



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 09:08 PM GMT

PDB ID : 1NMC  
Title : COMPLEX BETWEEN NC10 ANTI-INFLUENZA VIRUS NEURAMINIDASE SINGLE CHAIN ANTIBODY WITH A 15 RESIDUE LINKER AND INFLUENZA VIRUS NEURAMINIDASE  
Authors : Malby, R.L.; McCoy, A.J.; Kortt, A.A.; Hudson, P.J.; Colman, P.M.  
Deposited on : 1997-12-21  
Resolution : 2.50 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  
<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

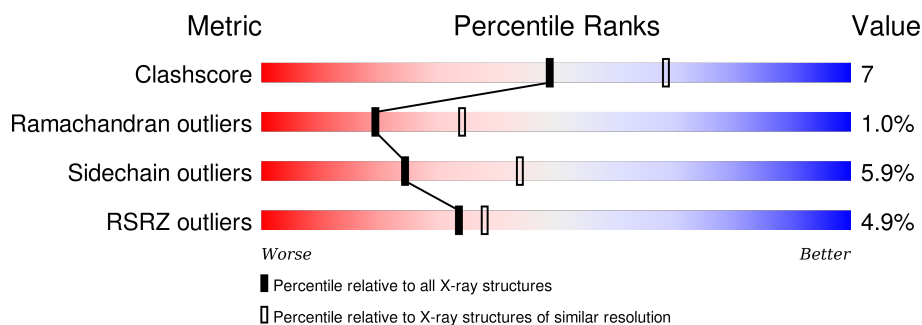
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.50 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	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)
RSRZ outliers	91569	3562 (2.50-2.50)

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>2%</div> <div>87%</div> <div>11%</div> <div>.</div> </div>
1	N	388	<div> <div>%</div> <div>88%</div> <div>10%</div> <div>.</div> </div>
2	B	122	<div> <div>2%</div> <div>75%</div> <div>19%</div> <div>6%</div> </div>
2	H	122	<div> <div>2%</div> <div>75%</div> <div>19%</div> <div>6%</div> </div>
3	C	109	<div> <div>19%</div> <div>71%</div> <div>28%</div> <div>.</div> </div>
3	L	109	<div> <div>22%</div> <div>71%</div> <div>28%</div> <div>.</div> </div>

## 2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 10138 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	N	388	Total	C	N	O	S	0	0	0
			3067	1914	538	592	23			
1	A	388	Total	C	N	O	S	0	0	0
			3067	1914	538	592	23			

- Molecule 2 is a protein called SINGLE CHAIN ANTIBODY.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	122	Total	C	N	O	S	0	0	0
			943	591	155	192	5			
2	B	122	Total	C	N	O	S	0	0	0
			943	591	155	192	5			

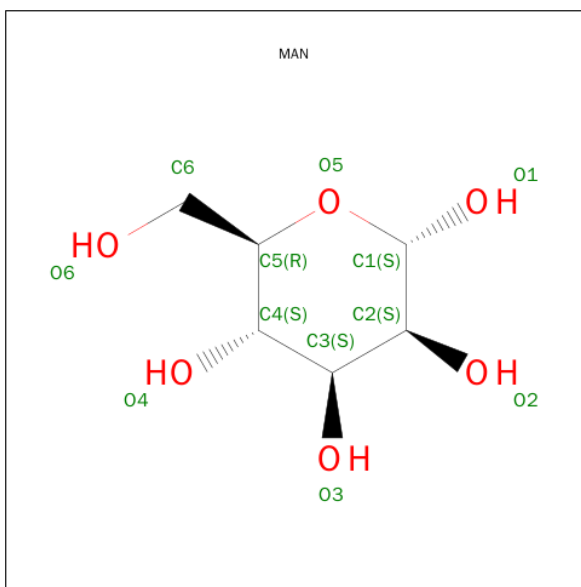
- Molecule 3 is a protein called SINGLE CHAIN ANTIBODY.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	L	109	Total	C	N	O	S	0	0	0
			857	535	138	182	2			
3	C	109	Total	C	N	O	S	0	0	0
			857	535	138	182	2			

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

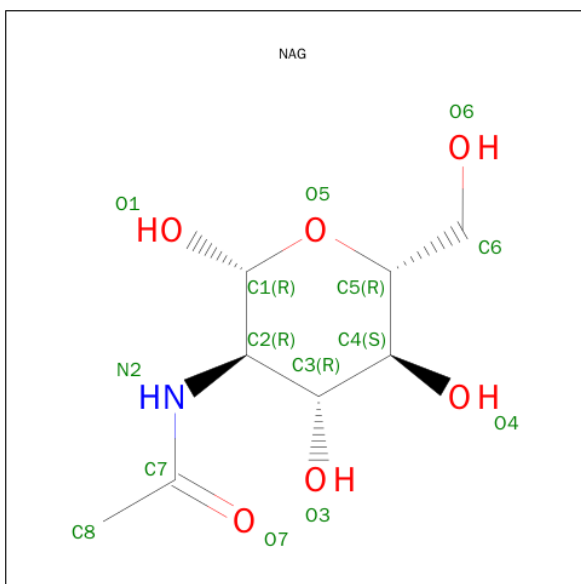
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	N	6	Total	C	N	O	0	0
			72	40	2	30		
4	A	6	Total	C	N	O	0	0
			72	40	2	30		

- Molecule 5 is SUGAR (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	N	1	Total	C	O	0	0
			11	6	5		
5	A	1	Total	C	O	0	0
			11	6	5		

- Molecule 6 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	N	1	Total	C	N	O	0	0
			14	8	1	5		

*Continued on next page...*

*Continued from previous page...*

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

- Molecule 7 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	1	Total	Ca	0	0
			1	1		
7	N	1	Total	Ca	0	0
			1	1		

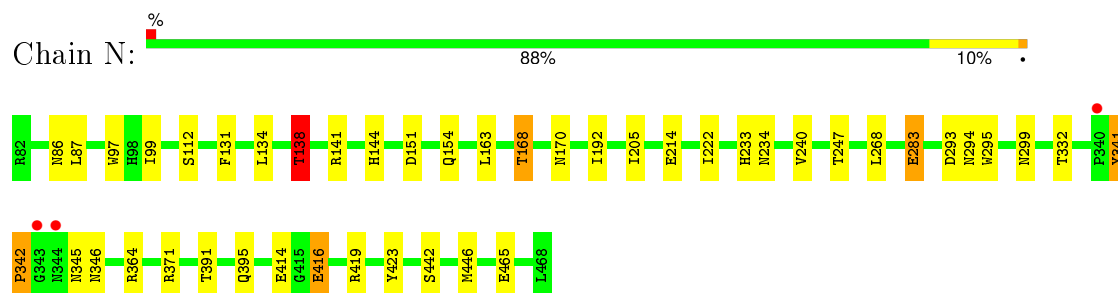
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	81	Total	O	0	0
			81	81		
8	B	6	Total	O	0	0
			6	6		
8	C	3	Total	O	0	0
			3	3		
8	H	6	Total	O	0	0
			6	6		
8	L	3	Total	O	0	0
			3	3		
8	N	81	Total	O	0	0
			81	81		

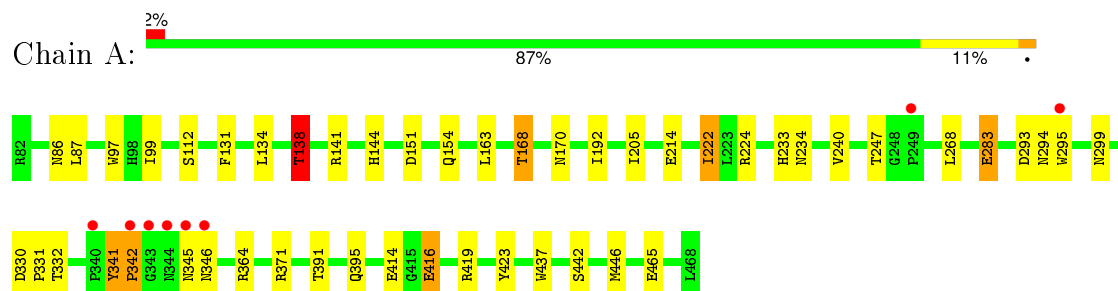
### 3 Residue-property plots

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 ( $\text{RSRZ} > 2$ ). 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.

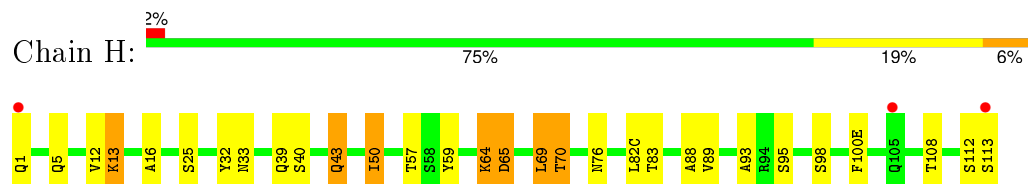
#### • Molecule 1: NEURAMINIDASE



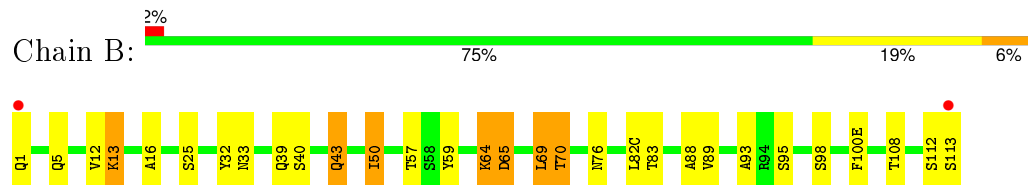
#### • Molecule 1: NEURAMINIDASE



#### • Molecule 2: SINGLE CHAIN ANTIBODY

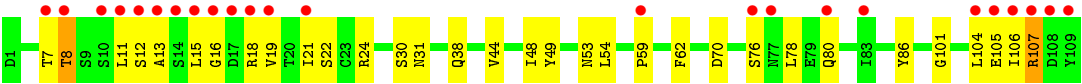


#### • Molecule 2: SINGLE CHAIN ANTIBODY



#### • Molecule 3: SINGLE CHAIN ANTIBODY





● Molecule 3: SINGLE CHAIN ANTIBODY



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 4 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	144.40 Å   144.40 Å   227.00 Å 90.00°   90.00°   90.00°	Depositor
Resolution (Å)	7.00 – 2.50 64.58 – 2.50	Depositor EDS
% Data completeness (in resolution range)	80.0 (7.00-2.50) 80.7 (64.58-2.50)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	185.30 (at 2.51 Å)	Xtrriage
Refinement program	X-PLOR 3.1	Depositor
R, $R_{free}$	0.220 ,   0.260 0.233 ,   (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	24.7	Xtrriage
Anisotropy	0.470	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 70.3	EDS
Estimated twinning fraction	No twinning to report.	Xtrriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtrriage
Outliers	1 of 67425 reflections (0.001%)	Xtrriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	10138	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	23.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 37.20 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 4.4472e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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: CA, BMA, NAG, 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	0.56	0/3150	0.83	1/4290 (0.0%)
1	N	0.56	0/3150	0.83	1/4290 (0.0%)
2	B	0.47	0/966	0.73	0/1306
2	H	0.47	0/966	0.73	0/1306
3	C	0.47	0/874	0.68	0/1187
3	L	0.47	0/874	0.68	0/1187
All	All	0.53	0/9980	0.78	2/13566 (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
1	A	0	1
1	N	0	1
All	All	0	2

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	N	138	THR	CB-CA-C	-5.50	96.76	111.60
1	A	138	THR	CB-CA-C	-5.49	96.77	111.60

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	423	TYR	Sidechain
1	N	423	TYR	Sidechain

## 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	3067	0	2893	27	1
1	N	3067	0	2893	24	1
2	B	943	0	880	21	0
2	H	943	0	880	21	0
3	C	857	0	805	23	0
3	L	857	0	805	23	0
4	A	72	0	61	0	0
4	N	72	0	61	0	0
5	A	11	0	10	0	0
5	N	11	0	10	0	0
6	A	28	0	26	1	0
6	N	28	0	26	0	0
7	A	1	0	0	0	0
7	N	1	0	0	0	0
8	A	81	0	0	3	0
8	B	6	0	0	1	0
8	C	3	0	0	0	0
8	H	6	0	0	1	0
8	L	3	0	0	0	0
8	N	81	0	0	3	0
All	All	10138	0	9350	139	2

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 (139) 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)
2:B:89:VAL:HG22	2:B:108:THR:HG22	1.57	0.87
2:H:89:VAL:HG22	2:H:108:THR:HG22	1.57	0.87

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:168:THR:HB	1:N:170:ASN:OD1	1.85	0.77
1:A:168:THR:HB	1:A:170:ASN:OD1	1.85	0.77
1:A:168:THR:HG22	1:A:170:ASN:H	1.49	0.77
1:N:168:THR:HG22	1:N:170:ASN:H	1.49	0.76
1:N:87:LEU:H	1:N:233:HIS:HD2	1.33	0.75
1:A:87:LEU:H	1:A:233:HIS:HD2	1.33	0.75
2:H:64:LYS:HE3	2:H:65:ASP:H	1.51	0.74
2:B:64:LYS:HE3	2:B:65:ASP:H	1.51	0.74
3:C:59:PRO:HG2	3:C:62:PHE:HE2	1.53	0.73
3:L:59:PRO:HG2	3:L:62:PHE:HE2	1.53	0.73
1:A:138:THR:HG23	1:A:144:HIS:HB2	1.73	0.69
3:C:59:PRO:HG2	3:C:62:PHE:CE2	2.27	0.69
1:N:138:THR:HG23	1:N:144:HIS:HB2	1.73	0.68
3:L:59:PRO:HG2	3:L:62:PHE:CE2	2.27	0.68
1:N:345:ASN:HA	8:N:543:HOH:O	2.00	0.61
1:A:345:ASN:HA	8:A:543:HOH:O	2.00	0.60
1:A:168:THR:HG22	1:A:170:ASN:N	2.16	0.60
1:N:168:THR:HG22	1:N:170:ASN:N	2.16	0.60
2:H:59:TYR:CE2	2:H:69:LEU:HD22	2.37	0.60
3:L:24:ARG:HG3	3:L:70:ASP:OD1	2.02	0.60
3:C:24:ARG:HG3	3:C:70:ASP:OD1	2.02	0.59
2:B:59:TYR:CE2	2:B:69:LEU:HD22	2.37	0.59
2:H:32:TYR:CD2	2:H:98:SER:HA	2.38	0.59
2:B:32:TYR:CD2	2:B:98:SER:HA	2.38	0.59
3:C:12:SER:HA	3:C:105:GLU:O	2.03	0.59
3:L:12:SER:HA	3:L:105:GLU:O	2.03	0.59
2:B:64:LYS:HE3	2:B:65:ASP:N	2.18	0.58
1:A:247:THR:HA	1:A:346:ASN:ND2	2.19	0.58
1:A:138:THR:CG2	1:A:144:HIS:HB2	2.34	0.58
1:N:138:THR:CG2	1:N:144:HIS:HB2	2.34	0.58
2:H:64:LYS:HE3	2:H:65:ASP:N	2.18	0.57
1:N:295:TRP:O	1:N:345:ASN:HB2	2.05	0.57
1:A:295:TRP:O	1:A:345:ASN:HB2	2.05	0.57
2:B:64:LYS:HE3	2:B:64:LYS:HA	1.86	0.57
1:N:247:THR:HA	1:N:346:ASN:ND2	2.19	0.56
1:N:416:GLU:CD	1:N:416:GLU:H	2.09	0.56
1:A:416:GLU:CD	1:A:416:GLU:H	2.09	0.56
2:H:64:LYS:HE3	2:H:64:LYS:HA	1.86	0.56
2:B:64:LYS:O	2:B:65:ASP:HB2	2.05	0.56
2:H:64:LYS:O	2:H:65:ASP:HB2	2.05	0.55
1:N:247:THR:HG22	1:N:346:ASN:HB3	1.88	0.55

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:247:THR:HG22	1:A:346:ASN:HB3	1.88	0.55
3:L:18:ARG:HB2	3:L:18:ARG:NH1	2.23	0.54
1:N:295:TRP:HA	1:N:346:ASN:ND2	2.23	0.54
1:A:295:TRP:HA	1:A:346:ASN:ND2	2.23	0.54
3:L:21:ILE:HD12	3:L:22:SER:H	1.73	0.53
3:C:21:ILE:HD12	3:C:22:SER:H	1.73	0.53
1:A:295:TRP:HD1	1:A:346:ASN:HD21	1.54	0.53
3:C:13:ALA:O	3:C:106:ILE:HA	2.08	0.53
1:N:295:TRP:HD1	1:N:346:ASN:HD21	1.55	0.53
3:C:18:ARG:HB2	3:C:18:ARG:NH1	2.22	0.53
1:N:86:ASN:OD1	1:N:234:ASN:HB2	2.09	0.53
3:L:13:ALA:O	3:L:106:ILE:HA	2.08	0.52
1:N:293:ASP:O	1:N:295:TRP:N	2.42	0.52
1:A:293:ASP:O	1:A:295:TRP:N	2.42	0.52
3:C:19:VAL:HG22	3:C:78:LEU:HD11	1.91	0.52
1:A:86:ASN:OD1	1:A:234:ASN:HB2	2.09	0.52
3:L:19:VAL:HG22	3:L:78:LEU:HD11	1.91	0.52
2:B:43:GLN:NE2	2:B:43:GLN:HA	2.24	0.52
3:C:48:ILE:CD1	3:C:54:LEU:HD12	2.40	0.51
2:H:43:GLN:NE2	2:H:43:GLN:HA	2.24	0.51
3:L:48:ILE:CD1	3:L:54:LEU:HD12	2.40	0.51
1:N:87:LEU:H	1:N:233:HIS:CD2	2.22	0.51
3:L:80:GLN:OE1	3:L:106:ILE:HD12	2.11	0.51
1:A:87:LEU:H	1:A:233:HIS:CD2	2.23	0.50
3:C:80:GLN:OE1	3:C:106:ILE:HD12	2.11	0.50
1:A:299:ASN:OD1	1:A:341:TYR:N	2.45	0.50
2:H:12:VAL:CG1	2:H:16:ALA:HB3	2.42	0.50
3:L:38:GLN:HG3	3:L:44:VAL:HG22	1.94	0.50
1:N:299:ASN:OD1	1:N:341:TYR:N	2.45	0.50
3:C:80:GLN:HA	3:C:80:GLN:OE1	2.12	0.49
2:B:40:SER:OG	2:B:43:GLN:HB3	2.12	0.49
2:H:40:SER:OG	2:H:43:GLN:HB3	2.12	0.49
3:L:11:LEU:O	3:L:104:LEU:HD12	2.12	0.49
3:C:38:GLN:HG3	3:C:44:VAL:HG22	1.94	0.49
2:B:12:VAL:CG1	2:B:16:ALA:HB3	2.42	0.49
1:A:295:TRP:HA	1:A:346:ASN:HD22	1.78	0.49
2:B:93:ALA:HB1	2:B:100(E):PHE:HB3	1.95	0.49
1:N:295:TRP:HA	1:N:346:ASN:HD22	1.78	0.49
3:L:80:GLN:HA	3:L:80:GLN:OE1	2.12	0.49
3:C:11:LEU:O	3:C:104:LEU:HD12	2.12	0.49
2:H:93:ALA:HB1	2:H:100(E):PHE:HB3	1.95	0.48

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:442:SER:HB2	8:A:519:HOH:O	2.14	0.48
2:H:13:LYS:HD2	2:H:113:SER:HA	1.95	0.48
2:B:33:ASN:HB2	2:B:95:SER:HB2	1.95	0.48
1:A:131:PHE:CE1	1:A:163:LEU:HD12	2.49	0.48
2:H:33:ASN:HB2	2:H:95:SER:HB2	1.95	0.48
2:H:64:LYS:O	2:H:65:ASP:CB	2.62	0.47
2:B:64:LYS:O	2:B:65:ASP:CB	2.62	0.47
2:B:13:LYS:HD2	2:B:113:SER:HA	1.95	0.47
1:N:442:SER:HB2	8:N:519:HOH:O	2.14	0.47
1:N:192:ILE:HG12	1:N:205:ILE:HG13	1.95	0.47
3:C:49:TYR:O	3:C:53:ASN:HB2	2.14	0.47
3:L:49:TYR:O	3:L:53:ASN:HB2	2.14	0.47
1:N:131:PHE:CE1	1:N:163:LEU:HD12	2.49	0.47
1:A:192:ILE:HG12	1:A:205:ILE:HG13	1.95	0.47
1:A:341:TYR:HA	1:A:342:PRO:HD3	1.76	0.47
3:C:12:SER:HB3	3:C:107:ARG:HB2	1.97	0.47
3:L:12:SER:HB3	3:L:107:ARG:HB2	1.97	0.46
2:H:12:VAL:HG13	2:H:16:ALA:HB3	1.97	0.46
2:B:12:VAL:HG13	2:B:16:ALA:HB3	1.97	0.46
3:C:48:ILE:HA	3:C:53:ASN:O	2.17	0.45
2:H:100(E):PHE:CD1	2:H:100(E):PHE:N	2.84	0.45
3:L:48:ILE:HA	3:L:53:ASN:O	2.17	0.45
2:B:100(E):PHE:CD1	2:B:100(E):PHE:N	2.84	0.45
1:N:97:TRP:HB2	1:N:395:GLN:NE2	2.32	0.44
1:A:97:TRP:HB2	1:A:395:GLN:NE2	2.32	0.44
2:H:50:ILE:O	2:H:57:THR:HA	2.18	0.43
2:B:50:ILE:O	2:B:57:THR:HA	2.18	0.43
1:N:341:TYR:HA	1:N:342:PRO:HD3	1.76	0.43
3:L:86:TYR:O	3:L:101:GLY:HA2	2.18	0.43
2:B:1:GLN:N	2:B:1:GLN:OE1	2.45	0.43
3:C:86:TYR:O	3:C:101:GLY:HA2	2.18	0.42
2:H:1:GLN:OE1	2:H:1:GLN:N	2.45	0.42
1:A:330:ASP:HA	1:A:331:PRO:HD2	1.95	0.42
3:L:21:ILE:HD12	3:L:22:SER:N	2.35	0.41
3:C:21:ILE:HD12	3:C:22:SER:N	2.35	0.41
1:A:222:ILE:O	1:A:224:ARG:HG2	2.21	0.41
2:B:39:GLN:O	2:B:88:ALA:HB1	2.21	0.41
2:H:39:GLN:O	2:H:88:ALA:HB1	2.21	0.41
3:C:7:THR:O	3:C:8:THR:HG22	2.21	0.41
1:A:283:GLU:HG3	8:A:535:HOH:O	2.21	0.41
3:C:15:LEU:HD23	3:C:16:GLY:N	2.36	0.41

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:11:LEU:HB3	3:L:104:LEU:HD12	2.02	0.41
2:H:12:VAL:CG1	2:H:13:LYS:N	2.84	0.40
2:H:70:THR:HB	8:H:116:HOH:O	2.21	0.40
3:L:7:THR:O	3:L:8:THR:HG22	2.21	0.40
1:A:437:TRP:CD1	6:A:476(A):NAG:H82	2.56	0.40
1:N:283:GLU:HG3	8:N:535:HOH:O	2.21	0.40
3:C:11:LEU:HB3	3:C:104:LEU:HD12	2.02	0.40
3:C:30:SER:O	3:C:31:ASN:HB2	2.21	0.40
3:L:18:ARG:HG3	3:L:76:SER:HA	2.03	0.40
3:C:18:ARG:HG3	3:C:76:SER:HA	2.03	0.40
3:L:15:LEU:HD23	3:L:16:GLY:N	2.36	0.40
2:B:12:VAL:CG1	2:B:13:LYS:N	2.84	0.40
3:L:30:SER:O	3:L:31:ASN:HB2	2.21	0.40
2:B:70:THR:HB	8:B:149:HOH:O	2.21	0.40

All (2) 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:A:214:GLU:OE2	1:A:419:ARG:NH2[4_555]	2.09	0.11
1:N:214:GLU:OE2	1:N:419:ARG:NH2[4_555]	2.09	0.11

## 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%)	357 (92%)	26 (7%)	3 (1%)	24 41
1	N	386/388 (100%)	357 (92%)	26 (7%)	3 (1%)	24 41
2	B	120/122 (98%)	114 (95%)	4 (3%)	2 (2%)	11 19
2	H	120/122 (98%)	114 (95%)	4 (3%)	2 (2%)	11 19

Continued on next page...

*Continued from previous page...*

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	C	107/109 (98%)	95 (89%)	11 (10%)	1 (1%)	21	37
3	L	107/109 (98%)	95 (89%)	11 (10%)	1 (1%)	21	37
All	All	1226/1238 (99%)	1132 (92%)	82 (7%)	12 (1%)	19	34

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	N	294	ASN
3	L	8	THR
1	A	294	ASN
3	C	8	THR
2	H	43	GLN
2	H	65	ASP
2	B	43	GLN
2	B	65	ASP
1	N	342	PRO
1	A	342	PRO
1	N	222	ILE
1	A	222	ILE

### 5.3.2 Protein sidechains ⓘ

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	341/341 (100%)	321 (94%)	20 (6%)	24	44
1	N	341/341 (100%)	321 (94%)	20 (6%)	24	44
2	B	100/100 (100%)	89 (89%)	11 (11%)	8	14
2	H	100/100 (100%)	89 (89%)	11 (11%)	8	14
3	C	98/98 (100%)	97 (99%)	1 (1%)	82	95
3	L	98/98 (100%)	97 (99%)	1 (1%)	82	95
All	All	1078/1078 (100%)	1014 (94%)	64 (6%)	24	44

All (64) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	N	99	ILE
1	N	112	SER
1	N	134	LEU
1	N	138	THR
1	N	141	ARG
1	N	151	ASP
1	N	154	GLN
1	N	168	THR
1	N	240	VAL
1	N	268	LEU
1	N	283	GLU
1	N	332	THR
1	N	341	TYR
1	N	364	ARG
1	N	371	ARG
1	N	391	THR
1	N	414	GLU
1	N	416	GLU
1	N	446	MET
1	N	465	GLU
2	H	5	GLN
2	H	13	LYS
2	H	25	SER
2	H	50	ILE
2	H	64	LYS
2	H	69	LEU
2	H	70	THR
2	H	76	ASN
2	H	82(C)	LEU
2	H	83	THR
2	H	112	SER
3	L	107	ARG
1	A	99	ILE
1	A	112	SER
1	A	134	LEU
1	A	138	THR
1	A	141	ARG
1	A	151	ASP
1	A	154	GLN
1	A	168	THR
1	A	240	VAL
1	A	268	LEU
1	A	283	GLU

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
1	A	332	THR
1	A	341	TYR
1	A	364	ARG
1	A	371	ARG
1	A	391	THR
1	A	414	GLU
1	A	416	GLU
1	A	446	MET
1	A	465	GLU
2	B	5	GLN
2	B	13	LYS
2	B	25	SER
2	B	50	ILE
2	B	64	LYS
2	B	69	LEU
2	B	70	THR
2	B	76	ASN
2	B	82(C)	LEU
2	B	83	THR
2	B	112	SER
3	C	107	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	N	233	HIS
1	N	296	GLN
1	N	345	ASN
1	N	346	ASN
2	H	43	GLN
2	H	76	ASN
3	L	53	ASN
1	A	233	HIS
1	A	296	GLN
1	A	345	ASN
1	A	346	ASN
2	B	43	GLN
2	B	76	ASN
3	C	53	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 ⓘ

12 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$
4	NAG	A	469(A)	1,4	14,14,15	1.38	3 (21%)	15,19,21	4.05	5 (33%)
4	NAG	A	470(B)	4	14,14,15	1.28	2 (14%)	15,19,21	1.42	2 (13%)
4	BMA	A	471(C)	4	11,11,12	1.11	1 (9%)	14,15,17	1.30	2 (14%)
4	MAN	A	472(D)	4	11,11,12	0.91	0	14,15,17	1.46	2 (14%)
4	MAN	A	473(E)	4	11,11,12	1.40	1 (9%)	14,15,17	1.36	2 (14%)
4	MAN	A	474(F)	4	11,11,12	1.76	2 (18%)	14,15,17	1.70	1 (7%)
4	NAG	N	469(A)	1,4	14,14,15	1.38	3 (21%)	15,19,21	4.04	5 (33%)
4	NAG	N	470(B)	4	14,14,15	1.28	1 (7%)	15,19,21	1.42	2 (13%)
4	BMA	N	471(C)	4	11,11,12	1.10	1 (9%)	14,15,17	1.31	2 (14%)
4	MAN	N	472(D)	4	11,11,12	0.92	0	14,15,17	1.46	2 (14%)
4	MAN	N	473(E)	4	11,11,12	1.41	1 (9%)	14,15,17	1.36	2 (14%)
4	MAN	N	474(F)	4	11,11,12	1.77	2 (18%)	14,15,17	1.70	1 (7%)

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
4	NAG	A	469(A)	1,4	-	0/6/23/26	0/1/1/1
4	NAG	A	470(B)	4	-	0/6/23/26	0/1/1/1
4	BMA	A	471(C)	4	-	0/2/19/22	0/1/1/1
4	MAN	A	472(D)	4	-	0/2/19/22	0/1/1/1
4	MAN	A	473(E)	4	-	0/2/19/22	0/1/1/1
4	MAN	A	474(F)	4	-	0/2/19/22	0/1/1/1
4	NAG	N	469(A)	1,4	-	0/6/23/26	0/1/1/1
4	NAG	N	470(B)	4	-	0/6/23/26	0/1/1/1
4	BMA	N	471(C)	4	-	0/2/19/22	0/1/1/1
4	MAN	N	472(D)	4	-	0/2/19/22	0/1/1/1
4	MAN	N	473(E)	4	-	0/2/19/22	0/1/1/1
4	MAN	N	474(F)	4	-	0/2/19/22	0/1/1/1

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	N	473(E)	MAN	C2-C3	-3.13	1.48	1.52
4	A	473(E)	MAN	C2-C3	-3.12	1.48	1.52
4	N	470(B)	NAG	C1-C2	-2.73	1.48	1.52
4	A	470(B)	NAG	C1-C2	-2.66	1.48	1.52
4	A	470(B)	NAG	O5-C1	-2.00	1.40	1.43
4	A	469(A)	NAG	C1-C2	2.18	1.55	1.52
4	N	469(A)	NAG	C1-C2	2.18	1.55	1.52
4	N	471(C)	BMA	C2-C3	2.18	1.55	1.52
4	N	474(F)	MAN	C6-C5	2.19	1.59	1.51
4	A	474(F)	MAN	C6-C5	2.20	1.59	1.51
4	A	471(C)	BMA	C2-C3	2.22	1.55	1.52
4	N	469(A)	NAG	O5-C5	2.34	1.48	1.43
4	A	469(A)	NAG	O5-C5	2.34	1.48	1.43
4	A	469(A)	NAG	C6-C5	2.41	1.60	1.51
4	N	469(A)	NAG	C6-C5	2.42	1.60	1.51
4	A	474(F)	MAN	O5-C5	4.32	1.53	1.43
4	N	474(F)	MAN	O5-C5	4.33	1.53	1.43

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	472(D)	MAN	C6-C5-C4	-3.31	104.85	113.02
4	N	472(D)	MAN	C6-C5-C4	-3.30	104.88	113.02
4	N	471(C)	BMA	O5-C1-C2	-2.59	106.65	110.86
4	A	471(C)	BMA	O5-C1-C2	-2.59	106.66	110.86
4	A	469(A)	NAG	C6-C5-C4	-2.48	106.90	113.02
4	N	469(A)	NAG	C6-C5-C4	-2.47	106.92	113.02

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	N	470(B)	NAG	O7-C7-C8	-2.30	117.84	122.06
4	A	470(B)	NAG	O7-C7-C8	-2.29	117.86	122.06
4	N	473(E)	MAN	O5-C5-C6	2.07	111.84	107.35
4	A	473(E)	MAN	O5-C5-C6	2.10	111.89	107.35
4	A	471(C)	BMA	O5-C5-C6	2.37	112.48	107.35
4	N	471(C)	BMA	O5-C5-C6	2.39	112.51	107.35
4	N	472(D)	MAN	C1-O5-C5	2.50	115.42	112.25
4	A	472(D)	MAN	C1-O5-C5	2.52	115.45	112.25
4	A	469(A)	NAG	O3-C3-C2	2.55	114.17	109.11
4	N	469(A)	NAG	O3-C3-C2	2.57	114.19	109.11
4	N	473(E)	MAN	C3-C4-C5	2.87	115.20	110.20
4	A	473(E)	MAN	C3-C4-C5	2.88	115.22	110.20
4	N	470(B)	NAG	C6-C5-C4	2.93	120.25	113.02
4	A	470(B)	NAG	C6-C5-C4	2.95	120.29	113.02
4	A	469(A)	NAG	C3-C4-C5	3.12	115.64	110.20
4	N	469(A)	NAG	C3-C4-C5	3.13	115.65	110.20
4	A	474(F)	MAN	C1-O5-C5	4.68	118.19	112.25
4	N	474(F)	MAN	C1-O5-C5	4.69	118.21	112.25
4	N	469(A)	NAG	C2-N2-C7	7.31	132.43	123.04
4	A	469(A)	NAG	C2-N2-C7	7.33	132.45	123.04
4	N	469(A)	NAG	C1-O5-C5	12.48	128.09	112.25
4	A	469(A)	NAG	C1-O5-C5	12.50	128.11	112.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.6 Ligand geometry

Of 8 ligands modelled in this entry, 2 are monoatomic - leaving 6 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
5	MAN	A	475(G)	-	11,11,12	1.82	3 (27%)	14,15,17	2.64	6 (42%)
6	NAG	A	476(A)	1	14,14,15	1.36	3 (21%)	15,19,21	0.86	0
6	NAG	A	477(A)	1	14,14,15	1.13	3 (21%)	15,19,21	1.44	4 (26%)
5	MAN	N	475(G)	-	11,11,12	1.82	3 (27%)	14,15,17	2.64	6 (42%)
6	NAG	N	476(A)	1	14,14,15	1.36	3 (21%)	15,19,21	0.86	0
6	NAG	N	477(A)	1	14,14,15	1.13	3 (21%)	15,19,21	1.44	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
5	MAN	A	475(G)	-	-	0/2/19/22	0/1/1/1
6	NAG	A	476(A)	1	-	0/6/23/26	0/1/1/1
6	NAG	A	477(A)	1	-	0/6/23/26	0/1/1/1
5	MAN	N	475(G)	-	-	0/2/19/22	0/1/1/1
6	NAG	N	476(A)	1	-	0/6/23/26	0/1/1/1
6	NAG	N	477(A)	1	-	0/6/23/26	0/1/1/1

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	475(G)	MAN	C4-C5	-4.32	1.43	1.53
5	N	475(G)	MAN	C4-C5	-4.32	1.43	1.53
6	N	476(A)	NAG	C1-C2	-3.08	1.48	1.52
6	A	476(A)	NAG	C1-C2	-3.07	1.48	1.52
5	N	475(G)	MAN	O4-C4	-2.37	1.37	1.43
5	A	475(G)	MAN	O4-C4	-2.35	1.37	1.43
6	N	476(A)	NAG	O3-C3	-2.18	1.37	1.43
6	A	476(A)	NAG	O3-C3	-2.18	1.37	1.43
5	A	475(G)	MAN	C1-C2	2.01	1.57	1.52
5	N	475(G)	MAN	C1-C2	2.02	1.57	1.52
6	N	477(A)	NAG	C4-C5	2.07	1.57	1.53
6	N	477(A)	NAG	C8-C7	2.07	1.54	1.50
6	A	477(A)	NAG	C8-C7	2.08	1.54	1.50
6	A	477(A)	NAG	C1-C2	2.08	1.55	1.52
6	N	477(A)	NAG	C1-C2	2.10	1.55	1.52
6	A	477(A)	NAG	C4-C5	2.10	1.57	1.53
6	A	476(A)	NAG	O5-C5	2.43	1.48	1.43
6	N	476(A)	NAG	O5-C5	2.46	1.48	1.43

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	N	475(G)	MAN	O3-C3-C4	-4.24	100.80	110.34
5	A	475(G)	MAN	O3-C3-C4	-4.23	100.82	110.34
5	A	475(G)	MAN	C1-C2-C3	-3.49	105.41	109.54
5	N	475(G)	MAN	C1-C2-C3	-3.46	105.45	109.54
6	N	477(A)	NAG	O7-C7-C8	-2.36	117.74	122.06
6	A	477(A)	NAG	O7-C7-C8	-2.36	117.74	122.06
6	A	477(A)	NAG	C8-C7-N2	2.12	120.15	116.11
6	N	477(A)	NAG	C8-C7-N2	2.13	120.18	116.11
6	N	477(A)	NAG	C1-O5-C5	2.27	115.12	112.25
6	A	477(A)	NAG	C1-O5-C5	2.29	115.15	112.25
6	N	477(A)	NAG	O3-C3-C2	2.37	113.81	109.11
6	A	477(A)	NAG	O3-C3-C2	2.38	113.83	109.11
5	N	475(G)	MAN	O5-C5-C6	2.60	112.98	107.35
5	A	475(G)	MAN	O5-C5-C6	2.61	113.00	107.35
5	A	475(G)	MAN	C1-O5-C5	3.35	116.50	112.25
5	N	475(G)	MAN	C1-O5-C5	3.37	116.52	112.25
5	N	475(G)	MAN	C2-C3-C4	4.52	118.72	111.04
5	A	475(G)	MAN	C2-C3-C4	4.53	118.74	111.04
5	A	475(G)	MAN	O2-C2-C1	5.10	119.43	109.21
5	N	475(G)	MAN	O2-C2-C1	5.10	119.44	109.21

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	476(A)	NAG	1	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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%)	-0.51	8 (2%) 67 71	3, 12, 43, 78	0
1	N	388/388 (100%)	-0.59	3 (0%) 87 89	3, 12, 43, 78	0
2	B	122/122 (100%)	-0.19	2 (1%) 74 78	13, 27, 50, 80	0
2	H	122/122 (100%)	-0.25	3 (2%) 61 65	13, 27, 50, 80	0
3	C	109/109 (100%)	0.82	21 (19%) 2 1	13, 38, 72, 102	0
3	L	109/109 (100%)	0.92	24 (22%) 1 1	13, 38, 72, 102	0
All	All	1238/1238 (100%)	-0.24	61 (4%) 33 38	3, 18, 64, 102	0

All (61) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	L	109	TYR	10.5
3	C	108	ASP	9.1
3	C	109	TYR	8.7
3	L	106	ILE	7.7
2	B	113	SER	6.8
1	A	343	GLY	6.8
3	L	108	ASP	6.7
3	L	107	ARG	6.3
2	H	113	SER	6.1
3	L	11	LEU	5.9
3	C	106	ILE	5.1
3	C	76	SER	5.0
3	C	80	GLN	5.0
3	C	107	ARG	5.0
1	A	295	TRP	4.9
3	L	76	SER	4.7
1	A	340	PRO	4.7
3	C	18	ARG	4.7
3	C	105	GLU	4.7

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	A	346	ASN	4.7
3	L	15	LEU	4.4
3	C	12	SER	4.3
1	A	342	PRO	4.2
3	L	18	ARG	4.2
3	L	13	ALA	3.9
1	A	344	ASN	3.9
3	C	19	VAL	3.8
3	L	80	GLN	3.7
3	L	19	VAL	3.6
3	L	7	THR	3.5
3	L	105	GLU	3.3
3	L	77	ASN	3.1
3	L	104	LEU	3.1
2	H	1	GLN	3.1
3	L	16	GLY	3.1
3	C	11	LEU	3.0
3	C	77	ASN	3.0
3	L	14	SER	3.0
3	L	8	THR	3.0
3	C	17	ASP	2.9
1	A	345	ASN	2.9
3	C	59	PRO	2.9
3	C	7	THR	2.9
3	C	10	SER	2.8
3	L	21	ILE	2.8
3	L	83	ILE	2.8
3	C	78	LEU	2.7
3	C	75	ILE	2.7
3	L	59	PRO	2.7
2	B	1	GLN	2.7
3	C	13	ALA	2.6
3	L	12	SER	2.6
3	C	1	ASP	2.3
1	N	343	GLY	2.2
3	C	83	ILE	2.2
1	N	340	PRO	2.1
3	L	17	ASP	2.1
3	L	10	SER	2.1
1	A	249	PRO	2.1
1	N	344	ASN	2.0
2	H	105	GLN	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 [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	N	474(F)	11/12	0.96	0.11	-0.21	10,12,15,17	0
4	NAG	N	469(A)	14/15	0.96	0.10	-0.28	5,15,25,29	0
4	MAN	A	474(F)	11/12	0.97	0.10	-0.54	10,12,15,17	0
4	NAG	A	469(A)	14/15	0.95	0.10	-0.69	5,15,25,29	0
4	MAN	A	473(E)	11/12	0.96	0.11	-0.80	9,16,20,27	0
4	BMA	A	471(C)	11/12	0.96	0.10	-0.93	11,13,17,23	0
4	NAG	A	470(B)	14/15	0.96	0.09	-1.40	7,12,19,28	0
4	MAN	N	473(E)	11/12	0.95	0.10	-1.64	9,16,20,27	0
4	BMA	N	471(C)	11/12	0.97	0.09	-1.70	11,13,17,23	0
4	NAG	N	470(B)	14/15	0.97	0.12	-	7,12,19,28	0
4	MAN	N	472(D)	11/12	0.96	0.09	-	12,14,17,24	0
4	MAN	A	472(D)	11/12	0.97	0.11	-	12,14,17,24	0

## 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
7	CA	N	478	1/1	0.72	0.17	-0.11	65,65,65,65	0
7	CA	A	478	1/1	0.85	0.09	-1.32	65,65,65,65	0
5	MAN	N	475(G)	11/12	0.91	0.14	-	34,36,40,42	0
6	NAG	N	476(A)	14/15	0.88	0.14	-	40,53,58,64	0
6	NAG	A	476(A)	14/15	0.86	0.20	-	40,53,58,64	0
6	NAG	N	477(A)	14/15	0.83	0.17	-	44,48,51,56	0
6	NAG	A	477(A)	14/15	0.86	0.19	-	44,48,51,56	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
5	MAN	A	475(G)	11/12	0.86	0.16	-	34,36,40,42	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.