



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 08:05 PM GMT

PDB ID : 1INY  
Title : A SIALIC ACID DERIVED PHOSPHONATE ANALOG INHIBITS DIFFERENT STRAINS OF INFLUENZA VIRUS NEURAMINIDASE WITH DIFFERENT EFFICIENCIES  
Authors : White, C.L.; Janakiraman, M.N.; Laver, W.G.; Philippon, C.; Vasella, A.; Air, G.M.; Luo, M.  
Deposited on : 1994-09-26  
Resolution : 2.40 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto: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

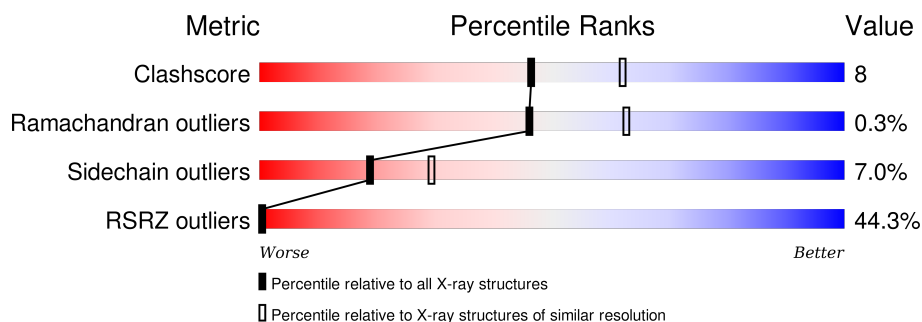
# 1 Overall quality at a glance

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  $\geq 3$ , 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	

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
3	NAG	A	473(B)	-	-	-	X

## 2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 4202 atoms, of which 945 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

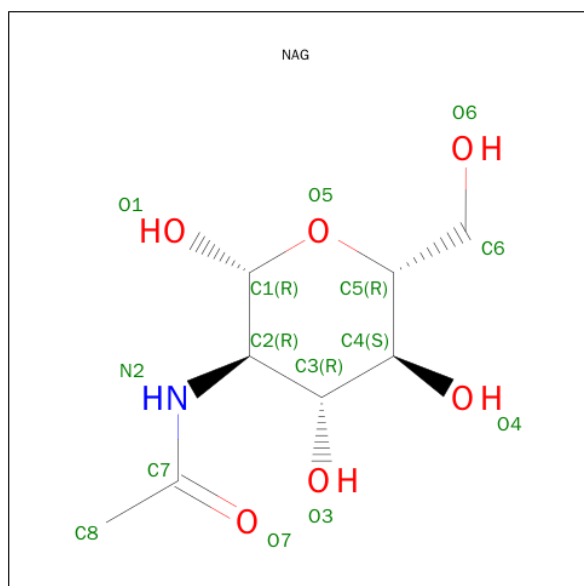
- Molecule 1 is a protein called INFLUENZA A SUBTYPE N9 NEURAMINIDASE.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	388	Total	C	H	N	O	S	0	0	0
			3780	1917	711	538	591	23			

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 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			

*Continued on next page...*

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	H	N	O	0	0
			27	8	13	1	5		

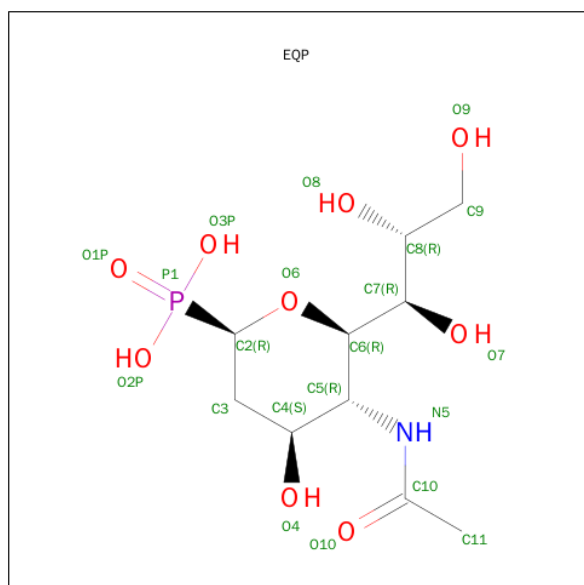
- Molecule 3 is a polymer of unknown type called SUGAR (7-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	6	Total	C	H	N	O	0	0
			133	38	64	1	30		

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

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

- Molecule 5 is (4-ACETAMIDO-2,4-DIDEOXY-D-GLYCERO-ALPHA-D-GALACTO-1-OC TOPYRANOSYL)PHOSPHONIC ACID (three-letter code: EQP) (formula: C<sub>10</sub>H<sub>20</sub>NO<sub>9</sub>P).



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

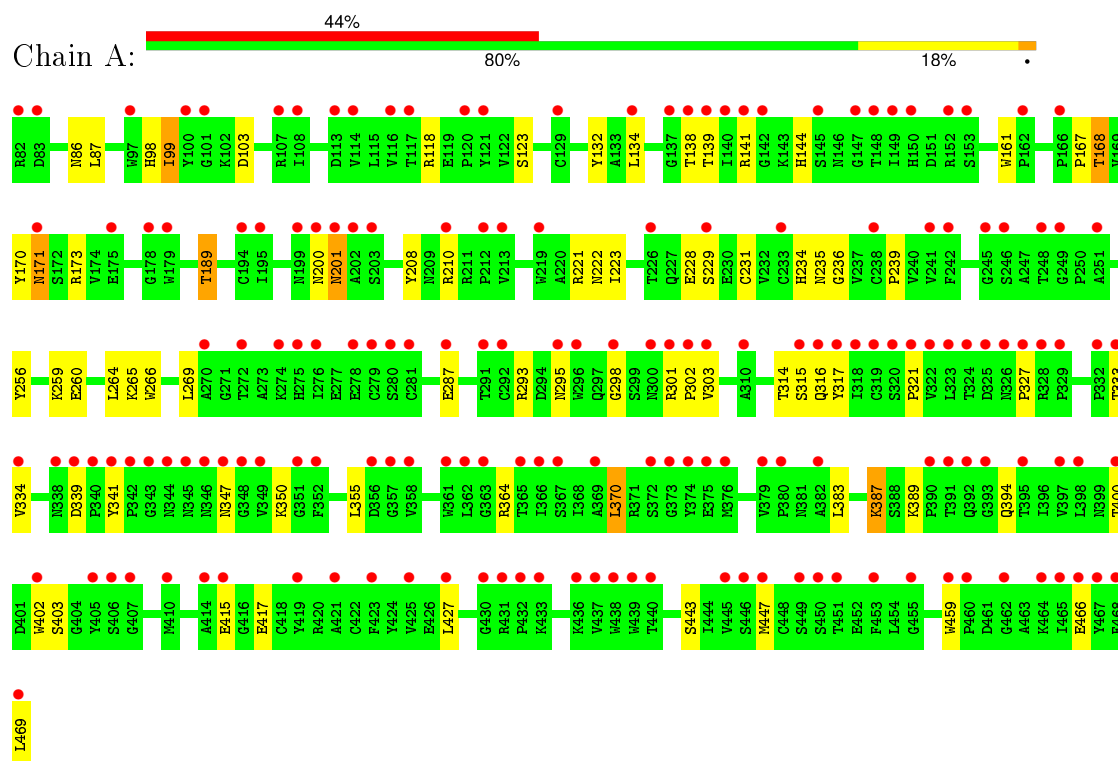
- Molecule 6 is water.

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

### 3 Residue-property plots

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 ( $RSRZ > 2$ ). 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



## 4 Data and refinement statistics

Property	Value	Source
Space group	I 4 3 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	184.86 Å   184.86 Å   184.86 Å 90.00°   90.00°   90.00°	Depositor
Resolution (Å)	8.00 – 2.40 28.52 – 2.39	Depositor EDS
% Data completeness (in resolution range)	(Not available) (8.00-2.40) 81.1 (28.52-2.39)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.04 (at 2.39 Å)	Xtriage
Refinement program	X-PLOR	Depositor
R, $R_{free}$	0.187 , (Not available) 0.399 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	20.8	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.24 , 12.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 17538 reflections	Xtriage
$F_o, F_c$ correlation	0.69	EDS
Total number of atoms	4202	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	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.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 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: EQP, CA, BMA, NAG, MAN

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.70	0/3152	0.84	0/4293

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3069	711	2900	46	2
2	A	42	41	38	3	0
3	A	69	64	58	0	0
4	A	1	0	0	0	0
5	A	21	19	17	0	0
6	A	55	110	0	1	0
All	All	3257	945	3013	46	2

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

All (46) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:200:ASN:HD21	2:A:472(A):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:A:472(A):NAG:C1	1.97	0.73
1:A:189:THR:HG22	1:A:208:TYR:CZ	2.26	0.71
1:A:201:ASN:HB3	1:A:221:ARG:NH1	2.07	0.69
1:A:327:PRO:HD2	1:A:347:ASN:HB3	1.75	0.69
1:A:168:THR:HG22	1:A:171:ASN:H	1.61	0.65
1:A:370:LEU:HD13	1:A:402:TRP:HZ3	1.62	0.64
1:A:293:ARG:HH21	1:A:295:ASN:ND2	1.98	0.62
1:A:87:LEU:H	1:A:234:HIS:CD2	2.17	0.60
1:A:98:HIS:HD2	1:A:99:ILE:O	1.85	0.59
1:A:86:ASN:OD1	1:A:235:ASN:HB2	2.03	0.59
1:A:355:LEU:HD13	1:A:383:LEU:HD13	1.88	0.56
1:A:259:LYS:HB2	1:A:264:LEU:HD11	1.87	0.55
1:A:236:GLY:HA3	1:A:259:LYS:HE3	1.89	0.54
1:A:99:ILE:HG12	1:A:459:TRP:CZ2	2.42	0.54
1:A:201:ASN:OD1	2:A:472(A):NAG:O5	2.26	0.53
1:A:321:PRO:HG2	1:A:389:LYS:HE2	1.91	0.53
1:A:201:ASN:N	1:A:201:ASN:HD22	2.07	0.53
1:A:161:TRP:CZ2	1:A:167:PRO:HG3	2.45	0.51
1:A:427:LEU:HB2	1:A:443:SER:HB3	1.95	0.48
1:A:123:SER:HB3	1:A:132:TYR:CE1	2.48	0.48
1:A:201:ASN:HB3	1:A:221:ARG:HH12	1.79	0.47
1:A:394:GLN:NE2	6:A:515:HOH:O	2.49	0.45
1:A:168:THR:CG2	1:A:170:TYR:H	2.30	0.45
1:A:168:THR:HG23	1:A:170:TYR:H	1.81	0.45
1:A:403:SER:HA	1:A:427:LEU:HD23	1.99	0.45
1:A:229:SER:HB3	1:A:350:LYS:HE2	1.98	0.44
1:A:168:THR:HG22	1:A:171:ASN:N	2.32	0.44
1:A:316:GLN:HG3	1:A:317:TYR:N	2.33	0.43
1:A:301:ARG:HA	1:A:302:PRO:HD3	1.93	0.43
1:A:138:THR:HG22	1:A:139:THR:N	2.33	0.43
1:A:138:THR:HG23	1:A:144:HIS:HB2	2.00	0.43
1:A:239:PRO:HA	1:A:256:TYR:O	2.19	0.43
1:A:466:GLU:HA	1:A:469:LEU:HG	2.01	0.42
1:A:265:LYS:HG2	1:A:266:TRP:N	2.35	0.42
1:A:138:THR:CG2	1:A:144:HIS:HB2	2.50	0.42
1:A:370:LEU:HD13	1:A:402:TRP:CZ3	2.50	0.42
1:A:264:LEU:HD23	1:A:264:LEU:HA	1.89	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:236:GLY:O	1:A:259:LYS:HD2	2.20	0.41
1:A:173:ARG:CD	1:A:210:ARG:HH22	2.23	0.41
1:A:303:VAL:O	1:A:315:SER:HA	2.21	0.41
1:A:298:GLY:HA2	1:A:341:TYR:O	2.20	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 ⓘ

### 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%)	354 (92%)	31 (8%)	1 (0%)	46 63

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	223	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	341/341 (100%)	317 (93%)	24 (7%)	19	29

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	99	ILE
1	A	103	ASP
1	A	118	ARG
1	A	134	LEU
1	A	141	ARG
1	A	168	THR
1	A	171	ASN
1	A	189	THR
1	A	201	ASN
1	A	222	ASN
1	A	228	GLU
1	A	231	CYS
1	A	260	GLU
1	A	269	LEU
1	A	287	GLU
1	A	314	THR
1	A	339	ASP
1	A	364	ARG
1	A	370	LEU
1	A	387	LYS
1	A	400	THR
1	A	415	GLU
1	A	417	GLU
1	A	447	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	95	ASN
1	A	98	HIS
1	A	171	ASN
1	A	200	ASN
1	A	201	ASN
1	A	222	ASN
1	A	234	HIS
1	A	295	ASN
1	A	346	ASN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
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 ⓘ

6 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	473(B)	3,2	14,14,15	3.03	5 (35%)	15,19,21	2.02	1 (6%)
3	BMA	A	474(C)	3	11,11,12	1.49	1 (9%)	14,15,17	1.99	3 (21%)
3	MAN	A	475(D)	3	11,11,12	2.41	3 (27%)	14,15,17	2.24	6 (42%)
3	MAN	A	476(E)	3	11,11,12	1.40	1 (9%)	14,15,17	1.79	3 (21%)
3	MAN	A	477(F)	3	11,11,12	1.73	3 (27%)	14,15,17	3.41	7 (50%)
3	MAN	A	478(G)	3	11,11,12	0.86	0	14,15,17	1.54	2 (14%)

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	473(B)	3,2	-	0/6/23/26	0/1/1/1
3	BMA	A	474(C)	3	-	0/2/19/22	0/1/1/1

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	MAN	A	475(D)	3	-	0/2/19/22	0/1/1/1
3	MAN	A	476(E)	3	-	0/2/19/22	0/1/1/1
3	MAN	A	477(F)	3	-	0/2/19/22	0/1/1/1
3	MAN	A	478(G)	3	-	0/2/19/22	0/1/1/1

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	477(F)	MAN	O5-C5	2.18	1.48	1.43
3	A	477(F)	MAN	C4-C3	2.29	1.58	1.52
3	A	473(B)	NAG	O4-C4	2.45	1.48	1.43
3	A	473(B)	NAG	C4-C5	2.60	1.58	1.53
3	A	475(D)	MAN	C4-C5	2.78	1.59	1.53
3	A	475(D)	MAN	O5-C5	2.94	1.49	1.43
3	A	474(C)	BMA	O5-C5	3.27	1.50	1.43
3	A	476(E)	MAN	O5-C1	3.36	1.49	1.43
3	A	473(B)	NAG	O5-C5	3.71	1.51	1.43
3	A	477(F)	MAN	C4-C5	4.01	1.61	1.53
3	A	473(B)	NAG	C3-C2	6.07	1.66	1.52
3	A	475(D)	MAN	C2-C3	6.68	1.61	1.52
3	A	473(B)	NAG	C1-C2	7.71	1.63	1.52

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	477(F)	MAN	C3-C4-C5	-4.29	102.72	110.20
3	A	475(D)	MAN	C3-C4-C5	-3.79	103.58	110.20
3	A	477(F)	MAN	O3-C3-C2	-3.44	103.79	110.00
3	A	476(E)	MAN	O2-C2-C3	-3.28	103.52	110.12
3	A	477(F)	MAN	O5-C5-C6	-2.68	101.54	107.35
3	A	478(G)	MAN	O5-C1-C2	-2.38	107.00	110.86
3	A	475(D)	MAN	O5-C1-C2	-2.20	107.28	110.86
3	A	477(F)	MAN	O2-C2-C1	2.24	113.70	109.21
3	A	475(D)	MAN	O4-C4-C5	2.63	116.22	109.24
3	A	474(C)	BMA	C6-C5-C4	2.67	119.60	113.02
3	A	474(C)	BMA	O5-C5-C6	2.85	113.51	107.35
3	A	477(F)	MAN	C2-C3-C4	3.10	116.30	111.04
3	A	475(D)	MAN	C1-C2-C3	3.12	113.23	109.54
3	A	476(E)	MAN	C1-O5-C5	3.29	116.43	112.25
3	A	477(F)	MAN	O4-C4-C5	3.30	118.00	109.24
3	A	476(E)	MAN	C1-C2-C3	3.60	113.80	109.54
3	A	475(D)	MAN	O3-C3-C2	3.68	116.64	110.00

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	475(D)	MAN	C1-O5-C5	3.85	117.14	112.25
3	A	478(G)	MAN	C1-O5-C5	4.53	118.00	112.25
3	A	474(C)	BMA	C1-O5-C5	5.85	119.67	112.25
3	A	473(B)	NAG	O3-C3-C2	6.49	121.97	109.11
3	A	477(F)	MAN	C1-O5-C5	9.54	124.35	112.25

There are no chirality outliers.

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	1.36	2 (14%)	15,19,21	1.63	3 (20%)
2	NAG	A	471(A)	1	14,14,15	1.39	3 (21%)	15,19,21	1.54	3 (20%)
2	NAG	A	472(A)	1,3	14,14,15	5.23	7 (50%)	15,19,21	3.97	8 (53%)
5	EQP	A	500	-	18,21,21	2.42	8 (44%)	22,31,31	2.44	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
2	NAG	A	472(A)	1,3	-	0/6/23/26	0/1/1/1
5	EQP	A	500	-	-	0/14/36/36	0/1/1/1

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	500	EQP	P1-O2P	-5.31	1.46	1.54
5	A	500	EQP	P1-O3P	-3.26	1.49	1.54
5	A	500	EQP	O4-C4	-3.17	1.36	1.43
5	A	500	EQP	P1-O1P	-2.39	1.45	1.49
5	A	500	EQP	C3-C4	-2.12	1.49	1.52
2	A	471(A)	NAG	C4-C3	2.00	1.57	1.52
2	A	471(A)	NAG	C4-C5	2.06	1.57	1.53
5	A	500	EQP	P1-C2	2.07	1.85	1.82
2	A	470(A)	NAG	C1-C2	2.23	1.55	1.52
2	A	472(A)	NAG	C4-C3	2.34	1.58	1.52
2	A	471(A)	NAG	C3-C2	3.42	1.60	1.52
2	A	470(A)	NAG	C4-C5	3.81	1.61	1.53
5	A	500	EQP	C6-C5	3.99	1.59	1.53
5	A	500	EQP	O6-C6	4.01	1.50	1.43
2	A	472(A)	NAG	O5-C5	6.27	1.57	1.43
2	A	472(A)	NAG	C1-C2	6.65	1.61	1.52
2	A	472(A)	NAG	C4-C5	6.76	1.67	1.53
2	A	472(A)	NAG	O4-C4	8.09	1.62	1.43
2	A	472(A)	NAG	C3-C2	8.69	1.72	1.52
2	A	472(A)	NAG	O5-C1	10.03	1.60	1.43

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	472(A)	NAG	C3-C4-C5	-7.63	96.89	110.20
5	A	500	EQP	O3P-P1-O1P	-7.43	93.73	113.49
2	A	472(A)	NAG	O3-C3-C4	-5.48	97.99	110.34
5	A	500	EQP	O6-C2-C3	-4.57	104.67	110.65
5	A	500	EQP	C8-C7-C6	-3.87	105.23	113.01
5	A	500	EQP	C3-C4-C5	-2.88	108.27	111.47
2	A	471(A)	NAG	C2-N2-C7	-2.44	119.91	123.04
2	A	470(A)	NAG	O4-C4-C3	-2.43	104.86	110.34
5	A	500	EQP	C9-C8-C7	-2.33	107.01	112.48
5	A	500	EQP	C4-C5-N5	-2.25	105.52	110.41
2	A	471(A)	NAG	C6-C5-C4	2.14	118.30	113.02
2	A	472(A)	NAG	O5-C5-C6	2.34	112.41	107.35
2	A	472(A)	NAG	O6-C6-C5	2.35	119.10	111.33
2	A	470(A)	NAG	O3-C3-C2	2.63	114.33	109.11
2	A	472(A)	NAG	O3-C3-C2	2.67	114.40	109.11
2	A	470(A)	NAG	C1-O5-C5	3.18	116.28	112.25
2	A	471(A)	NAG	O3-C3-C2	3.65	116.35	109.11
2	A	472(A)	NAG	O4-C4-C5	4.92	122.28	109.24

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	472(A)	NAG	C4-C3-C2	5.82	120.27	111.23
2	A	472(A)	NAG	C1-O5-C5	7.91	122.29	112.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	472(A)	NAG	3	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, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	388/388 (100%)	1.98	172 (44%) 0 0	2, 10, 19, 30	122 (31%)

All (172) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	317	TYR	5.7
1	A	347	ASN	5.3
1	A	114	VAL	4.7
1	A	390	PRO	4.6
1	A	280	SER	4.6
1	A	275	HIS	4.5
1	A	348	GLY	4.2
1	A	333	THR	4.1
1	A	342	PRO	4.1
1	A	343	GLY	4.1
1	A	202	ALA	4.1
1	A	440	THR	4.0
1	A	339	ASP	4.0
1	A	365	THR	4.0
1	A	199	ASN	4.0
1	A	345	ASN	4.0
1	A	400	THR	4.0
1	A	325	ASP	3.9
1	A	341	TYR	3.9
1	A	279	CYS	3.9
1	A	393	GLY	3.9
1	A	332	PRO	3.9
1	A	82	ARG	3.8
1	A	298	GLY	3.7
1	A	449	SER	3.7
1	A	295	ASN	3.7
1	A	300	ASN	3.7

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	A	296	TRP	3.7
1	A	315	SER	3.7
1	A	117	THR	3.7
1	A	147	GLY	3.6
1	A	344	ASN	3.6
1	A	414	ALA	3.6
1	A	322	VAL	3.6
1	A	138	THR	3.5
1	A	281	CYS	3.5
1	A	329	PRO	3.4
1	A	318	ILE	3.4
1	A	140	ILE	3.4
1	A	179	TRP	3.3
1	A	464	LYS	3.3
1	A	367	SER	3.3
1	A	374	TYR	3.3
1	A	139	THR	3.3
1	A	246	SER	3.3
1	A	439	TRP	3.2
1	A	310	ALA	3.2
1	A	379	VAL	3.2
1	A	361	TRP	3.2
1	A	346	ASN	3.2
1	A	438	TRP	3.2
1	A	358	VAL	3.1
1	A	251	ALA	3.1
1	A	450	SER	3.1
1	A	462	GLY	3.1
1	A	272	THR	3.1
1	A	380	PRO	3.0
1	A	398	LEU	3.0
1	A	466	GLU	3.0
1	A	366	ILE	3.0
1	A	459	TRP	3.0
1	A	467	TYR	2.9
1	A	301	ARG	2.9
1	A	248	THR	2.9
1	A	405	TYR	2.9
1	A	238	CYS	2.9
1	A	142	GLY	2.9
1	A	171	ASN	2.8
1	A	340	PRO	2.8

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	A	349	VAL	2.8
1	A	395	THR	2.8
1	A	108	ILE	2.8
1	A	219	TRP	2.8
1	A	397	VAL	2.8
1	A	338	ASN	2.8
1	A	423	PHE	2.7
1	A	372	SER	2.7
1	A	316	GLN	2.7
1	A	465	ILE	2.7
1	A	324	THR	2.7
1	A	326	ASN	2.7
1	A	242	PHE	2.7
1	A	200	ASN	2.7
1	A	201	ASN	2.6
1	A	469	LEU	2.6
1	A	213	VAL	2.6
1	A	327	PRO	2.6
1	A	363	GLY	2.6
1	A	291	THR	2.6
1	A	447	MET	2.6
1	A	453	PHE	2.6
1	A	425	VAL	2.6
1	A	352	PHE	2.6
1	A	145	SER	2.6
1	A	149	ILE	2.6
1	A	402	TRP	2.5
1	A	460	PRO	2.5
1	A	276	ILE	2.5
1	A	431	ARG	2.5
1	A	382	ALA	2.5
1	A	203	SER	2.5
1	A	362	LEU	2.5
1	A	323	LEU	2.5
1	A	83	ASP	2.5
1	A	137	GLY	2.5
1	A	320	SER	2.5
1	A	229	SER	2.4
1	A	97	TRP	2.4
1	A	430	GLY	2.4
1	A	113	ASP	2.4
1	A	274	LYS	2.4

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	A	436	LYS	2.4
1	A	245	GLY	2.4
1	A	302	PRO	2.4
1	A	406	SER	2.4
1	A	129	CYS	2.3
1	A	419	TYR	2.3
1	A	375	GLU	2.3
1	A	391	THR	2.3
1	A	328	ARG	2.3
1	A	356	ASP	2.3
1	A	437	VAL	2.3
1	A	451	THR	2.3
1	A	421	ALA	2.3
1	A	446	SER	2.3
1	A	357	GLY	2.3
1	A	373	GLY	2.3
1	A	410	MET	2.3
1	A	433	LYS	2.3
1	A	107	ARG	2.3
1	A	334	VAL	2.3
1	A	392	GLN	2.3
1	A	351	GLY	2.3
1	A	376	MET	2.2
1	A	153	SER	2.2
1	A	319	CYS	2.2
1	A	241	VAL	2.2
1	A	249	GLY	2.2
1	A	162	PRO	2.2
1	A	212	PRO	2.2
1	A	468	PHE	2.2
1	A	226	THR	2.2
1	A	303	VAL	2.2
1	A	178	GLY	2.2
1	A	175	GLU	2.2
1	A	321	PRO	2.2
1	A	369	ALA	2.1
1	A	432	PRO	2.1
1	A	292	CYS	2.1
1	A	270	ALA	2.1
1	A	148	THR	2.1
1	A	194	CYS	2.1
1	A	287	GLU	2.1

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	A	100	TYR	2.1
1	A	195	ILE	2.1
1	A	120	PRO	2.1
1	A	166	PRO	2.1
1	A	407	GLY	2.1
1	A	427	LEU	2.1
1	A	152	ARG	2.0
1	A	210	ARG	2.0
1	A	116	VAL	2.0
1	A	150	HIS	2.0
1	A	233	CYS	2.0
1	A	141	ARG	2.0
1	A	121	TYR	2.0
1	A	278	GLU	2.0
1	A	101	GLY	2.0
1	A	445	VAL	2.0
1	A	455	GLY	2.0
1	A	415	GLU	2.0
1	A	134	LEU	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 6.3 Carbohydrates ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
3	NAG	A	473(B)	14/15	0.47	0.41	2.59	0,0,57,61	6
3	MAN	A	476(E)	11/12	0.67	0.27	-0.90	0,0,56,58	0
3	BMA	A	474(C)	11/12	0.61	0.26	-1.27	0,2,50,52	0
3	MAN	A	477(F)	11/12	0.80	0.24	-2.14	0,0,32,69	0
3	MAN	A	478(G)	11/12	0.53	0.35	-	0,0,67,75	11
3	MAN	A	475(D)	11/12	0.72	0.29	-	0,0,41,56	0

## 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, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	NAG	A	472(A)	14/15	0.65	0.34	1.79	0,0,35,63	8
5	EQP	A	500	21/21	0.73	0.29	-0.09	0,2,28,34	7
4	CA	A	479	1/1	0.70	0.19	-2.01	12,12,12,12	0
2	NAG	A	471(A)	14/15	0.59	0.37	-	0,0,52,98	8
2	NAG	A	470(A)	14/15	0.82	0.25	-	0,0,74,80	5

## 6.5 Other polymers [i](#)

There are no such residues in this entry.