



# wwPDB X-ray Structure Validation Summary Report ⓘ

Jul 5, 2017 – 01:29 PM EDT

PDB ID : 1V0Z  
Title : Structure of Neuraminidase from English duck subtype N6  
Authors : Rudino-Pinera, E.; Tunnah, P.; Crennell, S.J.; Webster, R.G.; Laver, W.G.; Garman, E.F.  
Deposited on : unknown  
Resolution : 1.84 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.

---

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

MolProbity	:	4.02b-467
Mogul	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20029824
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
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)	:	rb-20029824

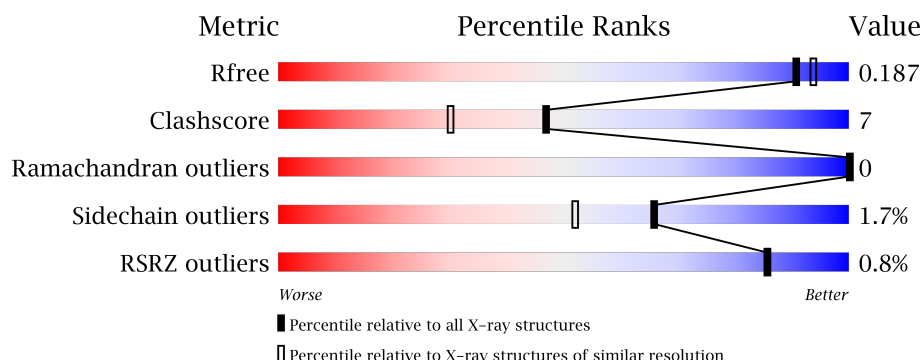
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.84 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))
$R_{free}$	100719	2964 (1.86-1.82)
Clashscore	112137	3197 (1.86-1.82)
Ramachandran outliers	110173	3164 (1.86-1.82)
Sidechain outliers	110143	3165 (1.86-1.82)
RSRZ outliers	101464	2973 (1.86-1.82)

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	389	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 1%, green 98%);"></div> <div style="display: flex; justify-content: space-between; width: 90%; margin: 0 auto;"> <span>1%</span> <span>91%</span> <span>8%</span> </div> </div>
1	B	389	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, orange 1%, yellow 1%, green 98%);"></div> <div style="display: flex; justify-content: space-between; width: 90%; margin: 0 auto;"> <span>1%</span> <span>92%</span> <span>7%</span> </div> </div>
1	C	389	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 2%, orange 1%, yellow 1%, green 96%);"></div> <div style="display: flex; justify-content: space-between; width: 90%; margin: 0 auto;"> <span>2%</span> <span>89%</span> <span>10%</span> </div> </div>
1	D	389	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 1%, green 98%);"></div> <div style="display: flex; justify-content: space-between; width: 90%; margin: 0 auto;"> <span>1%</span> <span>89%</span> <span>10%</span> </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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	CA	C	502	-	-	-	X
2	CA	D	504	-	-	-	X
3	GOL	A	502	-	-	-	X
3	GOL	B	502	-	-	-	X
3	GOL	C	504	-	-	-	X
3	GOL	D	505	-	-	-	X
4	NAG	A	506	-	-	X	X
4	NAG	A	512	-	-	-	X
4	NAG	A	515	-	-	-	X
4	NAG	B	508	-	-	-	X
4	NAG	C	507	-	-	-	X
4	NAG	D	508	-	-	X	X
5	MAN	A	507	-	-	-	X
5	MAN	A	509	-	-	-	X
5	MAN	A	514	-	-	-	X
5	MAN	A	520	-	-	-	X
5	MAN	A	521	-	-	-	X
5	MAN	B	509	-	-	-	X
7	PEG	C	503	-	-	X	X

## 2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 14347 atoms, of which 0 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 NEURAMINIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	389	Total	C	N	O	S	0	0	0
			3009	1875	535	572	27			
1	B	389	Total	C	N	O	S	0	0	0
			3009	1875	535	572	27			
1	C	389	Total	C	N	O	S	0	0	0
			3009	1875	535	572	27			
1	D	389	Total	C	N	O	S	0	0	0
			3009	1875	535	572	27			

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

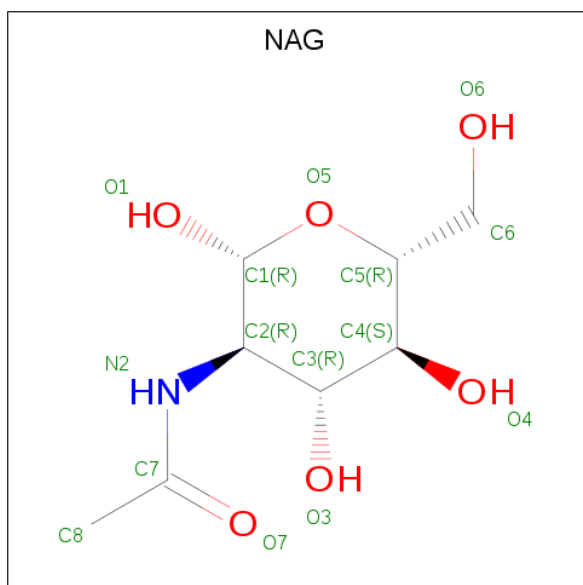
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Ca	0	0
			1	1		
2	A	1	Total	Ca	0	0
			1	1		
2	D	1	Total	Ca	0	0
			1	1		
2	C	1	Total	Ca	0	0
			1	1		

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



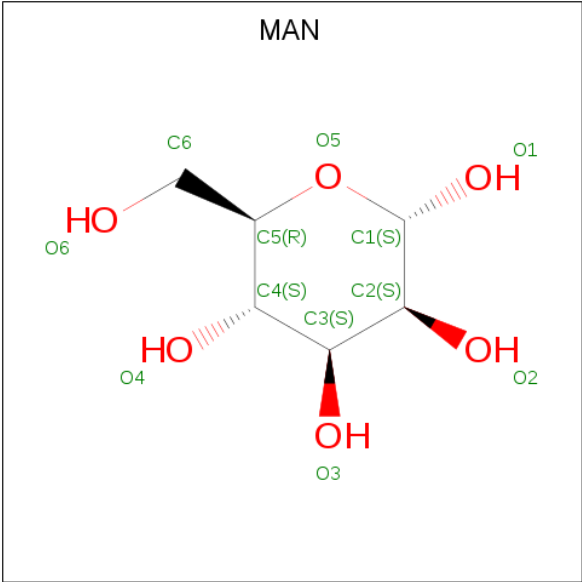
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		
3	C	1	Total	C	O	0	0
			6	3	3		
3	D	1	Total	C	O	0	0
			6	3	3		

- Molecule 4 is N-ACETYL-D-GLUCOSAMINE (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



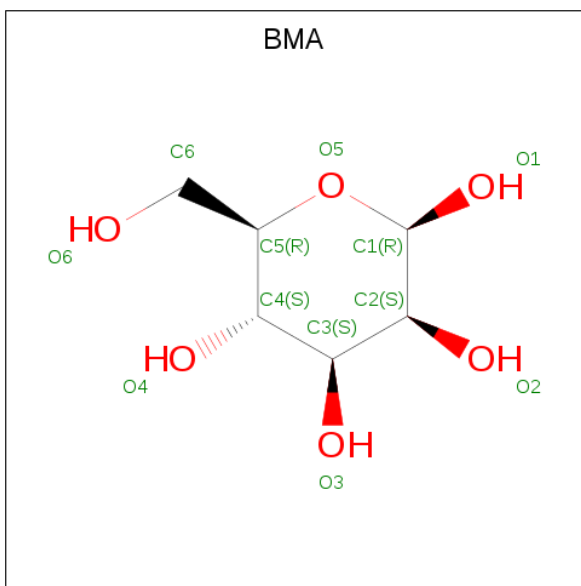
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	B	1	Total	C	N	O	0	0
			14	8	1	5		
4	B	1	Total	C	N	O	0	0
			14	8	1	5		
4	B	1	Total	C	N	O	0	0
			14	8	1	5		
4	C	1	Total	C	N	O	0	0
			14	8	1	5		
4	C	1	Total	C	N	O	0	0
			14	8	1	5		
4	C	1	Total	C	N	O	0	0
			14	8	1	5		
4	C	1	Total	C	N	O	0	0
			14	8	1	5		
4	C	1	Total	C	N	O	0	0
			14	8	1	5		
4	D	1	Total	C	N	O	0	0
			14	8	1	5		
4	D	1	Total	C	N	O	0	0
			14	8	1	5		
4	D	1	Total	C	N	O	0	0
			14	8	1	5		
4	D	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 5 is ALPHA-D-MANNOSE (three-letter code: MAN) (formula: C<sub>6</sub>H<sub>12</sub>O<sub>6</sub>).



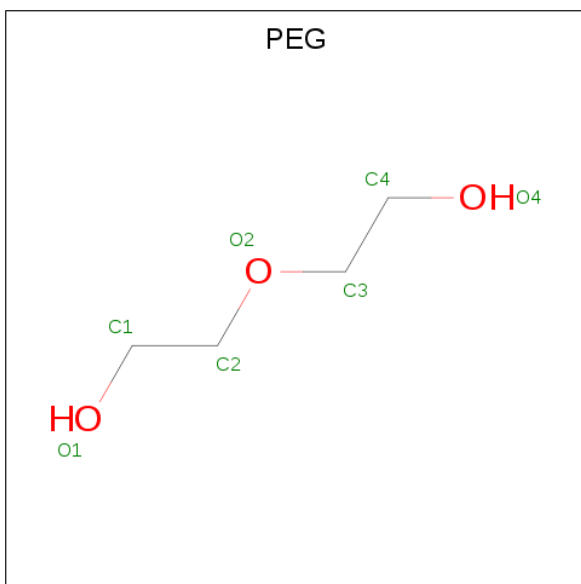
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			11	6	5		
5	A	1	Total	C	O	0	0
			11	6	5		
5	A	1	Total	C	O	0	0
			11	6	5		
5	A	1	Total	C	O	0	0
			11	6	5		
5	A	1	Total	C	O	0	0
			11	6	5		
5	A	1	Total	C	O	0	0
			11	6	5		
5	A	1	Total	C	O	0	0
			11	6	5		
5	B	1	Total	C	O	0	0
			11	6	5		
5	B	1	Total	C	O	0	0
			11	6	5		
5	B	1	Total	C	O	0	0
			11	6	5		
5	D	1	Total	C	O	0	0
			11	6	5		
5	D	1	Total	C	O	0	0
			11	6	5		

- Molecule 6 is BETA-D-MANNOSE (three-letter code: BMA) (formula:  $C_6H_{12}O_6$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			11	6	5		
6	A	1	Total	C	O	0	0
			11	6	5		
6	B	1	Total	C	O	0	0
			11	6	5		
6	D	1	Total	C	O	0	0
			11	6	5		

- Molecule 7 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula:  $C_4H_{10}O_3$ ).





Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	C	1	Total	C	O	0	0
			7	4	3		

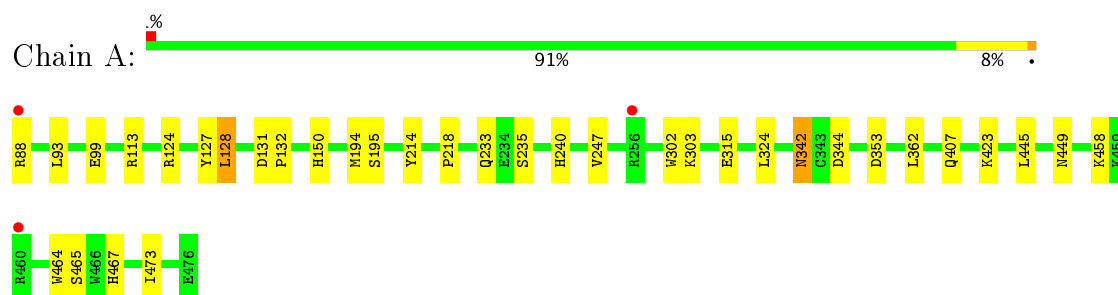
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	460	Total	O	0	0
			460	460		
8	B	442	Total	O	0	0
			442	442		
8	C	454	Total	O	0	0
			454	454		
8	D	442	Total	O	0	0
			442	442		

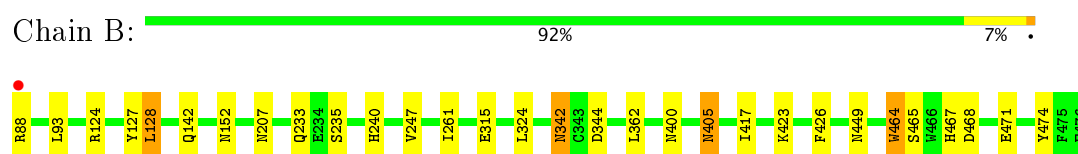
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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.

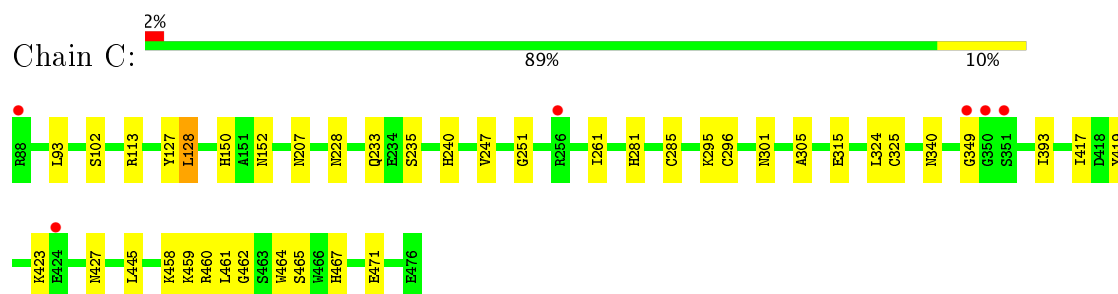
#### • Molecule 1: NEURAMINIDASE



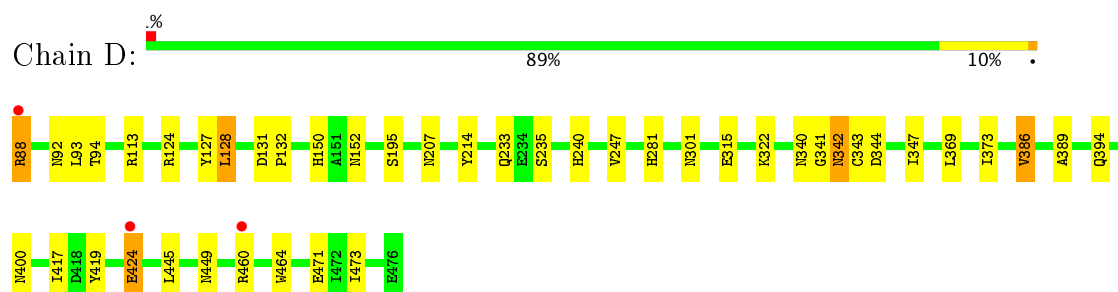
#### • Molecule 1: NEURAMINIDASE



#### • Molecule 1: NEURAMINIDASE



#### • Molecule 1: NEURAMINIDASE



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	106.48Å 73.75Å 106.81Å 90.00° 90.37° 90.00°	Depositor
Resolution (Å)	19.96 – 1.84 19.98 – 1.84	Depositor EDS
% Data completeness (in resolution range)	100.0 (19.96-1.84) 93.2 (19.98-1.84)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.28 (at 1.84Å)	Xtriage
Refinement program	REFMAC 5.0	Depositor
R, $R_{free}$	0.149 , 0.190 0.150 , 0.187	Depositor DCC
$R_{free}$ test set	6696 reflections (5.27%)	DCC
Wilson B-factor (Å <sup>2</sup> )	12.7	Xtriage
Anisotropy	1.044	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.39 , 61.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.006 for l,k,-h 0.016 for h,-k,-l 0.012 for l,-k,h	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	14347	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	15.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.12% 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, 0.333 respectively for untwinned datasets, and 0.375, 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: GOL, BMA, NAG, CA, PEG, 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	0.65	0/3084	0.67	1/4185 (0.0%)
1	B	0.65	1/3084 (0.0%)	0.67	1/4185 (0.0%)
1	C	0.66	0/3084	0.66	1/4185 (0.0%)
1	D	0.65	0/3084	0.69	1/4185 (0.0%)
All	All	0.65	1/12336 (0.0%)	0.67	4/16740 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	464	TRP	CB-CG	-5.11	1.41	1.50

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	128	LEU	CA-CB-CG	7.07	131.57	115.30
1	D	128	LEU	CA-CB-CG	6.70	130.71	115.30
1	B	128	LEU	CA-CB-CG	6.39	129.99	115.30
1	A	128	LEU	CA-CB-CG	6.12	129.38	115.30

There are no chirality outliers.

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	3009	0	2885	26	0
1	B	3009	0	2888	31	0
1	C	3009	0	2888	53	0
1	D	3009	0	2888	50	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	6	0	8	2	0
3	B	6	0	8	1	0
3	C	6	0	8	1	0
3	D	6	0	8	0	0
4	A	112	0	100	12	0
4	B	42	0	38	9	0
4	C	70	0	64	12	0
4	D	56	0	52	16	0
5	A	99	0	89	9	0
5	B	33	0	30	1	0
5	D	22	0	20	4	0
6	A	22	0	16	0	0
6	B	11	0	9	0	0
6	D	11	0	9	3	0
7	C	7	0	10	16	0
8	A	460	0	0	5	0
8	B	442	0	0	1	0
8	C	454	0	0	6	0
8	D	442	0	0	1	0
All	All	14347	0	12018	174	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 7.

The worst 5 of 174 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:D:207:ASN:HD21	4:D:508:NAG:C1	1.03	1.63
1:D:152:ASN:HD21	4:D:507:NAG:C1	1.01	1.55
1:B:152:ASN:HD21	4:B:504:NAG:C1	0.97	1.54
1:C:152:ASN:HD21	4:C:506:NAG:C1	0.92	1.53
1:C:207:ASN:HD21	4:C:507:NAG:C1	0.94	1.52

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	387/389 (100%)	375 (97%)	12 (3%)	0	100	100
1	B	387/389 (100%)	375 (97%)	12 (3%)	0	100	100
1	C	387/389 (100%)	374 (97%)	13 (3%)	0	100	100
1	D	387/389 (100%)	373 (96%)	14 (4%)	0	100	100
All	All	1548/1556 (100%)	1497 (97%)	51 (3%)	0	100	100

There are no Ramachandran outliers to report.

### 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	331/331 (100%)	327 (99%)	4 (1%)	75	67
1	B	331/331 (100%)	325 (98%)	6 (2%)	64	50
1	C	331/331 (100%)	327 (99%)	4 (1%)	75	67
1	D	331/331 (100%)	323 (98%)	8 (2%)	54	37
All	All	1324/1324 (100%)	1302 (98%)	22 (2%)	66	52

5 of 22 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	464	TRP
1	C	445	LEU
1	D	460	ARG

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	C	128	LEU
1	C	324	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 52 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	422	ASN
1	C	207	ASN
1	D	406	ASN
1	B	427	ASN
1	B	467	HIS

### 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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 47 ligands modelled in this entry, 4 are monoatomic - leaving 43 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	$\# Z  > 2$
3	GOL	A	502	-	5,5,5	1.20	0	5,5,5	1.75	1 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	NAG	A	503	1,4	14,14,15	0.64	0	15,19,21	0.93	0
4	NAG	A	504	4	14,14,15	0.55	0	15,19,21	0.85	1 (6%)
4	NAG	A	505	1	14,14,15	0.63	0	15,19,21	0.95	1 (6%)
4	NAG	A	506	-	14,14,15	0.57	0	15,19,21	1.64	2 (13%)
5	MAN	A	507	6	11,11,12	0.57	0	13,15,17	1.55	3 (23%)
5	MAN	A	508	-	11,11,12	0.37	0	13,15,17	1.53	2 (15%)
5	MAN	A	509	-	11,11,12	0.51	0	13,15,17	1.44	2 (15%)
6	BMA	A	510	5,4	11,11,12	0.26	0	13,15,17	1.25	1 (7%)
5	MAN	A	511	6	11,11,12	0.41	0	13,15,17	0.90	0
4	NAG	A	512	6	14,14,15	0.58	0	15,19,21	0.66	0
4	NAG	A	513	-	14,14,15	0.51	0	15,19,21	1.23	1 (6%)
5	MAN	A	514	-	11,11,12	0.43	0	13,15,17	1.64	2 (15%)
4	NAG	A	515	1,4	14,14,15	0.77	0	15,19,21	2.32	5 (33%)
4	NAG	A	516	4,6	14,14,15	0.61	0	15,19,21	1.47	2 (13%)
6	BMA	A	517	5,4	11,11,12	0.56	0	13,15,17	1.05	1 (7%)
5	MAN	A	518	5,6	11,11,12	0.51	0	13,15,17	0.81	0
5	MAN	A	519	5	11,11,12	0.44	0	13,15,17	0.97	1 (7%)
5	MAN	A	520	6	11,11,12	0.40	0	13,15,17	1.39	2 (15%)
5	MAN	A	521	-	11,11,12	0.60	0	13,15,17	1.89	4 (30%)
3	GOL	B	502	-	5,5,5	1.73	1 (20%)	5,5,5	2.05	1 (20%)
4	NAG	B	503	-	14,14,15	0.44	0	15,19,21	1.43	3 (20%)
4	NAG	B	504	-	14,14,15	0.70	0	15,19,21	0.97	1 (6%)
5	MAN	B	505	6	11,11,12	0.43	0	13,15,17	1.12	2 (15%)
5	MAN	B	506	-	11,11,12	0.38	0	13,15,17	1.22	2 (15%)
6	BMA	B	507	5,4	11,11,12	0.42	0	13,15,17	1.21	1 (7%)
4	NAG	B	508	6	14,14,15	0.67	0	15,19,21	2.74	6 (40%)
5	MAN	B	509	-	11,11,12	0.51	0	13,15,17	1.91	3 (23%)
4	NAG	C	501	-	14,14,15	0.53	0	15,19,21	1.32	2 (13%)
7	PEG	C	503	-	6,6,6	0.27	0	5,5,5	6.20	5 (100%)
3	GOL	C	504	-	5,5,5	1.63	1 (20%)	5,5,5	2.03	2 (40%)
4	NAG	C	505	-	14,14,15	0.55	0	15,19,21	1.54	4 (26%)
4	NAG	C	506	-	14,14,15	0.66	0	15,19,21	1.19	1 (6%)
4	NAG	C	507	4	14,14,15	0.61	0	15,19,21	1.58	3 (20%)
4	NAG	C	508	4	14,14,15	0.60	0	15,19,21	0.51	0
4	NAG	D	501	-	14,14,15	0.49	0	15,19,21	1.03	1 (6%)
6	BMA	D	502	5	11,11,12	0.44	0	13,15,17	1.05	1 (7%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	MAN	D	503	6	11,11,12	0.49	0	13,15,17	1.68	2 (15%)
3	GOL	D	505	-	5,5,5	1.39	0	5,5,5	1.81	1 (20%)
4	NAG	D	506	-	14,14,15	0.45	0	15,19,21	1.18	1 (6%)
4	NAG	D	507	-	14,14,15	0.59	0	15,19,21	1.10	1 (6%)
4	NAG	D	508	-	14,14,15	0.62	0	15,19,21	1.80	3 (20%)
5	MAN	D	509	-	11,11,12	0.60	0	13,15,17	1.29	2 (15%)

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	GOL	A	502	-	-	0/4/4/4	0/0/0/0
4	NAG	A	503	1,4	-	0/6/23/26	0/1/1/1
4	NAG	A	504	4	-	0/6/23/26	0/1/1/1
4	NAG	A	505	1	-	0/6/23/26	0/1/1/1
4	NAG	A	506	-	-	0/6/23/26	0/1/1/1
5	MAN	A	507	6	-	0/2/19/22	0/1/1/1
5	MAN	A	508	-	-	0/2/19/22	0/1/1/1
5	MAN	A	509	-	-	0/2/19/22	0/1/1/1
6	BMA	A	510	5,4	-	0/2/19/22	0/1/1/1
5	MAN	A	511	6	-	0/2/19/22	0/1/1/1
4	NAG	A	512	6	-	0/6/23/26	0/1/1/1
4	NAG	A	513	-	-	0/6/23/26	0/1/1/1
5	MAN	A	514	-	-	0/2/19/22	0/1/1/1
4	NAG	A	515	1,4	-	0/6/23/26	0/1/1/1
4	NAG	A	516	4,6	-	0/6/23/26	0/1/1/1
6	BMA	A	517	5,4	-	0/2/19/22	0/1/1/1
5	MAN	A	518	5,6	-	0/2/19/22	0/1/1/1
5	MAN	A	519	5	-	0/2/19/22	0/1/1/1
5	MAN	A	520	6	-	0/2/19/22	0/1/1/1
5	MAN	A	521	-	-	0/2/19/22	0/1/1/1
3	GOL	B	502	-	-	0/4/4/4	0/0/0/0
4	NAG	B	503	-	-	0/6/23/26	0/1/1/1
4	NAG	B	504	-	-	0/6/23/26	0/1/1/1
5	MAN	B	505	6	-	0/2/19/22	0/1/1/1
5	MAN	B	506	-	-	0/2/19/22	0/1/1/1
6	BMA	B	507	5,4	-	0/2/19/22	0/1/1/1
4	NAG	B	508	6	-	0/6/23/26	0/1/1/1
5	MAN	B	509	-	-	0/2/19/22	0/1/1/1

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	C	501	-	-	0/6/23/26	0/1/1/1
7	PEG	C	503	-	-	0/4/4/4	0/0/0/0
3	GOL	C	504	-	-	0/4/4/4	0/0/0/0
4	NAG	C	505	-	-	0/6/23/26	0/1/1/1
4	NAG	C	506	-	-	0/6/23/26	0/1/1/1
4	NAG	C	507	4	-	0/6/23/26	0/1/1/1
4	NAG	C	508	4	-	0/6/23/26	0/1/1/1
4	NAG	D	501	-	-	0/6/23/26	0/1/1/1
6	BMA	D	502	5	-	0/2/19/22	0/1/1/1
5	MAN	D	503	6	-	0/2/19/22	0/1/1/1
3	GOL	D	505	-	-	0/4/4/4	0/0/0/0
4	NAG	D	506	-	-	0/6/23/26	0/1/1/1
4	NAG	D	507	-	-	0/6/23/26	0/1/1/1
4	NAG	D	508	-	-	0/6/23/26	0/1/1/1
5	MAN	D	509	-	-	0/2/19/22	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	504	GOL	O3-C3	2.34	1.52	1.42
3	B	502	GOL	O3-C3	2.70	1.53	1.42

The worst 5 of 79 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	C	503	PEG	C3-O2-C2	-6.15	86.66	113.30
4	A	515	NAG	C3-C4-C5	-6.09	99.49	110.22
4	B	508	NAG	C4-C3-C2	-5.51	102.94	111.02
4	B	508	NAG	O5-C1-C2	-5.03	104.47	111.47
4	A	506	NAG	O5-C1-C2	-4.49	105.23	111.47

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

27 monomers are involved in 79 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	502	GOL	2	0
4	A	506	NAG	9	0
5	A	507	MAN	4	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	508	MAN	2	0
5	A	509	MAN	2	0
4	A	512	NAG	3	0
5	A	514	MAN	2	0
4	A	515	NAG	3	0
5	A	520	MAN	5	0
5	A	521	MAN	3	0
3	B	502	GOL	1	0
4	B	504	NAG	4	0
5	B	505	MAN	1	0
5	B	506	MAN	1	0
4	B	508	NAG	5	0
7	C	503	PEG	16	0
3	C	504	GOL	1	0
4	C	506	NAG	5	0
4	C	507	NAG	4	0
4	C	508	NAG	3	0
4	D	501	NAG	1	0
6	D	502	BMA	3	0
5	D	503	MAN	2	0
4	D	506	NAG	3	0
4	D	507	NAG	4	0
4	D	508	NAG	8	0
5	D	509	MAN	2	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	389/389 (100%)	-0.48	3 (0%) 86 86	7, 12, 20, 31	0
1	B	389/389 (100%)	-0.49	1 (0%) 93 93	7, 12, 18, 37	0
1	C	389/389 (100%)	-0.52	6 (1%) 74 73	7, 11, 19, 33	0
1	D	389/389 (100%)	-0.47	3 (0%) 86 86	7, 12, 18, 33	0
All	All	1556/1556 (100%)	-0.49	13 (0%) 86 86	7, 12, 19, 37	0

The worst 5 of 13 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	88	ARG	4.3
1	C	350	GLY	3.5
1	C	349	GLY	3.2
1	A	88	ARG	3.2
1	C	88	ARG	2.9

### 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 carbohydrates 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. 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	NAG	C	507	14/15	0.86	0.24	12.73	25,29,32,34	0
5	MAN	B	509	11/12	0.74	0.33	12.28	44,47,48,49	0
4	NAG	B	508	14/15	0.69	0.26	11.55	26,35,39,43	0
3	GOL	B	502	6/6	0.67	0.28	9.39	12,25,26,28	0
5	MAN	A	507	11/12	0.90	0.20	7.60	22,24,24,27	0
3	GOL	D	505	6/6	0.73	0.29	7.37	17,29,30,30	0
3	GOL	C	504	6/6	0.76	0.26	7.08	13,26,28,29	0
5	MAN	A	509	11/12	0.85	0.18	6.59	24,27,28,29	0
3	GOL	A	502	6/6	0.69	0.24	6.32	19,29,30,31	0
7	PEG	C	503	7/7	0.67	0.25	6.26	20,24,28,29	0
4	NAG	D	508	14/15	0.82	0.21	6.24	23,26,27,27	0
2	CA	C	502	1/1	0.98	0.17	5.33	19,19,19,19	0
5	MAN	A	520	11/12	0.94	0.14	5.28	14,15,16,19	0
4	NAG	A	515	14/15	0.81	0.32	4.26	26,31,35,38	0
2	CA	D	504	1/1	0.99	0.14	3.74	19,19,19,19	0
5	MAN	A	521	11/12	0.92	0.14	3.65	19,20,21,21	0
5	MAN	A	514	11/12	0.85	0.19	3.00	30,33,36,38	0
4	NAG	A	512	14/15	0.80	0.28	2.32	20,24,27,30	0
4	NAG	A	506	14/15	0.73	0.30	2.01	42,44,45,45	0
2	CA	B	501	1/1	0.99	0.09	1.70	19,19,19,19	0
4	NAG	C	508	14/15	0.81	0.21	1.60	18,24,29,33	0
2	CA	A	501	1/1	0.99	0.14	1.35	20,20,20,20	0
4	NAG	A	516	14/15	0.92	0.15	1.00	14,20,24,25	0
5	MAN	A	518	11/12	0.94	0.13	-	24,25,27,27	0
4	NAG	D	501	14/15	0.41	0.37	-	74,77,77,77	0
4	NAG	A	503	14/15	0.90	0.16	-	20,22,26,32	0
4	NAG	C	501	14/15	0.47	0.49	-	64,67,68,68	0
4	NAG	A	513	14/15	0.15	0.47	-	95,96,97,97	0
6	BMA	A	510	11/12	0.94	0.21	-	21,25,26,31	0
5	MAN	B	505	11/12	0.82	0.26	-	35,37,37,37	0
6	BMA	B	507	11/12	0.85	0.24	-	35,36,37,38	0
5	MAN	A	519	11/12	0.84	0.41	-	38,42,44,44	0
4	NAG	A	505	14/15	0.89	0.16	-	19,22,27,28	0
4	NAG	B	503	14/15	0.32	0.43	-	98,99,99,99	0
4	NAG	B	504	14/15	0.90	0.15	-	16,22,26,29	0
4	NAG	D	507	14/15	0.92	0.15	-	17,22,26,26	0
4	NAG	D	506	14/15	0.50	0.43	-	105,105,106,106	0
5	MAN	D	503	11/12	0.60	0.42	-	45,49,51,51	0
5	MAN	B	506	11/12	0.79	0.29	-	32,33,36,38	0
5	MAN	A	508	11/12	0.81	0.21	-	26,30,35,38	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
6	BMA	D	502	11/12	0.85	0.28	-	32,35,36,40	0
5	MAN	D	509	11/12	0.54	0.39	-	67,68,68,68	0
6	BMA	A	517	11/12	0.94	0.13	-	16,19,19,21	0
4	NAG	C	505	14/15	0.47	0.37	-	62,63,64,64	0
5	MAN	A	511	11/12	0.75	0.44	-	45,48,49,50	0
4	NAG	A	504	14/15	0.68	0.45	-	39,43,45,45	0
4	NAG	C	506	14/15	0.93	0.13	-	15,18,25,26	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.