



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 4, 2026 – 05:44 PM UTC

PDB ID : 4GRK / pdb_00004grk
Title : Crystal Structure of C-lobe of Bovine lactoferrin Complexed with ketorolac at 1.68 Å Resolution
Authors : Gautam, L.; Shukla, P.K.; Sinha, M.; Kaur, P.; Sharma, S.; Singh, T.P.
Deposited on : 2012-08-25
Resolution : 1.68 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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

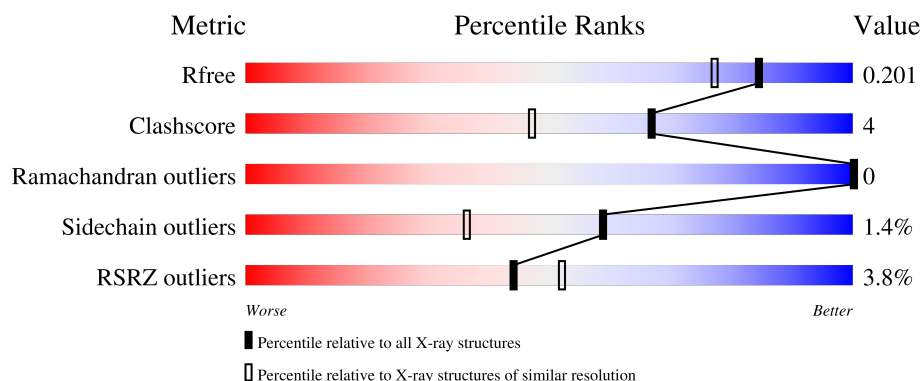
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.68 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1054 (1.68-1.68)
Clashscore	190562	1078 (1.68-1.68)
Ramachandran outliers	187476	1068 (1.68-1.68)
Sidechain outliers	187428	1067 (1.68-1.68)
RSRZ outliers	180081	1055 (1.68-1.68)

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 of 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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	335	3% 82% 17%
2	B	6	67% 67% 33%
3	C	3	33% 67%
4	D	2	100%

2 Entry composition [i](#)

There are 12 unique types of molecules in this entry. The entry contains 3095 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	335	Total	C	N	O	S	0	0	0
			2560	1593	448	499	20			

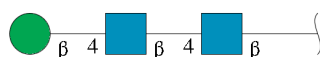
There are 2 discrepancies between the modelled and reference sequences:

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 2 is a protein called C-terminal peptide from Lactotransferrin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	6	Total	C	N	O	S	0	0	0
			44	29	6	8	1			

- Molecule 3 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



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

- Molecule 4 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
4	D	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



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

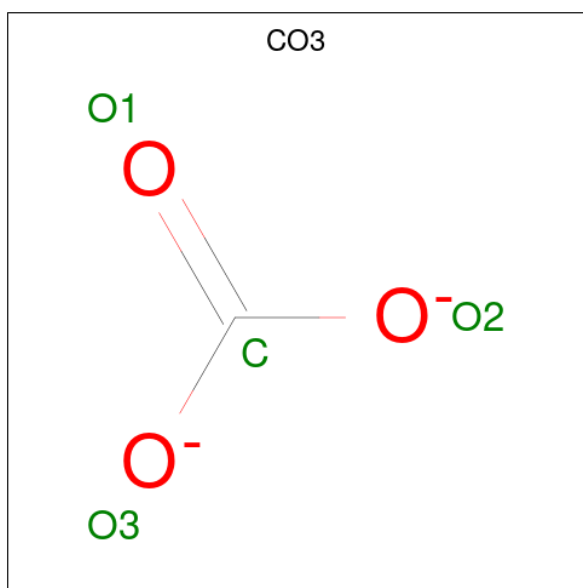
- Molecule 6 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

- Molecule 7 is FE (III) ION (CCD ID: FE) (formula: Fe).

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

- Molecule 8 is CARBONATE ION (CCD ID: CO3) (formula: CO_3).



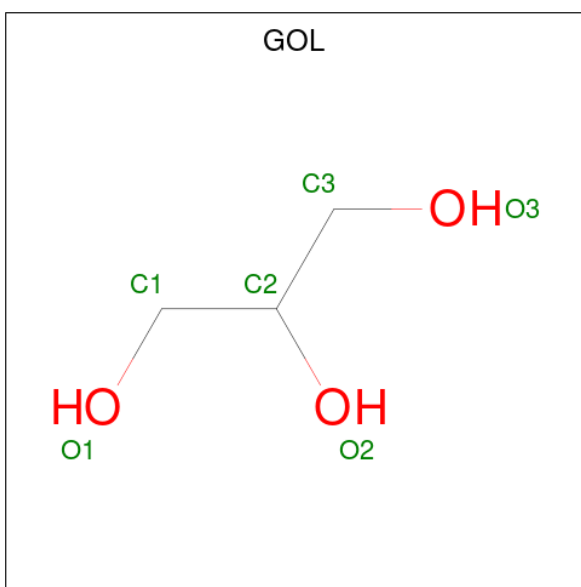
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	C	O	0	0
			4	1	3		

- Molecule 9 is SULFATE ION (CCD ID: SO4) (formula: O_4S).



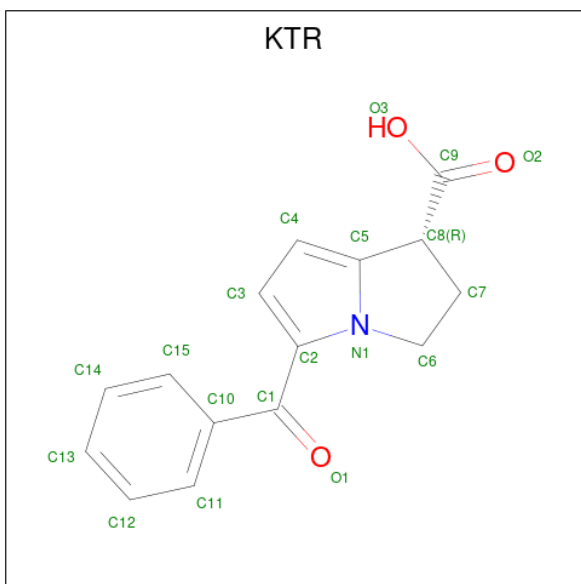
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	A	1	Total	O	S	0	0
			5	4	1		

- Molecule 10 is GLYCEROL (CCD ID: GOL) (formula: $\text{C}_3\text{H}_8\text{O}_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	A	1	Total	C	O	0	0
			6	3	3		
10	A	1	Total	C	O	0	0
			6	3	3		

- Molecule 11 is (1R)-5-benzoyl-2,3-dihydro-1H-pyrrolizine-1-carboxylic acid (CCD ID: KTR) (formula: $C_{15}H_{13}NO_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
11	A	1	Total	C	N	O	0	0
			19	15	1	3		

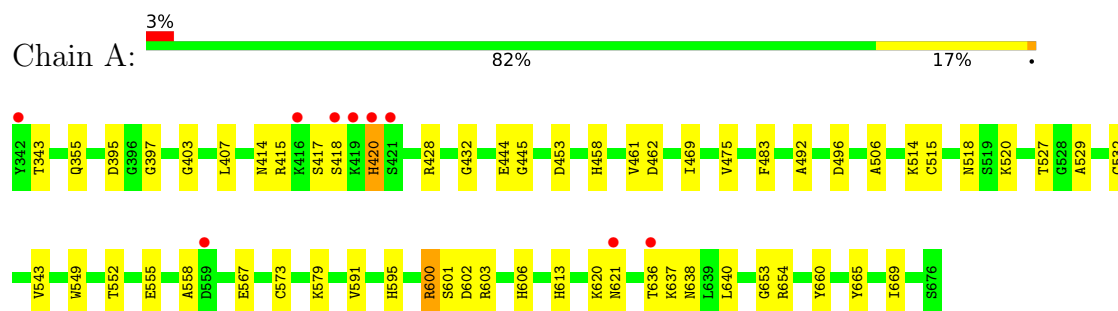
- Molecule 12 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	A	364	Total 364	O 364	0	0
12	B	3	Total 3	O 3	0	0

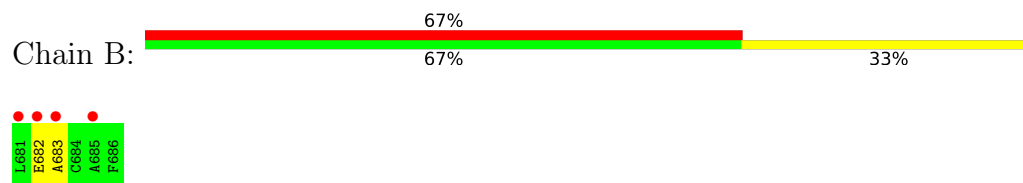
3 Residue-property plots [i](#)

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 and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Lactotransferrin



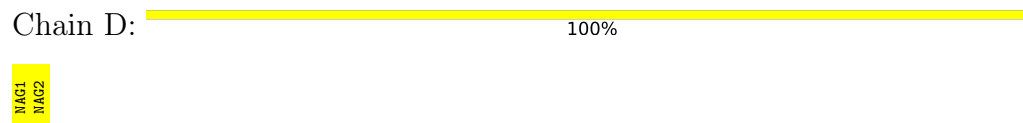
- Molecule 2: C-terminal peptide from Lactotransferrin



- Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



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



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	62.62Å 49.95Å 65.50Å 90.00° 107.22° 90.00°	Depositor
Resolution (Å)	62.57 – 1.68 62.57 – 1.68	Depositor EDS
% Data completeness (in resolution range)	99.5 (62.57-1.68) 99.5 (62.57-1.68)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.05	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.19 (at 1.68Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.155 , 0.205 0.155 , 0.201	Depositor DCC
R_{free} test set	2212 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	20.0	Xtriage
Anisotropy	0.449	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 47.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.017 for l,-k,h	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	3095	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.33% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: BMA, NAG, CO3, ZN, SO4, GOL, FE, KTR

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	1.76	29/2608 (1.1%)	1.48	10/3533 (0.3%)
2	B	1.90	0/44	1.45	2/58 (3.4%)
All	All	1.76	29/2652 (1.1%)	1.48	12/3591 (0.3%)

All (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	414	ASN	C-O	-8.06	1.15	1.24
1	A	492	ALA	N-CA	7.58	1.55	1.46
1	A	600	ARG	CD-NE	-6.92	1.36	1.46
1	A	600	ARG	CA-C	-6.59	1.44	1.52
1	A	403	GLY	C-O	6.46	1.31	1.24
1	A	529	ALA	N-CA	-6.40	1.38	1.46
1	A	603	ARG	CZ-NH1	6.20	1.41	1.32
1	A	638	ASN	N-CA	6.12	1.55	1.46
1	A	469	ILE	CA-C	6.10	1.59	1.52
1	A	621	ASN	N-CA	6.05	1.53	1.46
1	A	496	ASP	N-CA	6.02	1.54	1.46
1	A	601	SER	N-CA	-5.72	1.39	1.46
1	A	407	LEU	CA-C	5.67	1.60	1.53
1	A	420	HIS	CG-CD2	5.56	1.42	1.35
1	A	475	VAL	N-CA	5.55	1.53	1.46
1	A	532	CYS	C-O	-5.48	1.17	1.24
1	A	506	ALA	C-O	5.46	1.31	1.24
1	A	613	HIS	CG-CD2	5.46	1.41	1.35
1	A	420	HIS	CE1-NE2	5.37	1.38	1.32
1	A	458	HIS	ND1-CE1	5.36	1.38	1.32
1	A	518	ASN	CA-CB	5.36	1.63	1.53
1	A	445	GLY	CA-C	5.32	1.59	1.51
1	A	558	ALA	C-O	-5.26	1.17	1.23
1	A	640	LEU	N-CA	5.22	1.52	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	552	THR	N-CA	5.21	1.52	1.45
1	A	549	TRP	CA-C	-5.17	1.46	1.52
1	A	458	HIS	CA-C	-5.17	1.46	1.52
1	A	543	VAL	C-O	-5.14	1.18	1.24
1	A	514	LYS	C-O	-5.04	1.17	1.23

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	682	GLU	N-CA-C	6.91	120.59	112.72
1	A	444	GLU	CA-C-N	-6.48	110.95	122.16
1	A	444	GLU	C-N-CA	-6.48	110.95	122.16
1	A	453	ASP	N-CA-C	6.36	120.82	113.38
1	A	600	ARG	NE-CZ-NH1	-6.31	115.19	121.50
1	A	355	GLN	N-CA-C	-6.19	104.53	111.28
1	A	660	TYR	N-CA-C	-5.54	105.16	111.14
1	A	555	GLU	N-CA-C	-5.28	105.70	111.82
1	A	600	ARG	CB-CG-CD	-5.26	99.20	111.30
1	A	620	LYS	CA-C-N	-5.25	114.83	122.86
1	A	620	LYS	C-N-CA	-5.25	114.83	122.86
2	B	683	ALA	N-CA-C	5.04	117.92	110.46

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2560	0	2480	15	0
2	B	44	0	39	0	0
3	C	39	0	34	1	0
4	D	28	0	25	0	0
5	A	14	0	13	0	0
6	A	2	0	0	0	0
7	A	1	0	0	0	0
8	A	4	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	A	5	0	0	0	0
10	A	12	0	16	0	0
11	A	19	0	11	5	0
12	A	364	0	0	1	0
12	B	3	0	0	0	0
All	All	3095	0	2618	20	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 4.

All (20) 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)
11:A:713:KTR:H8	11:A:713:KTR:H13	1.78	0.65
11:A:713:KTR:H8	11:A:713:KTR:C3	2.29	0.61
1:A:415:ARG:NH2	1:A:432:GLY:O	2.32	0.58
11:A:713:KTR:H13	11:A:713:KTR:C11	2.33	0.58
3:C:2:NAG:H4	3:C:3:BMA:O2	2.08	0.53
1:A:395:ASP:HA	1:A:595:HIS:CD2	2.44	0.52
1:A:417:SER:OG	1:A:418:SER:N	2.41	0.51
11:A:713:KTR:C3	11:A:713:KTR:C11	2.86	0.49
1:A:573:CYS:SG	1:A:579:LYS:HG3	2.53	0.48
1:A:420:HIS:HB2	1:A:428:ARG:HD3	1.95	0.47
1:A:653:GLY:O	1:A:654:ARG:C	2.58	0.45
1:A:600:ARG:HB2	12:A:881:HOH:O	2.17	0.45
1:A:665:TYR:CZ	1:A:669:ILE:HD11	2.51	0.45
1:A:461:VAL:O	1:A:462:ASP:HB2	2.17	0.44
1:A:591:VAL:HG11	11:A:713:KTR:H13	2.00	0.44
1:A:483:PHE:C	1:A:483:PHE:CD2	2.96	0.43
1:A:343:THR:OG1	1:A:606:HIS:CD2	2.72	0.43
1:A:397:GLY:HA3	1:A:462:ASP:O	2.20	0.42
1:A:520:LYS:HD2	1:A:520:LYS:HA	1.93	0.40
1:A:527:THR:HG21	1:A:636:THR:O	2.22	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	333/335 (99%)	323 (97%)	10 (3%)	0	100	100
2	B	4/6 (67%)	4 (100%)	0	0	100	100
All	All	337/341 (99%)	327 (97%)	10 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	278/278 (100%)	274 (99%)	4 (1%)	59	36
2	B	4/4 (100%)	4 (100%)	0	100	100
All	All	282/282 (100%)	278 (99%)	4 (1%)	59	36

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	515	CYS
1	A	567	GLU
1	A	602	ASP
1	A	637	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	359	GLN
1	A	420	HIS
1	A	489	GLN
1	A	585	GLN
1	A	642	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 ⓘ

5 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$
3	NAG	C	1	3,1	14,14,15	0.95	0	17,19,21	1.35	2 (11%)
3	NAG	C	2	3	14,14,15	1.27	2 (14%)	17,19,21	2.11	4 (23%)
3	BMA	C	3	3	11,11,12	1.36	1 (9%)	15,15,17	2.45	5 (33%)
4	NAG	D	1	4,1	14,14,15	1.14	1 (7%)	17,19,21	1.66	3 (17%)
4	NAG	D	2	4	14,14,15	0.53	0	17,19,21	1.98	5 (29%)

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	C	1	3,1	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	C	2	3	-	0/6/23/26	0/1/1/1
3	BMA	C	3	3	-	2/2/19/22	0/1/1/1
4	NAG	D	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	D	2	4	-	2/6/23/26	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	2	NAG	O5-C1	-2.81	1.39	1.43
4	D	1	NAG	O5-C1	-2.47	1.39	1.43
3	C	2	NAG	O7-C7	-2.37	1.17	1.23
3	C	3	BMA	O5-C1	-2.33	1.39	1.43

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	3	BMA	O5-C5-C6	6.62	120.54	107.66
3	C	2	NAG	O5-C1-C2	-5.40	102.94	111.29
3	C	3	BMA	C6-C5-C4	-4.80	101.23	113.02
3	C	2	NAG	C2-N2-C7	4.68	129.17	122.90
4	D	2	NAG	C3-C4-C5	-4.15	102.70	110.23
4	D	2	NAG	C1-O5-C5	4.00	117.55	112.19
4	D	1	NAG	O5-C1-C2	-3.82	105.39	111.29
4	D	1	NAG	C1-O5-C5	3.66	117.08	112.19
4	D	2	NAG	C1-C2-N2	2.79	114.83	110.43
3	C	2	NAG	C3-C4-C5	-2.74	105.27	110.23
3	C	1	NAG	C1-C2-N2	-2.65	106.26	110.43
3	C	1	NAG	C1-O5-C5	2.59	115.65	112.19
3	C	2	NAG	O7-C7-C8	-2.54	117.53	122.05
4	D	2	NAG	O5-C1-C2	2.50	115.16	111.29
3	C	3	BMA	O6-C6-C5	2.46	119.71	111.33
4	D	2	NAG	O7-C7-C8	-2.31	117.95	122.05
3	C	3	BMA	O5-C1-C2	2.25	116.16	110.79
3	C	3	BMA	O4-C4-C5	-2.24	103.81	109.32
4	D	1	NAG	C1-C2-N2	-2.10	107.13	110.43

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	3	BMA	O5-C5-C6-O6

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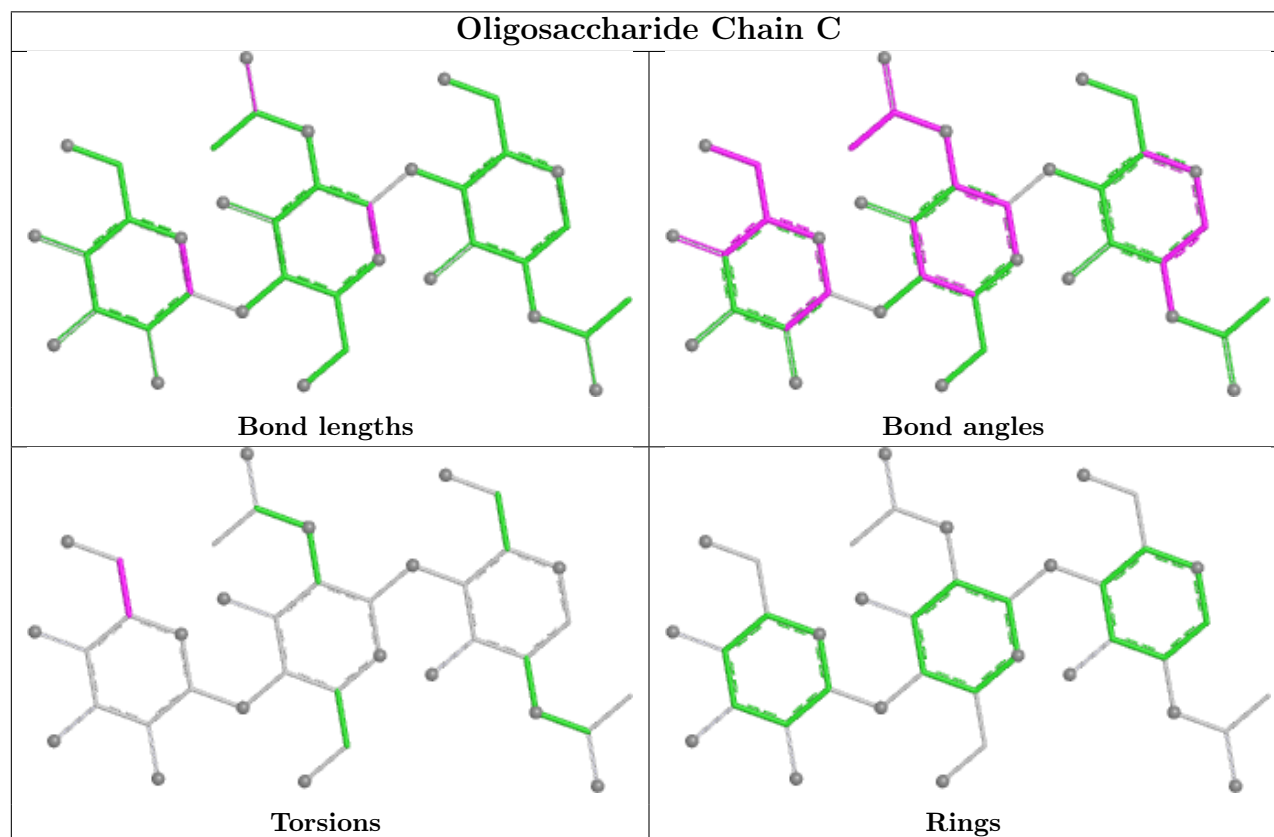
Mol	Chain	Res	Type	Atoms
3	C	3	BMA	C4-C5-C6-O6
4	D	2	NAG	O5-C5-C6-O6
4	D	2	NAG	C4-C5-C6-O6

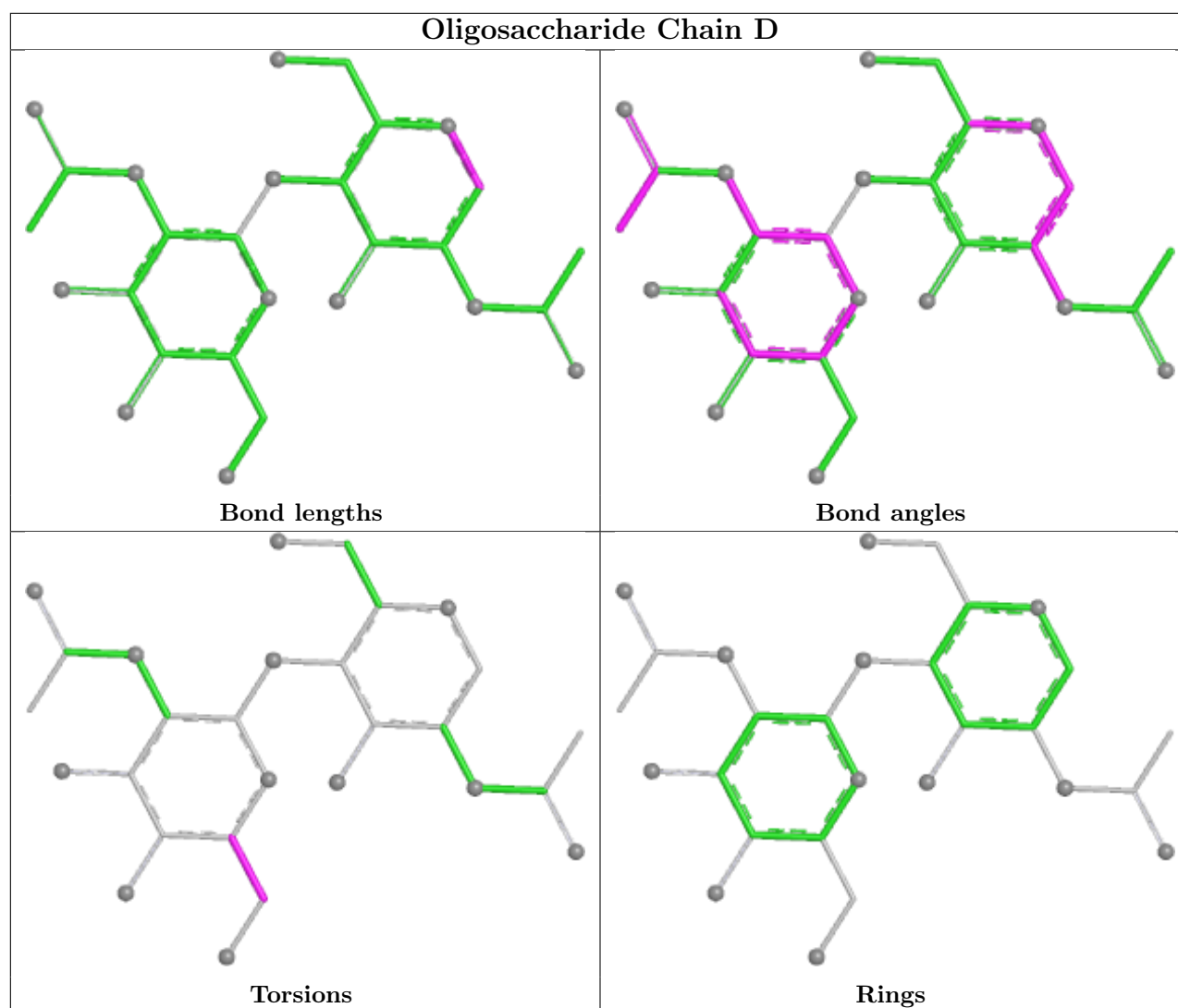
There are no ring outliers.

2 monomers are involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	2	NAG	1	0
3	C	3	BMA	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 9 ligands modelled in this entry, 3 are monoatomic - leaving 6 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	$\# Z > 2$
10	GOL	A	714	-	5,5,5	0.94	0	5,5,5	1.13	0
9	SO4	A	711	-	4,4,4	0.59	0	6,6,6	0.81	0
8	CO3	A	710	7	3,3,3	0.66	0	2,3,3	2.86	1 (50%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	NAG	A	701	1	14,14,15	0.97	1 (7%)	17,19,21	3.04	8 (47%)
11	KTR	A	713	-	20,21,21	1.00	2 (10%)	22,30,30	1.80	4 (18%)
10	GOL	A	712	-	5,5,5	0.73	0	5,5,5	2.01	3 (60%)

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
11	KTR	A	713	-	-	1/12/21/21	0/3/3/3
5	NAG	A	701	1	-	0/6/23/26	0/1/1/1
10	GOL	A	714	-	-	2/4/4/4	-
10	GOL	A	712	-	-	0/4/4/4	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	701	NAG	O7-C7	2.47	1.28	1.23
11	A	713	KTR	O2-C9	2.14	1.28	1.22
11	A	713	KTR	C8-C9	2.07	1.54	1.52

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	701	NAG	C1-O5-C5	5.84	120.02	112.19
5	A	701	NAG	O5-C1-C2	-5.81	102.31	111.29
5	A	701	NAG	C2-N2-C7	5.22	129.89	122.90
11	A	713	KTR	C6-N1-C2	4.97	140.58	135.46
5	A	701	NAG	O7-C7-N2	3.88	128.84	121.98
8	A	710	CO3	O3-C-O1	3.82	129.45	119.68
11	A	713	KTR	O3-C9-O2	-3.75	115.57	124.08
11	A	713	KTR	O2-C9-C8	3.69	132.50	120.19
5	A	701	NAG	O3-C3-C4	-3.51	102.09	110.38
5	A	701	NAG	C8-C7-N2	-3.12	110.94	116.12
11	A	713	KTR	C7-C6-N1	3.10	105.54	102.70
5	A	701	NAG	O5-C5-C6	2.98	113.46	107.66
5	A	701	NAG	C1-C2-N2	2.57	114.48	110.43
10	A	712	GOL	O3-C3-C2	2.43	121.31	110.38
10	A	712	GOL	O2-C2-C3	-2.43	99.14	109.18
10	A	712	GOL	C3-C2-C1	2.38	120.53	111.80

There are no chirality outliers.

All (3) torsion outliers are listed below:

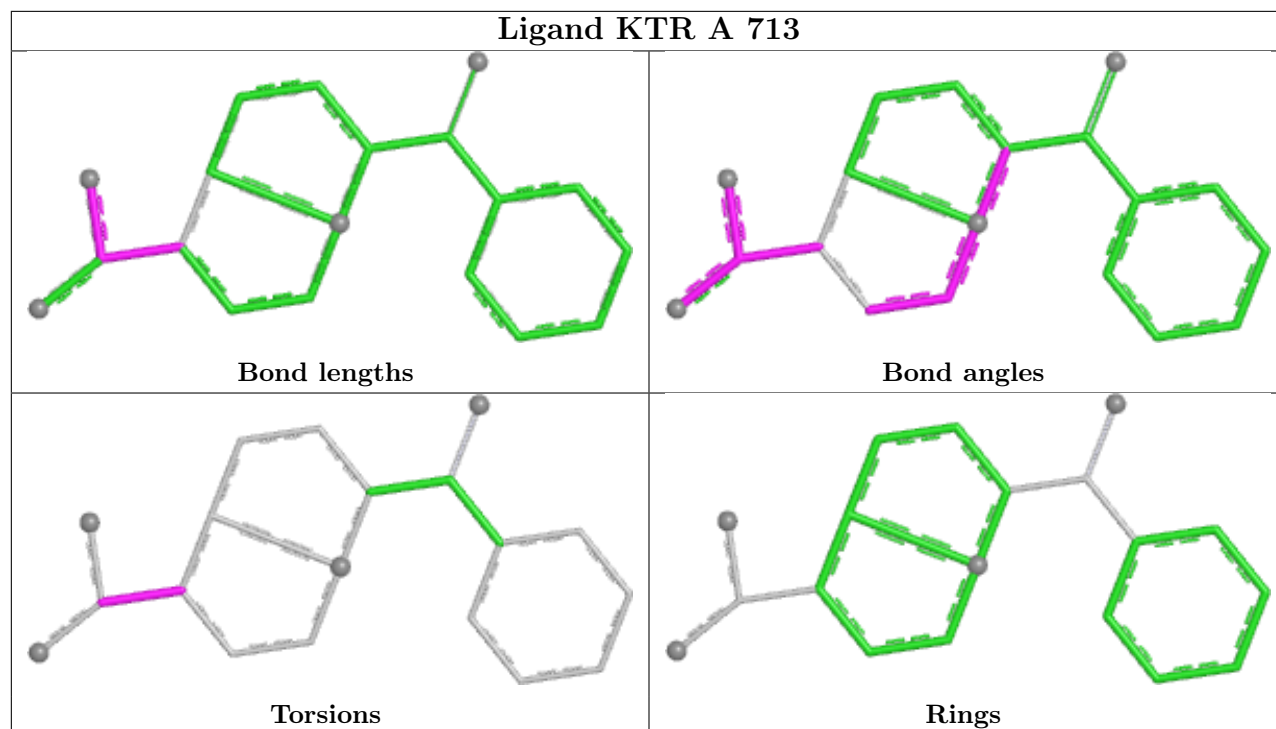
Mol	Chain	Res	Type	Atoms
10	A	714	GOL	C1-C2-C3-O3
10	A	714	GOL	O2-C2-C3-O3
11	A	713	KTR	C5-C8-C9-O3

There are no ring outliers.

1 monomer is involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	A	713	KTR	5	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	335/335 (100%)	-0.08	9 (2%) 56 63	13, 22, 47, 101	0
2	B	6/6 (100%)	2.66	4 (66%) 0 0	45, 50, 82, 88	0
All	All	341/341 (100%)	-0.04	13 (3%) 44 52	13, 22, 48, 101	0

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	681	LEU	4.5
1	A	342	TYR	4.3
1	A	420	HIS	4.1
1	A	621	ASN	3.4
2	B	685	ALA	2.9
1	A	419	LYS	2.8
2	B	683	ALA	2.7
1	A	636	THR	2.7
1	A	418	SER	2.5
1	A	416	LYS	2.4
2	B	682	GLU	2.4
1	A	421	SER	2.2
1	A	559	ASP	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

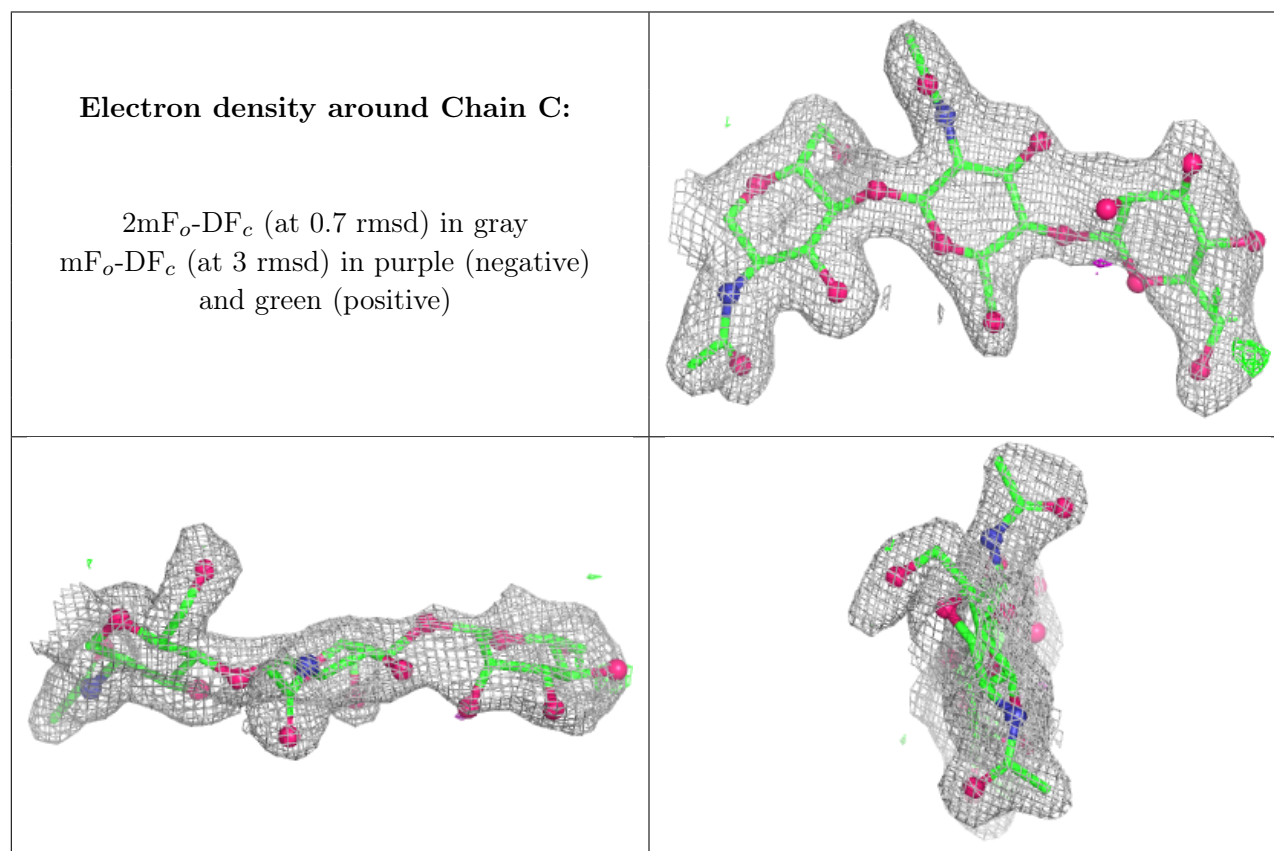
6.3 Carbohydrates [i](#)

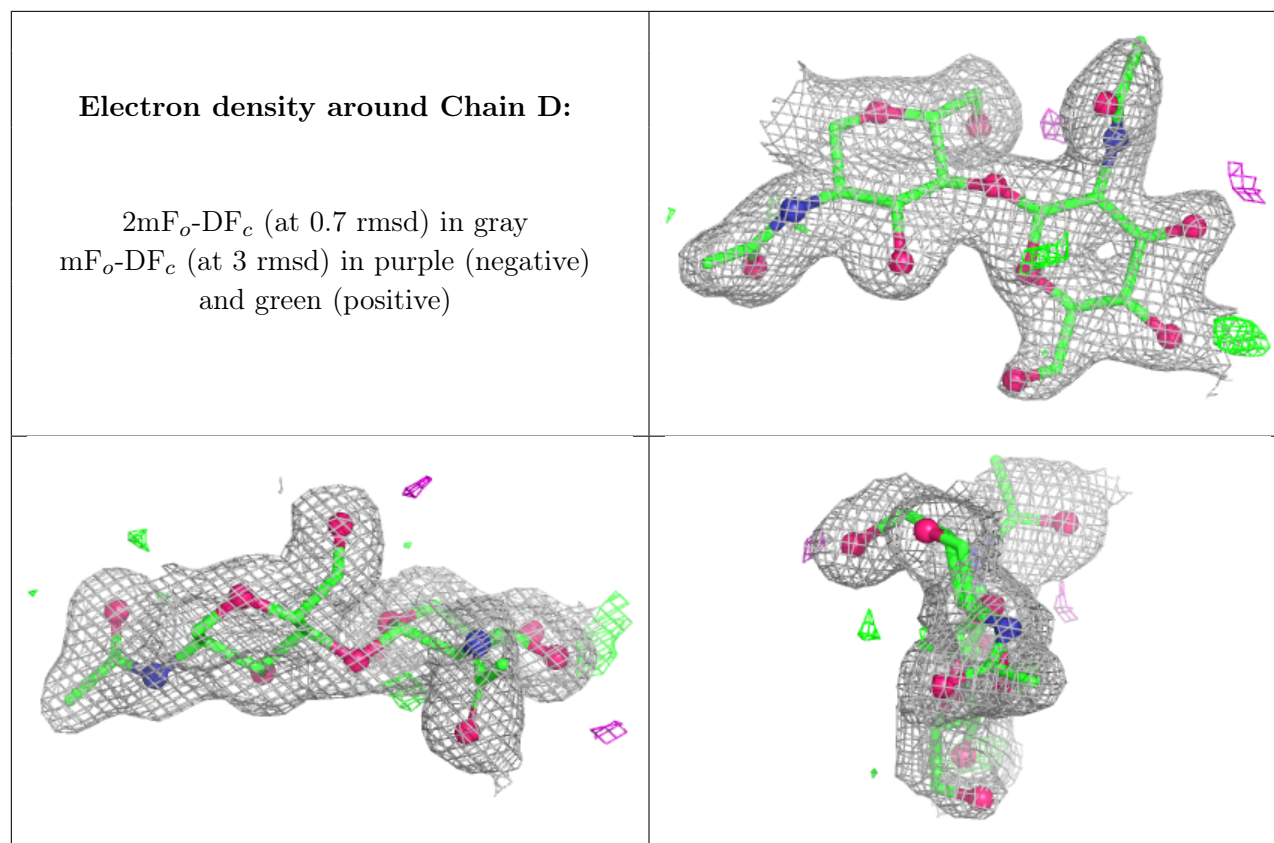
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	BMA	C	3	11/12	0.51	0.15	62,73,77,81	0
4	NAG	D	2	14/15	0.86	0.12	41,46,55,57	0
3	NAG	C	1	14/15	0.89	0.10	32,37,46,48	0
3	NAG	C	2	14/15	0.89	0.11	42,51,59,65	0
4	NAG	D	1	14/15	0.95	0.07	25,29,37,38	0

The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.



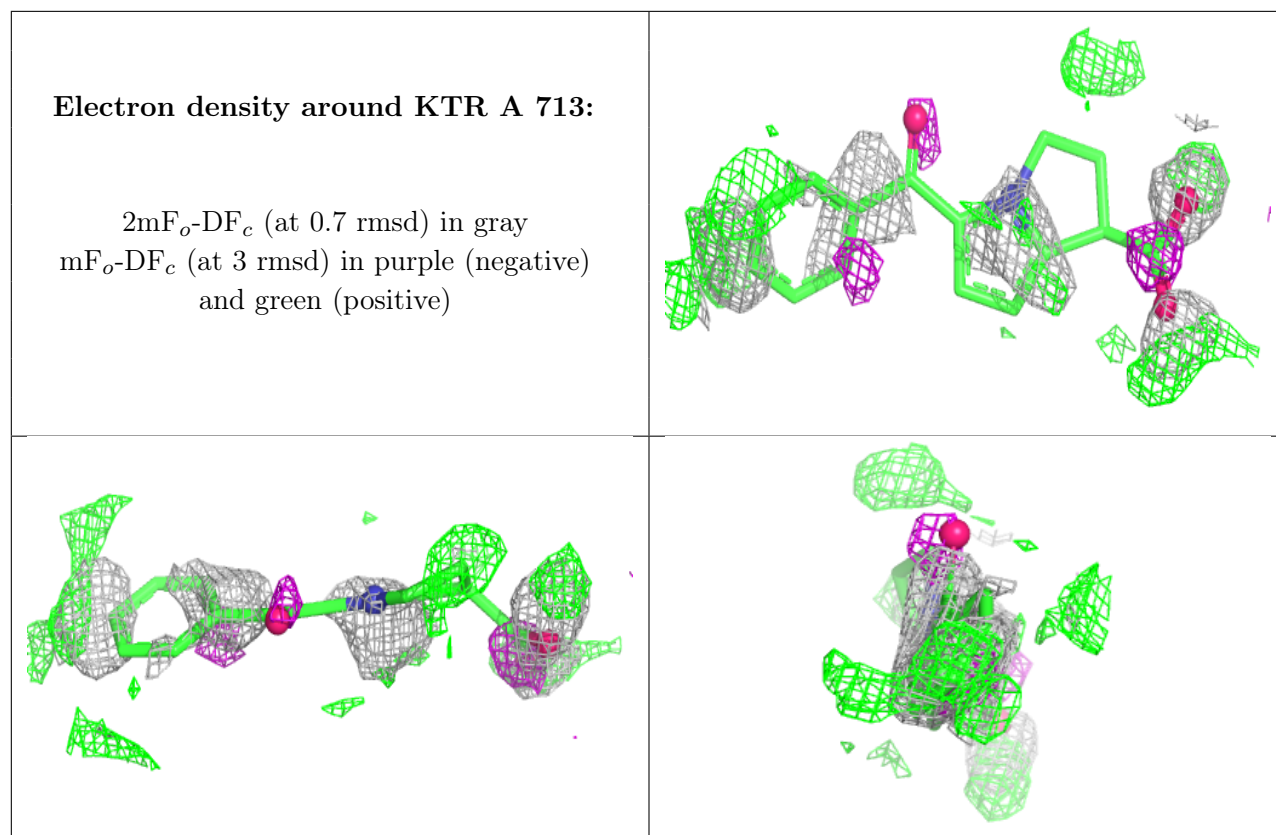


6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
11	KTR	A	713	19/19	0.43	0.26	40,52,58,59	19
10	GOL	A	712	6/6	0.83	0.14	29,44,45,49	0
5	NAG	A	701	14/15	0.83	0.11	36,46,52,59	0
10	GOL	A	714	6/6	0.89	0.14	22,38,41,42	0
9	SO4	A	711	5/5	0.95	0.07	48,48,52,56	0
6	ZN	A	708	1/1	0.97	0.04	24,24,24,24	0
6	ZN	A	707	1/1	0.99	0.04	22,22,22,22	0
8	CO3	A	710	4/4	0.99	0.03	12,15,15,15	0
7	FE	A	709	1/1	1.00	0.01	14,14,14,14	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



6.5 Other polymers [i](#)

There are no such residues in this entry.