



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 04:26 AM UTC

PDB ID : 2X8S / pdb_00002x8s
Title : Crystal Structure of the Abn2 D171A mutant in complex with arabinotriose
Authors : deSanctis, D.; Inacio, J.M.; Lindley, P.F.; de Sa-Nogueira, I.; Bento, I.
Deposited on : 2010-03-11
Resolution : 1.50 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 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
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

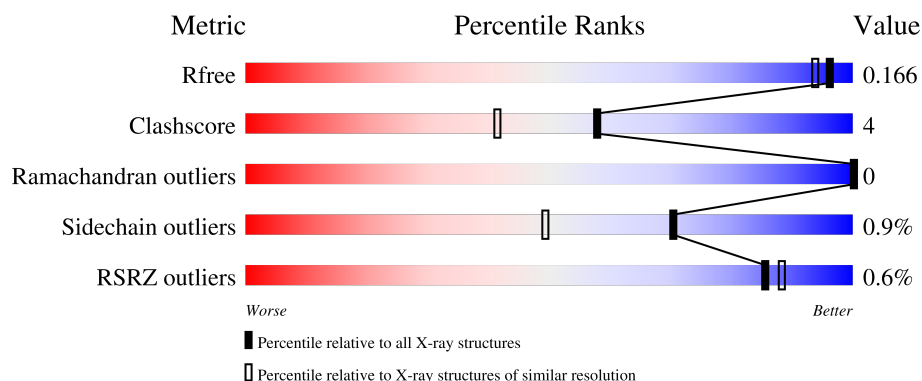
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.50 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))
R_{free}	180053	4037 (1.50-1.50)
Clashscore	190562	4235 (1.50-1.50)
Ramachandran outliers	187476	4153 (1.50-1.50)
Sidechain outliers	187428	4150 (1.50-1.50)
RSRZ outliers	180081	4039 (1.50-1.50)

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 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	470	
1	B	470	
2	C	3	
2	D	3	

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
4	GOL	A	1477	-	-	X	-
4	GOL	B	1480	-	-	X	-

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 7979 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.

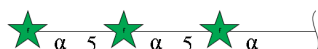
- Molecule 1 is a protein called ENDO-ALPHA-1,5-L-ARABINANASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	443	Total	C	N	O	S	0	10	0
			3577	2273	605	687	12			
1	B	443	Total	C	N	O	S	0	11	0
			3590	2283	607	687	13			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	171	ALA	ASP	engineered mutation	UNP B3FRL6
A	470	LEU	-	expression tag	UNP B3FRL6
B	171	ALA	ASP	engineered mutation	UNP B3FRL6
B	470	LEU	-	expression tag	UNP B3FRL6

- Molecule 2 is an oligosaccharide called alpha-L-arabinofuranose-(1-5)-alpha-L-arabinofuranose-(1-5)-alpha-L-arabinofuranose.



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
2	C	3	Total	C	O	0	1	0
			29	15	14			
2	D	3	Total	C	O	0	1	0
			29	15	14			

- Molecule 3 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Cl	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	2	Total	Cl	0	0
			2	2		

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 5 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (CCD ID: TRS) (formula: $C_4H_{12}NO_3$).



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

- Molecule 6 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	1	Total	Ca	0	0
			1	1		

- Molecule 7 is SODIUM ION (CCD ID: NA) (formula: Na).

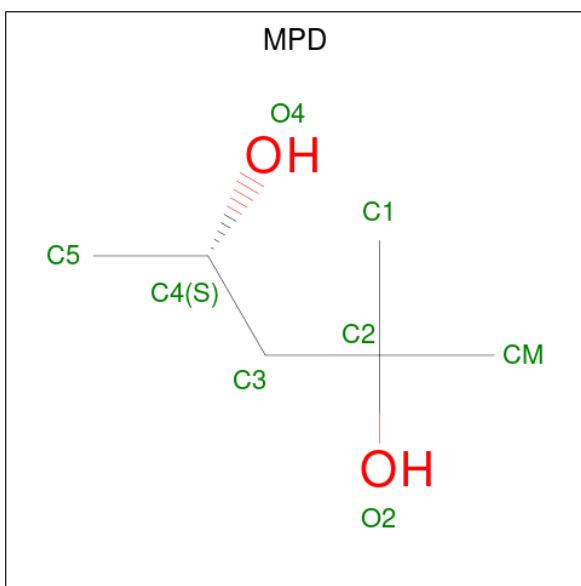
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	B	2	Total	Na	0	0
			2	2		

- Molecule 8 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	B	1	Total	O	P	0	0
			5	4	1		

- Molecule 9 is (4S)-2-METHYL-2,4-PENTANEDIOL (CCD ID: MPD) (formula: C₆H₁₄O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	B	1	Total	C	O	0	0
			8	6	2		

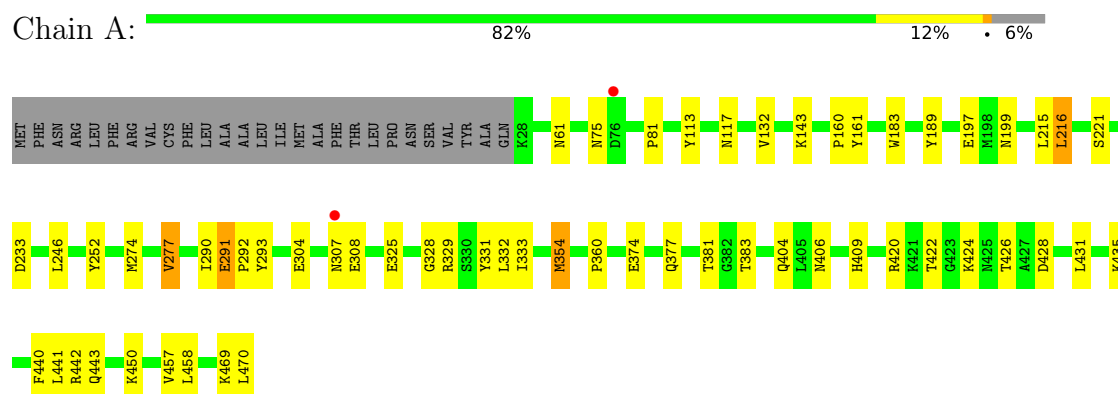
- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	326	Total 326	O 326	0	0
10	B	365	Total 365	O 365	0	0

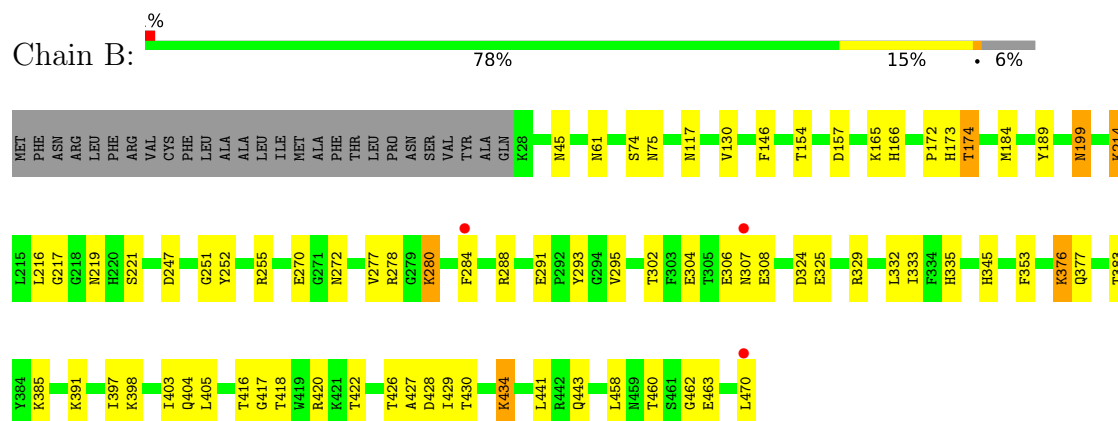
3 Residue-property plots

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 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.

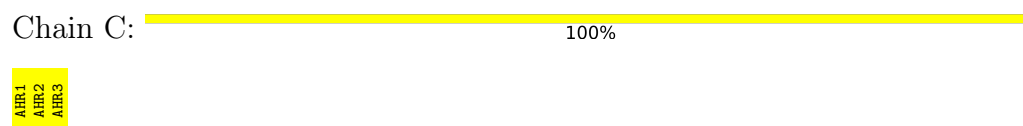
- Molecule 1: ENDO-ALPHA-1,5-L-ARABINANASE



- Molecule 1: ENDO-ALPHA-1,5-L-ARABINANASE



- Molecule 2: alpha-L-arabinofuranose-(1-5)-alpha-L-arabinofuranose-(1-5)-alpha-L-arabinofuranose



- Molecule 2: alpha-L-arabinofuranose-(1-5)-alpha-L-arabinofuranose-(1-5)-alpha-L-arabinofuranose

Chain D:

100%

AHR1
AHR2
AHR3

4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	51.95Å 57.98Å 85.59Å 96.14° 91.77° 117.34°	Depositor
Resolution (Å)	24.59 – 1.50 24.59 – 1.50	Depositor EDS
% Data completeness (in resolution range)	96.0 (24.59-1.50) 96.0 (24.59-1.50)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.44 (at 1.41Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.147 , 0.167 0.146 , 0.166	Depositor DCC
R_{free} test set	7784 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	11.6	Xtriage
Anisotropy	0.173	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 50.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.019 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	7979	wwPDB-VP
Average B, all atoms (Å ²)	15.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.51% 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: PO4, MPD, TRS, CA, GOL, NA, CL, AHR

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	1.01	30/3673 (0.8%)	0.77	3/4976 (0.1%)
1	B	1.15	46/3686 (1.2%)	0.79	5/4992 (0.1%)
All	All	1.08	76/7359 (1.0%)	0.78	8/9968 (0.1%)

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
1	B	1	0

All (76) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	325	GLU	C-N	-19.55	1.06	1.34
1	A	325	GLU	C-N	-19.23	1.05	1.33
1	A	81	PRO	C-N	-11.88	1.17	1.33
1	A	290	ILE	C-O	-11.29	1.12	1.24
1	B	429	ILE	C-O	-8.92	1.14	1.24
1	B	333	ILE	C-O	-8.70	1.14	1.24
1	B	441	LEU	C-O	-8.53	1.13	1.23
1	A	333	ILE	C-O	-8.46	1.15	1.24
1	B	353	PHE	C-O	-8.45	1.13	1.23
1	B	332	LEU	C-O	-8.43	1.14	1.24
1	B	427	ALA	C-O	-8.37	1.13	1.24
1	A	332	LEU	C-O	-8.13	1.14	1.24
1	A	431	LEU	C-O	-7.93	1.15	1.23
1	B	405	LEU	C-O	-7.85	1.14	1.24
1	A	304	GLU	C-O	-7.75	1.14	1.23
1	B	376	LYS	C-O	-7.53	1.15	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	441	LEU	C-N	-7.41	1.23	1.33
1	A	441	LEU	C-O	-7.20	1.15	1.23
1	B	403	ILE	C-O	-7.19	1.16	1.23
1	B	428	ASP	C-O	-7.08	1.15	1.23
1	B	458	LEU	C-O	-7.00	1.15	1.23
1	A	291	GLU	C-O	-6.99	1.15	1.24
1	B	434	LYS	C-O	-6.97	1.15	1.23
1	B	324	ASP	C-O	-6.90	1.15	1.24
1	B	306	GLU	C-O	-6.86	1.16	1.24
1	A	199	ASN	C-O	-6.74	1.15	1.24
1	B	284	PHE	C-O	-6.73	1.16	1.23
1	A	458	LEU	C-O	-6.67	1.16	1.23
1	A	216	LEU	C-O	-6.51	1.17	1.23
1	A	277[A]	VAL	C-O	-6.47	1.17	1.24
1	A	277[B]	VAL	C-O	-6.47	1.17	1.24
1	B	404	GLN	C-O	-6.35	1.15	1.24
1	B	154	THR	C-O	-6.22	1.16	1.23
1	B	199	ASN	C-O	-6.22	1.16	1.24
1	B	173	HIS	C-O	-6.17	1.16	1.24
1	B	166	HIS	C-O	-6.17	1.15	1.23
1	A	246	LEU	C-O	-6.00	1.16	1.24
1	B	251	GLY	C-O	-5.97	1.16	1.23
1	A	442	ARG	C-O	-5.91	1.16	1.24
1	A	233	ASP	C-O	-5.89	1.17	1.24
1	B	74	SER	C-O	-5.76	1.17	1.23
1	B	308	GLU	C-N	-5.73	1.25	1.33
1	B	165	LYS	C-O	-5.72	1.16	1.24
1	B	172	PRO	C-O	-5.65	1.17	1.23
1	B	174	THR	C-O	-5.63	1.17	1.24
1	B	270	GLU	CB-CG	-5.61	1.35	1.52
1	B	214	LYS	C-O	-5.60	1.17	1.23
1	B	247	ASP	C-O	-5.57	1.16	1.23
1	B	307	ASN	C-N	5.52	1.40	1.33
1	B	462	GLY	C-O	-5.50	1.15	1.24
1	B	443[A]	GLN	C-O	-5.47	1.16	1.23
1	B	443[B]	GLN	C-O	-5.47	1.16	1.23
1	A	308	GLU	C-O	-5.46	1.17	1.23
1	A	215	LEU	C-O	-5.37	1.17	1.24
1	A	75	ASN	CG-OD1	5.36	1.33	1.23
1	B	304	GLU	C-O	-5.34	1.17	1.23
1	A	409	HIS	ND1-CE1	5.28	1.37	1.32
1	B	45	ASN	CG-OD1	5.27	1.33	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	440	PHE	C-O	-5.26	1.17	1.23
1	B	75	ASN	CG-OD1	5.25	1.33	1.23
1	B	280	LYS	C-O	-5.24	1.17	1.23
1	B	398	LYS	C-O	-5.24	1.17	1.23
1	B	398	LYS	CG-CD	-5.20	1.36	1.52
1	A	328	GLY	C-O	-5.19	1.17	1.24
1	B	345	HIS	ND1-CE1	5.18	1.37	1.32
1	A	404	GLN	CD-OE1	5.17	1.33	1.23
1	A	457	VAL	C-O	-5.17	1.18	1.23
1	B	325	GLU	C-O	-5.17	1.17	1.24
1	B	377	GLN	CD-OE1	5.17	1.33	1.23
1	A	307	ASN	C-O	-5.15	1.17	1.24
1	A	377	GLN	CD-OE1	5.13	1.33	1.23
1	B	219	ASN	CG-OD1	5.11	1.33	1.23
1	A	61	ASN	CG-OD1	5.10	1.33	1.23
1	A	406	ASN	CG-OD1	5.06	1.33	1.23
1	B	61	ASN	CG-OD1	5.04	1.33	1.23
1	B	272	ASN	CG-OD1	5.02	1.33	1.23

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	354	MET	CG-SD-CE	-9.17	80.72	100.90
1	A	409	HIS	CB-CG-CD2	-6.57	122.66	131.20
1	B	345	HIS	CB-CG-CD2	-6.38	122.91	131.20
1	B	335	HIS	CB-CG-CD2	-5.79	123.67	131.20
1	B	307	ASN	N-CA-C	5.74	119.47	112.23
1	A	409	HIS	CB-CG-ND1	5.66	131.19	122.70
1	B	345	HIS	CB-CG-ND1	5.37	130.76	122.70
1	B	335	HIS	CB-CG-ND1	5.02	130.22	122.70

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	B	397[B]	ILE	CB

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	3577	0	3427	24	0
1	B	3590	0	3454	37	0
2	C	29	0	0	0	0
2	D	29	0	0	0	0
3	A	1	0	0	0	0
3	B	2	0	0	1	0
4	A	18	0	24	6	0
4	B	18	0	23	5	0
5	A	8	0	10	1	0
6	B	1	0	0	0	0
7	B	2	0	0	0	0
8	B	5	0	0	0	0
9	B	8	0	14	0	0
10	A	326	0	0	2	0
10	B	365	0	0	8	0
All	All	7979	0	6952	64	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 (64) 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:B:199:ASN:HD21	4:B:1480:GOL:H11	0.99	1.10
1:B:329[A]:ARG:HG2	1:B:329[A]:ARG:HH21	1.18	1.07
1:B:199:ASN:ND2	4:B:1480:GOL:H11	1.79	0.97
4:A:1477:GOL:H11	1:B:288:ARG:HG3	1.47	0.93
1:B:329[A]:ARG:HH21	1:B:329[A]:ARG:CG	1.81	0.92
1:B:199:ASN:HD21	4:B:1480:GOL:C1	1.90	0.79
1:A:277[B]:VAL:HG12	1:A:293:TYR:CG	2.24	0.73
1:B:329[A]:ARG:CG	1:B:329[A]:ARG:NH2	2.45	0.67
1:A:274:MET:O	1:A:277[B]:VAL:HG22	1.95	0.66
1:B:420:ARG:HD2	3:B:1478:CL:CL	2.33	0.65
1:B:434:LYS:HE2	10:B:2336:HOH:O	1.95	0.65
4:A:1475:GOL:H32	10:A:2014:HOH:O	1.96	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:277[A]:VAL:HG22	1:A:293:TYR:CG	2.33	0.64
1:B:329[A]:ARG:HG2	1:B:329[A]:ARG:NH2	2.00	0.64
4:B:1480:GOL:H2	10:B:2364:HOH:O	2.00	0.61
4:A:1477:GOL:H12	1:B:288:ARG:HB2	1.84	0.60
1:B:383:THR:HG22	1:B:470:LEU:HD23	1.86	0.58
1:A:132[B]:VAL:HG21	1:A:143:LYS:HD2	1.86	0.56
1:A:354:MET:HE1	1:A:360:PRO:HB3	1.88	0.56
1:B:418:THR:OG1	1:B:430[B]:THR:HG22	2.06	0.56
1:B:422:THR:HB	1:B:426:THR:HB	1.88	0.55
1:B:434:LYS:CE	10:B:2336:HOH:O	2.54	0.55
1:B:302:THR:HB	1:B:397[B]:ILE:HD11	1.88	0.54
1:A:160:PRO:HD3	4:A:1477:GOL:H32	1.90	0.54
1:A:381:THR:C	1:A:469:LYS:HZ1	2.16	0.53
1:B:418:THR:H	1:B:430[B]:THR:HG22	1.73	0.53
1:B:460:THR:HG23	10:B:2335:HOH:O	2.07	0.52
1:A:435:LYS:NZ	1:A:435:LYS:HB3	2.24	0.52
4:B:1480:GOL:H12	10:B:2365:HOH:O	2.10	0.51
1:B:277:VAL:HG22	1:B:293:TYR:CG	2.46	0.49
1:A:329[B]:ARG:NE	1:A:331:TYR:OH	2.43	0.49
1:B:417:GLY:HA3	1:B:430[A]:THR:O	2.13	0.49
1:A:277[B]:VAL:HG12	1:A:293:TYR:CD2	2.48	0.49
1:A:132[B]:VAL:CG2	1:A:143:LYS:HD2	2.43	0.48
1:B:418:THR:N	1:B:430[B]:THR:HG22	2.28	0.48
1:B:130[B]:VAL:HG23	1:B:146:PHE:CE1	2.50	0.47
1:B:278:ARG:NH1	10:B:2219:HOH:O	2.47	0.47
1:B:416[A]:THR:HG22	10:B:2317:HOH:O	2.15	0.47
1:B:329[A]:ARG:NH2	10:B:2247:HOH:O	2.48	0.46
1:A:113:TYR:CD2	1:A:132[B]:VAL:HG22	2.50	0.46
1:A:277[B]:VAL:O	1:A:277[B]:VAL:HG23	2.15	0.46
1:B:174:THR:OG1	1:B:184[B]:MET:HG3	2.16	0.45
1:A:420:ARG:HG3	1:A:428:ASP:HB3	1.99	0.45
1:B:288:ARG:HH21	1:B:291:GLU:CD	2.24	0.45
4:A:1477:GOL:H11	1:B:288:ARG:CG	2.32	0.45
1:A:291:GLU:N	1:A:292:PRO:CD	2.80	0.45
1:A:189:TYR:HA	1:A:221:SER:O	2.17	0.44
1:B:385:LYS:HG3	1:B:470:LEU:HD11	2.00	0.44
1:A:374:GLU:HA	1:A:424:LYS:HG2	1.99	0.44
1:B:189:TYR:HA	1:B:221:SER:O	2.20	0.42
1:A:443[B]:GLN:HB2	10:A:2251:HOH:O	2.19	0.42
1:B:214:LYS:CE	1:B:217:GLY:O	2.67	0.42
1:A:422:THR:HB	1:A:426:THR:HB	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:383:THR:HG22	1:A:470:LEU:HD12	2.02	0.41
1:A:383:THR:CG2	1:A:470:LEU:HD12	2.50	0.41
1:A:161:TYR:O	1:B:280:LYS:HE2	2.20	0.41
5:A:1478:TRS:O2	5:A:1478:TRS:O1	2.36	0.41
1:A:183:TRP:CZ3	1:A:197:GLU:HG2	2.56	0.41
4:A:1477:GOL:C1	1:B:288:ARG:HB2	2.50	0.41
1:B:391:LYS:HG2	1:B:463:GLU:HG2	2.03	0.41
1:B:157:ASP:OD1	1:B:157:ASP:C	2.63	0.41
1:B:418:THR:H	1:B:430[B]:THR:CG2	2.33	0.40
1:A:450:LYS:HB3	1:A:450:LYS:HE3	1.71	0.40
1:B:255:ARG:HA	1:B:295:VAL:O	2.21	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	451/470 (96%)	441 (98%)	10 (2%)	0	100	100
1	B	452/470 (96%)	442 (98%)	10 (2%)	0	100	100
All	All	903/940 (96%)	883 (98%)	20 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	380/394 (96%)	377 (99%)	3 (1%)	73	54
1	B	382/394 (97%)	378 (99%)	4 (1%)	68	45
All	All	762/788 (97%)	755 (99%)	7 (1%)	70	49

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	117	ASN
1	A	216	LEU
1	A	252	TYR
1	B	117	ASN
1	B	216	LEU
1	B	252	TYR
1	B	376	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	61	ASN
1	A	168	ASN
1	A	388	GLN
1	B	307	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 ⓘ

8 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	AHR	C	1	2	10,10,10	0.81	0	13,14,14	1.43	2 (15%)
2	AHR	C	2	2	9,9,10	0.88	1 (11%)	11,12,14	0.80	0
2	AHR	C	3[A]	-	9,9,10	0.49	0	11,12,14	1.24	1 (9%)
2	AHR	C	3[B]	-	9,9,10	0.51	0	11,12,14	1.02	1 (9%)
2	AHR	D	1	2	10,10,10	0.81	0	13,14,14	1.61	2 (15%)
2	AHR	D	2	2	9,9,10	0.83	1 (11%)	11,12,14	0.76	0
2	AHR	D	3[A]	-	9,9,10	1.71	1 (11%)	11,12,14	0.84	0
2	AHR	D	3[B]	-	9,9,10	0.56	0	11,12,14	1.19	1 (9%)

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	AHR	C	1	2	-	0/2/18/18	0/1/1/1
2	AHR	C	2	2	-	0/2/15/18	0/1/1/1
2	AHR	C	3[A]	-	-	0/2/15/18	0/1/1/1
2	AHR	C	3[B]	-	-	0/2/15/18	0/1/1/1
2	AHR	D	1	2	-	2/2/18/18	0/1/1/1
2	AHR	D	2	2	-	0/2/15/18	0/1/1/1
2	AHR	D	3[A]	-	-	0/2/15/18	0/1/1/1
2	AHR	D	3[B]	-	-	2/2/15/18	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	3[A]	AHR	O5-C5	-5.04	1.21	1.42
2	D	2	AHR	O5-C5	-2.04	1.33	1.42
2	C	2	AHR	O5-C5	-2.02	1.33	1.42

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	1	AHR	O5-C5-C4	-3.82	98.33	111.33
2	D	3[B]	AHR	O5-C5-C4	-3.19	100.48	111.33
2	C	3[A]	AHR	O5-C5-C4	-3.09	100.81	111.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1	AHR	C1-C2-C3	2.93	105.89	102.29
2	D	1	AHR	C1-C2-C3	2.61	105.50	102.29
2	C	1	AHR	O1-C1-O4	-2.36	108.11	111.12
2	C	3[B]	AHR	O5-C5-C4	2.01	118.17	111.33

There are no chirality outliers.

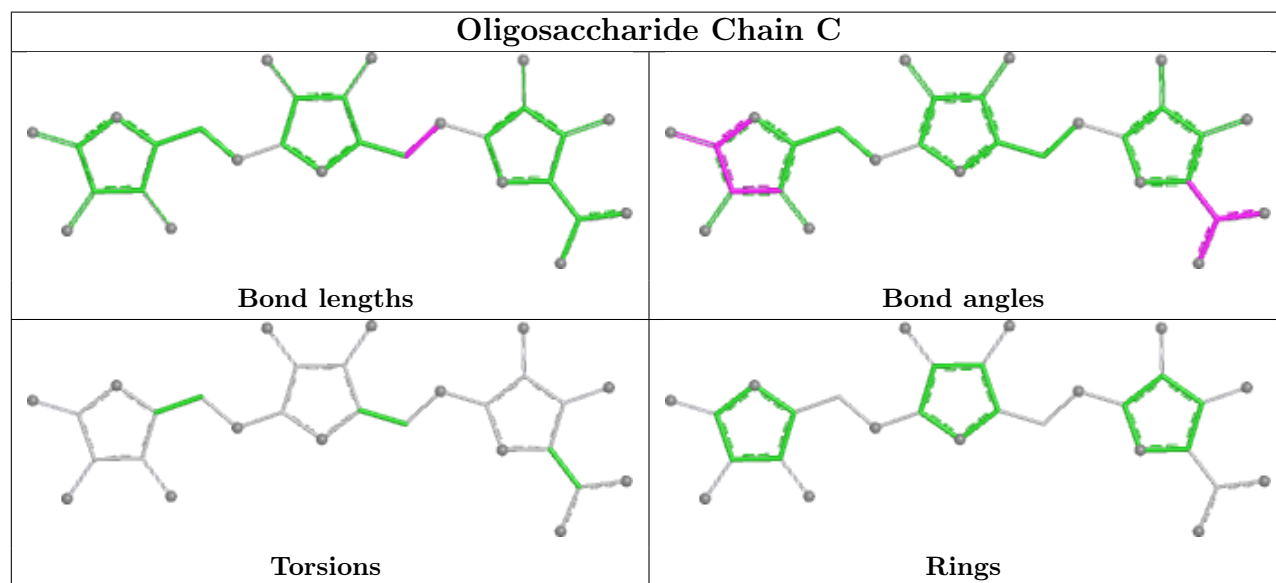
All (4) torsion outliers are listed below:

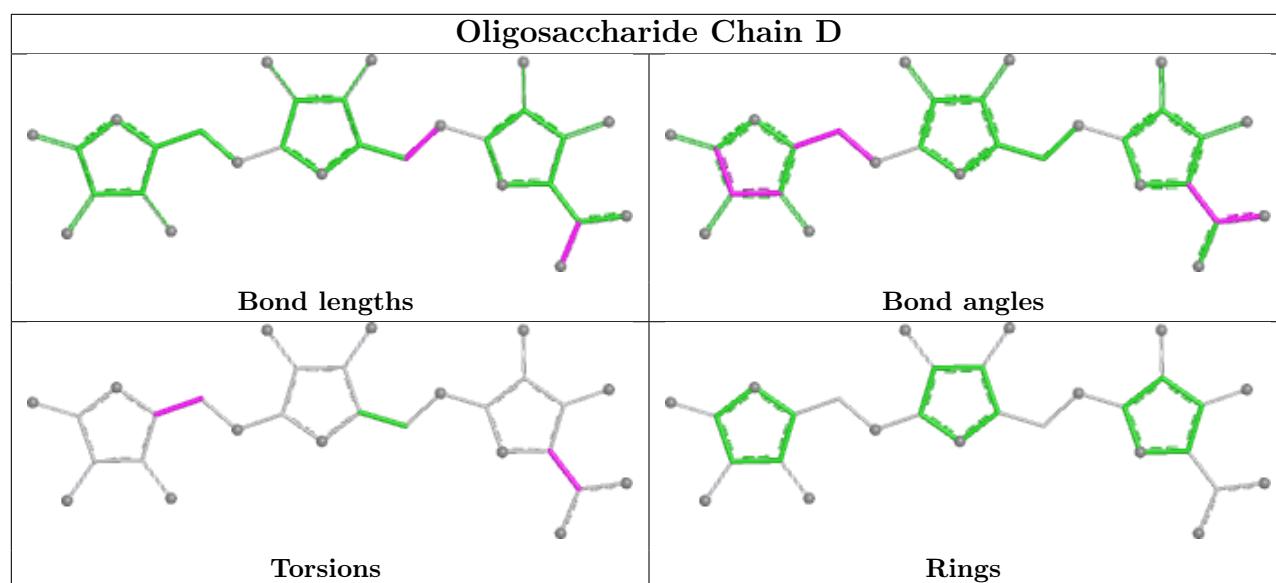
Mol	Chain	Res	Type	Atoms
2	D	1	AHR	C3-C4-C5-O5
2	D	3[B]	AHR	O4-C4-C5-O5
2	D	3[B]	AHR	C3-C4-C5-O5
2	D	1	AHR	O4-C4-C5-O5

There are no ring outliers.

No monomer is involved in short contacts.

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 15 ligands modelled in this entry, 6 are monoatomic - leaving 9 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	GOL	B	1482	-	5,5,5	0.63	0	5,5,5	0.68	0
4	GOL	A	1476	-	5,5,5	0.86	0	5,5,5	0.94	0
9	MPD	B	1483	-	7,7,7	0.30	0	9,10,10	0.26	0
4	GOL	A	1477	-	5,5,5	0.81	0	5,5,5	1.54	1 (20%)
4	GOL	B	1476	-	5,5,5	0.46	0	5,5,5	0.46	0
5	TRS	A	1478	-	7,7,7	1.43	1 (14%)	9,9,9	1.48	2 (22%)
8	PO4	B	1479	-	4,4,4	0.95	0	6,6,6	0.48	0
4	GOL	A	1475	-	5,5,5	0.44	0	5,5,5	0.55	0
4	GOL	B	1480	-	5,5,5	1.39	0	5,5,5	2.13	2 (40%)

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
4	GOL	B	1482	-	-	0/4/4/4	-
4	GOL	A	1476	-	-	0/4/4/4	-
9	MPD	B	1483	-	-	1/5/5/5	-
4	GOL	A	1477	-	-	4/4/4/4	-
4	GOL	B	1476	-	-	0/4/4/4	-
5	TRS	A	1478	-	-	6/9/9/9	-
4	GOL	A	1475	-	-	0/4/4/4	-
4	GOL	B	1480	-	-	2/4/4/4	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1478	TRS	O1-C1	-2.42	1.34	1.42

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1477	GOL	C3-C2-C1	3.21	123.57	111.80
4	B	1480	GOL	C3-C2-C1	-2.96	100.93	111.80
5	A	1478	TRS	O3-C3-C	-2.94	102.67	110.88
4	B	1480	GOL	O1-C1-C2	-2.87	97.47	110.38
5	A	1478	TRS	O1-C1-C	-2.61	103.61	110.88

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1477	GOL	O1-C1-C2-C3
4	A	1477	GOL	C1-C2-C3-O3
4	B	1480	GOL	C1-C2-C3-O3
5	A	1478	TRS	C2-C-C1-O1
5	A	1478	TRS	C3-C-C1-O1
5	A	1478	TRS	N-C-C1-O1
5	A	1478	TRS	C1-C-C3-O3
5	A	1478	TRS	C2-C-C3-O3
5	A	1478	TRS	N-C-C3-O3
4	A	1477	GOL	O1-C1-C2-O2
4	A	1477	GOL	O2-C2-C3-O3
4	B	1480	GOL	O2-C2-C3-O3
9	B	1483	MPD	C1-C2-C3-C4

There are no ring outliers.

4 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1477	GOL	5	0
5	A	1478	TRS	1	0
4	A	1475	GOL	1	0
4	B	1480	GOL	5	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	2
1	B	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	81:PRO	C	82:ASN	N	1.17
1	B	325:GLU	C	326:LYS	N	1.07
1	A	325:GLU	C	326:LYS	N	1.05

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	443/470 (94%)	-0.39	2 (0%) 87 89	4, 13, 28, 40	10 (2%)
1	B	443/470 (94%)	-0.49	3 (0%) 84 87	4, 11, 24, 39	11 (2%)
All	All	886/940 (94%)	-0.44	5 (0%) 85 88	4, 12, 27, 40	21 (2%)

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	284	PHE	3.8
1	A	307	ASN	2.5
1	A	76	ASP	2.3
1	B	307	ASN	2.2
1	B	470	LEU	2.1

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.

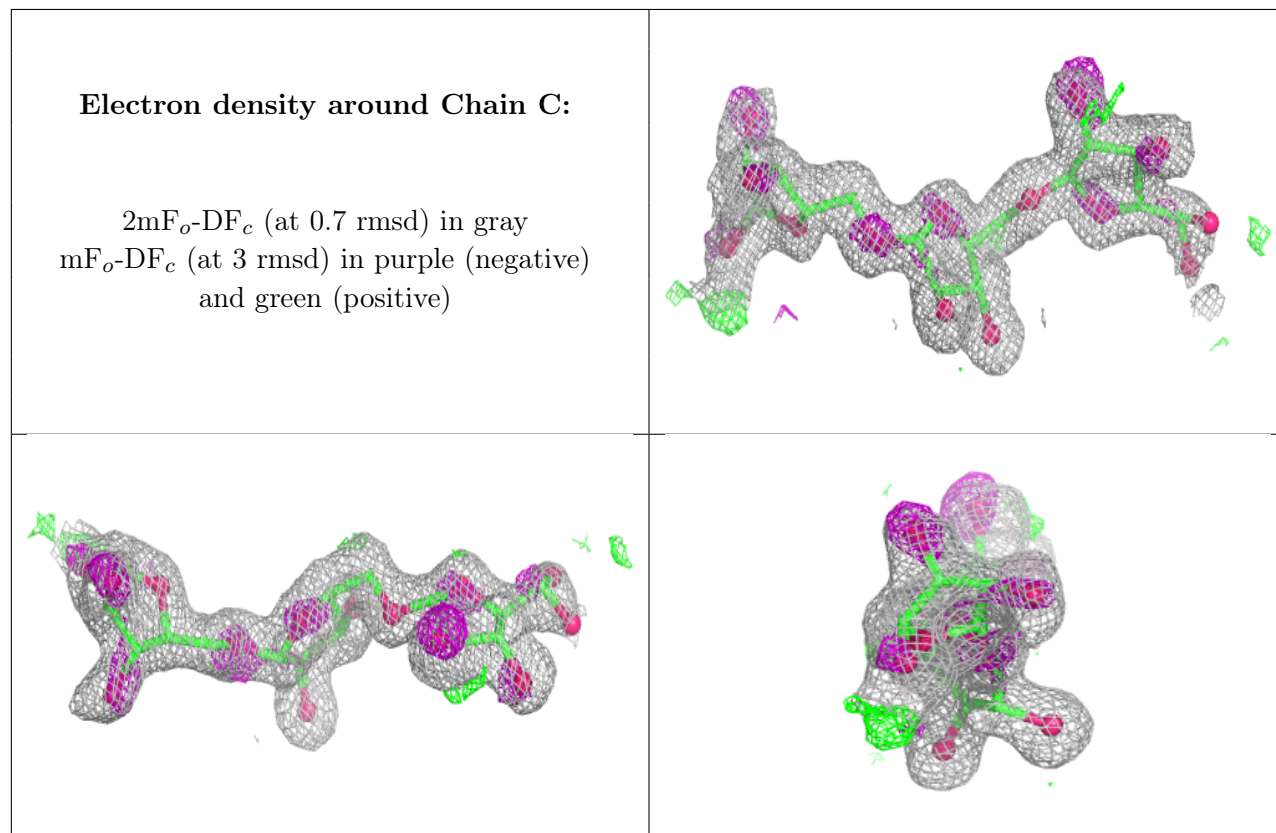
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	AHR	D	1	10/10	0.85	0.12	13,26,28,28	0
2	AHR	C	1	10/10	0.89	0.10	12,25,26,26	0
2	AHR	C	3[B]	9/10	0.92	0.08	17,17,19,20	1
2	AHR	C	3[A]	9/10	0.92	0.08	17,17,19,20	1

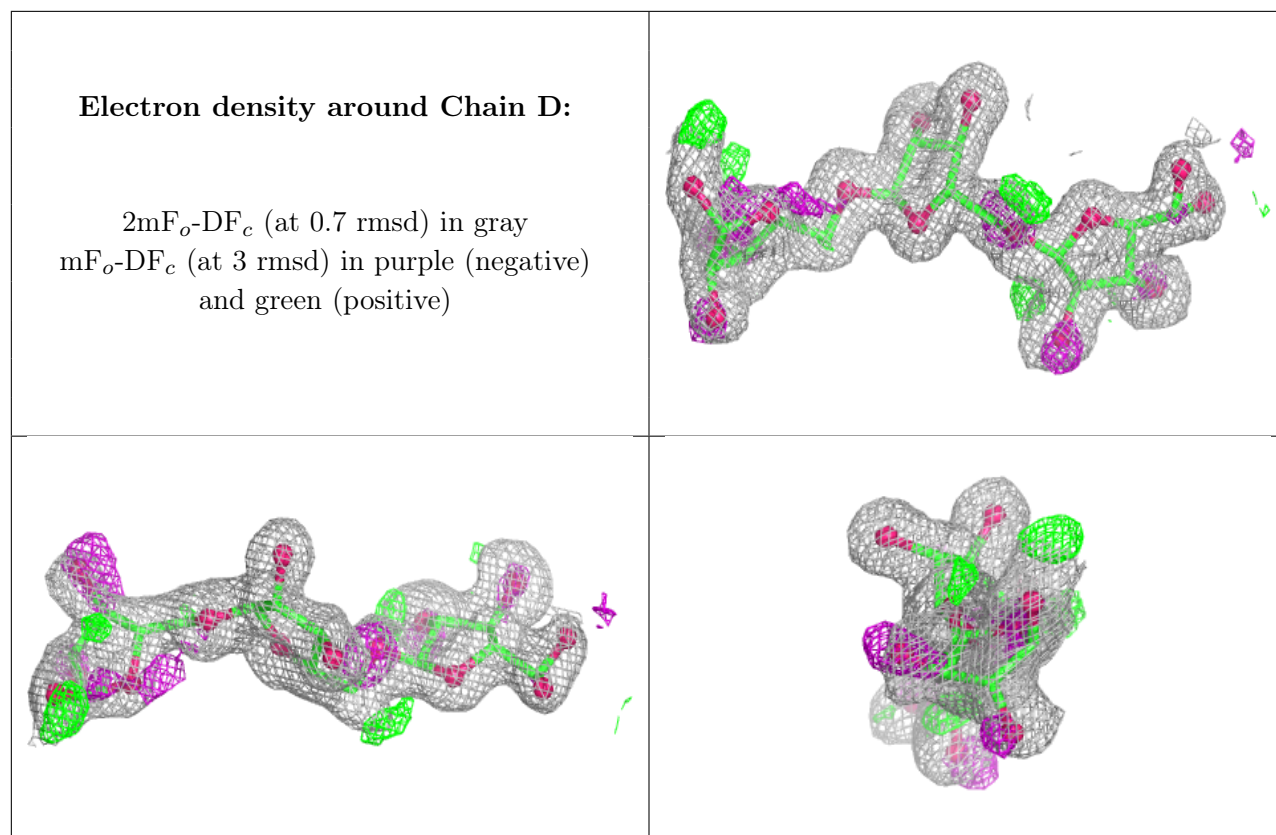
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	AHR	D	3[A]	9/10	0.95	0.06	11,12,14,16	1
2	AHR	D	3[B]	9/10	0.95	0.06	11,12,14,16	1
2	AHR	C	2	9/10	0.96	0.05	9,10,13,19	0
2	AHR	D	2	9/10	0.96	0.05	9,10,12,13	0

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($\text{\AA}^2$)	Q<0.9
4	GOL	A	1477	6/6	0.81	0.12	30,35,39,44	0
4	GOL	B	1480	6/6	0.82	0.15	23,31,46,49	0
5	TRS	A	1478	8/8	0.82	0.12	38,38,48,51	0
8	PO4	B	1479	5/5	0.82	0.10	43,51,52,67	0
9	MPD	B	1483	8/8	0.83	0.17	30,38,43,50	0
7	NA	B	1481	1/1	0.84	0.12	48,48,48,48	0
4	GOL	B	1482	6/6	0.90	0.11	13,27,34,36	0
4	GOL	A	1476	6/6	0.93	0.10	16,26,33,34	0
4	GOL	A	1475	6/6	0.93	0.10	14,22,29,32	0
4	GOL	B	1476	6/6	0.95	0.10	14,18,23,26	0
7	NA	B	1477	1/1	0.97	0.09	25,25,25,25	0
3	CL	B	1478	1/1	0.97	0.22	36,36,36,36	0
3	CL	A	1474	1/1	0.99	0.05	16,16,16,16	0
3	CL	B	1475	1/1	0.99	0.09	14,14,14,14	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	CA	B	1471	1/1	1.00	0.01	5,5,5,5	0

6.5 Other polymers [i](#)

There are no such residues in this entry.