



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 09:49 AM UTC

PDB ID : 3NBD / pdb_00003nbd
Title : Clitocybe nebularis ricin B-like lectin (CNL) in complex with lactose, crystallized at pH 7.1
Authors : Renko, M.; Pohleven, J.; Sabotic, J.; Kos, J.; Turk, D.
Deposited on : 2010-06-03
Resolution : 1.15 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

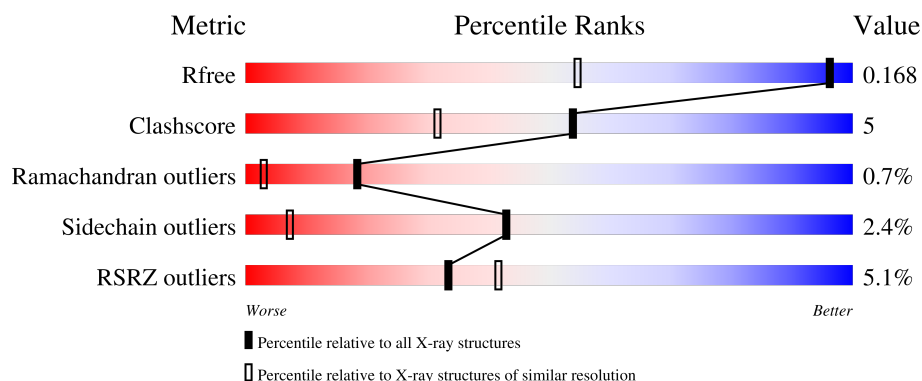
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.15 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	1380 (1.16-1.12)
Clashscore	190562	1393 (1.16-1.12)
Ramachandran outliers	187476	1369 (1.16-1.12)
Sidechain outliers	187428	1369 (1.16-1.12)
RSRZ outliers	180081	1379 (1.16-1.12)

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	148	5% 53% 45% .
1	B	148	5% 57% 39% ..
2	C	2	100%
2	D	2	100%

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 2937 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 Ricin B-like lectin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	148	Total	C	N	O	S	12	13	0
			1173	738	196	238	1			
1	B	148	Total	C	N	O	S	12	7	0
			1158	726	195	236	1			

- Molecule 2 is an oligosaccharide called beta-D-galactopyranose-(1-4)-alpha-D-glucopyranoside.



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
2	C	2	Total	C	O	0	0	0
			23	12	11			
2	D	2	Total	C	O	0	0	0
			23	12	11			

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

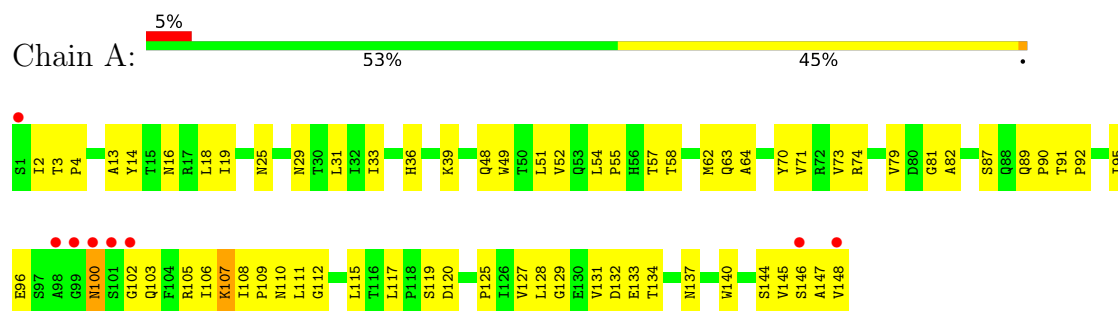
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	283	Total	O	0	0
			283	283		
4	B	252	Total	O	0	0
			252	252		

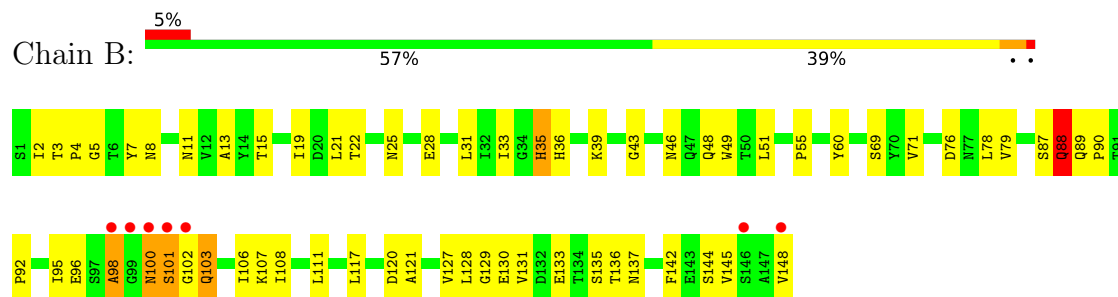
3 Residue-property plots [i](#)

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: Ricin B-like lectin



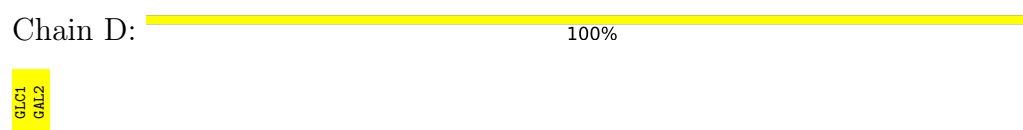
- Molecule 1: Ricin B-like lectin



- Molecule 2: beta-D-galactopyranose-(1-4)-alpha-D-glucopyranose



- Molecule 2: beta-D-galactopyranose-(1-4)-alpha-D-glucopyranose



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	43.12Å 85.08Å 97.63Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	23.03 – 1.15 23.03 – 1.15	Depositor EDS
% Data completeness (in resolution range)	99.5 (23.03-1.15) 99.9 (23.03-1.15)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.19 (at 1.15Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.138 , 0.160 (Not available) , 0.168	Depositor DCC
R_{free} test set	6456 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	10.6	Xtriage
Anisotropy	0.282	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 49.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	2937	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 5.35% 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: GLC, SO4, GAL

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	2.93	72/1235 (5.8%)	1.12	5/1693 (0.3%)
1	B	2.84	71/1208 (5.9%)	1.16	3/1655 (0.2%)
All	All	2.88	143/2443 (5.9%)	1.14	8/3348 (0.2%)

All (143) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	102	GLY	C-O	10.32	1.37	1.23
1	B	3	THR	CA-C	8.49	1.62	1.52
1	A	108	ILE	CA-C	8.22	1.59	1.53
1	A	112	GLY	CA-C	8.05	1.60	1.51
1	A	2	ILE	CA-C	7.91	1.62	1.52
1	B	111	LEU	CA-C	7.86	1.62	1.52
1	A	33	ILE	C-N	7.68	1.38	1.33
1	A	131	VAL	CA-CB	7.54	1.62	1.54
1	A	52	VAL	CA-C	7.43	1.61	1.52
1	A	112	GLY	N-CA	7.37	1.56	1.45
1	A	129	GLY	N-CA	7.28	1.51	1.45
1	B	121	ALA	N-CA	7.20	1.54	1.46
1	B	71	VAL	CA-CB	7.18	1.62	1.54
1	A	74	ARG	CD-NE	7.17	1.56	1.46
1	A	102	GLY	C-N	7.08	1.43	1.33
1	B	98	ALA	N-CA	7.05	1.54	1.46
1	A	117	LEU	C-N	7.04	1.41	1.34
1	B	35	HIS	ND1-CE1	7.01	1.39	1.32
1	A	109	PRO	CA-CB	6.75	1.62	1.53
1	A	146	SER	C-N	-6.72	1.24	1.33
1	B	49	TRP	C-O	6.61	1.31	1.24
1	A	111	LEU	C-O	6.60	1.32	1.24
1	A	16[A]	ASN	CA-CB	6.56	1.64	1.53
1	A	16[B]	ASN	CA-CB	6.56	1.64	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	133	GLU	C-O	6.53	1.32	1.24
1	A	36	HIS	ND1-CE1	6.52	1.39	1.32
1	A	125	PRO	C-O	6.52	1.30	1.23
1	B	95	ILE	N-CA	6.52	1.54	1.46
1	B	117	LEU	C-O	6.52	1.31	1.24
1	A	89	GLN	CA-C	6.51	1.58	1.52
1	B	130	GLU	CA-C	6.47	1.60	1.52
1	B	96	GLU	CA-C	6.46	1.60	1.52
1	B	127	VAL	CA-C	6.46	1.59	1.52
1	A	57	THR	CA-C	6.45	1.60	1.52
1	A	39[A]	LYS	CA-CB	6.44	1.64	1.53
1	A	39[B]	LYS	CA-CB	6.44	1.64	1.53
1	B	33	ILE	C-N	6.39	1.37	1.33
1	B	76	ASP	CA-C	6.32	1.61	1.53
1	A	54	LEU	CA-C	6.31	1.60	1.52
1	B	13	ALA	N-CA	6.25	1.53	1.46
1	A	105	ARG	NE-CZ	6.23	1.40	1.33
1	B	120	ASP	CA-C	6.20	1.61	1.52
1	A	145	VAL	C-O	6.17	1.30	1.24
1	A	3	THR	CA-CB	6.14	1.64	1.53
1	B	121	ALA	CA-C	6.12	1.60	1.52
1	A	71	VAL	CA-CB	6.11	1.61	1.54
1	A	92	PRO	N-CA	6.10	1.54	1.47
1	B	22	THR	CA-C	6.08	1.61	1.52
1	A	91	THR	CA-C	6.08	1.59	1.52
1	A	71	VAL	C-O	5.98	1.30	1.24
1	A	48	GLN	N-CA	5.95	1.53	1.46
1	B	31	LEU	N-CA	5.94	1.53	1.46
1	B	108	ILE	CA-CB	5.93	1.61	1.54
1	B	19	ILE	CA-C	5.92	1.59	1.52
1	A	79	VAL	C-O	5.89	1.30	1.23
1	B	15	THR	CA-C	5.89	1.61	1.52
1	B	79	VAL	N-CA	5.88	1.52	1.46
1	B	25	ASN	CA-C	5.83	1.59	1.52
1	B	8	ASN	C-O	5.83	1.31	1.23
1	A	13	ALA	CA-C	5.83	1.60	1.52
1	A	95	ILE	C-O	5.76	1.30	1.24
1	B	131	VAL	CA-C	5.75	1.59	1.52
1	A	62	MET	CA-C	5.73	1.59	1.52
1	A	29	ASN	CA-C	5.71	1.60	1.52
1	A	111	LEU	C-N	-5.70	1.27	1.33
1	B	46	ASN	CA-C	5.68	1.60	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	2	ILE	C-O	5.68	1.29	1.24
1	B	4	PRO	N-CA	5.65	1.53	1.47
1	B	135	SER	CA-C	5.64	1.59	1.52
1	A	96	GLU	N-CA	5.64	1.53	1.46
1	B	2	ILE	CA-CB	5.63	1.60	1.54
1	A	106	ILE	CA-CB	5.63	1.60	1.53
1	A	107[A]	LYS	C-N	5.63	1.38	1.33
1	A	107[B]	LYS	C-N	5.63	1.38	1.33
1	B	39	LYS	N-CA	5.62	1.52	1.46
1	B	95	ILE	C-O	5.62	1.30	1.24
1	B	55	PRO	N-CA	5.60	1.54	1.47
1	A	64	ALA	CA-C	5.58	1.60	1.52
1	B	60	TYR	CA-C	5.57	1.59	1.52
1	B	120	ASP	CG-OD2	5.56	1.35	1.25
1	A	134	THR	CA-C	5.55	1.59	1.52
1	A	55	PRO	CA-CB	5.53	1.60	1.53
1	A	2	ILE	CA-CB	5.53	1.60	1.54
1	B	11	ASN	N-CA	5.52	1.52	1.45
1	B	137	ASN	CA-C	5.50	1.60	1.52
1	B	136	THR	CA-C	5.50	1.60	1.52
1	A	109	PRO	CA-C	5.48	1.59	1.52
1	A	63	GLN	N-CA	5.47	1.53	1.46
1	A	145	VAL	CA-C	5.45	1.59	1.52
1	B	117	LEU	C-N	5.45	1.39	1.34
1	A	110	ASN	CG-OD1	5.44	1.33	1.23
1	A	36	HIS	CE1-NE2	5.42	1.38	1.32
1	B	145	VAL	CA-CB	5.42	1.60	1.53
1	A	31	LEU	C-O	5.41	1.30	1.23
1	B	48	GLN	N-CA	5.41	1.52	1.46
1	A	4	PRO	CA-CB	5.41	1.60	1.53
1	A	18	LEU	CA-C	5.39	1.59	1.52
1	B	49	TRP	N-CA	5.39	1.52	1.46
1	B	28	GLU	CA-C	5.38	1.59	1.52
1	A	25	ASN	CA-C	5.36	1.59	1.52
1	B	39	LYS	CA-CB	5.36	1.62	1.53
1	B	102	GLY	C-N	5.31	1.41	1.33
1	B	69	SER	CA-C	5.31	1.59	1.52
1	B	51	LEU	CA-CB	5.30	1.60	1.53
1	B	103	GLN	CA-C	5.30	1.59	1.52
1	A	19	ILE	CA-C	5.29	1.58	1.52
1	A	134	THR	CB-OG1	5.29	1.52	1.43
1	A	73	VAL	C-O	5.28	1.29	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	5	GLY	CA-C	5.27	1.57	1.52
1	B	129	GLY	N-CA	5.27	1.50	1.45
1	B	78	LEU	N-CA	5.26	1.53	1.46
1	B	90	PRO	CA-CB	5.26	1.60	1.53
1	B	142	PHE	CA-CB	5.24	1.60	1.53
1	A	70	TYR	C-N	5.23	1.40	1.33
1	B	92	PRO	N-CA	5.23	1.53	1.47
1	A	132	ASP	N-CA	5.22	1.52	1.46
1	B	128	LEU	C-O	5.22	1.30	1.23
1	A	140	TRP	C-O	5.21	1.30	1.23
1	A	144[A]	SER	CA-C	5.20	1.59	1.52
1	A	144[B]	SER	CA-C	5.20	1.59	1.52
1	B	11	ASN	C-O	5.18	1.30	1.23
1	B	108	ILE	C-N	5.18	1.39	1.33
1	A	54	LEU	N-CA	5.18	1.53	1.46
1	A	103	GLN	C-O	5.14	1.30	1.23
1	B	8	ASN	CG-OD1	5.14	1.33	1.23
1	B	106	ILE	CA-CB	5.14	1.59	1.53
1	A	119	SER	CA-CB	5.13	1.62	1.53
1	B	88[A]	GLN	C-O	5.13	1.30	1.24
1	B	88[B]	GLN	C-O	5.13	1.30	1.24
1	A	90	PRO	CA-C	5.09	1.58	1.52
1	A	115	LEU	C-O	5.09	1.30	1.23
1	A	49	TRP	N-CA	5.08	1.52	1.46
1	B	21	LEU	CA-C	5.08	1.59	1.52
1	B	43	GLY	N-CA	5.07	1.50	1.45
1	A	73	VAL	N-CA	5.06	1.51	1.46
1	A	87	SER	C-O	5.06	1.29	1.23
1	B	35	HIS	N-CA	5.06	1.52	1.45
1	B	7	TYR	CA-C	5.05	1.58	1.52
1	B	19	ILE	CA-CB	5.05	1.59	1.54
1	A	58	THR	N-CA	5.04	1.51	1.46
1	B	144[A]	SER	C-O	5.04	1.29	1.23
1	B	144[B]	SER	C-O	5.04	1.29	1.23
1	B	144[C]	SER	C-O	5.04	1.29	1.23

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	74	ARG	NE-CZ-NH1	7.09	128.59	121.50
1	B	102	GLY	O-C-N	6.53	131.18	122.70
1	A	102	GLY	CA-C-N	-5.99	111.83	122.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	102	GLY	C-N-CA	-5.99	111.83	122.74
1	B	103	GLN	N-CA-C	5.90	119.26	109.46
1	A	51	LEU	CB-CG-CD2	5.90	128.39	110.70
1	B	28	GLU	OE1-CD-OE2	5.74	136.68	122.90
1	A	111	LEU	N-CA-C	5.31	120.62	113.72

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	1173	0	1191	13	0
1	B	1158	0	1159	10	0
2	C	23	0	21	0	0
2	D	23	0	21	0	0
3	A	15	0	0	0	0
3	B	10	0	0	0	0
4	A	283	0	0	1	0
4	B	252	0	0	1	0
All	All	2937	0	2392	23	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 5.

All (23) 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:87:SER:OG	1:B:88[A]:GLN:OE1	2.03	0.76
1:B:88[A]:GLN:OE1	1:B:89:GLN:N	2.18	0.76
1:A:137[B]:ASN:OD1	4:A:208:HOH:O	2.07	0.72
1:B:100:ASN:O	1:B:101:SER:CB	2.36	0.72
1:A:127[B]:VAL:HG12	1:A:128:LEU:N	2.06	0.69
1:A:82:ALA:O	1:A:127[B]:VAL:HG13	1.92	0.69
1:B:100:ASN:O	1:B:101:SER:HB2	2.00	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:98:ALA:HB2	4:B:286:HOH:O	2.01	0.60
1:A:107[B]:LYS:HZ3	1:A:107[B]:LYS:HB3	1.69	0.58
1:A:81:GLY:C	1:A:127[B]:VAL:CG1	2.80	0.54
1:A:107[B]:LYS:HB3	1:A:107[B]:LYS:NZ	2.24	0.52
1:B:35:HIS:HD2	1:B:36:HIS:O	1.93	0.51
1:A:81:GLY:O	1:A:127[B]:VAL:HG11	2.11	0.50
1:A:107[B]:LYS:NZ	1:A:107[B]:LYS:CB	2.76	0.49
1:B:100:ASN:O	1:B:101:SER:OG	2.30	0.48
1:A:100:ASN:OD1	1:A:100:ASN:N	2.46	0.47
1:A:127[B]:VAL:CG1	1:A:128:LEU:N	2.75	0.47
1:A:81:GLY:C	1:A:127[B]:VAL:HG11	2.43	0.44
1:B:101:SER:C	1:B:103:GLN:H	2.26	0.44
1:A:81:GLY:O	1:A:127[B]:VAL:CG1	2.66	0.44
1:B:107[B]:LYS:HB3	1:B:107[B]:LYS:HE3	1.32	0.42
1:A:14:TYR:CD1	1:A:120[A]:ASP:HB3	2.57	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	158/148 (107%)	153 (97%)	4 (2%)	1 (1%)	21	4
1	B	155/148 (105%)	153 (99%)	1 (1%)	1 (1%)	21	4
All	All	313/296 (106%)	306 (98%)	5 (2%)	2 (1%)	18	4

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	147	ALA
1	B	101	SER

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	140/127 (110%)	138 (99%)	2 (1%)	59	21
1	B	136/127 (107%)	131 (96%)	5 (4%)	30	2
All	All	276/254 (109%)	269 (98%)	7 (2%)	43	7

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

Mol	Chain	Res	Type
1	A	100	ASN
1	A	148	VAL
1	B	88[A]	GLN
1	B	88[B]	GLN
1	B	100	ASN
1	B	133	GLU
1	B	148	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	36	HIS
1	A	48	GLN
1	B	29	ASN
1	B	35	HIS
1	B	48	GLN
1	B	100	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	GLC	C	1	2	12,12,12	1.09	0	17,17,17	1.55	5 (29%)
2	GAL	C	2	2	11,11,12	2.06	5 (45%)	15,15,17	0.58	0
2	GLC	D	1	2	12,12,12	1.28	2 (16%)	17,17,17	0.47	0
2	GAL	D	2	2	11,11,12	1.51	2 (18%)	15,15,17	0.41	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GLC	C	1	2	-	0/2/22/22	0/1/1/1
2	GAL	C	2	2	-	0/2/19/22	0/1/1/1
2	GLC	D	1	2	-	2/2/22/22	0/1/1/1
2	GAL	D	2	2	-	0/2/19/22	0/1/1/1

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	2	GAL	O5-C5	3.37	1.50	1.43
2	D	2	GAL	C1-C2	3.13	1.59	1.52
2	C	2	GAL	O5-C1	2.85	1.48	1.43
2	C	2	GAL	C2-C3	2.79	1.56	1.52
2	D	1	GLC	C4-C5	2.77	1.58	1.53
2	C	2	GAL	C1-C2	2.66	1.58	1.52
2	D	2	GAL	O5-C1	-2.26	1.39	1.43
2	C	2	GAL	O4-C4	2.19	1.48	1.43
2	D	1	GLC	O5-C5	2.17	1.49	1.44

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1	GLC	C3-C4-C5	3.09	115.83	110.23
2	C	1	GLC	O1-C1-O5	2.53	117.93	110.41
2	C	1	GLC	O3-C3-C4	2.41	116.06	110.38
2	C	1	GLC	C4-C3-C2	2.40	115.04	110.83
2	C	1	GLC	O2-C2-C1	2.20	114.32	109.25

There are no chirality outliers.

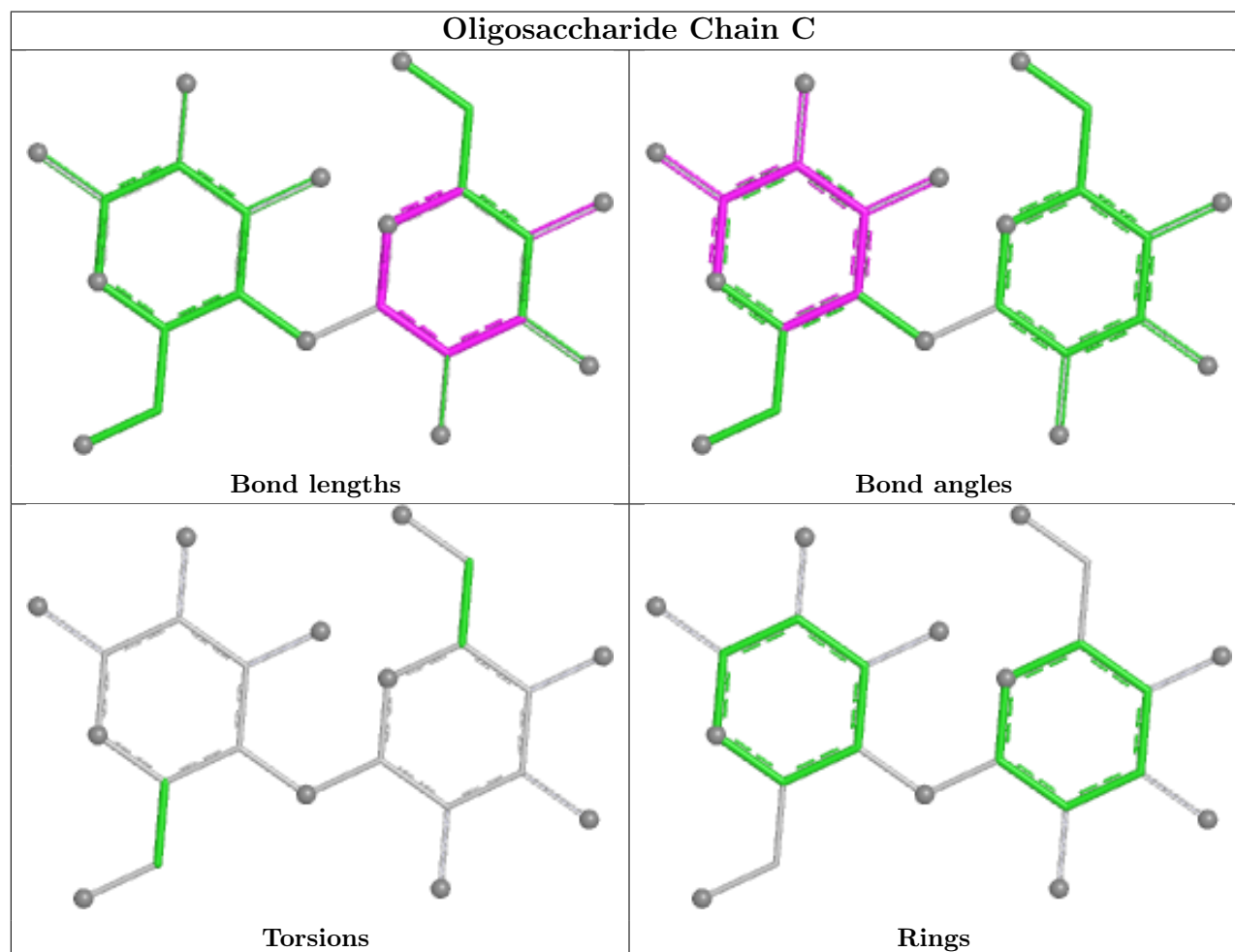
All (2) torsion outliers are listed below:

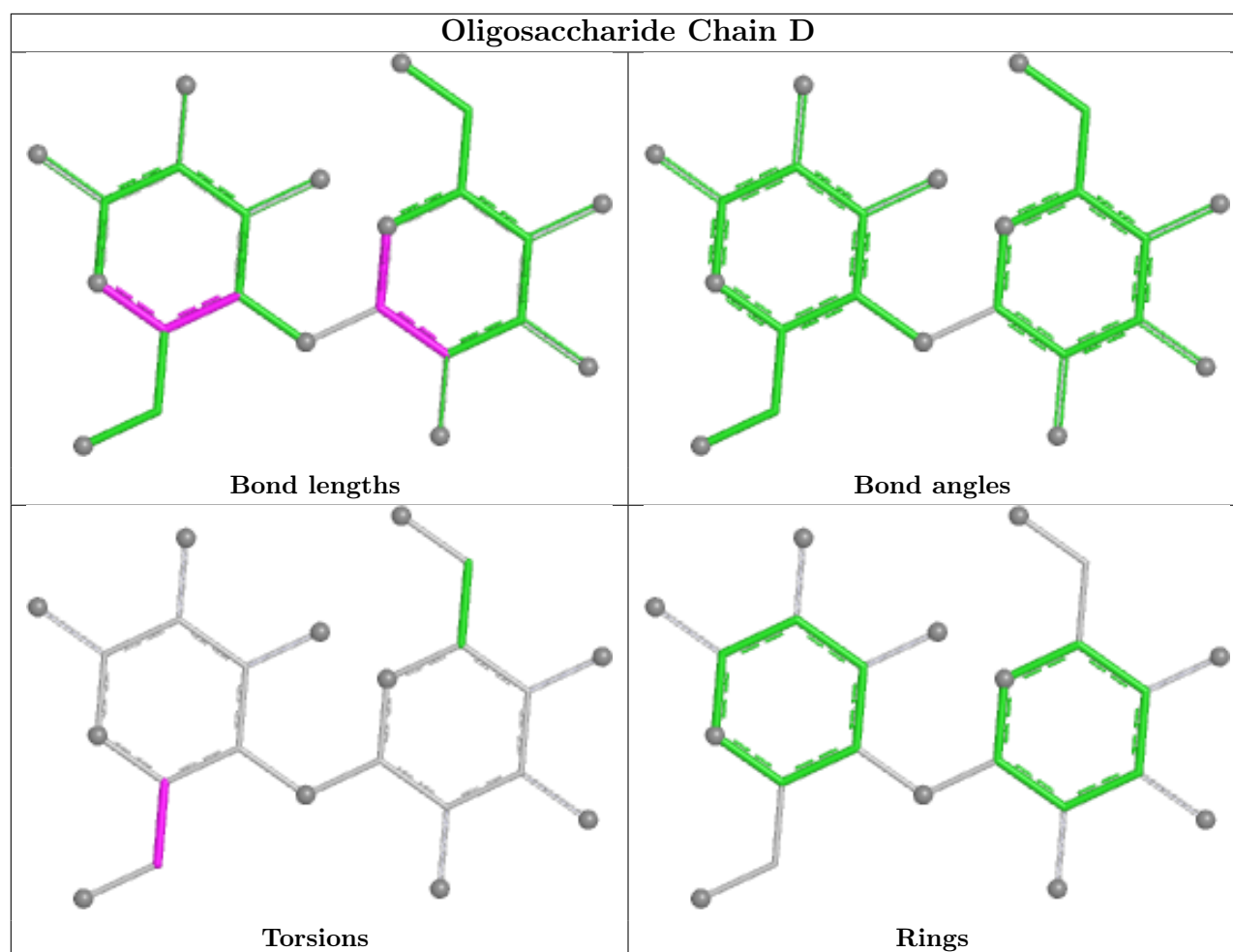
Mol	Chain	Res	Type	Atoms
2	D	1	GLC	C4-C5-C6-O6
2	D	1	GLC	O5-C5-C6-O6

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](#)

5 ligands 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	SO4	A	677	-	4,4,4	1.10	0	6,6,6	0.93	0
3	SO4	B	678	-	4,4,4	0.63	0	6,6,6	0.35	0
3	SO4	A	672	-	4,4,4	0.54	0	6,6,6	0.82	0
3	SO4	B	671	-	4,4,4	0.94	0	6,6,6	0.76	0
3	SO4	A	679	-	4,4,4	1.91	1 (25%)	6,6,6	1.82	2 (33%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	679	SO4	O1-S	3.42	1.65	1.44

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	679	SO4	O4-S-O2	-3.26	92.52	109.56
3	A	679	SO4	O2-S-O1	2.34	125.52	109.06

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 [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	147/148 (99%)	-0.20	8 (5%) 31 39	4, 9, 17, 50	14 (9%)
1	B	147/148 (99%)	0.17	7 (4%) 35 43	4, 12, 25, 54	8 (5%)
All	All	294/296 (99%)	-0.01	15 (5%) 33 41	4, 10, 25, 54	22 (7%)

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	148	VAL	12.6
1	B	99	GLY	9.4
1	A	100	ASN	8.6
1	A	148	VAL	7.0
1	B	101	SER	6.2
1	B	146	SER	5.9
1	B	100	ASN	5.7
1	A	99	GLY	5.2
1	A	101	SER	4.8
1	A	146	SER	3.9
1	B	102	GLY	3.4
1	A	98	ALA	3.3
1	B	98	ALA	3.2
1	A	1[A]	SER	3.1
1	A	102	GLY	2.0

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

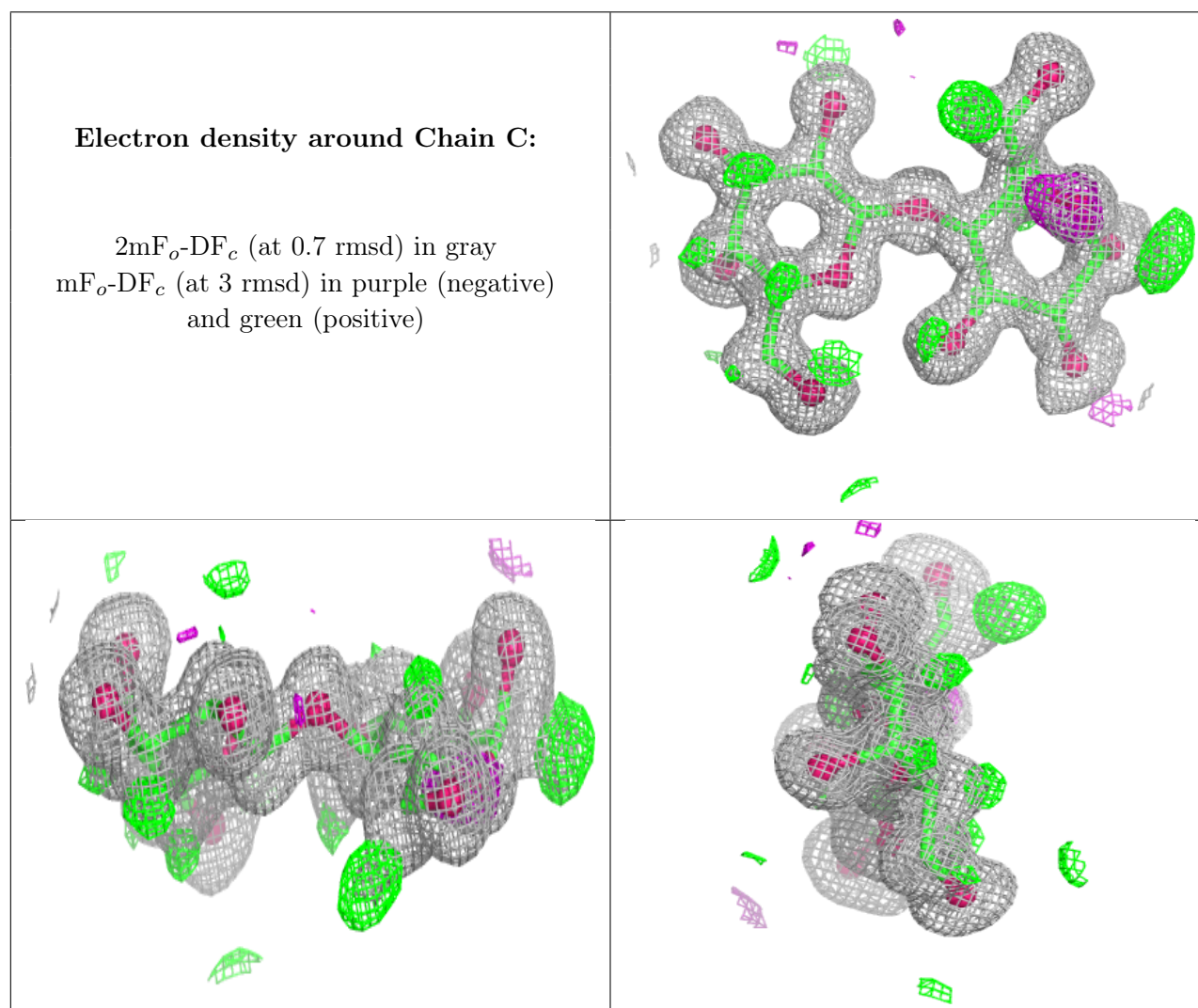
There are no non-standard protein/DNA/RNA residues in this entry.

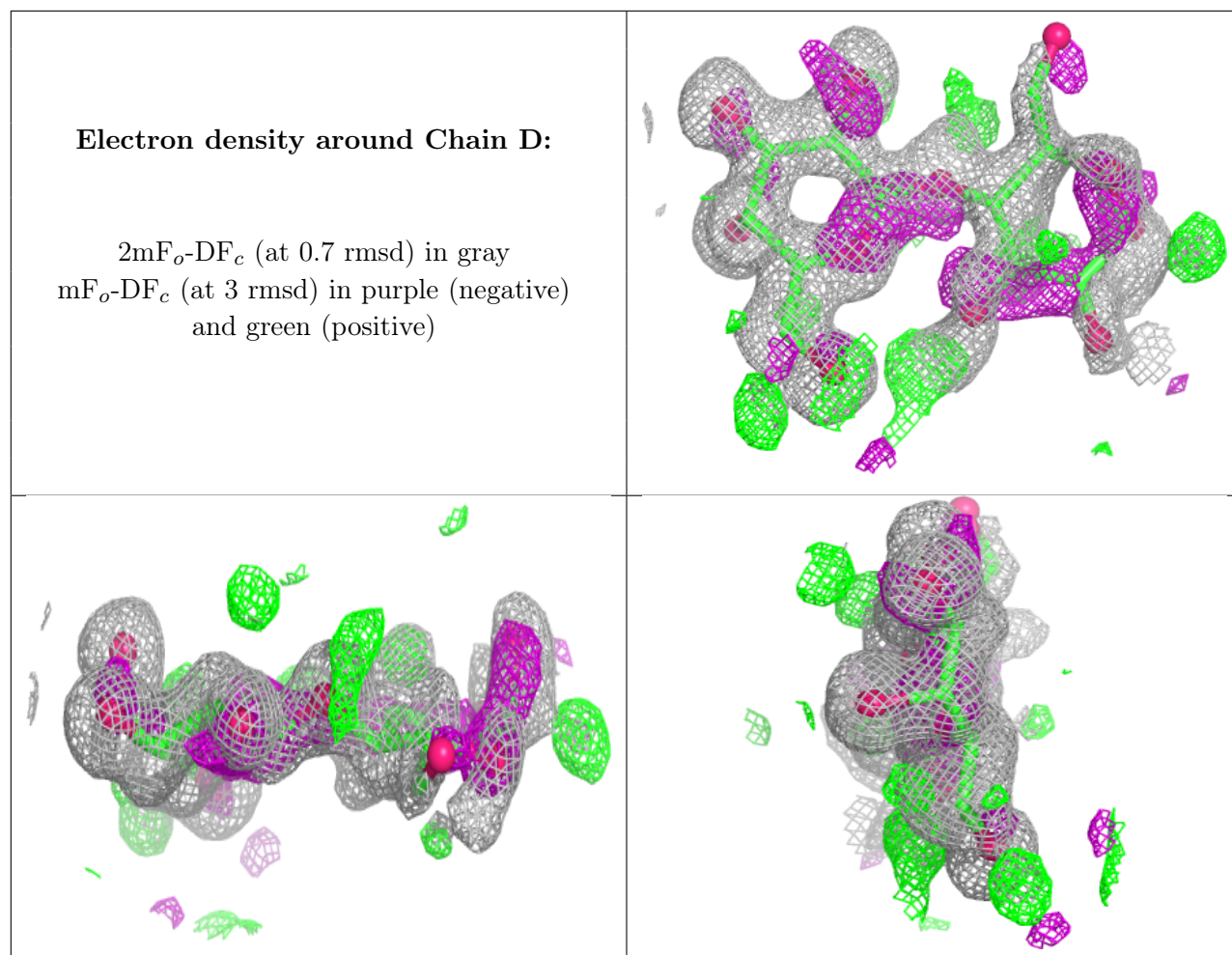
6.3 Carbohydrates [i](#)

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
2	GLC	D	1	12/12	0.71	0.17	22,40,47,49	0
2	GAL	D	2	11/12	0.93	0.09	12,16,20,20	0
2	GLC	C	1	12/12	0.97	0.06	8,12,16,17	0
2	GAL	C	2	11/12	0.99	0.03	6,7,8,12	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
3	SO4	B	678	5/5	0.70	0.14	64,66,67,68	0
3	SO4	B	671	5/5	0.93	0.10	24,26,34,35	0
3	SO4	A	672	5/5	0.93	0.12	22,25,32,34	0
3	SO4	A	679	5/5	0.95	0.08	14,21,23,24	0
3	SO4	A	677	5/5	0.99	0.05	19,20,25,28	0

6.5 Other polymers [i](#)

There are no such residues in this entry.