



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 02:26 PM UTC

PDB ID : 1INW / pdb_00001inw
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

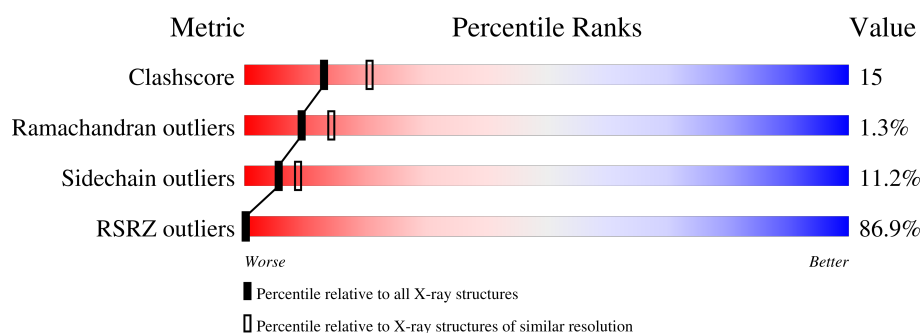
1 Overall quality at a glance

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	87% 59% 34% 6%
2	B	5	100%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	MAN	B	3	X	-	-	-
2	MAN	B	5	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	NAG	A	470(A)	-	-	-	X

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 4246 atoms, of which 1013 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.

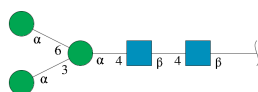
- Molecule 1 is a protein called INFLUENZA A SUBTYPE N2 NEURAMINIDASE.

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

There is a discrepancy between the modelled and reference sequences:

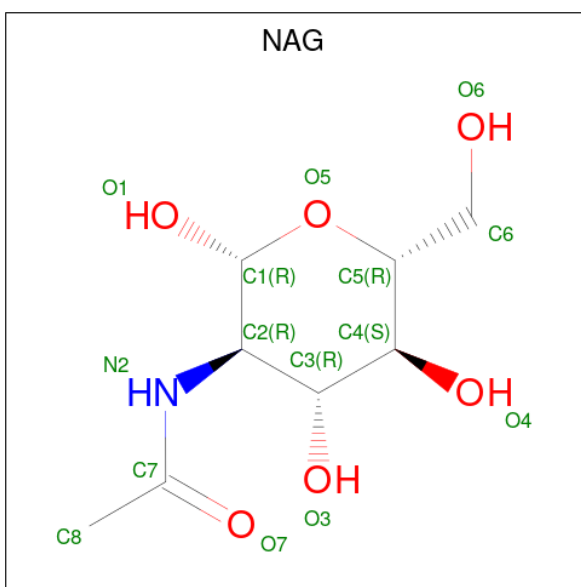
Chain	Residue	Modelled	Actual	Comment	Reference
A	339	ASP	ASN	conflict	UNP P06820

- Molecule 2 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



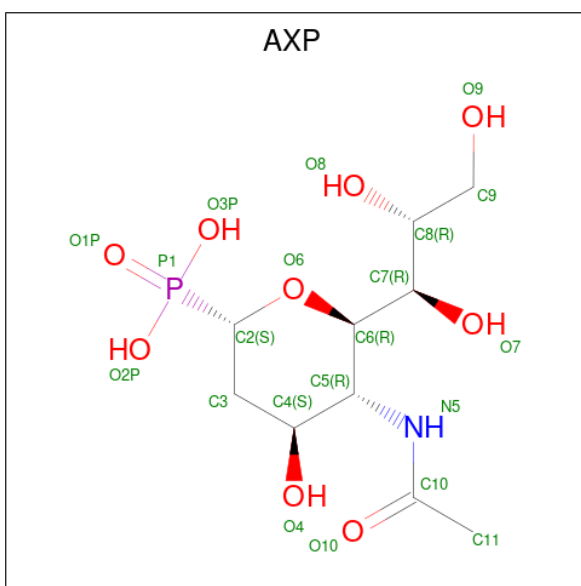
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	5	Total	C	H	N	O	0	0	0
			118	34	57	2	25			

- 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		
3	A	1	Total	C	H	N	O	0	0
			28	8	14	1	5		

- Molecule 4 is (1S)-4-acetamido-1,5-anhydro-2,4-dideoxy-1-phosphono-D-glycero-D-galacto-ocitol (CCD ID: AXP) (formula: $C_{10}H_{20}NO_9P$).



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

- Molecule 5 is CALCIUM ION (CCD ID: CA) (formula: Ca).

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

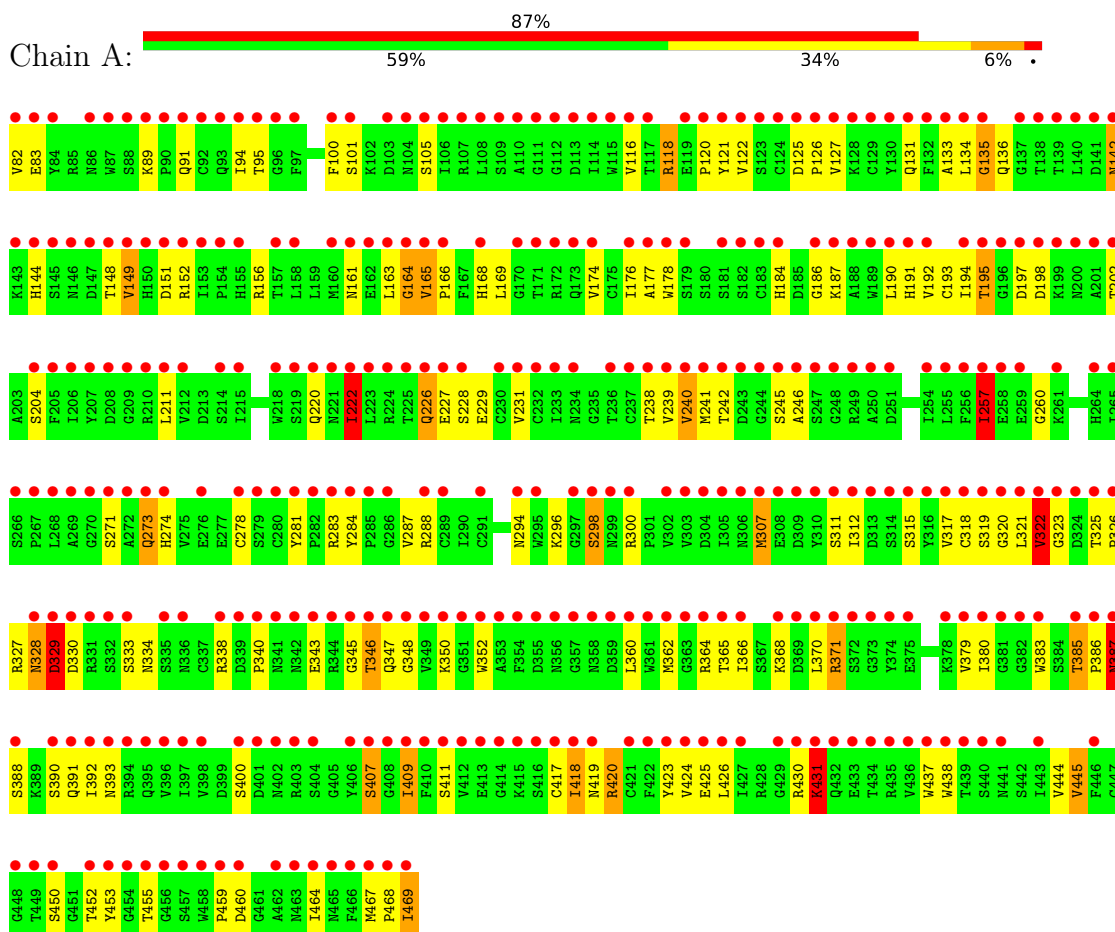
- Molecule 6 is water.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	86	Total	H	O		
			258	172	86	7	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)]alpha-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, α , β , γ	122.08Å 141.67Å 141.87Å 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) 63.0 (8.00-2.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.21 (at 2.41Å)	Xtriage
Refinement program	X-PLOR	Depositor
R, R_{free}	0.206 , (Not available) 0.518 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	27.9	Xtriage
Anisotropy	0.691	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.84 , 223.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.44	EDS
Total number of atoms	4246	wwPDB-VP
Average B, all atoms (Å ²)	10.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.26% 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, AXP, 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	0.99	6/3092 (0.2%)	1.22	30/4194 (0.7%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	121	TYR	C-O	-7.68	1.16	1.24
1	A	239	VAL	C-O	-7.03	1.16	1.24
1	A	281	TYR	C-O	-6.88	1.15	1.24
1	A	135	GLY	C-O	-6.43	1.15	1.23
1	A	101	SER	C-O	-5.91	1.16	1.23
1	A	307	MET	SD-CE	-5.31	1.66	1.79

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	328	ASN	N-CA-C	7.63	122.86	111.04
1	A	257	ILE	N-CA-C	7.49	118.60	108.11
1	A	164	GLY	CA-C-N	-7.46	117.22	122.59
1	A	164	GLY	C-N-CA	-7.46	117.22	122.59
1	A	226	GLN	N-CA-C	7.39	123.57	111.37
1	A	431	LYS	N-CA-C	-7.21	95.45	110.80
1	A	271	SER	N-CA-C	7.09	120.80	112.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	467	MET	N-CA-C	6.83	119.51	110.08
1	A	345	GLY	N-CA-C	6.71	122.04	113.24
1	A	387	ASN	N-CA-C	6.42	120.90	113.38
1	A	338	ARG	N-CA-C	6.42	121.78	113.88
1	A	298	SER	N-CA-C	-6.26	105.68	113.38
1	A	229	GLU	N-CA-C	6.18	119.22	110.50
1	A	444	VAL	N-CA-C	-6.08	100.33	108.35
1	A	197	ASP	N-CA-C	-6.02	101.57	110.48
1	A	318	CYS	N-CA-C	5.90	117.71	111.28
1	A	105	SER	N-CA-C	5.76	118.05	111.02
1	A	116	VAL	N-CA-C	-5.76	100.29	108.58
1	A	450	SER	N-CA-C	-5.58	106.14	113.17
1	A	222	ILE	N-CA-C	5.57	120.93	109.34
1	A	319	SER	N-CA-C	5.51	118.46	110.42
1	A	169	LEU	N-CA-C	5.50	119.08	112.38
1	A	273	GLN	N-CA-C	5.45	117.30	111.36
1	A	323	GLY	N-CA-C	5.26	125.65	113.18
1	A	296	LYS	N-CA-C	5.11	120.14	113.30
1	A	152	ARG	N-CA-C	5.09	116.61	107.80
1	A	287	VAL	N-CA-C	-5.07	100.94	108.45
1	A	300	ARG	CA-C-N	5.07	125.05	120.03
1	A	300	ARG	C-N-CA	5.07	125.05	120.03
1	A	329	ASP	N-CA-C	-5.03	100.10	110.80

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	423	TYR	Sidechain

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	3022	723	2852	91	0
2	B	61	57	52	0	0
3	A	42	42	39	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	21	19	18	1	0
5	A	1	0	0	0	0
6	A	86	172	0	5	0
All	All	3233	1013	2961	91	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 15.

All (91) 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	0.86
1:A:437:TRP:H	1:A:469:ILE:HG21	1.40	0.85
1:A:226:GLN:HE21	1:A:240:VAL:H	1.27	0.81
1:A:419:ASN:ND2	1:A:420:ARG:H	1.78	0.81
1:A:430:ARG:O	1:A:431:LYS:HB2	1.81	0.79
1:A:419:ASN:HD22	1:A:420:ARG:H	1.27	0.78
1:A:431:LYS:HA	1:A:431:LYS:HZ3	1.47	0.78
1:A:228:SER:HB3	1:A:350:LYS:HE2	1.71	0.72
1:A:184:HIS:CD2	1:A:186:GLY:H	2.10	0.70
1:A:177:ALA:HB2	1:A:193:CYS:HB3	1.76	0.68
1:A:274:HIS:HD2	1:A:294:ASN:H	1.43	0.67
1:A:135:GLY:O	1:A:156:ARG:HD2	1.96	0.66
1:A:184:HIS:HD2	1:A:186:GLY:H	1.43	0.64
1:A:142:ASN:HD22	1:A:144:HIS:H	1.46	0.64
1:A:419:ASN:ND2	1:A:420:ARG:N	2.46	0.64
1:A:317:VAL:HG23	6:A:549:HOH:O	1.99	0.63
1:A:380:ILE:HB	1:A:390:SER:HB2	1.81	0.62
1:A:131:GLN:HE21	1:A:163:LEU:HD12	1.63	0.62
1:A:437:TRP:N	1:A:469:ILE:HG21	2.13	0.61
1:A:273:GLN:HG3	1:A:340:PRO:HG3	1.84	0.60
1:A:198:ASP:HB3	1:A:222:ILE:HG12	1.85	0.59
1:A:149:VAL:HG22	6:A:509:HOH:O	2.02	0.59
1:A:328:ASN:O	1:A:329:ASP:HB2	2.01	0.59
1:A:194:ILE:HD11	1:A:241:MET:HE3	1.84	0.58
1:A:409:ILE:HD11	1:A:420:ARG:HD3	1.86	0.58
1:A:240:VAL:HG21	1:A:278:CYS:SG	2.44	0.57
1:A:118:ARG:HD2	1:A:425:GLU:OE2	2.03	0.57
1:A:419:ASN:HD22	1:A:420:ARG:N	2.02	0.56
1:A:131:GLN:NE2	1:A:164:GLY:H	2.04	0.56
1:A:288:ARG:NH1	1:A:383:TRP:CZ2	2.73	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:437:TRP:HD1	1:A:469:ILE:CG2	2.20	0.55
1:A:166:PRO:O	1:A:168:HIS:HD2	1.89	0.55
1:A:411:SER:HB3	1:A:418:ILE:CD1	2.37	0.54
1:A:95:THR:HG22	1:A:453:TYR:HE2	1.71	0.54
1:A:246:ALA:O	1:A:274:HIS:NE2	2.41	0.53
1:A:333:SER:HA	1:A:343:GLU:OE1	2.08	0.53
1:A:326:PRO:HA	1:A:368:LYS:O	2.09	0.52
1:A:468:PRO:O	1:A:469:ILE:HB	2.10	0.51
1:A:437:TRP:H	1:A:469:ILE:CG2	2.20	0.51
1:A:346:THR:O	1:A:347:GLN:HB2	2.11	0.51
1:A:283:ARG:O	1:A:284:TYR:C	2.53	0.50
1:A:311:SER:C	1:A:312:ILE:HD13	2.37	0.50
1:A:391:GLN:HG2	1:A:392:ILE:N	2.27	0.49
1:A:228:SER:HB3	1:A:350:LYS:CE	2.42	0.49
1:A:347:GLN:HB3	6:A:573:HOH:O	2.12	0.49
1:A:190:LEU:HD11	1:A:257:ILE:HD11	1.95	0.48
1:A:136:GLN:CD	1:A:156:ARG:HD3	2.39	0.48
1:A:238:THR:OG1	1:A:307:MET:HE1	2.13	0.48
1:A:366:ILE:HG21	1:A:400:SER:HB3	1.94	0.48
1:A:136:GLN:OE1	1:A:156:ARG:HD3	2.14	0.48
1:A:168:HIS:HB2	6:A:567:HOH:O	2.13	0.48
1:A:328:ASN:HB2	6:A:548:HOH:O	2.14	0.48
1:A:325:THR:O	1:A:348:GLY:HA2	2.14	0.48
1:A:321:LEU:HD12	1:A:379:VAL:HG22	1.94	0.47
1:A:320:GLY:HA3	1:A:387:ASN:HD22	1.79	0.47
1:A:385:THR:HA	1:A:386:PRO:HD2	1.81	0.46
1:A:174:VAL:HG11	1:A:191:HIS:CD2	2.51	0.46
1:A:418:ILE:HD11	1:A:420:ARG:NH2	2.31	0.45
1:A:245:SER:O	1:A:274:HIS:HE1	2.00	0.45
1:A:392:ILE:HG12	1:A:393:ASN:N	2.30	0.45
1:A:198:ASP:HB3	1:A:222:ILE:CG1	2.46	0.45
1:A:365:THR:HG21	1:A:371:ARG:HA	1.99	0.45
1:A:321:LEU:O	1:A:322:VAL:HB	2.17	0.45
1:A:334:ASN:HA	1:A:387:ASN:HD21	1.82	0.44
1:A:184:HIS:HD2	1:A:186:GLY:N	2.13	0.44
1:A:452:THR:CG2	1:A:453:TYR:N	2.81	0.43
1:A:151:ASP:HB3	4:A:500:AXP:O4	2.19	0.43
1:A:362:MET:CE	1:A:364:ARG:HD3	2.49	0.43
1:A:82:VAL:O	1:A:187:LYS:HE2	2.19	0.43
1:A:226:GLN:NE2	1:A:240:VAL:H	2.04	0.43
1:A:120:PRO:HA	1:A:133:ALA:HA	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:464:ILE:HD12	1:A:464:ILE:HA	1.86	0.42
1:A:352:TRP:CD1	1:A:407:SER:HG	2.38	0.42
1:A:438:TRP:HD1	1:A:469:ILE:HD12	1.84	0.42
1:A:459:PRO:O	1:A:460:ASP:C	2.61	0.42
1:A:89:LYS:HB2	1:A:418:ILE:CG2	2.50	0.42
1:A:204:SER:HB3	1:A:211:LEU:HD11	2.02	0.42
1:A:298:SER:O	1:A:322:VAL:HG13	2.19	0.42
1:A:329:ASP:O	1:A:330:ASP:C	2.62	0.42
1:A:89:LYS:HB3	1:A:417:CYS:HA	2.01	0.42
1:A:176:ILE:HG22	1:A:195:THR:HG21	2.02	0.42
1:A:91:GLN:HG3	1:A:420:ARG:NH1	2.35	0.41
1:A:100:PHE:HB3	1:A:445:VAL:O	2.20	0.41
1:A:321:LEU:HD23	1:A:321:LEU:HA	1.64	0.41
1:A:125:ASP:HB2	1:A:126:PRO:HD2	2.02	0.41
1:A:174:VAL:O	1:A:174:VAL:HG12	2.20	0.41
1:A:257:ILE:HD11	1:A:260:GLY:HA2	2.03	0.41
1:A:226:GLN:O	1:A:227:GLU:HB2	2.21	0.41
1:A:426:LEU:HD13	1:A:460:ASP:N	2.35	0.41
1:A:165:VAL:HA	1:A:166:PRO:HD2	1.94	0.41
1:A:100:PHE:HD2	1:A:445:VAL:CG2	2.34	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%)	342 (89%)	39 (10%)	5 (1%)	9 14

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	329	ASP

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Mol	Chain	Res	Type
1	A	431	LYS
1	A	220	GLN
1	A	322	VAL
1	A	222	ILE

5.3.2 Protein sidechains ⓘ

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%)	300 (89%)	38 (11%)	6 9

All (38) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	83	GLU
1	A	94	ILE
1	A	118	ARG
1	A	122	VAL
1	A	127	VAL
1	A	134	LEU
1	A	142	ASN
1	A	148	THR
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	240	VAL
1	A	242	THR
1	A	257	ILE
1	A	315	SER
1	A	322	VAL
1	A	327	ARG

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Mol	Chain	Res	Type
1	A	346	THR
1	A	360	LEU
1	A	370	LEU
1	A	371	ARG
1	A	385	THR
1	A	387	ASN
1	A	388	SER
1	A	407	SER
1	A	409	ILE
1	A	418	ILE
1	A	420	ARG
1	A	424	VAL
1	A	431	LYS
1	A	445	VAL
1	A	455	THR
1	A	469	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	93	GLN
1	A	131	GLN
1	A	142	ASN
1	A	155	HIS
1	A	168	HIS
1	A	184	HIS
1	A	226	GLN
1	A	274	HIS
1	A	334	ASN
1	A	356	ASN
1	A	387	ASN
1	A	391	GLN
1	A	393	ASN
1	A	419	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 ⓘ

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	1,2	14,14,15	1.07	0	17,19,21	1.35	2 (11%)
2	NAG	B	2	2	14,14,15	0.96	1 (7%)	17,19,21	1.15	1 (5%)
2	MAN	B	3	2	11,11,12	1.01	1 (9%)	15,15,17	1.12	1 (6%)
2	MAN	B	4	2	11,11,12	0.85	0	15,15,17	1.33	2 (13%)
2	MAN	B	5	2	11,11,12	0.83	1 (9%)	15,15,17	0.86	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	B	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	B	2	2	-	0/6/23/26	0/1/1/1
2	MAN	B	3	2	1/1/5/5	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 (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	3	MAN	C4-C5	2.76	1.58	1.53
2	B	5	MAN	C4-C5	2.07	1.57	1.53
2	B	2	NAG	C4-C5	2.07	1.57	1.53

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1	NAG	C1-C2-N2	-2.84	105.95	110.43
2	B	1	NAG	C1-O5-C5	2.49	115.52	112.19
2	B	2	NAG	O7-C7-C8	-2.28	118.00	122.05
2	B	4	MAN	C1-C2-C3	2.14	112.76	109.64
2	B	3	MAN	C2-C3-C4	-2.03	107.29	110.86
2	B	4	MAN	O2-C2-C1	2.00	113.81	109.22

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	B	3	MAN	C1

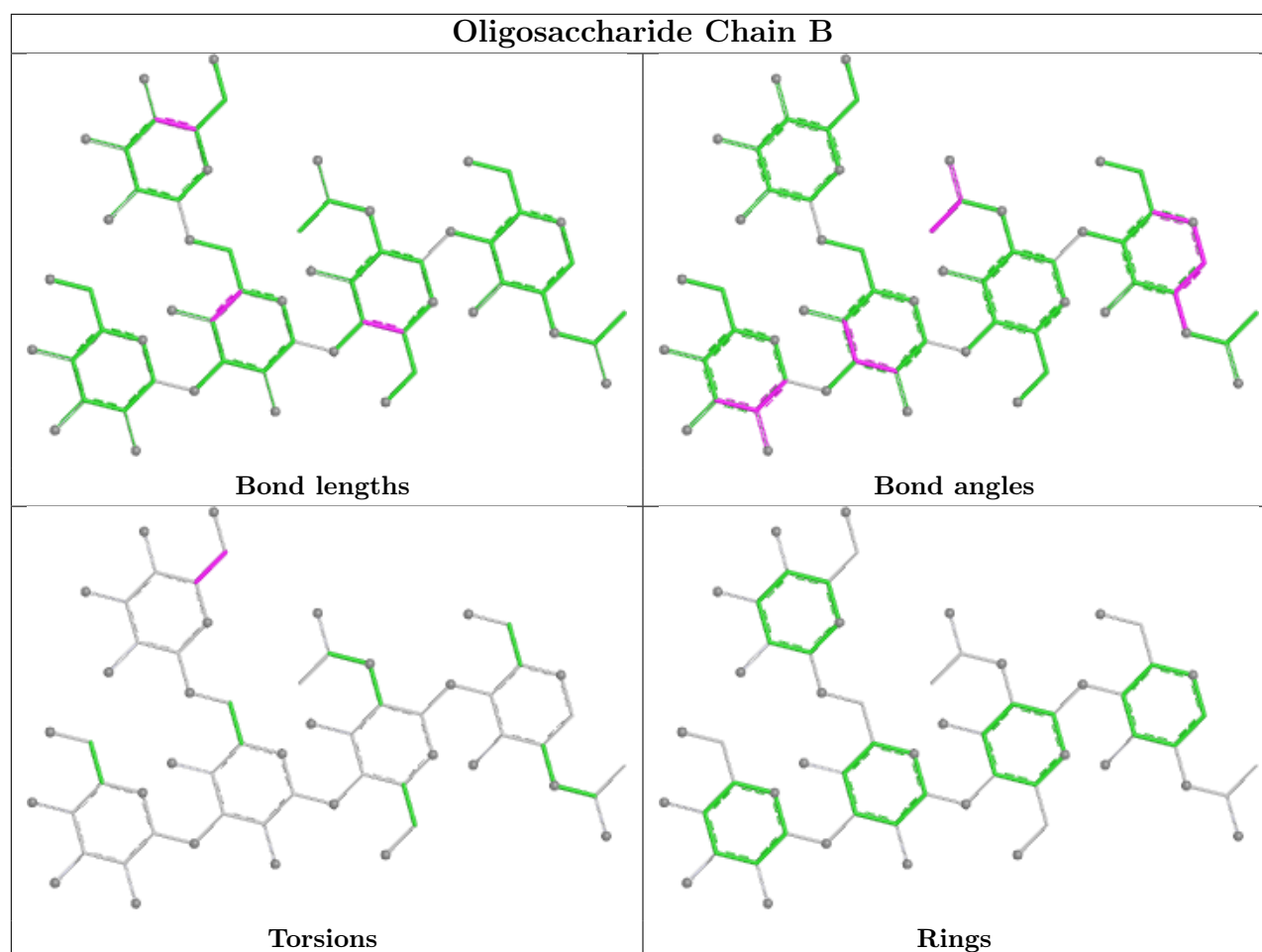
All (1) torsion outliers are listed below:

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	477(A)	1	14,14,15	1.00	1 (7%)	17,19,21	1.99	3 (17%)
3	NAG	A	471(A)	1	14,14,15	1.17	2 (14%)	17,19,21	1.70	3 (17%)
4	AXP	A	500	-	18,21,21	1.91	6 (33%)	22,31,31	2.33	8 (36%)
3	NAG	A	470(A)	1	14,14,15	1.05	1 (7%)	17,19,21	1.41	1 (5%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	A	477(A)	1	-	0/6/23/26	0/1/1/1
3	NAG	A	471(A)	1	-	2/6/23/26	0/1/1/1
4	AXP	A	500	-	-	2/14/36/36	0/1/1/1
3	NAG	A	470(A)	1	-	2/6/23/26	0/1/1/1

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	500	AXP	P1-O2P	-4.38	1.47	1.54
4	A	500	AXP	C8-C7	-3.30	1.47	1.53
4	A	500	AXP	P1-O3P	-3.26	1.49	1.54
3	A	477(A)	NAG	C1-C2	2.76	1.56	1.52
3	A	471(A)	NAG	C2-N2	-2.62	1.41	1.46
3	A	471(A)	NAG	C1-C2	-2.34	1.49	1.52
3	A	470(A)	NAG	C3-C2	-2.30	1.47	1.52
4	A	500	AXP	C6-C5	2.29	1.56	1.53
4	A	500	AXP	O6-C6	2.03	1.47	1.44
4	A	500	AXP	O8-C8	-2.01	1.39	1.43

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	477(A)	NAG	C1-O5-C5	5.90	120.09	112.19
4	A	500	AXP	C2-O6-C6	5.11	123.16	112.36
4	A	500	AXP	O3P-P1-O2P	-4.94	94.19	107.58
4	A	500	AXP	O3P-P1-O1P	-4.84	101.31	113.45
3	A	471(A)	NAG	C1-O5-C5	4.55	118.28	112.19
3	A	470(A)	NAG	C1-O5-C5	4.42	118.11	112.19
3	A	477(A)	NAG	C3-C4-C5	-3.33	104.20	110.23
4	A	500	AXP	O4-C4-C5	-3.11	102.78	109.84
4	A	500	AXP	O6-C2-C3	2.87	114.51	110.66
3	A	471(A)	NAG	C1-C2-N2	2.66	114.63	110.43
4	A	500	AXP	O8-C8-C7	-2.43	103.55	109.25
4	A	500	AXP	O7-C7-C6	-2.43	104.19	109.44
3	A	471(A)	NAG	O5-C1-C2	-2.17	107.93	111.29
4	A	500	AXP	O1P-P1-C2	2.17	118.24	113.34
3	A	477(A)	NAG	C1-C2-N2	2.03	113.63	110.43

There are no chirality outliers.

All (6) torsion outliers are listed below:

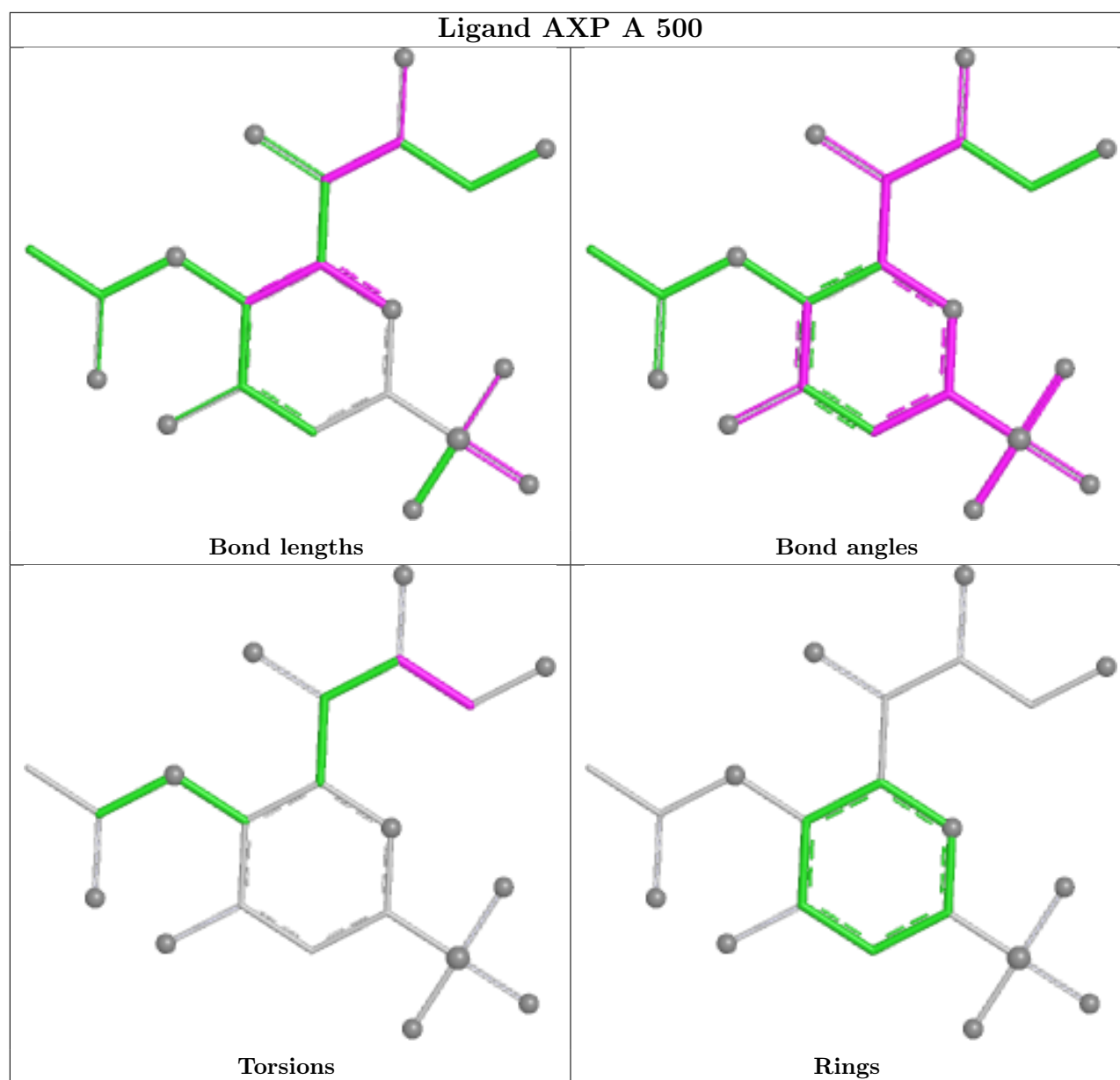
Mol	Chain	Res	Type	Atoms
4	A	500	AXP	C7-C8-C9-O9
4	A	500	AXP	O8-C8-C9-O9
3	A	471(A)	NAG	O5-C5-C6-O6
3	A	471(A)	NAG	C4-C5-C6-O6
3	A	470(A)	NAG	O5-C5-C6-O6
3	A	470(A)	NAG	C4-C5-C6-O6

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	500	AXP	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



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%)	3.50	337 (86%)  	1, 9, 17, 25	118 (30%)

All (337) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	320	GLY	9.0
1	A	339	ASP	7.3
1	A	372	SER	7.1
1	A	432	GLN	7.0
1	A	221	ASN	7.0
1	A	326	PRO	6.8
1	A	168	HIS	6.8
1	A	387	ASN	6.8
1	A	349	VAL	6.7
1	A	313	ASP	6.6
1	A	331	ARG	6.5
1	A	335	SER	6.5
1	A	332	SER	6.5
1	A	414	GLY	6.4
1	A	392	ILE	6.3
1	A	328	ASN	6.3
1	A	165	VAL	6.1
1	A	348	GLY	6.1
1	A	407	SER	6.1
1	A	456	GLY	6.0
1	A	86	ASN	5.9
1	A	234	ASN	5.9
1	A	469	ILE	5.9
1	A	210	ARG	5.9
1	A	265	ILE	5.9
1	A	322	VAL	5.8
1	A	346	THR	5.7

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Mol	Chain	Res	Type	RSRZ
1	A	261	LYS	5.7
1	A	243	ASP	5.7
1	A	249	ARG	5.7
1	A	274	HIS	5.6
1	A	202	THR	5.6
1	A	341	ASN	5.6
1	A	273	GLN	5.6
1	A	402	ASN	5.6
1	A	450	SER	5.5
1	A	214	SER	5.5
1	A	269	ALA	5.5
1	A	147	ASP	5.5
1	A	321	LEU	5.5
1	A	304	ASP	5.4
1	A	329	ASP	5.4
1	A	317	VAL	5.4
1	A	139	THR	5.3
1	A	189	TRP	5.3
1	A	220	GLN	5.3
1	A	431	LYS	5.3
1	A	201	ALA	5.2
1	A	181	SER	5.2
1	A	330	ASP	5.2
1	A	375	GLU	5.2
1	A	266	SER	5.2
1	A	199	LYS	5.2
1	A	416	SER	5.2
1	A	148	THR	5.1
1	A	336	ASN	5.1
1	A	351	GLY	5.1
1	A	358	ASN	5.1
1	A	162	GLU	5.0
1	A	194	ILE	5.0
1	A	312	ILE	5.0
1	A	184	HIS	5.0
1	A	425	GLU	4.9
1	A	177	ALA	4.9
1	A	406	TYR	4.9
1	A	123	SER	4.9
1	A	82	VAL	4.9
1	A	324	ASP	4.8
1	A	319	SER	4.8

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Mol	Chain	Res	Type	RSRZ
1	A	299	ASN	4.8
1	A	340	PRO	4.8
1	A	218	TRP	4.8
1	A	309	ASP	4.7
1	A	240	VAL	4.7
1	A	271	SER	4.7
1	A	310	TYR	4.7
1	A	353	ALA	4.7
1	A	279	SER	4.7
1	A	345	GLY	4.6
1	A	465	ASN	4.6
1	A	94	ILE	4.6
1	A	338	ARG	4.6
1	A	151	ASP	4.6
1	A	369	ASP	4.6
1	A	206	ILE	4.5
1	A	164	GLY	4.5
1	A	124	CYS	4.5
1	A	232	CYS	4.5
1	A	117	THR	4.5
1	A	231	VAL	4.5
1	A	225	THR	4.4
1	A	153	ILE	4.4
1	A	211	LEU	4.4
1	A	84	TYR	4.4
1	A	179	SER	4.4
1	A	359	ASP	4.4
1	A	90	PRO	4.4
1	A	154	PRO	4.4
1	A	264	HIS	4.4
1	A	239	VAL	4.4
1	A	237	CYS	4.4
1	A	200	ASN	4.3
1	A	363	GLY	4.3
1	A	295	TRP	4.3
1	A	227	GLU	4.3
1	A	286	GLY	4.3
1	A	398	VAL	4.3
1	A	258	GLU	4.3
1	A	390	SER	4.3
1	A	88	SER	4.2
1	A	347	GLN	4.2

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Mol	Chain	Res	Type	RSRZ
1	A	244	GLY	4.2
1	A	436	VAL	4.2
1	A	300	ARG	4.2
1	A	343	GLU	4.2
1	A	423	TYR	4.2
1	A	289	CYS	4.2
1	A	93	GLN	4.1
1	A	170	GLY	4.1
1	A	186	GLY	4.1
1	A	412	VAL	4.1
1	A	112	GLY	4.1
1	A	171	THR	4.1
1	A	108	LEU	4.1
1	A	437	TRP	4.1
1	A	413	GLU	4.1
1	A	125	ASP	4.1
1	A	360	LEU	4.1
1	A	130	TYR	4.0
1	A	342	ASN	4.0
1	A	344	ARG	4.0
1	A	383	TRP	4.0
1	A	257	ILE	4.0
1	A	116	VAL	4.0
1	A	308	GLU	4.0
1	A	357	GLY	4.0
1	A	396	VAL	4.0
1	A	267	PRO	3.9
1	A	371	ARG	3.9
1	A	333	SER	3.9
1	A	439	THR	3.9
1	A	366	ILE	3.9
1	A	176	ILE	3.8
1	A	397	ILE	3.8
1	A	111	GLY	3.8
1	A	370	LEU	3.8
1	A	100	PHE	3.8
1	A	306	ASN	3.8
1	A	138	THR	3.7
1	A	388	SER	3.7
1	A	391	GLN	3.7
1	A	113	ASP	3.7
1	A	284	TYR	3.7

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Mol	Chain	Res	Type	RSRZ
1	A	101	SER	3.7
1	A	311	SER	3.7
1	A	178	TRP	3.7
1	A	415	LYS	3.7
1	A	364	ARG	3.7
1	A	385	THR	3.7
1	A	424	VAL	3.7
1	A	144	HIS	3.7
1	A	464	ILE	3.7
1	A	368	LYS	3.7
1	A	131	GLN	3.6
1	A	105	SER	3.6
1	A	283	ARG	3.6
1	A	134	LEU	3.6
1	A	268	LEU	3.6
1	A	380	ILE	3.6
1	A	281	TYR	3.6
1	A	248	GLY	3.6
1	A	297	GLY	3.6
1	A	374	TYR	3.5
1	A	91	GLN	3.5
1	A	246	ALA	3.5
1	A	466	PHE	3.5
1	A	89	LYS	3.5
1	A	434	THR	3.5
1	A	188	ALA	3.5
1	A	291	CYS	3.5
1	A	204	SER	3.5
1	A	429	GLY	3.5
1	A	146	ASN	3.5
1	A	133	ALA	3.5
1	A	121	TYR	3.4
1	A	233	ILE	3.4
1	A	463	ASN	3.4
1	A	83	GLU	3.4
1	A	365	THR	3.4
1	A	141	ASP	3.4
1	A	197	ASP	3.4
1	A	198	ASP	3.4
1	A	401	ASP	3.4
1	A	212	VAL	3.4
1	A	303	VAL	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	298	SER	3.4
1	A	411	SER	3.4
1	A	302	VAL	3.3
1	A	427	ILE	3.3
1	A	400	SER	3.3
1	A	129	CYS	3.3
1	A	255	LEU	3.3
1	A	114	ILE	3.3
1	A	314	SER	3.3
1	A	278	CYS	3.3
1	A	96	GLY	3.3
1	A	106	ILE	3.3
1	A	250	ALA	3.3
1	A	352	TRP	3.2
1	A	97	PHE	3.2
1	A	222	ILE	3.2
1	A	440	SER	3.2
1	A	441	ASN	3.2
1	A	459	PRO	3.2
1	A	408	GLY	3.2
1	A	87	TRP	3.2
1	A	228	SER	3.2
1	A	208	ASP	3.1
1	A	449	THR	3.1
1	A	183	CYS	3.1
1	A	247	SER	3.1
1	A	467	MET	3.1
1	A	161	ASN	3.1
1	A	356	ASN	3.1
1	A	382	GLY	3.1
1	A	430	ARG	3.1
1	A	157	THR	3.1
1	A	457	SER	3.1
1	A	137	GLY	3.1
1	A	209	GLY	3.1
1	A	282	PRO	3.0
1	A	417	CYS	3.0
1	A	142	ASN	3.0
1	A	224	ARG	3.0
1	A	109	SER	3.0
1	A	381	GLY	3.0
1	A	272	ALA	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	152	ARG	3.0
1	A	230	CYS	3.0
1	A	110	ALA	3.0
1	A	126	PRO	3.0
1	A	373	GLY	3.0
1	A	174	VAL	2.9
1	A	143	LYS	2.9
1	A	223	LEU	2.9
1	A	195	THR	2.9
1	A	403	ARG	2.9
1	A	256	PHE	2.9
1	A	254	ILE	2.9
1	A	443	ILE	2.9
1	A	150	HIS	2.9
1	A	305	ILE	2.8
1	A	421	CYS	2.8
1	A	378	LYS	2.8
1	A	419	ASN	2.8
1	A	251	ASP	2.8
1	A	355	ASP	2.8
1	A	361	TRP	2.8
1	A	393	ASN	2.8
1	A	386	PRO	2.8
1	A	426	LEU	2.7
1	A	128	LYS	2.7
1	A	394	ARG	2.7
1	A	160	MET	2.7
1	A	462	ALA	2.7
1	A	446	PHE	2.7
1	A	448	GLY	2.7
1	A	192	VAL	2.7
1	A	245	SER	2.7
1	A	215	ILE	2.7
1	A	158	LEU	2.7
1	A	433	GLU	2.7
1	A	460	ASP	2.6
1	A	172	ARG	2.6
1	A	163	LEU	2.6
1	A	285	PRO	2.6
1	A	422	PHE	2.6
1	A	92	CYS	2.6
1	A	140	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	226	GLN	2.6
1	A	325	THR	2.6
1	A	120	PRO	2.6
1	A	187	LYS	2.6
1	A	149	VAL	2.6
1	A	145	SER	2.6
1	A	455	THR	2.6
1	A	468	PRO	2.5
1	A	132	PHE	2.5
1	A	205	PHE	2.5
1	A	219	SER	2.5
1	A	318	CYS	2.5
1	A	166	PRO	2.5
1	A	104	ASN	2.5
1	A	155	HIS	2.5
1	A	238	THR	2.5
1	A	242	THR	2.5
1	A	452	THR	2.5
1	A	280	CYS	2.4
1	A	207	TYR	2.4
1	A	270	GLY	2.4
1	A	418	ILE	2.4
1	A	127	VAL	2.4
1	A	362	MET	2.4
1	A	276	GLU	2.4
1	A	103	ASP	2.3
1	A	294	ASN	2.3
1	A	196	GLY	2.3
1	A	404	SER	2.3
1	A	307	MET	2.3
1	A	115	TRP	2.3
1	A	458	TRP	2.3
1	A	119	GLU	2.3
1	A	107	ARG	2.3
1	A	173	GLN	2.2
1	A	190	LEU	2.2
1	A	350	LYS	2.2
1	A	438	TRP	2.2
1	A	410	PHE	2.2
1	A	288	ARG	2.2
1	A	409	ILE	2.2
1	A	236	THR	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	453	TYR	2.2
1	A	122	VAL	2.2
1	A	316	TYR	2.2
1	A	315	SER	2.2
1	A	323	GLY	2.1
1	A	454	GLY	2.1
1	A	191	HIS	2.1
1	A	379	VAL	2.1
1	A	259	GLU	2.1
1	A	435	ARG	2.1
1	A	135	GLY	2.1
1	A	354	PHE	2.1
1	A	95	THR	2.1
1	A	395	GLN	2.0
1	A	241	MET	2.0
1	A	182	SER	2.0

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

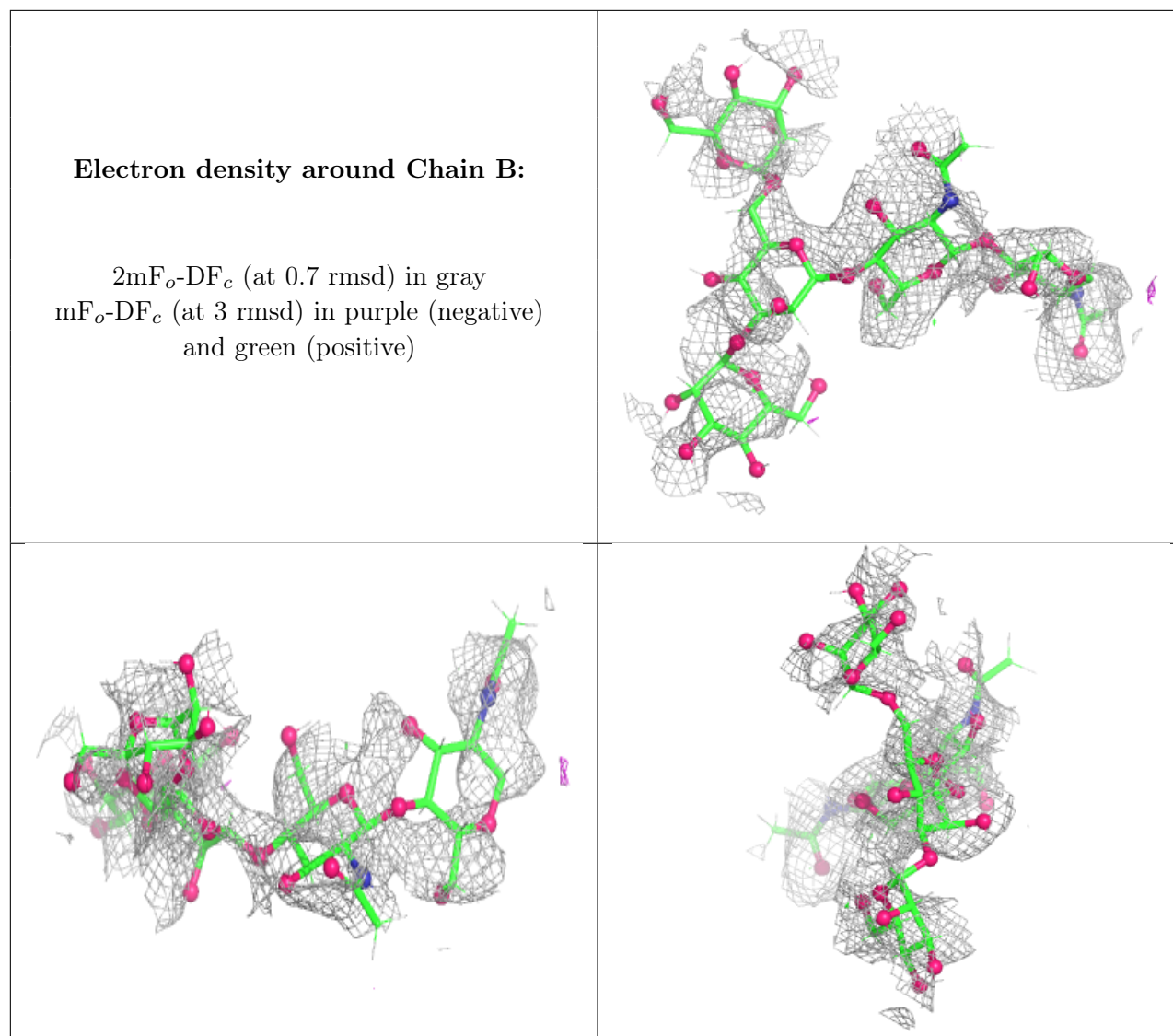
There are no non-standard protein/DNA/RNA residues in this entry.

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	MAN	B	5	11/12	0.21	0.41	0,0,59,61	11
2	NAG	B	2	14/15	0.41	0.33	0,0,34,34	5
2	MAN	B	4	11/12	0.44	0.31	0,0,54,56	5
2	MAN	B	3	11/12	0.53	0.27	0,16,39,39	5
2	NAG	B	1	14/15	0.65	0.24	0,0,36,43	13

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



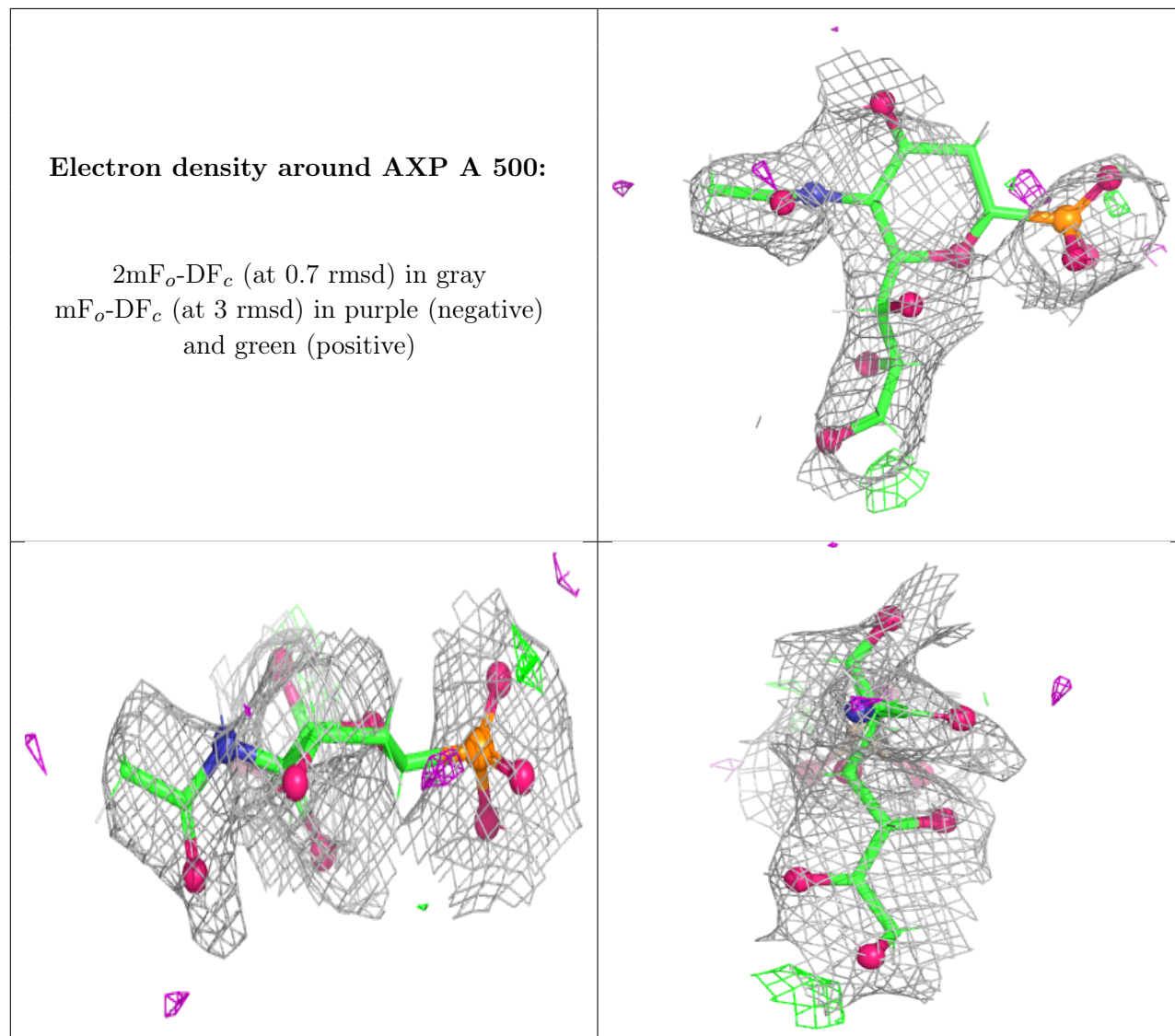
6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	NAG	A	470(A)	14/15	0.38	0.41	0,0,38,46	14
5	CA	A	501	1/1	0.45	0.28	11,11,11,11	0
3	NAG	A	477(A)	14/15	0.64	0.31	0,0,39,42	14
4	AXP	A	500	21/21	0.66	0.22	0,15,19,25	1
3	NAG	A	471(A)	14/15	0.69	0.30	0,0,43,52	13

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 ⓘ

There are no such residues in this entry.