



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 13, 2018 – 01:30 pm GMT

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 : 2004-03-12  
Resolution : 1.84 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/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 : 1.7.3 (157068), CSD as539be (2018)  
Xtriage (Phenix) : 1.13  
EDS : trunk31020  
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)  
Refmac : 5.8.0158  
CCP4 : 7.0 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk31020

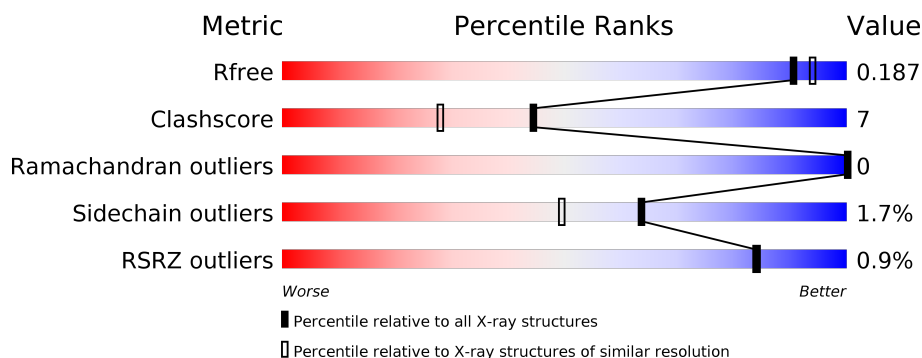
# 1 Overall quality at a glance

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))
$R_{free}$	111664	3313 (1.86-1.82)
Clashscore	122126	3530 (1.86-1.82)
Ramachandran outliers	120053	3495 (1.86-1.82)
Sidechain outliers	120020	3496 (1.86-1.82)
RSRZ outliers	108989	3265 (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: 91%;"></div> <div style="width: 8%;"></div> <div style="width: 1%;"></div> </div> <div>91% 8% .</div>
1	B	389	<div> <div style="width: 92%;"></div> <div style="width: 7%;"></div> <div style="width: 1%;"></div> </div> <div>92% 7% .</div>
1	C	389	<div> <div style="width: 89%;"></div> <div style="width: 10%;"></div> <div style="width: 1%;"></div> </div> <div>89% 10%</div>
1	D	389	<div> <div style="width: 89%;"></div> <div style="width: 10%;"></div> <div style="width: 1%;"></div> </div> <div>89% 10% .</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
4	NAG	A	504	-	-	-	X
4	NAG	A	506	-	-	X	-
4	NAG	A	513	-	-	-	X
4	NAG	B	503	-	-	-	X
4	NAG	C	501	-	-	-	X
4	NAG	D	506	-	-	-	X
4	NAG	D	508	-	-	X	-
5	MAN	A	511	-	-	-	X
5	MAN	D	503	-	-	-	X
7	PEG	C	503	-	-	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).

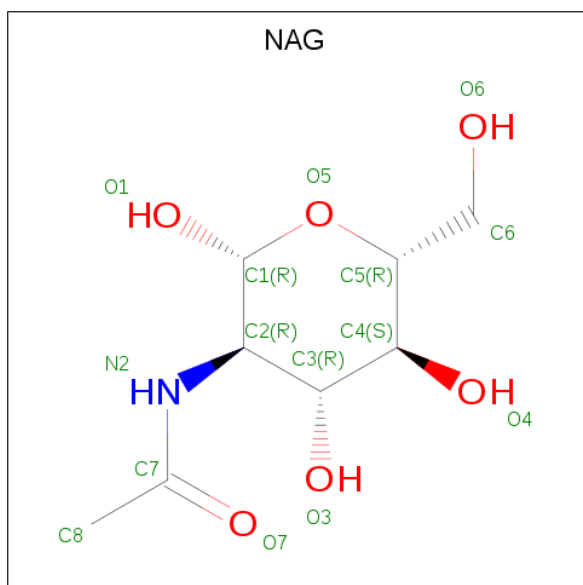
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Ca	0	0
			1	1		
2	A	1	Total	Ca	0	0
			1	1		
2	D	1	Total	Ca	0	0
			1	1		
2	C	1	Total	Ca	0	0
			1	1		

- 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:  $C_8H_{15}NO_6$ ).



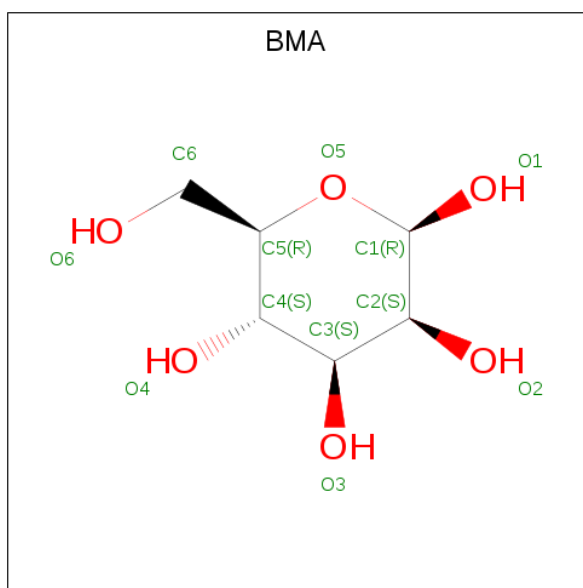
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	B	1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



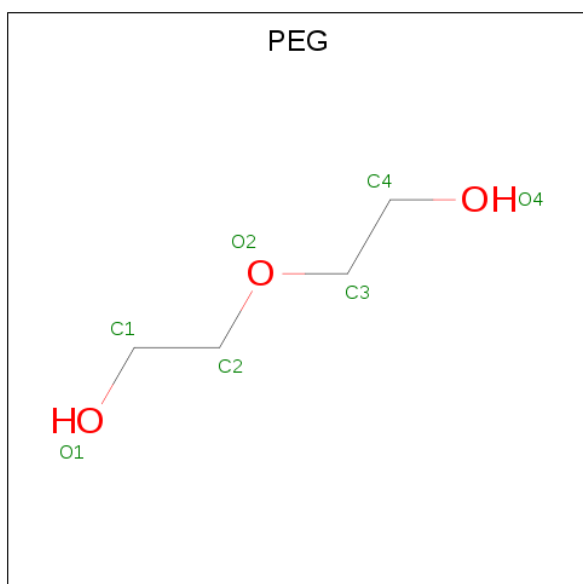
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			11	6	5		
5	A	1	Total	C	O	0	0
			11	6	5		
5	A	1	Total	C	O	0	0
			11	6	5		
5	A	1	Total	C	O	0	0
			11	6	5		
5	A	1	Total	C	O	0	0
			11	6	5		
5	A	1	Total	C	O	0	0
			11	6	5		
5	A	1	Total	C	O	0	0
			11	6	5		
5	B	1	Total	C	O	0	0
			11	6	5		
5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

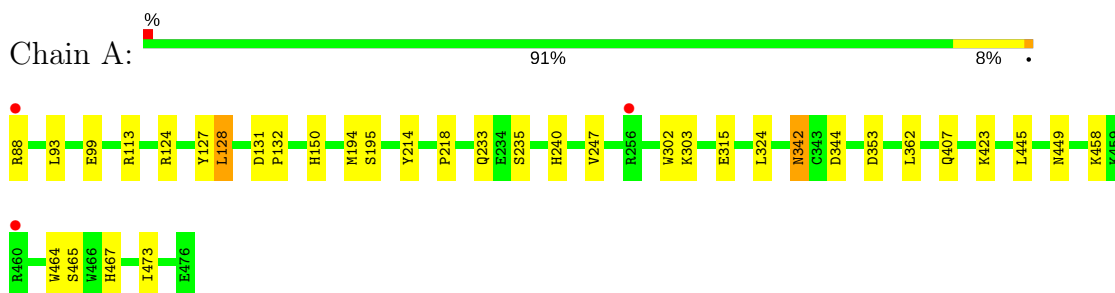
- Molecule 8 is water.

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		

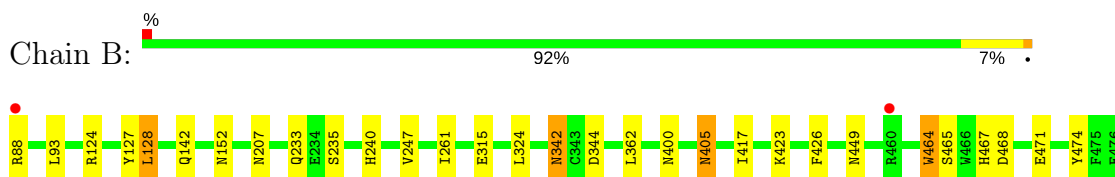
### 3 Residue-property plots

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.

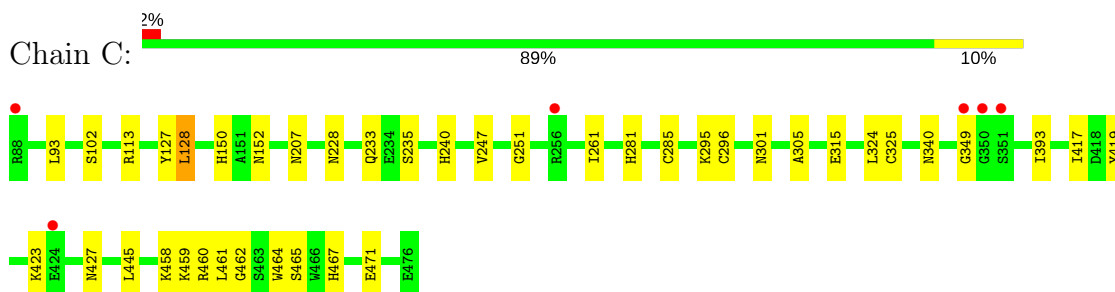
#### • Molecule 1: NEURAMINIDASE



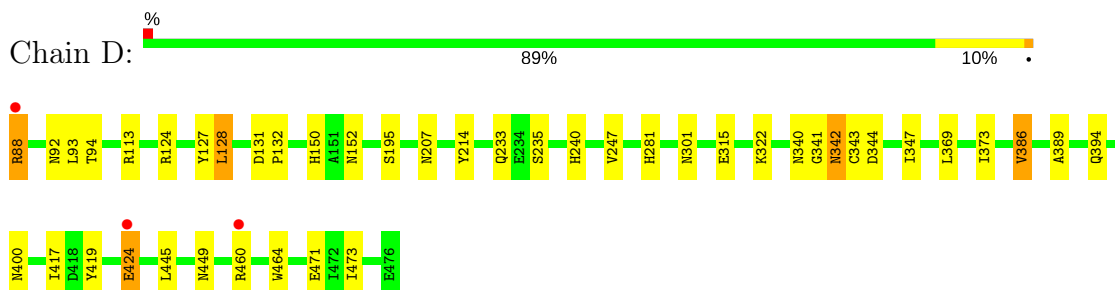
#### • Molecule 1: NEURAMINIDASE



#### • 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 (5.00%)	wwPDB-VP
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.

All (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
1:C:207:ASN:ND2	4:C:507:NAG:C1	1.75	1.44
1:C:152:ASN:ND2	4:C:506:NAG:C1	1.75	1.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:152:ASN:ND2	4:B:504:NAG:C1	1.82	1.39
1:D:152:ASN:ND2	4:D:507:NAG:C1	1.85	1.38
1:D:207:ASN:ND2	4:D:508:NAG:C1	1.89	1.33
1:C:460:ARG:NH1	8:C:603:HOH:O	1.60	1.27
5:A:520:MAN:O3	5:A:521:MAN:C1	1.81	1.27
5:A:507:MAN:O6	5:A:508:MAN:C1	1.85	1.24
5:B:505:MAN:O6	5:B:506:MAN:C1	1.90	1.19
5:A:514:MAN:C1	5:A:520:MAN:O6	1.92	1.17
4:A:506:NAG:O4	4:A:512:NAG:C1	1.94	1.16
5:A:507:MAN:O3	5:A:509:MAN:C1	1.92	1.16
1:D:88:ARG:HH11	1:D:88:ARG:HB2	0.98	1.08
1:D:88:ARG:HH11	1:D:88:ARG:CB	1.73	1.02
1:C:423:LYS:NZ	7:C:503:PEG:H32	1.76	1.00
1:B:93:LEU:H	1:B:240:HIS:HD2	1.12	0.98
1:C:423:LYS:NZ	7:C:503:PEG:C3	2.27	0.98
1:D:88:ARG:NH1	1:D:88:ARG:HB2	1.78	0.97
1:C:93:LEU:H	1:C:240:HIS:HD2	1.13	0.95
4:B:508:NAG:C1	4:D:508:NAG:O4	2.15	0.93
4:A:506:NAG:HO4	4:A:512:NAG:C1	1.78	0.92
1:C:423:LYS:NZ	7:C:503:PEG:H42	1.83	0.92
1:C:150:HIS:HE1	1:D:471:GLU:H	1.13	0.92
1:B:471:GLU:H	1:D:150:HIS:HE1	1.15	0.90
1:D:93:LEU:H	1:D:240:HIS:HD2	1.17	0.90
1:A:150:HIS:HE1	1:C:471:GLU:H	1.17	0.88
1:B:423:LYS:HE2	8:D:812:HOH:O	1.75	0.86
4:C:508:NAG:O4	6:D:502:BMA:C1	2.24	0.84
4:A:506:NAG:C1	1:B:207:ASN:HD21	1.90	0.84
1:B:93:LEU:H	1:B:240:HIS:CD2	1.98	0.82
1:B:468:ASP:O	8:B:602:HOH:O	1.97	0.82
4:B:508:NAG:C1	4:D:508:NAG:C4	2.59	0.81
1:C:423:LYS:NZ	7:C:503:PEG:C4	2.44	0.80
1:A:93:LEU:H	1:A:240:HIS:HD2	1.27	0.80
1:C:423:LYS:HZ1	7:C:503:PEG:C4	1.96	0.78
1:C:423:LYS:HZ1	7:C:503:PEG:C3	1.95	0.78
1:D:386:VAL:HG22	1:D:389:ALA:HB2	1.66	0.77
1:C:423:LYS:HZ1	7:C:503:PEG:H42	1.49	0.76
1:C:233:GLN:HE21	1:C:247:VAL:H	1.30	0.76
4:C:508:NAG:HO4	6:D:502:BMA:C1	2.00	0.74
5:A:520:MAN:C3	5:A:521:MAN:C1	2.66	0.73
1:C:207:ASN:HD21	4:C:507:NAG:C2	1.97	0.72
1:A:93:LEU:H	1:A:240:HIS:CD2	2.09	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:471:GLU:HG3	1:D:473:ILE:HG22	1.72	0.71
1:C:423:LYS:HZ3	7:C:503:PEG:H42	1.54	0.71
1:D:207:ASN:HD21	4:D:508:NAG:C2	2.00	0.69
1:C:423:LYS:HZ3	7:C:503:PEG:H32	1.57	0.68
1:B:233:GLN:HE21	1:B:247:VAL:H	1.42	0.67
1:D:471:GLU:CG	1:D:473:ILE:HG22	2.24	0.67
4:B:508:NAG:C1	4:D:508:NAG:H4	2.24	0.67
4:A:515:NAG:H61	1:C:461:LEU:O	1.95	0.67
1:D:233:GLN:HE21	1:D:247:VAL:H	1.42	0.66
1:A:233:GLN:HE21	1:A:247:VAL:H	1.42	0.66
4:A:506:NAG:C2	1:B:207:ASN:HD21	2.09	0.66
5:A:507:MAN:C3	5:A:509:MAN:C1	2.74	0.65
1:D:93:LEU:H	1:D:240:HIS:CD2	2.07	0.65
1:D:342:ASN:HD22	1:D:344:ASP:H	1.44	0.65
1:C:152:ASN:ND2	4:C:506:NAG:C2	2.60	0.64
1:C:93:LEU:H	1:C:240:HIS:CD2	2.04	0.64
1:B:405:ASN:HD22	1:B:405:ASN:C	2.02	0.63
1:C:150:HIS:CE1	1:D:471:GLU:H	2.06	0.62
1:D:400:ASN:HB3	5:D:503:MAN:H2	1.81	0.62
1:B:247:VAL:HG22	1:B:261:ILE:HD12	1.81	0.62
1:D:342:ASN:ND2	1:D:344:ASP:H	1.98	0.61
4:A:506:NAG:H2	1:B:207:ASN:HD21	1.65	0.61
1:C:465:SER:OG	1:C:467:HIS:HD2	1.84	0.60
1:C:423:LYS:HZ2	7:C:503:PEG:H32	1.64	0.60
1:D:152:ASN:ND2	4:D:507:NAG:C2	2.64	0.60
4:A:506:NAG:H2	1:B:207:ASN:ND2	2.17	0.59
1:C:458:LYS:HE3	8:C:778:HOH:O	2.03	0.59
1:C:152:ASN:ND2	4:C:506:NAG:O5	2.26	0.59
5:A:520:MAN:HO3	5:A:521:MAN:C1	2.12	0.59
1:C:427:ASN:OD1	7:C:503:PEG:H22	2.03	0.59
1:A:473:ILE:HG12	8:A:2607:HOH:O	2.03	0.58
1:D:88:ARG:HH11	1:D:88:ARG:CG	2.15	0.58
1:B:400:ASN:O	4:B:508:NAG:O7	2.21	0.58
1:C:207:ASN:ND2	4:C:507:NAG:C2	2.62	0.58
1:A:324:LEU:HD21	1:A:362:LEU:HD21	1.85	0.57
4:A:515:NAG:O5	1:C:462:GLY:HA2	2.05	0.57
5:A:507:MAN:HO6	5:A:508:MAN:C1	2.12	0.57
4:A:506:NAG:C1	1:B:207:ASN:ND2	2.65	0.56
1:C:152:ASN:CG	4:C:506:NAG:C1	2.68	0.56
3:A:502:GOL:H32	1:C:113:ARG:NH2	2.22	0.55
1:C:423:LYS:HZ3	7:C:503:PEG:C4	2.17	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:471:GLU:H	1:D:150:HIS:CE1	2.07	0.54
1:A:342:ASN:HD22	1:A:344:ASP:H	1.54	0.54
1:A:150:HIS:CE1	1:C:471:GLU:H	2.09	0.54
1:A:465:SER:OG	1:A:467:HIS:HD2	1.91	0.54
1:B:240:HIS:HE1	1:B:315:GLU:OE2	1.90	0.54
1:A:353:ASP:OD2	8:A:2301:HOH:O	0.53	0.53
1:B:127:TYR:CG	1:B:235:SER:HA	2.43	0.53
1:D:373:ILE:HD13	5:D:509:MAN:H61	1.89	0.53
7:C:503:PEG:H12	8:C:629:HOH:O	2.08	0.53
1:A:302:TRP:O	1:A:303:LYS:HE2	2.09	0.53
1:C:233:GLN:NE2	1:C:247:VAL:H	2.04	0.53
1:B:342:ASN:HD22	1:B:344:ASP:H	1.56	0.53
1:A:124:ARG:HA	1:A:449:ASN:ND2	2.24	0.53
1:D:92:ASN:HD21	4:D:506:NAG:C1	2.22	0.52
1:C:240:HIS:HE1	1:C:315:GLU:OE1	1.92	0.52
1:C:102:SER:HB2	1:C:459:LYS:O	2.09	0.52
1:A:467:HIS:H	1:A:467:HIS:CD2	2.28	0.52
1:B:152:ASN:ND2	4:B:504:NAG:C2	2.68	0.52
1:C:295:LYS:HE3	8:C:657:HOH:O	2.09	0.52
3:A:502:GOL:H32	1:C:113:ARG:HH22	1.75	0.51
1:A:93:LEU:N	1:A:240:HIS:HD2	2.02	0.51
1:D:400:ASN:CB	5:D:503:MAN:H2	2.39	0.51
4:A:506:NAG:C2	1:B:207:ASN:ND2	2.74	0.51
1:D:281:HIS:HD2	1:D:301:ASN:H	1.59	0.51
1:D:94:THR:HG21	4:D:506:NAG:H81	1.93	0.51
1:D:240:HIS:HE1	1:D:315:GLU:OE1	1.94	0.50
1:B:342:ASN:ND2	1:B:344:ASP:H	2.09	0.50
1:D:340:ASN:ND2	1:D:394:GLN:HE21	2.08	0.50
1:D:88:ARG:CB	1:D:88:ARG:NH1	2.54	0.50
4:A:506:NAG:C4	4:A:512:NAG:C1	2.89	0.50
1:C:127:TYR:CG	1:C:235:SER:HA	2.47	0.49
1:A:423:LYS:HE3	8:A:2668:HOH:O	2.12	0.49
4:C:508:NAG:C4	6:D:502:BMA:C1	2.91	0.49
1:D:473:ILE:HD13	4:D:501:NAG:H62	1.95	0.49
1:A:240:HIS:HE1	1:A:315:GLU:OE2	1.96	0.49
1:A:88:ARG:HH11	1:A:194:MET:HA	1.77	0.48
1:B:152:ASN:CG	4:B:504:NAG:C1	2.72	0.48
1:A:218:PRO:HG2	7:C:503:PEG:H11	1.94	0.48
1:D:92:ASN:ND2	4:D:506:NAG:C1	2.77	0.48
1:A:131:ASP:HB2	1:A:132:PRO:CD	2.44	0.47
1:D:127:TYR:CG	1:D:235:SER:HA	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:124:ARG:HA	1:B:449:ASN:ND2	2.30	0.47
1:A:407:GLN:NE2	8:A:2303:HOH:O	2.43	0.47
1:D:340:ASN:HD21	1:D:394:GLN:HE21	1.62	0.47
1:A:127:TYR:CG	1:A:235:SER:HA	2.50	0.47
1:C:340:ASN:ND2	8:C:608:HOH:O	2.47	0.46
1:C:281:HIS:HD2	1:C:301:ASN:H	1.63	0.46
1:C:423:LYS:HZ1	7:C:503:PEG:H31	1.78	0.46
1:C:247:VAL:HG22	1:C:261:ILE:HD12	1.97	0.46
4:A:515:NAG:H81	8:A:2634:HOH:O	2.15	0.46
1:D:322:LYS:HB2	1:D:343:CYS:O	2.16	0.45
1:B:324:LEU:HD21	1:B:362:LEU:HD21	1.98	0.45
1:D:373:ILE:HG21	5:D:509:MAN:H61	2.00	0.44
1:C:467:HIS:HE1	8:C:975:HOH:O	2.00	0.44
1:A:99:GLU:HB3	1:A:458:LYS:HD3	2.00	0.43
1:A:113:ARG:NH2	3:B:502:GOL:H32	2.33	0.43
1:A:342:ASN:ND2	1:A:344:ASP:H	2.15	0.43
1:B:465:SER:OG	1:B:467:HIS:HD2	2.01	0.43
1:C:417:ILE:HB	1:C:419:TYR:CZ	2.54	0.42
1:C:228:ASN:HB3	1:C:251:GLY:HA2	2.01	0.42
1:A:195:SER:HB2	1:A:214:TYR:CZ	2.54	0.42
4:B:508:NAG:O7	4:D:508:NAG:H61	2.19	0.42
1:C:427:ASN:OD1	7:C:503:PEG:C2	2.68	0.42
1:D:131:ASP:HB2	1:D:132:PRO:CD	2.49	0.42
1:D:341:GLY:HA2	1:D:347:ILE:HD11	2.01	0.42
1:C:150:HIS:HE1	1:D:471:GLU:N	1.97	0.42
1:C:285:CYS:HB3	1:C:296:CYS:HB3	2.01	0.42
1:D:369:LEU:HG	1:D:386:VAL:HG13	2.02	0.41
1:D:424:GLU:O	1:D:424:GLU:HG2	2.20	0.41
1:C:305:ALA:HB2	1:C:349:GLY:HA2	2.01	0.41
1:D:195:SER:HB2	1:D:214:TYR:CZ	2.55	0.41
1:D:342:ASN:C	1:D:342:ASN:HD22	2.24	0.41
1:D:152:ASN:CG	4:D:507:NAG:C1	2.77	0.41
1:B:471:GLU:HB2	1:B:474:TYR:CD1	2.56	0.41
1:D:417:ILE:HB	1:D:419:TYR:CZ	2.56	0.41
1:A:150:HIS:HE1	1:C:471:GLU:N	1.99	0.41
3:C:504:GOL:H32	1:D:113:ARG:NH2	2.35	0.41
1:D:471:GLU:OE2	1:D:473:ILE:HG22	2.21	0.41
1:D:124:ARG:HA	1:D:449:ASN:ND2	2.35	0.41
5:A:514:MAN:C1	5:A:520:MAN:HO6	2.23	0.40
1:B:342:ASN:C	1:B:342:ASN:HD22	2.24	0.40
1:B:417:ILE:HG21	1:B:426:PHE:HB3	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:467:HIS:CD2	1:B:467:HIS:H	2.38	0.40
1:C:325:CYS:O	1:C:393:ILE:HA	2.21	0.40
1:D:207:ASN:ND2	4:D:508:NAG:C2	2.70	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	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%)	74	64
1	B	331/331 (100%)	325 (98%)	6 (2%)	62	47

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	331/331 (100%)	327 (99%)	4 (1%)	74	64
1	D	331/331 (100%)	323 (98%)	8 (2%)	52	35
All	All	1324/1324 (100%)	1302 (98%)	22 (2%)	63	49

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	128	LEU
1	A	342	ASN
1	A	445	LEU
1	A	464	TRP
1	B	88	ARG
1	B	128	LEU
1	B	142	GLN
1	B	342	ASN
1	B	405	ASN
1	B	464	TRP
1	C	128	LEU
1	C	324	LEU
1	C	445	LEU
1	C	464	TRP
1	D	88	ARG
1	D	128	LEU
1	D	342	ASN
1	D	386	VAL
1	D	424	GLU
1	D	445	LEU
1	D	460	ARG
1	D	464	TRP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (52) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	150	HIS
1	A	233	GLN
1	A	240	HIS
1	A	340	ASN
1	A	342	ASN
1	A	400	ASN
1	A	406	ASN

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Mol	Chain	Res	Type
1	A	407	GLN
1	A	408	ASN
1	A	422	ASN
1	A	427	ASN
1	A	449	ASN
1	A	467	HIS
1	B	142	GLN
1	B	152	ASN
1	B	207	ASN
1	B	233	GLN
1	B	240	HIS
1	B	340	ASN
1	B	342	ASN
1	B	405	ASN
1	B	406	ASN
1	B	408	ASN
1	B	422	ASN
1	B	427	ASN
1	B	449	ASN
1	B	467	HIS
1	C	150	HIS
1	C	152	ASN
1	C	207	ASN
1	C	233	GLN
1	C	240	HIS
1	C	281	HIS
1	C	340	ASN
1	C	394	GLN
1	C	406	ASN
1	C	408	ASN
1	C	422	ASN
1	C	449	ASN
1	C	467	HIS
1	D	150	HIS
1	D	152	ASN
1	D	207	ASN
1	D	233	GLN
1	D	240	HIS
1	D	281	HIS
1	D	340	ASN
1	D	342	ASN
1	D	406	ASN

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Mol	Chain	Res	Type
1	D	422	ASN
1	D	427	ASN
1	D	449	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 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	1.21	0	5,5,5	1.81	1 (20%)
4	NAG	A	503	1,4	14,14,15	0.63	0	17,19,21	0.97	0
4	NAG	A	504	4	14,14,15	0.55	0	17,19,21	0.81	1 (5%)
4	NAG	A	505	1	14,14,15	0.63	0	17,19,21	0.95	1 (5%)
4	NAG	A	506	-	14,14,15	0.56	0	17,19,21	1.76	3 (17%)
5	MAN	A	507	6	11,11,12	0.54	0	15,15,17	1.43	2 (13%)
5	MAN	A	508	-	11,11,12	0.37	0	15,15,17	1.43	2 (13%)
5	MAN	A	509	-	11,11,12	0.51	0	15,15,17	1.38	2 (13%)
6	BMA	A	510	5,4	11,11,12	0.25	0	15,15,17	1.18	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	MAN	A	511	6	11,11,12	0.40	0	15,15,17	0.86	0
4	NAG	A	512	6	14,14,15	0.57	0	17,19,21	0.66	0
4	NAG	A	513	-	14,14,15	0.51	0	17,19,21	1.20	1 (5%)
5	MAN	A	514	-	11,11,12	0.43	0	15,15,17	1.53	2 (13%)
4	NAG	A	515	1,4	14,14,15	0.77	0	17,19,21	2.50	6 (35%)
4	NAG	A	516	4,6	14,14,15	0.61	0	17,19,21	1.39	2 (11%)
6	BMA	A	517	5,4	11,11,12	0.54	0	15,15,17	0.98	1 (6%)
5	MAN	A	518	5,6	11,11,12	0.50	0	15,15,17	0.86	0
5	MAN	A	519	5	11,11,12	0.43	0	15,15,17	0.93	1 (6%)
5	MAN	A	520	6	11,11,12	0.38	0	15,15,17	1.32	2 (13%)
5	MAN	A	521	-	11,11,12	0.58	0	15,15,17	1.77	4 (26%)
3	GOL	B	502	-	5,5,5	1.74	1 (20%)	5,5,5	2.12	3 (60%)
4	NAG	B	503	-	14,14,15	0.44	0	17,19,21	1.40	3 (17%)
4	NAG	B	504	-	14,14,15	0.70	0	17,19,21	1.06	2 (11%)
5	MAN	B	505	6	11,11,12	0.41	0	15,15,17	1.06	1 (6%)
5	MAN	B	506	-	11,11,12	0.37	0	15,15,17	1.13	2 (13%)
6	BMA	B	507	5,4	11,11,12	0.41	0	15,15,17	1.15	1 (6%)
4	NAG	B	508	6	14,14,15	0.66	0	17,19,21	2.61	6 (35%)
5	MAN	B	509	-	11,11,12	0.50	0	15,15,17	1.84	3 (20%)
4	NAG	C	501	-	14,14,15	0.53	0	17,19,21	1.30	2 (11%)
7	PEG	C	503	-	6,6,6	0.27	0	5,5,5	6.19	5 (100%)
3	GOL	C	504	-	5,5,5	1.63	1 (20%)	5,5,5	2.10	2 (40%)
4	NAG	C	505	-	14,14,15	0.54	0	17,19,21	1.54	5 (29%)
4	NAG	C	506	-	14,14,15	0.66	0	17,19,21	1.11	1 (5%)
4	NAG	C	507	4	14,14,15	0.61	0	17,19,21	1.56	3 (17%)
4	NAG	C	508	4	14,14,15	0.59	0	17,19,21	0.64	0
4	NAG	D	501	-	14,14,15	0.49	0	17,19,21	1.02	1 (5%)
6	BMA	D	502	5	11,11,12	0.44	0	15,15,17	1.12	2 (13%)
5	MAN	D	503	6	11,11,12	0.49	0	15,15,17	1.60	2 (13%)
3	GOL	D	505	-	5,5,5	1.39	0	5,5,5	1.86	1 (20%)
4	NAG	D	506	-	14,14,15	0.44	0	17,19,21	1.14	1 (5%)
4	NAG	D	507	-	14,14,15	0.59	0	17,19,21	1.20	2 (11%)
4	NAG	D	508	-	14,14,15	0.62	0	17,19,21	1.72	3 (17%)
5	MAN	D	509	-	11,11,12	0.58	0	15,15,17	1.20	2 (13%)

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
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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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	2.33	1.52	1.42
3	B	502	GOL	O3-C3	2.69	1.53	1.42

All (85) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	C	503	PEG	C3-O2-C2	-6.07	86.66	113.30
4	A	515	NAG	C3-C4-C5	-6.01	99.49	110.24
4	B	508	NAG	C4-C3-C2	-5.51	102.94	111.02
4	B	508	NAG	O5-C1-C2	-5.10	104.47	111.52
4	A	506	NAG	O5-C1-C2	-4.56	105.23	111.52
4	D	508	NAG	C1-O5-C5	-4.26	106.32	112.19
4	C	507	NAG	C1-O5-C5	-4.13	106.50	112.19
4	A	515	NAG	C1-O5-C5	-3.63	107.20	112.19
4	C	501	NAG	O5-C1-C2	-3.60	106.55	111.52
4	D	507	NAG	C1-O5-C5	-3.47	107.42	112.19
5	D	503	MAN	C2-C3-C4	-3.34	105.07	110.87
4	A	513	NAG	O5-C1-C2	-3.31	106.95	111.52
4	B	503	NAG	O5-C1-C2	-3.27	107.01	111.52
4	D	501	NAG	O5-C1-C2	-3.00	107.38	111.52
4	D	506	NAG	O5-C1-C2	-2.96	107.43	111.52
5	A	507	MAN	O6-C6-C5	-2.90	101.18	111.29
4	C	505	NAG	O5-C1-C2	-2.82	107.62	111.52
4	D	508	NAG	O5-C1-C2	-2.65	107.87	111.52
5	A	520	MAN	O6-C6-C5	-2.62	102.14	111.29
5	A	521	MAN	O2-C2-C1	-2.58	103.98	109.17
6	D	502	BMA	C1-C2-C3	-2.51	106.49	109.66
4	C	506	NAG	C1-O5-C5	-2.48	108.78	112.19
4	A	516	NAG	O4-C4-C5	-2.38	103.33	109.31
4	A	506	NAG	C4-C3-C2	-2.37	107.55	111.02
4	A	515	NAG	O6-C6-C5	-2.34	103.13	111.29
4	C	507	NAG	C2-N2-C7	-2.32	119.55	122.94
5	B	505	MAN	O6-C6-C5	-2.28	103.33	111.29
5	A	507	MAN	O5-C1-C2	-2.26	107.26	110.78
4	B	508	NAG	O4-C4-C5	-2.20	103.79	109.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	508	MAN	O2-C2-C1	-2.11	104.93	109.17
4	C	505	NAG	C4-C3-C2	-2.10	107.94	111.02
4	A	505	NAG	O5-C1-C2	-2.08	108.64	111.52
4	A	515	NAG	C1-C2-N2	-2.04	107.01	110.49
4	B	504	NAG	C1-O5-C5	-2.03	109.39	112.19
5	B	506	MAN	O2-C2-C1	-2.02	105.10	109.17
7	C	503	PEG	O4-C4-C3	2.01	123.69	111.91
4	A	504	NAG	C1-O5-C5	2.02	114.97	112.19
3	B	502	GOL	C3-C2-C1	2.03	119.45	111.63
3	B	502	GOL	O1-C1-C2	2.04	120.01	110.11
4	B	504	NAG	O5-C5-C6	2.06	110.40	107.15
6	D	502	BMA	O5-C5-C6	2.10	110.47	107.15
4	C	505	NAG	O5-C5-C4	2.16	116.08	110.83
4	B	508	NAG	C1-O5-C5	2.16	115.16	112.19
5	A	519	MAN	C1-O5-C5	2.20	115.21	112.19
4	C	507	NAG	C3-C4-C5	2.26	114.29	110.24
5	D	509	MAN	C3-C4-C5	2.31	114.36	110.24
4	B	503	NAG	C3-C4-C5	2.42	114.57	110.24
4	D	507	NAG	O5-C5-C6	2.46	111.03	107.15
3	C	504	GOL	O1-C1-C2	2.48	122.13	110.11
4	C	505	NAG	C3-C4-C5	2.56	114.82	110.24
5	A	521	MAN	O5-C1-C2	2.64	114.89	110.78
4	A	515	NAG	O4-C4-C3	2.65	116.53	110.34
5	A	514	MAN	O5-C1-C2	2.68	114.96	110.78
5	A	509	MAN	O5-C1-C2	2.68	114.96	110.78
4	C	501	NAG	C3-C4-C5	2.72	115.10	110.24
5	A	520	MAN	C1-O5-C5	2.73	115.94	112.19
4	C	505	NAG	C1-O5-C5	2.75	115.97	112.19
4	B	503	NAG	C1-O5-C5	2.88	116.15	112.19
5	D	503	MAN	C1-O5-C5	2.92	116.21	112.19
6	A	517	BMA	C1-O5-C5	3.11	116.46	112.19
5	B	509	MAN	C1-C2-C3	3.13	113.62	109.66
5	B	506	MAN	C1-O5-C5	3.13	116.50	112.19
5	A	521	MAN	C1-C2-C3	3.13	113.62	109.66
5	D	509	MAN	C1-C2-C3	3.24	113.75	109.66
3	A	502	GOL	O3-C3-C2	3.29	126.05	110.11
7	C	503	PEG	O2-C3-C4	3.33	125.01	110.10
3	C	504	GOL	O3-C3-C2	3.40	126.59	110.11
6	B	507	BMA	C1-O5-C5	3.40	116.87	112.19
4	A	506	NAG	O5-C5-C6	3.41	112.55	107.15
6	A	510	BMA	C1-O5-C5	3.55	117.08	112.19
5	B	509	MAN	O5-C1-C2	3.58	116.35	110.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	505	GOL	O3-C3-C2	3.61	127.62	110.11
3	B	502	GOL	O3-C3-C2	3.65	127.82	110.11
4	D	508	NAG	C3-C4-C5	3.77	116.99	110.24
5	A	509	MAN	C1-O5-C5	3.82	117.44	112.19
5	A	508	MAN	C1-O5-C5	3.94	117.61	112.19
4	A	516	NAG	C1-O5-C5	4.14	117.88	112.19
4	B	508	NAG	C1-C2-N2	4.23	117.71	110.49
4	B	508	NAG	C2-N2-C7	4.35	129.29	122.94
5	A	521	MAN	C1-O5-C5	4.36	118.19	112.19
5	A	514	MAN	C1-O5-C5	4.66	118.59	112.19
5	B	509	MAN	C1-O5-C5	4.85	118.86	112.19
4	A	515	NAG	O5-C5-C6	5.16	115.32	107.15
7	C	503	PEG	O2-C2-C1	7.67	144.49	110.10
7	C	503	PEG	O1-C1-C2	9.00	164.65	111.91

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
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

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
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	2 (0%) 90 90	7, 12, 18, 37	0
1	C	389/389 (100%)	-0.52	6 (1%) 73 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	14 (0%) 84 84	7, 12, 19, 37	0

All (14) 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
1	D	88	ARG	2.9
1	A	460	ARG	2.8
1	C	256	ARG	2.6
1	D	424	GLU	2.6
1	D	460	ARG	2.2
1	A	256	ARG	2.2
1	C	424	GLU	2.1
1	C	351	SER	2.0
1	B	460	ARG	2.0

### 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 ⓘ

There are no carbohydrates in this entry.

## 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. 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	B-factors(Å <sup>2</sup> )	Q<0.9
4	NAG	A	513	14/15	0.15	0.47	95,96,97,97	0
4	NAG	B	503	14/15	0.31	0.43	98,99,99,99	0
4	NAG	D	501	14/15	0.42	0.37	74,77,77,77	0
4	NAG	C	505	14/15	0.46	0.37	62,63,64,64	0
4	NAG	C	501	14/15	0.47	0.49	64,67,68,68	0
4	NAG	D	506	14/15	0.50	0.43	105,105,106,106	0
5	MAN	D	509	11/12	0.53	0.39	67,68,68,68	0
5	MAN	D	503	11/12	0.60	0.42	45,49,51,51	0
3	GOL	B	502	6/6	0.67	0.29	12,25,26,28	0
7	PEG	C	503	7/7	0.67	0.25	20,24,28,29	0
4	NAG	A	504	14/15	0.68	0.45	39,43,45,45	0
4	NAG	B	508	14/15	0.69	0.26	26,35,39,43	0
3	GOL	A	502	6/6	0.69	0.25	19,29,30,31	0
4	NAG	A	506	14/15	0.73	0.30	42,44,45,45	0
3	GOL	D	505	6/6	0.73	0.29	17,29,30,30	0
5	MAN	B	509	11/12	0.74	0.33	44,47,48,49	0
5	MAN	A	511	11/12	0.75	0.44	45,48,49,50	0
3	GOL	C	504	6/6	0.76	0.26	13,26,28,29	0
5	MAN	B	506	11/12	0.79	0.29	32,33,36,38	0
4	NAG	A	512	14/15	0.80	0.28	20,24,27,30	0
4	NAG	A	515	14/15	0.81	0.32	26,31,35,38	0
5	MAN	A	508	11/12	0.81	0.20	26,30,35,38	0
4	NAG	C	508	14/15	0.81	0.21	18,24,29,33	0
4	NAG	D	508	14/15	0.82	0.21	23,26,27,27	0
5	MAN	B	505	11/12	0.82	0.26	35,37,37,37	0
5	MAN	A	519	11/12	0.84	0.41	38,42,44,44	0
6	BMA	B	507	11/12	0.85	0.24	35,36,37,38	0
5	MAN	A	514	11/12	0.85	0.19	30,33,36,38	0
5	MAN	A	509	11/12	0.85	0.18	24,27,28,29	0
6	BMA	D	502	11/12	0.85	0.28	32,35,36,40	0
4	NAG	C	507	14/15	0.86	0.24	25,29,32,34	0
4	NAG	A	505	14/15	0.89	0.16	19,22,27,28	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
5	MAN	A	507	11/12	0.90	0.20	22,24,24,27	0
4	NAG	A	503	14/15	0.90	0.16	20,22,26,32	0
4	NAG	B	504	14/15	0.90	0.15	16,22,26,29	0
5	MAN	A	521	11/12	0.91	0.14	19,20,21,21	0
4	NAG	D	507	14/15	0.92	0.15	17,22,26,26	0
4	NAG	A	516	14/15	0.92	0.15	14,20,24,25	0
4	NAG	C	506	14/15	0.93	0.13	15,18,25,26	0
5	MAN	A	520	11/12	0.94	0.14	14,15,16,19	0
5	MAN	A	518	11/12	0.94	0.13	24,25,27,27	0
6	BMA	A	517	11/12	0.94	0.13	16,19,19,21	0
6	BMA	A	510	11/12	0.94	0.21	21,25,26,31	0
2	CA	C	502	1/1	0.98	0.17	19,19,19,19	0
2	CA	D	504	1/1	0.99	0.14	19,19,19,19	0
2	CA	A	501	1/1	0.99	0.14	20,20,20,20	0
2	CA	B	501	1/1	0.99	0.09	19,19,19,19	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.