



Full wwPDB X-ray Structure Validation Report i

Nov 25, 2024 – 03:11 PM EST

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the i symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references \(1\)](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.21
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.004 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.40

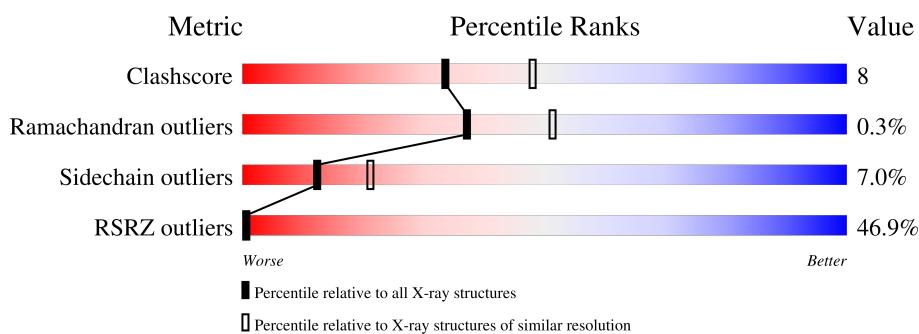
1 Overall quality at a glance [\(i\)](#)

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

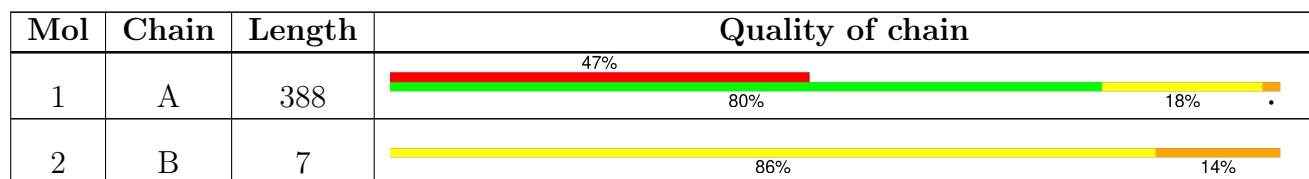
The reported resolution of this entry is 2.40 Å.

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	180529	5218 (2.40-2.40)
Ramachandran outliers	177936	5158 (2.40-2.40)
Sidechain outliers	177891	5159 (2.40-2.40)
RSRZ outliers	164620	4642 (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 >=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 <=5%



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.

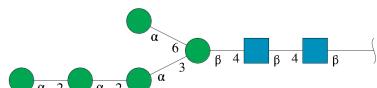
- Molecule 1 is a protein called INFLUENZA A SUBTYPE N9 NEURAMINIDASE.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	388	Total	C	H	N	O	S	0	0	0

There is a discrepancy between the modelled and reference sequences:

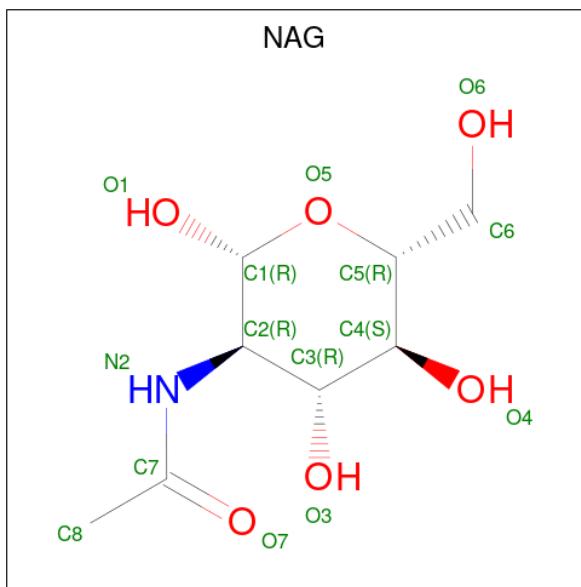
Chain	Residue	Modelled	Actual	Comment	Reference
A	370	LEU	SER	conflict	UNP P03472

- 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
2	B	7	Total	C	H	N	O		0	0	0

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C₈H₁₅NO₆).

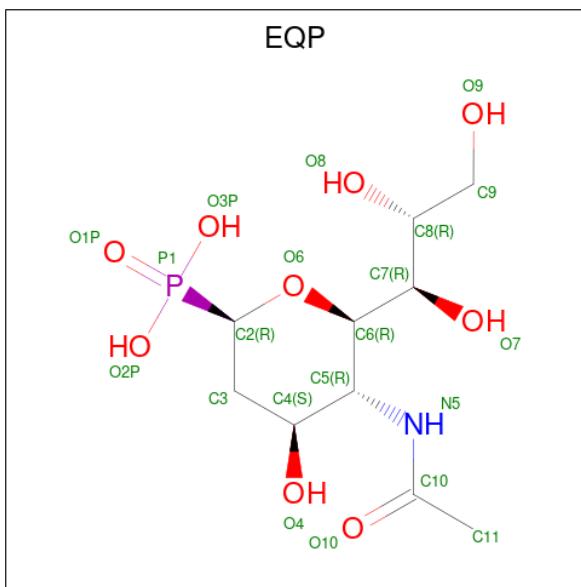


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total C H N O					0	0
			28 8 14 1 5						
3	A	1	Total C H N O					0	0
			28 8 14 1 5						

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

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

- Molecule 5 is (1R)-4-acetamido-1,5-anhydro-2,4-dideoxy-1-phosphono-D-glycero-D-galacto-octitol (three-letter code: EQP) (formula: C₁₀H₂₀NO₉P).



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

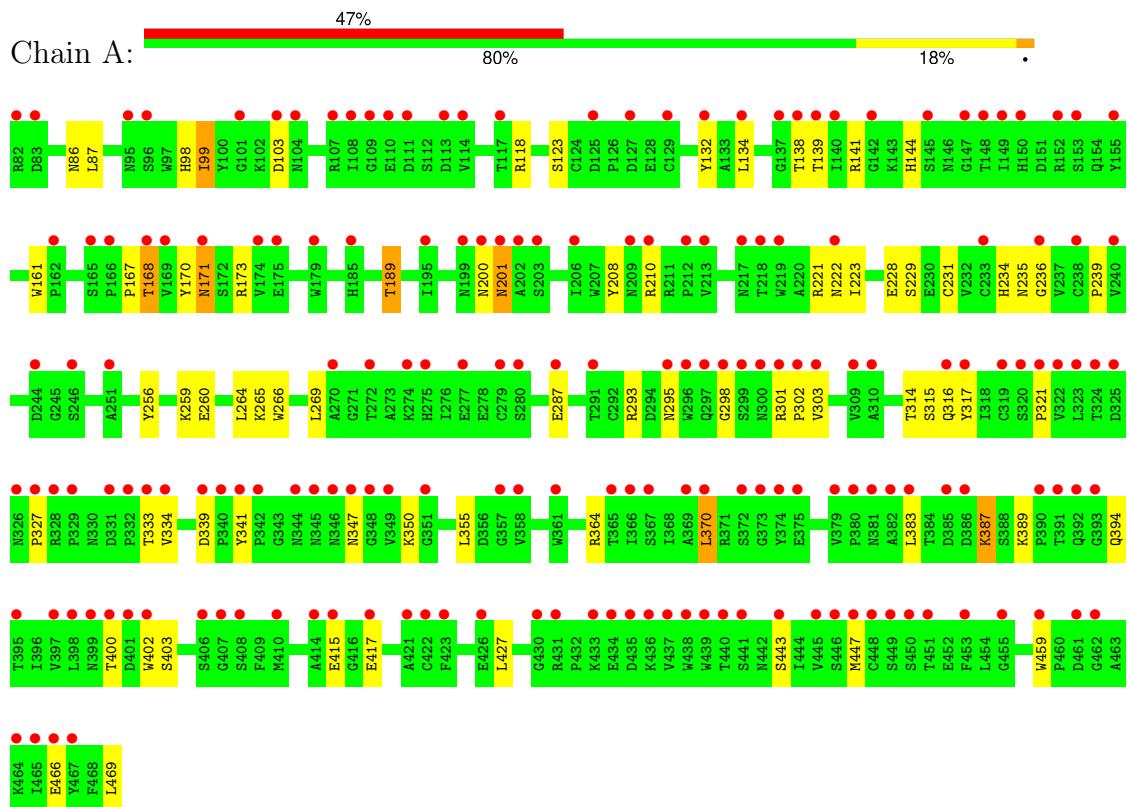
- Molecule 6 is water.

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

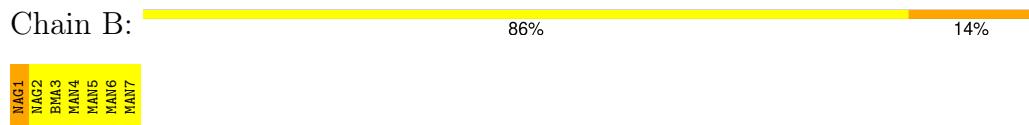
3 Residue-property plots

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 i

Property	Value	Source
Space group	I 4 3 2	Depositor
Cell constants a, b, c, α , β , γ	184.86 Å 184.86 Å 184.86 Å 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) 79.0 (8.00-2.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ ¹	1.04 (at 2.39 Å)	Xtriage
Refinement program	X-PLOR	Depositor
R , R_{free}	0.187 , (Not available) 0.396 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	20.8	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 15.0	EDS
L-test for twinning ²	$< L > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.68	EDS
Total number of atoms	4202	wwPDB-VP
Average B, all atoms (Å ²)	8.0	wwPDB-VP

Xtriage'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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $< |L| >$, $< L^2 >$ 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, BMA, CA, MAN, 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	0.70	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:298:GLY:HA2	1:A:341:TYR:O	2.20	0.41
1:A:303:VAL:O	1:A:315:SER:HA	2.21	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%)	37 / 51

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%)	12 21

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

Sometimes 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	2,1	14,14,15	5.40	7 (50%)	17,19,21	4.31	10 (58%)
2	NAG	B	2	2	14,14,15	3.20	5 (35%)	17,19,21	2.36	2 (11%)
2	BMA	B	3	2	11,11,12	1.57	1 (9%)	15,15,17	2.00	4 (26%)
2	MAN	B	4	2	11,11,12	2.30	3 (27%)	15,15,17	2.00	5 (33%)
2	MAN	B	5	2	11,11,12	1.42	1 (9%)	15,15,17	1.61	3 (20%)
2	MAN	B	6	2	11,11,12	1.77	3 (27%)	15,15,17	3.20	6 (40%)
2	MAN	B	7	2	11,11,12	0.87	0	15,15,17	1.35	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	-	4/6/23/26	0/1/1/1
2	NAG	B	2	2	-	1/6/23/26	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	10.00	1.60	1.43
2	B	1	NAG	C3-C2	9.59	1.72	1.52
2	B	2	NAG	C1-C2	7.93	1.63	1.52
2	B	1	NAG	O4-C4	7.83	1.62	1.43
2	B	1	NAG	O5-C5	7.11	1.57	1.43
2	B	1	NAG	C1-C2	6.84	1.61	1.52
2	B	1	NAG	C4-C5	6.75	1.67	1.53
2	B	2	NAG	C3-C2	6.68	1.66	1.52
2	B	4	MAN	C2-C3	6.00	1.61	1.52
2	B	2	NAG	O5-C5	4.21	1.51	1.43
2	B	6	MAN	C4-C5	4.01	1.61	1.53
2	B	3	BMA	O5-C5	3.71	1.50	1.43
2	B	5	MAN	O5-C1	3.36	1.49	1.43
2	B	4	MAN	O5-C5	3.33	1.49	1.43
2	B	4	MAN	C4-C5	2.79	1.59	1.53
2	B	2	NAG	C4-C5	2.61	1.58	1.53
2	B	6	MAN	O5-C5	2.47	1.48	1.43
2	B	1	NAG	C4-C3	2.39	1.58	1.52
2	B	2	NAG	O4-C4	2.38	1.48	1.43
2	B	6	MAN	C4-C3	2.34	1.58	1.52

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	6	MAN	C1-O5-C5	9.08	124.35	112.19
2	B	1	NAG	O5-C1-C2	-7.99	98.93	111.29
2	B	1	NAG	C1-O5-C5	7.54	122.29	112.19
2	B	1	NAG	C3-C4-C5	-7.36	96.89	110.23
2	B	2	NAG	O5-C1-C2	-6.34	101.49	111.29
2	B	1	NAG	C4-C3-C2	6.32	120.27	111.02
2	B	2	NAG	O3-C3-C2	6.05	121.97	109.40
2	B	3	BMA	C1-O5-C5	5.58	119.67	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1	NAG	O4-C4-C5	5.26	122.28	109.32
2	B	1	NAG	O3-C3-C4	-5.25	97.99	110.38
2	B	7	MAN	C1-O5-C5	4.33	118.00	112.19
2	B	1	NAG	C1-C2-N2	-4.22	103.78	110.43
2	B	6	MAN	C3-C4-C5	-4.14	102.72	110.23
2	B	4	MAN	C1-O5-C5	3.69	117.14	112.19
2	B	4	MAN	C3-C4-C5	-3.67	103.58	110.23
2	B	6	MAN	O4-C4-C5	3.52	118.00	109.32
2	B	4	MAN	O3-C3-C2	3.23	116.64	110.05
2	B	5	MAN	O2-C2-C3	-3.20	103.52	110.15
2	B	5	MAN	C1-O5-C5	3.16	116.43	112.19
2	B	6	MAN	O5-C5-C6	-3.15	101.54	107.66
2	B	6	MAN	C2-C3-C4	3.09	116.30	110.86
2	B	6	MAN	O3-C3-C2	-3.07	103.79	110.05
2	B	3	BMA	O5-C5-C6	3.00	113.51	107.66
2	B	5	MAN	C1-C2-C3	2.85	113.80	109.64
2	B	4	MAN	O4-C4-C5	2.80	116.22	109.32
2	B	3	BMA	C6-C5-C4	2.68	119.60	113.02
2	B	3	BMA	O5-C5-C4	-2.59	104.53	110.83
2	B	4	MAN	C1-C2-C3	2.46	113.23	109.64
2	B	1	NAG	O5-C5-C6	2.44	112.41	107.66
2	B	1	NAG	O3-C3-C2	2.41	114.40	109.40
2	B	1	NAG	O6-C6-C5	2.28	119.10	111.33

There are no chirality outliers.

All (9) torsion outliers are listed below:

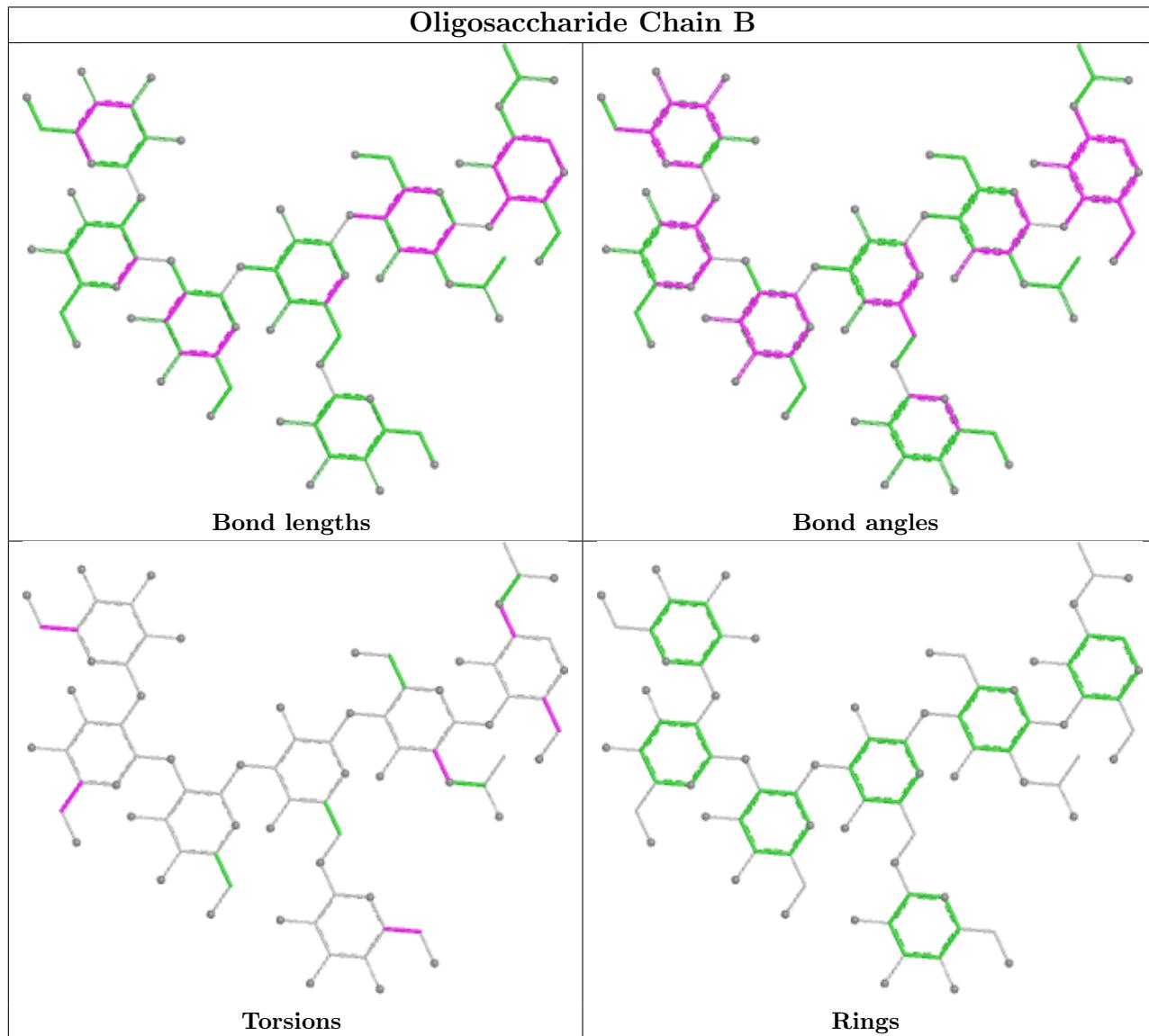
Mol	Chain	Res	Type	Atoms
2	B	1	NAG	C4-C5-C6-O6
2	B	1	NAG	O5-C5-C6-O6
2	B	6	MAN	C4-C5-C6-O6
2	B	1	NAG	C1-C2-N2-C7
2	B	6	MAN	O5-C5-C6-O6
2	B	1	NAG	C3-C2-N2-C7
2	B	2	NAG	C3-C2-N2-C7
2	B	7	MAN	C4-C5-C6-O6
2	B	5	MAN	C4-C5-C6-O6

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 (i)

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	470(A)	1	14,14,15	1.39	2 (14%)	17,19,21	1.47	4 (23%)
3	NAG	A	471(A)	1	14,14,15	1.47	3 (21%)	17,19,21	1.46	3 (17%)
5	EQP	A	500	-	18,21,21	2.50	6 (33%)	22,31,31	2.56	8 (36%)

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	470(A)	1	-	2/6/23/26	0/1/1/1
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

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	500	EQP	P1-O2P	-5.56	1.46	1.54
5	A	500	EQP	O6-C6	4.25	1.50	1.44
5	A	500	EQP	C6-C5	4.14	1.59	1.53
3	A	470(A)	NAG	C4-C5	3.81	1.61	1.53
3	A	471(A)	NAG	C3-C2	3.74	1.60	1.52
5	A	500	EQP	P1-O3P	-3.43	1.49	1.54
5	A	500	EQP	O4-C4	-3.39	1.36	1.43
5	A	500	EQP	P1-O1P	-2.55	1.45	1.49
3	A	470(A)	NAG	C1-C2	2.35	1.55	1.52
3	A	471(A)	NAG	C4-C5	2.08	1.57	1.53
3	A	471(A)	NAG	C4-C3	2.05	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	-7.87	93.73	113.45
5	A	500	EQP	O6-C2-C3	-4.46	104.67	110.66
5	A	500	EQP	C8-C7-C6	-4.16	105.23	113.05
3	A	471(A)	NAG	O3-C3-C2	3.35	116.35	109.40
5	A	500	EQP	O1P-P1-C2	-3.15	106.20	113.34
3	A	470(A)	NAG	C1-O5-C5	3.05	116.28	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	500	EQP	C9-C8-C7	-2.53	107.01	112.17
5	A	500	EQP	C4-C5-N5	-2.49	105.52	110.44
3	A	470(A)	NAG	O3-C3-C2	2.37	114.33	109.40
5	A	500	EQP	C2-O6-C6	2.35	117.32	112.36
3	A	470(A)	NAG	O4-C4-C3	-2.34	104.86	110.38
3	A	470(A)	NAG	O5-C5-C6	-2.28	103.22	107.66
3	A	471(A)	NAG	C2-N2-C7	-2.23	119.91	122.90
3	A	471(A)	NAG	C6-C5-C4	2.15	118.30	113.02
5	A	500	EQP	O7-C7-C8	2.08	113.65	108.93

There are no chirality outliers.

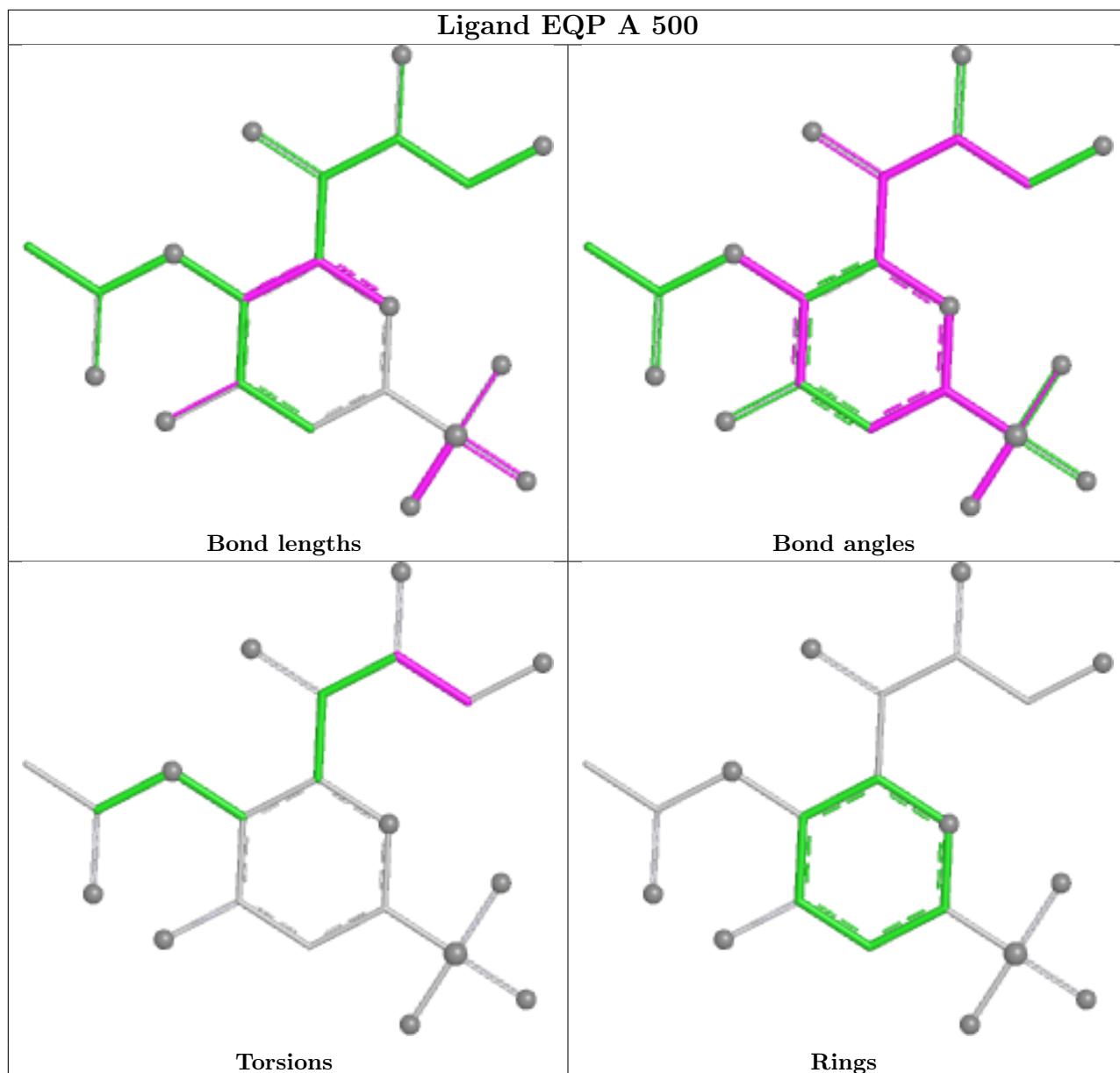
All (3) torsion outliers are listed below:

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

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 [\(i\)](#)

Warning: The R factor obtained from EDS is 0.4027, which does not match the depositor's R factor of 0.187. Please interpret the results in this section carefully.

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	388/388 (100%)	2.09	182 (46%) 0 0	1, 7, 13, 20	115 (29%)

All (182) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	171	ASN	6.9
1	A	82	ARG	5.0
1	A	393	GLY	5.0
1	A	325	ASP	4.7
1	A	466	GLU	4.6
1	A	400	THR	4.6
1	A	317	TYR	4.4
1	A	342	PRO	4.4
1	A	346	ASN	4.4
1	A	339	ASP	4.4
1	A	199	ASN	4.3
1	A	329	PRO	4.2
1	A	332	PRO	4.2
1	A	310	ALA	4.2
1	A	175	GLU	4.2
1	A	298	GLY	4.2
1	A	398	LEU	4.2
1	A	390	PRO	4.1
1	A	347	ASN	4.0
1	A	440	THR	4.0
1	A	142	GLY	4.0
1	A	367	SER	4.0
1	A	168	THR	4.0
1	A	450	SER	3.9

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Mol	Chain	Res	Type	RSRZ
1	A	449	SER	3.9
1	A	127	ASP	3.8
1	A	147	GLY	3.8
1	A	365	THR	3.7
1	A	113	ASP	3.7
1	A	345	ASN	3.7
1	A	417	GLU	3.7
1	A	251	ALA	3.7
1	A	316	GLN	3.6
1	A	326	ASN	3.6
1	A	101	GLY	3.6
1	A	331	ASP	3.6
1	A	137	GLY	3.6
1	A	348	GLY	3.6
1	A	438	TRP	3.6
1	A	319	CYS	3.6
1	A	200	ASN	3.5
1	A	117	THR	3.5
1	A	414	ALA	3.4
1	A	209	ASN	3.4
1	A	333	THR	3.4
1	A	300	ASN	3.4
1	A	341	TYR	3.4
1	A	145	SER	3.3
1	A	375	GLU	3.3
1	A	275	HIS	3.3
1	A	114	VAL	3.3
1	A	370	LEU	3.3
1	A	185	HIS	3.3
1	A	279	CYS	3.2
1	A	95	ASN	3.1
1	A	358	VAL	3.1
1	A	372	SER	3.1
1	A	111	ASP	3.1
1	A	166	PRO	3.1
1	A	462	GLY	3.0
1	A	374	TYR	3.0
1	A	439	TRP	3.0
1	A	379	VAL	3.0
1	A	277	GLU	2.9
1	A	150	HIS	2.9
1	A	421	ALA	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	291	THR	2.9
1	A	361	TRP	2.9
1	A	464	LYS	2.9
1	A	373	GLY	2.9
1	A	107	ARG	2.9
1	A	212	PRO	2.9
1	A	334	VAL	2.9
1	A	270	ALA	2.9
1	A	295	ASN	2.9
1	A	210	ARG	2.9
1	A	246	SER	2.9
1	A	296	TRP	2.9
1	A	455	GLY	2.8
1	A	139	THR	2.8
1	A	344	ASN	2.8
1	A	83	ASP	2.8
1	A	201	ASN	2.8
1	A	383	LEU	2.8
1	A	297	GLN	2.8
1	A	244	ASP	2.8
1	A	380	PRO	2.8
1	A	433	LYS	2.8
1	A	301	ARG	2.7
1	A	320	SER	2.7
1	A	322	VAL	2.7
1	A	435	ASP	2.7
1	A	447	MET	2.7
1	A	179	TRP	2.7
1	A	222	ASN	2.7
1	A	108	ILE	2.7
1	A	436	LYS	2.7
1	A	274	LYS	2.7
1	A	357	GLY	2.7
1	A	134	LEU	2.6
1	A	386	ASP	2.6
1	A	445	VAL	2.6
1	A	423	PHE	2.6
1	A	323	LEU	2.6
1	A	437	VAL	2.6
1	A	129	CYS	2.6
1	A	381	ASN	2.6
1	A	299	SER	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	125	ASP	2.6
1	A	351	GLY	2.6
1	A	202	ALA	2.5
1	A	340	PRO	2.5
1	A	430	GLY	2.5
1	A	410	MET	2.5
1	A	138	THR	2.5
1	A	103	ASP	2.5
1	A	431	ARG	2.5
1	A	238	CYS	2.5
1	A	303	VAL	2.5
1	A	406	SER	2.5
1	A	324	THR	2.5
1	A	391	THR	2.5
1	A	385	ASP	2.5
1	A	104	ASN	2.5
1	A	415	GLU	2.5
1	A	407	GLY	2.5
1	A	213	VAL	2.4
1	A	280	SER	2.4
1	A	408	SER	2.4
1	A	434	GLU	2.4
1	A	109	GLY	2.4
1	A	327	PRO	2.4
1	A	148	THR	2.4
1	A	382	ALA	2.4
1	A	392	GLN	2.4
1	A	272	THR	2.4
1	A	467	TYR	2.4
1	A	174	VAL	2.4
1	A	110	GLU	2.4
1	A	401	ASP	2.3
1	A	140	ILE	2.3
1	A	369	ALA	2.3
1	A	459	TRP	2.3
1	A	366	ILE	2.3
1	A	236	GLY	2.3
1	A	397	VAL	2.3
1	A	195	ILE	2.3
1	A	219	TRP	2.3
1	A	328	ARG	2.3
1	A	132	TYR	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	218	THR	2.2
1	A	155	TYR	2.2
1	A	448	CYS	2.2
1	A	165	SER	2.2
1	A	395	THR	2.2
1	A	402	TRP	2.2
1	A	426	GLU	2.2
1	A	422	CYS	2.2
1	A	96	SER	2.2
1	A	453	PHE	2.2
1	A	153	SER	2.2
1	A	203	SER	2.2
1	A	233	CYS	2.2
1	A	441	SER	2.2
1	A	287	GLU	2.2
1	A	321	PRO	2.1
1	A	206	ILE	2.1
1	A	240	VAL	2.1
1	A	349	VAL	2.1
1	A	302	PRO	2.1
1	A	399	ASN	2.1
1	A	461	ASP	2.1
1	A	309	VAL	2.1
1	A	451	THR	2.1
1	A	443	SER	2.0
1	A	446	SER	2.0
1	A	465	ILE	2.0
1	A	169	VAL	2.0
1	A	162	PRO	2.0
1	A	149	ILE	2.0
1	A	152	ARG	2.0
1	A	217	ASN	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.

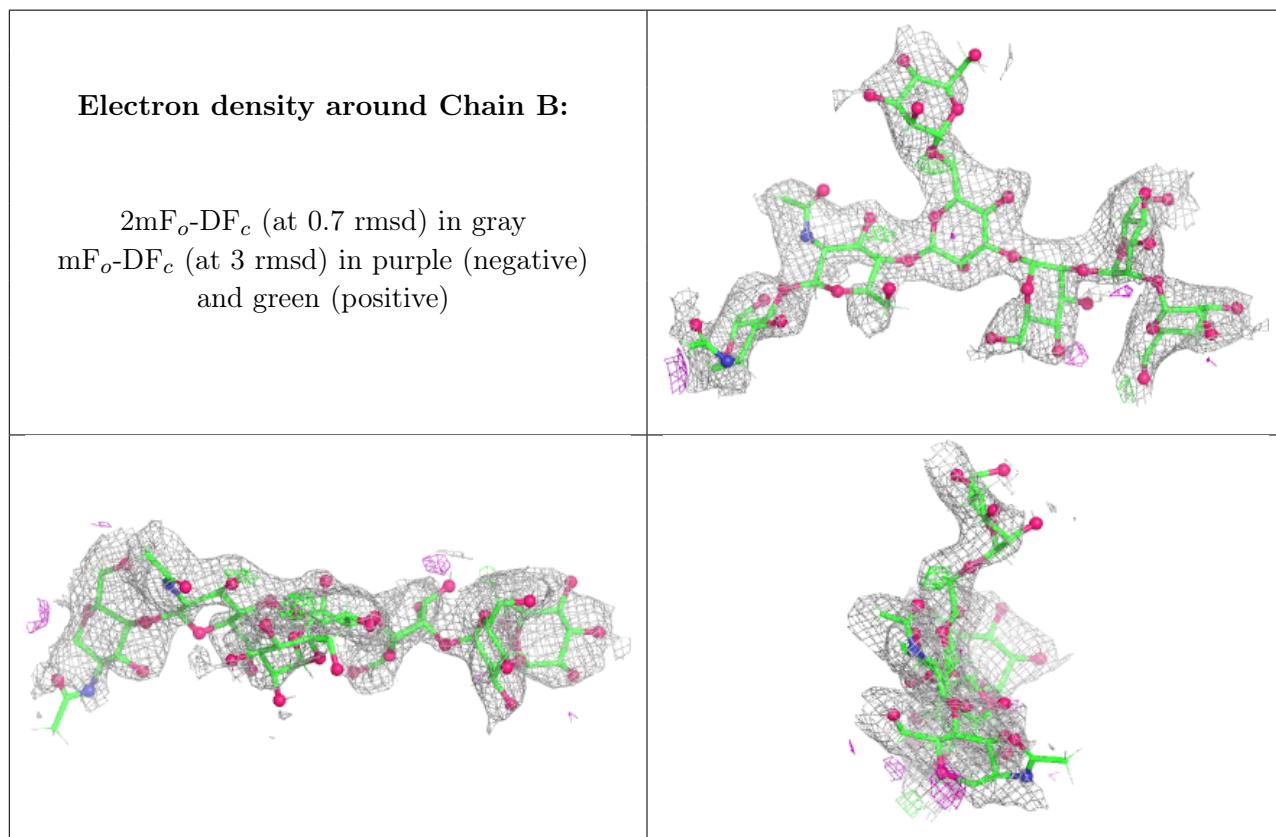
6.3 Carbohydrates [\(i\)](#)

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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	NAG	B	2	14/15	0.43	0.27	0,0,57,61	6
2	BMA	B	3	11/12	0.49	0.19	0,2,50,52	0
2	MAN	B	7	11/12	0.50	0.28	0,0,67,75	11
2	MAN	B	4	11/12	0.67	0.23	0,0,41,56	0
2	MAN	B	6	11/12	0.68	0.21	0,0,32,69	0
2	NAG	B	1	14/15	0.70	0.24	0,0,35,63	8
2	MAN	B	5	11/12	0.70	0.17	0,0,56,58	0

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

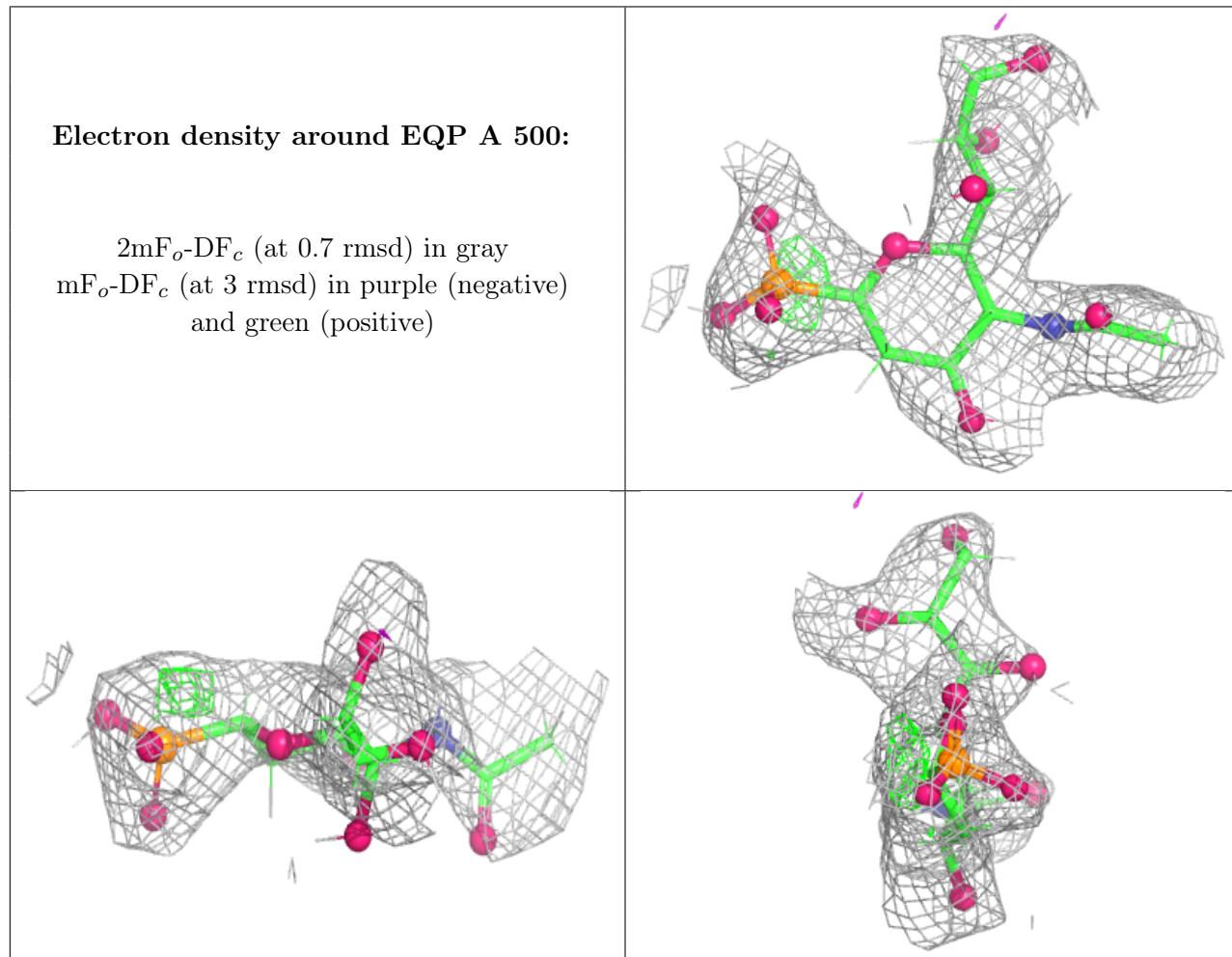


6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	NAG	A	471(A)	14/15	0.43	0.23	0,0,52,98	8
4	CA	A	479	1/1	0.70	0.13	12,12,12,12	0
5	EQP	A	500	21/21	0.70	0.17	0,2,28,34	7
3	NAG	A	470(A)	14/15	0.75	0.21	0,0,74,80	5

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.