



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 04:45 AM GMT

PDB ID : 2O51  
Title : Crystal structure of bovine C-lobe with fructose at 3.0 Å resolution  
Authors : Mir, R.; Ethayathulla, A.S.; Sinha, M.; Singh, N.; Sharma, S.; Singh, T.P.  
Deposited on : 2006-12-05  
Resolution : 3.00 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) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

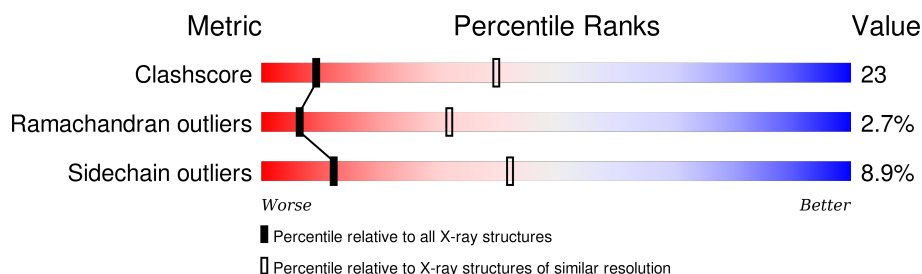
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.00 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	1912 (3.00-3.00)
Ramachandran outliers	100387	1853 (3.00-3.00)
Sidechain outliers	100360	1856 (3.00-3.00)

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	NAG	A	687	-	-	X	-
3	NAG	A	688	X	-	-	-
4	NAG	A	690	X	-	-	-

## 2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 2936 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
1	A	341	Total	C	N	O	S	0	0	0
			2605	1622	454	508	21			

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

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

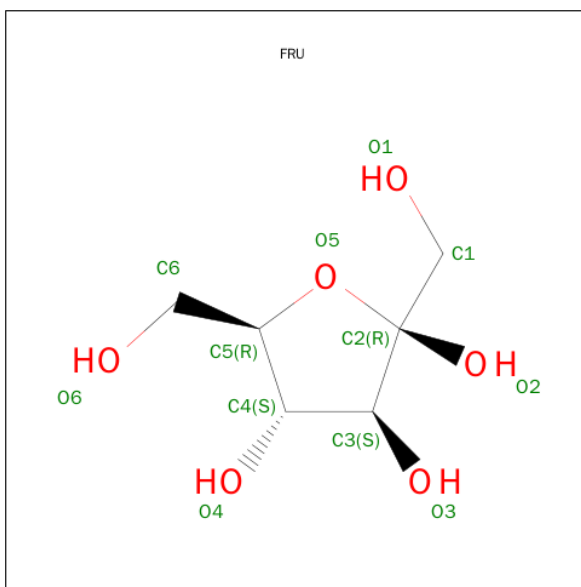
- Molecule 3 is a polymer of unknown type called SUGAR (2-MER).

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

- 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 SUGAR (FRUCTOSE) (three-letter code: FRU) (formula: C<sub>6</sub>H<sub>12</sub>O<sub>6</sub>).

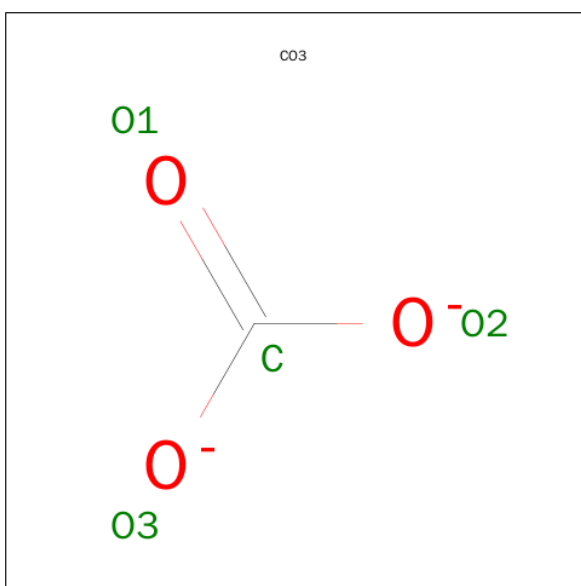


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			12	6	6		

- Molecule 6 is FE (III) ION (three-letter code: FE) (formula: Fe).

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

- Molecule 7 is CARBONATE ION (three-letter code: CO3) (formula: CO<sub>3</sub>).

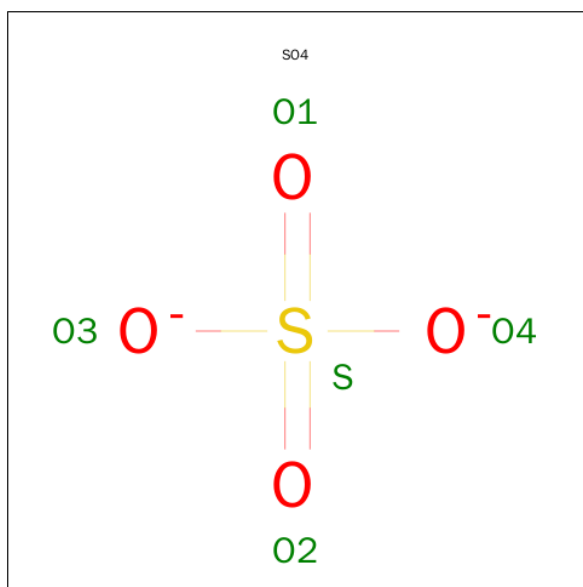


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			4	1	3		

- Molecule 8 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- 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.

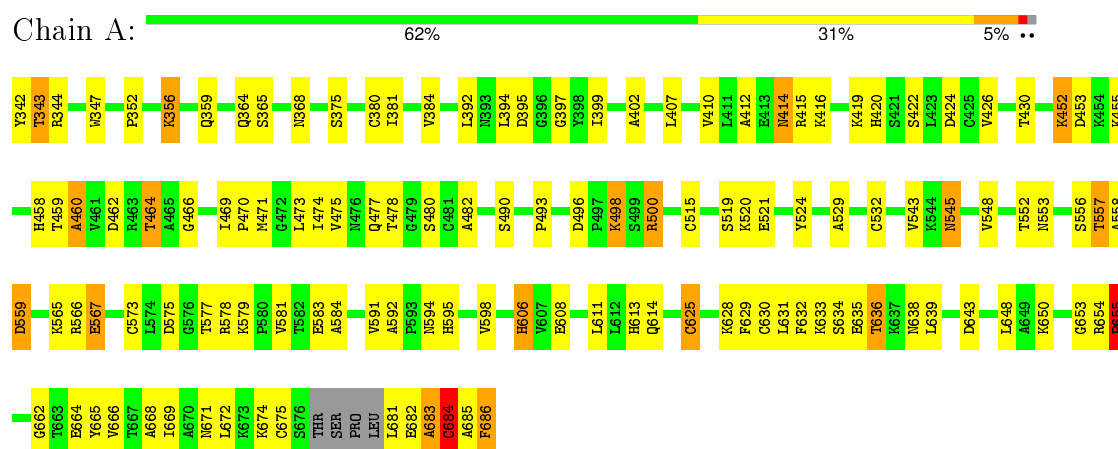
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	179	Total	O	0	0
			179	179		

### 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.

Note EDS was not executed.

#### • Molecule 1: Lactotransferrin



## 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, $\alpha$ , $\beta$ , $\gamma$	63.58 Å 50.33 Å 66.08 Å 90.00° 107.94° 90.00°	Depositor
Resolution (Å)	19.84 – 3.00	Depositor
% Data completeness (in resolution range)	95.9 (19.84-3.00)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.13	Depositor
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.180 , 0.202	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2936	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	31.0	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: CO3, BMA, NAG, ZN, FE, FRU, 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	0.58	1/2653 (0.0%)	0.72	1/3591 (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
3	A	1	0
4	A	1	0
All	All	2	0

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	686	PHE	C-OXT	22.34	1.65	1.23

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	655	PRO	CA-N-CD	-9.80	97.78	111.50

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	688	NAG	C1
4	A	690	NAG	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	2521	116	0
2	A	50	0	43	2	0
3	A	28	0	25	8	0
4	A	50	0	43	9	0
5	A	12	0	12	0	0
6	A	1	0	0	0	0
7	A	4	0	0	0	0
8	A	2	0	0	0	0
9	A	5	0	0	0	0
10	A	179	0	0	16	0
All	All	2936	0	2644	121	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 23.

All (121) 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:545:ASN:HD21	4:A:689:NAG:C1	1.34	1.38
1:A:686:PHE:C	1:A:686:PHE:OXT	1.65	1.33
1:A:368:ASN:HD21	3:A:687:NAG:C1	1.44	1.28
1:A:368:ASN:HD21	3:A:687:NAG:C2	1.81	0.92
1:A:416:LYS:HG3	10:A:765:HOH:O	1.72	0.89
1:A:545:ASN:CG	4:A:689:NAG:C1	2.50	0.80
1:A:545:ASN:HD21	4:A:689:NAG:C2	1.96	0.79
1:A:682:GLU:O	1:A:683:ALA:HB2	1.83	0.79
1:A:430:THR:HB	1:A:594:ASN:ND2	2.00	0.77
3:A:688:NAG:H82	10:A:775:HOH:O	1.86	0.76
1:A:653:GLY:C	1:A:655:PRO:HD3	2.05	0.76
1:A:545:ASN:OD1	4:A:689:NAG:C1	2.34	0.75
1:A:343:THR:O	1:A:343:THR:HG23	1.86	0.75
1:A:368:ASN:CG	3:A:687:NAG:C1	2.54	0.74
1:A:683:ALA:O	1:A:684:CYS:HB3	1.87	0.74
1:A:683:ALA:HB1	10:A:785:HOH:O	1.90	0.72
1:A:686:PHE:OXT	1:A:686:PHE:CB	2.38	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:430:THR:HB	1:A:594:ASN:HD22	1.53	0.71
4:A:690:NAG:H61	4:A:691:MAN:O2	1.90	0.71
4:A:691:MAN:H4	4:A:692:BMA:O2	1.91	0.69
1:A:686:PHE:OXT	1:A:686:PHE:CA	2.41	0.68
1:A:419:LYS:O	1:A:420:HIS:HB2	1.94	0.67
3:A:687:NAG:H2	10:A:766:HOH:O	1.95	0.67
1:A:653:GLY:O	1:A:655:PRO:HD3	1.94	0.66
1:A:653:GLY:O	1:A:654:ARG:C	2.33	0.66
1:A:565:LYS:HD3	1:A:567:GLU:HG2	1.79	0.64
1:A:395:ASP:HA	1:A:595:HIS:CD2	2.32	0.64
1:A:632:PHE:O	1:A:633:LYS:HD2	1.99	0.63
1:A:548:VAL:HG11	1:A:581:VAL:HG11	1.79	0.63
1:A:636:THR:HG23	1:A:636:THR:O	1.97	0.62
1:A:473:LEU:O	1:A:477:GLN:HG3	1.99	0.62
1:A:625:CYS:C	1:A:630:CYS:SG	2.78	0.62
1:A:368:ASN:ND2	3:A:687:NAG:C2	2.53	0.62
1:A:478:THR:HG22	1:A:480:SER:HB3	1.82	0.61
1:A:683:ALA:CB	10:A:725:HOH:O	2.47	0.61
1:A:368:ASN:OD1	3:A:687:NAG:C1	2.49	0.61
1:A:635:GLU:O	1:A:636:THR:HG22	2.01	0.60
1:A:653:GLY:C	1:A:655:PRO:CD	2.69	0.60
1:A:577:THR:HG22	1:A:578:ARG:N	2.16	0.60
1:A:352:PRO:HG3	1:A:520:LYS:HD2	1.82	0.60
1:A:577:THR:CG2	1:A:578:ARG:N	2.66	0.58
1:A:414:ASN:HD21	1:A:430:THR:HA	1.69	0.58
1:A:415:ARG:HH11	1:A:415:ARG:HG2	1.69	0.57
1:A:475:VAL:HG13	1:A:480:SER:O	2.04	0.57
1:A:415:ARG:NH1	1:A:415:ARG:HG2	2.19	0.57
1:A:662:GLY:O	1:A:666:VAL:HG23	2.04	0.57
1:A:686:PHE:HB3	1:A:686:PHE:OXT	2.05	0.55
1:A:638:ASN:HD22	1:A:643:ASP:H	1.54	0.54
1:A:584:ALA:HB3	4:A:689:NAG:H82	1.90	0.54
1:A:552:THR:OG1	1:A:566:ARG:HG2	2.07	0.54
1:A:577:THR:HG21	1:A:579:LYS:HZ3	1.73	0.54
1:A:682:GLU:O	1:A:683:ALA:CB	2.51	0.53
1:A:500:ARG:HB3	10:A:776:HOH:O	2.09	0.53
1:A:416:LYS:HD2	4:A:690:NAG:O4	2.08	0.53
1:A:424:ASP:HB2	10:A:711:HOH:O	2.08	0.53
1:A:638:ASN:ND2	1:A:643:ASP:H	2.07	0.52
1:A:460:ALA:HA	1:A:493:PRO:HD2	1.92	0.52
1:A:459:THR:OG1	1:A:466:GLY:HA3	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:690:NAG:C6	4:A:691:MAN:O2	2.59	0.51
1:A:625:CYS:HA	1:A:629:PHE:O	2.10	0.51
1:A:529:ALA:O	1:A:532:CYS:HB3	2.10	0.51
1:A:452:LYS:O	1:A:453:ASP:HB2	2.12	0.50
1:A:683:ALA:O	1:A:684:CYS:CB	2.57	0.50
1:A:426:VAL:HG12	1:A:650:LYS:HG3	1.93	0.50
1:A:459:THR:O	1:A:460:ALA:HB2	2.11	0.50
1:A:577:THR:HG21	1:A:579:LYS:NZ	2.26	0.50
1:A:671:ASN:HB3	10:A:742:HOH:O	2.12	0.50
1:A:464:THR:HG21	1:A:592:ALA:CB	2.41	0.49
1:A:365:SER:O	1:A:368:ASN:ND2	2.45	0.49
1:A:521:GLU:HB3	1:A:524:TYR:HB2	1.95	0.49
1:A:674:LYS:HD3	1:A:681:LEU:HD21	1.95	0.49
1:A:682:GLU:HG3	1:A:682:GLU:O	2.13	0.49
1:A:668:ALA:HB1	2:A:1:NAG:H83	1.95	0.48
1:A:567:GLU:H	1:A:567:GLU:CD	2.16	0.48
1:A:464:THR:HG21	1:A:592:ALA:HB1	1.96	0.48
1:A:665:TYR:CZ	1:A:669:ILE:HD11	2.49	0.48
1:A:381:ILE:HD11	1:A:394:LEU:HD11	1.94	0.48
1:A:634:SER:O	1:A:635:GLU:HB2	2.14	0.48
1:A:606:HIS:HB3	10:A:716:HOH:O	2.13	0.48
1:A:556:SER:C	1:A:557:THR:HG23	2.34	0.47
1:A:392:LEU:HD11	1:A:394:LEU:HD21	1.96	0.47
1:A:672:LEU:O	1:A:675:CYS:HB2	2.16	0.46
1:A:410:VAL:CG1	1:A:608:GLU:HB2	2.46	0.46
1:A:496:ASP:OD1	1:A:498:LYS:HD3	2.16	0.46
1:A:668:ALA:CB	2:A:1:NAG:H83	2.46	0.45
1:A:683:ALA:HA	10:A:725:HOH:O	2.16	0.45
1:A:343:THR:O	1:A:343:THR:CG2	2.58	0.45
1:A:356:LYS:HE3	1:A:356:LYS:HB2	1.74	0.45
1:A:614:GLN:NE2	10:A:766:HOH:O	2.49	0.45
1:A:683:ALA:CA	10:A:725:HOH:O	2.65	0.45
1:A:469:ILE:N	1:A:470:PRO:HD2	2.33	0.44
1:A:470:PRO:O	1:A:474:ILE:HG13	2.17	0.44
1:A:394:LEU:HD12	1:A:598:VAL:HG21	1.98	0.44
1:A:553:ASN:OD1	1:A:566:ARG:HG3	2.17	0.44
1:A:500:ARG:HD2	10:A:776:HOH:O	2.18	0.44
1:A:558:ALA:O	1:A:559:ASP:C	2.56	0.44
1:A:364:GLN:OE1	1:A:628:LYS:HE2	2.18	0.43
1:A:455:LYS:HE2	10:A:738:HOH:O	2.17	0.43
1:A:653:GLY:O	1:A:655:PRO:CD	2.65	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:458:HIS:HB3	1:A:466:GLY:O	2.18	0.43
1:A:557:THR:OG1	1:A:557:THR:O	2.37	0.43
1:A:556:SER:O	1:A:557:THR:HG23	2.18	0.43
1:A:402:ALA:HB1	1:A:407:LEU:HD12	1.99	0.43
1:A:380:CYS:HB3	1:A:392:LEU:HD13	2.00	0.43
1:A:565:LYS:HD3	1:A:567:GLU:CG	2.47	0.43
1:A:634:SER:HB2	1:A:639:LEU:HD12	1.99	0.42
1:A:478:THR:O	1:A:478:THR:CG2	2.67	0.42
1:A:347:TRP:CZ3	1:A:611:LEU:HD11	2.54	0.42
1:A:478:THR:O	1:A:478:THR:HG22	2.18	0.42
1:A:613:HIS:CD2	3:A:687:NAG:O6	2.73	0.42
1:A:359:GLN:HG2	10:A:807:HOH:O	2.19	0.42
1:A:395:ASP:O	1:A:399:ILE:HG12	2.21	0.41
1:A:632:PHE:C	1:A:633:LYS:HD2	2.41	0.41
1:A:380:CYS:O	1:A:384:VAL:HG23	2.19	0.41
1:A:397:GLY:HA3	1:A:462:ASP:O	2.20	0.41
1:A:636:THR:CG2	1:A:636:THR:O	2.67	0.41
1:A:577:THR:CG2	1:A:578:ARG:H	2.34	0.41
1:A:575:ASP:OD1	1:A:577:THR:HB	2.20	0.41
1:A:412:ALA:O	1:A:648:LEU:HA	2.21	0.40
1:A:682:GLU:HB3	10:A:824:HOH:O	2.21	0.40
1:A:573:CYS:HB2	1:A:575:ASP:OD1	2.22	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%)	306 (91%)	22 (6%)	9 (3%)	6	32

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	683	ALA
1	A	685	ALA
1	A	460	ALA
1	A	684	CYS
1	A	464	THR
1	A	519	SER
1	A	559	ASP
1	A	482	ALA
1	A	543	VAL

### 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%)	257 (91%)	25 (9%)	12	42

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	342	TYR
1	A	343	THR
1	A	344	ARG
1	A	356	LYS
1	A	375	SER
1	A	414	ASN
1	A	422	SER
1	A	452	LYS
1	A	471	MET
1	A	490	SER
1	A	498	LYS
1	A	500	ARG
1	A	515	CYS
1	A	545	ASN
1	A	557	THR
1	A	567	GLU
1	A	583	GLU
1	A	591	VAL

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Mol	Chain	Res	Type
1	A	606	HIS
1	A	625	CYS
1	A	631	LEU
1	A	636	THR
1	A	655	PRO
1	A	664	GLU
1	A	684	CYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	368	ASN
1	A	414	ASN
1	A	420	HIS
1	A	545	ASN
1	A	585	GLN
1	A	594	ASN
1	A	613	HIS
1	A	621	ASN
1	A	638	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 ⓘ

10 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	$\# Z  > 2$
2	NAG	A	1	1,2	14,14,15	0.63	0	15,19,21	0.62	0
2	NAG	A	2	2	14,14,15	0.90	0	15,19,21	1.42	1 (6%)
2	BMA	A	3	2	11,11,12	0.66	0	14,15,17	1.14	1 (7%)
2	MAN	A	4	2	11,11,12	0.66	0	14,15,17	2.21	3 (21%)
3	NAG	A	687	1,3	14,14,15	0.79	0	15,19,21	1.96	4 (26%)
3	NAG	A	688	3	14,14,15	0.83	1 (7%)	15,19,21	1.25	2 (13%)
4	NAG	A	689	1,4	14,14,15	0.71	0	15,19,21	3.55	2 (13%)
4	NAG	A	690	4	14,14,15	0.75	0	15,19,21	1.77	5 (33%)
4	MAN	A	691	4	11,11,12	1.37	3 (27%)	14,15,17	3.21	4 (28%)
4	BMA	A	692	4	11,11,12	1.24	2 (18%)	14,15,17	1.65	3 (21%)

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	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	2	2	-	0/6/23/26	0/1/1/1
2	BMA	A	3	2	-	0/2/19/22	0/1/1/1
2	MAN	A	4	2	-	0/2/19/22	0/1/1/1
3	NAG	A	687	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	688	3	1/1/5/7	0/6/23/26	0/1/1/1
4	NAG	A	689	1,4	-	0/6/23/26	0/1/1/1
4	NAG	A	690	4	1/1/5/7	0/6/23/26	0/1/1/1
4	MAN	A	691	4	-	0/2/19/22	1/1/1/1
4	BMA	A	692	4	-	0/2/19/22	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	688	NAG	C1-C2	-2.17	1.49	1.52
4	A	691	MAN	O5-C5	2.13	1.48	1.43
4	A	692	BMA	C1-C2	2.26	1.57	1.52
4	A	691	MAN	O4-C4	2.50	1.48	1.43
4	A	691	MAN	C2-C3	2.58	1.56	1.52
4	A	692	BMA	C2-C3	2.97	1.56	1.52

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	689	NAG	C2-N2-C7	-12.88	106.49	123.04
4	A	691	MAN	C3-C4-C5	-10.43	92.01	110.20
4	A	692	BMA	C6-C5-C4	-3.36	104.73	113.02
3	A	688	NAG	C4-C3-C2	-2.96	106.62	111.23
3	A	688	NAG	C2-N2-C7	-2.91	119.30	123.04
3	A	687	NAG	O4-C4-C3	-2.65	104.37	110.34
4	A	690	NAG	C1-O5-C5	-2.27	109.37	112.25
3	A	687	NAG	C6-C5-C4	2.15	118.32	113.02
4	A	692	BMA	C2-C3-C4	2.26	114.88	111.04
2	A	3	BMA	C3-C4-C5	2.33	114.25	110.20
4	A	692	BMA	C1-O5-C5	2.62	115.57	112.25
4	A	690	NAG	O4-C4-C3	2.65	116.31	110.34
4	A	691	MAN	C1-O5-C5	2.73	115.72	112.25
4	A	690	NAG	C4-C3-C2	2.75	115.51	111.23
3	A	687	NAG	C4-C3-C2	2.83	115.62	111.23
4	A	691	MAN	O3-C3-C2	2.95	115.33	110.00
4	A	690	NAG	C3-C4-C5	3.07	115.55	110.20
4	A	689	NAG	C1-O5-C5	3.23	116.34	112.25
4	A	691	MAN	C6-C5-C4	3.33	121.24	113.02
4	A	690	NAG	O4-C4-C5	3.35	118.12	109.24
2	A	4	MAN	O5-C1-C2	3.73	116.91	110.86
2	A	4	MAN	C1-O5-C5	3.81	117.09	112.25
2	A	2	NAG	C4-C3-C2	4.68	118.51	111.23
3	A	687	NAG	C3-C4-C5	5.22	119.30	110.20
2	A	4	MAN	C1-C2-C3	5.84	116.44	109.54

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	688	NAG	C1
4	A	690	NAG	C1

There are no torsion outliers.

All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	691	MAN	C1-C2-C3-C4-C5-O5

7 monomers are involved in 19 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1	NAG	2	0
3	A	687	NAG	7	0
3	A	688	NAG	1	0
4	A	689	NAG	5	0
4	A	690	NAG	3	0
4	A	691	MAN	3	0
4	A	692	BMA	1	0

## 5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 3 are monoatomic - leaving 3 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	FRU	A	693	-	11,12,12	1.53	2 (18%)	10,18,18	4.14	2 (20%)
7	CO3	A	695	6	0,3,3	0.00	-	0,3,3	0.00	-
9	SO4	A	698	-	4,4,4	0.39	0	6,6,6	0.17	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
5	FRU	A	693	-	-	0/5/24/24	0/1/1/1
7	CO3	A	695	6	-	0/0/0/0	0/0/0/0
9	SO4	A	698	-	-	0/0/0/0	0/0/0/0

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	693	FRU	O5-C5	2.00	1.48	1.43
5	A	693	FRU	C1-C2	3.97	1.59	1.52

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
5	A	693	FRU	O2-C2-O5	4.94	119.57	109.37
5	A	693	FRU	O1-C1-C2	11.58	133.90	111.39

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 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 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.