



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 6, 2020 – 11:17 PM BST

PDB ID : 1INF
Title : INFLUENZA VIRUS B/LEE/40 NEURAMINIDASE COMPLEXED WITH
BANA113 INHIBITOR
Authors : Jedrzejewski, M.J.; Luo, M.
Deposited on : 1995-07-07
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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.13.1
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.13.1

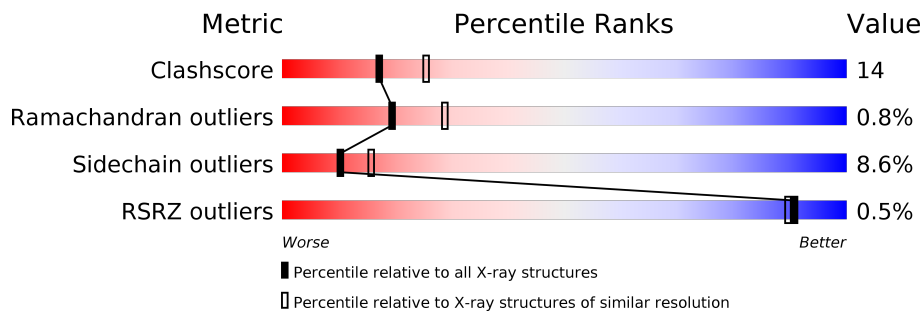
1 Overall quality at a glance

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	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (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 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	390	

2 Entry composition i

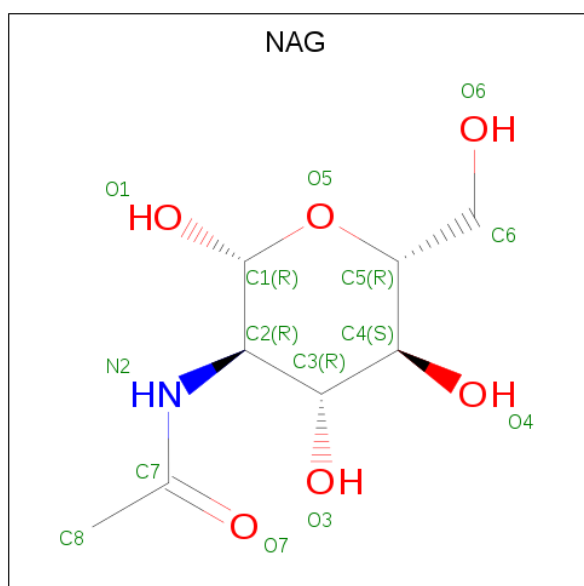
There are 5 unique types of molecules in this entry. The entry contains 4157 atoms, of which 962 are hydrogens and 0 are deuteriums.

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 VIRUS B/LEE/40 NEURAMINIDASE.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	A	390	3732	1907	694	529	574	28	0	0	0

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

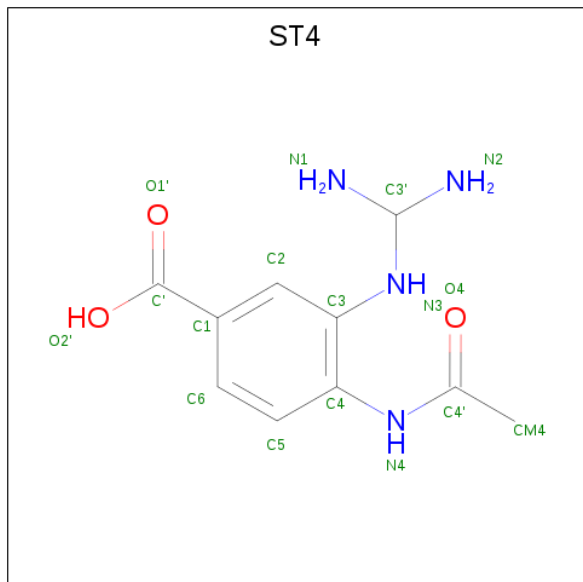


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	H	N	O		
2	A	1	28	8	14	1	5	0	0

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	2	Total	Ca	0	0
			2	2		

- Molecule 4 is 4-(ACETYLAMINO)-3-GUANIDINOBENZOIC ACID (three-letter code: ST4) (formula: $C_{10}H_{14}N_4O_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	H	N	O		
4	A	1	23	10	6	4	3	0	0

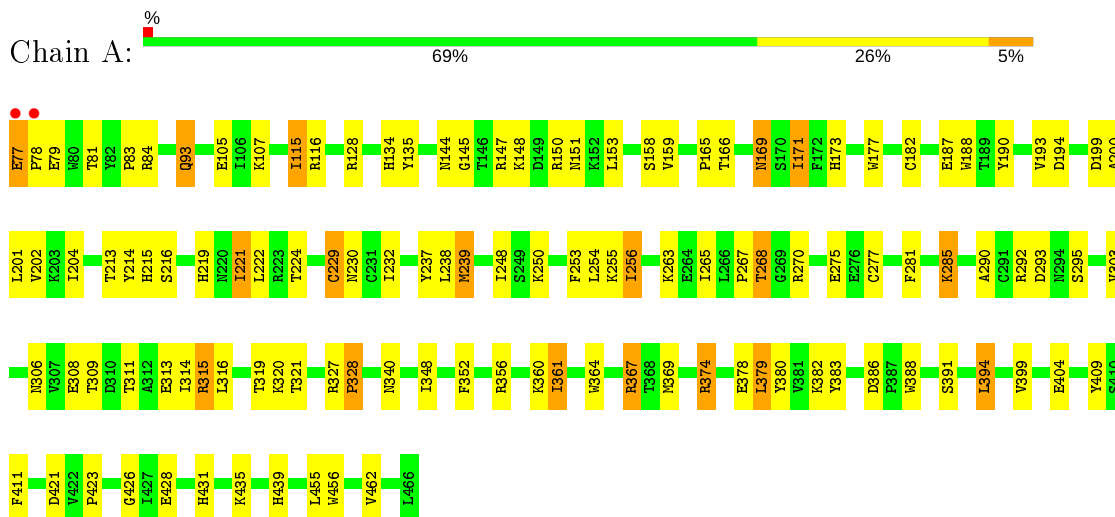
- Molecule 5 is water.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	H	O		
5	A	124	372	248	124	0	0

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 VIRUS B/LEE/40 NEURAMINIDASE



4 Data and refinement statistics

Property	Value	Source
Space group	P 4 21 2	Depositor
Cell constants a, b, c, α , β , γ	124.25Å 124.25Å 71.35Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	6.50 – 2.40 34.29 – 2.21	Depositor EDS
% Data completeness (in resolution range)	(Not available) (6.50-2.40) 62.1 (34.29-2.21)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.02 (at 2.22Å)	Xtrriage
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.159 , (Not available) 0.175 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	15.5	Xtrriage
Anisotropy	0.458	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 64.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.26$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	4157	wwPDB-VP
Average B, all atoms (Å ²)	13.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.82% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ST4, 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	0.55	0/3112	0.86	2/4207 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	290	ALA	N-CA-C	-5.14	97.13	111.00
1	A	293	ASP	N-CA-C	-5.09	97.25	111.00

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	3038	694	2934	82	0
2	A	14	14	13	1	0
3	A	2	0	0	0	0
4	A	17	6	12	0	0
5	A	124	248	0	8	0
All	All	3195	962	2959	82	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 (82) 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:369:MET:HE1	1:A:399:VAL:HG22	1.67	0.77
1:A:166:THR:OG1	1:A:169:ASN:HB2	1.89	0.71
1:A:309:THR:O	1:A:311:THR:HG23	1.91	0.70
1:A:268:THR:HG22	1:A:313:GLU:HG3	1.79	0.65
1:A:230:ASN:HB3	1:A:281:PHE:CE2	2.32	0.63
1:A:148:LYS:HE3	1:A:151:ASN:HD22	1.64	0.62
1:A:107:LYS:HG2	5:A:625:HOH:O	1.99	0.61
1:A:147:ARG:HG2	1:A:147:ARG:HH11	1.64	0.61
1:A:237:TYR:CE2	1:A:255:LYS:HG3	2.37	0.60
1:A:367:ARG:HD2	1:A:380:TYR:CE1	2.36	0.60
1:A:275:GLU:OE2	1:A:292:ARG:HD2	2.02	0.59
1:A:303:VAL:HG22	1:A:314:ILE:HG12	1.85	0.58
1:A:159:VAL:HG11	1:A:165:PRO:HA	1.86	0.58
1:A:147:ARG:HD3	1:A:435:LYS:HG3	1.85	0.58
1:A:201:LEU:HD11	1:A:213:THR:HB	1.88	0.56
1:A:248:ILE:CG2	1:A:250:LYS:HZ2	2.18	0.56
1:A:232:ILE:HB	1:A:281:PHE:CZ	2.41	0.55
1:A:116:ARG:HD2	1:A:428:GLU:OE2	2.07	0.55
1:A:248:ILE:HG21	1:A:250:LYS:HZ2	1.71	0.55
1:A:285:LYS:HG2	1:A:308:GLU:CG	2.37	0.55
1:A:158:SER:O	1:A:171:ILE:HG22	2.07	0.54
1:A:369:MET:HE1	1:A:399:VAL:CG2	2.37	0.54
1:A:193:VAL:HG22	1:A:202:VAL:HG22	1.90	0.54
1:A:201:LEU:HD12	1:A:214:TYR:O	2.09	0.53
1:A:150:ARG:HG2	1:A:177:TRP:CD2	2.44	0.53
1:A:321:THR:HG23	5:A:589:HOH:O	2.09	0.52
1:A:348:ILE:HD12	1:A:374:ARG:CD	2.40	0.52
1:A:265:ILE:O	1:A:267:PRO:HD3	2.09	0.52
1:A:128:ARG:NH1	1:A:158:SER:OG	2.43	0.52
1:A:224:THR:OG1	1:A:238:LEU:HD11	2.09	0.52
1:A:105:GLU:HB3	5:A:625:HOH:O	2.11	0.51
1:A:327:ARG:HD2	5:A:588:HOH:O	2.10	0.51
1:A:215:HIS:HD2	5:A:546:HOH:O	1.92	0.51
1:A:128:ARG:HG3	1:A:188:TRP:CZ2	2.46	0.51
1:A:364:TRP:HE3	1:A:379:LEU:HD22	1.76	0.51
1:A:93:GLN:HE22	1:A:455:LEU:H	1.58	0.50
1:A:275:GLU:HG3	1:A:292:ARG:HB3	1.94	0.50
1:A:348:ILE:HD12	1:A:374:ARG:HD2	1.95	0.49
1:A:360:LYS:HD3	1:A:383:TYR:CD2	2.48	0.49
1:A:77:GLU:HG2	1:A:78:PRO:O	2.13	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:84:ARG:O	1:A:356:ARG:NH1	2.47	0.48
1:A:431:HIS:CE1	1:A:462:VAL:HB	2.48	0.48
1:A:202:VAL:O	1:A:213:THR:HA	2.13	0.48
1:A:159:VAL:HG21	1:A:165:PRO:HG3	1.97	0.47
1:A:215:HIS:CD2	5:A:546:HOH:O	2.65	0.47
1:A:239:MET:SD	1:A:277:CYS:SG	3.13	0.47
1:A:237:TYR:CZ	1:A:255:LYS:HG3	2.49	0.47
1:A:83:PRO:O	2:A:467:NAG:N2	2.48	0.47
1:A:319:THR:HB	5:A:600:HOH:O	2.13	0.47
1:A:423:PRO:HD3	5:A:593:HOH:O	2.14	0.47
1:A:320:LYS:HG2	1:A:391:SER:O	2.15	0.47
1:A:382:LYS:HB2	1:A:394:LEU:HD12	1.96	0.46
1:A:182:CYS:HB3	1:A:229:CYS:O	2.15	0.46
1:A:369:MET:HE2	1:A:378:GLU:CG	2.46	0.45
1:A:316:LEU:HD11	1:A:340:ASN:ND2	2.32	0.45
1:A:177:TRP:NE1	1:A:194:ASP:HA	2.31	0.45
1:A:292:ARG:NH2	1:A:409:TYR:OH	2.49	0.45
1:A:221:ILE:O	1:A:221:ILE:HG22	2.17	0.44
1:A:147:ARG:HG3	1:A:439:HIS:ND1	2.33	0.44
1:A:150:ARG:HG2	1:A:177:TRP:CE3	2.52	0.43
1:A:145:GLY:O	1:A:148:LYS:HG2	2.18	0.43
1:A:360:LYS:HG2	1:A:361:ILE:N	2.33	0.43
1:A:315:ARG:HG3	1:A:388:TRP:CD2	2.54	0.43
1:A:200:ALA:HB3	1:A:222:LEU:HB3	2.01	0.43
1:A:411:PHE:CZ	1:A:426:GLY:HA3	2.53	0.43
1:A:115:ILE:HD13	1:A:115:ILE:H	1.84	0.43
1:A:77:GLU:HB2	1:A:78:PRO:HD2	2.01	0.43
1:A:84:ARG:HD3	1:A:421:ASP:OD1	2.20	0.42
1:A:367:ARG:HD2	1:A:380:TYR:HE1	1.83	0.42
1:A:239:MET:HB2	1:A:253:PHE:CE2	2.55	0.42
1:A:237:TYR:HA	1:A:254:LEU:O	2.19	0.42
1:A:306:ASN:OD1	1:A:308:GLU:HB2	2.20	0.42
1:A:204:ILE:HD13	1:A:256:ILE:HD12	2.02	0.42
1:A:173:HIS:CE1	1:A:190:TYR:CE1	3.08	0.42
1:A:352:PHE:HA	1:A:364:TRP:O	2.19	0.41
1:A:348:ILE:HD12	1:A:374:ARG:HD3	2.02	0.41
1:A:147:ARG:HD2	1:A:435:LYS:HA	2.00	0.41
1:A:216:SER:OG	1:A:219:HIS:HA	2.21	0.41
1:A:316:LEU:HD11	1:A:340:ASN:HD22	1.86	0.41
1:A:263:LYS:HB2	1:A:263:LYS:NZ	2.36	0.40
1:A:386:ASP:OD1	1:A:388:TRP:HB2	2.21	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:314:ILE:C	1:A:315:ARG:HG2	2.42	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	388/390 (100%)	361 (93%)	24 (6%)	3 (1%)	19 29

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	199	ASP
1	A	221	ILE
1	A	328	PRO

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	326/326 (100%)	298 (91%)	28 (9%)	10 16

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	77	GLU
1	A	79	GLU
1	A	81	THR
1	A	93	GLN
1	A	115	ILE
1	A	134	HIS
1	A	135	TYR
1	A	144	ASN
1	A	153	LEU
1	A	169	ASN
1	A	171	ILE
1	A	187	GLU
1	A	229	CYS
1	A	239	MET
1	A	256	ILE
1	A	268	THR
1	A	270	ARG
1	A	285	LYS
1	A	295	SER
1	A	315	ARG
1	A	328	PRO
1	A	361	ILE
1	A	367	ARG
1	A	374	ARG
1	A	379	LEU
1	A	394	LEU
1	A	404	GLU
1	A	456	TRP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	93	GLN
1	A	144	ASN
1	A	169	ASN
1	A	215	HIS
1	A	220	ASN
1	A	230	ASN
1	A	340	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 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	467	1	14,14,15	1.19	2 (14%)	17,19,21	1.73	3 (17%)
4	ST4	A	471	-	14,17,17	2.23	1 (7%)	16,23,23	1.15	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	A	467	1	-	1/6/23/26	0/1/1/1
4	ST4	A	471	-	-	2/6/12/12	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	471	ST4	C1-C'	-8.00	1.39	1.47

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	467	NAG	O5-C5	2.19	1.47	1.43
2	A	467	NAG	O3-C3	-2.05	1.38	1.43

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	467	NAG	C3-C4-C5	3.84	117.08	110.24
2	A	467	NAG	C1-O5-C5	3.44	116.86	112.19
4	A	471	ST4	CM4-C4'-N4	2.90	119.24	114.98
2	A	467	NAG	C2-N2-C7	-2.87	118.82	122.90

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	471	ST4	C4-C3-N3-C3'
4	A	471	ST4	C2-C3-N3-C3'
2	A	467	NAG	C1-C2-N2-C7

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	467	NAG	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	390/390 (100%)	-0.71	2 (0%) 91 89	3, 12, 27, 57	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	77	GLU	4.6
1	A	78	PRO	3.5

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](#)

There are no monosaccharides in this entry.

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	CA	A	501	1/1	0.68	0.11	28,28,28,28	1
2	NAG	A	467	14/15	0.85	0.24	15,15,35,45	0
4	ST4	A	471	17/17	0.94	0.12	15,18,25,31	0
3	CA	A	500	1/1	0.99	0.03	19,19,19,19	0

6.5 Other polymers [i](#)

There are no such residues in this entry.