



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 7, 2020 – 11:23 PM BST

PDB ID : 5JST  
Title : MBP fused MDV1 coiled coil  
Authors : Kim, B.-W.; Song, H.K.  
Deposited on : 2016-05-09  
Resolution : 2.20 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](mailto: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.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.13.1  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.13.1

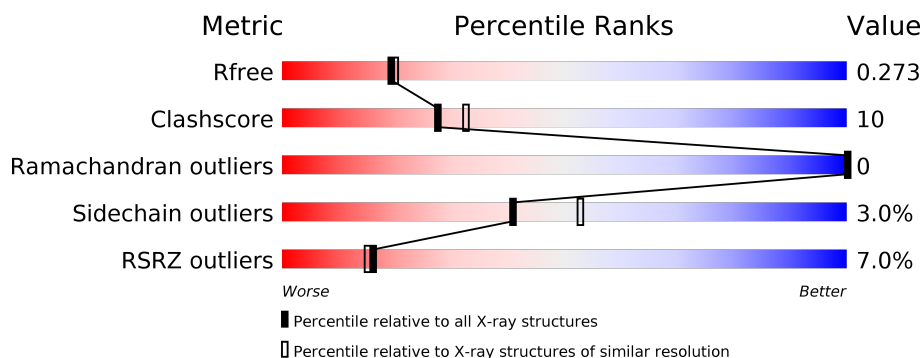
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.20 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))
$R_{free}$	130704	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	443	<div> <div>3%</div> <div> <div></div> <div>82%</div> <div>14%</div> <div>••</div> </div> </div>
1	B	443	<div> <div>10%</div> <div> <div></div> <div>74%</div> <div>23%</div> <div>•</div> </div> </div>
2	C	2	<div> <div>100%</div> </div>
2	D	2	<div> <div>50%</div> <div>50%</div> </div>

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	GLC	C	1	-	-	X	-
3	ACT	A	503	-	-	X	-

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 6836 atoms, of which 14 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 Maltose-binding periplasmic protein, Mitochondrial division protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	428	Total	C	N	O	S	0	0	0
			3250	2084	534	626	6			
1	B	432	Total	C	N	O	S	0	0	0
			3279	2100	540	633	6			

There are 24 discrepancies between the modelled and reference sequences:

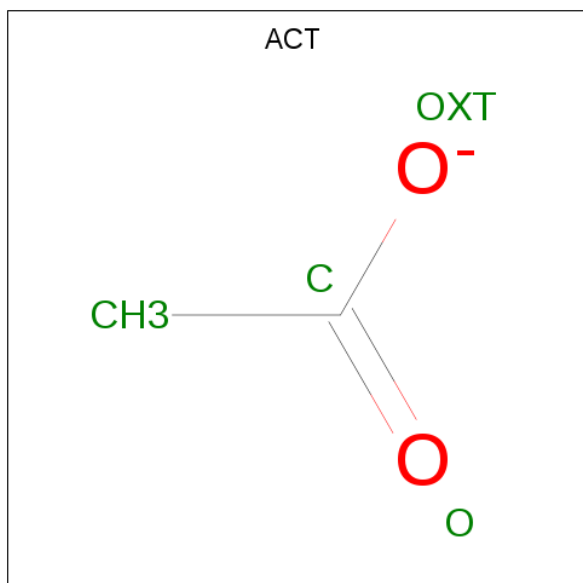
Chain	Residue	Modelled	Actual	Comment	Reference
A	0	MET	-	initiating methionine	UNP P0AEX9
A	82	ALA	ASP	engineered mutation	UNP P0AEX9
A	83	ALA	LYS	engineered mutation	UNP P0AEX9
A	239	ALA	LYS	engineered mutation	UNP P0AEX9
A	359	ALA	GLU	engineered mutation	UNP P0AEX9
A	362	ALA	LYS	engineered mutation	UNP P0AEX9
A	363	ALA	ASP	engineered mutation	UNP P0AEX9
A	367	ASN	-	linker	UNP P0AEX9
A	368	ALA	-	linker	UNP P0AEX9
A	369	ALA	-	linker	UNP P0AEX9
A	370	ALA	-	linker	UNP P0AEX9
A	371	GLY	-	linker	UNP P0AEX9
B	0	MET	-	initiating methionine	UNP P0AEX9
B	82	ALA	ASP	engineered mutation	UNP P0AEX9
B	83	ALA	LYS	engineered mutation	UNP P0AEX9
B	239	ALA	LYS	engineered mutation	UNP P0AEX9
B	359	ALA	GLU	engineered mutation	UNP P0AEX9
B	362	ALA	LYS	engineered mutation	UNP P0AEX9
B	363	ALA	ASP	engineered mutation	UNP P0AEX9
B	367	ASN	-	linker	UNP P0AEX9
B	368	ALA	-	linker	UNP P0AEX9
B	369	ALA	-	linker	UNP P0AEX9
B	370	ALA	-	linker	UNP P0AEX9
B	371	GLY	-	linker	UNP P0AEX9

- 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 (three-letter code: ACT) (formula: C<sub>2</sub>H<sub>3</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	O		0	0
			4	2	2			
3	A	1	Total	C	O		0	0
			4	2	2			
3	A	1	Total	C	H	O	0	0
			7	2	3	2		
3	A	1	Total	C	H	O	0	0
			7	2	3	2		
3	B	1	Total	C	O		0	0
			4	2	2			

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	H	O	0	0
			14	3	8	3		

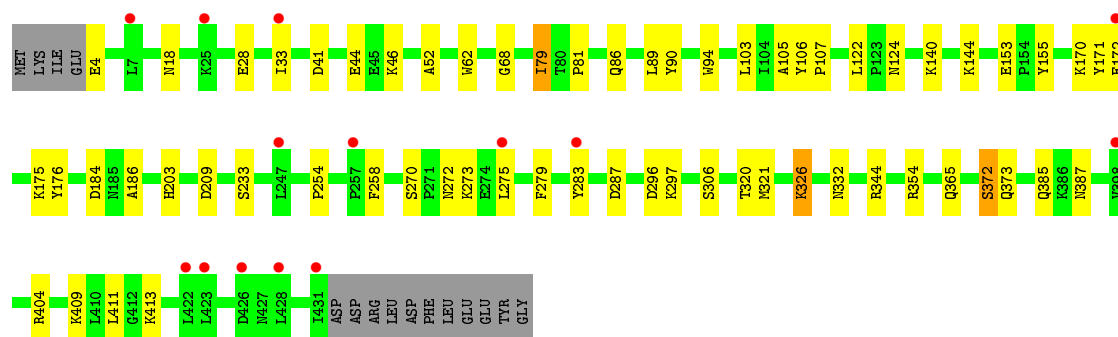
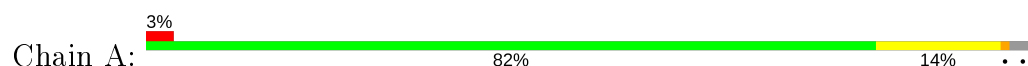
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	137	Total	O	0	0
			137	137		
5	B	84	Total	O	0	0
			84	84		

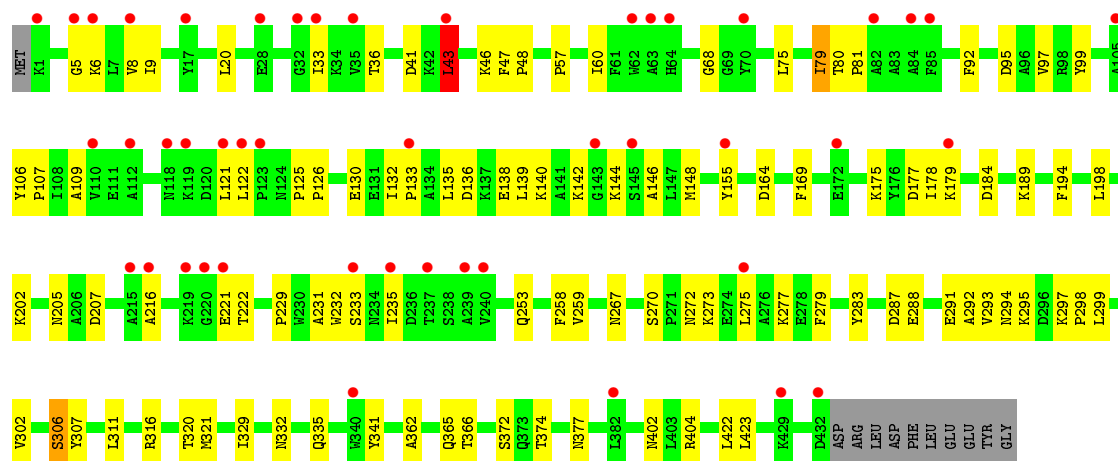
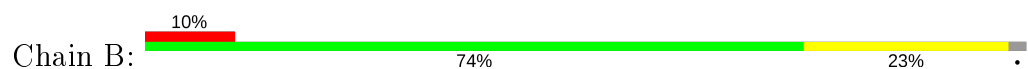
### 3 Residue-property plots [i](#)

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: Maltose-binding periplasmic protein,Mitochondrial division protein 1



- Molecule 1: Maltose-binding periplasmic protein,Mitochondrial division protein 1



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



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

Chain D:





## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	128.51Å 102.94Å 79.27Å 90.00° 102.51° 90.00°	Depositor
Resolution (Å)	36.85 – 2.20 36.85 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.1 (36.85-2.20) 93.2 (36.85-2.20)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.87 (at 2.20Å)	Xtriage
Refinement program	PHENIX 1.10.1_2155	Depositor
R, $R_{free}$	0.225 , 0.274 0.225 , 0.273	Depositor DCC
$R_{free}$ test set	2011 reflections (3.96%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	47.8	Xtriage
Anisotropy	0.149	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 50.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.012 for -1/2*h+1/2*k+1,1/2*h-1/2*k+1,1/2*h+1/2*k 0.015 for -1/2*h-1/2*k+1,-1/2*h-1/2*k-1,1/2*h-1/2*k	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	6836	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.40% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: GOL, GLC, ACT

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	0.40	0/3320	0.53	0/4519
1	B	0.35	0/3349	0.51	1/4560 (0.0%)
All	All	0.38	0/6669	0.52	1/9079 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	43	LEU	CA-CB-CG	5.28	127.44	115.30

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	3250	0	3182	58	0
1	B	3279	0	3201	72	0
2	C	23	0	21	7	0
2	D	23	0	21	2	0
3	A	16	6	12	2	0
3	B	4	0	3	0	0
4	A	6	8	8	0	0
5	A	137	0	0	13	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	B	84	0	0	6	1
All	All	6822	14	6448	131	1

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 10.

All (131) 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:A:79:ILE:HG23	1:A:81:PRO:HD3	1.35	1.03
1:A:175:LYS:HD2	1:A:176:TYR:H	1.25	1.01
1:B:404:ARG:NH1	5:B:602:HOH:O	2.07	0.86
1:A:79:ILE:HD11	1:A:106:TYR:CD1	2.11	0.85
1:B:79:ILE:HG23	1:B:81:PRO:HD3	1.60	0.83
1:B:140:LYS:NZ	1:B:202:LYS:O	2.13	0.81
1:B:402:ASN:OD1	5:B:601:HOH:O	1.99	0.81
1:A:33:ILE:HD13	1:A:275:LEU:HD13	1.63	0.80
1:A:79:ILE:HG22	1:A:103:LEU:HB2	1.63	0.80
1:A:86:GLN:NE2	5:A:605:HOH:O	2.14	0.80
1:B:92:PHE:HA	1:B:95:ASP:OD2	1.84	0.78
1:B:164:ASP:OD1	1:B:253:GLN:NE2	2.16	0.78
1:A:413:LYS:NZ	5:A:607:HOH:O	2.19	0.75
1:A:411:LEU:O	5:A:601:HOH:O	2.03	0.74
1:A:79:ILE:HD11	1:A:106:TYR:CG	2.22	0.74
1:A:155:TYR:HB2	2:C:1:GLC:C6	2.19	0.73
1:A:175:LYS:HD2	1:A:176:TYR:N	2.02	0.69
1:A:270:SER:O	1:A:273:LYS:NZ	2.26	0.69
1:A:203:HIS:NE2	5:A:609:HOH:O	2.26	0.68
1:A:155:TYR:HB2	2:C:1:GLC:H62	1.75	0.67
5:A:603:HOH:O	2:C:2:GLC:O3	2.12	0.66
1:A:287:ASP:OD1	1:A:306:SER:OG	2.14	0.65
1:A:79:ILE:HD11	1:A:106:TYR:CE1	2.31	0.65
1:A:44:GLU:OE2	5:A:604:HOH:O	2.13	0.64
1:A:372:SER:N	5:A:612:HOH:O	2.30	0.64
1:B:79:ILE:HG13	1:B:106:TYR:CE1	2.34	0.63
1:A:153:GLU:OE1	1:A:344:ARG:NH1	2.32	0.61
1:B:335:GLN:HA	1:B:374:THR:HG21	1.82	0.60
1:B:292:ALA:HA	1:B:295:LYS:NZ	2.16	0.60
1:A:175:LYS:CD	1:A:176:TYR:H	2.07	0.60
1:B:287:ASP:OD1	1:B:306:SER:OG	2.19	0.59
1:A:41:ASP:O	1:A:46:LYS:HE2	2.01	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:89:LEU:HD22	1:A:94:TRP:CZ2	2.37	0.58
1:B:99:TYR:OH	5:B:603:HOH:O	2.15	0.58
1:A:155:TYR:HB2	2:C:1:GLC:H5	1.85	0.58
1:B:5:GLY:O	1:B:33:ILE:HG23	2.02	0.58
1:B:307:TYR:CE2	1:B:311:LEU:HD11	2.39	0.57
1:B:140:LYS:HA	1:B:144:LYS:O	2.04	0.57
1:B:148:MET:SD	1:B:222:THR:HG21	2.44	0.57
1:B:80:THR:O	1:B:277:LYS:NZ	2.30	0.57
1:B:341:TYR:OH	5:B:604:HOH:O	2.17	0.57
1:B:8:VAL:HG12	1:B:36:THR:HB	1.86	0.56
1:A:186:ALA:H	3:A:503:ACT:H2	1.69	0.56
1:A:89:LEU:HD23	1:A:107:PRO:HG2	1.88	0.56
1:B:6:LYS:O	1:B:272:ASN:ND2	2.39	0.56
1:A:4:GLU:N	1:A:272:ASN:HD21	2.04	0.55
1:B:109:ALA:HA	1:B:302:VAL:HA	1.88	0.55
1:B:47:PHE:HB2	1:B:60:ILE:HD12	1.88	0.55
1:B:177:ASP:OD1	1:B:179:LYS:HG2	2.06	0.55
1:A:68:GLY:HA3	1:A:332:ASN:O	2.06	0.55
1:A:155:TYR:HB2	2:C:1:GLC:C5	2.37	0.54
1:B:33:ILE:HD13	1:B:275:LEU:HD13	1.90	0.54
1:B:122:LEU:HD21	1:B:126:PRO:HD3	1.91	0.53
1:B:92:PHE:HB2	5:B:657:HOH:O	2.09	0.53
1:A:254:PRO:HB3	1:A:326:LYS:HD3	1.90	0.52
1:A:86:GLN:CD	5:A:605:HOH:O	2.42	0.52
1:A:4:GLU:N	1:A:4:GLU:OE1	2.42	0.52
1:A:33:ILE:HD13	1:A:275:LEU:CD1	2.37	0.52
1:B:279:PHE:O	1:B:283:TYR:HB2	2.10	0.52
1:A:18:ASN:HB2	1:A:296:ASP:OD2	2.10	0.52
1:B:270:SER:O	1:B:273:LYS:NZ	2.44	0.51
1:B:205:ASN:OD1	1:B:207:ASP:HB2	2.10	0.51
1:B:216:ALA:HB1	1:B:222:THR:HG23	1.93	0.51
1:B:68:GLY:HA3	1:B:332:ASN:O	2.10	0.51
1:A:387:ASN:ND2	5:A:606:HOH:O	2.18	0.51
5:B:605:HOH:O	2:D:1:GLC:O2	2.18	0.50
1:A:33:ILE:CD1	1:A:275:LEU:HD22	2.42	0.49
1:A:52:ALA:O	1:A:385:GLN:HG3	2.11	0.49
1:B:320:THR:HG22	1:B:321:MET:CE	2.43	0.49
1:B:155:TYR:HB2	2:D:2:GLC:H62	1.95	0.49
1:B:216:ALA:HB1	1:B:222:THR:CG2	2.43	0.48
1:A:140:LYS:HD3	1:A:144:LYS:O	2.13	0.48
1:A:79:ILE:HD11	1:A:106:TYR:CD2	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:288:GLU:OE1	1:B:288:GLU:N	2.30	0.47
1:A:90:TYR:CE1	5:A:608:HOH:O	2.56	0.47
1:B:142:LYS:HG2	1:B:142:LYS:O	2.14	0.47
1:A:90:TYR:OH	5:A:608:HOH:O	2.21	0.46
1:B:41:ASP:O	1:B:46:LYS:HE2	2.16	0.46
1:B:320:THR:HG22	1:B:321:MET:HE2	1.97	0.46
1:B:292:ALA:HA	1:B:295:LYS:HZ2	1.81	0.46
1:B:292:ALA:HA	1:B:295:LYS:HZ3	1.81	0.46
1:B:135:LEU:O	1:B:139:LEU:HG	2.15	0.45
1:A:155:TYR:CB	2:C:1:GLC:H62	2.43	0.45
1:A:90:TYR:HE1	5:A:608:HOH:O	1.98	0.45
1:B:122:LEU:HD13	1:B:135:LEU:HD11	1.98	0.45
1:B:291:GLU:O	1:B:295:LYS:HG2	2.16	0.45
1:A:184:ASP:HB2	1:A:365:GLN:OE1	2.17	0.45
1:B:135:LEU:HG	1:B:139:LEU:CD1	2.47	0.45
1:B:130:GLU:N	1:B:130:GLU:OE1	2.44	0.45
1:A:79:ILE:HG22	1:A:103:LEU:CB	2.42	0.45
1:A:171:TYR:O	1:A:172:GLU:HG3	2.18	0.44
1:B:229:PRO:HA	1:B:232:TRP:CE2	2.53	0.44
1:A:62:TRP:HE1	2:C:1:GLC:H2	1.83	0.44
1:B:8:VAL:HG23	1:B:57:PRO:HA	1.99	0.44
1:A:79:ILE:HD12	1:A:105:ALA:C	2.37	0.44
1:A:413:LYS:HB3	1:A:413:LYS:HE2	1.71	0.44
1:A:186:ALA:N	3:A:503:ACT:H2	2.32	0.43
1:B:43:LEU:HD23	1:B:43:LEU:C	2.38	0.43
1:B:144:LYS:HD2	1:B:221:GLU:HA	2.00	0.43
1:B:169:PHE:CD1	1:B:178:ILE:HA	2.53	0.43
1:A:320:THR:HG22	1:A:321:MET:HE2	2.00	0.43
1:A:321:MET:CE	1:A:321:MET:HA	2.49	0.43
1:B:132:ILE:N	1:B:133:PRO:CD	2.81	0.43
1:A:209:ASP:HB2	5:A:693:HOH:O	2.18	0.43
1:B:121:LEU:CD2	1:B:142:LYS:HE3	2.48	0.43
1:B:184:ASP:HB2	1:B:365:GLN:OE1	2.19	0.43
1:B:231:ALA:O	1:B:235:ILE:HG13	2.19	0.43
1:B:177:ASP:OD1	1:B:179:LYS:CG	2.67	0.43
1:B:362:ALA:O	1:B:366:THR:HG23	2.19	0.42
1:B:259:VAL:HB	1:B:329:ILE:HA	2.02	0.42
1:B:233:SER:OG	1:B:298:PRO:HD3	2.19	0.42
1:B:9:ILE:HG21	1:B:20:LEU:HD21	2.01	0.42
1:B:233:SER:OG	1:B:297:LYS:HA	2.19	0.42
1:A:79:ILE:HD12	1:A:105:ALA:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:293:VAL:HG11	1:B:299:LEU:HD21	2.02	0.42
1:B:48:PRO:HA	1:B:75:LEU:HD13	2.01	0.41
1:B:232:TRP:CH2	1:B:316:ARG:HB3	2.55	0.41
1:B:122:LEU:HD21	1:B:125:PRO:HA	2.02	0.41
1:A:354:ARG:NH2	1:B:46:LYS:HD3	2.35	0.41
1:B:97:VAL:HG21	1:B:107:PRO:HD3	2.02	0.41
1:B:294:ASN:OD1	1:B:298:PRO:HA	2.19	0.41
1:A:233:SER:HB3	1:A:297:LYS:HD3	2.01	0.41
1:B:288:GLU:H	1:B:288:GLU:CD	2.17	0.41
1:A:279:PHE:O	1:A:283:TYR:HB2	2.20	0.41
1:A:28:GLU:HG3	1:A:33:ILE:O	2.21	0.41
1:B:194:PHE:CE2	1:B:198:LEU:HD11	2.56	0.41
1:B:184:ASP:HB2	1:B:365:GLN:CD	2.41	0.41
1:A:33:ILE:HD12	1:A:275:LEU:HD22	2.03	0.41
1:B:57:PRO:O	1:B:267:ASN:HB2	2.21	0.41
1:B:184:ASP:O	1:B:189:LYS:HE3	2.21	0.40
1:B:136:ASP:HA	1:B:146:ALA:HB2	2.03	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:688:HOH:O	5:B:634:HOH:O[3_455]	2.05	0.15

## 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	426/443 (96%)	415 (97%)	11 (3%)	0	100	100
1	B	430/443 (97%)	418 (97%)	12 (3%)	0	100	100
All	All	856/886 (97%)	833 (97%)	23 (3%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	328/357 (92%)	318 (97%)	10 (3%)	41	53
1	B	330/357 (92%)	320 (97%)	10 (3%)	41	53
All	All	658/714 (92%)	638 (97%)	20 (3%)	41	53

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	79	ILE
1	A	122	LEU
1	A	124	ASN
1	A	170	LYS
1	A	258	PHE
1	A	326	LYS
1	A	372	SER
1	A	373	GLN
1	A	404	ARG
1	A	409	LYS
1	B	43	LEU
1	B	79	ILE
1	B	138	GLU
1	B	175	LYS
1	B	258	PHE
1	B	306	SER
1	B	372	SER
1	B	377	ASN
1	B	422	LEU
1	B	423	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 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	0.80	0	17,17,17	2.35	6 (35%)
2	GLC	C	2	2	11,11,12	0.87	0	15,15,17	2.32	5 (33%)
2	GLC	D	1	2	12,12,12	0.46	0	17,17,17	0.85	0
2	GLC	D	2	2	11,11,12	0.74	0	15,15,17	1.19	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	-	0/2/22/22	0/1/1/1
2	GLC	C	2	2	-	2/2/19/22	0/1/1/1
2	GLC	D	1	2	-	0/2/22/22	0/1/1/1
2	GLC	D	2	2	-	2/2/19/22	0/1/1/1

There are no bond length outliers.

All (12) bond angle outliers are listed below:



Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1	GLC	C4-C3-C2	-6.37	99.70	110.82
2	C	2	GLC	O5-C1-C2	4.44	117.62	110.77
2	C	1	GLC	O5-C5-C4	-4.04	102.36	109.69
2	C	2	GLC	C1-O5-C5	3.95	117.55	112.19
2	C	2	GLC	C3-C4-C5	-3.75	103.55	110.24
2	C	2	GLC	C1-C2-C3	3.63	114.13	109.67
2	C	1	GLC	O2-C2-C1	3.00	116.11	109.16
2	C	1	GLC	O4-C4-C5	2.94	116.59	109.30
2	C	1	GLC	C1-C2-C3	-2.46	105.22	110.31
2	C	1	GLC	O1-C1-C2	2.41	115.81	109.03
2	C	2	GLC	O5-C5-C6	-2.30	103.61	107.20
2	D	2	GLC	O6-C6-C5	-2.11	104.04	111.29

There are no chirality outliers.

All (4) torsion outliers are listed below:

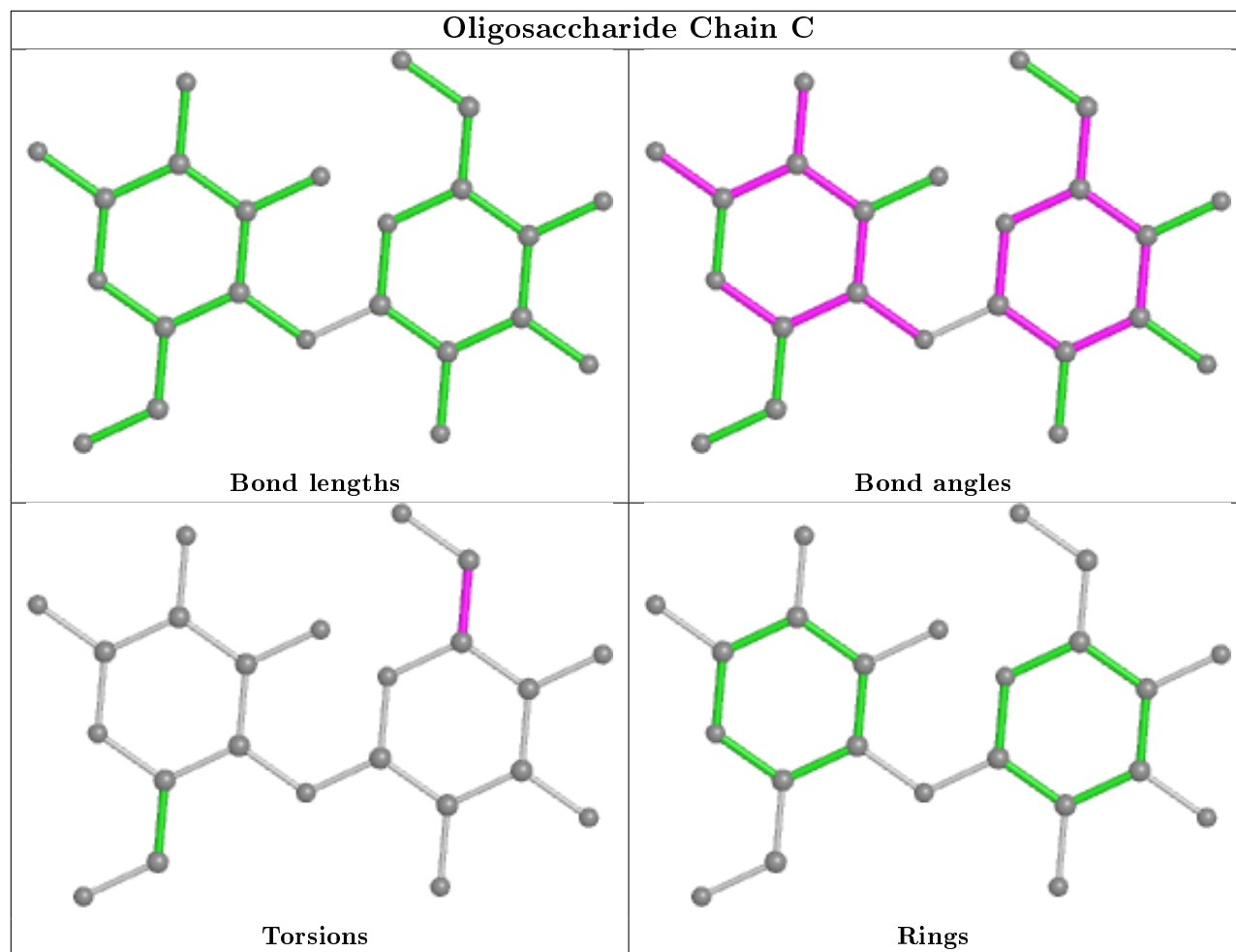
Mol	Chain	Res	Type	Atoms
2	D	2	GLC	C4-C5-C6-O6
2	C	2	GLC	O5-C5-C6-O6
2	D	2	GLC	O5-C5-C6-O6
2	C	2	GLC	C4-C5-C6-O6

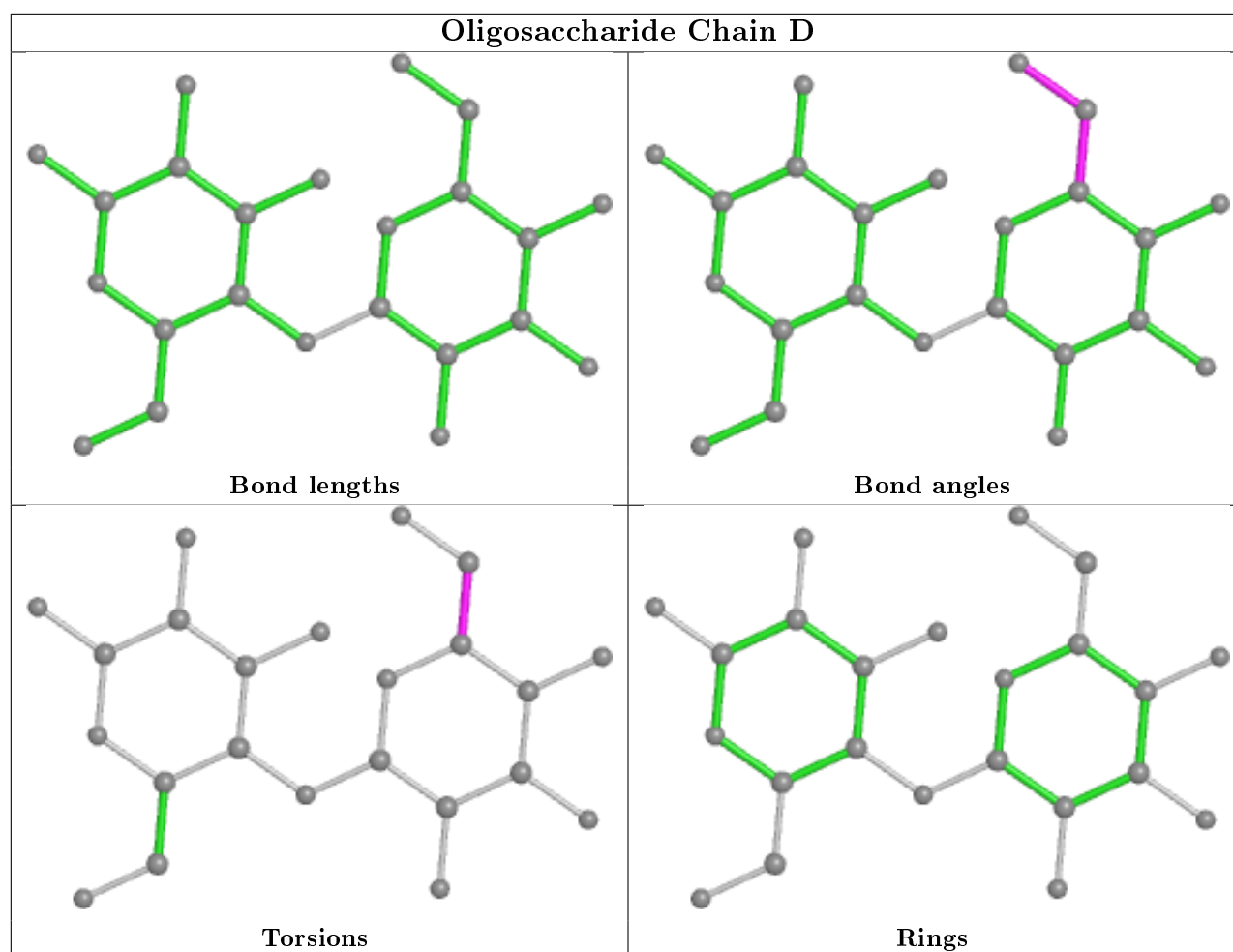
There are no ring outliers.

4 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	1	GLC	1	0
2	C	1	GLC	6	0
2	C	2	GLC	1	0
2	D	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](#)

6 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	ACT	A	503	-	1,3,3	2.30	1 (100%)	0,3,3	0.00	-
3	ACT	A	504	-	1,3,3	1.91	0	0,3,3	0.00	-
3	ACT	A	502	-	1,3,3	1.54	0	0,3,3	0.00	-
4	GOL	A	506	-	5,5,5	0.38	0	5,5,5	0.09	0
3	ACT	A	505	-	1,3,3	1.40	0	0,3,3	0.00	-
3	ACT	B	502	-	1,3,3	1.84	0	0,3,3	0.00	-

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	A	506	-	-	2/4/4/4	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	503	ACT	CH3-C	2.30	1.51	1.48

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	506	GOL	C1-C2-C3-O3
4	A	506	GOL	O2-C2-C3-O3

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	503	ACT	2	0

## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	428/443 (96%)	0.40	14 (3%) 46 44	35, 54, 84, 101	0
1	B	432/443 (97%)	0.75	46 (10%) 6 5	37, 63, 95, 117	0
All	All	860/886 (97%)	0.58	60 (6%) 16 15	35, 58, 92, 117	0

All (60) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	240	VAL	6.1
1	B	35	VAL	5.1
1	B	32	GLY	4.5
1	A	426	ASP	4.2
1	B	121	LEU	4.1
1	B	216	ALA	4.1
1	A	428	LEU	4.1
1	A	423	LEU	3.7
1	B	239	ALA	3.4
1	B	235	ILE	3.4
1	B	33	ILE	3.4
1	B	145	SER	3.3
1	A	283	TYR	3.3
1	B	5	GLY	3.3
1	B	6	LYS	3.2
1	A	33	ILE	3.2
1	B	123	PRO	3.2
1	B	17	TYR	3.2
1	B	432	ASP	3.0
1	B	275	LEU	3.0
1	B	429	LYS	2.9
1	B	122	LEU	2.9
1	B	179	LYS	2.9
1	B	143	GLY	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	219	LYS	2.8
1	B	220	GLY	2.8
1	B	63	ALA	2.7
1	B	340	TRP	2.7
1	A	247	LEU	2.7
1	A	422	LEU	2.6
1	B	62	TRP	2.6
1	B	70	TYR	2.5
1	B	172	GLU	2.5
1	B	8	VAL	2.3
1	A	25	LYS	2.3
1	B	119	LYS	2.3
1	B	215	ALA	2.2
1	B	84	ALA	2.2
1	B	237	THR	2.2
1	B	43	LEU	2.2
1	B	105	ALA	2.2
1	B	382	LEU	2.2
1	B	85	PHE	2.2
1	B	155	TYR	2.2
1	B	64	HIS	2.2
1	A	7	LEU	2.2
1	A	275	LEU	2.2
1	A	398	VAL	2.1
1	B	1	LYS	2.1
1	B	28	GLU	2.1
1	A	431	ILE	2.1
1	B	118	ASN	2.1
1	B	82	ALA	2.1
1	A	172	GLU	2.0
1	B	233	SER	2.0
1	B	133	PRO	2.0
1	B	221	GLU	2.0
1	A	257	PRO	2.0
1	B	112	ALA	2.0
1	B	110	VAL	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

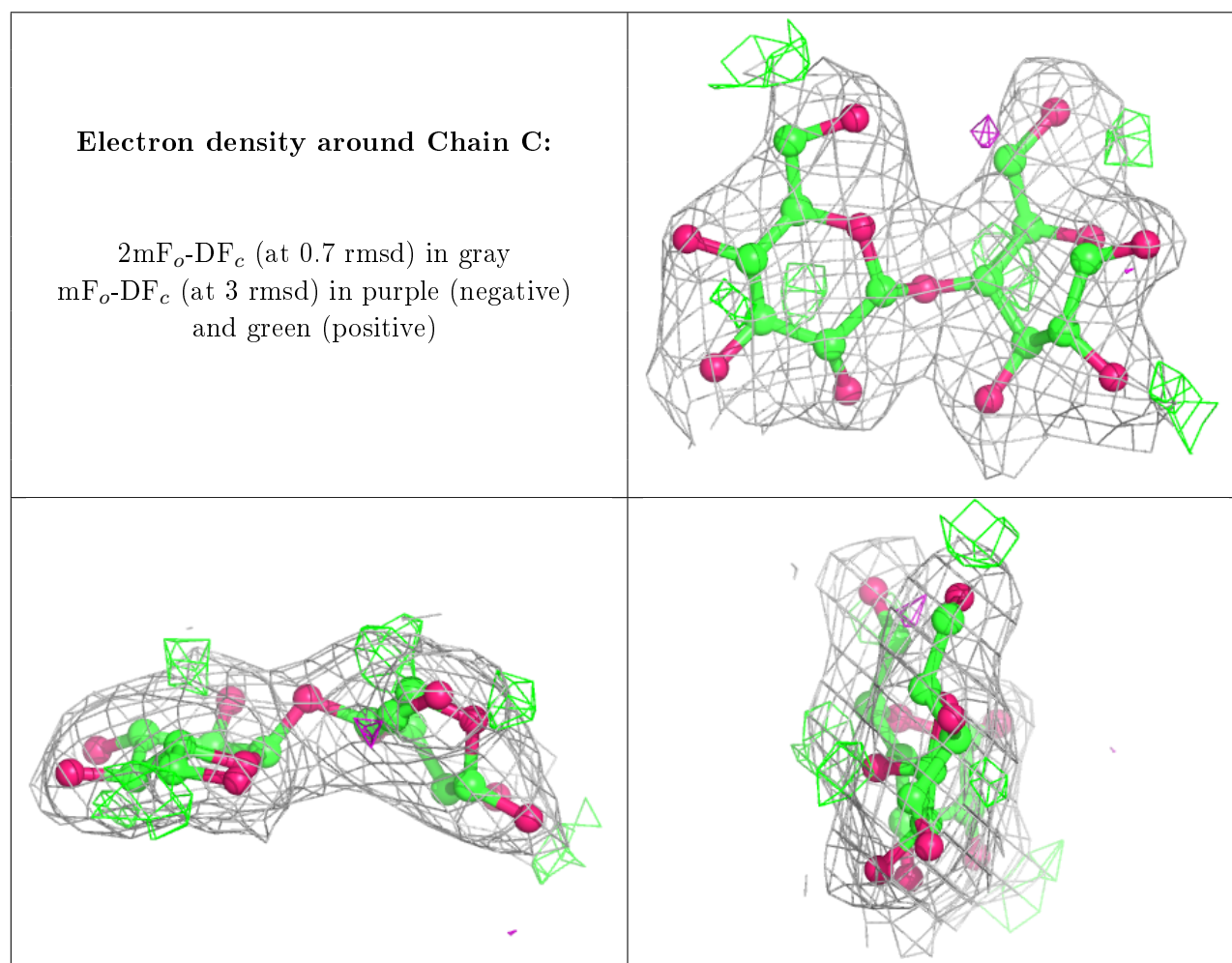
There are no non-standard protein/DNA/RNA residues in this entry.

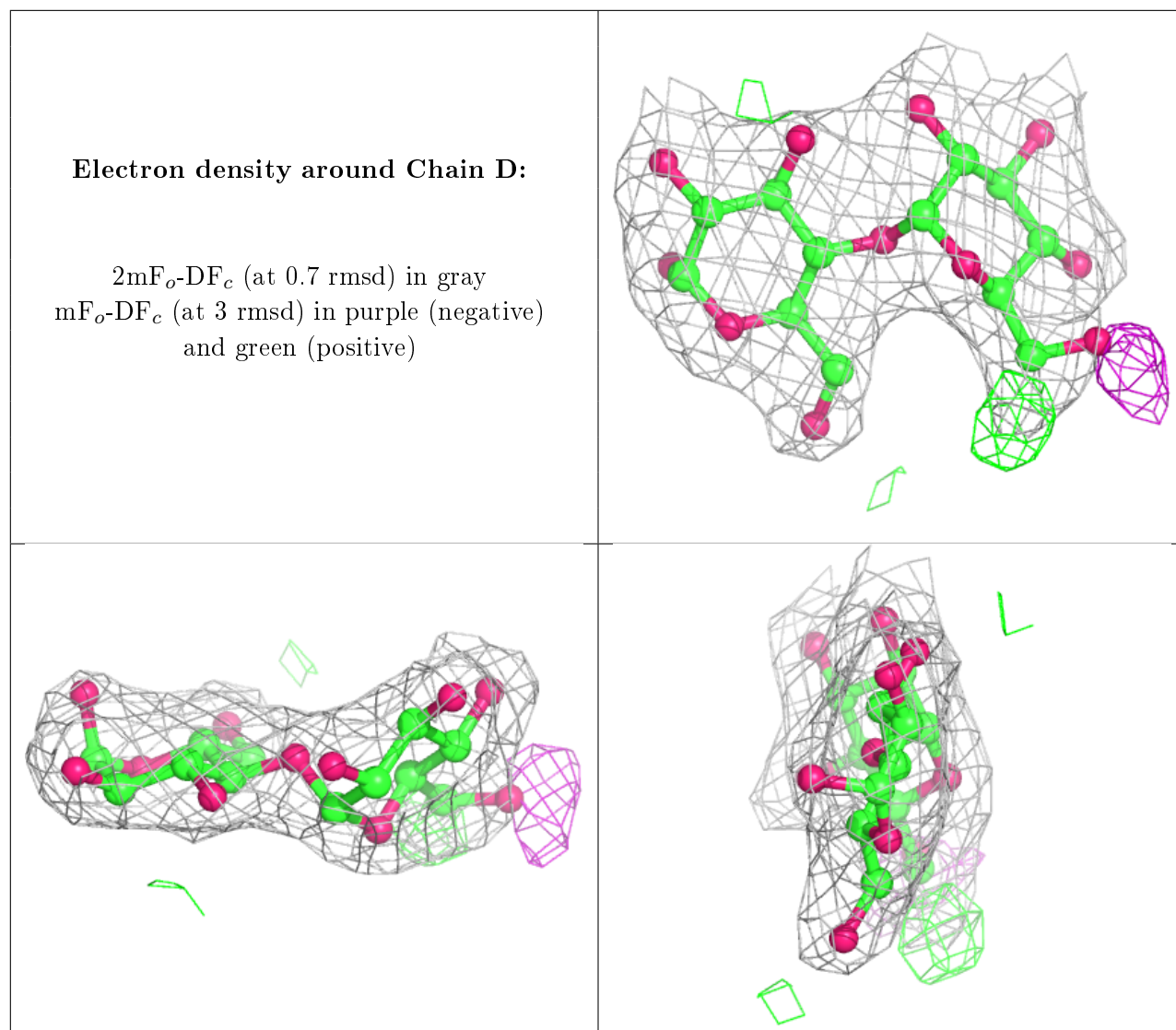
### 6.3 Carbohydrates ⓘ

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, 95<sup>th</sup> 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	C	1	12/12	0.92	0.17	42,45,55,55	0
2	GLC	D	1	12/12	0.93	0.20	50,55,58,59	0
2	GLC	D	2	11/12	0.93	0.28	44,48,50,54	0
2	GLC	C	2	11/12	0.95	0.17	46,49,56,61	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 ⓘ

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
3	ACT	A	503	4/4	0.73	0.26	53,61,62,66	0
3	ACT	A	505	4/4	0.73	0.30	105,113,126,126	0
4	GOL	A	506	6/6	0.76	0.21	68,82,98,99	0
3	ACT	A	504	4/4	0.84	0.19	62,67,75,75	0
3	ACT	B	502	4/4	0.84	0.44	74,75,77,79	0
3	ACT	A	502	4/4	0.88	0.21	73,81,84,88	0



## 6.5 Other polymers [i](#)

There are no such residues in this entry.