



# wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 31, 2016 – 08:07 PM GMT

PDB ID : 1IVD  
Title : STRUCTURES OF AROMATIC INHIBITORS OF INFLUENZA VIRUS  
NEURAMINIDASE  
Authors : Jedrzejewski, M.J.; Luo, M.  
Deposited on : 1994-12-12  
Resolution : 1.90 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](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.

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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

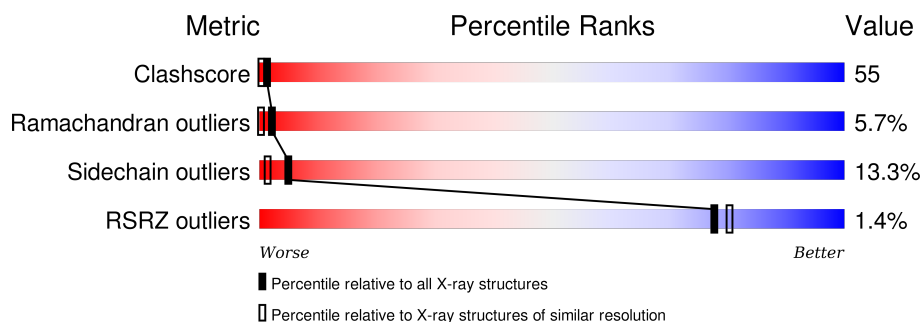
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.90 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	5398 (1.90-1.90)
Ramachandran outliers	100387	5338 (1.90-1.90)
Sidechain outliers	100360	5339 (1.90-1.90)
RSRZ outliers	91569	4766 (1.90-1.90)

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	<div> <div>29%</div> <div>58%</div> <div>12%</div> </div>
1	B	388	<div> <div>28%</div> <div>60%</div> <div>11%</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	B	484	-	-	-	X
4	NAG	A	478	-	-	X	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	MAN	A	483	-	-	X	X
4	NAG	B	478	-	-	-	X
4	MAN	B	483	-	-	-	X
5	FUC	B	477	X	-	-	-

## 2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 8595 atoms, of which 2036 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	6	Total	C	H	N	O	0	0
			139	40	67	2	30		
4	B	6	Total	C	H	N	O	0	0
			139	40	67	2	30		

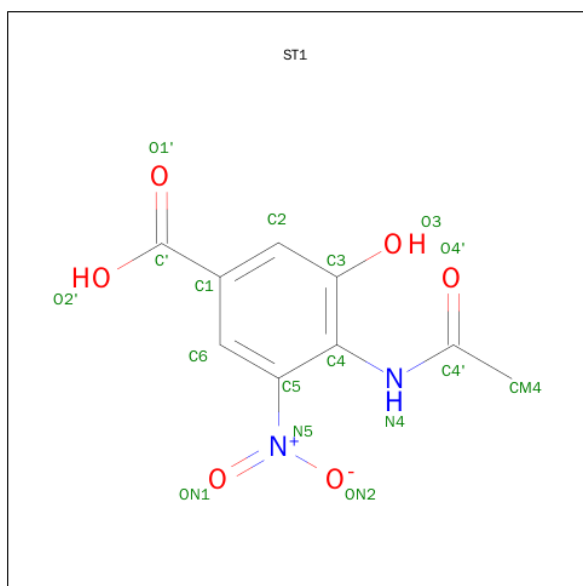
- Molecule 5 is a polymer of unknown type called SUGAR (4-MER).

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

- Molecule 6 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

- Molecule 7 is 4-(ACETYLAMINO)-3-HYDROXY-5-NITROBENZOIC ACID (three-letter code: ST1) (formula: C<sub>9</sub>H<sub>8</sub>N<sub>2</sub>O<sub>6</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	A	1	Total	C	H	N	O	0	0
			19	9	2	2	6		
7	B	1	Total	C	H	N	O	0	0
			19	9	2	2	6		

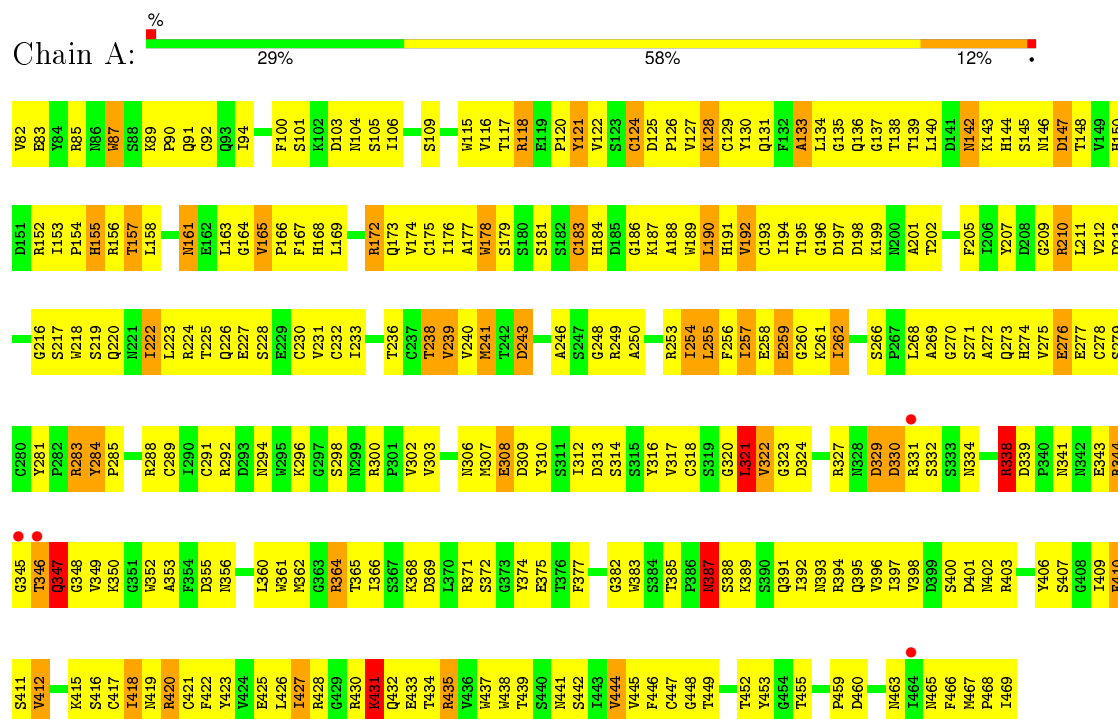
- Molecule 8 is water.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	121	Total	H	O	1	0
			363	242	121		
8	B	4	Total	H	O	0	0
			12	8	4		

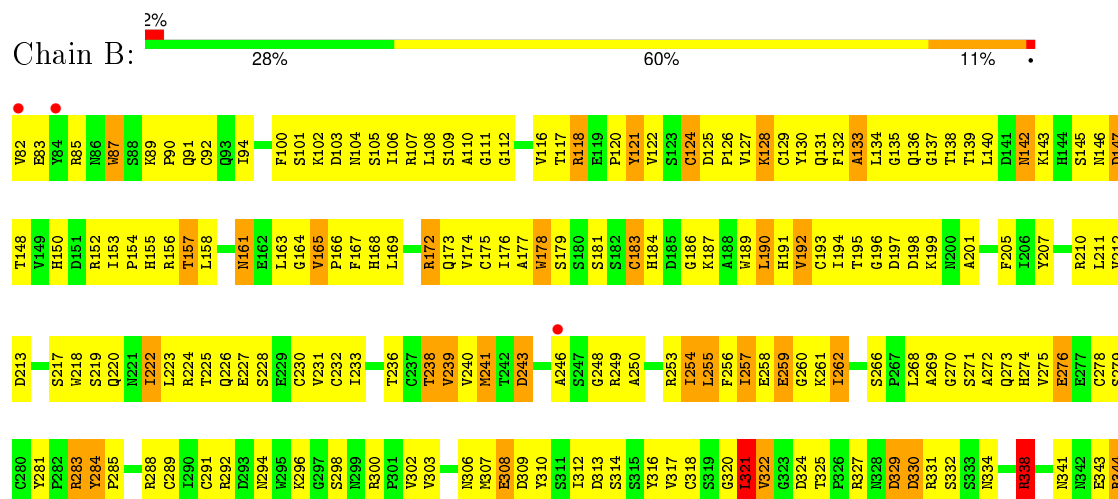
### 3 Residue-property plots

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, $\alpha$ , $\beta$ , $\gamma$	120.42Å 139.83Å 140.07Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	5.00 – 1.90 25.93 – 1.76	Depositor EDS
% Data completeness (in resolution range)	(Not available) (5.00-1.90) 28.4 (25.93-1.76)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.71 (at 1.76Å)	Xtriage
Refinement program	X-PLOR	Depositor
R, $R_{free}$	0.225 , (Not available) 0.287 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	4.1	Xtriage
Anisotropy	3.656	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 65.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.42$ , $\langle L^2 \rangle = 0.24$	Xtriage
Outliers	0 of 33261 reflections	Xtriage
$F_o, F_c$ correlation	0.72	EDS
Total number of atoms	8595	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	7.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.53% 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: BMA, NAG, ST1, CA, 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	0.64	0/3092	0.94	4/4194 (0.1%)
1	B	0.64	0/3092	0.94	4/4194 (0.1%)
All	All	0.64	0/6184	0.94	8/8388 (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
5	B	1	0

There are no bond length outliers.

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	243	ASP	N-CA-C	-5.70	95.60	111.00
1	B	243	ASP	N-CA-C	-5.70	95.60	111.00
1	A	338	ARG	NE-CZ-NH1	5.12	122.86	120.30
1	B	338	ARG	NE-CZ-NH1	5.12	122.86	120.30
1	A	444	VAL	N-CA-C	-5.06	97.35	111.00

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	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	2850	335	5
1	B	3022	723	2850	352	4
2	A	56	54	50	9	0
2	B	56	54	50	8	0
3	A	49	47	42	2	4
4	A	72	67	60	26	5
4	B	72	67	60	3	4
5	B	49	47	42	0	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
7	A	17	2	7	1	0
7	B	17	2	7	1	0
8	A	121	242	0	27	2
8	B	4	8	0	5	0
All	All	6559	2036	6018	678	12

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 55.

The worst 5 of 678 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)
4:A:478:NAG:H61	1:B:455:THR:CG2	1.57	1.35
1:B:107:ARG:CZ	8:B:497:HOH:O	1.78	1.31
8:A:515:HOH:O	1:B:100:PHE:CZ	1.83	1.31
4:A:478:NAG:C6	1:B:455:THR:CG2	2.15	1.24
1:B:205:PHE:HD2	1:B:257:ILE:HD12	1.08	1.17

The worst 5 of 12 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:463:ASN:HD22	4:A:482:MAN:H62[3_654]	1.02	0.58
3:A:477:FUL:H1	4:A:481:MAN:O3[3_654]	1.02	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:477:FUL:H3	4:A:481:MAN:HO3[3_654]	1.04	0.56
1:A:455:THR:OG1	4:B:478:NAG:H1[4_555]	1.42	0.18
1:A:455:THR:CG2	4:B:478:NAG:H61[4_555]	1.43	0.17

## 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%)	294 (76%)	70 (18%)	22 (6%)	2	0
1	B	386/388 (100%)	294 (76%)	70 (18%)	22 (6%)	2	0
All	All	772/776 (100%)	588 (76%)	140 (18%)	44 (6%)	2	0

5 of 44 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	145	SER
1	A	284	TYR
1	A	329	ASP
1	A	346	THR
1	A	347	GLN

### 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%)	293 (87%)	45 (13%)	5	1

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	338/338 (100%)	293 (87%)	45 (13%)	5	1
All	All	676/676 (100%)	586 (87%)	90 (13%)	5	1

5 of 90 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	420	ARG
1	B	142	ASN
1	B	410	PHE
1	A	427	ILE
1	B	83	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 27 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	402	ASN
1	B	131	GLN
1	B	393	ASN
1	A	419	ASN
1	A	161	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 ⓘ

28 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	1.67	3 (21%)	15,19,21	2.56	8 (53%)
2	NAG	A	473	2	14,14,15	1.99	4 (28%)	15,19,21	2.64	3 (20%)
3	NAG	A	474	1,3	14,14,15	1.96	3 (21%)	15,19,21	2.04	5 (33%)
3	NAG	A	475	3	14,14,15	1.77	1 (7%)	15,19,21	3.32	6 (40%)
3	BMA	A	476	3	11,11,12	2.18	5 (45%)	14,15,17	2.43	3 (21%)
3	FUL	A	477	3,4	10,10,11	2.56	4 (40%)	14,14,16	2.79	8 (57%)
4	NAG	A	478	1,4	14,14,15	4.63	9 (64%)	15,19,21	3.51	8 (53%)
4	NAG	A	479	4	14,14,15	1.86	4 (28%)	15,19,21	2.08	6 (40%)
4	BMA	A	480	4	11,11,12	2.42	2 (18%)	14,15,17	3.06	5 (35%)
4	MAN	A	481	3,4	11,11,12	2.89	5 (45%)	14,15,17	2.08	5 (35%)
4	MAN	A	482	4	11,11,12	2.37	3 (27%)	14,15,17	3.04	4 (28%)
4	MAN	A	483	4	11,11,12	3.17	5 (45%)	14,15,17	2.84	8 (57%)
2	NAG	A	484	1,2	14,14,15	2.08	5 (35%)	15,19,21	2.62	5 (33%)
2	NAG	A	485	2	14,14,15	1.44	3 (21%)	15,19,21	3.71	11 (73%)
2	NAG	B	472	1,2	14,14,15	1.67	3 (21%)	15,19,21	2.56	8 (53%)
2	NAG	B	473	2	14,14,15	1.99	4 (28%)	15,19,21	2.64	3 (20%)
5	NAG	B	474	1,5	14,14,15	1.96	3 (21%)	15,19,21	2.04	5 (33%)
5	NAG	B	475	5	14,14,15	1.77	1 (7%)	15,19,21	3.32	6 (40%)
5	BMA	B	476	5	11,11,12	2.18	5 (45%)	14,15,17	2.43	3 (21%)
5	FUC	B	477	5	10,10,11	2.56	4 (40%)	14,14,16	2.79	8 (57%)
4	NAG	B	478	1,4	14,14,15	4.63	9 (64%)	15,19,21	3.51	8 (53%)
4	NAG	B	479	4	14,14,15	1.86	4 (28%)	15,19,21	2.08	6 (40%)
4	BMA	B	480	4	11,11,12	2.42	2 (18%)	14,15,17	3.06	5 (35%)
4	MAN	B	481	4	11,11,12	2.89	5 (45%)	14,15,17	2.08	5 (35%)
4	MAN	B	482	4	11,11,12	2.37	3 (27%)	14,15,17	3.04	4 (28%)
4	MAN	B	483	4	11,11,12	3.17	5 (45%)	14,15,17	2.84	8 (57%)
2	NAG	B	484	1,2	14,14,15	2.08	5 (35%)	15,19,21	2.62	5 (33%)
2	NAG	B	485	2	14,14,15	1.44	3 (21%)	15,19,21	3.71	11 (73%)

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	1/1/1/1
3	FUL	A	477	3,4	-	0/0/17/20	0/1/1/1
4	NAG	A	478	1,4	-	0/6/23/26	0/1/1/1
4	NAG	A	479	4	-	0/6/23/26	0/1/1/1
4	BMA	A	480	4	-	0/2/19/22	0/1/1/1
4	MAN	A	481	3,4	-	0/2/19/22	0/1/1/1
4	MAN	A	482	4	-	0/2/19/22	0/1/1/1
4	MAN	A	483	4	-	0/2/19/22	1/1/1/1
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
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
5	NAG	B	474	1,5	-	0/6/23/26	0/1/1/1
5	NAG	B	475	5	-	0/6/23/26	0/1/1/1
5	BMA	B	476	5	-	0/2/19/22	1/1/1/1
5	FUC	B	477	5	1/1/5/5	0/0/17/20	0/1/1/1
4	NAG	B	478	1,4	-	0/6/23/26	0/1/1/1
4	NAG	B	479	4	-	0/6/23/26	0/1/1/1
4	BMA	B	480	4	-	0/2/19/22	0/1/1/1
4	MAN	B	481	4	-	0/2/19/22	0/1/1/1
4	MAN	B	482	4	-	0/2/19/22	0/1/1/1
4	MAN	B	483	4	-	0/2/19/22	1/1/1/1
2	NAG	B	484	1,2	-	0/6/23/26	0/1/1/1
2	NAG	B	485	2	-	0/6/23/26	0/1/1/1

The worst 5 of 112 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	477	FUC	O2-C2	-3.39	1.35	1.43
3	A	477	FUL	O2-C2	-3.39	1.35	1.43
4	B	481	MAN	O4-C4	-3.24	1.35	1.43
4	A	481	MAN	O4-C4	-3.24	1.35	1.43
4	A	479	NAG	O5-C1	-2.44	1.39	1.43

The worst 5 of 170 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	478	NAG	O7-C7-C8	-7.90	107.56	122.06
4	A	478	NAG	O7-C7-C8	-7.90	107.56	122.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	485	NAG	C2-N2-C7	-7.27	113.70	123.04
2	A	485	NAG	C2-N2-C7	-7.27	113.70	123.04
4	A	483	MAN	C3-C4-C5	-6.01	99.72	110.20

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	B	477	FUC	C1

There are no torsion outliers.

All (4) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	483	MAN	C1-C2-C3-C4-C5-O5
4	B	483	MAN	C1-C2-C3-C4-C5-O5
5	B	476	BMA	C1-C2-C3-C4-C5-O5
3	A	476	BMA	C1-C2-C3-C4-C5-O5

21 monomers are involved in 57 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	472	NAG	5	0
2	A	473	NAG	3	0
3	A	475	NAG	2	0
3	A	476	BMA	2	0
3	A	477	FUL	0	4
4	A	478	NAG	19	0
4	A	479	NAG	3	0
4	A	480	BMA	1	0
4	A	481	MAN	0	4
4	A	482	MAN	0	1
4	A	483	MAN	6	0
2	A	484	NAG	3	0
2	A	485	NAG	5	0
2	B	472	NAG	4	0
2	B	473	NAG	3	0
4	B	478	NAG	1	3
4	B	479	NAG	3	0
4	B	480	BMA	1	0
4	B	483	MAN	1	1
2	B	484	NAG	3	0
2	B	485	NAG	4	0

## 5.6 Ligand geometry

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	$\# Z  > 2$
7	ST1	A	471	-	12,17,17	1.05	1 (8%)	13,24,24	3.02	3 (23%)
7	ST1	B	471	-	12,17,17	1.05	1 (8%)	13,24,24	3.02	3 (23%)

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
7	ST1	A	471	-	-	1/7/12/12	0/1/1/1
7	ST1	B	471	-	-	1/7/12/12	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	B	471	ST1	C4-C5	-2.16	1.38	1.42
7	A	471	ST1	C4-C5	-2.16	1.38	1.42

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	B	471	ST1	C4-N4-C4'	-9.70	110.54	123.33
7	A	471	ST1	C4-N4-C4'	-9.70	110.54	123.33
7	B	471	ST1	C5-C4-N4	-2.10	119.07	123.28
7	A	471	ST1	C5-C4-N4	-2.10	119.07	123.28
7	B	471	ST1	CM4-C4'-N4	3.23	119.56	114.97

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	B	471	ST1	CM4-C4'-N4-C4
7	A	471	ST1	CM4-C4'-N4-C4

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	471	ST1	1	0
7	B	471	ST1	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, 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%)	0.28	4 (1%) 84 86	2, 8, 19, 43	0
1	B	388/388 (100%)	0.28	7 (1%) 71 74	2, 8, 19, 43	0
All	All	776/776 (100%)	0.28	11 (1%) 78 80	2, 8, 20, 43	0

The worst 5 of 11 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	345	GLY	5.2
1	B	345	GLY	3.3
1	A	346	THR	2.9
1	A	464	ILE	2.8
1	B	84	TYR	2.8

### 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, 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
4	MAN	A	483	11/12	0.88	0.34	11.24	0,0,19,20	0
4	MAN	B	483	11/12	0.91	0.28	7.48	0,0,19,20	0
2	NAG	B	484	14/15	0.90	0.18	4.07	0,0,12,16	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
4	NAG	A	478	14/15	0.87	0.19	3.58	0,2,14,17	0
4	NAG	B	478	14/15	0.86	0.18	2.70	0,2,14,17	0
2	NAG	A	484	14/15	0.91	0.17	1.73	0,0,12,16	0
2	NAG	B	472	14/15	0.94	0.16	0.22	0,0,12,16	0
2	NAG	A	472	14/15	0.95	0.13	-0.25	0,0,12,16	0
5	FUC	B	477	10/11	0.85	0.30	-	0,0,17,21	0
5	BMA	B	476	11/12	0.87	0.30	-	0,0,18,25	0
4	BMA	B	480	11/12	0.68	0.29	-	0,0,27,29	0
3	FUL	A	477	10/11	0.90	0.24	-	0,0,17,21	0
4	MAN	B	481	11/12	0.87	0.29	-	0,0,22,25	0
4	NAG	A	479	14/15	0.87	0.33	-	0,0,22,23	0
2	NAG	B	473	14/15	0.91	0.24	-	0,0,21,22	0
5	NAG	B	475	14/15	0.84	0.22	-	0,0,35,38	0
3	NAG	A	474	14/15	0.87	0.16	-	0,6,19,22	0
4	MAN	B	482	11/12	0.79	0.27	-	0,0,26,30	0
3	NAG	A	475	14/15	0.87	0.17	-	0,0,35,38	0
2	NAG	B	485	14/15	0.95	0.16	-	0,0,9,14	0
4	MAN	A	481	11/12	0.90	0.34	-	0,0,22,25	0
3	BMA	A	476	11/12	0.88	0.29	-	0,0,18,25	0
4	BMA	A	480	11/12	0.80	0.33	-	0,0,27,29	0
2	NAG	A	485	14/15	0.94	0.20	-	0,0,9,14	0
4	MAN	A	482	11/12	0.78	0.33	-	0,0,26,30	0
2	NAG	A	473	14/15	0.86	0.17	-	0,0,21,22	0
5	NAG	B	474	14/15	0.85	0.15	-	0,6,19,22	0
4	NAG	B	479	14/15	0.91	0.31	-	0,0,22,23	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, 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
7	ST1	A	471	17/17	0.89	0.14	0.85	0,10,19,22	0
7	ST1	B	471	17/17	0.92	0.12	-0.69	0,10,19,22	0
6	CA	A	470	1/1	1.00	0.03	-1.63	15,15,15,15	0
6	CA	B	470	1/1	0.99	0.05	-1.86	15,15,15,15	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.