



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 02:40 PM UTC

PDB ID : 1INY / pdb_00001iny
Title : A SIALIC ACID DERIVED PHOSPHONATE ANALOG INHIBITS DIFFERENT STRAINS OF INFLUENZA VIRUS NEURAMINIDASE WITH DIFFERENT EFFICIENCIES
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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 ⓘ 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	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (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

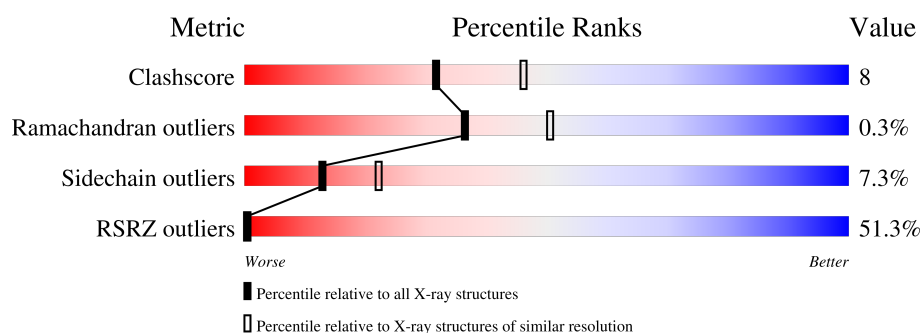
1 Overall quality at a glance

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 ≥ 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	51% 72% 24% .
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.

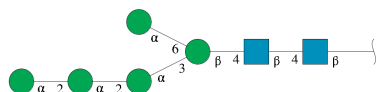
- Molecule 1 is a protein called INFLUENZA A SUBTYPE N9 NEURAMINIDASE.

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 (CCD ID: NAG) (formula: C₈H₁₅NO₆).

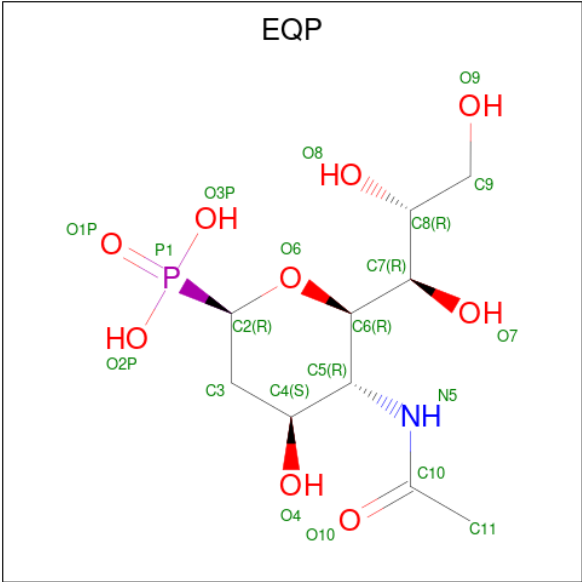


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	H	N	O	0	0
			28	8	14	1	5		
3	A	1	Total	C	H	N	O	0	0
			28	8	14	1	5		

- Molecule 4 is CALCIUM ION (CCD ID: 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 (CCD ID: EQP) (formula: C₁₀H₂₀NO₉P).



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

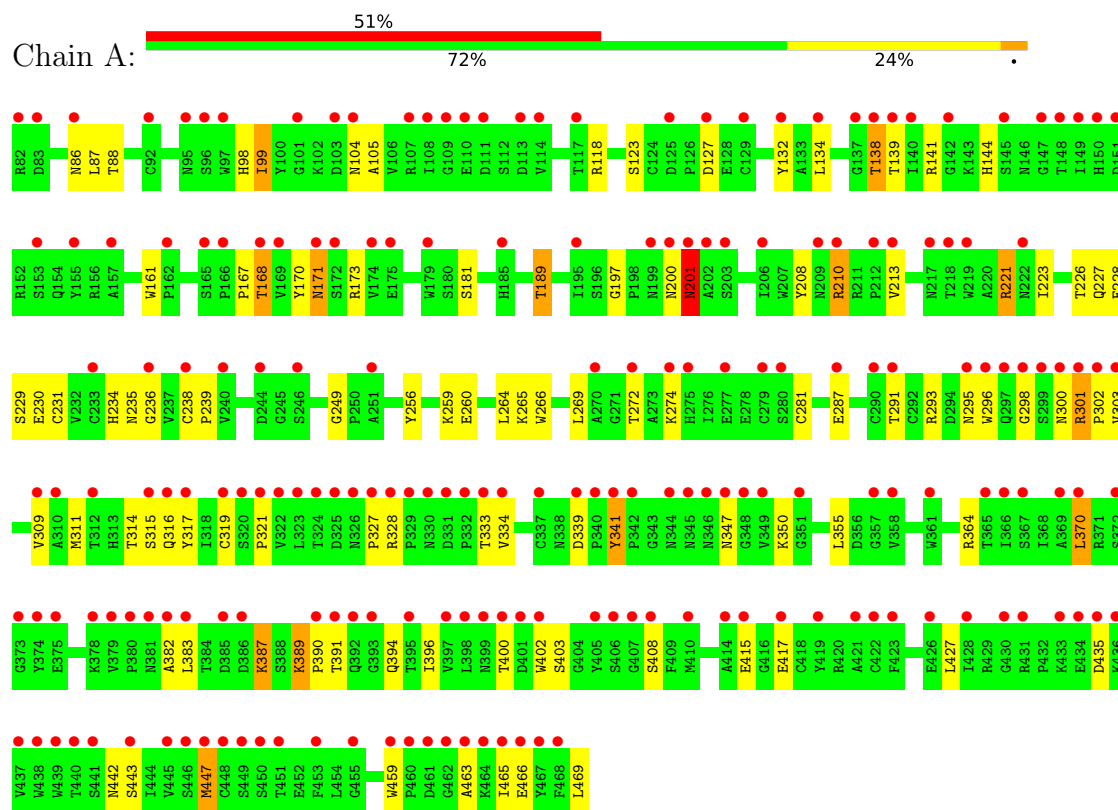
- Molecule 6 is water.

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

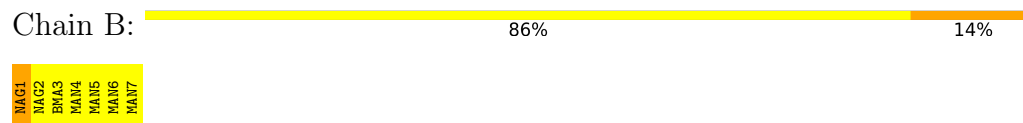
3 Residue-property plots [i](#)

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: 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, α , β , γ	184.86Å 184.86Å 184.86Å 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
$\langle I/\sigma(I) \rangle$ ¹	1.04 (at 2.39Å)	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	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	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 $\langle |L| \rangle$, $\langle L^2 \rangle$ 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: CA, MAN, NAG, EQP, BMA

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	0.96	4/3152 (0.1%)	1.20	34/4293 (0.8%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	238	CYS	C-O	-6.71	1.18	1.24
1	A	311	MET	SD-CE	-5.68	1.65	1.79
1	A	296	TRP	C-O	5.49	1.30	1.24
1	A	309	VAL	C-O	-5.22	1.18	1.24

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	227	GLN	N-CA-C	10.22	123.70	111.33
1	A	435	ASP	N-CA-C	8.86	123.70	113.15
1	A	181	SER	N-CA-C	8.73	120.17	108.38
1	A	105	ALA	N-CA-C	8.32	119.98	111.07
1	A	201	ASN	N-CA-C	7.80	120.94	107.28
1	A	221	ARG	N-CA-C	7.33	121.51	111.54
1	A	249	GLY	CA-C-N	7.21	127.64	119.93
1	A	249	GLY	C-N-CA	7.21	127.64	119.93
1	A	138	THR	CB-CA-C	-6.53	99.46	110.43
1	A	328	ARG	N-CA-C	6.44	114.02	108.22
1	A	213	VAL	N-CA-C	6.44	117.79	111.67
1	A	226	THR	N-CA-C	6.40	116.91	108.07
1	A	291	THR	N-CA-C	-6.38	98.84	109.24
1	A	319	CYS	N-CA-C	6.30	117.81	111.07
1	A	210	ARG	N-CA-C	6.14	120.35	112.86
1	A	230	GLU	N-CA-C	6.06	119.04	110.50
1	A	301	ARG	N-CA-C	6.03	119.42	110.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	341	TYR	CA-C-N	5.93	126.43	120.14
1	A	341	TYR	C-N-CA	5.93	126.43	120.14
1	A	390	PRO	N-CA-C	5.86	120.81	111.26
1	A	197	GLY	CA-C-N	5.73	126.19	120.52
1	A	197	GLY	C-N-CA	5.73	126.19	120.52
1	A	300	ASN	N-CA-C	-5.66	102.15	110.52
1	A	389	LYS	CA-C-N	5.52	125.84	119.93
1	A	389	LYS	C-N-CA	5.52	125.84	119.93
1	A	382	ALA	N-CA-C	5.43	117.63	111.11
1	A	272	THR	N-CA-C	5.43	119.60	112.92
1	A	104	ASN	N-CA-C	-5.30	106.11	112.58
1	A	127	ASP	N-CA-C	5.25	120.68	113.97
1	A	281	CYS	N-CA-C	5.23	118.09	109.72
1	A	274	LYS	N-CA-C	5.16	119.63	113.23
1	A	463	ALA	N-CA-C	5.12	117.31	110.35
1	A	408	SER	N-CA-C	5.10	118.38	110.17
1	A	442	ASN	N-CA-C	5.05	116.66	109.14

There are no chirality outliers.

There are no planarity outliers.

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	3069	711	2900	49	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	49	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 (49) 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:396:ILE:HD12	1:A:447:MET:HE2	1.87	0.57
1:A:396:ILE:CD1	1:A:447:MET:HE2	2.35	0.56
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:171:ASN:C	1:A:171:ASN:ND2	2.75	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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%)	36	50

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%)	316 (93%)	25 (7%)	13	22

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	88	THR
1	A	99	ILE
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	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	391	THR
1	A	400	THR
1	A	415	GLU
1	A	417	GLU
1	A	447	MET
1	A	465	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	95	ASN
1	A	98	HIS
1	A	171	ASN
1	A	200	ASN
1	A	201	ASN

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Mol	Chain	Res	Type
1	A	222	ASN
1	A	227	GLN
1	A	234	HIS
1	A	235	ASN
1	A	295	ASN
1	A	344	ASN
1	A	346	ASN
1	A	381	ASN
1	A	394	GLN
1	A	399	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 ⓘ

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	5.40	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	1,2	-	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

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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
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:

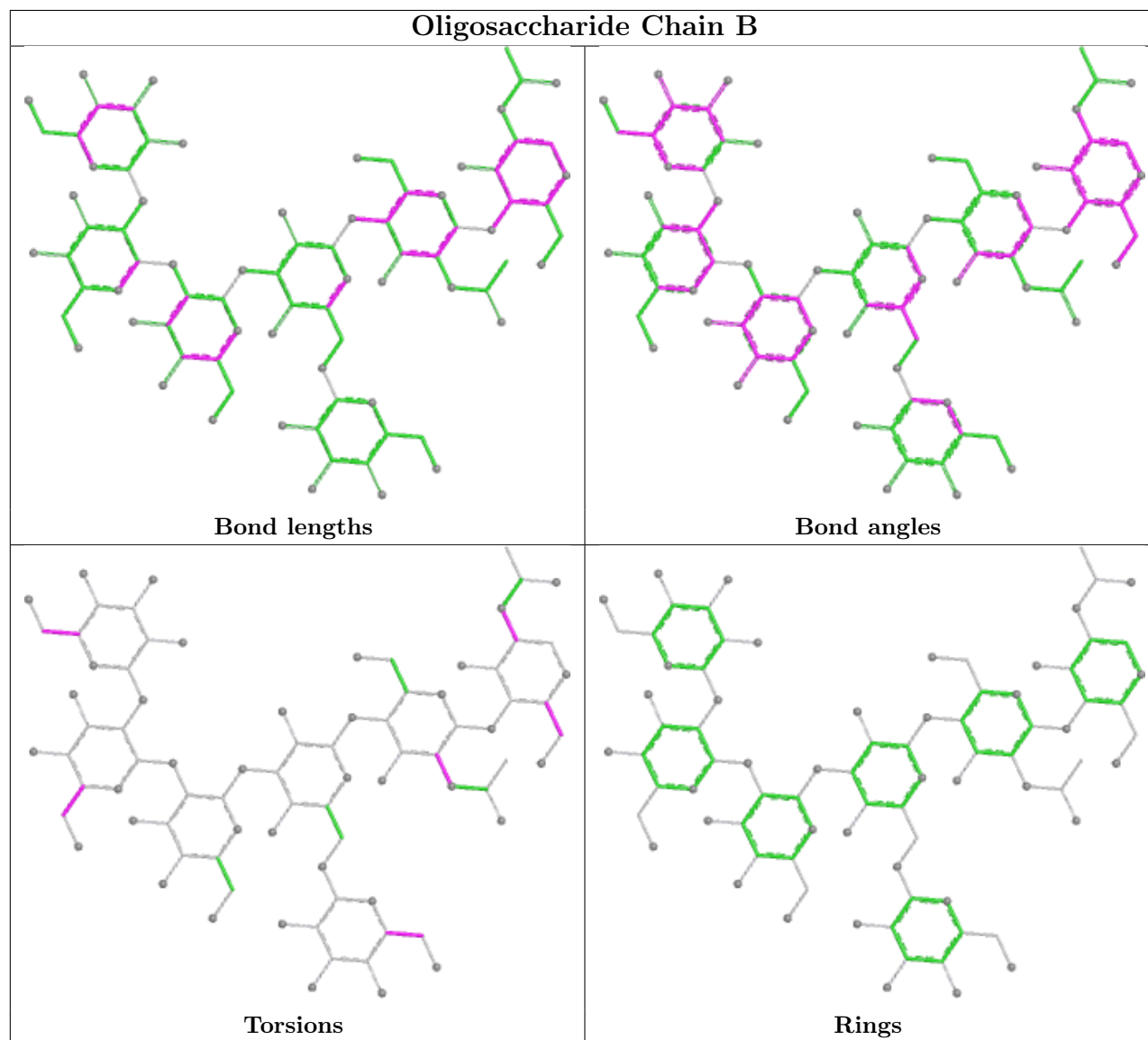
Mol	Chain	Res	Type	Atoms
2	B	1	NAG	C4-C5-C6-O6
2	B	1	NAG	O5-C5-C6-O6
2	B	6	MAN	C4-C5-C6-O6
2	B	1	NAG	C1-C2-N2-C7
2	B	6	MAN	O5-C5-C6-O6
2	B	1	NAG	C3-C2-N2-C7
2	B	2	NAG	C3-C2-N2-C7
2	B	7	MAN	C4-C5-C6-O6
2	B	5	MAN	C4-C5-C6-O6

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
5	EQP	A	500	-	18,21,21	2.50	6 (33%)	22,31,31	2.56	8 (36%)
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%)

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	EQP	A	500	-	-	1/14/36/36	0/1/1/1
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

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

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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
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.

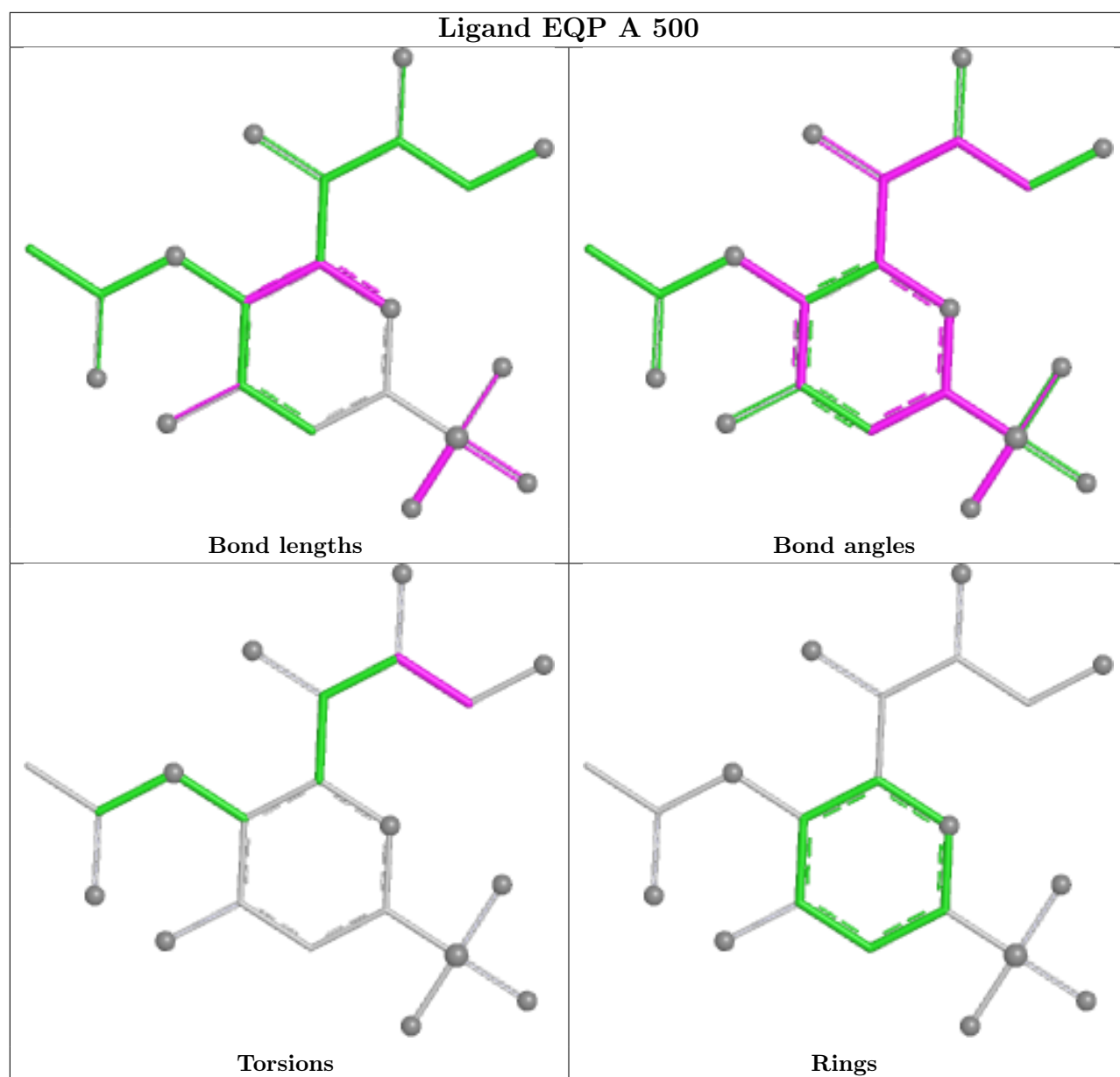
All (3) torsion outliers are listed below:

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

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, 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%)	2.15	199 (51%) 0 0	1, 7, 13, 20	115 (29%)

All (199) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	171	ASN	6.9
1	A	393	GLY	5.0
1	A	82	ARG	4.9
1	A	325	ASP	4.6
1	A	400	THR	4.6
1	A	466	GLU	4.5
1	A	317	TYR	4.5
1	A	342	PRO	4.4
1	A	346	ASN	4.4
1	A	199	ASN	4.3
1	A	339	ASP	4.3
1	A	310	ALA	4.3
1	A	398	LEU	4.3
1	A	329	PRO	4.3
1	A	332	PRO	4.3
1	A	298	GLY	4.2
1	A	175	GLU	4.1
1	A	390	PRO	4.1
1	A	440	THR	4.1
1	A	347	ASN	4.0
1	A	142	GLY	4.0
1	A	367	SER	4.0
1	A	168	THR	4.0
1	A	450	SER	4.0
1	A	449	SER	3.9
1	A	147	GLY	3.8
1	A	365	THR	3.8

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Mol	Chain	Res	Type	RSRZ
1	A	345	ASN	3.8
1	A	127	ASP	3.8
1	A	438	TRP	3.7
1	A	251	ALA	3.7
1	A	319	CYS	3.7
1	A	113	ASP	3.7
1	A	101	GLY	3.7
1	A	316	GLN	3.7
1	A	326	ASN	3.7
1	A	137	GLY	3.6
1	A	348	GLY	3.6
1	A	417	GLU	3.6
1	A	331	ASP	3.6
1	A	200	ASN	3.5
1	A	117	THR	3.5
1	A	414	ALA	3.5
1	A	333	THR	3.5
1	A	341	TYR	3.5
1	A	209	ASN	3.4
1	A	300	ASN	3.4
1	A	145	SER	3.4
1	A	370	LEU	3.4
1	A	114	VAL	3.3
1	A	275	HIS	3.3
1	A	279	CYS	3.3
1	A	185	HIS	3.3
1	A	375	GLU	3.2
1	A	358	VAL	3.2
1	A	372	SER	3.2
1	A	95	ASN	3.2
1	A	374	TYR	3.1
1	A	166	PRO	3.1
1	A	439	TRP	3.1
1	A	462	GLY	3.1
1	A	111	ASP	3.1
1	A	361	TRP	3.1
1	A	379	VAL	3.0
1	A	296	TRP	3.0
1	A	291	THR	3.0
1	A	421	ALA	3.0
1	A	150	HIS	3.0
1	A	373	GLY	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	334	VAL	2.9
1	A	270	ALA	2.9
1	A	212	PRO	2.9
1	A	246	SER	2.9
1	A	295	ASN	2.9
1	A	455	GLY	2.9
1	A	277	GLU	2.9
1	A	139	THR	2.9
1	A	464	LYS	2.9
1	A	383	LEU	2.9
1	A	344	ASN	2.9
1	A	179	TRP	2.9
1	A	107	ARG	2.8
1	A	201	ASN	2.8
1	A	297	GLN	2.8
1	A	210	ARG	2.8
1	A	380	PRO	2.8
1	A	83	ASP	2.8
1	A	320	SER	2.8
1	A	322	VAL	2.8
1	A	447	MET	2.8
1	A	244	ASP	2.8
1	A	108	ILE	2.8
1	A	433	LYS	2.8
1	A	222	ASN	2.7
1	A	134	LEU	2.7
1	A	129	CYS	2.7
1	A	435	ASP	2.7
1	A	357	GLY	2.7
1	A	423	PHE	2.7
1	A	301	ARG	2.7
1	A	436	LYS	2.7
1	A	445	VAL	2.7
1	A	323	LEU	2.7
1	A	274	LYS	2.7
1	A	437	VAL	2.7
1	A	386	ASP	2.6
1	A	238	CYS	2.6
1	A	381	ASN	2.6
1	A	299	SER	2.6
1	A	351	GLY	2.6
1	A	202	ALA	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	430	GLY	2.6
1	A	340	PRO	2.6
1	A	410	MET	2.6
1	A	138	THR	2.6
1	A	125	ASP	2.6
1	A	303	VAL	2.6
1	A	406	SER	2.6
1	A	324	THR	2.6
1	A	391	THR	2.6
1	A	104	ASN	2.5
1	A	103	ASP	2.5
1	A	407	GLY	2.5
1	A	213	VAL	2.5
1	A	280	SER	2.5
1	A	408	SER	2.5
1	A	109	GLY	2.5
1	A	385	ASP	2.5
1	A	431	ARG	2.5
1	A	148	THR	2.5
1	A	327	PRO	2.5
1	A	467	TYR	2.5
1	A	459	TRP	2.5
1	A	382	ALA	2.5
1	A	272	THR	2.5
1	A	415	GLU	2.4
1	A	392	GLN	2.4
1	A	174	VAL	2.4
1	A	434	GLU	2.4
1	A	140	ILE	2.4
1	A	219	TRP	2.4
1	A	369	ALA	2.4
1	A	366	ILE	2.4
1	A	236	GLY	2.4
1	A	195	ILE	2.4
1	A	401	ASP	2.4
1	A	448	CYS	2.4
1	A	132	TYR	2.4
1	A	397	VAL	2.4
1	A	110	GLU	2.4
1	A	402	TRP	2.4
1	A	422	CYS	2.3
1	A	155	TYR	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	218	THR	2.3
1	A	233	CYS	2.3
1	A	453	PHE	2.3
1	A	395	THR	2.3
1	A	165	SER	2.3
1	A	96	SER	2.3
1	A	328	ARG	2.3
1	A	153	SER	2.2
1	A	203	SER	2.2
1	A	441	SER	2.2
1	A	206	ILE	2.2
1	A	426	GLU	2.2
1	A	240	VAL	2.2
1	A	321	PRO	2.2
1	A	349	VAL	2.2
1	A	302	PRO	2.2
1	A	399	ASN	2.2
1	A	287	GLU	2.2
1	A	309	VAL	2.1
1	A	451	THR	2.1
1	A	337	CYS	2.1
1	A	461	ASP	2.1
1	A	465	ILE	2.1
1	A	290	CYS	2.1
1	A	443	SER	2.1
1	A	446	SER	2.1
1	A	169	VAL	2.1
1	A	149	ILE	2.1
1	A	405	TYR	2.1
1	A	92	CYS	2.1
1	A	162	PRO	2.1
1	A	97	TRP	2.1
1	A	217	ASN	2.1
1	A	312	THR	2.1
1	A	428	ILE	2.1
1	A	172	SER	2.1
1	A	468	PHE	2.0
1	A	330	ASN	2.0
1	A	151	ASP	2.0
1	A	460	PRO	2.0
1	A	157	ALA	2.0
1	A	463	ALA	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	86	ASN	2.0
1	A	378	LYS	2.0
1	A	315	SER	2.0
1	A	419	TYR	2.0

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

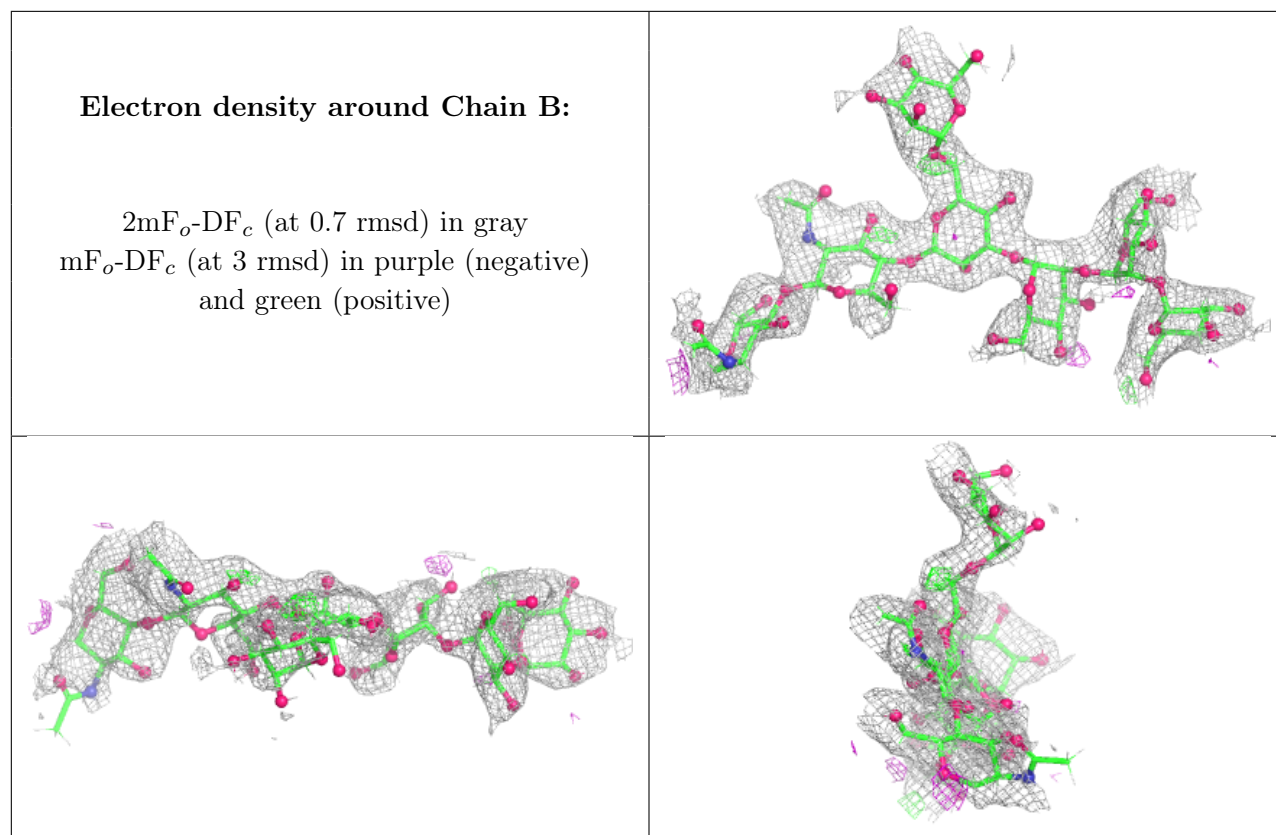
There are no non-standard protein/DNA/RNA residues in this entry.

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, 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($\text{\AA}^2$)	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.

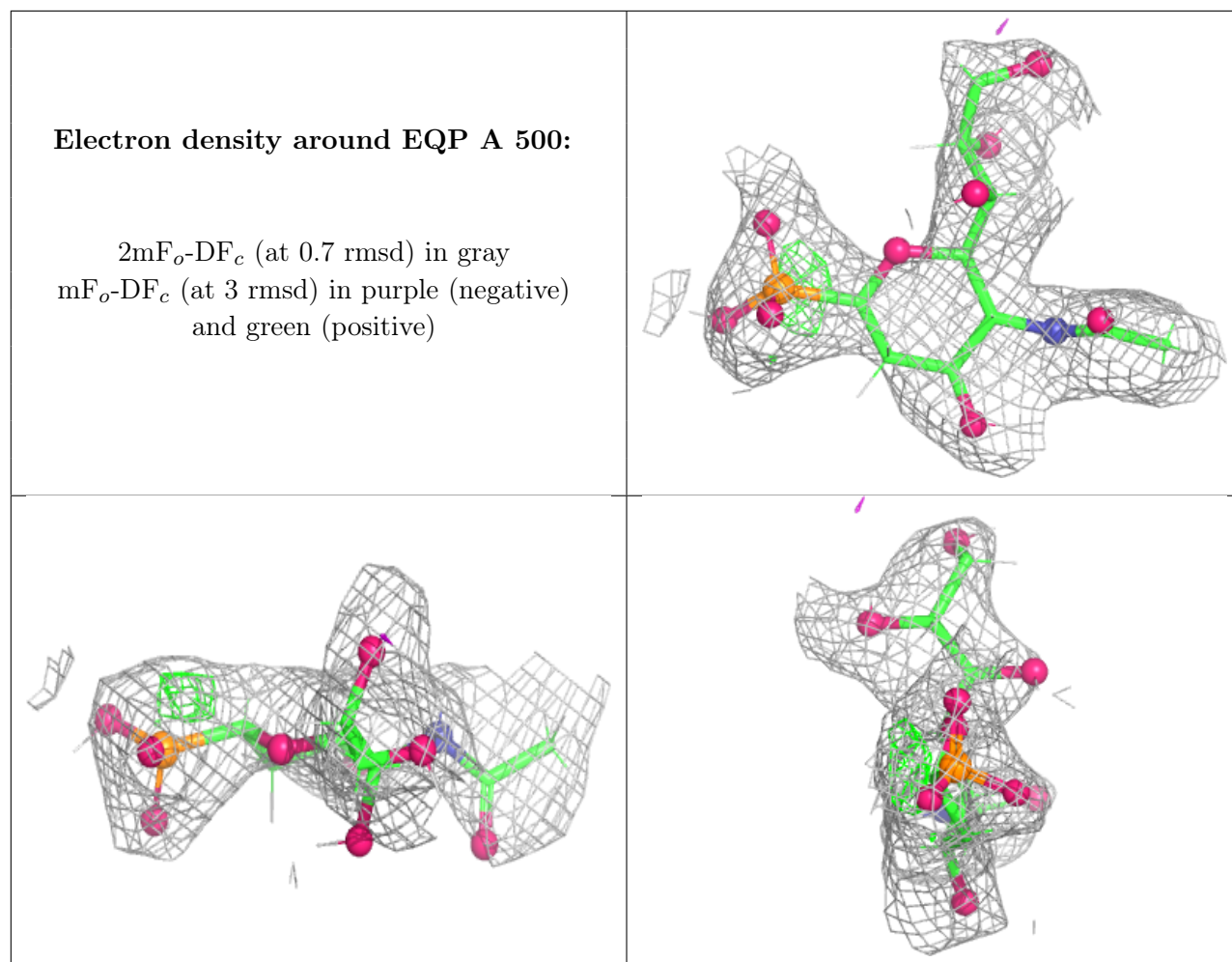


6.4 Ligands [i](#)

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.