



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 06:00 AM UTC

PDB ID : 5TIB / pdb_00005tib
Title : Gasdermin-B C-terminal domain containing the polymorphism residues
Arg299:Ser306 fused to maltose binding protein
Authors : Chao, K.; Herzberg, O.
Deposited on : 2016-10-01
Resolution : 2.60 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

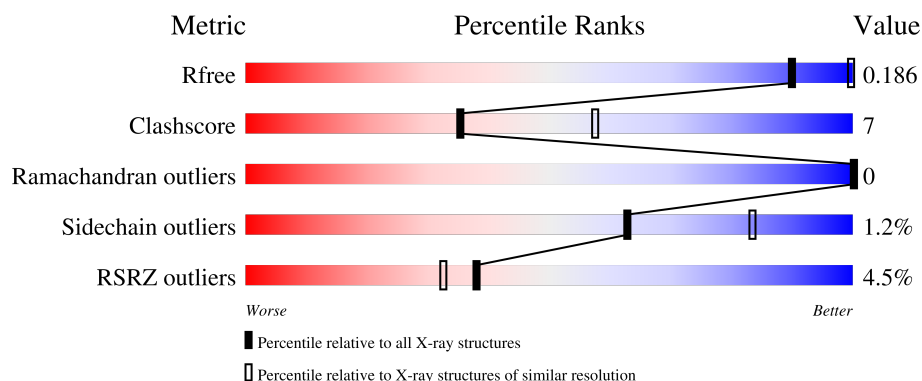
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

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	557	
1	B	557	
2	C	2	
2	D	2	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 8238 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 Sugar ABC transporter substrate-binding protein, Gasdermin-B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	533	Total	C	N	O	S	0	0	0
			4056	2600	661	782	13			
1	B	530	Total	C	N	O	S	0	0	0
			3845	2464	635	734	12			

There are 26 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	82	ALA	ASP	see remark 999	UNP A0A178SBV6
A	83	ALA	LYS	see remark 999	UNP A0A178SBV6
A	172	ALA	GLU	see remark 999	UNP A0A178SBV6
A	173	ALA	ASN	see remark 999	UNP A0A178SBV6
A	239	ALA	LYS	see remark 999	UNP A0A178SBV6
A	362	ALA	LYS	see remark 999	UNP A0A178SBV6
A	363	ALA	ASP	see remark 999	UNP A0A178SBV6
A	367	ASN	-	linker	UNP A0A178SBV6
A	368	ALA	-	linker	UNP A0A178SBV6
A	369	ALA	-	linker	UNP A0A178SBV6
A	370	ALA	-	linker	UNP A0A178SBV6
A	1299	ARG	GLY	see remark 999	UNP Q8TAX9
A	1306	SER	PRO	see remark 999	UNP Q8TAX9
B	82	ALA	ASP	see remark 999	UNP A0A178SBV6
B	83	ALA	LYS	see remark 999	UNP A0A178SBV6
B	172	ALA	GLU	see remark 999	UNP A0A178SBV6
B	173	ALA	ASN	see remark 999	UNP A0A178SBV6
B	239	ALA	LYS	see remark 999	UNP A0A178SBV6
B	362	ALA	LYS	see remark 999	UNP A0A178SBV6
B	363	ALA	ASP	see remark 999	UNP A0A178SBV6
B	367	ASN	-	linker	UNP A0A178SBV6
B	368	ALA	-	linker	UNP A0A178SBV6
B	369	ALA	-	linker	UNP A0A178SBV6
B	370	ALA	-	linker	UNP A0A178SBV6

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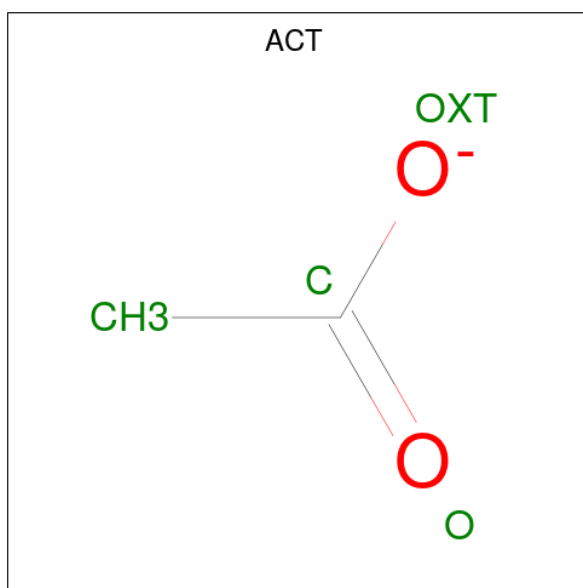
Chain	Residue	Modelled	Actual	Comment	Reference
B	1299	ARG	GLY	see remark 999	UNP Q8TAX9
B	1306	SER	PRO	see remark 999	UNP Q8TAX9

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



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 ACETATE ION (CCD ID: ACT) (formula: C₂H₃O₂).



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

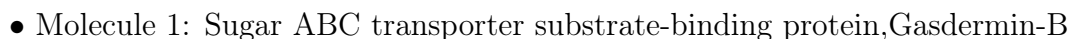
- Molecule 4 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Na	0	0
			1	1		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	232	Total 232	O 232	0	0
5	B	54	Total 54	O 54	0	0

- Molecule 1: Sugar ABC transporter substrate-binding protein, Gasdermin-B



GLC1
GLC2

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

Chain D:

50%

50%

GLC1
GLC2

4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	104.06Å 104.06Å 252.21Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	96.19 – 2.60 96.19 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.9 (96.19-2.60) 99.9 (96.19-2.60)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.10 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, R_{free}	0.184 , 0.233 0.191 , 0.186	Depositor DCC
R_{free} test set	2168 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	39.6	Xtriage
Anisotropy	0.019	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 66.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	8238	wwPDB-VP
Average B, all atoms (Å ²)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.62% 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: ACT, NA, 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	1.28	6/4136 (0.1%)	0.98	3/5617 (0.1%)
1	B	0.94	1/3924 (0.0%)	1.03	3/5362 (0.1%)
All	All	1.13	7/8060 (0.1%)	1.01	6/10979 (0.1%)

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	95	ASP	C-O	-6.92	1.16	1.24
1	A	94	TRP	C-O	-5.72	1.17	1.24
1	A	72	GLN	C-O	-5.60	1.17	1.24
1	A	90	TYR	C-O	-5.52	1.17	1.24
1	A	109	ALA	C-O	-5.31	1.17	1.23
1	B	1294	GLU	CA-C	5.03	1.59	1.52
1	A	351	ALA	C-O	-5.02	1.18	1.24

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1230	GLY	N-CA-C	6.51	121.10	112.77
1	B	228	GLY	CA-C-N	6.11	126.28	119.32
1	B	228	GLY	C-N-CA	6.11	126.28	119.32
1	A	1296	LEU	N-CA-C	5.95	117.76	111.28
1	A	1232	THR	N-CA-C	5.28	116.83	108.96
1	A	189	LYS	N-CA-C	5.00	116.73	111.28

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	4056	0	3993	25	0
1	B	3845	0	3599	91	0
2	C	23	0	21	0	0
2	D	23	0	21	1	0
3	A	4	0	3	0	0
4	A	1	0	0	0	0
5	A	232	0	0	1	0
5	B	54	0	0	3	0
All	All	8238	0	7637	115	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 7.

All (115) 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:331:PRO:HB2	1:B:336:MET:HE2	1.65	0.78
1:B:1301:LEU:HG	1:B:1315:PHE:CE2	2.26	0.71
1:B:355:GLN:NE2	1:B:360:ALA:HA	2.07	0.70
1:A:1366:MET:HE1	1:A:1393:TYR:HB2	1.77	0.67
1:A:153:GLU:CD	1:A:344:ARG:HH12	2.04	0.66
1:B:139:LEU:O	1:B:144:LYS:HB2	1.97	0.65
1:B:331:PRO:CB	1:B:336:MET:HE2	2.27	0.65
1:B:28:GLU:O	1:B:32:GLY:N	2.30	0.64
1:B:1315:PHE:CE1	1:B:1321:LEU:HB2	2.33	0.63
1:B:178:ILE:HD11	1:B:333:ILE:HD12	1.80	0.63
1:B:130:GLU:OE1	1:B:130:GLU:N	2.29	0.62
1:B:189:LYS:NZ	1:B:358:ASP:OD2	2.32	0.62
1:B:154:PRO:HA	1:B:157:THR:CG2	2.30	0.62
1:B:65:ASP:HB3	1:B:330:MET:HE3	1.82	0.61
1:B:154:PRO:HA	1:B:157:THR:HG22	1.83	0.61
1:B:331:PRO:CG	1:B:336:MET:HE2	2.31	0.61
1:B:1248:ASN:OD1	1:B:1249:MET:N	2.33	0.61
1:B:117:TYR:CE2	1:B:125:PRO:HG3	2.37	0.59
1:B:157:THR:HG21	1:B:347:VAL:HG11	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1301:LEU:HD11	1:B:1315:PHE:CD2	2.38	0.58
1:B:1301:LEU:CD1	1:B:1315:PHE:CD2	2.87	0.58
1:B:118:ASN:ND2	1:B:240:VAL:HG13	2.20	0.57
1:B:178:ILE:HD12	1:B:335:GLN:HG2	1.86	0.57
1:B:270:SER:O	1:B:273:LYS:HD2	2.04	0.57
1:B:331:PRO:HD2	1:B:336:MET:CE	2.35	0.56
1:B:19:GLY:N	1:B:296:ASP:OD2	2.35	0.56
1:B:301:ALA:CB	1:B:321:MET:HE1	2.36	0.55
1:A:1274:SER:HB2	1:A:1310:LEU:HB2	1.89	0.55
1:B:132:ILE:N	1:B:133:PRO:CD	2.70	0.55
1:B:331:PRO:HG2	1:B:336:MET:HE2	1.89	0.54
1:B:1255:ASP:O	1:B:1259:VAL:HG23	2.07	0.54
1:A:1384:PRO:HB3	1:B:101:GLY:HA3	1.89	0.54
1:B:331:PRO:CG	1:B:336:MET:CE	2.85	0.54
1:B:18:ASN:HB2	1:B:296:ASP:OD2	2.08	0.54
1:B:51:ALA:HB3	1:B:75:LEU:HD13	1.90	0.54
1:B:1365:VAL:O	1:B:1365:VAL:HG12	2.06	0.54
1:A:158:TRP:N	1:A:159:PRO:CD	2.71	0.53
1:B:44:GLU:HG2	1:B:45:GLU:HG3	1.88	0.53
1:B:117:TYR:CD2	1:B:125:PRO:HG3	2.43	0.53
1:B:273:LYS:O	1:B:276:ALA:N	2.42	0.53
1:B:1237:GLU:CB	1:B:1334:ASP:OD2	2.57	0.52
1:B:117:TYR:CE1	1:B:243:GLY:HA3	2.44	0.52
1:B:181:VAL:O	1:B:365:GLN:NE2	2.43	0.52
1:B:233:SER:O	1:B:236:ASP:HB2	2.10	0.52
1:B:331:PRO:CD	1:B:336:MET:CE	2.88	0.52
1:B:178:ILE:HG22	1:B:178:ILE:O	2.09	0.52
1:A:1366:MET:HE1	1:A:1393:TYR:CB	2.39	0.51
1:B:126:PRO:CB	1:B:131:GLU:OE1	2.59	0.51
1:B:1291:ARG:NH1	1:B:1305:ASP:OD1	2.44	0.51
1:B:314:ASP:OD1	1:B:315:PRO:HD2	2.11	0.51
1:B:130:GLU:O	1:B:133:PRO:HD2	2.11	0.50
1:B:178:ILE:HG22	1:B:1221:SER:OG	2.12	0.50
1:B:14:ASP:O	1:B:230:TRP:HB2	2.12	0.50
1:B:1355:LEU:N	1:B:1356:PRO:CD	2.75	0.49
1:B:199:ILE:HG21	1:B:206:ALA:HB2	1.94	0.49
1:B:1303:MET:O	1:B:1306:SER:CB	2.61	0.48
1:B:1264:THR:HG22	1:B:1266:GLU:H	1.78	0.48
1:A:195:LEU:CD1	1:A:204:MET:HE1	2.44	0.48
1:B:128:THR:HG22	1:B:249:THR:OG1	2.14	0.47
1:B:131:GLU:C	1:B:133:PRO:HD2	2.38	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:158:TRP:N	1:B:159:PRO:CD	2.77	0.47
1:B:132:ILE:HD13	1:B:147:LEU:HD22	1.97	0.47
1:B:190:ALA:HB1	1:B:251:LYS:HE3	1.96	0.47
1:A:1383:ASP:HB3	1:A:1386:ALA:HB3	1.97	0.46
1:A:153:GLU:OE1	1:A:344:ARG:NH1	2.47	0.46
1:B:153:GLU:OE1	1:B:344:ARG:NH1	2.49	0.46
1:B:331:PRO:HG2	1:B:336:MET:CE	2.45	0.46
1:B:1302:HIS:HB3	5:B:1618:HOH:O	2.15	0.46
1:A:132:ILE:N	1:A:133:PRO:CD	2.79	0.46
1:A:68:GLY:HA3	1:A:332:ASN:O	2.16	0.46
1:A:1355:LEU:N	1:A:1356:PRO:CD	2.78	0.45
1:B:118:ASN:CG	1:B:121:LEU:HD13	2.41	0.45
1:B:349:ASN:HB3	1:B:355:GLN:HB2	1.98	0.45
1:A:58:ASP:OD1	1:A:270:SER:OG	2.34	0.45
1:B:199:ILE:HA	1:B:204:MET:O	2.16	0.45
1:A:291:GLU:OE2	1:A:295:LYS:HE2	2.16	0.45
1:B:189:LYS:NZ	1:B:358:ASP:CG	2.75	0.45
1:B:51:ALA:HA	1:B:55:ASP:O	2.16	0.45
1:B:92:PHE:HD2	5:B:1636:HOH:O	2.00	0.45
1:B:65:ASP:OD1	1:B:330:MET:HE1	2.17	0.44
1:B:44:GLU:OE1	1:B:44:GLU:N	2.49	0.44
1:B:189:LYS:HZ1	1:B:358:ASP:CG	2.24	0.44
1:B:1233:LYS:HG2	1:B:1387:ARG:CZ	2.48	0.44
1:A:1366:MET:CE	1:A:1393:TYR:HB2	2.46	0.44
1:B:1303:MET:O	1:B:1306:SER:HB2	2.18	0.44
1:B:279:PHE:CD1	1:B:279:PHE:C	2.96	0.44
1:A:1310:LEU:C	1:A:1310:LEU:HD23	2.43	0.43
1:B:259:VAL:HB	1:B:329:ILE:HA	2.01	0.43
1:A:151:LEU:HD13	1:A:199:ILE:HD11	1.99	0.43
1:B:1307:ASP:C	1:B:1309:PRO:HD3	2.44	0.43
1:A:1229:ARG:HD3	5:A:1752:HOH:O	2.19	0.43
1:A:153:GLU:CD	1:A:344:ARG:NH1	2.75	0.43
1:B:273:LYS:O	1:B:276:ALA:HB3	2.19	0.43
1:B:1357:LEU:O	1:B:1361:GLN:HG3	2.19	0.43
1:B:111:GLU:OE1	2:D:1:GLC:O2	2.30	0.42
1:B:346:ALA:HB2	1:B:364:ALA:HB2	2.01	0.42
1:B:1310:LEU:C	1:B:1310:LEU:HD23	2.44	0.42
1:A:217:PHE:HA	1:A:222:THR:HG22	2.01	0.42
1:B:28:GLU:O	1:B:32:GLY:CA	2.68	0.42
1:B:178:ILE:CG2	1:B:1221:SER:OG	2.67	0.42
1:A:229:PRO:HA	1:A:232:TRP:CE2	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:195:LEU:HD12	1:A:204:MET:HE1	2.02	0.41
1:B:296:ASP:OD1	1:B:296:ASP:C	2.63	0.41
1:B:1263:LEU:HD21	1:B:1325:ARG:HD3	2.01	0.41
1:B:1383:ASP:OD1	1:B:1384:PRO:HD2	2.21	0.41
1:B:111:GLU:HG3	5:B:1611:HOH:O	2.20	0.41
1:B:245:THR:OG1	1:B:246:VAL:N	2.54	0.41
1:B:314:ASP:HA	1:B:315:PRO:HD3	1.93	0.41
1:B:80:THR:N	1:B:81:PRO:HD3	2.36	0.40
1:A:1310:LEU:O	1:A:1313:SER:HB2	2.21	0.40
1:B:331:PRO:HD2	1:B:336:MET:HE3	2.03	0.40
1:A:89:LEU:HD22	1:A:94:TRP:CZ2	2.56	0.40
1:A:340:TRP:CE3	1:A:340:TRP:HA	2.56	0.40
1:B:28:GLU:O	1:B:32:GLY:HA2	2.21	0.40
1:B:331:PRO:HB2	1:B:336:MET:CE	2.45	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	527/557 (95%)	521 (99%)	6 (1%)	0	100	100
1	B	524/557 (94%)	515 (98%)	9 (2%)	0	100	100
All	All	1051/1114 (94%)	1036 (99%)	15 (1%)	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	411/451 (91%)	409 (100%)	2 (0%)	81	92
1	B	358/451 (79%)	351 (98%)	7 (2%)	48	74
All	All	769/902 (85%)	760 (99%)	9 (1%)	63	83

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	60	ILE
1	A	258	PHE
1	B	8	VAL
1	B	175	LYS
1	B	258	PHE
1	B	326	LYS
1	B	345	THR
1	B	366	THR
1	B	1404	GLU

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	367	ASN
1	A	1248	ASN
1	A	1302	HIS
1	A	1361	GLN
1	B	152	GLN
1	B	201	ASN
1	B	205	ASN
1	B	253	GLN
1	B	325	GLN
1	B	349	ASN
1	B	355	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 ⓘ

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	0.63	0	17,17,17	1.16	2 (11%)
2	GLC	C	2	2	11,11,12	1.19	1 (9%)	15,15,17	0.53	0
2	GLC	D	1	2	12,12,12	0.86	0	17,17,17	0.89	1 (5%)
2	GLC	D	2	2	11,11,12	0.64	0	15,15,17	1.17	1 (6%)

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	-	2/2/22/22	0/1/1/1
2	GLC	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	GLC	D	2	2	-	2/2/19/22	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	2	GLC	C2-C3	3.34	1.57	1.52

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	2	GLC	C1-O5-C5	3.17	116.44	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1	GLC	O1-C1-O5	-2.71	102.36	110.41
2	C	1	GLC	O2-C2-C3	-2.58	104.29	110.38
2	D	1	GLC	C3-C4-C5	2.09	114.03	110.23

There are no chirality outliers.

All (6) torsion outliers are listed below:

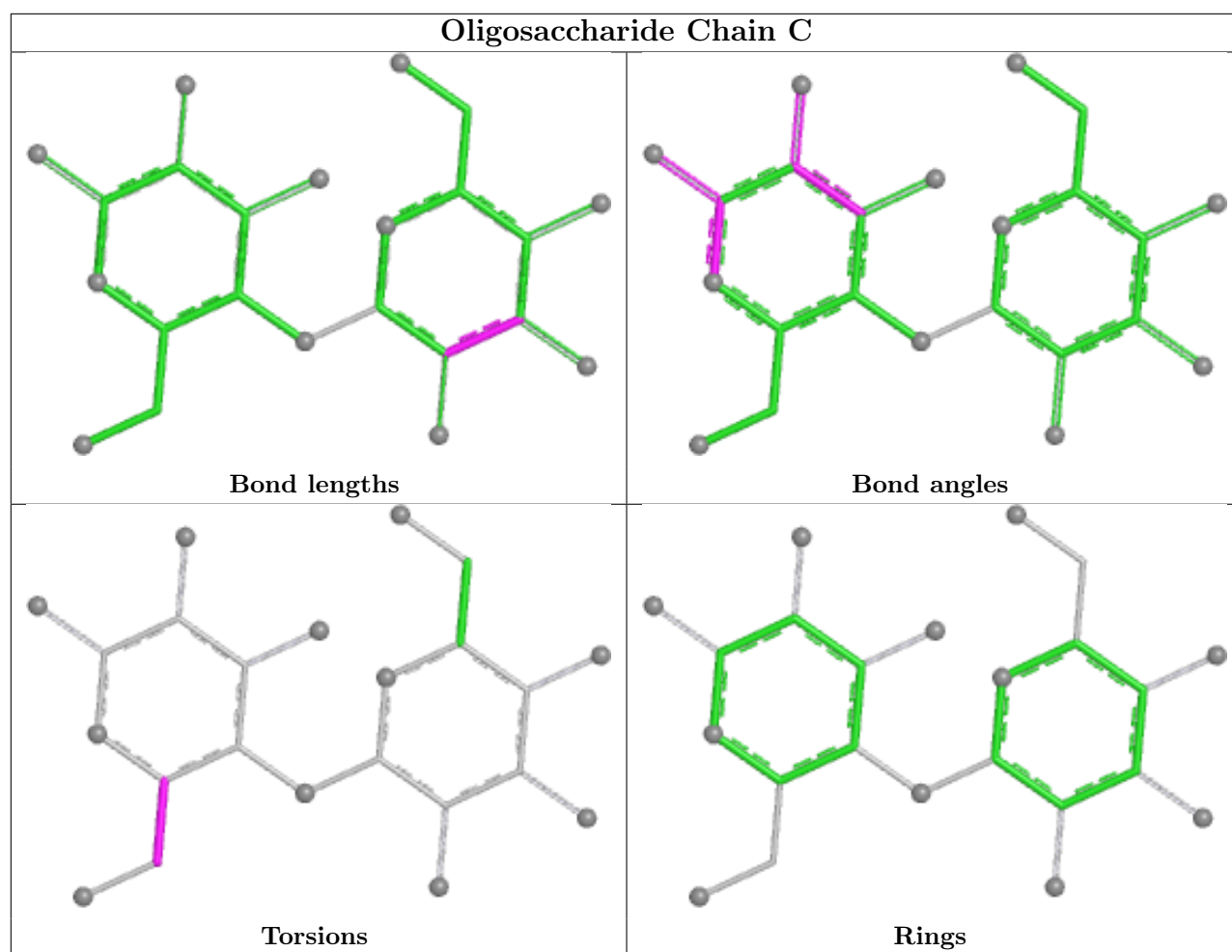
Mol	Chain	Res	Type	Atoms
2	D	1	GLC	C4-C5-C6-O6
2	D	1	GLC	O5-C5-C6-O6
2	D	2	GLC	C4-C5-C6-O6
2	D	2	GLC	O5-C5-C6-O6
2	C	1	GLC	C4-C5-C6-O6
2	C	1	GLC	O5-C5-C6-O6

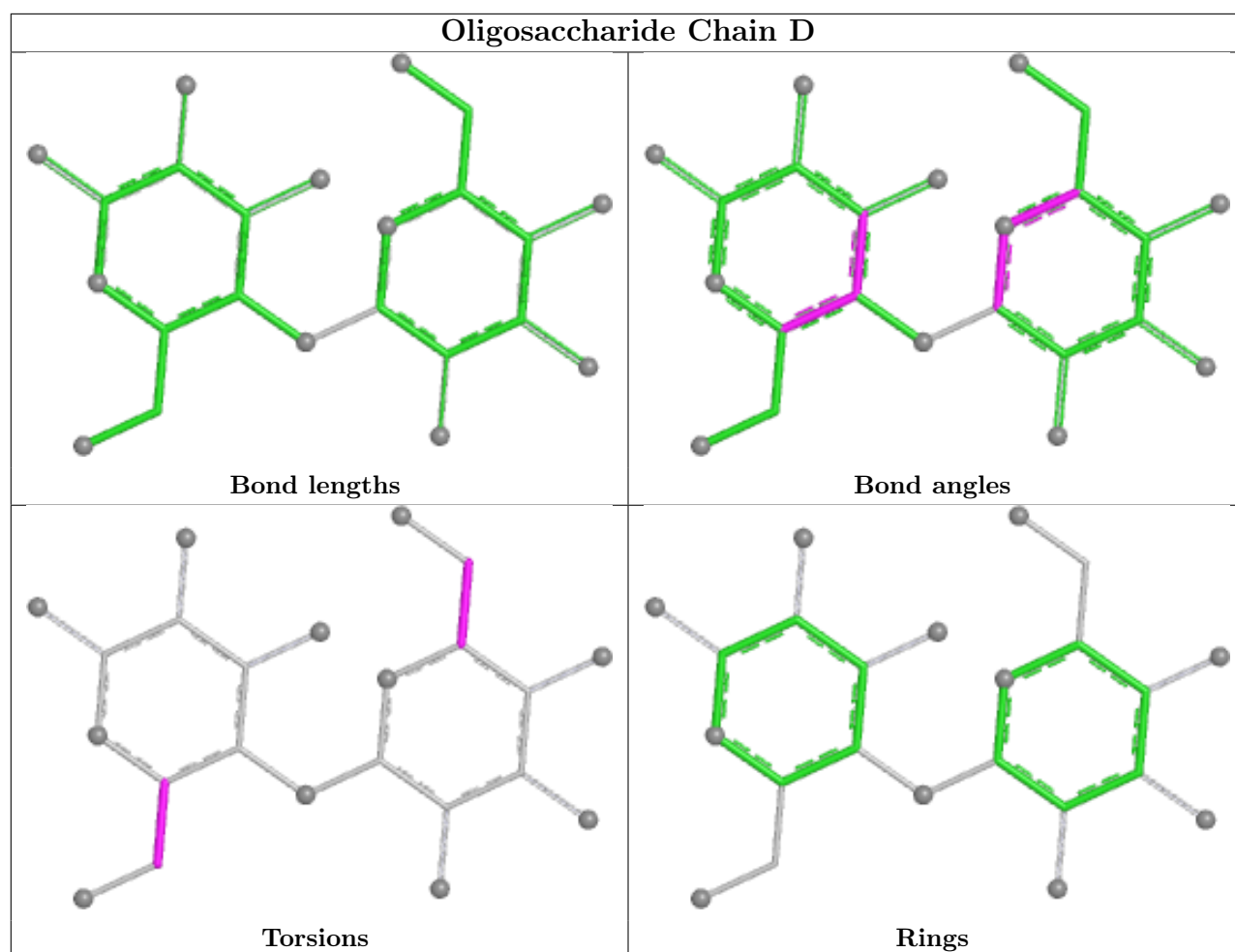
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	1	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](#)

Of 2 ligands modelled in this entry, 1 is monoatomic - leaving 1 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	$\# Z > 2$
3	ACT	A	1502	-	3,3,3	0.83	0	3,3,3	0.83	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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	533/557 (95%)	-0.56	6 (1%) 78 74	16, 29, 55, 97	0
1	B	530/557 (95%)	0.62	42 (7%) 18 14	30, 63, 95, 110	0
All	All	1063/1114 (95%)	0.03	48 (4%) 38 32	16, 45, 87, 110	0

All (48) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	243	GLY	4.7
1	B	1404	GLU	4.2
1	B	33	ILE	3.7
1	B	173	ALA	3.6
1	B	1405	GLY	3.5
1	B	3	GLU	3.3
1	B	124	ASN	3.3
1	A	239	ALA	3.1
1	B	351	ALA	3.1
1	A	1246	SER	3.1
1	A	1232	THR	3.0
1	B	239	ALA	2.9
1	A	1406	PRO	2.8
1	B	269	ALA	2.8
1	B	53	THR	2.8
1	B	210	TYR	2.7
1	B	1302	HIS	2.7
1	B	28	GLU	2.7
1	B	148	MET	2.6
1	B	205	ASN	2.5
1	B	240	VAL	2.5
1	B	141	ALA	2.4
1	B	92	PHE	2.4
1	B	52	ALA	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	1247	ARG	2.4
1	B	1248	ASN	2.3
1	B	1320	VAL	2.3
1	B	250	PHE	2.3
1	B	1318	ALA	2.2
1	B	55	ASP	2.2
1	A	1370	TRP	2.2
1	B	223	ALA	2.2
1	B	31	THR	2.2
1	B	1317	ALA	2.1
1	B	29	LYS	2.1
1	B	132	ILE	2.1
1	B	359	ALA	2.1
1	A	1233	LYS	2.1
1	B	295	LYS	2.1
1	B	117	TYR	2.1
1	B	1305	ASP	2.1
1	B	119	LYS	2.1
1	B	1364	SER	2.0
1	B	32	GLY	2.0
1	B	357	VAL	2.0
1	B	146	ALA	2.0
1	B	350	ALA	2.0
1	B	1360	ASP	2.0

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

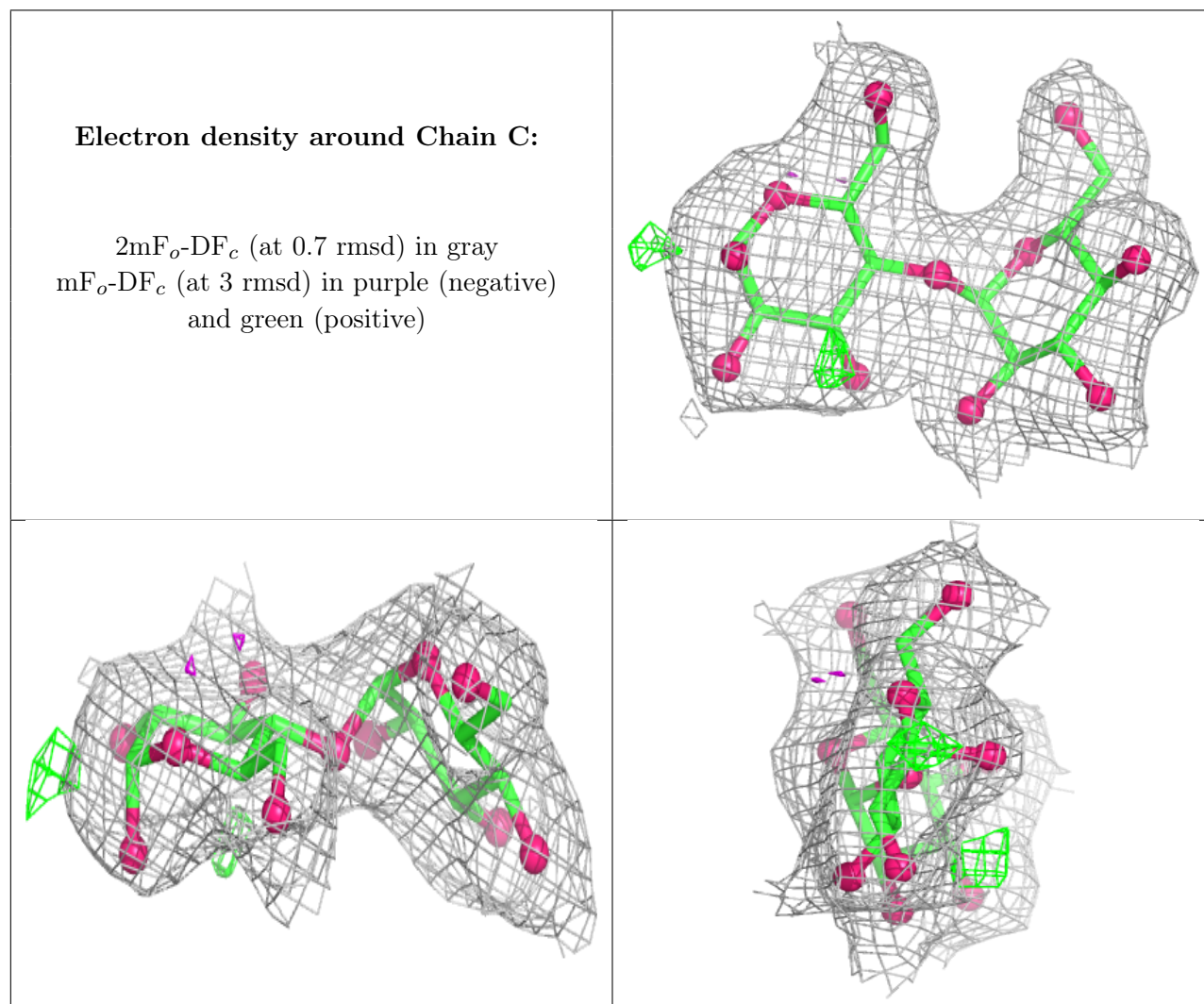
There are no non-standard protein/DNA/RNA residues in this entry.

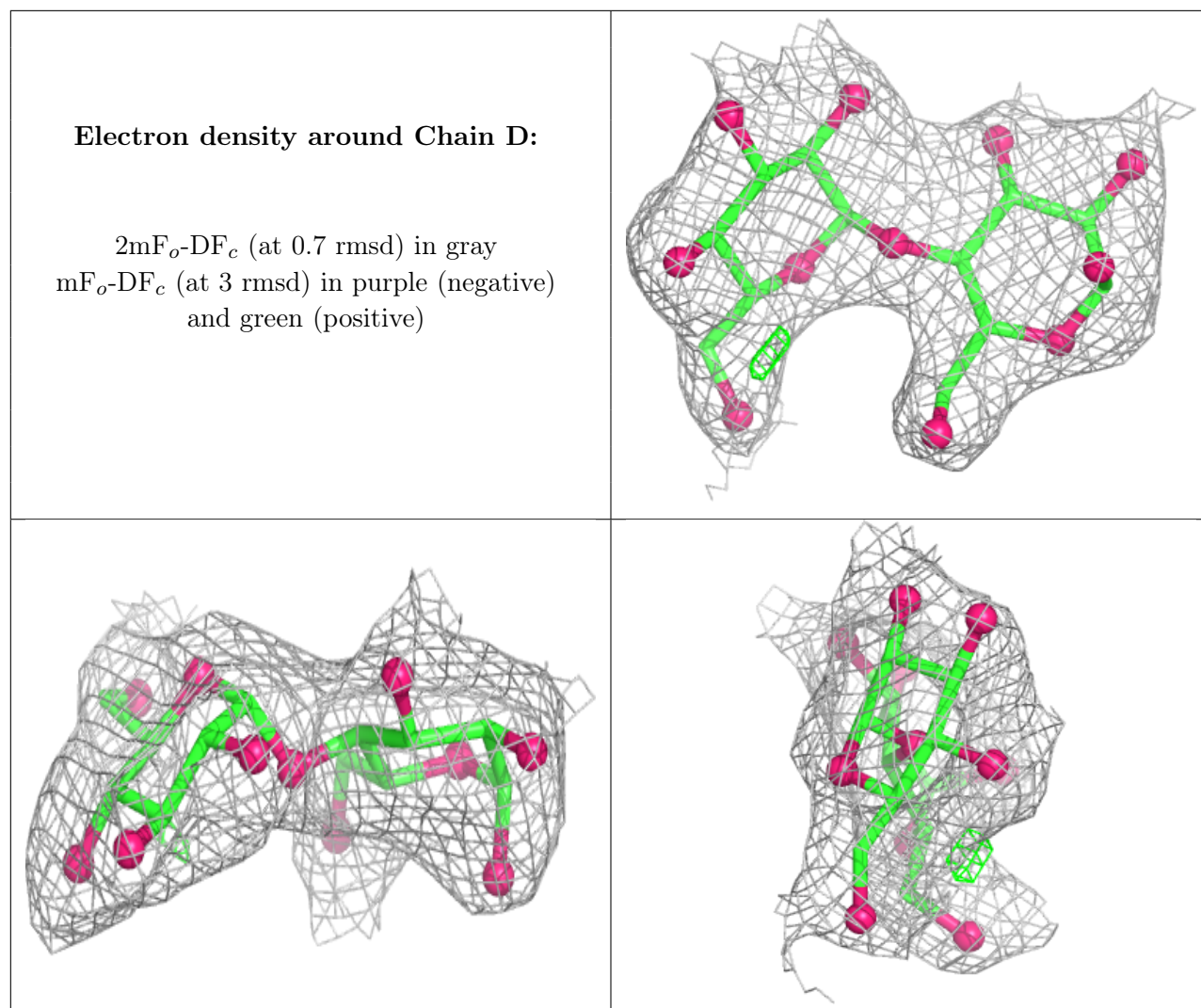
6.3 Carbohydrates [i](#)

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($\text{\AA}^2$)	Q<0.9
2	GLC	D	1	12/12	0.90	0.08	46,53,58,58	0
2	GLC	D	2	11/12	0.91	0.08	42,51,53,54	0
2	GLC	C	1	12/12	0.94	0.07	20,25,27,33	0
2	GLC	C	2	11/12	0.98	0.04	16,17,18,18	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	ACT	A	1502	4/4	0.79	0.18	47,48,49,58	0
4	NA	A	1503	1/1	0.95	0.05	37,37,37,37	0

6.5 Other polymers [i](#)

There are no such residues in this entry.