



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 10:06 AM GMT

PDB ID : 3KW7  
Title : Crystal structure of LacB from Trametes sp. AH28-2  
Authors : Ge, H.H.; Teng, M.K.; Niu, L.W.  
Deposited on : 2009-12-01  
Resolution : 3.44 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.

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

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

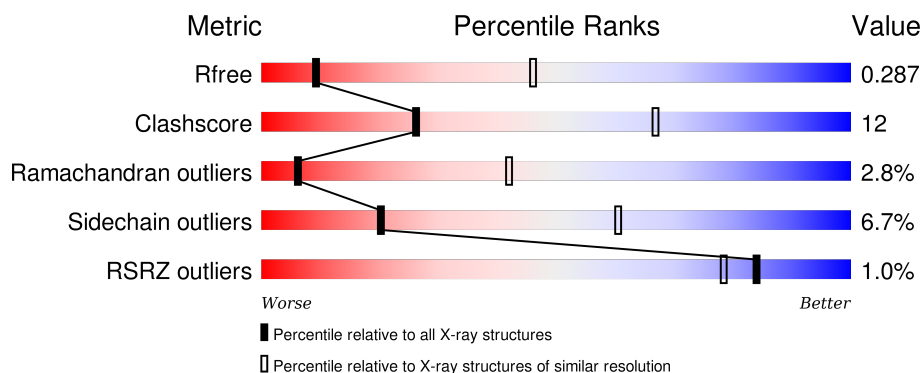
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*



The reported resolution of this entry is 3.44 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))
$R_{free}$	91344	1007 (3.54-3.34)
Clashscore	102246	1044 (3.52-3.36)
Ramachandran outliers	100387	1013 (3.52-3.36)
Sidechain outliers	100360	1014 (3.52-3.36)
RSRZ outliers	91569	1012 (3.54-3.34)

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	502	 70% 26% •
1	B	502	 2% 72% 25% •

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 7825 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.

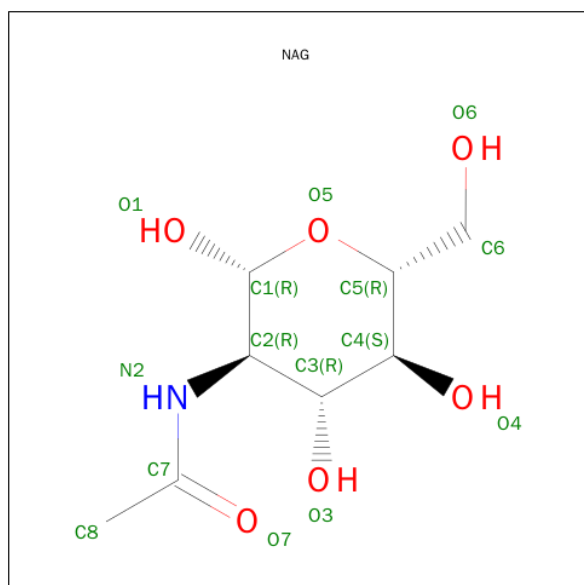
- Molecule 1 is a protein called Laccase B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	502	Total	C	N	O	S	5	0	0
			3809	2416	631	753	9			
1	B	502	Total	C	N	O	S	18	0	0
			3808	2416	631	752	9			

- Molecule 2 is COPPER (II) ION (three-letter code: CU) (formula: Cu).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	4	Total	Cu	0	0
			4	4		
2	A	4	Total	Cu	0	0
			4	4		

- Molecule 3 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).



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

- Molecule 4 is a polymer of unknown type called SUGAR (2-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	2	Total	C	N	O	0	0
			28	16	2	10		
4	A	2	Total	C	N	O	0	0
			28	16	2	10		
4	B	2	Total	C	N	O	0	0
			28	16	2	10		
4	B	2	Total	C	N	O	0	0
			28	16	2	10		

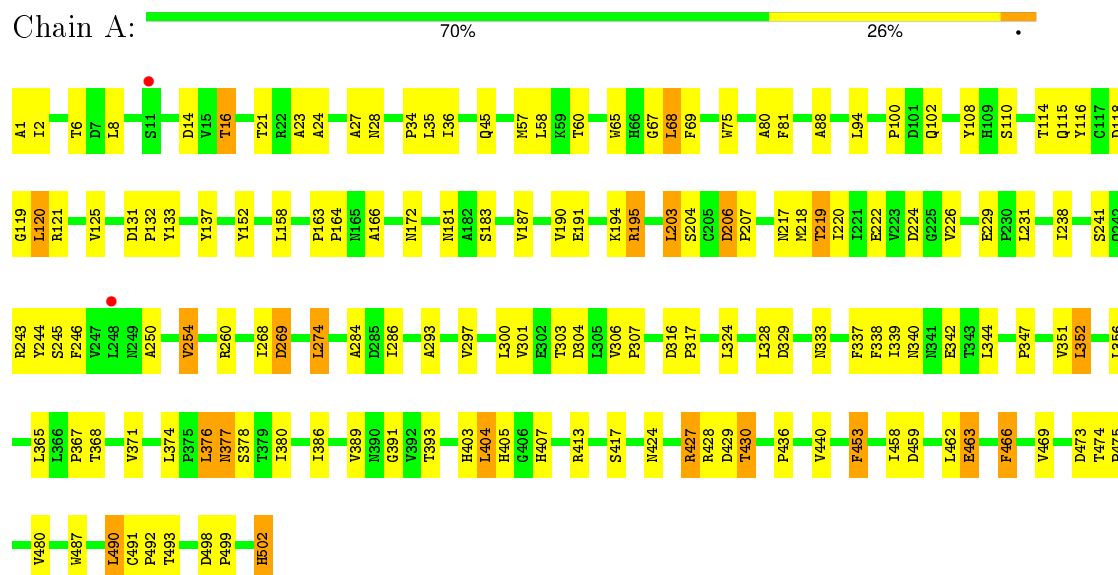
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	19	Total	O	0	0
			19	19		
5	B	13	Total	O	0	0
			13	13		

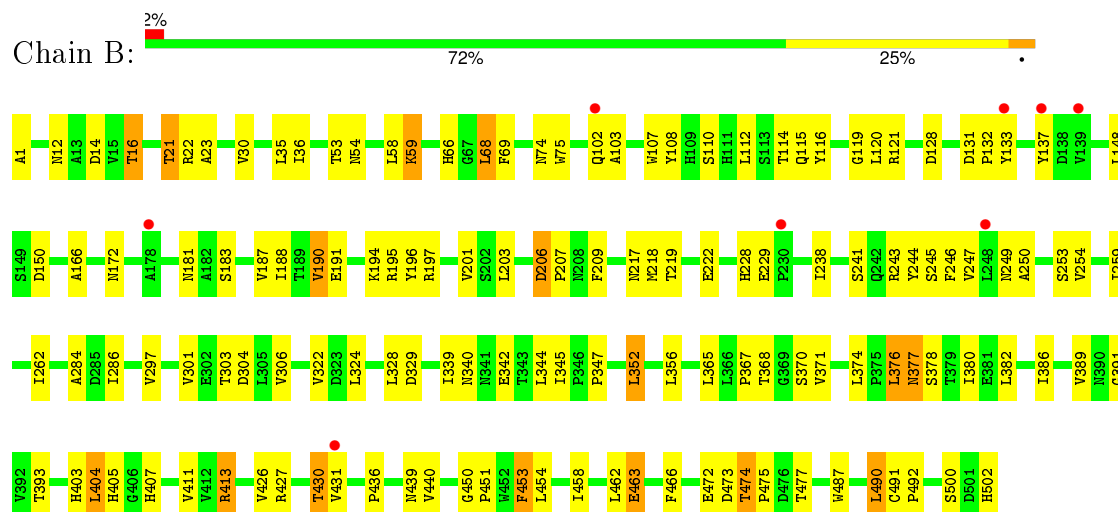
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

#### • Molecule 1: Laccase B



#### • Molecule 1: Laccase B



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 41	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	98.78 Å 98.78 Å 149.96 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 3.44 44.60 – 3.44	Depositor EDS
% Data completeness (in resolution range)	98.9 (30.00-3.44) 99.0 (44.60-3.44)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.73 (at 3.40 Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.223 , 0.292 0.222 , 0.287	Depositor DCC
$R_{free}$ test set	974 reflections (5.42%)	DCC
Wilson B-factor (Å <sup>2</sup> )	67.7	Xtriage
Anisotropy	0.441	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 19.8	EDS
Estimated twinning fraction	0.448 for h,-k,-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 18997 reflections	Xtriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	7825	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.00% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: NAG, CU

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	0.74	2/3919 (0.1%)	0.74	3/5396 (0.1%)
1	B	0.90	5/3918 (0.1%)	0.81	5/5396 (0.1%)
All	All	0.82	7/7837 (0.1%)	0.77	8/10792 (0.1%)

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	500	SER	CB-OG	-26.65	1.07	1.42
1	B	30	VAL	CB-CG1	-17.97	1.15	1.52
1	B	21	THR	CB-CG2	-7.42	1.27	1.52
1	A	274	LEU	CG-CD2	-7.29	1.24	1.51
1	A	417	SER	CB-OG	6.80	1.51	1.42
1	B	59	LYS	CE-NZ	6.38	1.65	1.49
1	B	112	LEU	CG-CD1	-5.05	1.33	1.51

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	30	VAL	CG1-CB-CG2	15.94	136.40	110.90
1	B	30	VAL	CA-CB-CG2	-15.80	87.19	110.90
1	B	112	LEU	CD1-CG-CD2	7.51	133.03	110.50
1	B	253	SER	N-CA-CB	6.82	120.73	110.50
1	A	427	ARG	NE-CZ-NH2	-6.19	117.21	120.30
1	A	274	LEU	CB-CG-CD2	5.41	120.20	111.00
1	A	304	ASP	CB-CG-OD2	5.22	123.00	118.30
1	B	304	ASP	CB-CG-OD2	5.18	122.96	118.30

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	3809	0	3600	94	0
1	B	3808	0	3600	84	0
2	A	4	0	0	0	0
2	B	4	0	0	0	0
3	A	28	0	26	3	0
3	B	28	0	26	3	0
4	A	56	0	50	2	0
4	B	56	0	50	1	0
5	A	19	0	0	3	0
5	B	13	0	0	3	0
All	All	7825	0	7352	181	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 12.

All (181) 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:A:217:ASN:HD21	3:A:701:NAG:C1	1.67	1.08
1:B:1:ALA:HB3	1:B:35:LEU:O	1.52	1.07
1:A:1:ALA:HB3	1:A:35:LEU:O	1.57	1.03
1:B:23:ALA:HB1	5:B:515:HOH:O	1.61	0.98
1:B:376:LEU:O	1:B:378:SER:N	1.98	0.96
1:A:376:LEU:O	1:A:378:SER:N	2.01	0.92
1:B:217:ASN:HD21	3:B:705:NAG:C1	1.82	0.91
1:A:376:LEU:HD12	1:A:473:ASP:CB	2.01	0.91
1:B:376:LEU:CD1	1:B:473:ASP:OD2	2.20	0.90
1:B:376:LEU:HD12	1:B:473:ASP:CG	1.95	0.87
4:B:704:NAG:H82	5:B:510:HOH:O	1.75	0.85
1:B:376:LEU:HD12	1:B:473:ASP:CB	2.07	0.84
1:A:376:LEU:HD12	1:A:473:ASP:CG	1.97	0.83
1:B:1:ALA:CB	1:B:35:LEU:O	2.26	0.83
1:B:376:LEU:HD12	1:B:473:ASP:OD2	1.79	0.82
1:A:376:LEU:CD1	1:A:473:ASP:OD2	2.28	0.82
1:B:328:LEU:HD23	1:B:339:ILE:HG21	1.61	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:217:ASN:ND2	3:A:701:NAG:C1	2.46	0.79
1:B:427:ARG:HG2	1:B:427:ARG:HH11	1.46	0.79
1:A:376:LEU:HD12	1:A:473:ASP:HB2	1.65	0.78
1:A:328:LEU:HD23	1:A:339:ILE:HG21	1.65	0.77
1:B:181:ASN:HD22	1:B:183:SER:HB3	1.50	0.75
1:B:254:VAL:HG12	1:B:284:ALA:HB2	1.67	0.75
1:A:222:GLU:HB3	1:A:245:SER:HB2	1.70	0.72
1:B:222:GLU:HB3	1:B:245:SER:HB2	1.72	0.71
1:A:206:ASP:HB3	1:A:207:PRO:HD3	1.73	0.71
1:B:23:ALA:CB	5:B:515:HOH:O	2.30	0.70
1:A:181:ASN:HD22	1:A:183:SER:HB3	1.56	0.69
1:B:427:ARG:HG2	1:B:427:ARG:NH1	2.07	0.68
1:A:254:VAL:HG12	1:A:284:ALA:HB2	1.74	0.68
1:A:376:LEU:HD12	1:A:473:ASP:OD2	1.91	0.66
1:B:228:HIS:NE2	1:B:426:VAL:HG23	2.11	0.66
1:B:229:GLU:HB2	1:B:306:VAL:HG23	1.78	0.66
1:B:206:ASP:HB3	1:B:207:PRO:HD3	1.77	0.66
1:A:352:LEU:HD22	1:A:356:LEU:CD1	2.25	0.65
1:B:376:LEU:HD12	1:B:473:ASP:HB2	1.78	0.64
1:A:347:PRO:HD3	1:A:367:PRO:HD3	1.78	0.64
1:B:217:ASN:ND2	3:B:705:NAG:C1	2.58	0.64
1:B:328:LEU:HD23	1:B:339:ILE:CG2	2.29	0.62
1:B:12:ASN:HD22	1:B:53:THR:H	1.47	0.62
1:B:103:ALA:HB1	1:B:128:ASP:HB2	1.81	0.62
1:B:386:ILE:O	1:B:436:PRO:HA	2.00	0.62
1:B:191:GLU:HB2	1:B:194:LYS:HD2	1.82	0.61
1:A:386:ILE:O	1:A:436:PRO:HA	1.99	0.61
1:A:328:LEU:HD23	1:A:339:ILE:CG2	2.30	0.61
1:A:203:LEU:H	1:A:203:LEU:HD12	1.65	0.61
1:A:203:LEU:N	1:A:203:LEU:HD12	2.15	0.60
1:B:12:ASN:ND2	1:B:54:ASN:H	2.00	0.60
1:B:352:LEU:HD22	1:B:356:LEU:CD1	2.30	0.60
1:B:218:MET:HG2	1:B:246:PHE:CD1	2.37	0.60
1:B:352:LEU:HD22	1:B:356:LEU:HD12	1.84	0.59
1:B:376:LEU:C	1:B:378:SER:H	2.06	0.59
1:A:365:LEU:HD13	1:A:371:VAL:HG11	1.85	0.59
1:B:487:TRP:HA	1:B:490:LEU:HD22	1.84	0.59
1:A:376:LEU:O	1:A:377:ASN:C	2.41	0.59
1:A:8:LEU:HD22	1:A:27:ALA:HB1	1.83	0.59
1:B:75:TRP:HB2	1:B:487:TRP:CD1	2.38	0.58
1:A:220:ILE:CD1	1:A:300:LEU:HD13	2.33	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:413:ARG:NH1	1:B:439:ASN:HB3	2.19	0.58
1:A:191:GLU:HB2	1:A:194:LYS:HD2	1.86	0.58
1:B:203:LEU:N	1:B:203:LEU:HD12	2.19	0.57
1:A:137:TYR:HA	1:A:195:ARG:HB2	1.85	0.57
1:B:195:ARG:HG2	1:B:249:ASN:OD1	2.05	0.56
1:A:218:MET:HG2	1:A:246:PHE:CD1	2.40	0.56
1:B:68:LEU:HA	1:B:102:GLN:HE22	1.71	0.56
1:A:352:LEU:HD22	1:A:356:LEU:HD12	1.87	0.55
4:A:705:NAG:C8	5:A:519:HOH:O	2.55	0.55
1:A:376:LEU:C	1:A:378:SER:H	2.10	0.54
1:A:352:LEU:HD22	1:A:356:LEU:HD11	1.87	0.54
1:B:324:LEU:HB3	1:B:380:ILE:HG13	1.90	0.54
1:B:491:CYS:N	1:B:492:PRO:HD2	2.23	0.54
1:B:181:ASN:ND2	1:B:183:SER:HB3	2.21	0.54
1:B:403:HIS:HB2	1:B:430:THR:HB	1.88	0.54
1:B:188:ILE:HD12	1:B:259:ILE:HD13	1.90	0.54
1:B:196:TYR:O	1:B:247:VAL:HA	2.08	0.54
4:A:705:NAG:H82	5:A:519:HOH:O	2.07	0.53
1:B:217:ASN:HD21	3:B:705:NAG:C2	2.21	0.53
1:A:329:ASP:H	1:A:340:ASN:ND2	2.07	0.53
1:B:329:ASP:H	1:B:340:ASN:ND2	2.07	0.53
1:A:224:ASP:OD2	1:A:428:ARG:HB2	2.09	0.52
1:A:376:LEU:C	1:A:378:SER:N	2.62	0.52
1:A:238:ILE:HG23	1:A:238:ILE:O	2.08	0.52
1:A:45:GLN:HB3	1:A:94:LEU:HD11	1.92	0.52
1:A:1:ALA:CB	1:A:35:LEU:O	2.46	0.51
1:B:376:LEU:HD13	1:B:473:ASP:OD2	2.05	0.51
1:A:14:ASP:HA	1:A:23:ALA:HA	1.91	0.51
1:A:119:GLY:O	1:A:121:ARG:N	2.42	0.50
1:A:487:TRP:HA	1:A:490:LEU:HD22	1.92	0.50
1:A:429:ASP:OD1	1:A:430:THR:HG22	2.11	0.50
1:A:241:SER:OG	1:A:430:THR:HG21	2.11	0.50
1:A:268:ILE:O	1:A:269:ASP:HB2	2.12	0.49
1:A:68:LEU:HA	1:A:102:GLN:HE22	1.77	0.49
1:A:491:CYS:N	1:A:492:PRO:HD2	2.28	0.49
1:A:376:LEU:HD13	1:A:473:ASP:OD2	2.11	0.49
1:B:203:LEU:H	1:B:203:LEU:HD12	1.77	0.49
1:B:474:THR:HG23	1:B:475:PRO:HD3	1.93	0.49
1:A:75:TRP:HB2	1:A:487:TRP:CD1	2.48	0.48
1:A:229:GLU:HB2	1:A:306:VAL:HG23	1.94	0.48
1:B:238:ILE:HG23	1:B:238:ILE:O	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:365:LEU:HD13	1:B:371:VAL:HG11	1.95	0.48
1:A:301:VAL:HG12	1:A:303:THR:HG22	1.96	0.48
1:B:238:ILE:HD12	1:B:244:TYR:HD2	1.78	0.48
1:A:28:ASN:HD22	1:A:34:PRO:HG3	1.79	0.48
1:A:405:HIS:CD2	1:A:453:PHE:HB3	2.48	0.48
1:A:24:ALA:HB1	1:A:118:ASP:O	2.14	0.47
1:A:324:LEU:HB3	1:A:380:ILE:HG13	1.96	0.47
1:B:407:HIS:NE2	1:B:472:GLU:OE1	2.41	0.47
1:B:188:ILE:HD12	1:B:259:ILE:CD1	2.44	0.47
1:A:333:ASN:HB3	1:A:338:PHE:HE2	1.80	0.47
1:B:137:TYR:CG	1:B:197:ARG:HB2	2.50	0.47
1:B:376:LEU:HD23	1:B:377:ASN:H	1.80	0.47
1:A:226:VAL:HG11	1:A:427:ARG:HD2	1.95	0.47
1:A:403:HIS:HB2	1:A:430:THR:HB	1.97	0.47
1:A:16:THR:HB	1:A:21:THR:HA	1.97	0.47
1:A:260:ARG:CZ	1:A:293:ALA:HB2	2.45	0.47
1:A:206:ASP:HA	1:A:458:ILE:HG23	1.97	0.46
1:B:16:THR:HB	1:B:21:THR:HA	1.98	0.46
1:A:35:LEU:HD11	1:A:125:VAL:HG23	1.98	0.46
1:A:376:LEU:HD23	1:A:377:ASN:H	1.81	0.46
1:B:206:ASP:HA	1:B:458:ILE:HG23	1.98	0.45
1:A:490:LEU:HA	1:A:493:THR:HG22	1.98	0.45
1:B:53:THR:O	1:B:59:LYS:HE3	2.17	0.45
1:A:23:ALA:HB1	5:A:507:HOH:O	2.17	0.45
1:A:131:ASP:O	1:A:133:TYR:N	2.49	0.45
1:B:119:GLY:O	1:B:121:ARG:N	2.48	0.45
1:B:66:HIS:CE1	1:B:241:SER:HB2	2.52	0.44
1:A:337:PHE:HB3	1:A:466:PHE:CD1	2.53	0.44
1:B:131:ASP:O	1:B:133:TYR:N	2.50	0.44
1:A:217:ASN:HD21	3:A:701:NAG:C2	2.26	0.44
1:A:163:PRO:HA	1:A:164:PRO:HD3	1.85	0.44
1:A:65:TRP:HB3	1:A:68:LEU:HD23	2.00	0.44
1:B:450:GLY:HA2	1:B:477:THR:HG23	1.98	0.44
1:A:474:THR:HG23	1:A:475:PRO:HD3	1.99	0.44
1:A:67:GLY:O	1:A:102:GLN:NE2	2.51	0.44
1:B:69:PHE:HD2	1:B:102:GLN:CD	2.21	0.44
1:A:351:VAL:HG11	1:A:469:VAL:HG11	1.99	0.43
1:A:238:ILE:HD12	1:A:244:TYR:HD2	1.83	0.43
1:A:158:LEU:HD23	1:A:158:LEU:HA	1.83	0.43
1:B:150:ASP:HB2	1:B:166:ALA:HB2	2.01	0.43
1:A:110:SER:HB2	1:A:120:LEU:HD23	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:206:ASP:HB3	1:B:207:PRO:CD	2.46	0.43
1:A:8:LEU:HD23	1:A:8:LEU:HA	1.93	0.43
1:A:60:THR:HG22	1:A:88:ALA:HA	2.00	0.43
1:B:218:MET:HG2	1:B:246:PHE:CE1	2.53	0.43
1:A:69:PHE:HD2	1:A:102:GLN:CD	2.22	0.43
1:A:306:VAL:HA	1:A:307:PRO:HD3	1.82	0.43
1:B:376:LEU:O	1:B:377:ASN:C	2.52	0.43
1:A:219:THR:HA	1:A:231:LEU:O	2.19	0.43
1:A:80:ALA:O	1:A:81:PHE:HB2	2.19	0.43
1:A:204:SER:OG	1:A:207:PRO:HD2	2.19	0.42
1:B:426:VAL:HG22	1:B:427:ARG:N	2.35	0.42
1:B:110:SER:OG	1:B:115:GLN:HB3	2.20	0.42
1:A:480:VAL:HG12	1:A:480:VAL:O	2.19	0.42
1:B:301:VAL:HG12	1:B:303:THR:HG22	2.01	0.42
1:A:376:LEU:CD1	1:A:473:ASP:CG	2.74	0.42
1:B:131:ASP:C	1:B:133:TYR:H	2.22	0.42
1:B:36:ILE:HD12	1:B:108:TYR:CD1	2.55	0.42
1:B:411:VAL:HG11	1:B:431:VAL:HG21	2.02	0.42
1:B:148:LEU:HB3	1:B:209:PHE:CE2	2.54	0.42
1:B:190:VAL:HG12	1:B:196:TYR:CE1	2.54	0.41
1:A:499:PRO:O	1:A:502:HIS:HB2	2.20	0.41
1:A:404:LEU:HD13	1:A:407:HIS:HB2	2.01	0.41
1:B:367:PRO:HG2	1:B:370:SER:HB2	2.02	0.41
1:B:114:THR:HG23	1:B:463:GLU:HG3	2.03	0.41
1:B:107:TRP:HB3	1:B:201:VAL:HG11	2.03	0.41
1:A:131:ASP:C	1:A:133:TYR:H	2.23	0.41
1:B:352:LEU:HD22	1:B:356:LEU:HD11	1.99	0.41
1:A:36:ILE:HD12	1:A:108:TYR:CD1	2.55	0.41
1:A:23:ALA:O	1:A:57:MET:HE1	2.20	0.41
1:A:114:THR:HG23	1:A:463:GLU:HG3	2.03	0.41
1:A:2:ILE:HB	1:A:6:THR:HG21	2.02	0.41
1:B:328:LEU:HD11	1:B:382:LEU:HD22	2.03	0.41
1:A:28:ASN:HB2	1:A:34:PRO:HG3	2.02	0.41
1:A:110:SER:OG	1:A:115:GLN:HB3	2.21	0.41
1:B:347:PRO:HD3	1:B:367:PRO:HD3	2.02	0.41
1:A:152:TYR:CE2	1:A:166:ALA:HA	2.56	0.41
1:B:74:ASN:CG	1:B:451:PRO:HD2	2.41	0.41
1:B:404:LEU:HG	1:B:454:LEU:HD13	2.04	0.40
1:A:114:THR:HA	1:A:459:ASP:OD1	2.21	0.40
1:A:424:ASN:O	1:A:424:ASN:OD1	2.40	0.40
1:B:405:HIS:CD2	1:B:453:PHE:HB3	2.56	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	500/502 (100%)	455 (91%)	29 (6%)	16 (3%)	5	39
1	B	500/502 (100%)	455 (91%)	33 (7%)	12 (2%)	7	46
All	All	1000/1004 (100%)	910 (91%)	62 (6%)	28 (3%)	6	42

All (28) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	377	ASN
1	A	389	VAL
1	B	377	ASN
1	B	389	VAL
1	A	269	ASP
1	B	250	ALA
1	B	286	ILE
1	B	393	THR
1	A	206	ASP
1	A	250	ALA
1	A	286	ILE
1	B	172	ASN
1	B	206	ASP
1	A	120	LEU
1	A	172	ASN
1	A	317	PRO
1	B	58	LEU
1	A	58	LEU
1	A	393	THR
1	A	440	VAL
1	B	120	LEU
1	A	132	PRO

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Mol	Chain	Res	Type
1	A	391	GLY
1	B	391	GLY
1	A	254	VAL
1	B	440	VAL
1	B	132	PRO
1	A	100	PRO

### 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	423/423 (100%)	395 (93%)	28 (7%)	21	61
1	B	423/423 (100%)	394 (93%)	29 (7%)	19	59
All	All	846/846 (100%)	789 (93%)	57 (7%)	20	60

All (57) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	16	THR
1	A	68	LEU
1	A	116	TYR
1	A	187	VAL
1	A	190	VAL
1	A	195	ARG
1	A	203	LEU
1	A	219	THR
1	A	243	ARG
1	A	274	LEU
1	A	297	VAL
1	A	316	ASP
1	A	342	GLU
1	A	344	LEU
1	A	352	LEU
1	A	368	THR
1	A	374	LEU

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Mol	Chain	Res	Type
1	A	376	LEU
1	A	404	LEU
1	A	413	ARG
1	A	430	THR
1	A	453	PHE
1	A	462	LEU
1	A	463	GLU
1	A	466	PHE
1	A	490	LEU
1	A	498	ASP
1	A	502	HIS
1	B	14	ASP
1	B	16	THR
1	B	22	ARG
1	B	68	LEU
1	B	116	TYR
1	B	187	VAL
1	B	190	VAL
1	B	219	THR
1	B	243	ARG
1	B	262	ILE
1	B	297	VAL
1	B	322	VAL
1	B	342	GLU
1	B	344	LEU
1	B	345	ILE
1	B	352	LEU
1	B	368	THR
1	B	374	LEU
1	B	376	LEU
1	B	404	LEU
1	B	413	ARG
1	B	430	THR
1	B	453	PHE
1	B	462	LEU
1	B	463	GLU
1	B	466	PHE
1	B	474	THR
1	B	490	LEU
1	B	502	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	70	GLN
1	A	91	ASN
1	A	115	GLN
1	A	181	ASN
1	A	217	ASN
1	A	275	ASN
1	A	327	ASN
1	A	340	ASN
1	A	481	ASN
1	B	12	ASN
1	B	70	GLN
1	B	91	ASN
1	B	115	GLN
1	B	181	ASN
1	B	217	ASN
1	B	275	ASN
1	B	327	ASN
1	B	340	ASN
1	B	360	GLN
1	B	481	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](#)

8 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	702	1,4	14,14,15	0.70	0	15,19,21	2.06	2 (13%)
4	NAG	A	703	4	14,14,15	0.59	0	15,19,21	1.52	2 (13%)
4	NAG	A	704	1,4	14,14,15	0.56	0	15,19,21	1.49	3 (20%)
4	NAG	A	705	4	14,14,15	0.64	0	15,19,21	1.79	5 (33%)
4	NAG	B	701	1,4	14,14,15	0.83	1 (7%)	15,19,21	1.53	2 (13%)
4	NAG	B	702	4	14,14,15	0.54	0	15,19,21	2.00	2 (13%)
4	NAG	B	703	1,4	14,14,15	0.66	0	15,19,21	1.51	3 (20%)
4	NAG	B	704	4	14,14,15	0.57	0	15,19,21	2.28	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
4	NAG	A	702	1,4	-	0/6/23/26	0/1/1/1
4	NAG	A	703	4	-	0/6/23/26	0/1/1/1
4	NAG	A	704	1,4	-	0/6/23/26	0/1/1/1
4	NAG	A	705	4	-	0/6/23/26	0/1/1/1
4	NAG	B	701	1,4	-	0/6/23/26	0/1/1/1
4	NAG	B	702	4	-	0/6/23/26	0/1/1/1
4	NAG	B	703	1,4	-	0/6/23/26	0/1/1/1
4	NAG	B	704	4	-	0/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	701	NAG	C1-C2	2.52	1.55	1.52

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	702	NAG	C2-N2-C7	-7.03	114.01	123.04
4	B	704	NAG	C4-C3-C2	-6.16	101.65	111.23
4	B	703	NAG	O4-C4-C3	-2.69	104.27	110.34
4	A	705	NAG	O7-C7-C8	-2.47	117.54	122.06
4	B	701	NAG	C3-C2-N2	-2.39	104.83	110.56
4	A	705	NAG	C3-C4-C5	-2.23	106.32	110.20
4	A	704	NAG	C2-N2-C7	-2.15	120.28	123.04
4	A	703	NAG	C2-N2-C7	-2.10	120.34	123.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	703	NAG	C2-N2-C7	-2.07	120.38	123.04
4	A	702	NAG	O7-C7-C8	-2.03	118.34	122.06
4	B	704	NAG	C3-C2-N2	2.34	116.18	110.56
4	A	705	NAG	C8-C7-N2	2.42	120.73	116.11
4	B	704	NAG	O4-C4-C5	2.44	115.70	109.24
4	B	702	NAG	C4-C3-C2	2.46	115.06	111.23
4	A	705	NAG	C2-N2-C7	2.60	126.38	123.04
4	A	704	NAG	O3-C3-C2	2.72	114.51	109.11
4	B	703	NAG	O3-C3-C2	2.96	114.99	109.11
4	A	704	NAG	C1-O5-C5	3.02	116.08	112.25
4	A	703	NAG	C1-O5-C5	3.29	116.43	112.25
4	A	705	NAG	O4-C4-C5	3.48	118.46	109.24
4	B	704	NAG	C1-O5-C5	3.52	116.72	112.25
4	B	701	NAG	C1-O5-C5	4.37	117.79	112.25
4	B	702	NAG	C1-O5-C5	6.38	120.35	112.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	705	NAG	2	0
4	B	704	NAG	1	0

## 5.6 Ligand geometry

Of 12 ligands modelled in this entry, 8 are monoatomic - leaving 4 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
3	NAG	A	701	-	14,14,15	0.58	0	15,19,21	1.34	2 (13%)
3	NAG	A	706	1	14,14,15	0.68	0	15,19,21	1.94	5 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	NAG	B	705	-	14,14,15	0.55	0	15,19,21	1.25	1 (6%)
3	NAG	B	706	1	14,14,15	0.99	1 (7%)	15,19,21	1.92	6 (40%)

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	NAG	A	701	-	-	0/6/23/26	0/1/1/1
3	NAG	A	706	1	-	0/6/23/26	0/1/1/1
3	NAG	B	705	-	-	0/6/23/26	0/1/1/1
3	NAG	B	706	1	-	0/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	706	NAG	O6-C6	2.08	1.51	1.42

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	706	NAG	O3-C3-C4	-3.42	102.65	110.34
3	A	701	NAG	C1-O5-C5	-3.10	108.31	112.25
3	B	706	NAG	C2-N2-C7	-3.08	119.08	123.04
3	A	706	NAG	C2-N2-C7	-3.08	119.08	123.04
3	B	706	NAG	O7-C7-C8	-2.48	117.51	122.06
3	B	706	NAG	O3-C3-C4	-2.36	105.03	110.34
3	A	706	NAG	O7-C7-C8	-2.10	118.21	122.06
3	B	706	NAG	C8-C7-N2	2.01	119.94	116.11
3	A	701	NAG	C3-C4-C5	2.24	114.11	110.20
3	A	706	NAG	C3-C2-N2	2.47	116.47	110.56
3	A	706	NAG	O3-C3-C2	2.52	114.11	109.11
3	B	706	NAG	C4-C3-C2	2.69	115.41	111.23
3	B	705	NAG	C3-C4-C5	3.05	115.51	110.20
3	B	706	NAG	O4-C4-C5	3.31	118.02	109.24

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	701	NAG	3	0
3	B	705	NAG	3	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	502/502 (100%)	0.28	2 (0%) 93 90	23, 49, 72, 82	26 (5%)
1	B	502/502 (100%)	0.26	8 (1%) 74 69	22, 49, 72, 80	31 (6%)
All	All	1004/1004 (100%)	0.27	10 (0%) 84 78	22, 49, 72, 82	57 (5%)

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	248	LEU	3.6
1	B	178	ALA	3.6
1	B	230	PRO	3.4
1	A	11	SER	2.8
1	B	139	VAL	2.6
1	A	248	LEU	2.5
1	B	133	TYR	2.2
1	B	102	GLN	2.2
1	B	137	TYR	2.1
1	B	431	VAL	2.1

### 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

### 6.3 Carbohydrates ⓘ

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( $\text{\AA}^2$ )	Q<0.9
4	NAG	B	703	14/15	0.95	0.26	0.49	51,54,57,63	0
4	NAG	A	702	14/15	0.94	0.24	-0.10	63,66,70,71	0
4	NAG	B	701	14/15	0.93	0.24	-0.41	64,66,71,73	0
4	NAG	A	703	14/15	0.90	0.20	-0.79	45,55,59,60	0
4	NAG	B	702	14/15	0.89	0.22	-0.88	54,62,64,65	0
4	NAG	A	704	14/15	0.96	0.23	-1.35	53,58,64,65	0
4	NAG	A	705	14/15	0.86	0.27	-	68,70,72,74	0
4	NAG	B	704	14/15	0.90	0.23	-	67,70,74,74	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( $\text{\AA}^2$ )	Q<0.9
3	NAG	A	701	14/15	0.84	0.33	0.36	87,88,89,90	0
3	NAG	B	706	14/15	0.85	0.23	0.23	50,54,58,59	0
3	NAG	B	705	14/15	0.81	0.30	0.18	93,94,95,96	0
3	NAG	A	706	14/15	0.89	0.24	0.11	41,47,49,51	0
2	CU	A	601	1/1	0.99	0.12	-1.90	46,46,46,46	0
2	CU	A	603	1/1	0.98	0.14	-2.15	53,53,53,53	0
2	CU	B	604	1/1	0.95	0.13	-2.17	67,67,67,67	0
2	CU	B	601	1/1	0.99	0.12	-2.18	52,52,52,52	0
2	CU	A	602	1/1	0.97	0.11	-2.22	58,58,58,58	0
2	CU	B	602	1/1	0.98	0.13	-2.47	60,60,60,60	0
2	CU	B	603	1/1	0.98	0.12	-2.67	51,51,51,51	0
2	CU	A	604	1/1	0.98	0.13	-3.85	61,61,61,61	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.