



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 12:19 AM UTC

PDB ID : 3ZST / pdb_00003zst
Title : GlgE isoform 1 from Streptomyces coelicolor with alpha-cyclodextrin bound
Authors : Syson, K.; Stevenson, C.E.M.; Rejzek, M.; Fairhurst, S.A.; Nair, A.; Bruton, C.J.; Field, R.A.; Chater, K.F.; Lawson, D.M.; Bornemann, S.
Deposited on : 2011-06-30
Resolution : 2.30 Å(reported)

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

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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

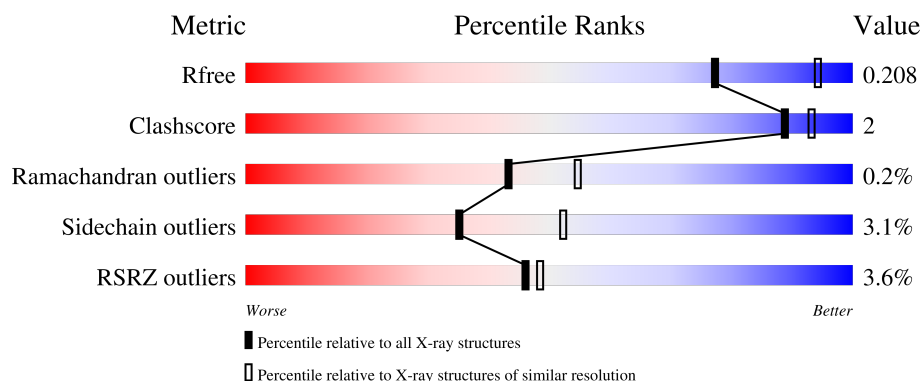
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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	695	% 89% 7%
1	B	695	6% 87% 5% • 7%
2	C	6	83% 17%
2	D	6	100%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 11175 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 PUTATIVE GLUCANOHYDROLASE PEP1A GLGE ISO-FORM 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	649	Total	C	N	O	S	0	5	0
			5157	3260	937	950	10			
1	B	649	Total	C	N	O	S	0	5	0
			5151	3257	936	948	10			

There are 40 discrepancies between the modelled and reference sequences:

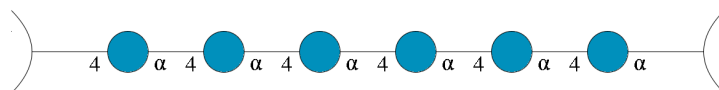
Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	expression tag	UNP Q9L1K2
A	-18	GLY	-	expression tag	UNP Q9L1K2
A	-17	SER	-	expression tag	UNP Q9L1K2
A	-16	SER	-	expression tag	UNP Q9L1K2
A	-15	HIS	-	expression tag	UNP Q9L1K2
A	-14	HIS	-	expression tag	UNP Q9L1K2
A	-13	HIS	-	expression tag	UNP Q9L1K2
A	-12	HIS	-	expression tag	UNP Q9L1K2
A	-11	HIS	-	expression tag	UNP Q9L1K2
A	-10	HIS	-	expression tag	UNP Q9L1K2
A	-9	SER	-	expression tag	UNP Q9L1K2
A	-8	SER	-	expression tag	UNP Q9L1K2
A	-7	GLY	-	expression tag	UNP Q9L1K2
A	-6	LEU	-	expression tag	UNP Q9L1K2
A	-5	VAL	-	expression tag	UNP Q9L1K2
A	-4	PRO	-	expression tag	UNP Q9L1K2
A	-3	ARG	-	expression tag	UNP Q9L1K2
A	-2	GLY	-	expression tag	UNP Q9L1K2
A	-1	SER	-	expression tag	UNP Q9L1K2
A	0	HIS	-	expression tag	UNP Q9L1K2
B	-19	MET	-	expression tag	UNP Q9L1K2
B	-18	GLY	-	expression tag	UNP Q9L1K2
B	-17	SER	-	expression tag	UNP Q9L1K2
B	-16	SER	-	expression tag	UNP Q9L1K2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-15	HIS	-	expression tag	UNP Q9L1K2
B	-14	HIS	-	expression tag	UNP Q9L1K2
B	-13	HIS	-	expression tag	UNP Q9L1K2
B	-12	HIS	-	expression tag	UNP Q9L1K2
B	-11	HIS	-	expression tag	UNP Q9L1K2
B	-10	HIS	-	expression tag	UNP Q9L1K2
B	-9	SER	-	expression tag	UNP Q9L1K2
B	-8	SER	-	expression tag	UNP Q9L1K2
B	-7	GLY	-	expression tag	UNP Q9L1K2
B	-6	LEU	-	expression tag	UNP Q9L1K2
B	-5	VAL	-	expression tag	UNP Q9L1K2
B	-4	PRO	-	expression tag	UNP Q9L1K2
B	-3	ARG	-	expression tag	UNP Q9L1K2
B	-2	GLY	-	expression tag	UNP Q9L1K2
B	-1	SER	-	expression tag	UNP Q9L1K2
B	0	HIS	-	expression tag	UNP Q9L1K2

- Molecule 2 is an oligosaccharide called Cyclohexakis-(1-4)-(alpha-D-glucopyranose).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
2	C	6	Total	C	O	0	0	0
			66	36	30			
2	D	6	Total	C	O	0	0	0
			66	36	30			

- Molecule 3 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			4	2	2		

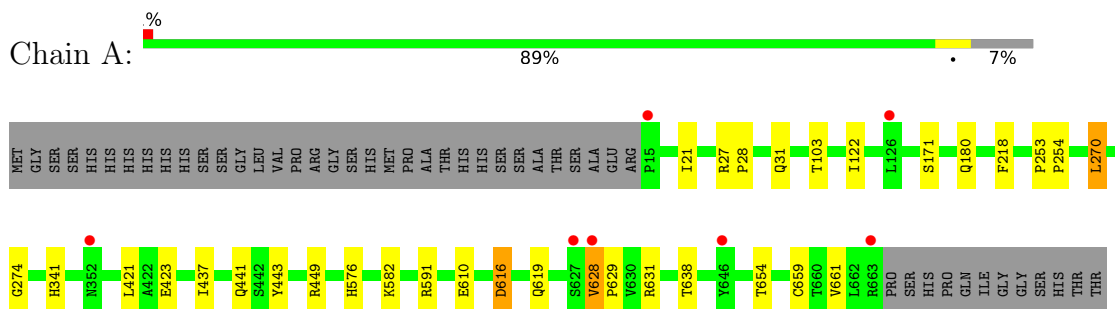
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	488	Total	O	0	0
			488	488		
4	B	243	Total	O	0	0
			243	243		

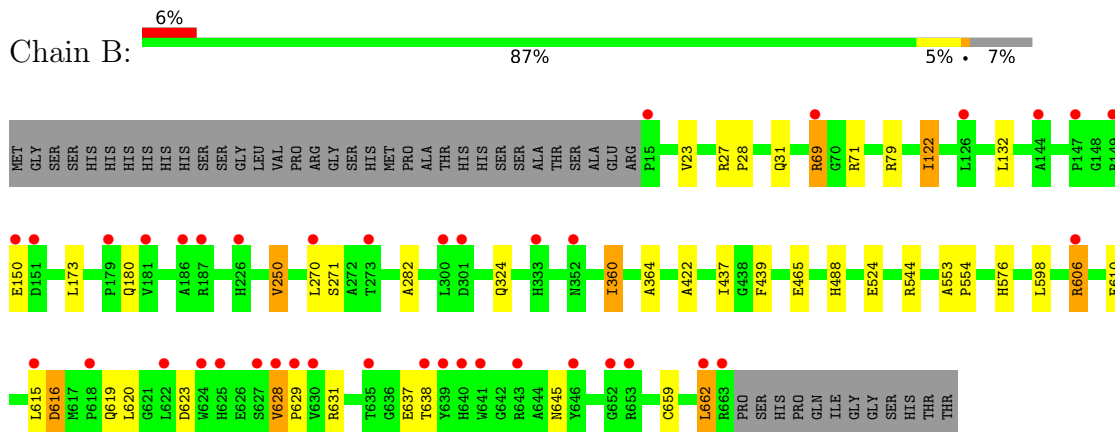
3 Residue-property plots [i](#)

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.

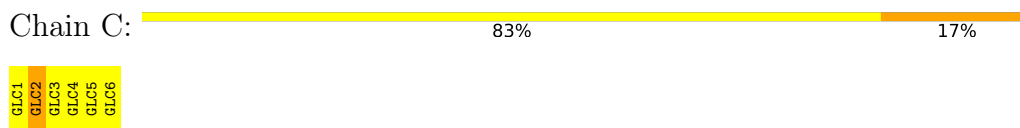
- Molecule 1: PUTATIVE GLUCANOHYDROLASE PEP1A GLGE ISOFORM 1



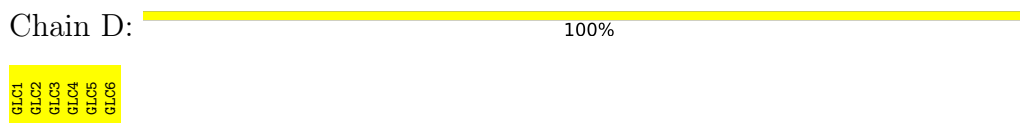
- Molecule 1: PUTATIVE GLUCANOHYDROLASE PEP1A GLGE ISOFORM 1



- Molecule 2: Cyclohexakis-(1-4)-(alpha-D-glucopyranose)



- Molecule 2: Cyclohexakis-(1-4)-(alpha-D-glucopyranose)



4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	113.24Å 113.24Å 314.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	106.54 – 2.30 106.54 – 2.30	Depositor EDS
% Data completeness (in resolution range)	93.4 (106.54-2.30) 93.4 (106.54-2.30)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	7.16 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.6.0101	Depositor
R, R_{free}	0.173 , 0.201 0.180 , 0.208	Depositor DCC
R_{free} test set	4305 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	27.2	Xtriage
Anisotropy	0.445	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 37.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	11175	wwPDB-VP
Average B, all atoms (Å ²)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.92% 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: EDO, GLC

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	0.99	1/5324 (0.0%)	0.89	2/7280 (0.0%)
1	B	0.89	0/5319	0.87	0/7275
All	All	0.94	1/10643 (0.0%)	0.88	2/14555 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	21	ILE	CA-CB	5.15	1.59	1.53

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	274	GLY	N-CA-C	5.07	118.81	112.73
1	A	218	PHE	CB-CA-C	-5.02	105.20	110.17

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	5157	0	5002	15	0
1	B	5151	0	4990	24	0
2	C	66	0	54	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	66	0	54	0	0
3	A	4	0	6	0	0
4	A	488	0	0	3	0
4	B	243	0	0	1	0
All	All	11175	0	10106	39	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 2.

All (39) 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:615:LEU:HD23	1:B:620:LEU:HD11	1.52	0.90
1:B:628:VAL:HG13	1:B:629:PRO:HD2	1.63	0.78
1:B:282:ALA:HA	1:B:360:ILE:HD13	1.69	0.73
1:B:122:ILE:CD1	1:B:132:LEU:HD21	2.19	0.72
1:A:628:VAL:HG13	1:A:629:PRO:HD2	1.77	0.66
1:B:122:ILE:HD11	1:B:132:LEU:HD21	1.78	0.65
1:B:122:ILE:HD11	1:B:132:LEU:CD2	2.35	0.56
1:B:364:ALA:HB1	4:B:2175:HOH:O	2.07	0.54
1:A:103:THR:HG21	4:A:2119:HOH:O	2.07	0.54
1:B:437:ILE:C	1:B:437:ILE:HD12	2.34	0.52
1:B:615:LEU:HD23	1:B:620:LEU:CD1	2.33	0.52
1:B:615:LEU:HD13	1:B:645:ASN:ND2	2.26	0.51
1:A:576:HIS:CG	1:A:619:GLN:HG2	2.48	0.49
1:A:437:ILE:HD12	1:A:437:ILE:C	2.38	0.49
1:B:576:HIS:CG	1:B:619:GLN:HG2	2.47	0.49
1:B:282:ALA:HA	1:B:360:ILE:CD1	2.40	0.48
1:A:27:ARG:HB3	1:A:28:PRO:HA	1.97	0.47
1:B:324:GLN:NE2	1:B:360:ILE:HD12	2.31	0.46
1:B:488:HIS:HB3	1:B:606[B]:ARG:HH21	1.81	0.45
1:A:591:ARG:HD3	4:A:2459:HOH:O	2.15	0.45
1:B:422:ALA:HB2	1:B:439:PHE:CD1	2.52	0.45
1:B:553:ALA:HB3	1:B:554:PRO:HD3	1.98	0.44
1:B:27:ARG:HB3	1:B:28:PRO:HA	1.99	0.44
1:B:662:LEU:HD12	1:B:662:LEU:H	1.83	0.43
1:B:250:VAL:O	1:B:250:VAL:HG12	2.17	0.43
1:A:423:GLU:HA	1:A:443:TYR:CD1	2.54	0.42
1:A:270:LEU:HD12	1:A:270:LEU:HA	1.80	0.42
1:A:341:HIS:HE1	4:A:2301:HOH:O	2.02	0.42
1:A:582:LYS:HG3	1:A:610:GLU:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:421:LEU:HD13	1:A:441:GLN:HB3	2.01	0.41
1:B:615:LEU:N	1:B:615:LEU:HD12	2.36	0.41
1:B:628:VAL:HG13	1:B:629:PRO:CD	2.43	0.41
1:B:122:ILE:HD12	1:B:173:LEU:HB2	2.03	0.41
1:A:628:VAL:CG1	1:A:661:VAL:HG13	2.51	0.41
1:A:449:ARG:HH22	2:C:2:GLC:HO2	1.69	0.40
1:A:631:ARG:O	1:A:659:CYS:HA	2.21	0.40
1:B:631:ARG:O	1:B:659:CYS:HA	2.22	0.40
1:A:253:PRO:O	1:A:254:PRO:C	2.64	0.40
1:B:69:ARG:HE	1:B:69:ARG:HB2	1.74	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	652/695 (94%)	640 (98%)	11 (2%)	1 (0%)	43	55
1	B	652/695 (94%)	641 (98%)	10 (2%)	1 (0%)	43	55
All	All	1304/1390 (94%)	1281 (98%)	21 (2%)	2 (0%)	43	55

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	616	ASP
1	A	616	ASP

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	539/575 (94%)	530 (98%)	9 (2%)	53	72
1	B	538/575 (94%)	513 (95%)	25 (5%)	24	36
All	All	1077/1150 (94%)	1043 (97%)	34 (3%)	35	51

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	31	GLN
1	A	122	ILE
1	A	171	SER
1	A	180	GLN
1	A	270	LEU
1	A	616	ASP
1	A	628	VAL
1	A	638	THR
1	A	654	THR
1	B	23	VAL
1	B	31	GLN
1	B	69	ARG
1	B	71	ARG
1	B	79	ARG
1	B	122	ILE
1	B	150	GLU
1	B	180	GLN
1	B	250	VAL
1	B	270	LEU
1	B	271	SER
1	B	360	ILE
1	B	465	GLU
1	B	524	GLU
1	B	544	ARG
1	B	598	LEU
1	B	606[A]	ARG
1	B	606[B]	ARG
1	B	610	GLU
1	B	616	ASP
1	B	623	ASP
1	B	628	VAL
1	B	637	GLU
1	B	638	THR

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Mol	Chain	Res	Type
1	B	662	LEU

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

Mol	Chain	Res	Type
1	A	31	GLN
1	A	188	HIS
1	A	262	HIS
1	A	352	ASN
1	A	397	HIS
1	A	436	GLN
1	B	31	GLN
1	B	188	HIS
1	B	262	HIS
1	B	395	ASN
1	B	436	GLN

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 ⓘ

12 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	11,11,12	1.03	1 (9%)	15,15,17	1.69	4 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	GLC	C	2	2	11,11,12	1.77	3 (27%)	15,15,17	2.08	6 (40%)
2	GLC	C	3	2	11,11,12	1.34	1 (9%)	15,15,17	1.60	4 (26%)
2	GLC	C	4	2	11,11,12	1.40	1 (9%)	15,15,17	1.88	3 (20%)
2	GLC	C	5	2	11,11,12	1.00	0	15,15,17	2.07	3 (20%)
2	GLC	C	6	2	11,11,12	1.76	4 (36%)	15,15,17	1.80	4 (26%)
2	GLC	D	1	2	11,11,12	1.43	3 (27%)	15,15,17	1.37	0
2	GLC	D	2	2	11,11,12	1.81	3 (27%)	15,15,17	1.75	2 (13%)
2	GLC	D	3	2	11,11,12	1.27	1 (9%)	15,15,17	1.80	3 (20%)
2	GLC	D	4	2	11,11,12	1.77	3 (27%)	15,15,17	1.11	1 (6%)
2	GLC	D	5	2	11,11,12	1.42	3 (27%)	15,15,17	1.59	5 (33%)
2	GLC	D	6	2	11,11,12	1.73	2 (18%)	15,15,17	1.93	4 (26%)

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	-	2/2/19/22	0/1/1/1
2	GLC	C	2	2	-	2/2/19/22	0/1/1/1
2	GLC	C	3	2	-	2/2/19/22	0/1/1/1
2	GLC	C	4	2	-	2/2/19/22	0/1/1/1
2	GLC	C	5	2	-	1/2/19/22	0/1/1/1
2	GLC	C	6	2	-	0/2/19/22	0/1/1/1
2	GLC	D	1	2	-	2/2/19/22	0/1/1/1
2	GLC	D	2	2	-	0/2/19/22	0/1/1/1
2	GLC	D	3	2	-	2/2/19/22	0/1/1/1
2	GLC	D	4	2	-	2/2/19/22	0/1/1/1
2	GLC	D	5	2	-	0/2/19/22	0/1/1/1
2	GLC	D	6	2	-	2/2/19/22	0/1/1/1

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	6	GLC	O5-C1	4.44	1.51	1.43
2	C	2	GLC	O5-C1	3.73	1.50	1.43
2	D	2	GLC	O5-C5	3.58	1.50	1.43
2	D	2	GLC	O5-C1	3.49	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	4	GLC	C4-C5	3.29	1.60	1.53
2	C	6	GLC	O5-C1	2.82	1.48	1.43
2	C	4	GLC	O5-C5	2.79	1.48	1.43
2	C	6	GLC	O5-C5	2.77	1.48	1.43
2	C	6	GLC	C4-C5	2.62	1.58	1.53
2	D	1	GLC	O5-C5	2.62	1.48	1.43
2	D	5	GLC	C2-C3	2.50	1.56	1.52
2	C	1	GLC	O4-C4	2.50	1.49	1.43
2	C	2	GLC	O2-C2	2.48	1.48	1.43
2	D	4	GLC	O5-C5	2.44	1.48	1.43
2	D	3	GLC	O5-C5	2.28	1.47	1.43
2	D	1	GLC	O4-C4	2.27	1.48	1.43
2	D	6	GLC	O5-C5	2.19	1.47	1.43
2	C	3	GLC	C4-C5	2.18	1.57	1.53
2	D	5	GLC	O4-C4	2.14	1.48	1.43
2	D	2	GLC	C4-C5	2.12	1.57	1.53
2	C	2	GLC	C2-C3	-2.11	1.49	1.52
2	D	4	GLC	O5-C1	2.11	1.47	1.43
2	D	1	GLC	C4-C5	2.08	1.57	1.53
2	D	5	GLC	O5-C1	2.06	1.47	1.43
2	C	6	GLC	C1-C2	2.02	1.57	1.52

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	5	GLC	O4-C4-C3	-6.04	96.14	110.38
2	D	2	GLC	C1-O5-C5	4.78	118.59	112.19
2	C	4	GLC	C1-O5-C5	4.63	118.39	112.19
2	D	6	GLC	C1-O5-C5	4.02	117.57	112.19
2	C	6	GLC	C3-C4-C5	4.00	117.49	110.23
2	C	1	GLC	C6-C5-C4	-3.97	103.26	113.02
2	D	6	GLC	C3-C4-C5	3.86	117.23	110.23
2	D	3	GLC	O5-C5-C6	3.79	115.03	107.66
2	C	2	GLC	C1-O5-C5	3.62	117.03	112.19
2	C	4	GLC	O5-C5-C4	3.50	119.35	110.83
2	C	3	GLC	C3-C4-C5	3.50	116.58	110.23
2	C	2	GLC	O4-C4-C3	-3.35	102.47	110.38
2	D	3	GLC	O4-C4-C3	-3.31	102.58	110.38
2	D	3	GLC	C1-O5-C5	-3.28	107.78	112.19
2	C	5	GLC	C1-O5-C5	3.25	116.54	112.19
2	D	6	GLC	O4-C4-C3	-3.09	103.09	110.38
2	C	2	GLC	C3-C4-C5	3.09	115.83	110.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	5	GLC	C3-C4-C5	3.07	115.81	110.23
2	C	2	GLC	C1-C2-C3	-3.07	105.17	109.64
2	C	6	GLC	O4-C4-C3	-3.07	103.14	110.38
2	D	2	GLC	O5-C5-C4	3.02	118.18	110.83
2	C	3	GLC	O4-C4-C3	-2.95	103.41	110.38
2	C	2	GLC	C2-C3-C4	2.92	116.00	110.86
2	C	6	GLC	O5-C5-C6	2.89	113.28	107.66
2	C	1	GLC	O5-C5-C4	-2.81	104.00	110.83
2	D	4	GLC	C3-C4-C5	2.74	115.20	110.23
2	C	4	GLC	C6-C5-C4	-2.71	106.35	113.02
2	D	5	GLC	O5-C5-C4	-2.53	104.67	110.83
2	C	1	GLC	O5-C1-C2	-2.52	104.77	110.79
2	C	1	GLC	C3-C4-C5	2.49	114.75	110.23
2	C	2	GLC	O5-C1-C2	2.43	116.59	110.79
2	D	5	GLC	C3-C4-C5	2.37	114.54	110.23
2	C	3	GLC	O5-C5-C4	2.29	116.39	110.83
2	D	5	GLC	O5-C5-C6	2.25	112.04	107.66
2	D	6	GLC	O5-C5-C6	2.19	111.93	107.66
2	C	6	GLC	C1-C2-C3	2.15	112.77	109.64
2	D	5	GLC	O3-C3-C4	-2.13	105.35	110.38
2	C	3	GLC	O5-C1-C2	2.06	115.69	110.79
2	D	5	GLC	C1-O5-C5	2.01	114.88	112.19

There are no chirality outliers.

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	3	GLC	O5-C5-C6-O6
2	D	1	GLC	O5-C5-C6-O6
2	C	1	GLC	O5-C5-C6-O6
2	D	6	GLC	O5-C5-C6-O6
2	D	1	GLC	C4-C5-C6-O6
2	D	4	GLC	C4-C5-C6-O6
2	D	6	GLC	C4-C5-C6-O6
2	C	2	GLC	O5-C5-C6-O6
2	C	1	GLC	C4-C5-C6-O6
2	C	3	GLC	C4-C5-C6-O6
2	C	4	GLC	C4-C5-C6-O6
2	D	4	GLC	O5-C5-C6-O6
2	D	3	GLC	C4-C5-C6-O6
2	C	2	GLC	C4-C5-C6-O6
2	D	3	GLC	O5-C5-C6-O6

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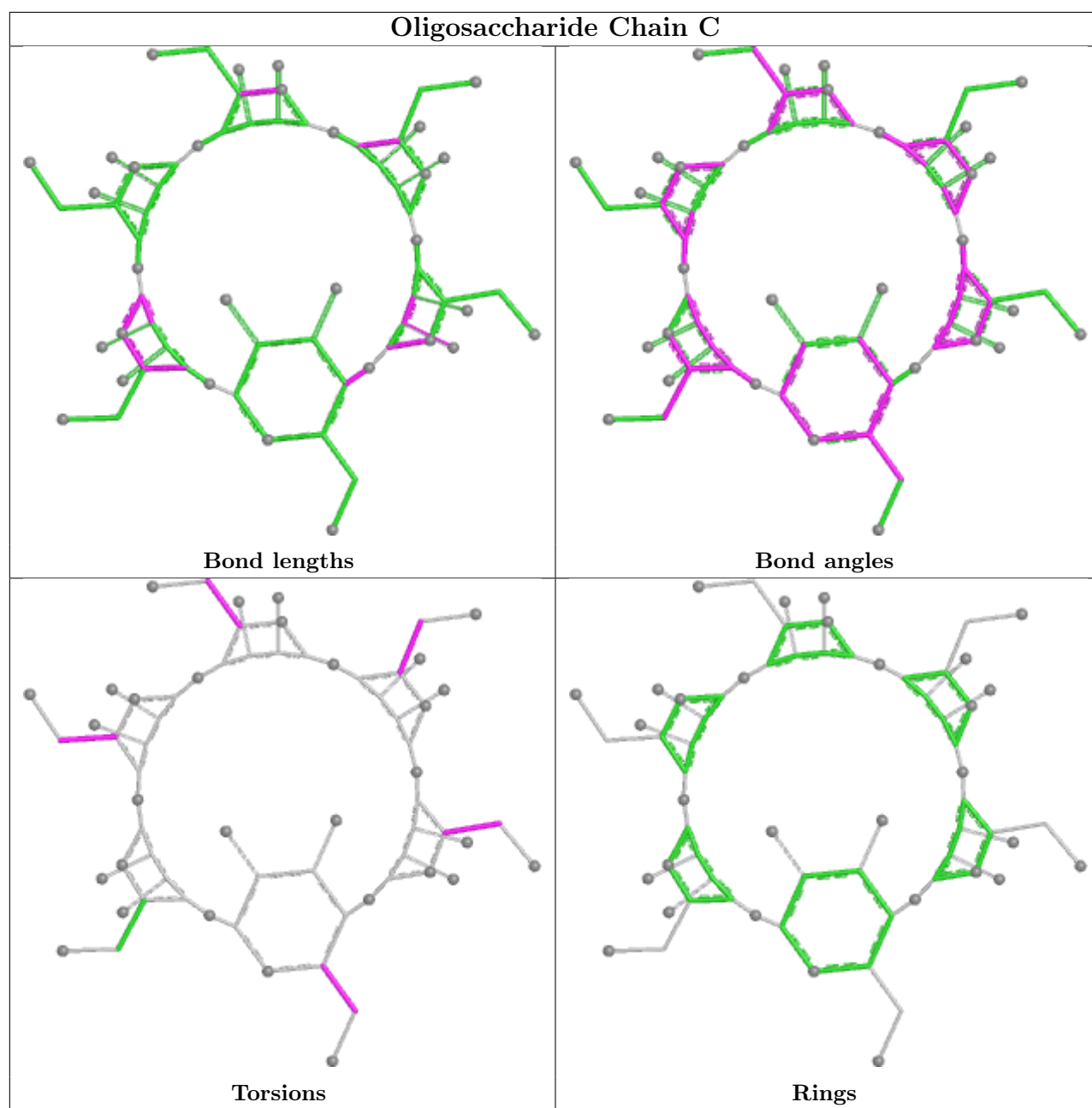
Mol	Chain	Res	Type	Atoms
2	C	5	GLC	C4-C5-C6-O6
2	C	4	GLC	O5-C5-C6-O6

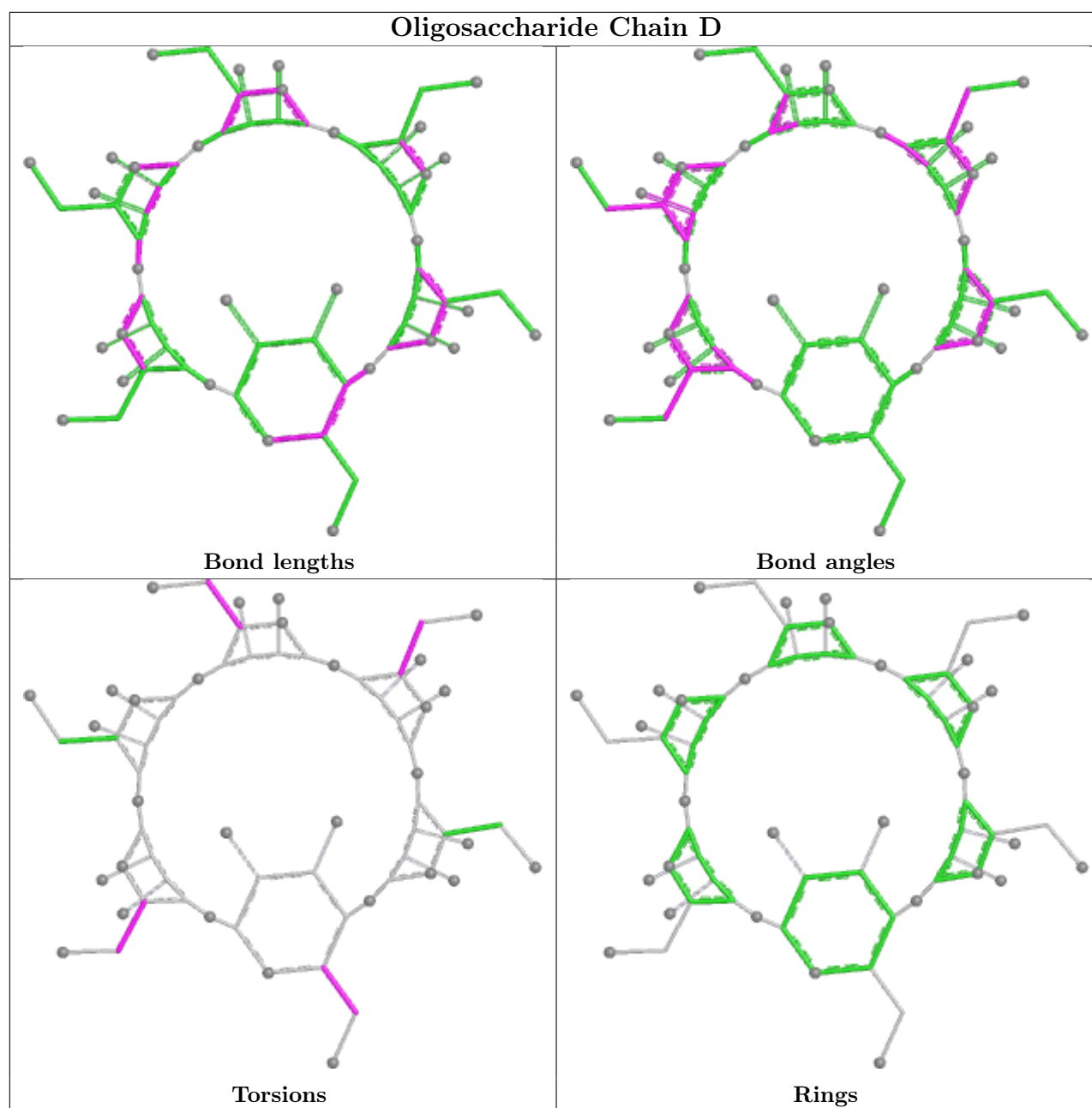
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	2	GLC	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](#)

1 ligand is 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	EDO	A	750	-	3,3,3	0.80	0	2,2,2	0.12	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
3	EDO	A	750	-	-	0/1/1/1	-

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 [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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	649/695 (93%)	-0.32	7 (1%) 78 79	22, 36, 64, 103	5 (0%)
1	B	649/695 (93%)	0.64	40 (6%) 26 28	26, 53, 86, 121	5 (0%)
All	All	1298/1390 (93%)	0.16	47 (3%) 46 48	22, 45, 78, 121	10 (0%)

All (47) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	663	ARG	7.2
1	B	15	PRO	6.3
1	A	663	ARG	5.0
1	B	187[A]	ARG	4.6
1	A	15	PRO	4.4
1	B	606[A]	ARG	3.9
1	B	333[A]	HIS	3.9
1	B	628	VAL	3.6
1	B	270	LEU	3.5
1	B	126	LEU	3.5
1	B	226	HIS	3.4
1	B	352	ASN	3.4
1	B	640	HIS	3.3
1	B	144	ALA	3.3
1	A	352	ASN	3.2
1	B	662	LEU	3.2
1	B	69	ARG	3.2
1	B	643	ARG	3.1
1	B	186	ALA	3.1
1	B	653	ARG	2.9
1	B	618	PRO	2.9
1	B	652	GLY	2.8
1	B	624	TRP	2.8
1	B	627	SER	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	646	TYR	2.8
1	B	638	THR	2.7
1	A	126	LEU	2.7
1	B	622	LEU	2.6
1	B	641	TRP	2.5
1	A	628	VAL	2.5
1	B	149	ARG	2.5
1	B	273	THR	2.4
1	B	179	PRO	2.4
1	B	630	VAL	2.3
1	B	301	ASP	2.3
1	A	646	TYR	2.3
1	B	639	TYR	2.3
1	B	147	PRO	2.2
1	B	625	HIS	2.2
1	B	635	THR	2.1
1	B	629	PRO	2.1
1	B	150	GLU	2.1
1	B	181	VAL	2.1
1	B	300	LEU	2.1
1	B	615	LEU	2.0
1	A	627	SER	2.0
1	B	151	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.

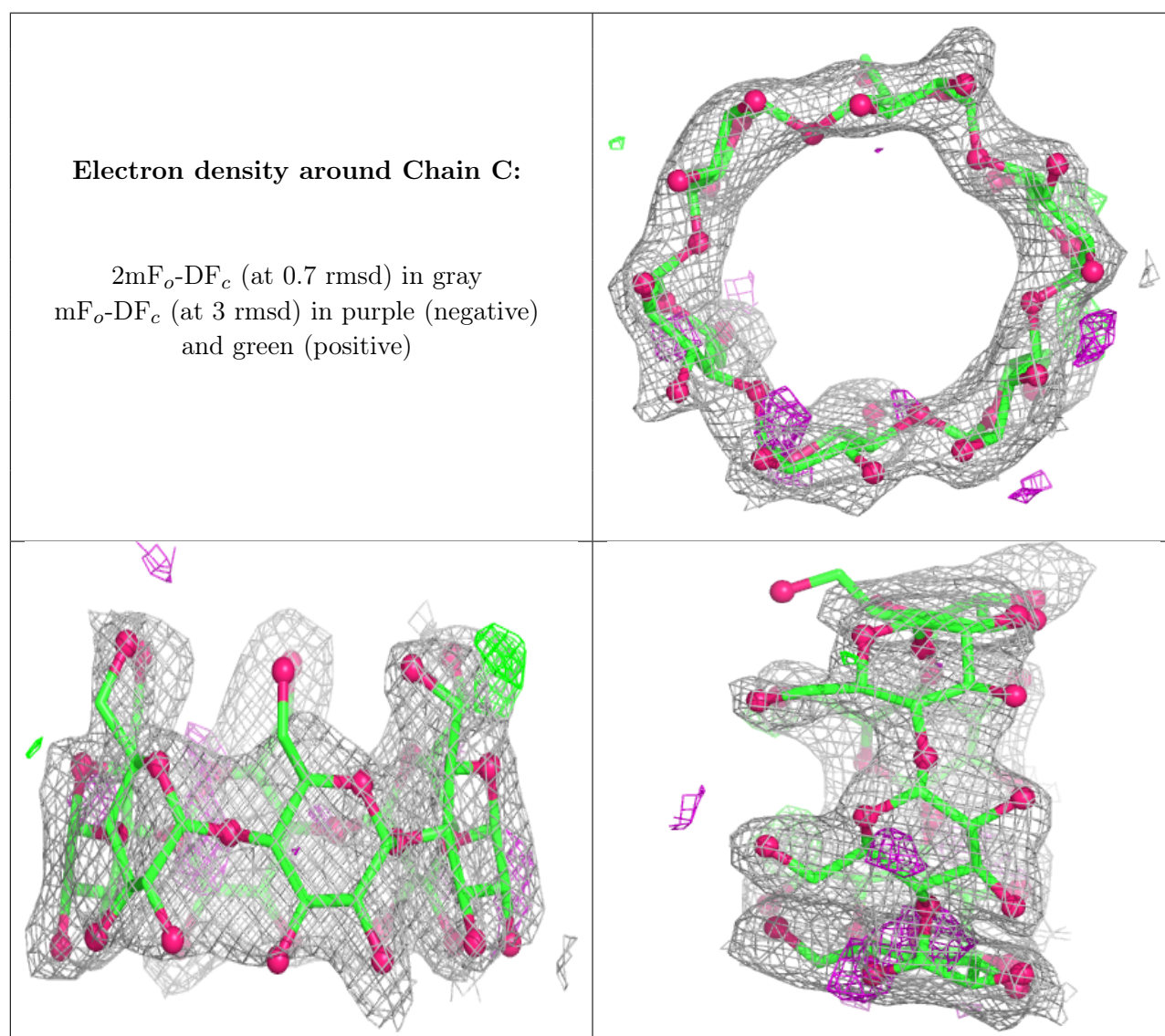
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	GLC	D	2	11/12	0.57	0.17	99,106,114,118	0
2	GLC	D	3	11/12	0.64	0.15	82,97,100,106	0
2	GLC	C	4	11/12	0.74	0.15	86,99,102,102	0
2	GLC	D	1	11/12	0.75	0.17	77,87,94,102	0
2	GLC	C	3	11/12	0.83	0.14	66,73,81,88	0

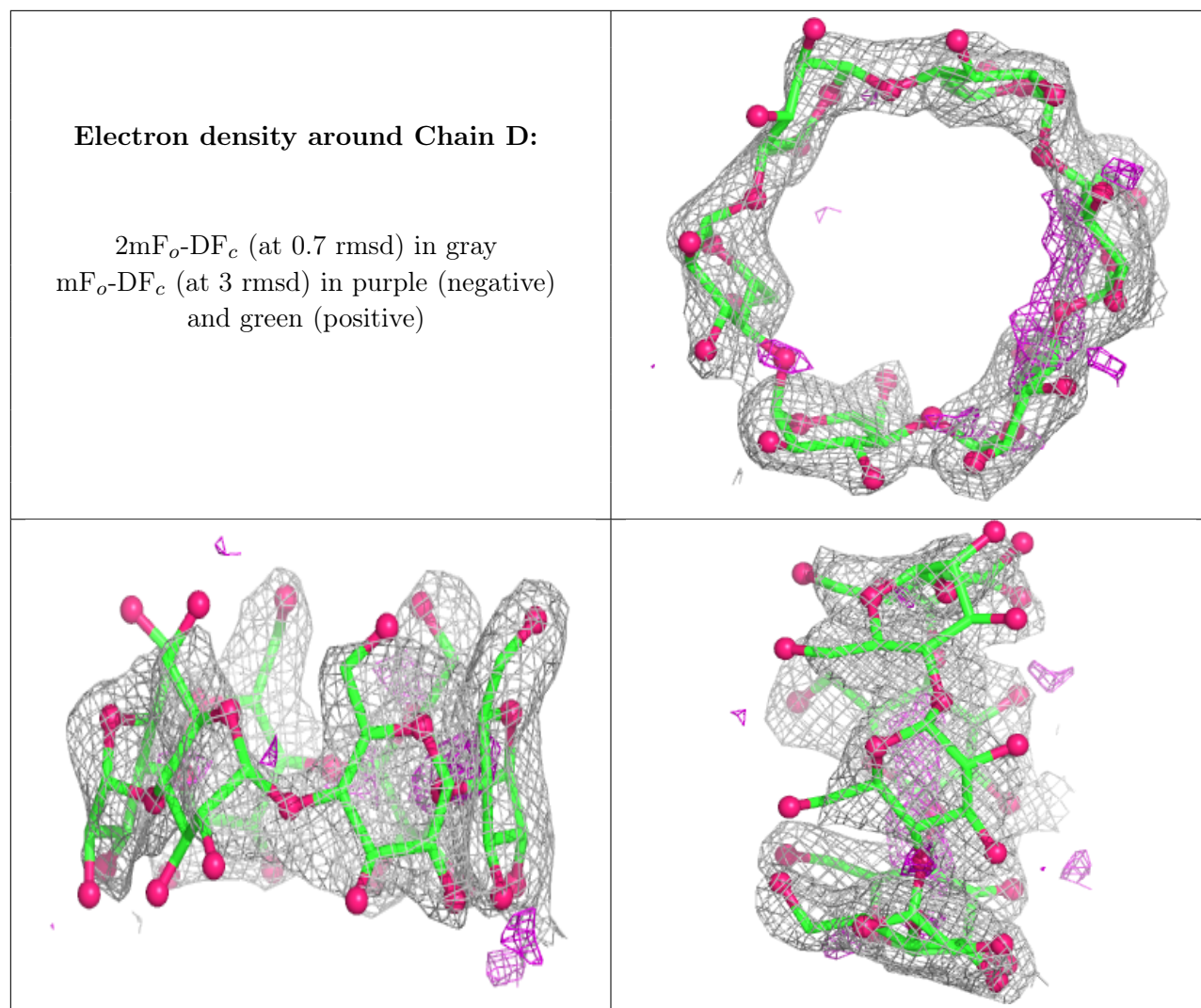
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	GLC	D	4	11/12	0.85	0.12	74,78,81,87	0
2	GLC	C	5	11/12	0.86	0.10	75,82,90,92	0
2	GLC	D	6	11/12	0.86	0.15	60,67,74,83	0
2	GLC	D	5	11/12	0.88	0.14	62,65,73,74	0
2	GLC	C	2	11/12	0.88	0.12	46,51,59,64	0
2	GLC	C	1	11/12	0.91	0.13	50,53,59,61	0
2	GLC	C	6	11/12	0.91	0.11	55,66,70,70	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	EDO	A	750	4/4	0.91	0.15	42,46,52,58	0

6.5 Other polymers [i](#)

There are no such residues in this entry.