



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 08:04 PM GMT

PDB ID : 1INW
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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

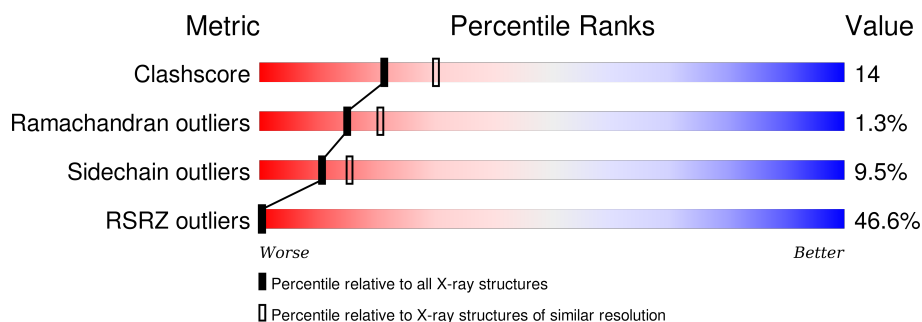
1 Overall quality at a glance

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	102246	3407 (2.40-2.40)
Ramachandran outliers	100387	3351 (2.40-2.40)
Sidechain outliers	100360	3352 (2.40-2.40)
RSRZ outliers	91569	2928 (2.40-2.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	<div> <div>47%</div> <div>66%</div> <div>29%</div> <div>.</div> </div>

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	NAG	A	477(A)	-	-	-	X
3	MAN	A	474(C)	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 SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

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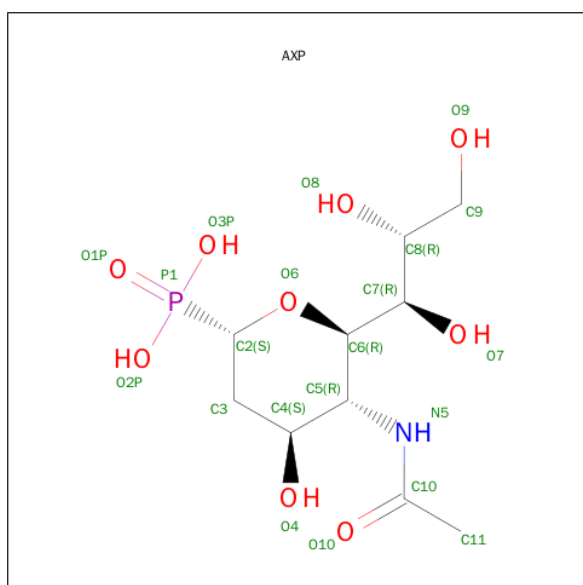
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	H	N	O	0	0
			28	8	14	1	5		

- Molecule 3 is a polymer of unknown type called SUGAR (5-MER).

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

- Molecule 4 is SUGAR (4-ACETAMIDO-2,4-DIDEXOY-D-GLYCERO-BETA-D-GALACTO-O-OCTOPYRANOSYLPHOSPHONIC ACID (AN AXIAL PHOSPHONATE)) (three-letter code: 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

- Molecule 5 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

- Molecule 6 is water.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	86	Total	H	O	7	0
			258	172	86		

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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 ($\text{RSRZ} > 2$). 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



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	122.08 Å 141.67 Å 141.87 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	8.00 – 2.40 21.05 – 2.40	Depositor EDS
% Data completeness (in resolution range)	(Not available) (8.00-2.40) 65.4 (21.05-2.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.21 (at 2.41 Å)	Xtriage
Refinement program	X-PLOR	Depositor
R, R_{free}	0.206 , (Not available) (Not available) , (Not available)	Depositor DCC
R_{free} test set	NotAvailable	DCC
Wilson B-factor (Å ²)	27.9	Xtriage
Anisotropy	0.691	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.23 , 54.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	1 of 31623 reflections (0.003%)	Xtriage
F_o, F_c correlation	0.45	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, 0.375 respectively for untwinned datasets, and 0.333, 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: AXP, MAN, CA, NAG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.71	0/3092	0.89	3/4194 (0.1%)

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
3	A	1	0
All	All	1	1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	431	LYS	N-CA-C	-5.76	95.45	111.00
1	A	292	ARG	NE-CZ-NH1	5.51	123.06	120.30
1	A	323	GLY	N-CA-C	5.02	125.65	113.10

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	474(C)	MAN	C1

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	87	0
2	A	42	42	39	0	0
3	A	61	57	52	0	0
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	87	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 14.

All (87) 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:NZ	1:A:431:LYS:HA	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:HZ3	1:A:431:LYS:HA	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:328:ASN:O	1:A:329:ASP:HB2	2.01	0.59
1:A:149:VAL:HG22	6:A:509:HOH:O	2.02	0.59
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
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: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: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:328:ASN:HB2	6:A:548:HOH:O	2.14	0.48
1:A:168:HIS:HB2	6:A:567:HOH:O	2.13	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:283:ARG:O	1:A:284:TYR:C	2.53	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:311:SER:C	1:A:312:ILE:HD13	2.37	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:136:GLN:CD	1:A:156:ARG:HD3	2.39	0.43
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:226:GLN:NE2	1:A:240:VAL:H	2.04	0.43
1:A:82:VAL:O	1:A:187:LYS:HE2	2.19	0.43
1:A:120:PRO:HA	1:A:133:ALA:HA	2.00	0.42
1:A:464:ILE:HA	1:A:464:ILE:HD12	1.86	0.42
1:A:438:TRP:HD1	1:A:469:ILE:HD12	1.84	0.42
1:A:89:LYS:HB2	1:A:418:ILE:CG2	2.50	0.42
1:A:298:SER:O	1:A:322:VAL:HG13	2.19	0.42
1:A:204:SER:HB3	1:A:211:LEU:HD11	2.02	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:HA	1:A:321:LEU:HD23	1.64	0.41
1:A:125:ASP:HB2	1:A:126:PRO:HD2	2.02	0.41
1:A:257:ILE:HD11	1:A:260:GLY:HA2	2.03	0.41
1:A:174:VAL:O	1:A:174:VAL:HG12	2.20	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
1:A:352:TRP:HD1	1:A:407:SER:HG	1.69	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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%)	15 21

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	329	ASP
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%)	306 (90%)	32 (10%)	11 15

All (32) 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	283	ARG

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Mol	Chain	Res	Type
1	A	315	SER
1	A	327	ARG
1	A	346	THR
1	A	370	LEU
1	A	385	THR
1	A	387	ASN
1	A	388	SER
1	A	407	SER
1	A	418	ILE
1	A	424	VAL
1	A	431	LYS
1	A	455	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	131	GLN
1	A	142	ASN
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	358	ASN
1	A	387	ASN
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 carbohydrates 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$
3	NAG	A	472(A)	1,3	14,14,15	1.03	0	15,19,21	1.21	1 (6%)
3	NAG	A	473(B)	3	14,14,15	0.95	1 (7%)	15,19,21	1.23	1 (6%)
3	MAN	A	474(C)	3	11,11,12	1.00	1 (9%)	14,15,17	1.29	2 (14%)
3	MAN	A	475(D)	3	11,11,12	0.85	0	14,15,17	1.51	4 (28%)
3	MAN	A	476(F)	3	11,11,12	0.82	1 (9%)	14,15,17	0.97	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
3	NAG	A	472(A)	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	473(B)	3	-	0/6/23/26	0/1/1/1
3	MAN	A	474(C)	3	1/1/5/5	0/2/19/22	0/1/1/1
3	MAN	A	475(D)	3	-	0/2/19/22	0/1/1/1
3	MAN	A	476(F)	3	-	0/2/19/22	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	473(B)	NAG	C4-C5	2.05	1.57	1.53
3	A	476(F)	MAN	C4-C5	2.06	1.57	1.53
3	A	474(C)	MAN	C4-C5	2.75	1.58	1.53

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	473(B)	NAG	O7-C7-C8	-2.21	118.00	122.06
3	A	474(C)	MAN	C2-C3-C4	-2.21	107.29	111.04
3	A	475(D)	MAN	O2-C2-C3	-2.04	106.02	110.12
3	A	475(D)	MAN	C1-O5-C5	2.05	114.86	112.25
3	A	474(C)	MAN	O5-C1-C2	2.11	114.28	110.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	475(D)	MAN	O2-C2-C1	2.30	113.81	109.21
3	A	472(A)	NAG	C1-O5-C5	2.58	115.52	112.25
3	A	475(D)	MAN	C1-C2-C3	2.72	112.76	109.54

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	474(C)	MAN	C1

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	$\# Z > 2$
2	NAG	A	470(A)	1	14,14,15	1.00	1 (7%)	15,19,21	1.50	1 (6%)
2	NAG	A	471(A)	1	14,14,15	1.13	2 (14%)	15,19,21	1.78	4 (26%)
2	NAG	A	477(A)	1	14,14,15	0.96	1 (7%)	15,19,21	2.08	2 (13%)
4	AXP	A	500	-	18,21,21	1.81	4 (22%)	22,31,31	1.95	6 (27%)

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	A	470(A)	1	-	0/6/23/26	0/1/1/1
2	NAG	A	471(A)	1	-	0/6/23/26	0/1/1/1

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

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	500	AXP	P1-O2P	-4.17	1.47	1.54
4	A	500	AXP	P1-O3P	-3.10	1.49	1.54
4	A	500	AXP	C8-C7	-2.84	1.47	1.53
2	A	471(A)	NAG	C2-N2	-2.48	1.41	1.46
2	A	471(A)	NAG	C1-C2	-2.38	1.49	1.52
2	A	470(A)	NAG	C3-C2	-2.02	1.47	1.52
4	A	500	AXP	C6-C5	2.20	1.56	1.53
2	A	477(A)	NAG	C1-C2	2.63	1.56	1.52

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	500	AXP	O3P-P1-O1P	-4.58	101.31	113.49
4	A	500	AXP	O3P-P1-O2P	-4.45	94.19	107.57
2	A	477(A)	NAG	C3-C4-C5	-3.44	104.20	110.20
2	A	471(A)	NAG	C3-C2-N2	-2.87	103.70	110.56
4	A	500	AXP	O7-C7-C6	-2.26	104.19	109.43
4	A	500	AXP	O8-C8-C7	-2.17	103.55	109.02
2	A	471(A)	NAG	O4-C4-C3	-2.07	105.67	110.34
2	A	471(A)	NAG	O3-C3-C2	2.15	113.37	109.11
4	A	500	AXP	O6-C2-C3	2.95	114.51	110.65
4	A	500	AXP	C3-C4-C5	3.80	115.70	111.47
2	A	470(A)	NAG	C1-O5-C5	4.61	118.11	112.25
2	A	471(A)	NAG	C1-O5-C5	4.75	118.28	112.25
2	A	477(A)	NAG	C1-O5-C5	6.18	120.09	112.25

There are no chirality outliers.

There are no torsion outliers.

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

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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%)	2.09	181 (46%) 0 0	2, 11, 23, 53	125 (32%)

All (181) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	392	ILE	9.7
1	A	469	ILE	6.8
1	A	141	ASP	5.7
1	A	189	TRP	5.6
1	A	456	GLY	5.5
1	A	82	VAL	5.3
1	A	218	TRP	5.3
1	A	400	SER	5.3
1	A	432	GLN	5.0
1	A	269	ALA	5.0
1	A	221	ASN	5.0
1	A	390	SER	4.9
1	A	330	ASP	4.9
1	A	296	LYS	4.9
1	A	439	THR	4.8
1	A	466	PHE	4.8
1	A	154	PRO	4.8
1	A	317	VAL	4.7
1	A	87	TRP	4.6
1	A	297	GLY	4.5
1	A	194	ILE	4.5
1	A	339	ASP	4.2
1	A	115	TRP	4.2
1	A	210	ARG	4.1
1	A	450	SER	4.1
1	A	273	GLN	4.1
1	A	406	TYR	4.1

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Mol	Chain	Res	Type	RSRZ
1	A	148	THR	4.0
1	A	84	TYR	4.0
1	A	245	SER	3.8
1	A	202	THR	3.8
1	A	348	GLY	3.7
1	A	139	THR	3.7
1	A	464	ILE	3.7
1	A	331	ARG	3.7
1	A	111	GLY	3.7
1	A	257	ILE	3.6
1	A	335	SER	3.6
1	A	274	HIS	3.6
1	A	326	PRO	3.6
1	A	249	ARG	3.6
1	A	113	ASP	3.6
1	A	352	TRP	3.5
1	A	397	ILE	3.5
1	A	371	ARG	3.5
1	A	158	LEU	3.4
1	A	116	VAL	3.4
1	A	186	GLY	3.4
1	A	192	VAL	3.3
1	A	97	PHE	3.3
1	A	200	ASN	3.3
1	A	190	LEU	3.3
1	A	285	PRO	3.3
1	A	196	GLY	3.3
1	A	240	VAL	3.3
1	A	423	TYR	3.3
1	A	261	LYS	3.2
1	A	165	VAL	3.2
1	A	441	ASN	3.2
1	A	176	ILE	3.2
1	A	458	TRP	3.2
1	A	236	THR	3.2
1	A	271	SER	3.1
1	A	106	ILE	3.1
1	A	322	VAL	3.1
1	A	325	THR	3.1
1	A	222	ILE	3.1
1	A	199	LYS	3.1
1	A	123	SER	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	448	GLY	3.0
1	A	328	ASN	3.0
1	A	225	THR	3.0
1	A	124	CYS	3.0
1	A	133	ALA	3.0
1	A	391	GLN	3.0
1	A	357	GLY	2.9
1	A	381	GLY	2.9
1	A	272	ALA	2.9
1	A	134	LEU	2.9
1	A	437	TRP	2.9
1	A	299	ASN	2.9
1	A	140	LEU	2.8
1	A	147	ASP	2.8
1	A	320	GLY	2.8
1	A	298	SER	2.8
1	A	372	SER	2.8
1	A	212	VAL	2.8
1	A	380	ILE	2.8
1	A	280	CYS	2.8
1	A	289	CYS	2.8
1	A	112	GLY	2.8
1	A	354	PHE	2.8
1	A	333	SER	2.8
1	A	291	CYS	2.7
1	A	412	VAL	2.7
1	A	237	CYS	2.7
1	A	304	ASP	2.7
1	A	217	SER	2.7
1	A	238	THR	2.7
1	A	232	CYS	2.7
1	A	353	ALA	2.7
1	A	153	ILE	2.7
1	A	278	CYS	2.7
1	A	184	HIS	2.6
1	A	438	TRP	2.6
1	A	268	LEU	2.6
1	A	321	LEU	2.6
1	A	122	VAL	2.6
1	A	445	VAL	2.6
1	A	162	GLU	2.6
1	A	215	ILE	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	375	GLU	2.6
1	A	267	PRO	2.6
1	A	117	THR	2.6
1	A	223	LEU	2.6
1	A	435	ARG	2.5
1	A	468	PRO	2.5
1	A	94	ILE	2.5
1	A	254	ILE	2.5
1	A	347	GLN	2.5
1	A	149	VAL	2.5
1	A	239	VAL	2.5
1	A	256	PHE	2.5
1	A	93	GLN	2.5
1	A	86	ASN	2.5
1	A	90	PRO	2.5
1	A	282	PRO	2.5
1	A	362	MET	2.4
1	A	230	CYS	2.4
1	A	324	ASP	2.4
1	A	416	SER	2.4
1	A	383	TRP	2.4
1	A	415	LYS	2.4
1	A	300	ARG	2.4
1	A	436	VAL	2.4
1	A	131	GLN	2.4
1	A	341	ASN	2.3
1	A	345	GLY	2.3
1	A	144	HIS	2.3
1	A	120	PRO	2.3
1	A	351	GLY	2.3
1	A	452	THR	2.3
1	A	83	GLU	2.3
1	A	214	SER	2.3
1	A	453	TYR	2.3
1	A	157	THR	2.3
1	A	374	TYR	2.3
1	A	205	PHE	2.3
1	A	402	ASN	2.3
1	A	382	GLY	2.2
1	A	195	THR	2.2
1	A	231	VAL	2.2
1	A	343	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	142	ASN	2.2
1	A	265	ILE	2.2
1	A	467	MET	2.2
1	A	313	ASP	2.2
1	A	336	ASN	2.2
1	A	340	PRO	2.2
1	A	100	PHE	2.1
1	A	178	TRP	2.1
1	A	346	THR	2.1
1	A	286	GLY	2.1
1	A	430	ARG	2.1
1	A	446	PHE	2.1
1	A	349	VAL	2.1
1	A	108	LEU	2.1
1	A	159	LEU	2.1
1	A	360	LEU	2.1
1	A	105	SER	2.1
1	A	216	GLY	2.1
1	A	386	PRO	2.1
1	A	143	LYS	2.0
1	A	295	TRP	2.0
1	A	429	GLY	2.0
1	A	114	ILE	2.0
1	A	443	ILE	2.0
1	A	197	ASP	2.0
1	A	411	SER	2.0
1	A	344	ARG	2.0
1	A	310	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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(\AA^2)	Q<0.9
3	MAN	A	474(C)	11/12	0.75	0.41	-	0,16,39,39	5
3	MAN	A	476(F)	11/12	0.33	0.74	-	0,0,59,61	11
3	NAG	A	472(A)	14/15	0.73	0.33	-	0,0,36,43	13
3	NAG	A	473(B)	14/15	0.75	0.31	-	0,0,34,34	5
3	MAN	A	475(D)	11/12	0.66	0.33	-	0,0,54,56	5

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(\AA^2)	Q<0.9
2	NAG	A	477(A)	14/15	0.57	0.39	2.75	0,0,39,42	14
2	NAG	A	470(A)	14/15	0.64	0.34	0.79	0,0,38,46	14
4	AXP	A	500	21/21	0.76	0.28	-0.35	0,15,19,25	1
5	CA	A	501	1/1	0.83	0.09	-3.94	11,11,11,11	0
2	NAG	A	471(A)	14/15	0.77	0.28	-	0,0,43,52	13

6.5 Other polymers [i](#)

There are no such residues in this entry.