



wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 31, 2016 – 08:04 PM GMT

PDB ID : 1INH
Title : INFLUENZA A SUBTYPE N2 NEURAMINIDASE COMPLEXED WITH AROMATIC BANA111 INHIBITOR
Authors : Jedrzejewski, M.J.; Luo, M.
Deposited on : 1995-07-07
Resolution : 2.40 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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

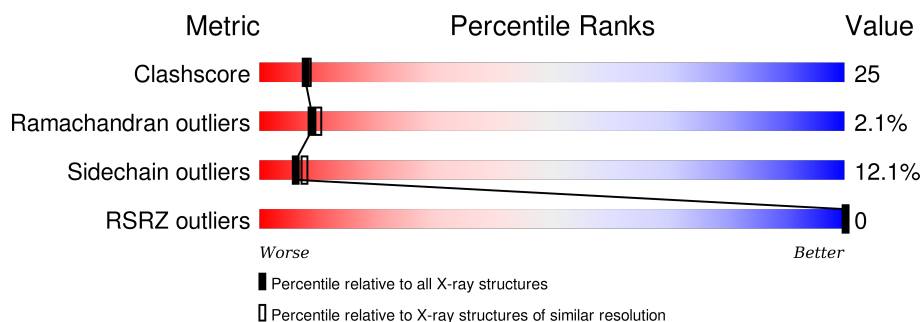
1 Overall quality at a glance

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>50%</div> <div>43%</div> <div>7%</div> </div>
1	B	388	<div> <div>49%</div> <div>44%</div> <div>7%</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
10	ST6	A	471	-	-	-	X
10	ST6	B	489	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	NAG	A	484	-	-	-	X
3	FUL	A	477	-	-	-	X
4	NAG	A	478	-	-	-	X
4	MAN	A	483	-	-	-	X
4	NAG	B	478	-	-	X	X
4	MAN	B	483	-	-	-	X
6	MAN	B	481	-	-	X	X
6	BMA	B	482	X	-	X	X
7	FUC	B	477	X	-	-	X
8	MAN	B	484	-	-	X	X
8	MAN	B	485	-	-	X	X

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 8232 atoms, of which 1796 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			
1	B	388	Total	C	H	N	O	S	0	0	0
			3745	1866	723	545	588	23			

There are 2 discrepancies between the modelled and reference sequences:

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

- Molecule 2 is a polymer of unknown type called SUGAR (2-MER).

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	2	Total	C	H	N	O		0	0
			55	16	27	2	10			
2	A	2	Total	C	H	N	O		0	0
			55	16	27	2	10			
2	B	2	Total	C	H	N	O		0	0
			55	16	27	2	10			
2	B	2	Total	C	H	N	O		0	0
			55	16	27	2	10			

- Molecule 3 is a polymer of unknown type called SUGAR (4-MER).

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	4	Total	C	H	N	O		0	0
			96	28	47	2	19			

- Molecule 4 is a polymer of unknown type called SUGAR (6-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	2	Total	C	H	N	O	0	0
			48	14	23	1	10		
4	B	2	Total	C	H	N	O	0	0
			48	14	23	1	10		

- Molecule 5 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

- Molecule 6 is a polymer of unknown type called SUGAR (3-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	B	3	Total	C	H	O	0	0
			64	18	31	15		

- Molecule 7 is a polymer of unknown type called SUGAR (4-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	B	4	Total	C	H	N	O	0	0
			96	28	47	2	19		

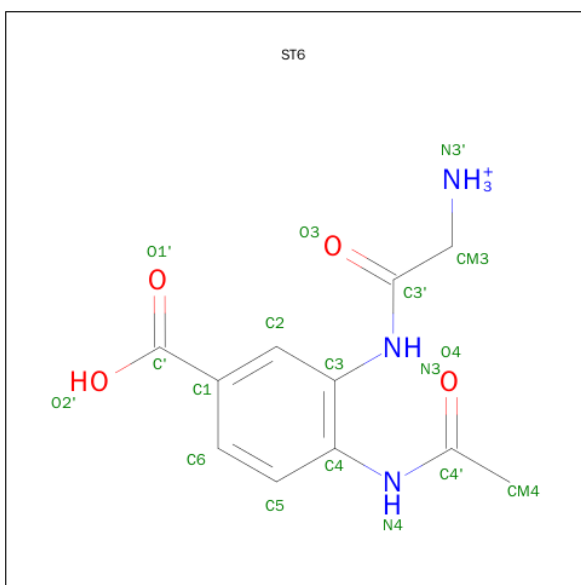
- Molecule 8 is a polymer of unknown type called SUGAR (3-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	B	3	Total	C	H	O	0	0
			64	18	31	15		

- Molecule 9 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	B	1	Total	Ca	0	0
			1	1		
9	A	1	Total	Ca	0	0
			1	1		

- Molecule 10 is 4-(ACETYLAMINO)-3-[(AMINOACETYL)AMINO]BENZOIC ACID (three-letter code: ST6) (formula: C₁₁H₁₄N₃O₄).

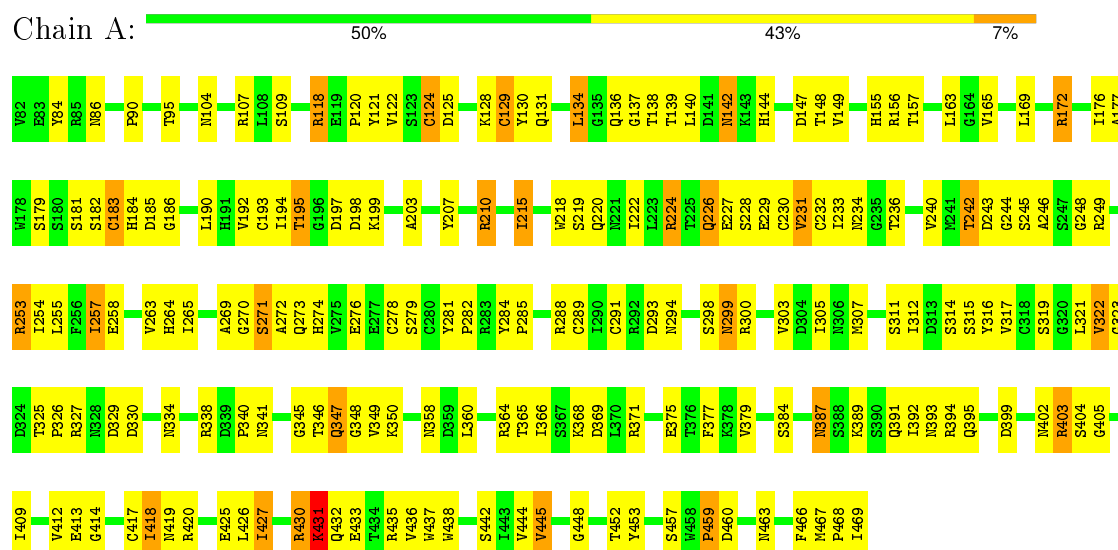


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
10	A	1	Total	C	H	N	O	0	0
			25	11	7	3	4		
10	B	1	Total	C	H	N	O	0	0
			25	11	7	3	4		

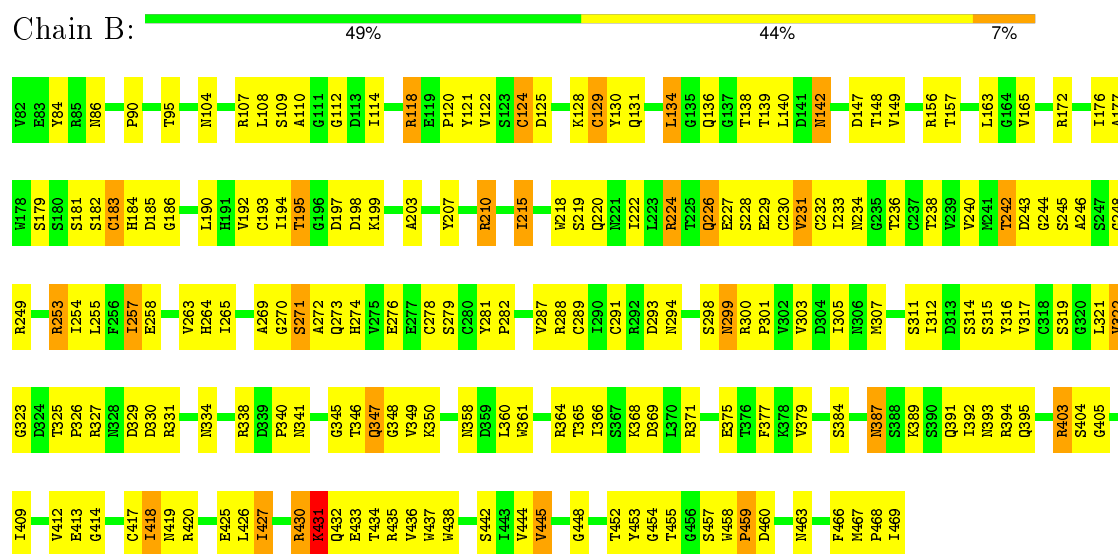
3 Residue-property plots

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 N2 NEURAMINIDASE



• 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	119.74Å 141.02Å 141.78Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	6.50 – 2.40 23.80 – 2.43	Depositor EDS
% Data completeness (in resolution range)	(Not available) (6.50-2.40) 47.3 (23.80-2.43)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.67 (at 2.44Å)	Xtriage
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.184 , (Not available) 0.205 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å ²)	16.0	Xtriage
Anisotropy	1.500	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 72.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.40$, $\langle L^2 \rangle = 0.22$	Xtriage
Outliers	0 of 21384 reflections	Xtriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	8232	wwPDB-VP
Average B, all atoms (Å ²)	12.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.04% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: BMA, NAG, CA, ST6, FUC, FUL, 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	0.63	0/3092	0.90	1/4194 (0.0%)
1	B	0.63	0/3092	0.90	1/4194 (0.0%)
All	All	0.63	0/6184	0.90	2/8388 (0.0%)

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
6	B	1	0
7	B	1	0
All	All	2	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	248	GLY	N-CA-C	-6.25	97.47	113.10
1	B	248	GLY	N-CA-C	-6.25	97.47	113.10

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
6	B	482	BMA	C1
7	B	477	FUC	C1

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3022	723	2851	138	63
1	B	3022	723	2849	172	9
2	A	56	54	50	0	0
2	B	56	54	50	0	0
3	A	49	47	43	1	0
4	A	25	23	18	6	0
4	B	25	23	21	4	4
5	B	28	26	24	4	0
6	B	33	31	22	35	0
7	B	49	47	43	1	0
8	B	33	31	27	2	59
9	A	1	0	0	0	0
9	B	1	0	0	0	0
10	A	18	7	13	1	0
10	B	18	7	13	1	0
All	All	6436	1796	6024	310	72

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 25.

The worst 5 of 310 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:B:391:GLN:OE1	6:B:481:MAN:C4	1.68	1.39
1:B:395:GLN:HG3	6:B:482:BMA:C5	1.62	1.29
1:B:377:PHE:CB	6:B:481:MAN:H3	1.64	1.27
1:B:395:GLN:CG	6:B:482:BMA:H5	1.67	1.25
1:B:453:TYR:OH	6:B:482:BMA:H4	1.32	1.23

The worst 5 of 72 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:B:331:ARG:NH2	1:B:434:THR:CG2[3_654]	0.72	1.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:394:ARG:N	8:B:485:MAN:C1[4_555]	0.73	1.47
1:A:394:ARG:N	8:B:484:MAN:O2[4_555]	0.84	1.36
1:A:393:ASN:CA	8:B:485:MAN:O2[4_555]	0.84	1.36
1:A:393:ASN:CB	8:B:485:MAN:HO3[4_555]	0.26	1.34

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%)	325 (84%)	53 (14%)	8 (2%)	9	10
1	B	386/388 (100%)	325 (84%)	53 (14%)	8 (2%)	9	10
All	All	772/776 (100%)	650 (84%)	106 (14%)	16 (2%)	9	10

5 of 16 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	322	VAL
1	A	431	LYS
1	B	322	VAL
1	B	431	LYS
1	A	345	GLY

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	338/338 (100%)	297 (88%)	41 (12%)	6	8
1	B	338/338 (100%)	297 (88%)	41 (12%)	6	8
All	All	676/676 (100%)	594 (88%)	82 (12%)	6	8

5 of 82 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	431	LYS
1	B	134	LEU
1	B	426	LEU
1	A	442	SER
1	B	122	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 19 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	419	ASN
1	B	104	ASN
1	B	393	ASN
1	A	402	ASN
1	B	402	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 ⓘ

26 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	$\# Z > 2$
2	NAG	A	472	1,2	14,14,15	1.16	1 (7%)	15,19,21	3.15	6 (40%)
2	NAG	A	473	2	14,14,15	2.20	4 (28%)	15,19,21	2.65	5 (33%)
3	NAG	A	474	1,3	14,14,15	1.42	3 (21%)	15,19,21	3.69	8 (53%)
3	NAG	A	475	3	14,14,15	2.86	6 (42%)	15,19,21	2.51	6 (40%)
3	BMA	A	476	3	11,11,12	2.15	4 (36%)	14,15,17	2.80	8 (57%)
3	FUL	A	477	3	10,10,11	3.49	5 (50%)	14,14,16	2.79	6 (42%)
4	NAG	A	478	1,5,4	14,14,15	3.49	6 (42%)	15,19,21	2.75	7 (46%)
4	MAN	A	483	4	11,11,12	3.41	5 (45%)	14,15,17	3.19	3 (21%)
2	NAG	A	484	1,2	14,14,15	1.50	3 (21%)	15,19,21	3.21	5 (33%)
2	NAG	A	485	2	14,14,15	2.21	7 (50%)	15,19,21	2.24	4 (26%)
8	BMA	B	471	8,5	11,11,12	5.22	5 (45%)	14,15,17	3.16	9 (64%)
2	NAG	B	472	1,2	14,14,15	1.16	1 (7%)	15,19,21	3.15	6 (40%)
2	NAG	B	473	2	14,14,15	2.20	4 (28%)	15,19,21	2.65	5 (33%)
7	NAG	B	474	1,7	14,14,15	1.42	3 (21%)	15,19,21	3.69	8 (53%)
7	NAG	B	475	7	14,14,15	2.86	6 (42%)	15,19,21	2.51	6 (40%)
7	BMA	B	476	7	11,11,12	2.15	4 (36%)	14,15,17	2.80	8 (57%)
7	FUC	B	477	7	10,10,11	3.49	5 (50%)	14,14,16	2.79	6 (42%)
4	NAG	B	478	1,5,4	14,14,15	3.49	6 (42%)	15,19,21	2.75	7 (46%)
6	BMA	B	480	5,6	11,11,12	5.22	5 (45%)	14,15,17	3.16	9 (64%)
6	MAN	B	481	6	11,11,12	2.53	4 (36%)	14,15,17	3.66	3 (21%)
6	BMA	B	482	6	11,11,12	2.57	4 (36%)	14,15,17	2.56	6 (42%)
4	MAN	B	483	4	11,11,12	3.41	5 (45%)	14,15,17	3.19	3 (21%)
8	MAN	B	484	8	11,11,12	2.53	4 (36%)	14,15,17	3.66	3 (21%)
8	MAN	B	485	8	11,11,12	2.57	4 (36%)	14,15,17	2.56	6 (42%)
2	NAG	B	486	1,2	14,14,15	1.50	3 (21%)	15,19,21	3.21	5 (33%)
2	NAG	B	487	2	14,14,15	2.21	7 (50%)	15,19,21	2.24	4 (26%)

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	472	1,2	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	A	473	2	-	0/6/23/26	0/1/1/1
3	NAG	A	474	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	475	3	-	0/6/23/26	0/1/1/1
3	BMA	A	476	3	-	0/2/19/22	0/1/1/1
3	FUL	A	477	3	-	0/0/17/20	0/1/1/1
4	NAG	A	478	1,5,4	-	0/6/23/26	0/1/1/1
4	MAN	A	483	4	-	0/2/19/22	0/1/1/1
2	NAG	A	484	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	485	2	-	0/6/23/26	0/1/1/1
8	BMA	B	471	8,5	-	0/2/19/22	1/1/1/1
2	NAG	B	472	1,2	-	0/6/23/26	0/1/1/1
2	NAG	B	473	2	-	0/6/23/26	0/1/1/1
7	NAG	B	474	1,7	-	0/6/23/26	0/1/1/1
7	NAG	B	475	7	-	0/6/23/26	0/1/1/1
7	BMA	B	476	7	-	0/2/19/22	0/1/1/1
7	FUC	B	477	7	1/1/5/5	0/0/17/20	0/1/1/1
4	NAG	B	478	1,5,4	-	0/6/23/26	0/1/1/1
6	BMA	B	480	5,6	-	0/2/19/22	1/1/1/1
6	MAN	B	481	6	-	0/2/19/22	1/1/1/1
6	BMA	B	482	6	1/1/5/5	0/2/19/22	0/1/1/1
4	MAN	B	483	4	-	0/2/19/22	0/1/1/1
8	MAN	B	484	8	-	0/2/19/22	1/1/1/1
8	MAN	B	485	8	-	0/2/19/22	0/1/1/1
2	NAG	B	486	1,2	-	0/6/23/26	0/1/1/1
2	NAG	B	487	2	-	0/6/23/26	0/1/1/1

The worst 5 of 114 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	487	NAG	C1-C2	-2.64	1.48	1.52
2	A	485	NAG	C1-C2	-2.64	1.48	1.52
2	B	486	NAG	O5-C5	-2.47	1.38	1.43
2	A	484	NAG	O5-C5	-2.47	1.38	1.43
4	A	478	NAG	O3-C3	-2.29	1.37	1.43

The worst 5 of 152 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	480	BMA	C3-C4-C5	-6.13	99.51	110.20
8	B	471	BMA	C3-C4-C5	-6.13	99.51	110.20
2	B	472	NAG	O4-C4-C3	-4.90	99.29	110.34
2	A	472	NAG	O4-C4-C3	-4.90	99.29	110.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	486	NAG	O3-C3-C2	-4.30	100.60	109.11

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
6	B	482	BMA	C1
7	B	477	FUC	C1

There are no torsion outliers.

All (4) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	B	480	BMA	C1-C2-C3-C4-C5-O5
8	B	471	BMA	C1-C2-C3-C4-C5-O5
6	B	481	MAN	C1-C2-C3-C4-C5-O5
8	B	484	MAN	C1-C2-C3-C4-C5-O5

14 monomers are involved in 112 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	475	NAG	1	0
3	A	476	BMA	1	0
4	A	478	NAG	5	0
4	A	483	MAN	4	0
8	B	471	BMA	2	0
7	B	475	NAG	1	0
7	B	476	BMA	1	0
4	B	478	NAG	4	4
6	B	480	BMA	3	0
6	B	481	MAN	15	0
6	B	482	BMA	17	0
4	B	483	MAN	3	0
8	B	484	MAN	0	25
8	B	485	MAN	0	34

5.6 Ligand geometry

Of 6 ligands modelled in this entry, 2 are 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
10	ST6	A	471	-	15,18,18	1.50	2 (13%)	20,24,24	1.57	5 (25%)
5	NAG	B	470	8,4	14,14,15	3.73	8 (57%)	15,19,21	4.58	10 (66%)
5	NAG	B	479	4,6	14,14,15	3.73	8 (57%)	15,19,21	4.58	10 (66%)
10	ST6	B	489	-	15,18,18	1.50	2 (13%)	20,24,24	1.57	5 (25%)

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
10	ST6	A	471	-	-	0/10/14/14	0/1/1/1
5	NAG	B	470	8,4	-	0/6/23/26	0/1/1/1
5	NAG	B	479	4,6	-	0/6/23/26	0/1/1/1
10	ST6	B	489	-	-	0/10/14/14	0/1/1/1

The worst 5 of 20 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	A	471	ST6	CM3-C3'	-3.62	1.48	1.52
10	B	489	ST6	CM3-C3'	-3.62	1.48	1.52
10	A	471	ST6	C3-N3	-2.86	1.36	1.41
10	B	489	ST6	C3-N3	-2.86	1.36	1.41
5	B	470	NAG	O5-C5	2.91	1.49	1.43

The worst 5 of 30 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	A	471	ST6	C3'-CM3-N3'	-3.74	105.39	109.87
10	B	489	ST6	C3'-CM3-N3'	-3.74	105.39	109.87
5	B	470	NAG	C4-C3-C2	-2.76	106.93	111.23
5	B	479	NAG	C4-C3-C2	-2.76	106.93	111.23
10	A	471	ST6	C3-N3-C3'	-2.48	116.47	126.55

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	A	471	ST6	1	0
5	B	470	NAG	2	0
5	B	479	NAG	2	0
10	B	489	ST6	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	388/388 (100%)	-0.54	0 100 100	2, 8, 25, 37	0
1	B	388/388 (100%)	-0.49	0 100 100	2, 8, 25, 37	0
All	All	776/776 (100%)	-0.52	0 100 100	2, 8, 26, 37	0

There are no RSRZ outliers to report.

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(Å ²)	Q<0.9
4	MAN	A	483	11/12	0.82	0.55	32.21	15,15,25,30	11
7	FUC	B	477	10/11	0.70	0.44	28.33	15,15,29,30	10
4	MAN	B	483	11/12	0.80	0.45	16.51	15,15,25,30	11
3	FUL	A	477	10/11	0.76	0.37	9.61	15,15,29,30	10
6	BMA	B	482	11/12	0.95	0.21	5.81	2,13,15,15	0
4	NAG	A	478	14/15	0.83	0.18	5.15	13,15,22,26	0
4	NAG	B	478	14/15	0.91	0.18	4.48	13,15,22,26	0
6	MAN	B	481	11/12	0.97	0.24	3.93	2,11,15,15	0
8	MAN	B	484	11/12	0.97	0.27	3.80	2,11,15,15	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
8	MAN	B	485	11/12	0.95	0.20	2.58	2,13,15,15	0
2	NAG	A	484	14/15	0.88	0.20	2.44	15,15,34,36	0
2	NAG	A	472	14/15	0.91	0.18	1.27	15,15,20,21	14
2	NAG	B	472	14/15	0.88	0.17	0.66	15,15,20,21	14
2	NAG	B	486	14/15	0.90	0.14	0.23	15,15,34,36	0
7	NAG	B	475	14/15	0.73	0.32	-	15,15,42,42	14
6	BMA	B	480	11/12	0.73	0.22	-	4,15,19,21	0
2	NAG	B	487	14/15	0.87	0.31	-	15,15,35,36	14
3	BMA	A	476	11/12	0.73	0.49	-	15,15,45,46	11
8	BMA	B	471	11/12	0.74	0.25	-	4,15,19,21	0
7	NAG	B	474	14/15	0.85	0.16	-	15,25,32,35	0
2	NAG	B	473	14/15	0.79	0.31	-	15,15,34,36	14
2	NAG	A	473	14/15	0.80	0.34	-	15,15,34,36	14
2	NAG	A	485	14/15	0.78	0.46	-	15,15,35,36	14
3	NAG	A	475	14/15	0.77	0.21	-	15,15,42,42	14
7	BMA	B	476	11/12	0.64	0.42	-	15,15,45,46	11
3	NAG	A	474	14/15	0.93	0.15	-	15,25,32,35	0

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. 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
10	ST6	A	471	18/18	0.79	0.33	9.68	0,61,64,65	18
10	ST6	B	489	18/18	0.76	0.31	5.29	0,61,64,65	18
9	CA	B	488	1/1	0.92	0.13	-0.20	24,24,24,24	0
9	CA	A	470	1/1	0.98	0.11	-1.33	24,24,24,24	0
5	NAG	B	470	14/15	0.76	0.24	-	2,15,23,25	0
5	NAG	B	479	14/15	0.76	0.25	-	2,15,23,25	0

6.5 Other polymers ⓘ

There are no such residues in this entry.