



# Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 10:48 AM GMT

PDB ID : 2DSF  
Title : Structure of the complex of C-terminal lobe of bovine lactoferrin with xylose at 2.8Å resolution  
Authors : Mir, R.; Singh, N.; Sinha, M.; Sharma, S.; Bhushan, A.; Singh, T.P.  
Deposited on : 2006-06-29  
Resolution : 2.80 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

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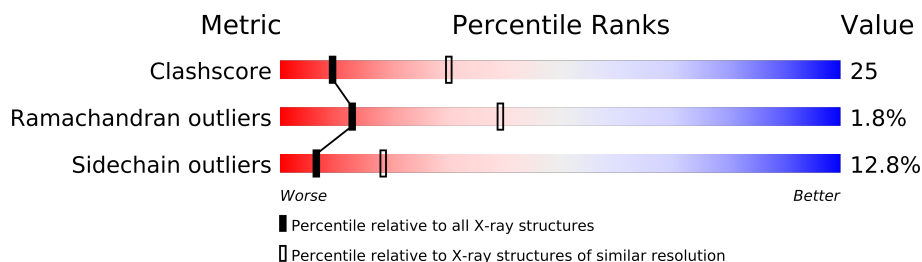
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 21963  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 2.80 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	79885	2295 (2.80-2.80)
Ramachandran outliers	78287	2252 (2.80-2.80)
Sidechain outliers	78261	2254 (2.80-2.80)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	345	

## 2 Entry composition i

There are 10 unique types of molecules in this entry. The entry contains 2921 atoms, of which 0 are hydrogen and 0 are deuterium.

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.

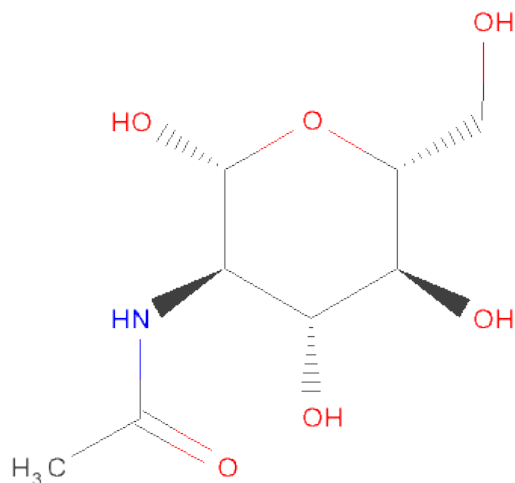
- Molecule 1 is a protein called Lactotransferrin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	341	2604	1622	454	507	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		

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

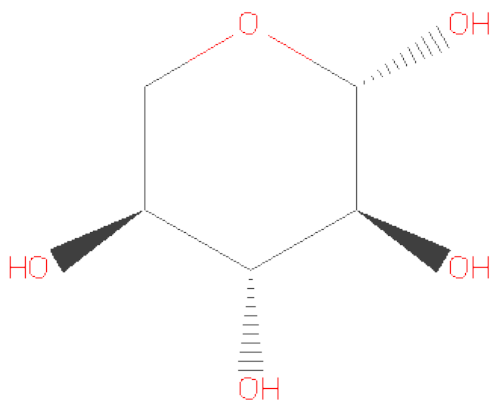
- Molecule 4 is a polymer of unknown type called SUGAR (4-MER).

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

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 5 is BETA-L-XYLOPYRANOSE (three-letter code: LXC) (formula: C<sub>5</sub>H<sub>10</sub>O<sub>5</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			10	5	5		

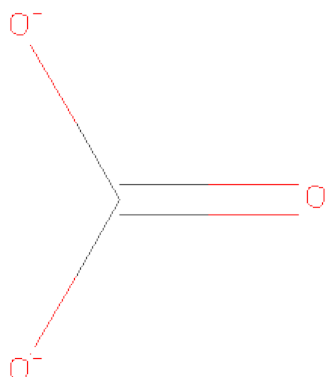
- Molecule 6 is ZINC ION (three-letter code: ZN) (formula: Zn).

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).

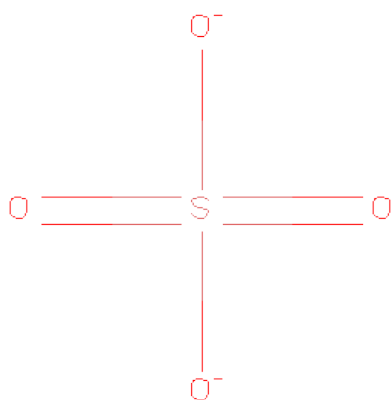
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	1	Total	Fe	0	0
			1	1		

- 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	192	Total	O	0	0
			192	192		

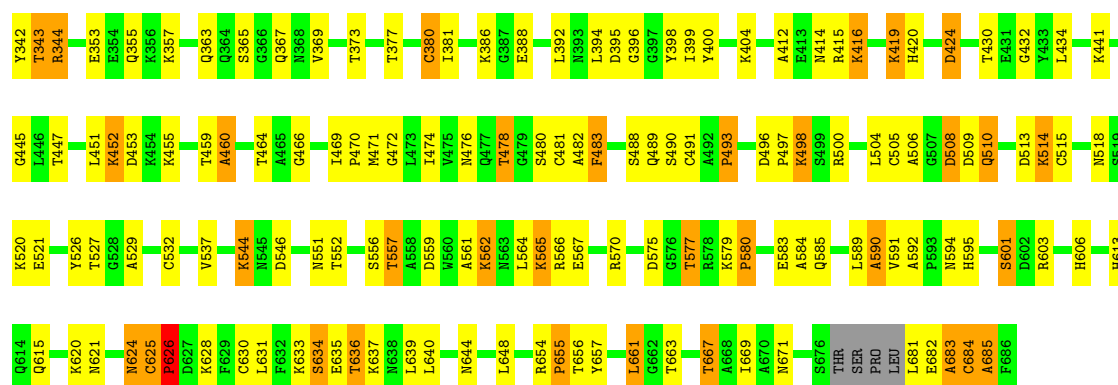
### 3 Residue-property plots

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.

Note EDS was not executed.

#### • Molecule 1: Lactotransferrin

Chain A: 



## 4 Data and refinement statistics

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

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	63.45Å 50.44Å 65.87Å 90.00° 107.80° 90.00°	Depositor
Resolution (Å)	19.94 – 2.80	Depositor
% Data completeness (in resolution range)	92.9 (19.94-2.80)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	CNS 0.9	Depositor
R, $R_{free}$	0.201 , 0.231	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2921	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	29.0	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, BMA, NAG, CO3, NDG, LXC, SO4, MAN, FE

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	0.57	2/2652 (0.1%)	1.07	14/3591 (0.4%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	683	ALA	CA-CB	-5.56	1.40	1.52
1	A	510	GLN	CA-CB	-5.01	1.43	1.53

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	625	CYS	C-N-CD	-22.02	72.15	120.60
1	A	683	ALA	N-CA-C	13.13	146.44	111.00
1	A	625	CYS	C-N-CA	8.49	157.66	122.00
1	A	656	THR	N-CA-C	-8.45	88.20	111.00
1	A	626	PRO	CA-N-CD	-6.66	102.18	111.50
1	A	682	GLU	N-CA-CB	6.58	122.45	110.60
1	A	681	LEU	CA-CB-CG	6.35	129.91	115.30
1	A	684	CYS	N-CA-C	-6.28	94.04	111.00
1	A	683	ALA	N-CA-CB	-6.05	101.63	110.10
1	A	683	ALA	CB-CA-C	-5.82	101.37	110.10
1	A	625	CYS	N-CA-C	-5.74	95.51	111.00
1	A	682	GLU	CA-CB-CG	-5.71	100.84	113.40
1	A	682	GLU	C-N-CA	-5.50	107.94	121.70
1	A	419	LYS	N-CA-C	-5.14	97.12	111.00

There are no chirality outliers.

There are no planarity outliers.

## 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2604	0	2518	131	0
2	A	14	0	13	0	0
3	A	39	0	34	2	0
4	A	50	0	43	2	0
5	A	10	0	7	0	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	192	0	0	22	0
All	All	2921	0	2615	132	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 25.

All (132) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:625:CYS:SG	1:A:626:PRO:HD3	1.71	1.28
1:A:395:ASP:HA	1:A:595:HIS:CD2	2.00	0.96
1:A:625:CYS:SG	1:A:626:PRO:CD	2.62	0.88
1:A:685:ALA:HB2	10:A:4026:HOH:O	1.75	0.85
1:A:474:ILE:O	1:A:478:THR:HB	1.76	0.85
1:A:620:LYS:C	1:A:621:ASN:HD22	1.86	0.78
1:A:355:GLN:HG3	1:A:373:THR:OG1	1.87	0.74
1:A:635:GLU:O	1:A:637:LYS:HG3	1.89	0.73
1:A:419:LYS:NZ	1:A:420:HIS:NE2	2.36	0.71
1:A:404:LYS:HD3	1:A:683:ALA:HB3	1.72	0.71
1:A:419:LYS:HZ2	1:A:420:HIS:CD2	2.08	0.71
1:A:552:THR:OG1	1:A:566:ARG:HG2	1.90	0.71
1:A:472:GLY:O	1:A:476:ASN:HB2	1.91	0.70
1:A:478:THR:HG22	1:A:480:SER:H	1.57	0.69
1:A:342:TYR:O	1:A:606:HIS:NE2	2.28	0.67
1:A:565:LYS:NZ	1:A:567:GLU:HB2	2.09	0.67
1:A:424:ASP:HB2	10:A:4020:HOH:O	1.94	0.66

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:343:THR:HA	1:A:606:HIS:NE2	2.11	0.66
1:A:584:ALA:HB3	4:A:5:NAG:H82	1.76	0.66
1:A:685:ALA:CB	10:A:4026:HOH:O	2.38	0.66
1:A:603:ARG:NH2	10:A:4036:HOH:O	2.27	0.66
1:A:585:GLN:HG2	10:A:3958:HOH:O	1.98	0.64
1:A:419:LYS:HZ2	1:A:420:HIS:CE1	2.15	0.63
1:A:606:HIS:HD2	10:A:4036:HOH:O	1.82	0.63
1:A:357:LYS:HG3	10:A:4022:HOH:O	1.99	0.62
1:A:478:THR:CG2	1:A:480:SER:H	2.12	0.62
1:A:478:THR:CG2	1:A:480:SER:HB3	2.30	0.61
1:A:471:MET:HE1	1:A:474:ILE:HD12	1.82	0.60
1:A:404:LYS:HB3	1:A:684:CYS:H	1.64	0.60
1:A:380:CYS:HB3	1:A:392:LEU:HD13	1.83	0.60
1:A:363:GLN:HA	10:A:4068:HOH:O	2.00	0.60
3:A:4:BMA:H4	10:A:4085:HOH:O	2.01	0.60
1:A:626:PRO:HD3	1:A:630:CYS:SG	2.42	0.59
1:A:601:SER:C	1:A:603:ARG:H	2.04	0.59
1:A:488:SER:HA	1:A:500:ARG:NH2	2.19	0.58
1:A:529:ALA:O	1:A:532:CYS:HB3	2.03	0.58
1:A:565:LYS:HZ2	1:A:567:GLU:HB2	1.68	0.58
1:A:654:ARG:N	1:A:655:PRO:HD3	2.19	0.57
1:A:513:ASP:OD2	1:A:520:LYS:HD3	2.04	0.57
1:A:489:GLN:HB3	1:A:504:LEU:HD13	1.85	0.57
1:A:518:ASN:OD1	1:A:520:LYS:HB2	2.04	0.57
1:A:399:ILE:CG2	1:A:661:LEU:HD11	2.35	0.56
1:A:685:ALA:HA	10:A:4080:HOH:O	2.06	0.56
1:A:654:ARG:NH2	10:A:4042:HOH:O	2.39	0.56
1:A:430:THR:HB	1:A:594:ASN:ND2	2.19	0.56
1:A:399:ILE:HG22	1:A:661:LEU:HD11	1.87	0.55
1:A:575:ASP:OD1	1:A:577:THR:HB	2.06	0.55
1:A:452:LYS:O	1:A:453:ASP:HB2	2.07	0.55
1:A:357:LYS:HD3	1:A:640:LEU:HG	1.88	0.55
1:A:532:CYS:O	1:A:537:VAL:HB	2.07	0.54
1:A:565:LYS:HZ3	1:A:567:GLU:H	1.56	0.54
1:A:589:LEU:O	1:A:590:ALA:HB2	2.09	0.53
1:A:394:LEU:O	1:A:595:HIS:HA	2.09	0.52
1:A:445:GLY:O	1:A:447:THR:HG23	2.10	0.52
1:A:469:ILE:N	1:A:470:PRO:HD2	2.25	0.52
1:A:478:THR:HG23	1:A:480:SER:HB3	1.91	0.52
1:A:496:ASP:OD1	1:A:498:LYS:HD3	2.09	0.52
1:A:357:LYS:O	1:A:357:LYS:HG2	2.10	0.51
1:A:556:SER:C	1:A:557:THR:HG23	2.30	0.51

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:654:ARG:N	1:A:655:PRO:CD	2.74	0.51
1:A:464:THR:HG21	1:A:592:ALA:CB	2.41	0.51
1:A:459:THR:OG1	1:A:466:GLY:HA3	2.12	0.50
1:A:634:SER:OG	1:A:639:LEU:HG	2.10	0.50
1:A:526:TYR:CE2	1:A:544:LYS:HE2	2.45	0.50
1:A:455:LYS:HB3	1:A:504:LEU:HD21	1.95	0.49
1:A:570:ARG:NH1	1:A:580:PRO:HA	2.27	0.49
1:A:464:THR:HG21	1:A:592:ALA:HB1	1.94	0.49
1:A:367:GLN:HB2	10:A:4056:HOH:O	2.13	0.49
1:A:601:SER:C	1:A:603:ARG:N	2.66	0.49
1:A:639:LEU:O	1:A:640:LEU:HB2	2.13	0.49
1:A:657:TYR:O	1:A:661:LEU:HD12	2.13	0.48
1:A:419:LYS:HD3	1:A:420:HIS:N	2.28	0.48
1:A:482:ALA:HA	10:A:4097:HOH:O	2.13	0.48
1:A:342:TYR:O	1:A:606:HIS:CD2	2.66	0.48
1:A:544:LYS:HG3	1:A:546:ASP:H	1.79	0.48
1:A:490:SER:C	1:A:504:LEU:HB2	2.34	0.48
1:A:667:THR:O	1:A:671:ASN:ND2	2.47	0.48
1:A:415:ARG:HH11	1:A:415:ARG:HG2	1.78	0.47
1:A:551:ASN:HA	1:A:556:SER:HB2	1.96	0.47
1:A:620:LYS:O	1:A:621:ASN:ND2	2.41	0.47
1:A:559:ASP:HB3	10:A:3962:HOH:O	2.14	0.47
1:A:505:CYS:HB3	1:A:521:GLU:OE1	2.15	0.47
1:A:344:ARG:HB2	10:A:4032:HOH:O	2.13	0.47
1:A:506:ALA:HA	1:A:514:LYS:HE2	1.96	0.47
1:A:483:PHE:C	1:A:483:PHE:CD2	2.88	0.47
1:A:434:LEU:HD12	1:A:584:ALA:HB1	1.96	0.46
1:A:634:SER:C	1:A:635:GLU:HG3	2.36	0.46
1:A:546:ASP:HA	4:A:5:NAG:H62	1.96	0.46
1:A:505:CYS:O	1:A:514:LYS:HE2	2.14	0.46
1:A:353:GLU:OE1	1:A:637:LYS:HE2	2.15	0.46
1:A:498:LYS:HE2	1:A:498:LYS:HB2	1.63	0.46
1:A:671:ASN:ND2	3:A:2:NDG:H3	2.31	0.46
1:A:459:THR:O	1:A:460:ALA:HB2	2.15	0.46
1:A:419:LYS:O	1:A:420:HIS:HB2	2.14	0.45
1:A:377:THR:HG21	1:A:398:TYR:CD2	2.52	0.45
1:A:377:THR:O	1:A:381:ILE:HG12	2.16	0.45
1:A:416:LYS:HG2	1:A:416:LYS:H	1.47	0.45
1:A:671:ASN:HB3	10:A:4019:HOH:O	2.16	0.45
1:A:559:ASP:HA	1:A:562:LYS:HG3	1.99	0.45
1:A:624:ASN:HB3	1:A:628:LYS:HB2	1.98	0.45
1:A:633:LYS:HA	1:A:633:LYS:HD3	1.88	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:561:ALA:HA	1:A:564:LEU:HG	1.98	0.44
1:A:577:THR:HG21	1:A:579:LYS:HZ3	1.82	0.44
1:A:396:GLY:HA2	1:A:399:ILE:HD12	2.00	0.44
1:A:451:LEU:HD12	10:A:3994:HOH:O	2.18	0.43
1:A:400:TYR:CD2	1:A:669:ILE:HG21	2.53	0.43
1:A:464:THR:O	1:A:469:ILE:HG12	2.18	0.43
1:A:395:ASP:HA	1:A:595:HIS:CG	2.52	0.43
1:A:685:ALA:CB	10:A:4080:HOH:O	2.65	0.43
1:A:565:LYS:C	1:A:565:LYS:HD3	2.39	0.43
1:A:365:SER:C	1:A:367:GLN:N	2.71	0.43
1:A:367:GLN:C	1:A:369:VAL:N	2.71	0.43
1:A:481:CYS:C	1:A:483:PHE:H	2.23	0.42
1:A:471:MET:HE1	1:A:474:ILE:CD1	2.49	0.42
1:A:636:THR:HG22	10:A:3971:HOH:O	2.18	0.42
1:A:613:HIS:HD2	10:A:4015:HOH:O	2.01	0.42
1:A:491:CYS:SG	1:A:493:PRO:HD3	2.59	0.42
1:A:518:ASN:OD1	1:A:518:ASN:C	2.59	0.42
1:A:565:LYS:HZ3	1:A:567:GLU:HB2	1.83	0.41
1:A:469:ILE:H	1:A:470:PRO:HD2	1.85	0.41
1:A:412:ALA:O	1:A:648:LEU:HA	2.20	0.41
1:A:480:SER:OG	1:A:481:CYS:N	2.53	0.41
1:A:526:TYR:CZ	1:A:544:LYS:HE2	2.56	0.41
1:A:367:GLN:C	1:A:369:VAL:H	2.20	0.41
1:A:683:ALA:HB1	1:A:684:CYS:O	2.21	0.41
1:A:386:LYS:HD2	1:A:388:GLU:OE1	2.19	0.41
1:A:577:THR:CG2	1:A:579:LYS:HZ3	2.34	0.41
1:A:415:ARG:NH2	1:A:432:GLY:O	2.48	0.41
1:A:644:ASN:N	10:A:3952:HOH:O	2.53	0.40
1:A:606:HIS:CD2	10:A:4036:HOH:O	2.66	0.40
1:A:508:ASP:OD1	1:A:508:ASP:N	2.53	0.40
1:A:544:LYS:HD2	1:A:546:ASP:OD1	2.21	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone ⓘ

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%)	302 (90%)	29 (9%)	6 (2%)	13	39

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	508	ASP
1	A	626	PRO
1	A	685	ALA
1	A	590	ALA
1	A	636	THR
1	A	460	ALA

### 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	282/286 (99%)	246 (87%)	36 (13%)	6	18

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	343	THR
1	A	344	ARG
1	A	380	CYS
1	A	414	ASN
1	A	416	LYS
1	A	424	ASP
1	A	441	LYS
1	A	452	LYS
1	A	478	THR
1	A	483	PHE
1	A	493	PRO
1	A	497	PRO
1	A	498	LYS
1	A	509	ASP
1	A	510	GLN
1	A	514	LYS
1	A	515	CYS

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Mol	Chain	Res	Type
1	A	527	THR
1	A	544	LYS
1	A	557	THR
1	A	562	LYS
1	A	565	LYS
1	A	577	THR
1	A	580	PRO
1	A	583	GLU
1	A	591	VAL
1	A	601	SER
1	A	615	GLN
1	A	624	ASN
1	A	626	PRO
1	A	631	LEU
1	A	634	SER
1	A	655	PRO
1	A	661	LEU
1	A	663	THR
1	A	667	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	355	GLN
1	A	363	GLN
1	A	414	ASN
1	A	458	HIS
1	A	510	GLN
1	A	585	GLN
1	A	621	ASN
1	A	671	ASN

### 5.3.3 RNA ⓘ

There are no RNA chains 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	NDG	A	2	1,3	12,14,15	0.95	0	15,19,21	1.21	1 (6%)
3	NAG	A	3	3	12,14,15	0.70	0	15,19,21	1.26	2 (13%)
3	BMA	A	4	3	10,11,12	0.67	0	11,15,17	0.96	1 (9%)
4	NAG	A	5	1,4	12,14,15	0.90	0	15,19,21	0.79	0
4	NAG	A	6	4	12,14,15	0.90	0	15,19,21	1.16	2 (13%)
4	MAN	A	7	4	10,11,12	0.99	0	11,15,17	1.54	2 (18%)
4	BMA	A	8	4	10,11,12	0.66	0	11,15,17	1.55	2 (18%)

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	NDG	A	2	1,3	-	0/6/23/26	1/1/1/1
3	NAG	A	3	3	-	0/6/23/26	0/1/1/1
3	BMA	A	4	3	-	0/2/19/22	0/1/1/1
4	NAG	A	5	1,4	-	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	0/1/1/1
4	BMA	A	8	4	-	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(°)
4	A	8	BMA	C3-C4-C5	3.95	117.26	110.20
4	A	7	MAN	C3-C4-C5	3.82	117.02	110.20
4	A	6	NAG	C3-C2-N2	-2.74	107.58	111.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	4	BMA	C4-C3-C2	2.58	113.96	110.50
3	A	3	NAG	C2-N2-C7	-2.43	119.02	123.09
4	A	7	MAN	C6-C5-C4	-2.38	107.25	113.00
3	A	2	NDG	C3-C4-C5	-2.37	105.97	110.20
4	A	8	BMA	O5-C5-C4	2.19	113.43	110.65
4	A	6	NAG	C3-C4-C5	-2.13	106.39	110.20
3	A	3	NAG	O5-C5-C6	-2.03	104.85	106.98

There are no chirality outliers.

There are no torsion outliers.

All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	2	NDG	C1-C2-C3-C4-C5-O

## 5.6 Ligand geometry ⓘ

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	$\# Z  > 2$
2	NAG	A	1001	1	12,14,15	0.65	0	15,19,21	1.96	5 (33%)
8	CO3	A	1999	7	0,3,3	0.00	-	0,3,3	0.00	-
5	LXC	A	3937	-	10,10,10	1.24	0	14,14,14	5.10	12 (85%)
9	SO4	A	3938	-	4,4,4	0.16	0	6,6,6	0.08	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
2	NAG	A	1001	1	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	CO3	A	1999	7	-	0/0/0/0	0/0/0/0
5	LXC	A	3937	-	3/3/4/4	0/0/17/17	0/1/1/1
9	SO4	A	3938	-	-	0/0/0/0	0/0/0/0

There are no bond length outliers.

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	3937	LXC	O5-C1-C2	8.92	122.00	109.24
5	A	3937	LXC	O3-C3-C4	7.70	123.94	110.03
5	A	3937	LXC	C5-C4-C3	7.35	118.97	109.71
5	A	3937	LXC	O2-C2-C1	6.54	123.80	109.89
5	A	3937	LXC	O4-C4-C5	5.18	119.87	109.14
5	A	3937	LXC	C1-C2-C3	4.83	118.19	110.53
5	A	3937	LXC	O4-C4-C3	4.31	118.60	110.23
5	A	3937	LXC	O1-C1-O5	4.19	121.33	109.88
2	A	1001	NAG	C3-C4-C5	4.08	117.50	110.20
5	A	3937	LXC	O3-C3-C2	3.52	118.25	110.35
5	A	3937	LXC	O2-C2-C3	3.41	118.00	110.35
2	A	1001	NAG	C6-C5-C4	-3.33	104.95	113.00
5	A	3937	LXC	C4-C3-C2	2.88	115.98	110.89
2	A	1001	NAG	C2-N2-C7	-2.83	118.33	123.09
2	A	1001	NAG	C3-C2-N2	-2.78	107.53	111.76
2	A	1001	NAG	O5-C5-C4	2.71	114.09	110.65
5	A	3937	LXC	O1-C1-C2	2.28	115.92	109.47

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	A	3937	LXC	C3
5	A	3937	LXC	C2
5	A	3937	LXC	C1

There are no torsion outliers.

There are no ring outliers.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

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 will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

### 6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

### 6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

### 6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.