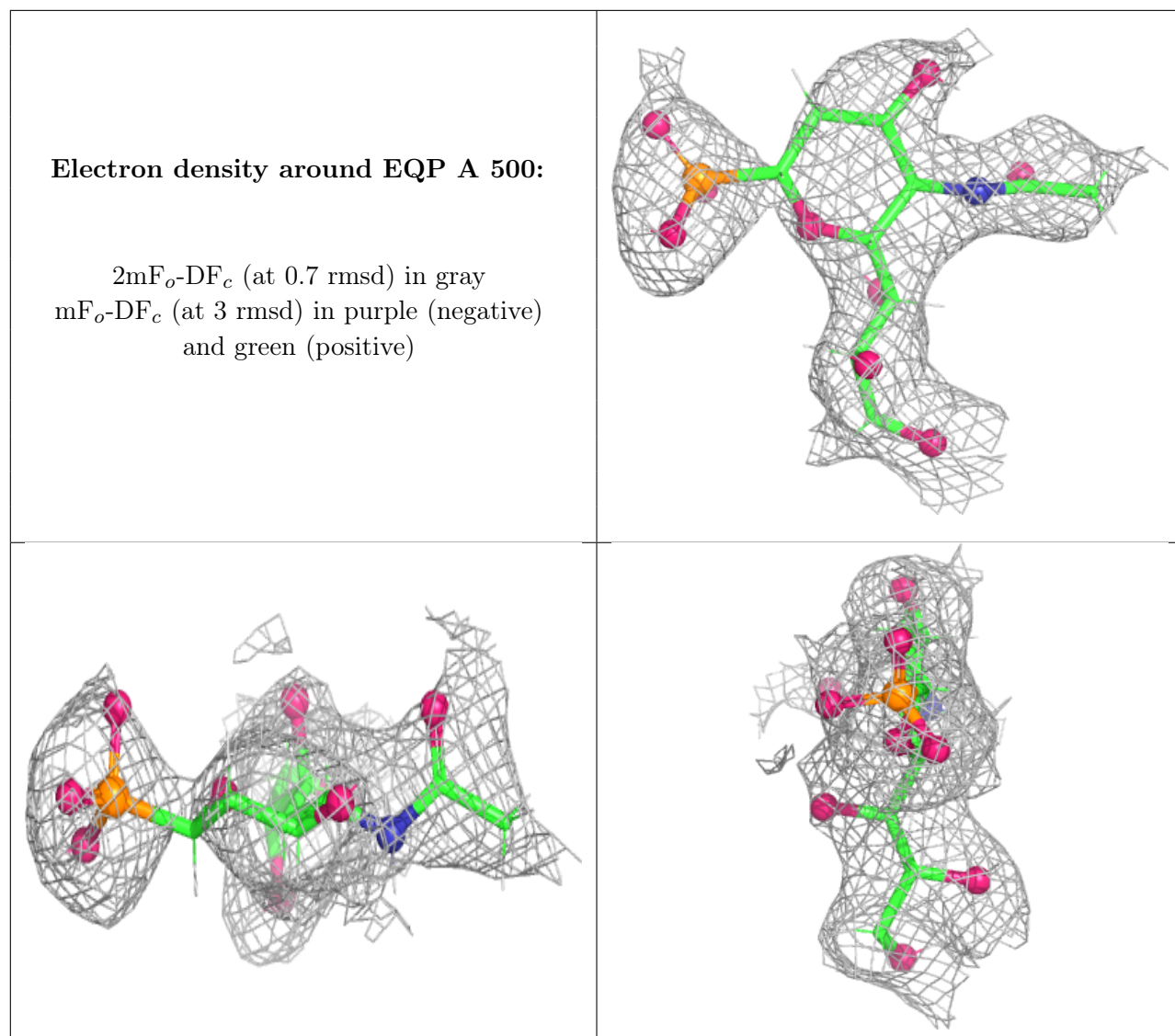


## 6.4 Ligands

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, 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( $\text{\AA}^2$ )	Q<0.9
3	NAG	A	471(A)	14/15	0.53	0.37	0,0,38,44	13
3	NAG	A	477(A)	14/15	0.62	0.22	0,0,33,39	14
3	NAG	A	470(A)	14/15	0.72	0.20	0,0,33,37	14
5	EQP	A	500	21/21	0.89	0.13	0,2,10,17	0
4	CA	A	478	1/1	0.96	0.04	11,11,11,11	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.



## 6.5 Other polymers [i](#)

There are no such residues in this entry.