



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 9, 2020 – 01:18 PM BST

PDB ID : 1SQY
Title : Structure of human diferric lactoferrin at 2.5Å resolution using crystals grown at pH 6.5
Authors : Vikram, P.; Prem Kumar, R.; Singh, N.; Kumar, J.; Ethayathulla, A.S.; Sharma, S.; Kaur, P.; Singh, T.P.
Deposited on : 2004-03-22
Resolution : 2.50 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.13.1

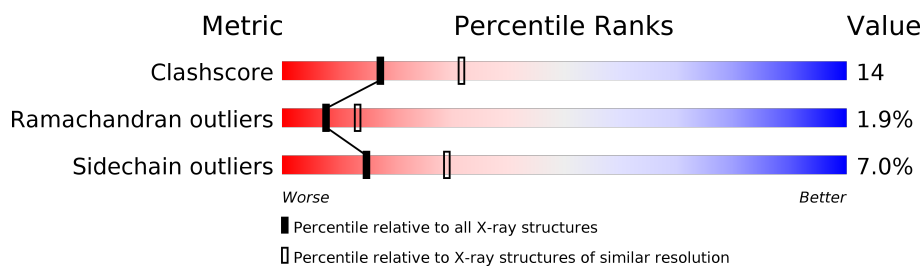
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	691	
2	B	2	
2	C	2	

2 Entry composition [i](#)

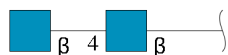
There are 5 unique types of molecules in this entry. The entry contains 5719 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 lactoferrin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	691	Total	C	N	O	S	0	0	0
			5347	3335	961	1014	37			

- Molecule 2 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

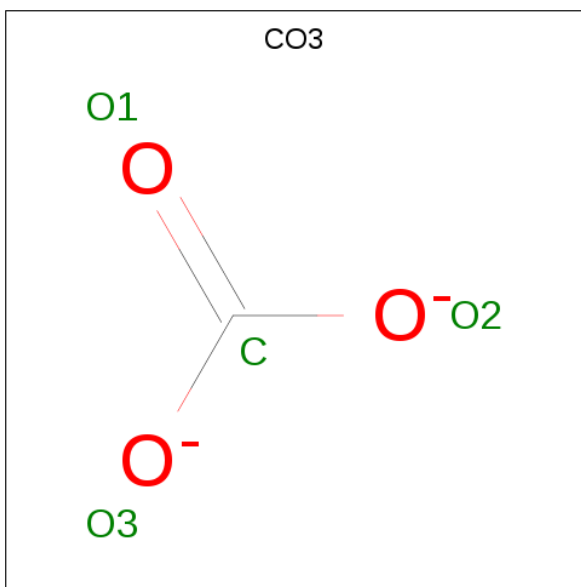


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	C	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 3 is FE (III) ION (three-letter code: FE) (formula: Fe).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	2	Total	Fe	0	0
			2	2		

- Molecule 4 is CARBONATE ION (three-letter code: CO3) (formula: CO₃).



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

- Molecule 5 is water.

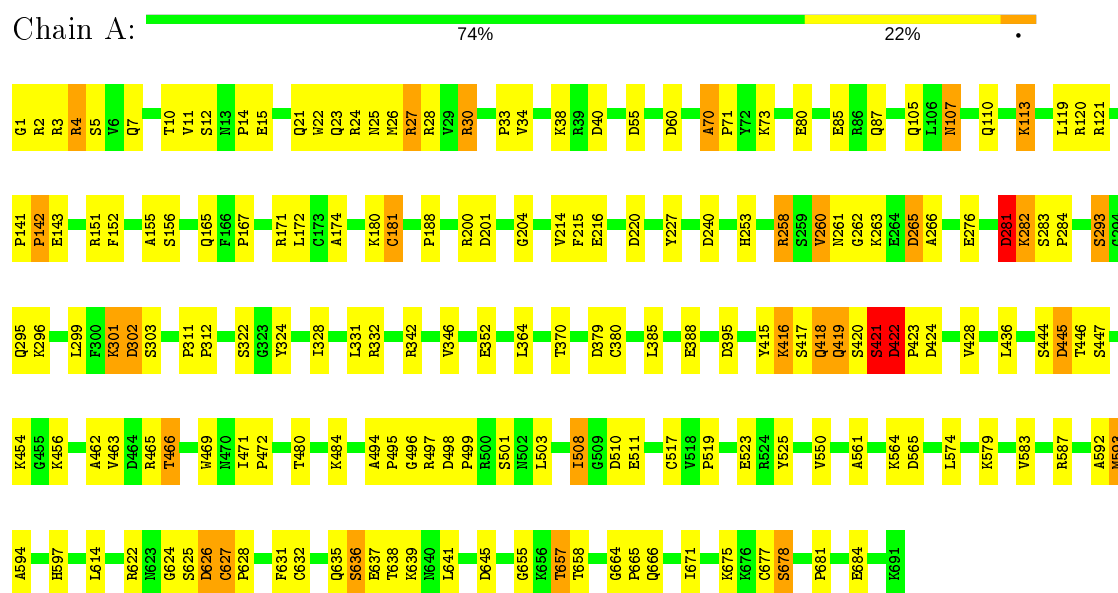
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	306	Total	O	0	0
			306	306		

3 Residue-property plots

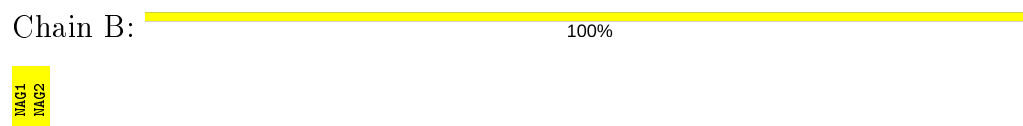
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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. 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: lactoferrin



- Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	56.16 Å 98.09 Å 157.04 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.73 – 2.50	Depositor
% Data completeness (in resolution range)	100.0 (19.73-2.50)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
Refinement program	REFMAC 5.0	Depositor
R, R_{free}	0.204 , 0.215	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	5719	wwPDB-VP
Average B, all atoms (Å ²)	53.0	wwPDB-VP

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: CO3, NAG, 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	0.66	0/5461	0.81	10/7387 (0.1%)

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	445	ASP	CB-CG-OD2	6.50	124.16	118.30
1	A	302	ASP	CB-CG-OD2	6.13	123.81	118.30
1	A	421	SER	N-CA-C	5.72	126.45	111.00
1	A	40	ASP	CB-CG-OD2	5.56	123.31	118.30
1	A	201	ASP	CB-CG-OD2	5.41	123.17	118.30
1	A	281	ASP	CB-CG-OD2	5.40	123.16	118.30
1	A	240	ASP	CB-CG-OD2	5.33	123.10	118.30
1	A	422	ASP	CB-CG-OD2	5.10	122.89	118.30
1	A	645	ASP	CB-CG-OD2	5.03	122.82	118.30
1	A	379	ASP	CB-CG-OD2	5.00	122.80	118.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	5347	0	5199	146	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	28	0	25	0	0
2	C	28	0	25	1	0
3	A	2	0	0	0	0
4	A	8	0	0	0	0
5	A	306	0	0	32	0
All	All	5719	0	5249	147	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 14.

All (147) 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:142:PRO:HA	5:A:736:HOH:O	1.65	0.95
1:A:107:ASN:HD22	1:A:107:ASN:H	1.18	0.89
1:A:70:ALA:HB3	1:A:71:PRO:HD3	1.58	0.85
1:A:24:ARG:HB3	1:A:27:ARG:NH1	1.98	0.79
1:A:24:ARG:HA	1:A:27:ARG:HD2	1.65	0.78
1:A:636:SER:O	1:A:639:LYS:HG3	1.86	0.76
1:A:70:ALA:CB	1:A:71:PRO:HD3	2.16	0.76
1:A:456:LYS:HD2	1:A:456:LYS:N	2.01	0.74
1:A:497:ARG:HE	1:A:497:ARG:HA	1.51	0.74
1:A:260:VAL:HG23	1:A:261:ASN:H	1.52	0.73
1:A:418:GLN:O	1:A:420:SER:N	2.21	0.72
1:A:632:CYS:HB3	5:A:750:HOH:O	1.91	0.71
1:A:511:GLU:HG3	5:A:885:HOH:O	1.89	0.71
1:A:508:ILE:H	1:A:508:ILE:HD13	1.55	0.71
1:A:258:ARG:HG2	5:A:787:HOH:O	1.90	0.71
1:A:303:SER:HB2	5:A:803:HOH:O	1.92	0.70
1:A:322:SER:HB3	1:A:385:LEU:O	1.92	0.70
1:A:658:THR:HB	5:A:947:HOH:O	1.91	0.70
1:A:10:THR:HG22	1:A:299:LEU:HD21	1.74	0.69
1:A:684:GLU:HG3	5:A:936:HOH:O	1.95	0.65
1:A:282:LYS:HA	5:A:811:HOH:O	1.97	0.65
1:A:510:ASP:HB2	5:A:885:HOH:O	1.96	0.64
1:A:496:GLY:HA2	1:A:519:PRO:HG3	1.79	0.64
1:A:70:ALA:HB3	1:A:71:PRO:CD	2.28	0.64
1:A:422:ASP:O	1:A:424:ASP:N	2.32	0.62
1:A:1:GLY:CA	1:A:4:ARG:HD3	2.30	0.62
1:A:444:SER:O	1:A:446:THR:N	2.33	0.61
1:A:281:ASP:HA	5:A:717:HOH:O	1.99	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:262:GLY:O	1:A:263:LYS:HB2	2.00	0.61
1:A:331:LEU:HB2	5:A:939:HOH:O	1.99	0.61
1:A:24:ARG:HB3	1:A:27:ARG:HH11	1.66	0.59
1:A:70:ALA:CB	1:A:71:PRO:CD	2.79	0.59
1:A:508:ILE:HD12	1:A:525:TYR:CD2	2.38	0.59
1:A:110:GLN:HG3	1:A:152:PHE:CE1	2.38	0.58
1:A:258:ARG:NH1	1:A:261:ASN:O	2.35	0.58
1:A:564:LYS:HD3	5:A:958:HOH:O	2.03	0.58
1:A:415:TYR:O	1:A:417:SER:N	2.37	0.58
1:A:4:ARG:HD2	1:A:4:ARG:H	1.69	0.58
1:A:261:ASN:ND2	5:A:840:HOH:O	2.35	0.57
1:A:174:ALA:HB3	1:A:188:PRO:HG2	1.86	0.57
1:A:107:ASN:N	1:A:107:ASN:HD22	1.95	0.57
1:A:105:GLN:HA	1:A:105:GLN:NE2	2.19	0.56
1:A:497:ARG:NE	1:A:497:ARG:HA	2.17	0.56
1:A:346:VAL:HG22	1:A:370:THR:CG2	2.36	0.56
1:A:497:ARG:HD3	1:A:503:LEU:HD13	1.88	0.56
1:A:466:THR:HG21	1:A:594:ALA:HB1	1.86	0.56
1:A:141:PRO:O	1:A:142:PRO:C	2.44	0.55
1:A:462:ALA:HB3	1:A:465:ARG:HD3	1.89	0.55
1:A:85:GLU:HG3	5:A:797:HOH:O	2.06	0.55
1:A:496:GLY:CA	1:A:519:PRO:HG3	2.36	0.55
1:A:677:CYS:O	1:A:678:SER:HB3	2.06	0.54
1:A:105:GLN:NE2	5:A:747:HOH:O	2.41	0.54
1:A:671:ILE:O	1:A:675:LYS:HG2	2.07	0.54
1:A:681:PRO:HD2	5:A:897:HOH:O	2.06	0.54
1:A:302:ASP:O	1:A:303:SER:HB2	2.08	0.54
1:A:33:PRO:HD2	5:A:826:HOH:O	2.08	0.53
1:A:7:GLN:HG3	1:A:55:ASP:OD2	2.09	0.53
1:A:70:ALA:O	1:A:73:LYS:HG2	2.08	0.53
1:A:15:GLU:HG2	1:A:299:LEU:CD2	2.39	0.53
1:A:388:GLU:HG2	5:A:870:HOH:O	2.08	0.53
1:A:635:GLN:HG2	5:A:920:HOH:O	2.09	0.53
1:A:471:ILE:HD13	1:A:592:ALA:HB3	1.90	0.52
1:A:324:TYR:CE1	1:A:328:ILE:HD11	2.45	0.52
1:A:200:ARG:HG2	1:A:227:TYR:OH	2.10	0.52
1:A:564:LYS:HE3	1:A:565:ASP:OD2	2.09	0.52
1:A:107:ASN:ND2	1:A:107:ASN:H	1.97	0.51
1:A:395:ASP:HA	1:A:597:HIS:CD2	2.45	0.51
1:A:281:ASP:HB2	5:A:802:HOH:O	2.09	0.51
1:A:216:GLU:OE1	1:A:301:LYS:NZ	2.44	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:499:PRO:HB3	5:A:878:HOH:O	2.11	0.51
1:A:265:ASP:HB2	5:A:864:HOH:O	2.11	0.50
1:A:655:GLY:O	1:A:657:THR:HG22	2.11	0.50
1:A:626:ASP:N	1:A:626:ASP:OD1	2.45	0.50
1:A:60:ASP:HA	1:A:253:HIS:CD2	2.47	0.50
1:A:156:SER:HA	1:A:172:LEU:HD12	1.94	0.50
1:A:466:THR:HG21	1:A:594:ALA:CB	2.42	0.49
1:A:638:THR:CG2	5:A:884:HOH:O	2.60	0.49
1:A:260:VAL:HG23	1:A:261:ASN:N	2.25	0.49
1:A:497:ARG:CD	1:A:503:LEU:HD13	2.42	0.49
1:A:3:ARG:HG2	1:A:266:ALA:CB	2.43	0.49
1:A:508:ILE:HD13	1:A:523:GLU:OE2	2.12	0.49
1:A:3:ARG:HG2	1:A:266:ALA:HB2	1.94	0.49
1:A:418:GLN:NE2	1:A:587:ARG:HD2	2.27	0.49
1:A:1:GLY:HA2	1:A:4:ARG:HD3	1.94	0.48
1:A:12:SER:OG	1:A:14:PRO:HD2	2.13	0.48
1:A:498:ASP:O	1:A:501:SER:HB3	2.12	0.48
1:A:415:TYR:O	1:A:416:LYS:C	2.52	0.48
1:A:80:GLU:OE1	1:A:253:HIS:HB2	2.13	0.48
1:A:4:ARG:HD2	1:A:4:ARG:N	2.29	0.47
1:A:262:GLY:O	1:A:263:LYS:CB	2.62	0.47
1:A:508:ILE:N	1:A:508:ILE:HD13	2.24	0.47
1:A:23:GLN:HG3	1:A:34:VAL:O	2.14	0.47
1:A:456:LYS:HD2	1:A:456:LYS:H	1.76	0.47
1:A:511:GLU:HG2	5:A:719:HOH:O	2.15	0.47
1:A:550:VAL:HG11	1:A:583:VAL:HG21	1.97	0.46
1:A:627:CYS:O	1:A:628:PRO:C	2.54	0.46
1:A:627:CYS:HA	1:A:631:PHE:O	2.15	0.46
1:A:497:ARG:HD3	1:A:503:LEU:CD1	2.46	0.45
1:A:113:LYS:HB3	1:A:204:GLY:HA2	1.97	0.45
1:A:24:ARG:O	1:A:27:ARG:HD3	2.17	0.45
1:A:463:VAL:HG23	1:A:495:PRO:O	2.16	0.45
1:A:499:PRO:C	5:A:904:HOH:O	2.55	0.45
1:A:498:ASP:HB2	5:A:933:HOH:O	2.16	0.45
1:A:11:VAL:HG22	1:A:15:GLU:OE1	2.17	0.45
2:C:2:NAG:C7	2:C:2:NAG:O3	2.65	0.44
1:A:281:ASP:C	1:A:282:LYS:HD2	2.38	0.44
1:A:214:VAL:HG13	1:A:215:PHE:CD1	2.52	0.44
1:A:21:GLN:O	1:A:25:ASN:ND2	2.50	0.44
1:A:24:ARG:CA	1:A:27:ARG:HD2	2.40	0.44
1:A:3:ARG:O	1:A:4:ARG:C	2.56	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:419:GLN:C	1:A:421:SER:H	2.03	0.43
1:A:469:TRP:O	1:A:472:PRO:HD2	2.18	0.43
1:A:636:SER:O	1:A:637:GLU:HG2	2.19	0.43
1:A:664:GLY:HA2	1:A:665:PRO:HD3	1.88	0.43
1:A:7:GLN:N	1:A:55:ASP:OD2	2.38	0.43
1:A:180:LYS:O	1:A:181:CYS:CB	2.66	0.43
1:A:561:ALA:O	1:A:564:LYS:HG2	2.19	0.43
1:A:30:ARG:HA	5:A:722:HOH:O	2.18	0.42
1:A:346:VAL:HG13	1:A:370:THR:HG23	2.01	0.42
1:A:27:ARG:O	1:A:27:ARG:HG2	2.19	0.42
1:A:627:CYS:HB3	1:A:628:PRO:HD3	2.01	0.42
1:A:639:LYS:HB3	1:A:639:LYS:HE2	1.93	0.42
1:A:295:GLN:O	1:A:296:LYS:HG2	2.19	0.42
1:A:436:LEU:HD23	1:A:593:MET:HG3	2.02	0.42
1:A:494:ALA:HB3	1:A:497:ARG:HG3	1.99	0.42
1:A:497:ARG:HG3	1:A:503:LEU:HB3	2.02	0.42
1:A:165:GLN:C	1:A:167:PRO:HD3	2.40	0.42
1:A:664:GLY:HA3	5:A:772:HOH:O	2.19	0.42
1:A:113:LYS:HG3	1:A:155:ALA:HB3	2.01	0.42
1:A:511:GLU:HB3	5:A:891:HOH:O	2.19	0.42
1:A:311:PRO:HA	1:A:312:PRO:HD3	1.74	0.42
1:A:283:SER:HA	1:A:284:PRO:HD3	1.93	0.41
1:A:428:VAL:O	1:A:428:VAL:HG12	2.20	0.41
1:A:30:ARG:CD	5:A:788:HOH:O	2.68	0.41
1:A:22:TRP:O	1:A:26:MET:HG2	2.20	0.41
1:A:276:GLU:O	1:A:282:LYS:HG2	2.21	0.41
1:A:105:GLN:HE21	1:A:105:GLN:CA	2.34	0.41
1:A:508:ILE:HD12	1:A:525:TYR:CE2	2.55	0.41
1:A:624:GLY:O	1:A:625:SER:C	2.57	0.41
1:A:119:LEU:O	1:A:120:ARG:HB2	2.21	0.41
1:A:508:ILE:N	1:A:508:ILE:CD1	2.84	0.41
1:A:143:GLU:CD	1:A:151:ARG:HH22	2.25	0.40
1:A:614:LEU:HD23	1:A:614:LEU:HA	1.93	0.40
1:A:331:LEU:HA	1:A:331:LEU:HD23	1.94	0.40
1:A:10:THR:HB	1:A:15:GLU:HB3	2.04	0.40
1:A:262:GLY:HA2	5:A:787:HOH:O	2.21	0.40
1:A:480:THR:CG2	5:A:931:HOH:O	2.68	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	689/691 (100%)	630 (91%)	46 (7%)	13 (2%)	8 13

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	70	ALA
1	A	419	GLN
1	A	421	SER
1	A	422	ASP
1	A	260	VAL
1	A	293	SER
1	A	416	LYS
1	A	423	PRO
1	A	445	ASP
1	A	466	THR
1	A	627	CYS
1	A	636	SER
1	A	678	SER

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	574/574 (100%)	534 (93%)	40 (7%)	15 29

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	ARG
1	A	4	ARG
1	A	5	SER
1	A	27	ARG
1	A	28	ARG
1	A	30	ARG
1	A	38	LYS
1	A	87	GLN
1	A	107	ASN
1	A	113	LYS
1	A	121	ARG
1	A	142	PRO
1	A	171	ARG
1	A	181	CYS
1	A	220	ASP
1	A	258	ARG
1	A	265	ASP
1	A	281	ASP
1	A	282	LYS
1	A	293	SER
1	A	301	LYS
1	A	332	ARG
1	A	342	ARG
1	A	352	GLU
1	A	364	LEU
1	A	380	CYS
1	A	418	GLN
1	A	447	SER
1	A	454	LYS
1	A	484	LYS
1	A	508	ILE
1	A	517	CYS
1	A	574	LEU
1	A	579	LYS
1	A	593	MET
1	A	622	ARG
1	A	626	ASP
1	A	641	LEU
1	A	657	THR
1	A	666	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	21	GLN
1	A	47	GLN
1	A	105	GLN
1	A	107	ASN
1	A	287	GLN
1	A	329	GLN
1	A	330	ASN
1	A	353	GLN
1	A	418	GLN
1	A	419	GLN
1	A	559	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 ⓘ

4 monosaccharides 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	B	1	1,2	14,14,15	0.88	1 (7%)	17,19,21	2.42	8 (47%)
2	NAG	B	2	2	14,14,15	0.74	0	17,19,21	1.41	3 (17%)
2	NAG	C	1	1,2	14,14,15	0.72	0	17,19,21	2.26	7 (41%)
2	NAG	C	2	2	14,14,15	1.11	0	17,19,21	3.05	8 (47%)

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	B	1	1,2	-	4/6/23/26	0/1/1/1
2	NAG	B	2	2	-	0/6/23/26	0/1/1/1
2	NAG	C	1	1,2	-	4/6/23/26	0/1/1/1
2	NAG	C	2	2	-	4/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1	NAG	C3-C2	2.12	1.57	1.52

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	2	NAG	C1-C2-N2	5.92	120.60	110.49
2	C	2	NAG	C3-C4-C5	5.84	120.66	110.24
2	C	2	NAG	C1-O5-C5	-5.28	105.04	112.19
2	B	1	NAG	C1-C2-N2	4.81	118.70	110.49
2	C	1	NAG	C1-C2-N2	-4.38	103.01	110.49
2	B	1	NAG	C4-C3-C2	-4.03	105.12	111.02
2	B	1	NAG	O4-C4-C3	3.90	119.35	110.35
2	C	1	NAG	O4-C4-C5	-3.79	99.88	109.30
2	C	2	NAG	O7-C7-N2	-3.72	115.11	121.95
2	C	1	NAG	C3-C4-C5	-3.54	103.93	110.24
2	C	2	NAG	C8-C7-N2	3.44	121.93	116.10
2	C	2	NAG	O4-C4-C5	-3.40	100.85	109.30
2	B	2	NAG	O5-C1-C2	3.30	116.50	111.29
2	B	1	NAG	O5-C1-C2	-2.85	106.79	111.29
2	C	2	NAG	C4-C3-C2	-2.71	107.04	111.02
2	B	1	NAG	C1-O5-C5	2.57	115.67	112.19
2	B	1	NAG	C8-C7-N2	-2.45	111.95	116.10
2	C	2	NAG	O5-C5-C4	2.44	116.77	110.83
2	C	1	NAG	O4-C4-C3	-2.41	104.78	110.35
2	C	1	NAG	O7-C7-C8	-2.34	117.71	122.06
2	B	1	NAG	C6-C5-C4	-2.21	107.82	113.00
2	B	2	NAG	C1-C2-N2	-2.15	106.81	110.49
2	C	1	NAG	C8-C7-N2	2.12	119.69	116.10
2	B	2	NAG	C1-O5-C5	2.08	115.01	112.19
2	C	1	NAG	O5-C5-C4	2.06	115.84	110.83
2	B	1	NAG	O3-C3-C4	-2.00	105.72	110.35

There are no chirality outliers.

All (12) torsion outliers are listed below:

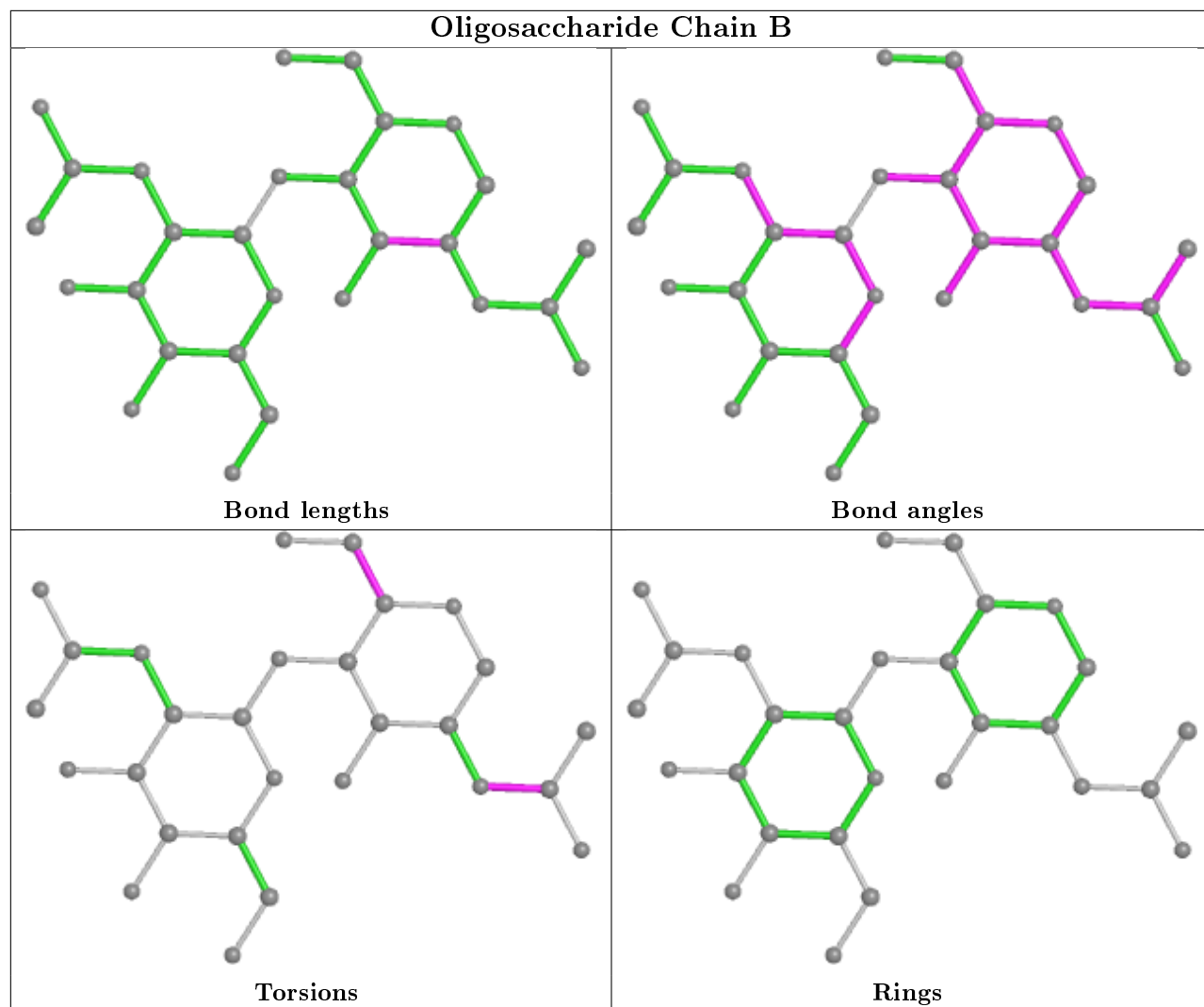
Mol	Chain	Res	Type	Atoms
2	C	2	NAG	C3-C2-N2-C7
2	C	2	NAG	C8-C7-N2-C2
2	C	2	NAG	O7-C7-N2-C2
2	C	1	NAG	O5-C5-C6-O6
2	B	1	NAG	C4-C5-C6-O6
2	C	1	NAG	C4-C5-C6-O6
2	C	1	NAG	C8-C7-N2-C2
2	C	1	NAG	O7-C7-N2-C2
2	B	1	NAG	C8-C7-N2-C2
2	B	1	NAG	O7-C7-N2-C2
2	B	1	NAG	O5-C5-C6-O6
2	C	2	NAG	C1-C2-N2-C7

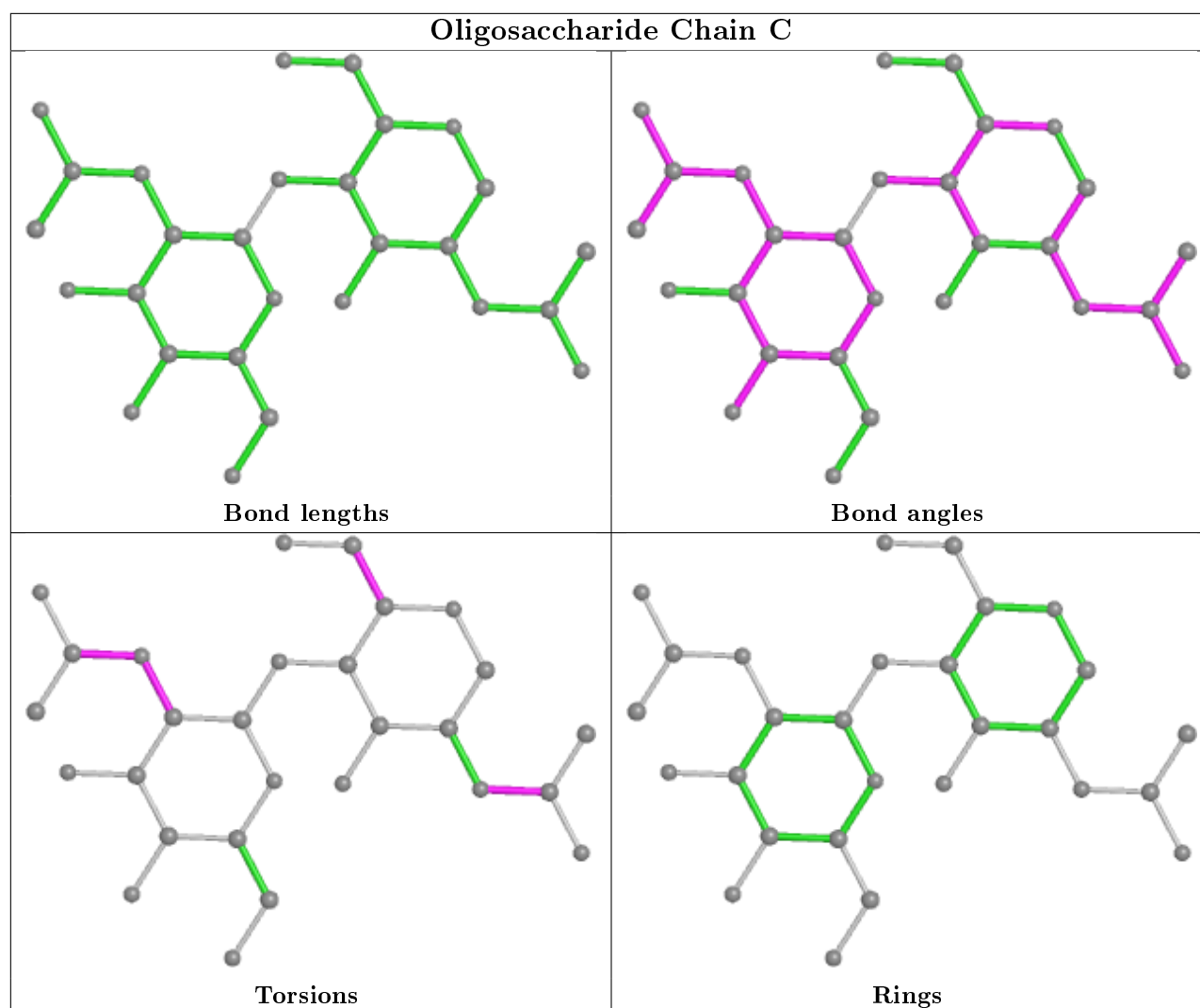
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	2	NAG	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.





5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 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	$\# Z > 2$
4	CO3	A	704	3	0,3,3	0.00	-	0,3,3	0.00	-
4	CO3	A	703	3	0,3,3	0.00	-	0,3,3	0.00	-

There are no bond length outliers.

There are no bond angle outliers.

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

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 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.