



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 13, 2017 – 02:50 am GMT

PDB ID : 2NUV  
Title : Crystal structure of the complex of C-terminal lobe of bovine lactoferrin with atenolol at 2.25 Å resolution  
Authors : Mir, R.; Singh, N.; Sinha, M.; Sharma, S.; Kaur, P.; Singh, T.P.  
Deposited on : 2006-11-10  
Resolution : 2.25 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	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	recalc28949

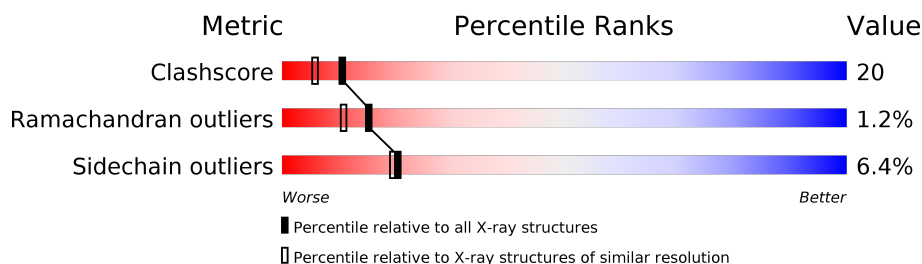
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.25 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	112137	1178 (2.26-2.26)
Ramachandran outliers	110173	1145 (2.26-2.26)
Sidechain outliers	110143	1146 (2.26-2.26)

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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	345	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	MAN	A	4	X	-	-	-
4	MAN	A	8	X	-	-	-

## 2 Entry composition [i](#)

There are 10 unique types of molecules in this entry. The entry contains 2982 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.

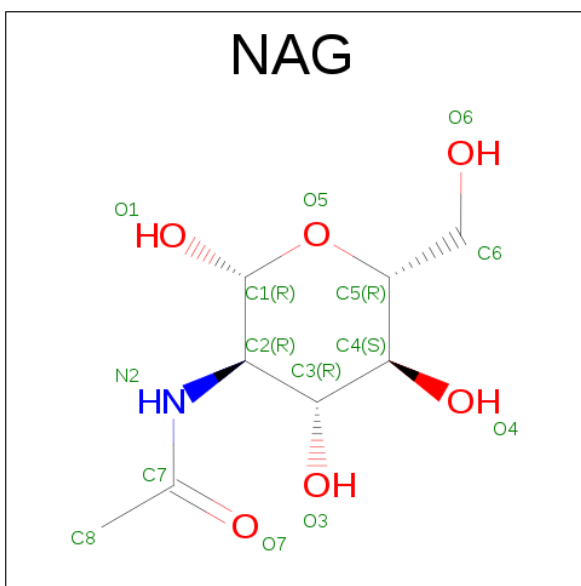
- Molecule 1 is a protein called Lactotransferrin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	341	2605	1622	454	508	21	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	565	LYS	ASN	SEE REMARK 999	UNP P24627
A	608	GLU	LYS	SEE REMARK 999	UNP P24627

- Molecule 2 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



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

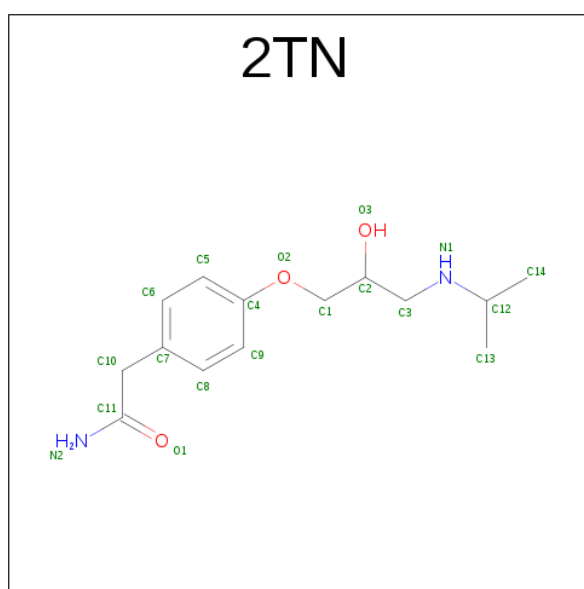
- Molecule 3 is a polymer of unknown type called SUGAR (3-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	3	Total	C	N	O	0	0
			39	22	2	15		

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	4	Total	C	N	O	0	0
			50	28	2	20		

- Molecule 5 is 2-(4-(2-HYDROXY-3-(ISOPROPYLAMINO)PROPOXY)PHENYL)ETHANAMIDE (three-letter code: 2TN) (formula:  $C_{14}H_{22}N_2O_3$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			19	14	2	3		

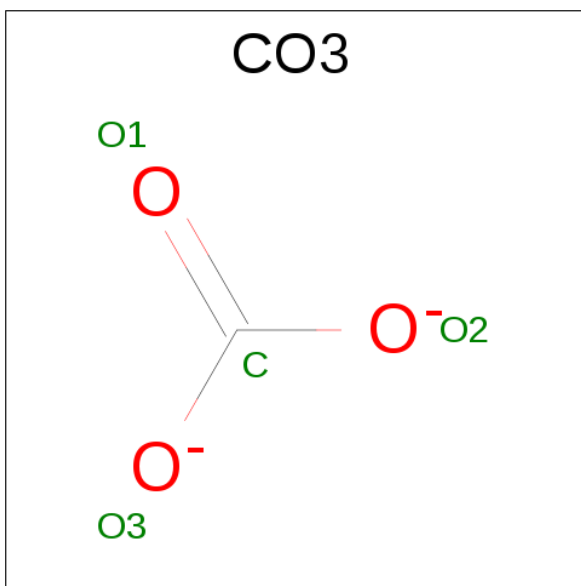
- Molecule 6 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	2	Total	Zn	0	0
			2	2		

- Molecule 7 is FE (III) ION (three-letter code: FE) (formula: Fe).

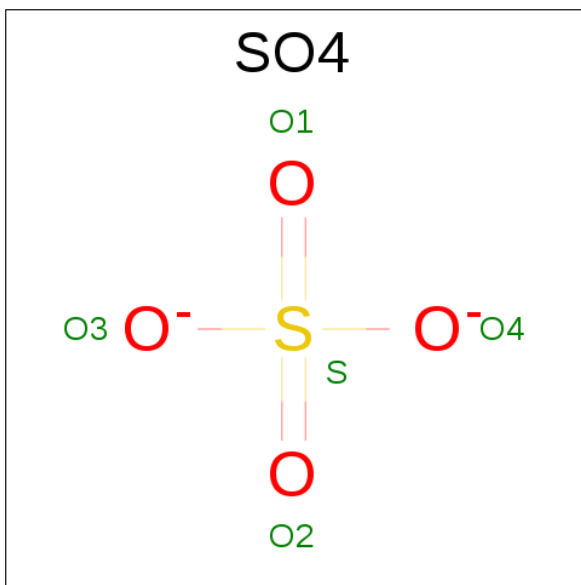
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	1	Total	Fe	0	0
			1	1		

- Molecule 8 is CARBONATE ION (three-letter code: CO3) (formula: CO<sub>3</sub>).



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

- Molecule 9 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	A	1	Total	O	S	0	0
			5	4	1		

- Molecule 10 is water.

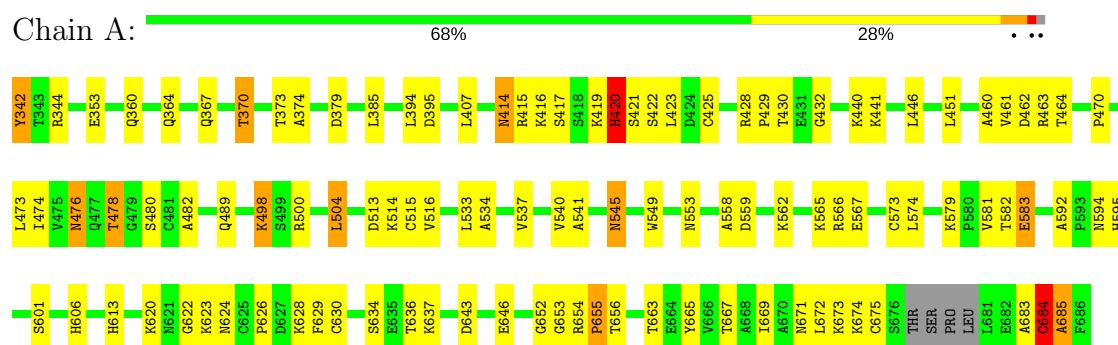
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	243	Total 243	O 243	0	0

### 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.

Note EDS was not executed.

#### • Molecule 1: Lactotransferrin



## 4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	60.65 Å   49.86 Å   64.99 Å 90.00°   106.30°   90.00°	Depositor
Resolution (Å)	19.82 – 2.25	Depositor
% Data completeness (in resolution range)	100.0 (19.82-2.25)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	CNS 0.9	Depositor
R, $R_{free}$	0.206 , 0.235	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2982	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	46.0	wwPDB-VP



## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, NAG, 2TN, CO3, FE, MAN, SO4

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	0.35	0/2653	0.74	6/3591 (0.2%)

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
3	A	1	0
4	A	1	0
All	All	2	0

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	420	HIS	N-CA-C	-6.19	94.28	111.00
1	A	656	THR	N-CA-C	-6.06	94.65	111.00
1	A	684	CYS	N-CA-C	-5.74	95.51	111.00
1	A	683	ALA	N-CA-C	5.66	126.28	111.00
1	A	394	LEU	CA-CB-CG	5.29	127.46	115.30
1	A	417	SER	N-CA-C	-5.20	96.97	111.00

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	4	MAN	C1
4	A	8	MAN	C1

There are no planarity outliers.

## 5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2605	0	2520	107	0
2	A	14	0	13	0	0
3	A	39	0	34	2	0
4	A	50	0	43	3	0
5	A	19	0	21	2	0
6	A	2	0	0	0	0
7	A	1	0	0	0	0
8	A	4	0	0	0	0
9	A	5	0	0	0	0
10	A	243	0	0	28	0
All	All	2982	0	2631	110	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 20.

All (110) 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:623:LYS:HB3	10:A:3233:HOH:O	1.42	1.19
1:A:545:ASN:HD21	4:A:5:NAG:C1	1.56	1.18
1:A:416:LYS:HD2	10:A:3200:HOH:O	1.65	0.95
1:A:545:ASN:ND2	4:A:5:NAG:C1	2.37	0.86
1:A:415:ARG:HG2	1:A:416:LYS:N	1.91	0.85
1:A:419:LYS:O	1:A:420:HIS:HB2	1.77	0.85
1:A:416:LYS:NZ	1:A:620:LYS:HE3	1.92	0.84
1:A:415:ARG:HG2	1:A:416:LYS:H	1.42	0.83
1:A:565:LYS:HG2	10:A:3245:HOH:O	1.80	0.81
1:A:344:ARG:HH11	1:A:344:ARG:HB3	1.49	0.77
1:A:565:LYS:HD3	1:A:567:GLU:H	1.48	0.77
1:A:620:LYS:HD3	1:A:646:GLU:HG3	1.71	0.73
1:A:416:LYS:HZ1	1:A:620:LYS:HE3	1.54	0.70
1:A:624:ASN:HB3	1:A:628:LYS:HB2	1.74	0.70
1:A:565:LYS:HD2	1:A:567:GLU:HB2	1.74	0.69
1:A:579:LYS:HD2	1:A:583:GLU:HG2	1.75	0.69
1:A:684:CYS:HB3	10:A:3223:HOH:O	1.93	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:344:ARG:HD2	1:A:367:GLN:O	1.94	0.67
1:A:416:LYS:NZ	1:A:620:LYS:CE	2.58	0.66
1:A:620:LYS:CD	1:A:646:GLU:HG3	2.24	0.66
1:A:613:HIS:CE1	10:A:3122:HOH:O	2.49	0.66
1:A:504:LEU:HG	1:A:537:VAL:HG12	1.78	0.64
1:A:646:GLU:HB2	10:A:3200:HOH:O	1.98	0.63
1:A:344:ARG:HB3	1:A:344:ARG:NH1	2.14	0.62
1:A:478:THR:HG23	1:A:480:SER:H	1.64	0.61
1:A:441:LYS:HE3	1:A:567:GLU:O	2.01	0.61
1:A:395:ASP:HA	1:A:595:HIS:CD2	2.35	0.60
1:A:416:LYS:HZ2	1:A:620:LYS:HE3	1.64	0.60
1:A:634:SER:O	1:A:637:LYS:HD3	2.02	0.60
1:A:624:ASN:ND2	10:A:3233:HOH:O	2.35	0.58
1:A:461:VAL:O	1:A:462:ASP:HB2	2.03	0.58
1:A:673:LYS:HE3	10:A:3030:HOH:O	2.03	0.58
1:A:637:LYS:CE	10:A:3170:HOH:O	2.51	0.57
1:A:342:TYR:HB2	10:A:3159:HOH:O	2.03	0.57
5:A:2001:2TN:H11	10:A:3141:HOH:O	2.04	0.57
1:A:416:LYS:HZ2	1:A:620:LYS:CE	2.18	0.56
1:A:514:LYS:HD3	10:A:3065:HOH:O	2.04	0.56
1:A:566:ARG:HG2	1:A:581:VAL:CG2	2.36	0.55
1:A:353:GLU:CD	10:A:3170:HOH:O	2.45	0.55
1:A:654:ARG:N	1:A:655:PRO:HD3	2.21	0.55
1:A:428:ARG:HD3	10:A:3086:HOH:O	2.07	0.54
1:A:637:LYS:NZ	10:A:3170:HOH:O	2.40	0.54
1:A:344:ARG:NH1	1:A:344:ARG:CB	2.71	0.53
1:A:373:THR:HG22	10:A:3047:HOH:O	2.07	0.53
1:A:652:GLY:O	1:A:654:ARG:N	2.37	0.52
1:A:626:PRO:HA	1:A:630:CYS:SG	2.50	0.52
1:A:423:LEU:HD12	1:A:423:LEU:H	1.75	0.52
1:A:565:LYS:CD	1:A:567:GLU:H	2.19	0.52
1:A:423:LEU:CD1	1:A:423:LEU:H	2.23	0.51
1:A:513:ASP:O	1:A:516:VAL:HG22	2.11	0.51
1:A:566:ARG:HG2	1:A:581:VAL:HG21	1.93	0.51
1:A:663:THR:O	1:A:667:THR:HG23	2.10	0.51
1:A:464:THR:HG21	1:A:592:ALA:HB1	1.93	0.51
1:A:606:HIS:HD2	10:A:3079:HOH:O	1.93	0.51
1:A:637:LYS:HE3	10:A:3170:HOH:O	2.10	0.50
1:A:636:THR:HA	1:A:643:ASP:OD2	2.12	0.50
1:A:476:ASN:OD1	3:A:2:NAG:H2	2.12	0.50
1:A:430:THR:HB	1:A:594:ASN:ND2	2.27	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:4:MAN:H5	10:A:3163:HOH:O	2.09	0.50
1:A:533:LEU:HB2	1:A:541:ALA:HB2	1.93	0.50
1:A:565:LYS:C	1:A:565:LYS:HD3	2.33	0.49
1:A:553:ASN:HD21	1:A:565:LYS:HE2	1.76	0.49
1:A:549:TRP:CZ2	1:A:582:THR:HG22	2.47	0.49
1:A:652:GLY:C	1:A:654:ARG:H	2.16	0.49
1:A:671:ASN:O	1:A:674:LYS:HG2	2.13	0.49
1:A:415:ARG:NH2	1:A:432:GLY:O	2.45	0.48
1:A:653:GLY:C	1:A:655:PRO:HD3	2.34	0.48
1:A:654:ARG:N	1:A:655:PRO:CD	2.76	0.48
1:A:478:THR:CG2	1:A:480:SER:H	2.27	0.48
1:A:624:ASN:CG	10:A:3233:HOH:O	2.51	0.48
1:A:482:ALA:CB	10:A:3235:HOH:O	2.63	0.47
1:A:558:ALA:O	1:A:562:LYS:HG3	2.14	0.47
1:A:685:ALA:N	10:A:3223:HOH:O	2.47	0.47
1:A:514:LYS:HG2	10:A:3042:HOH:O	2.15	0.46
1:A:464:THR:HG21	1:A:592:ALA:CB	2.45	0.46
1:A:646:GLU:CG	10:A:3200:HOH:O	2.63	0.46
1:A:385:LEU:HD23	1:A:407:LEU:HD21	1.98	0.46
1:A:549:TRP:CH2	1:A:582:THR:HG22	2.51	0.46
1:A:416:LYS:HZ1	1:A:620:LYS:CE	2.20	0.46
1:A:498:LYS:HE2	1:A:498:LYS:HB2	1.75	0.46
1:A:636:THR:HG21	10:A:3069:HOH:O	2.16	0.46
1:A:565:LYS:HD3	1:A:566:ARG:N	2.31	0.46
1:A:489:GLN:HB3	1:A:504:LEU:HD13	1.99	0.45
4:A:6:NAG:H4	4:A:7:MAN:H2	1.46	0.45
1:A:429:PRO:HB3	5:A:2001:2TN:HN21	1.83	0.44
1:A:482:ALA:HB1	10:A:3235:HOH:O	2.17	0.44
1:A:414:ASN:HB3	1:A:425:CYS:SG	2.57	0.44
1:A:470:PRO:O	1:A:474:ILE:HG12	2.17	0.44
1:A:419:LYS:HD3	1:A:419:LYS:HA	1.50	0.44
1:A:364:GLN:HG3	1:A:629:PHE:HB2	2.00	0.44
1:A:374:ALA:HB1	1:A:379:ASP:HB3	2.00	0.44
1:A:440:LYS:HE3	1:A:534:ALA:HA	1.99	0.44
1:A:460:ALA:HB3	1:A:463:ARG:HD3	1.99	0.44
1:A:672:LEU:O	1:A:675:CYS:HB2	2.18	0.44
1:A:414:ASN:HD22	1:A:414:ASN:HA	1.57	0.43
1:A:473:LEU:HD13	1:A:574:LEU:HD21	2.00	0.43
1:A:423:LEU:HD12	1:A:423:LEU:N	2.34	0.43
1:A:665:TYR:CZ	1:A:669:ILE:HD11	2.54	0.43
1:A:653:GLY:O	1:A:654:ARG:C	2.57	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:373:THR:CG2	10:A:3047:HOH:O	2.67	0.42
1:A:646:GLU:HG3	10:A:3200:HOH:O	2.20	0.42
1:A:344:ARG:HH11	1:A:344:ARG:CB	2.24	0.42
1:A:652:GLY:C	1:A:654:ARG:N	2.73	0.41
1:A:344:ARG:HH12	1:A:370:THR:HB	1.85	0.41
1:A:620:LYS:HD2	1:A:646:GLU:HG3	1.99	0.41
1:A:553:ASN:ND2	1:A:565:LYS:HE2	2.35	0.41
1:A:414:ASN:HD21	1:A:430:THR:HA	1.85	0.41
1:A:573:CYS:SG	1:A:579:LYS:HG3	2.61	0.41
1:A:446:LEU:HD11	1:A:451:LEU:HD23	2.03	0.40
1:A:540:VAL:HG22	1:A:541:ALA:N	2.36	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	337/345 (98%)	312 (93%)	21 (6%)	4 (1%)	15 11

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	420	HIS
1	A	685	ALA
1	A	684	CYS
1	A	622	GLY

### 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	282/286 (99%)	264 (94%)	18 (6%)	20	19

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	342	TYR
1	A	360	GLN
1	A	370	THR
1	A	414	ASN
1	A	420	HIS
1	A	421	SER
1	A	422	SER
1	A	476	ASN
1	A	478	THR
1	A	498	LYS
1	A	500	ARG
1	A	504	LEU
1	A	515	CYS
1	A	545	ASN
1	A	559	ASP
1	A	583	GLU
1	A	601	SER
1	A	655	PRO

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	359	GLN
1	A	393	ASN
1	A	414	ASN
1	A	545	ASN
1	A	585	GLN
1	A	624	ASN
1	A	671	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 ⓘ

7 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	$\# Z  > 2$
3	NAG	A	2	1,3	14,14,15	0.84	0	15,19,21	1.37	2 (13%)
3	NAG	A	3	3	14,14,15	0.72	0	15,19,21	0.92	1 (6%)
3	MAN	A	4	3	11,11,12	0.42	0	13,15,17	0.36	0
4	NAG	A	5	4	14,14,15	0.52	0	15,19,21	1.07	1 (6%)
4	NAG	A	6	4	14,14,15	0.71	0	15,19,21	1.29	2 (13%)
4	MAN	A	7	4	11,11,12	0.80	0	13,15,17	1.77	3 (23%)
4	MAN	A	8	4	11,11,12	0.65	0	13,15,17	1.04	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
3	NAG	A	2	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	3	3	-	0/6/23/26	0/1/1/1
3	MAN	A	4	3	1/1/4/5	0/2/19/22	0/1/1/1
4	NAG	A	5	4	-	0/6/23/26	0/1/1/1
4	NAG	A	6	4	-	0/6/23/26	0/1/1/1
4	MAN	A	7	4	-	0/2/19/22	1/1/1/1
4	MAN	A	8	4	1/1/4/5	0/2/19/22	0/1/1/1

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	3	NAG	C1-C2-N2	-2.75	105.79	110.49
4	A	5	NAG	C2-N2-C7	-2.14	119.82	122.94
4	A	7	MAN	O5-C1-C2	2.23	114.28	110.79
4	A	6	NAG	C3-C4-C5	2.23	114.16	110.22
4	A	8	MAN	C3-C4-C5	2.44	114.52	110.22
4	A	7	MAN	C3-C4-C5	2.55	114.71	110.22
3	A	2	NAG	O5-C1-C2	2.69	115.22	111.47
4	A	6	NAG	C4-C3-C2	3.45	116.07	111.02
3	A	2	NAG	C1-O5-C5	3.58	117.10	112.17
4	A	7	MAN	C1-O5-C5	4.64	118.56	112.17

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	A	8	MAN	C1
3	A	4	MAN	C1

There are no torsion outliers.

All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	7	MAN	C1-C2-C3-C4-C5-O5

5 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	2	NAG	1	0
3	A	4	MAN	1	0
4	A	5	NAG	2	0
4	A	6	NAG	1	0
4	A	7	MAN	1	0

## 5.6 Ligand geometry [i](#)

Of 7 ligands modelled in this entry, 3 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
9	SO4	A	1001	-	4,4,4	1.54	1 (25%)	6,6,6	0.80	0
8	CO3	A	1999	7	0,3,3	0.00	-	0,3,3	0.00	-
5	2TN	A	2001	-	19,19,19	1.56	3 (15%)	23,24,24	4.08	12 (52%)
2	NAG	A	3001	1	14,14,15	0.60	0	15,19,21	0.71	0

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
9	SO4	A	1001	-	-	0/0/0/0	0/0/0/0
8	CO3	A	1999	7	-	0/0/0/0	0/0/0/0
5	2TN	A	2001	-	-	0/14/14/14	0/1/1/1
2	NAG	A	3001	1	-	0/6/23/26	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	A	1001	SO4	O1-S	2.59	1.59	1.45
5	A	2001	2TN	C9-C4	2.97	1.44	1.38
5	A	2001	2TN	C6-C5	3.12	1.44	1.38
5	A	2001	2TN	C9-C8	3.22	1.44	1.38

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	2001	2TN	C5-C4-C9	-7.93	107.70	120.19
5	A	2001	2TN	C8-C7-C6	-4.99	110.26	118.16
5	A	2001	2TN	C10-C7-C6	2.21	124.07	120.89
5	A	2001	2TN	C6-C5-C4	2.39	122.74	119.74
5	A	2001	2TN	O2-C4-C5	2.71	133.31	119.94
5	A	2001	2TN	C14-C12-N1	2.96	120.02	110.37
5	A	2001	2TN	C10-C7-C8	3.31	125.66	120.89
5	A	2001	2TN	O3-C2-C1	3.41	121.92	109.34
5	A	2001	2TN	O3-C2-C3	5.26	128.49	109.35
5	A	2001	2TN	C5-C6-C7	5.66	128.82	121.02

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Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
5	A	2001	2TN	C8-C9-C4	8.48	130.36	119.74
5	A	2001	2TN	O2-C1-C2	10.01	127.21	107.63

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	2001	2TN	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

### 6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

### 6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

### 6.4 Ligands

EDS was not executed - this section is therefore empty.

### 6.5 Other polymers

EDS was not executed - this section is therefore empty.