



# Full wwPDB X-ray Structure Validation Report ⓘ

Jul 26, 2023 – 01:50 AM EDT

PDB ID : 1AF6  
Title : MALTOPORIN SUCROSE COMPLEX  
Authors : Dutzler, R.; Schirmer, T.  
Deposited on : 1997-03-21  
Resolution : 2.40 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.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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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)  
Xtrriage (Phenix) : 1.13  
EDS : 2.34  
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) : 2.34

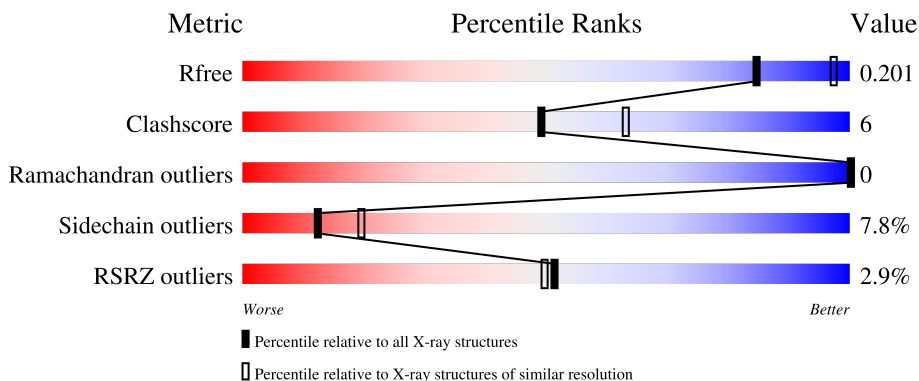
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.40 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	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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  $\geq 3$ , 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	421	<div style="display: flex; align-items: center;"> <div style="width: 2%; height: 10px; background-color: red; margin-right: 2px;"></div> <div style="width: 83%; height: 10px; background-color: green; margin-right: 2px;"></div> <div style="width: 14%; height: 10px; background-color: yellow; margin-right: 2px;"></div> <div style="width: 1%; height: 10px; background-color: orange; margin-right: 2px;"></div> <div style="width: 1%; height: 10px; background-color: grey;"></div> </div> <p style="margin-left: 20px;">2%      83%      14%      •</p>
1	B	421	<div style="display: flex; align-items: center;"> <div style="width: 3%; height: 10px; background-color: red; margin-right: 2px;"></div> <div style="width: 85%; height: 10px; background-color: green; margin-right: 2px;"></div> <div style="width: 12%; height: 10px; background-color: yellow; margin-right: 2px;"></div> <div style="width: 1%; height: 10px; background-color: orange; margin-right: 2px;"></div> <div style="width: 1%; height: 10px; background-color: grey;"></div> </div> <p style="margin-left: 20px;">3%      85%      12%      •</p>
1	C	421	<div style="display: flex; align-items: center;"> <div style="width: 3%; height: 10px; background-color: red; margin-right: 2px;"></div> <div style="width: 83%; height: 10px; background-color: green; margin-right: 2px;"></div> <div style="width: 14%; height: 10px; background-color: yellow; margin-right: 2px;"></div> <div style="width: 1%; height: 10px; background-color: orange; margin-right: 2px;"></div> <div style="width: 1%; height: 10px; background-color: grey;"></div> </div> <p style="margin-left: 20px;">3%      83%      14%      •</p>
2	D	2	<div style="display: flex; align-items: center;"> <div style="width: 50%; height: 10px; background-color: yellow; margin-right: 2px;"></div> <div style="width: 50%; height: 10px; background-color: orange;"></div> </div> <p style="margin-left: 20px;">50%      50%</p>
2	E	2	<div style="display: flex; align-items: center;"> <div style="width: 100%; height: 10px; background-color: yellow;"></div> </div> <p style="margin-left: 20px;">100%</p>

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Mol	Chain	Length	Quality of chain
2	F	2	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	MG	A	424	-	-	-	X
3	MG	B	424	-	-	-	X
3	MG	C	424	-	-	-	X

## 2 Entry composition [i](#)

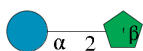
There are 4 unique types of molecules in this entry. The entry contains 10517 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 MALTOPORIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	421	3350	2110	571	655	14	0	0	0
1	B	421	3350	2110	571	655	14	0	0	0
1	C	421	3350	2110	571	655	14	0	0	0

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



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

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
3	A	2	2	2	0	0
3	B	1	1	1	0	0
3	C	1	1	1	0	0

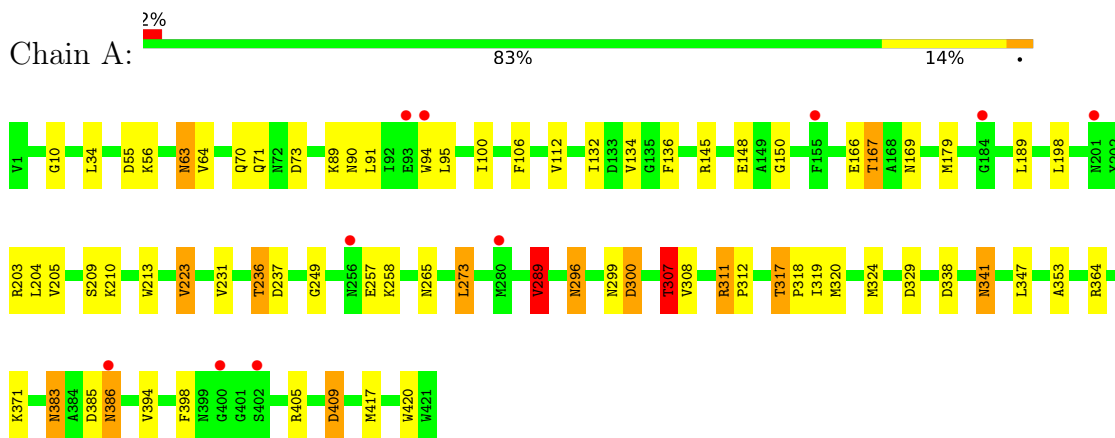
- Molecule 4 is water.

<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>		<b>ZeroOcc</b>	<b>AltConf</b>
4	A	130	Total 130	O 130	0	0
4	B	131	Total 131	O 131	0	0
4	C	133	Total 133	O 133	0	0

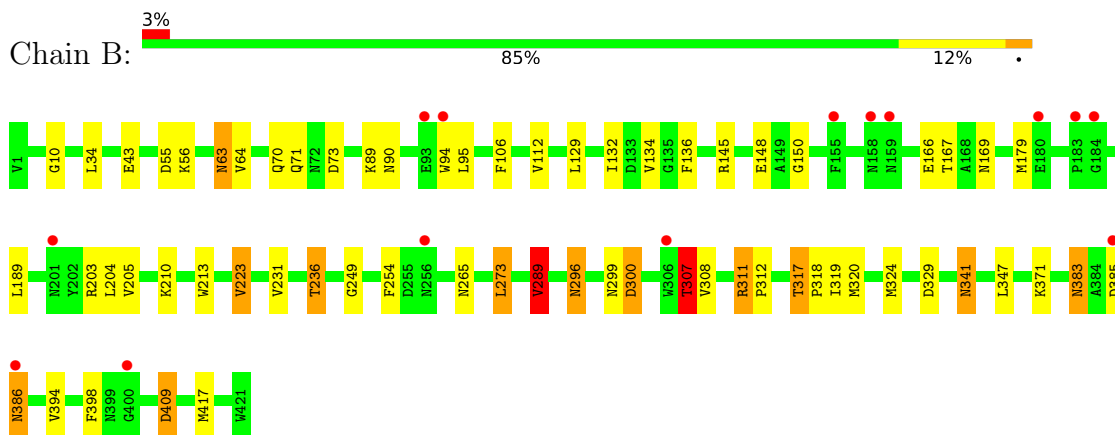
### 3 Residue-property plots [i](#)

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.

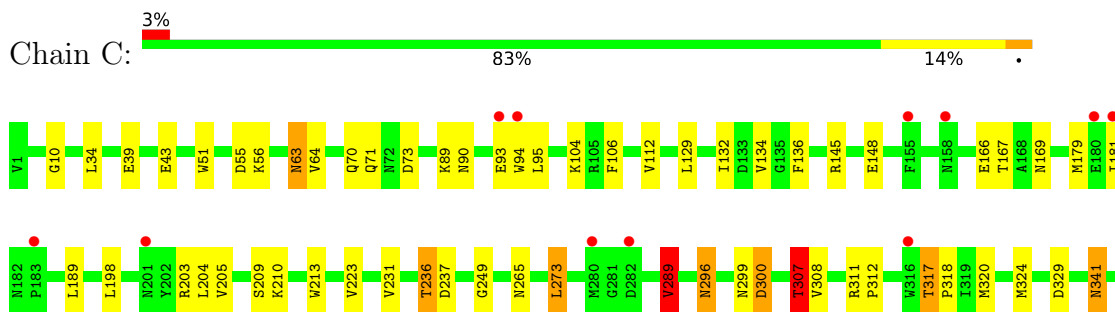
#### • Molecule 1: MALTOPORIN

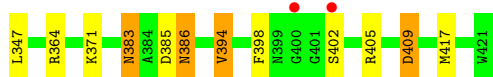


#### • Molecule 1: MALTOPORIN



#### • Molecule 1: MALTOPORIN





- Molecule 2: beta-D-fructofuranose-(2-1)-alpha-D-glucopyranose



- Molecule 2: beta-D-fructofuranose-(2-1)-alpha-D-glucopyranose



- Molecule 2: beta-D-fructofuranose-(2-1)-alpha-D-glucopyranose



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	129.66Å 211.51Å 217.91Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	8.00 – 2.40 19.99 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.0 (8.00-2.40) 99.0 (19.99-2.40)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	6.10 (at 2.41Å)	Xtrriage
Refinement program	PROLSQ	Depositor
R, $R_{free}$	0.195 , 0.214 0.183 , 0.201	Depositor DCC
$R_{free}$ test set	11446 reflections (9.93%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	37.0	Xtrriage
Anisotropy	0.388	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 63.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	0.007 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l 0.014 for 1/2*h+1/2*k,3/2*h-1/2*k,-l	Xtrriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	10517	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	41.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.64% 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: FRU, MG, 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	0.47	0/3443	0.92	7/4668 (0.1%)
1	B	0.48	0/3443	0.92	3/4668 (0.1%)
1	C	0.47	0/3443	0.91	5/4668 (0.1%)
All	All	0.47	0/10329	0.91	15/14004 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	6
1	B	0	5
1	C	0	6
All	All	0	17

There are no bond length outliers.

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	311	ARG	NE-CZ-NH2	-8.50	116.05	120.30
1	A	289	VAL	CB-CA-C	-7.36	97.41	111.40
1	B	289	VAL	CB-CA-C	-6.78	98.51	111.40
1	C	289	VAL	CB-CA-C	-6.74	98.59	111.40
1	A	311	ARG	NE-CZ-NH2	-6.37	117.11	120.30
1	C	364	ARG	NE-CZ-NH1	-5.80	117.40	120.30
1	A	364	ARG	NE-CZ-NH1	-5.78	117.41	120.30
1	A	338	ASP	CB-CG-OD1	-5.58	113.28	118.30
1	B	311	ARG	NE-CZ-NH2	-5.35	117.63	120.30
1	A	311	ARG	CD-NE-CZ	5.32	131.05	123.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	405	ARG	CD-NE-CZ	5.17	130.83	123.60
1	B	223	VAL	CB-CA-C	-5.16	101.61	111.40
1	A	223	VAL	CB-CA-C	-5.11	101.70	111.40
1	C	311	ARG	NE-CZ-NH1	5.06	122.83	120.30
1	C	405	ARG	CD-NE-CZ	5.03	130.65	123.60

There are no chirality outliers.

All (17) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	106	PHE	Mainchain
1	A	289	VAL	Mainchain
1	A	307	THR	Mainchain
1	A	386	ASN	Mainchain
1	A	409	ASP	Mainchain
1	A	420	TRP	Mainchain
1	B	106	PHE	Mainchain
1	B	289	VAL	Mainchain
1	B	307	THR	Mainchain
1	B	386	ASN	Mainchain
1	B	409	ASP	Mainchain
1	C	106	PHE	Mainchain
1	C	289	VAL	Mainchain
1	C	307	THR	Mainchain
1	C	386	ASN	Mainchain
1	C	402	SER	Mainchain
1	C	409	ASP	Mainchain

## 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	3350	0	3070	43	0
1	B	3350	0	3070	39	0
1	C	3350	0	3070	39	0
2	D	23	0	21	1	0
2	E	23	0	21	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	F	23	0	21	1	0
3	A	2	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
4	A	130	0	0	3	0
4	B	131	0	0	2	0
4	C	133	0	0	3	0
All	All	10517	0	9273	114	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 6.

All (114) 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:169:ASN:HD21	1:A:249:GLY:H	1.26	0.83
1:B:169:ASN:HD21	1:B:249:GLY:H	1.27	0.82
1:C:169:ASN:HD21	1:C:249:GLY:H	1.29	0.81
1:A:317:THR:HG22	1:A:320:MET:H	1.46	0.81
1:C:317:THR:HG22	1:C:320:MET:H	1.49	0.78
1:B:317:THR:HG22	1:B:320:MET:H	1.51	0.75
1:A:71:GLN:HE22	1:C:145:ARG:HH11	1.36	0.72
1:A:145:ARG:HH11	1:B:71:GLN:HE22	1.40	0.69
1:B:145:ARG:HH11	1:C:71:GLN:HE22	1.41	0.68
1:C:307:THR:HG23	1:C:329:ASP:OD1	1.98	0.64
1:B:307:THR:HG23	1:B:329:ASP:OD1	1.99	0.62
1:A:307:THR:HG23	1:A:329:ASP:OD1	1.99	0.62
4:C:425:HOH:O	2:F:2:FRU:O6	2.16	0.61
1:B:383:ASN:ND2	1:B:386:ASN:H	1.99	0.60
1:B:383:ASN:HD22	1:B:385:ASP:H	1.51	0.58
4:A:552:HOH:O	1:B:73:ASP:HA	2.04	0.58
1:B:148:GLU:O	1:B:166:GLU:HG3	2.03	0.57
1:A:383:ASN:HD22	1:A:385:ASP:H	1.51	0.57
1:C:204:LEU:HD12	1:C:210:LYS:HE2	1.86	0.57
1:A:317:THR:HG22	1:A:320:MET:N	2.17	0.56
1:C:383:ASN:HD22	1:C:385:ASP:H	1.53	0.56
1:A:94:TRP:CD1	1:A:95:LEU:HG	2.40	0.55
1:C:10:GLY:H	1:C:70:GLN:HE22	1.55	0.55
1:C:383:ASN:ND2	1:C:386:ASN:H	2.04	0.55
1:A:204:LEU:HD12	1:A:210:LYS:HE2	1.89	0.55
1:A:299:ASN:O	1:A:300:ASP:HB2	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:317:THR:HG22	1:C:320:MET:N	2.20	0.55
1:B:136:PHE:HE2	1:B:179:MET:HE3	1.72	0.54
1:B:10:GLY:H	1:B:70:GLN:HE22	1.55	0.54
1:B:317:THR:HG22	1:B:320:MET:N	2.22	0.54
1:C:94:TRP:CD1	1:C:95:LEU:HG	2.43	0.54
1:B:204:LEU:HD12	1:B:210:LYS:HE2	1.90	0.54
1:B:94:TRP:CD1	1:B:95:LEU:HG	2.43	0.53
1:C:299:ASN:O	1:C:300:ASP:HB2	2.09	0.52
1:C:148:GLU:O	1:C:166:GLU:HG3	2.10	0.52
1:A:383:ASN:ND2	1:A:386:ASN:H	2.08	0.52
1:A:341:ASN:ND2	4:A:515:HOH:O	2.43	0.51
1:C:341:ASN:ND2	4:C:521:HOH:O	2.43	0.51
1:B:136:PHE:CE2	1:B:179:MET:HE3	2.45	0.51
1:A:10:GLY:H	1:A:70:GLN:HE22	1.60	0.50
4:B:555:HOH:O	1:C:73:ASP:HA	2.12	0.50
1:A:112:VAL:HG11	1:A:289:VAL:HG13	1.94	0.50
1:C:136:PHE:HE2	1:C:179:MET:HE3	1.75	0.50
1:C:231:VAL:HB	1:C:273:LEU:HB3	1.94	0.50
1:A:231:VAL:HB	1:A:273:LEU:HB3	1.92	0.49
1:A:136:PHE:HE2	1:A:179:MET:HE3	1.77	0.49
1:A:136:PHE:CE2	1:A:179:MET:HE3	2.46	0.49
1:A:148:GLU:O	1:A:166:GLU:HG3	2.12	0.49
1:C:317:THR:HG23	1:C:318:PRO:HD2	1.95	0.49
1:B:10:GLY:H	1:B:70:GLN:NE2	2.10	0.49
1:C:56:LYS:HG2	1:C:90:ASN:O	2.12	0.48
1:A:73:ASP:HA	4:C:427:HOH:O	2.13	0.48
1:B:299:ASN:O	1:B:300:ASP:HB2	2.12	0.48
1:B:63:ASN:HD22	1:B:64:VAL:N	2.11	0.48
1:A:312:PRO:HD2	1:A:324:MET:O	2.14	0.48
1:B:383:ASN:HD22	1:B:385:ASP:N	2.10	0.48
1:A:383:ASN:HD22	1:A:385:ASP:N	2.12	0.48
1:B:112:VAL:HG11	1:B:289:VAL:HG13	1.95	0.48
1:A:10:GLY:H	1:A:70:GLN:NE2	2.12	0.48
1:A:71:GLN:NE2	1:C:145:ARG:HD2	2.29	0.47
1:C:10:GLY:H	1:C:70:GLN:NE2	2.12	0.47
1:B:63:ASN:HD22	1:B:63:ASN:C	2.17	0.47
1:B:317:THR:HG23	1:B:318:PRO:HD2	1.97	0.47
1:C:43:GLU:HB3	1:C:63:ASN:HD21	1.80	0.47
1:B:296:ASN:C	1:B:296:ASN:HD22	2.18	0.47
1:A:150:GLY:O	1:A:167:THR:HG23	2.15	0.47
1:B:169:ASN:ND2	1:B:249:GLY:H	2.03	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:213:TRP:H	1:C:236:THR:HG22	1.80	0.46
1:A:63:ASN:HD22	1:A:64:VAL:N	2.13	0.46
1:B:43:GLU:HB3	1:B:63:ASN:HD21	1.80	0.46
1:B:317:THR:HG22	1:B:319:ILE:H	1.80	0.46
1:C:383:ASN:HD22	1:C:385:ASP:N	2.13	0.46
1:B:341:ASN:ND2	4:B:517:HOH:O	2.49	0.46
1:C:169:ASN:ND2	1:C:249:GLY:H	2.07	0.46
1:C:136:PHE:CE2	1:C:179:MET:HE3	2.51	0.46
1:A:296:ASN:HD22	1:A:296:ASN:C	2.20	0.45
1:B:231:VAL:HB	1:B:273:LEU:HB3	1.98	0.45
1:A:145:ARG:HD2	1:B:71:GLN:NE2	2.31	0.45
1:A:91:LEU:HD12	1:A:100:ILE:HD11	1.98	0.45
1:A:56:LYS:HG2	1:A:90:ASN:O	2.17	0.45
1:A:63:ASN:HD22	1:A:63:ASN:C	2.19	0.45
1:B:145:ARG:HD2	1:C:71:GLN:NE2	2.32	0.45
1:A:353:ALA:HB1	1:C:51:TRP:CG	2.53	0.44
1:B:112:VAL:HG11	1:B:289:VAL:CG1	2.47	0.44
1:A:95:LEU:HD22	1:A:132:ILE:HG23	1.99	0.44
1:A:394:VAL:HG13	1:A:398:PHE:CB	2.48	0.44
1:C:129:LEU:HG	1:C:132:ILE:HD11	1.98	0.44
1:A:169:ASN:ND2	1:A:249:GLY:H	2.05	0.44
1:C:296:ASN:C	1:C:296:ASN:HD22	2.22	0.44
1:A:317:THR:HG23	1:A:318:PRO:HD2	2.00	0.44
1:C:112:VAL:HG11	1:C:289:VAL:HG13	2.00	0.43
1:B:312:PRO:HD2	1:B:324:MET:O	2.18	0.43
1:B:129:LEU:HG	1:B:132:ILE:HD11	2.01	0.43
1:A:317:THR:HG22	1:A:319:ILE:H	1.84	0.43
1:C:63:ASN:HD22	1:C:64:VAL:N	2.16	0.43
4:A:551:HOH:O	2:D:2:FRU:O6	2.21	0.43
1:A:198:LEU:HD21	1:A:204:LEU:CD2	2.48	0.43
1:B:95:LEU:HD22	1:B:132:ILE:HG23	2.01	0.43
1:B:56:LYS:HG2	1:B:90:ASN:O	2.18	0.42
1:A:213:TRP:H	1:A:236:THR:HG22	1.84	0.42
1:C:198:LEU:HD21	1:C:204:LEU:CD2	2.49	0.42
1:A:257:GLU:O	1:A:258:LYS:HB2	2.20	0.41
1:A:394:VAL:HG13	1:A:398:PHE:HB2	2.02	0.41
1:B:394:VAL:HG13	1:B:398:PHE:CB	2.50	0.41
1:C:93:GLU:H	1:C:93:GLU:HG3	1.71	0.41
1:C:209:SER:HB2	1:C:237:ASP:HB3	2.03	0.41
1:C:312:PRO:HD2	1:C:324:MET:O	2.20	0.41
1:A:209:SER:HB2	1:A:237:ASP:HB3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:150:GLY:HA3	1:B:254:PHE:CE2	2.55	0.41
1:B:213:TRP:H	1:B:236:THR:HG22	1.86	0.41
1:C:181:ILE:HD13	1:C:181:ILE:HA	1.95	0.41
1:A:145:ARG:HD2	1:B:71:GLN:HE21	1.86	0.40
1:C:394:VAL:HG13	1:C:398:PHE:CB	2.52	0.40
1:A:71:GLN:HE21	1:C:145:ARG:HD2	1.86	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	419/421 (100%)	406 (97%)	13 (3%)	0	100	100
1	B	419/421 (100%)	407 (97%)	12 (3%)	0	100	100
1	C	419/421 (100%)	406 (97%)	13 (3%)	0	100	100
All	All	1257/1263 (100%)	1219 (97%)	38 (3%)	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	340/340 (100%)	314 (92%)	26 (8%)	13	20

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	340/340 (100%)	314 (92%)	26 (8%)	13	20
1	C	340/340 (100%)	312 (92%)	28 (8%)	11	17
All	All	1020/1020 (100%)	940 (92%)	80 (8%)	12	19

All (80) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	34	LEU
1	A	55	ASP
1	A	63	ASN
1	A	89	LYS
1	A	134	VAL
1	A	167	THR
1	A	189	LEU
1	A	203	ARG
1	A	205	VAL
1	A	223	VAL
1	A	236	THR
1	A	265	ASN
1	A	273	LEU
1	A	289	VAL
1	A	296	ASN
1	A	300	ASP
1	A	307	THR
1	A	308	VAL
1	A	311	ARG
1	A	317	THR
1	A	341	ASN
1	A	347	LEU
1	A	371	LYS
1	A	383	ASN
1	A	409	ASP
1	A	417	MET
1	B	34	LEU
1	B	55	ASP
1	B	63	ASN
1	B	89	LYS
1	B	134	VAL
1	B	167	THR
1	B	189	LEU
1	B	203	ARG

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	B	205	VAL
1	B	223	VAL
1	B	236	THR
1	B	265	ASN
1	B	273	LEU
1	B	289	VAL
1	B	296	ASN
1	B	300	ASP
1	B	307	THR
1	B	308	VAL
1	B	311	ARG
1	B	317	THR
1	B	341	ASN
1	B	347	LEU
1	B	371	LYS
1	B	383	ASN
1	B	409	ASP
1	B	417	MET
1	C	34	LEU
1	C	39	GLU
1	C	55	ASP
1	C	63	ASN
1	C	89	LYS
1	C	104	LYS
1	C	134	VAL
1	C	167	THR
1	C	189	LEU
1	C	203	ARG
1	C	205	VAL
1	C	223	VAL
1	C	236	THR
1	C	265	ASN
1	C	273	LEU
1	C	289	VAL
1	C	296	ASN
1	C	300	ASP
1	C	307	THR
1	C	308	VAL
1	C	317	THR
1	C	341	ASN
1	C	347	LEU
1	C	371	LYS

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Mol	Chain	Res	Type
1	C	383	ASN
1	C	394	VAL
1	C	409	ASP
1	C	417	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (41) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	29	GLN
1	A	63	ASN
1	A	70	GLN
1	A	71	GLN
1	A	159	ASN
1	A	169	ASN
1	A	248	GLN
1	A	265	ASN
1	A	266	ASN
1	A	296	ASN
1	A	341	ASN
1	A	349	GLN
1	A	383	ASN
1	A	386	ASN
1	B	29	GLN
1	B	63	ASN
1	B	70	GLN
1	B	71	GLN
1	B	159	ASN
1	B	169	ASN
1	B	248	GLN
1	B	265	ASN
1	B	266	ASN
1	B	296	ASN
1	B	341	ASN
1	B	349	GLN
1	B	383	ASN
1	B	386	ASN
1	C	29	GLN
1	C	63	ASN
1	C	70	GLN
1	C	71	GLN
1	C	159	ASN
1	C	169	ASN

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Mol	Chain	Res	Type
1	C	248	GLN
1	C	265	ASN
1	C	296	ASN
1	C	341	ASN
1	C	349	GLN
1	C	383	ASN
1	C	386	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

6 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	D	1	2	11,11,12	0.83	0	15,15,17	1.27	1 (6%)
2	FRU	D	2	2	11,12,12	1.48	2 (18%)	10,18,18	0.64	0
2	GLC	E	1	2	11,11,12	0.96	0	15,15,17	1.23	1 (6%)
2	FRU	E	2	2	11,12,12	1.46	2 (18%)	10,18,18	0.66	0
2	GLC	F	1	2	11,11,12	0.85	0	15,15,17	1.34	1 (6%)
2	FRU	F	2	2	11,12,12	1.43	2 (18%)	10,18,18	0.59	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	D	1	2	-	0/2/19/22	0/1/1/1
2	FRU	D	2	2	-	0/5/24/24	0/1/1/1
2	GLC	E	1	2	-	0/2/19/22	0/1/1/1
2	FRU	E	2	2	-	0/5/24/24	0/1/1/1
2	GLC	F	1	2	-	0/2/19/22	0/1/1/1
2	FRU	F	2	2	-	0/5/24/24	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	2	FRU	O2-C2	3.26	1.46	1.40
2	E	2	FRU	O2-C2	3.22	1.46	1.40
2	F	2	FRU	O2-C2	3.04	1.46	1.40
2	F	2	FRU	O5-C2	2.69	1.47	1.43
2	D	2	FRU	O5-C2	2.69	1.47	1.43
2	E	2	FRU	O5-C2	2.67	1.47	1.43

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	1	GLC	C1-O5-C5	3.67	117.16	112.19
2	D	1	GLC	C1-O5-C5	3.39	116.78	112.19
2	E	1	GLC	C1-O5-C5	3.16	116.48	112.19

There are no chirality outliers.

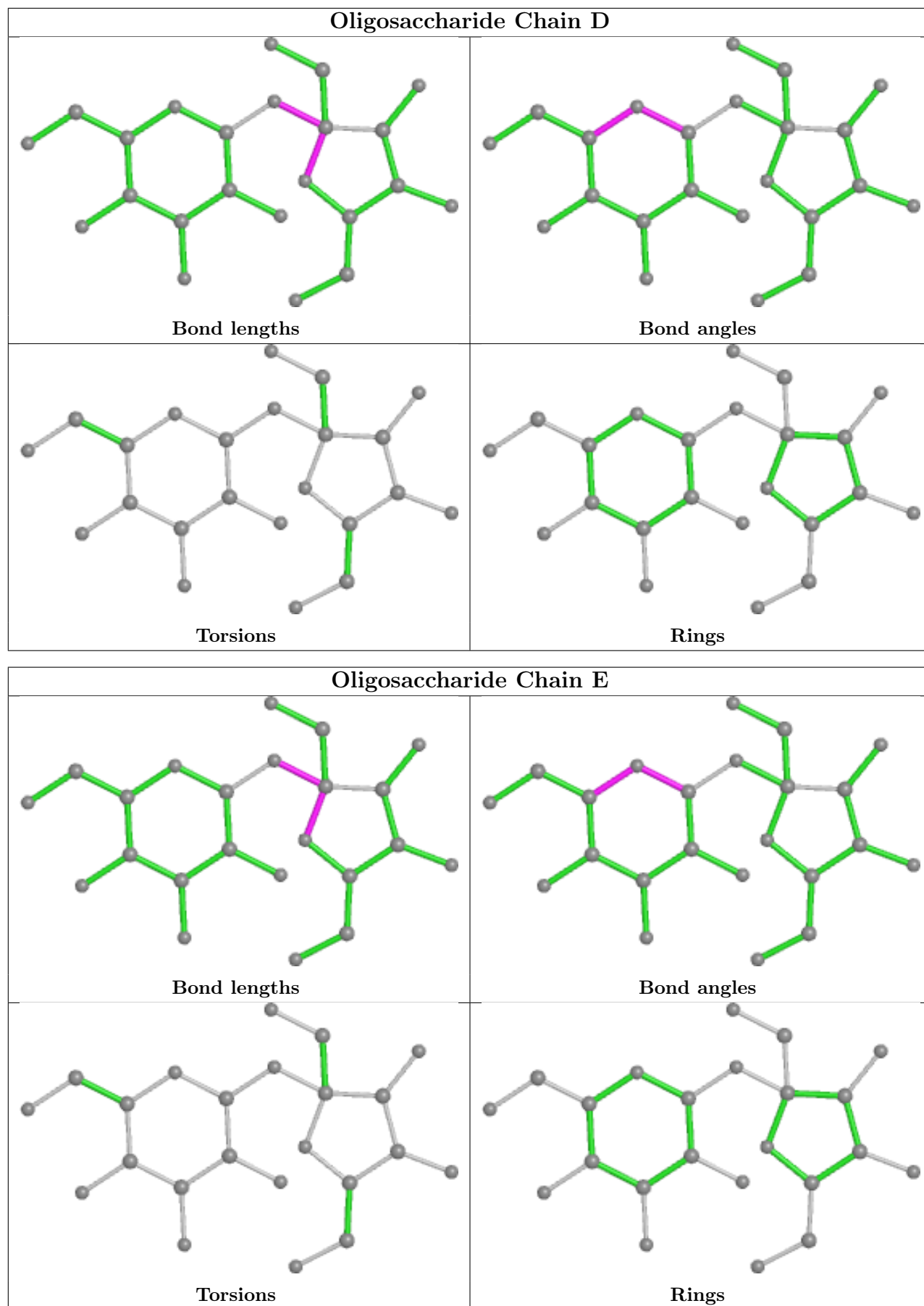
There are no torsion outliers.

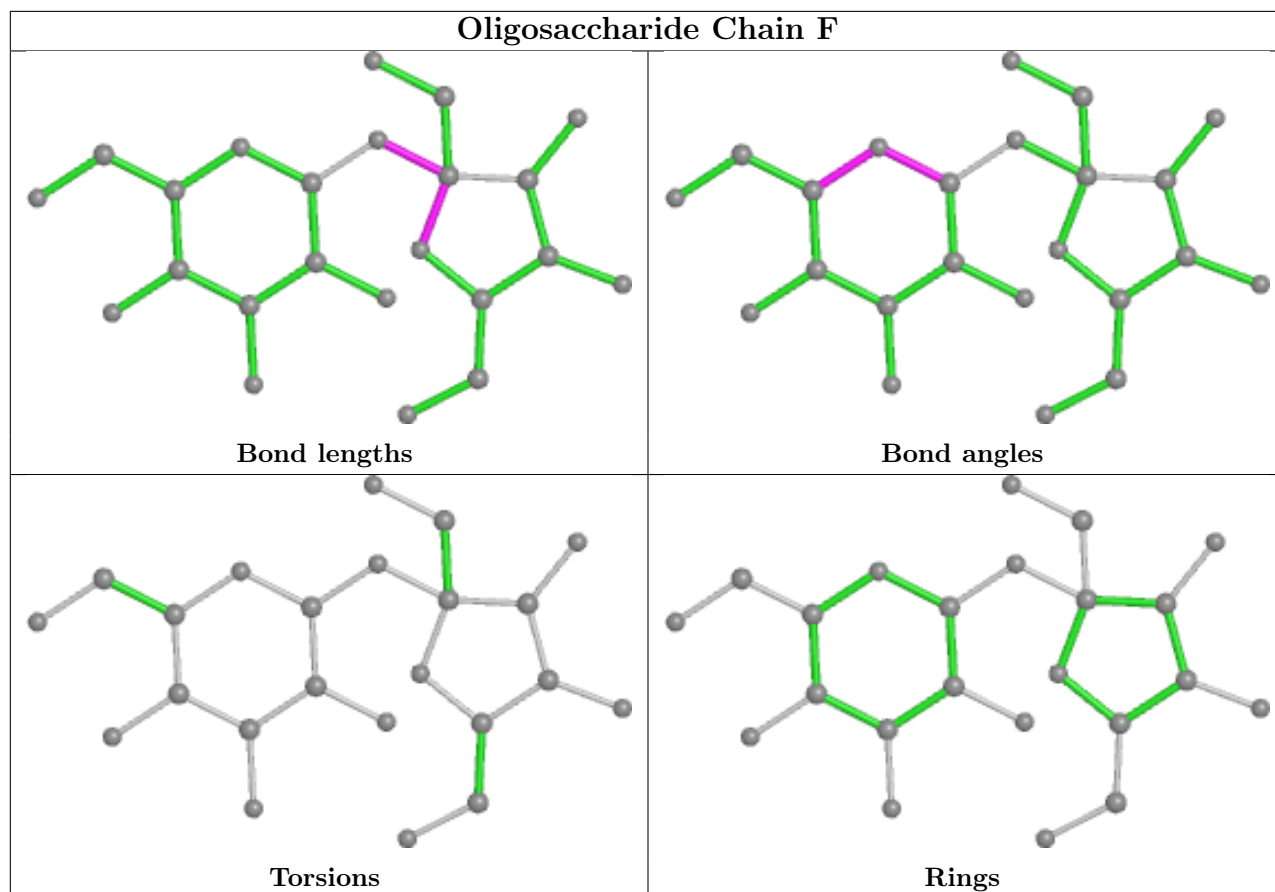
There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	2	FRU	1	0
2	D	2	FRU	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 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

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, 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	421/421 (100%)	-0.39	10 (2%) 59 57	22, 38, 66, 91	0
1	B	421/421 (100%)	-0.29	14 (3%) 46 45	23, 38, 67, 91	0
1	C	421/421 (100%)	-0.38	13 (3%) 49 47	23, 38, 66, 91	0
All	All	1263/1263 (100%)	-0.35	37 (2%) 51 50	22, 38, 67, 91	0

All (37) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	94	TRP	5.3
1	B	385	ASP	4.5
1	B	386	ASN	3.7
1	C	158	ASN	3.6
1	B	180	GLU	3.4
1	A	94	TRP	3.3
1	A	256	ASN	3.3
1	B	94	TRP	3.3
1	B	158	ASN	3.1
1	B	256	ASN	3.0
1	B	183	PRO	2.9
1	A	93	GLU	2.9
1	C	183	PRO	2.7
1	B	159	ASN	2.7
1	A	201	ASN	2.7
1	B	306	TRP	2.7
1	A	280	MET	2.6
1	C	280	MET	2.6
1	B	155	PHE	2.5
1	C	400	GLY	2.5
1	B	201	ASN	2.5
1	A	184	GLY	2.4
1	C	316	TRP	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	180	GLU	2.3
1	A	386	ASN	2.3
1	B	93	GLU	2.3
1	C	93	GLU	2.3
1	A	402	SER	2.3
1	B	184	GLY	2.2
1	A	155	PHE	2.2
1	B	400	GLY	2.2
1	C	402	SER	2.2
1	C	282	ASP	2.2
1	C	201	ASN	2.2
1	A	400	GLY	2.1
1	C	155	PHE	2.1
1	C	181	ILE	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](#)

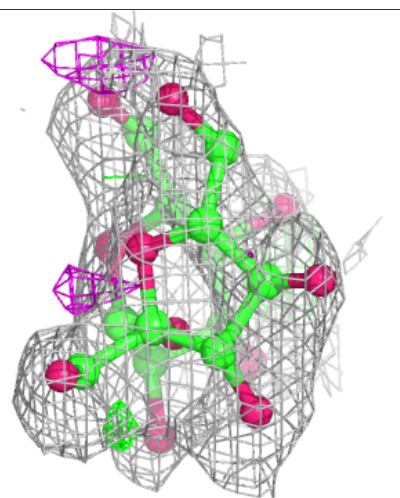
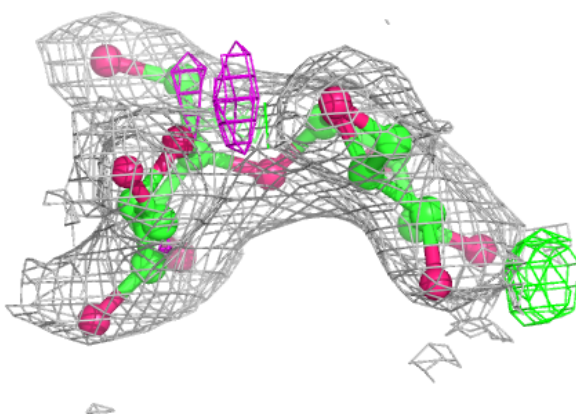
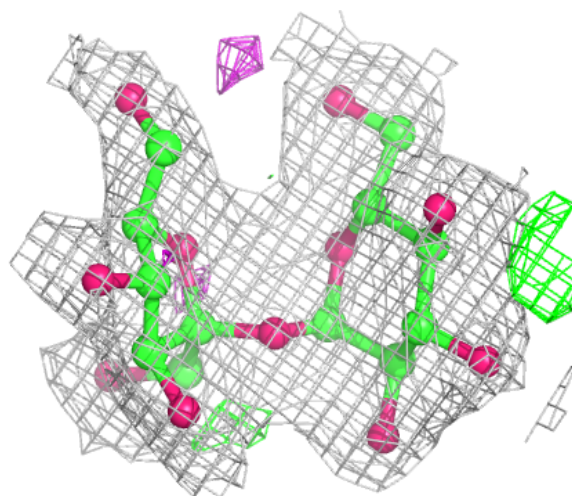
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 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
2	FRU	E	2	12/12	0.87	0.21	52,55,59,60	0
2	FRU	F	2	12/12	0.87	0.22	52,55,60,61	0
2	FRU	D	2	12/12	0.91	0.19	53,55,60,60	0
2	GLC	D	1	11/12	0.92	0.16	38,53,56,58	0
2	GLC	F	1	11/12	0.94	0.13	38,52,57,57	0
2	GLC	E	1	11/12	0.94	0.11	35,52,56,58	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.

**Electron density around Chain D:**

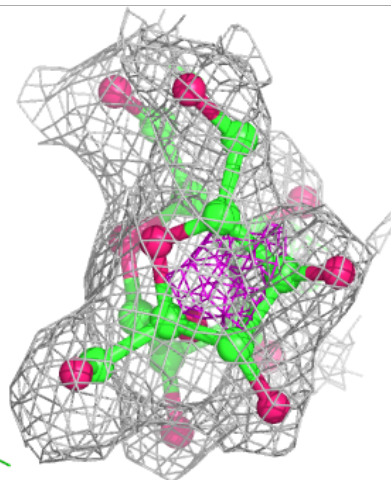
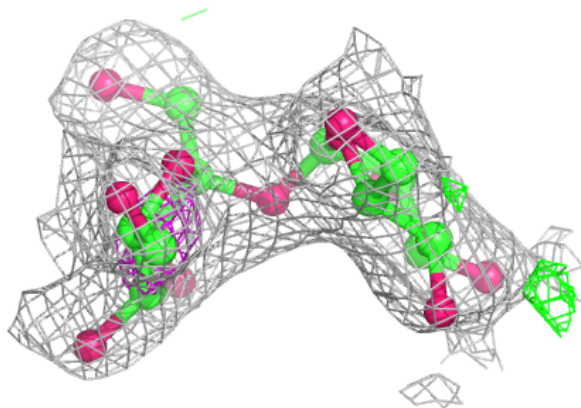
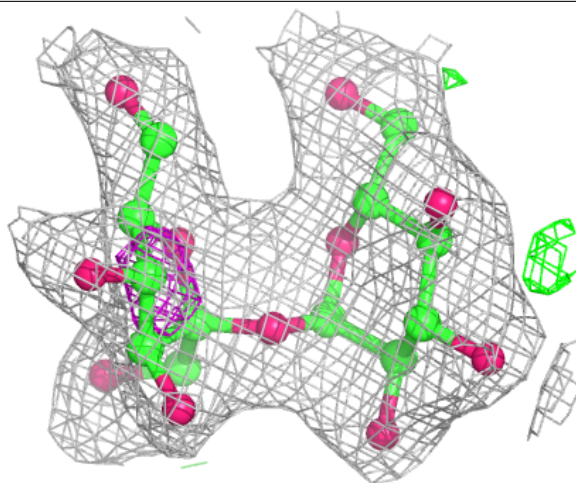
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

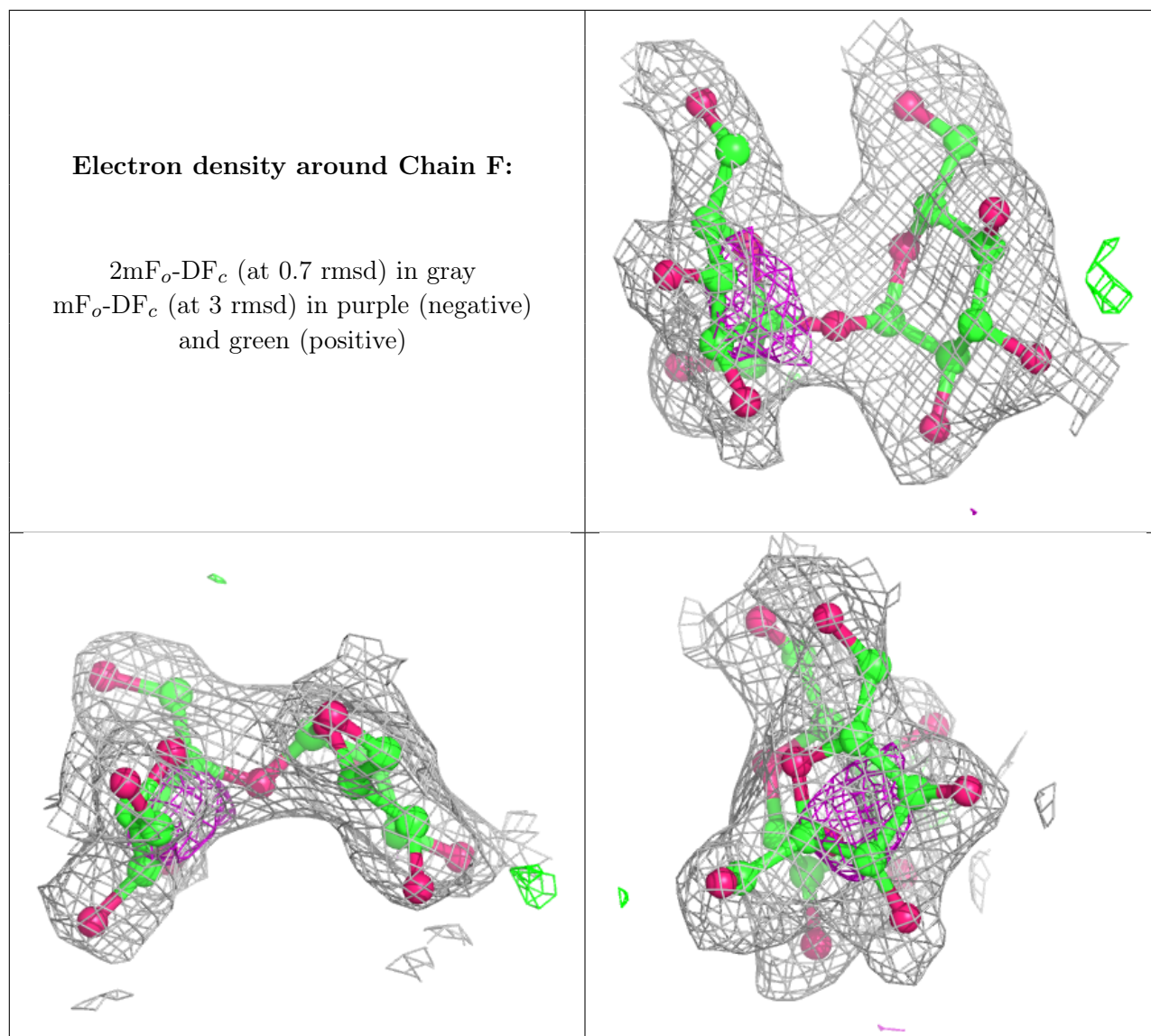




**Electron density around Chain E:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





## 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, 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	MG	A	424	1/1	0.24	0.83	93,93,93,93	0
3	MG	B	424	1/1	0.53	0.80	97,97,97,97	0
3	MG	C	424	1/1	0.56	0.53	96,96,96,96	0
3	MG	A	425	1/1	0.72	0.22	56,56,56,56	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.