



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2022 – 06:11 PM JST

PDB ID : 7FIR
Title : The crystal structure of beta-1,2-mannobiose phosphorylase in complex with 1,4-mannobiose
Authors : Dai, L.; Chang, Z.; Yang, J.; Liu, W.; Yang, Y.; Chen, C.-C.; Zhang, L.; Huang, J.; Sun, Y.; Guo, R.-T.
Deposited on : 2021-08-01
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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

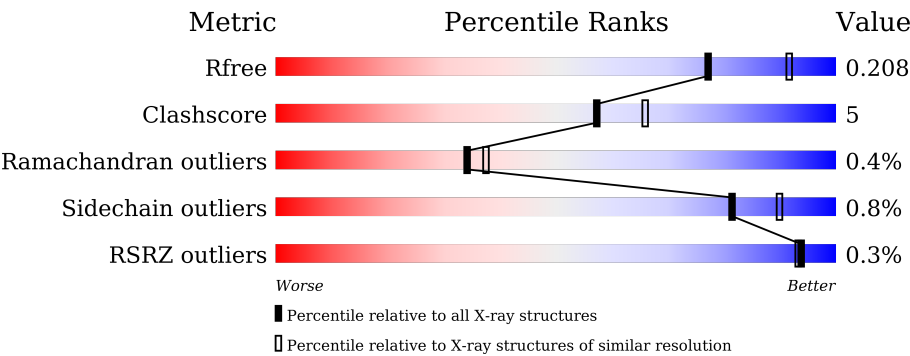
MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.27
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.27

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 2.20 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 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	313	<div><div></div><div></div><div></div><div></div><div></div></div> <div>85%12%.</div>
1	B	313	<div><div></div><div></div><div></div><div></div><div></div></div> <div>83%13%.</div>
1	C	313	<div><div></div><div></div><div></div><div></div><div></div></div> <div>86%10%..</div>
1	D	313	<div><div></div><div></div><div></div><div></div><div></div></div> <div>%84%12%.<div></div></div>
2	F	2	<div><div></div></div> <div>100%</div>
2	G	2	<div><div></div><div></div></div> <div>50%50%</div>

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Mol	Chain	Length	Quality of chain
2	H	2	 50%50%
2	I	2	 50%50%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 11348 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 Beta-1,2-mannobiose phosphorylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	302	Total	C	N	O	S	0	0	0
			2485	1615	415	447	8			
1	B	302	Total	C	N	O	S	0	0	0
			2485	1615	415	447	8			
1	C	304	Total	C	N	O	S	0	0	0
			2493	1619	417	449	8			
1	D	301	Total	C	N	O	S	0	0	0
			2477	1610	414	446	7			

There are 44 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-10	GLY	-	expression tag	UNP B0K2C3
A	-9	ALA	-	expression tag	UNP B0K2C3
A	-8	GLY	-	expression tag	UNP B0K2C3
A	-7	ALA	-	expression tag	UNP B0K2C3
A	-6	GLY	-	expression tag	UNP B0K2C3
A	-5	ALA	-	expression tag	UNP B0K2C3
A	-4	GLY	-	expression tag	UNP B0K2C3
A	-3	ALA	-	expression tag	UNP B0K2C3
A	-2	GLY	-	expression tag	UNP B0K2C3
A	-1	ALA	-	expression tag	UNP B0K2C3
A	0	GLY	-	expression tag	UNP B0K2C3
B	-10	GLY	-	expression tag	UNP B0K2C3
B	-9	ALA	-	expression tag	UNP B0K2C3
B	-8	GLY	-	expression tag	UNP B0K2C3
B	-7	ALA	-	expression tag	UNP B0K2C3
B	-6	GLY	-	expression tag	UNP B0K2C3
B	-5	ALA	-	expression tag	UNP B0K2C3
B	-4	GLY	-	expression tag	UNP B0K2C3
B	-3	ALA	-	expression tag	UNP B0K2C3
B	-2	GLY	-	expression tag	UNP B0K2C3
B	-1	ALA	-	expression tag	UNP B0K2C3

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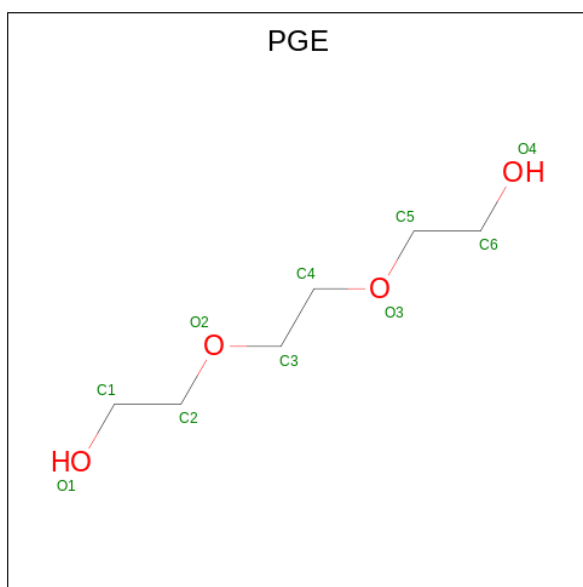
Chain	Residue	Modelled	Actual	Comment	Reference
B	0	GLY	-	expression tag	UNP B0K2C3
C	-10	GLY	-	expression tag	UNP B0K2C3
C	-9	ALA	-	expression tag	UNP B0K2C3
C	-8	GLY	-	expression tag	UNP B0K2C3
C	-7	ALA	-	expression tag	UNP B0K2C3
C	-6	GLY	-	expression tag	UNP B0K2C3
C	-5	ALA	-	expression tag	UNP B0K2C3
C	-4	GLY	-	expression tag	UNP B0K2C3
C	-3	ALA	-	expression tag	UNP B0K2C3
C	-2	GLY	-	expression tag	UNP B0K2C3
C	-1	ALA	-	expression tag	UNP B0K2C3
C	0	GLY	-	expression tag	UNP B0K2C3
D	-10	GLY	-	expression tag	UNP B0K2C3
D	-9	ALA	-	expression tag	UNP B0K2C3
D	-8	GLY	-	expression tag	UNP B0K2C3
D	-7	ALA	-	expression tag	UNP B0K2C3
D	-6	GLY	-	expression tag	UNP B0K2C3
D	-5	ALA	-	expression tag	UNP B0K2C3
D	-4	GLY	-	expression tag	UNP B0K2C3
D	-3	ALA	-	expression tag	UNP B0K2C3
D	-2	GLY	-	expression tag	UNP B0K2C3
D	-1	ALA	-	expression tag	UNP B0K2C3
D	0	GLY	-	expression tag	UNP B0K2C3

- Molecule 2 is an oligosaccharide called alpha-L-gulopyranose-(1-4)-alpha-L-allopyranose.



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
2	F	2	Total	C	O	0	0	0
			23	12	11			
2	G	2	Total	C	O	0	0	0
			23	12	11			
2	H	2	Total	C	O	0	0	0
			23	12	11			
2	I	2	Total	C	O	0	0	0
			23	12	11			

- Molecule 3 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: C₆H₁₄O₄).

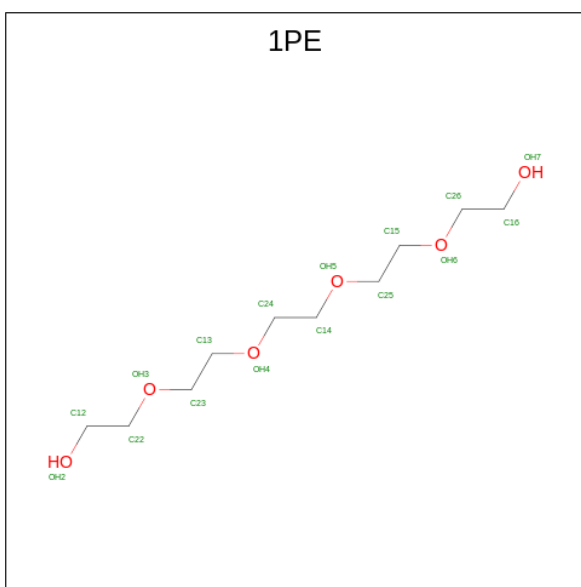


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			10	6	4		

- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	6	Total	Zn	0	0
			6	6		
4	B	4	Total	Zn	0	0
			4	4		
4	C	4	Total	Zn	0	0
			4	4		
4	D	3	Total	Zn	0	0
			3	3		

- Molecule 5 is PENTAETHYLENE GLYCOL (three-letter code: 1PE) (formula: C₁₀H₂₂O₆).

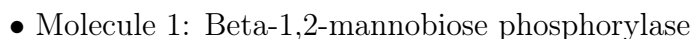
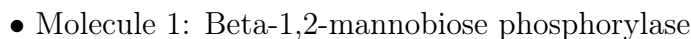


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	C	1	Total	C	O	0	0
			16	10	6		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	363	Total O 363 363	0	0
6	B	323	Total O 323 323	0	0
6	C	314	Total O 314 314	0	0
6	D	273	Total O 273 273	0	0

- Molecule 1: Beta-1,2-mannobiose phosphorylase





- Molecule 2: alpha-L-gulopyranose-(1-4)-alpha-L-allopyranose

Chain F: 100%



- Molecule 2: alpha-L-gulopyranose-(1-4)-alpha-L-allopyranose

Chain G: 50% 50%



- Molecule 2: alpha-L-gulopyranose-(1-4)-alpha-L-allopyranose

Chain H: 50% 50%



- Molecule 2: alpha-L-gulopyranose-(1-4)-alpha-L-allopyranose

Chain I: 50% 50%



4 Data and refinement statistics

Property	Value	Source
Space group	I 4	Depositor
Cell constants a, b, c, α , β , γ	205.30Å 205.30Å 78.65Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	36.29 – 2.20 36.29 – 2.20	Depositor EDS
% Data completeness (in resolution range)	98.8 (36.29-2.20) 87.2 (36.29-2.20)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.49 (at 2.20Å)	Xtriage
Refinement program	PHENIX 1.17.1	Depositor
R, R_{free}	0.170 , 0.206 0.170 , 0.208	Depositor DCC
R_{free} test set	2000 reflections (2.44%)	wwPDB-VP
Wilson B-factor (Å ²)	20.9	Xtriage
Anisotropy	0.263	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 45.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.012 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	11348	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.49% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 1PE, GUP, PGE, Z2D, ZN

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	1/2556 (0.0%)	0.59	0/3465
1	B	0.42	0/2556	0.57	0/3465
1	C	0.45	2/2564 (0.1%)	0.60	0/3475
1	D	0.41	1/2548 (0.0%)	0.55	0/3455
All	All	0.44	4/10224 (0.0%)	0.58	0/13860

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	270	CYS	CB-SG	-6.68	1.70	1.82
1	A	270	CYS	CB-SG	-6.37	1.71	1.82
1	C	270	CYS	CB-SG	-6.04	1.72	1.82
1	C	231	VAL	CB-CG2	-6.02	1.40	1.52

There are no bond angle outliers.

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	2485	0	2452	23	0
1	B	2485	0	2452	25	0
1	C	2493	0	2456	29	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	2477	0	2440	23	0
2	F	23	0	10	0	0
2	G	23	0	10	1	0
2	H	23	0	10	2	0
2	I	23	0	10	1	0
3	A	10	0	14	0	0
4	A	6	0	0	0	0
4	B	4	0	0	0	0
4	C	4	0	0	0	0
4	D	3	0	0	0	0
5	C	16	0	22	1	0
6	A	363	0	0	3	1
6	B	323	0	0	3	0
6	C	314	0	0	6	0
6	D	273	0	0	3	0
All	All	11348	0	9876	98	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 5.

All (98) 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:C:189:MET:SD	6:C:898:HOH:O	2.38	0.81
1:A:278:MET:HE3	1:A:294:VAL:HB	1.62	0.81
1:B:3:ARG:NH1	6:B:501:HOH:O	2.15	0.79
1:A:216:LEU:HD13	1:A:234:LEU:HD11	1.74	0.69
1:C:59:LYS:HE3	1:C:60:TYR:CE2	2.31	0.64
1:C:247:LYS:NZ	6:C:603:HOH:O	2.29	0.64
1:A:207:PRO:HG3	1:A:216:LEU:HD12	1.81	0.63
1:D:34:GLU:OE1	1:D:108:TYR:OH	2.09	0.62
1:A:278:MET:HE3	1:A:294:VAL:CB	2.32	0.59
1:C:83:PRO:O	5:C:501:1PE:H121	2.04	0.57
1:A:1:MET:HE1	1:A:247:LYS:HB3	1.88	0.56
1:C:231:VAL:HG23	1:C:250:ILE:HG21	1.88	0.56
1:C:119:ASP:HB3	6:C:683:HOH:O	2.05	0.56
1:C:231:VAL:CG2	1:C:250:ILE:HD13	2.35	0.56
1:D:99:PRO:O	1:D:270:CYS:HB3	2.06	0.55
1:C:59:LYS:HE3	1:C:60:TYR:CZ	2.41	0.55
1:D:61:LYS:HA	1:D:94:TRP:CH2	2.42	0.54
1:D:12:ILE:HG13	1:D:13:LEU:HD12	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:2:PHE:CZ	1:D:231:VAL:HG11	2.43	0.53
1:D:3:ARG:O	1:D:295:ILE:HD13	2.09	0.53
1:A:36:ASN:ND2	6:A:602:HOH:O	2.22	0.53
1:A:121:LEU:HB2	1:C:59:LYS:HE2	1.90	0.52
1:D:2:PHE:N	6:D:507:HOH:O	2.43	0.52
1:D:3:ARG:O	1:D:295:ILE:CD1	2.58	0.52
1:A:1:MET:HE3	6:A:846:HOH:O	2.09	0.52
1:D:216:LEU:HD22	1:D:234:LEU:HD21	1.93	0.51
1:C:176:SER:HB2	1:C:182:TRP:CE3	2.47	0.50
1:A:1:MET:HE2	1:A:248:GLU:H	1.76	0.50
1:A:1:MET:CE	1:A:248:GLU:H	2.25	0.49
1:C:148:LYS:HZ1	2:H:2:GUP:H5	1.76	0.49
1:C:27:PHE:CD2	1:C:287:ASP:HA	2.47	0.49
1:C:23:LYS:NZ	6:C:611:HOH:O	2.45	0.49
1:B:35:GLY:N	6:B:511:HOH:O	2.46	0.49
1:C:61:LYS:HA	1:C:94:TRP:CH2	2.48	0.49
1:C:124:ARG:NE	6:C:602:HOH:O	2.27	0.48
1:D:148:LYS:HZ1	2:I:2:GUP:H5	1.78	0.48
1:A:248:GLU:OE1	6:A:601:HOH:O	2.20	0.48
1:B:91:GLN:HG2	1:B:124:ARG:CZ	2.44	0.48
1:A:31:VAL:HG13	1:A:273:VAL:HG13	1.96	0.48
1:A:176:SER:HB2	1:A:182:TRP:CE3	2.49	0.48
1:C:7:LEU:HB2	1:C:292:VAL:HG13	1.95	0.48
1:A:1:MET:HE2	1:A:246:GLN:HG3	1.96	0.47
1:B:61:LYS:HA	1:B:94:TRP:CH2	2.49	0.47
1:B:25:ALA:HB2	1:B:262:LEU:HD12	1.97	0.47
1:D:289:HIS:HE1	6:D:741:HOH:O	1.98	0.47
1:A:66:ILE:HG12	1:A:96:VAL:HG23	1.96	0.47
1:C:8:SER:OG	1:C:10:LYS:O	2.32	0.47
1:C:231:VAL:CG2	1:C:250:ILE:HG21	2.44	0.46
1:D:11:PRO:HB3	1:D:289:HIS:HB3	1.97	0.46
1:D:32:ILE:HD11	1:D:133:LEU:HD11	1.96	0.46
1:C:231:VAL:HG22	1:C:250:ILE:HD13	1.97	0.46
1:C:37:LYS:HE3	1:C:39:HIS:NE2	2.31	0.46
1:B:7:LEU:HB2	1:B:292:VAL:HG13	1.97	0.46
1:A:11:PRO:HB3	1:A:289:HIS:HB3	1.98	0.46
1:B:216:LEU:HD13	1:B:234:LEU:HD11	1.98	0.45
1:C:156:LYS:HE2	1:C:161:TYR:CZ	2.51	0.45
1:D:15:PRO:HG3	1:D:25:ALA:HA	1.98	0.45
1:D:73:ASP:O	6:D:501:HOH:O	2.20	0.45
1:D:150:ALA:HA	1:D:164:PHE:O	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:61:LYS:HA	1:A:94:TRP:CH2	2.52	0.45
1:C:33:TYR:HB2	1:C:273:VAL:HG21	1.98	0.45
1:A:101:ILE:HD11	1:A:110:MET:CE	2.47	0.45
1:B:148:LYS:NZ	2:G:2:GUP:H5	2.31	0.45
1:B:278:MET:HG2	1:B:296:GLU:HA	1.97	0.45
1:B:91:GLN:HG2	1:B:124:ARG:NH1	2.33	0.44
1:D:167:ARG:HB2	1:D:172:TRP:NE1	2.33	0.44
1:A:99:PRO:O	1:A:270:CYS:HB3	2.18	0.44
1:C:148:LYS:NZ	2:H:2:GUP:H5	2.32	0.44
1:C:214:TRP:HB2	1:C:234:LEU:HB2	1.99	0.44
1:D:214:TRP:HB2	1:D:234:LEU:HB2	1.98	0.44
1:C:37:LYS:HE3	1:C:39:HIS:CE1	2.53	0.44
1:B:2:PHE:CZ	1:B:231:VAL:HG11	2.52	0.43
1:B:224:ASN:OD1	1:C:168:MET:HG2	2.18	0.43
1:B:176:SER:HB2	1:B:182:TRP:CE3	2.53	0.43
1:C:11:PRO:HB3	1:C:289:HIS:HB3	2.01	0.43
1:A:129:TRP:CH2	1:A:137:LYS:HE3	2.54	0.43
1:B:150:ALA:HA	1:B:164:PHE:O	2.18	0.43
1:B:40:LEU:HD13	1:B:77:PHE:CE2	2.54	0.42
1:B:168:MET:HA	1:B:169:PRO:HA	1.89	0.42
1:B:6:ARG:HD3	1:B:255:LEU:HD11	2.01	0.42
1:B:61:LYS:HG3	1:B:94:TRP:CE2	2.55	0.42
1:B:127:MET:O	1:B:139:HIS:HA	2.20	0.42
1:D:30:ALA:HB2	1:D:99:PRO:O	2.20	0.42
1:A:2:PHE:CZ	1:A:231:VAL:HG11	2.56	0.41
1:A:27:PHE:CD2	1:A:287:ASP:HA	2.55	0.41
1:D:7:LEU:HD13	1:D:75:ILE:HD11	2.01	0.41
1:B:248:GLU:OE2	6:B:502:HOH:O	2.22	0.41
1:B:11:PRO:HB3	1:B:289:HIS:HB3	2.01	0.41
1:C:215:LEU:HD12	1:C:215:LEU:HA	1.94	0.41
1:D:13:LEU:HB2	1:D:290:ILE:HB	2.03	0.41
1:B:91:GLN:O	1:B:124:ARG:NH1	2.47	0.41
1:B:241:LYS:HB2	1:B:241:LYS:HE3	1.93	0.40
1:D:101:ILE:HA	1:D:109:TYR:O	2.21	0.40
1:A:25:ALA:HB2	1:A:262:LEU:HD12	2.03	0.40
1:B:156:LYS:HE3	1:B:161:TYR:CZ	2.56	0.40
1:D:82:LYS:HA	1:D:82:LYS:HD2	1.91	0.40
1:B:221:VAL:HA	1:B:226:VAL:O	2.21	0.40
1:C:17:LYS:HE3	6:C:741:HOH:O	2.21	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)
6:A:701:HOH:O	6:A:868:HOH:O[6_554]	2.19	0.01

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	300/313 (96%)	290 (97%)	9 (3%)	1 (0%)	41	46
1	B	300/313 (96%)	290 (97%)	8 (3%)	2 (1%)	22	22
1	C	302/313 (96%)	289 (96%)	13 (4%)	0	100	100
1	D	299/313 (96%)	286 (96%)	11 (4%)	2 (1%)	22	22
All	All	1201/1252 (96%)	1155 (96%)	41 (3%)	5 (0%)	34	37

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	204	ALA
1	B	28	ASN
1	D	28	ASN
1	B	204	ALA
1	D	204	ALA

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	267/267 (100%)	264 (99%)	3 (1%)	73	85

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	267/267 (100%)	265 (99%)	2 (1%)	84	91
1	C	267/267 (100%)	265 (99%)	2 (1%)	84	91
1	D	266/267 (100%)	264 (99%)	2 (1%)	81	90
All	All	1067/1068 (100%)	1058 (99%)	9 (1%)	81	90

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

Mol	Chain	Res	Type
1	A	124	ARG
1	A	241	LYS
1	A	301	LYS
1	B	1	MET
1	B	277	ASP
1	C	59	LYS
1	C	124	ARG
1	D	10	LYS
1	D	27	PHE

Sometimes 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 ⓘ

8 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	Z2D	F	1	2	12,12,12	0.83	0	17,17,17	1.70	3 (17%)
2	GUP	F	2	2	11,11,12	1.43	2 (18%)	15,15,17	1.77	4 (26%)
2	Z2D	G	1	2	12,12,12	0.95	0	17,17,17	1.70	3 (17%)
2	GUP	G	2	2	11,11,12	1.41	1 (9%)	15,15,17	1.75	3 (20%)
2	Z2D	H	1	2	12,12,12	0.97	1 (8%)	17,17,17	1.59	4 (23%)
2	GUP	H	2	2	11,11,12	1.53	2 (18%)	15,15,17	1.60	3 (20%)
2	Z2D	I	1	2	12,12,12	0.92	0	17,17,17	1.35	3 (17%)
2	GUP	I	2	2	11,11,12	1.60	2 (18%)	15,15,17	1.61	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	Z2D	F	1	2	-	2/2/22/22	0/1/1/1
2	GUP	F	2	2	-	2/2/19/22	0/1/1/1
2	Z2D	G	1	2	-	2/2/22/22	0/1/1/1
2	GUP	G	2	2	-	2/2/19/22	0/1/1/1
2	Z2D	H	1	2	-	2/2/22/22	0/1/1/1
2	GUP	H	2	2	-	2/2/19/22	0/1/1/1
2	Z2D	I	1	2	-	2/2/22/22	0/1/1/1
2	GUP	I	2	2	-	2/2/19/22	0/1/1/1

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	I	2	GUP	C2-C3	-3.44	1.47	1.52
2	H	2	GUP	C2-C3	-3.22	1.47	1.52
2	G	2	GUP	C2-C3	-2.94	1.48	1.52
2	F	2	GUP	C2-C3	-2.81	1.48	1.52
2	I	2	GUP	C4-C3	-2.33	1.46	1.52
2	H	2	GUP	C4-C3	-2.23	1.46	1.52
2	H	1	Z2D	C3-C2	-2.14	1.46	1.52
2	F	2	GUP	O5-C1	2.11	1.47	1.43

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	1	Z2D	O4-C4-C3	4.27	120.23	110.35
2	F	1	Z2D	O4-C4-C3	4.22	120.11	110.35
2	G	2	GUP	O6-C6-C5	-4.00	97.58	111.29
2	F	2	GUP	C1-O5-C5	3.77	117.30	112.19
2	F	2	GUP	O6-C6-C5	-3.66	98.73	111.29
2	G	1	Z2D	O3-C3-C4	3.66	118.80	110.35
2	I	1	Z2D	O4-C4-C3	3.55	118.55	110.35
2	H	2	GUP	O6-C6-C5	-3.52	99.21	111.29
2	G	2	GUP	C1-O5-C5	3.42	116.83	112.19
2	F	1	Z2D	O3-C3-C4	3.40	118.22	110.35
2	H	1	Z2D	O4-C4-C3	3.33	118.06	110.35
2	I	2	GUP	O6-C6-C5	-3.17	100.42	111.29
2	H	2	GUP	C1-O5-C5	2.92	116.15	112.19
2	I	1	Z2D	O3-C3-C4	2.70	116.58	110.35
2	I	2	GUP	C1-O5-C5	2.57	115.67	112.19
2	G	1	Z2D	O3-C3-C2	-2.50	104.58	110.35
2	H	1	Z2D	O3-C3-C4	2.48	116.08	110.35
2	I	2	GUP	O5-C5-C4	2.44	116.77	110.83
2	G	2	GUP	O5-C5-C4	2.42	116.71	110.83
2	F	1	Z2D	C3-C4-C5	2.39	114.50	110.24
2	H	1	Z2D	O2-C2-C3	-2.31	105.02	110.35
2	I	2	GUP	O5-C1-C2	2.27	114.28	110.77
2	H	1	Z2D	O3-C3-C2	-2.25	105.15	110.35
2	F	2	GUP	O5-C5-C4	2.19	116.15	110.83
2	H	2	GUP	O5-C5-C6	2.19	110.63	107.20
2	F	2	GUP	O5-C5-C6	2.11	110.51	107.20
2	I	1	Z2D	O4-C4-C5	2.01	114.30	109.30

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	G	2	GUP	O5-C5-C6-O6
2	F	2	GUP	O5-C5-C6-O6
2	I	1	Z2D	O5-C5-C6-O6
2	G	1	Z2D	O5-C5-C6-O6
2	F	1	Z2D	O5-C5-C6-O6
2	H	1	Z2D	O5-C5-C6-O6
2	F	1	Z2D	C4-C5-C6-O6
2	G	1	Z2D	C4-C5-C6-O6
2	H	2	GUP	O5-C5-C6-O6
2	I	2	GUP	O5-C5-C6-O6
2	H	2	GUP	C4-C5-C6-O6

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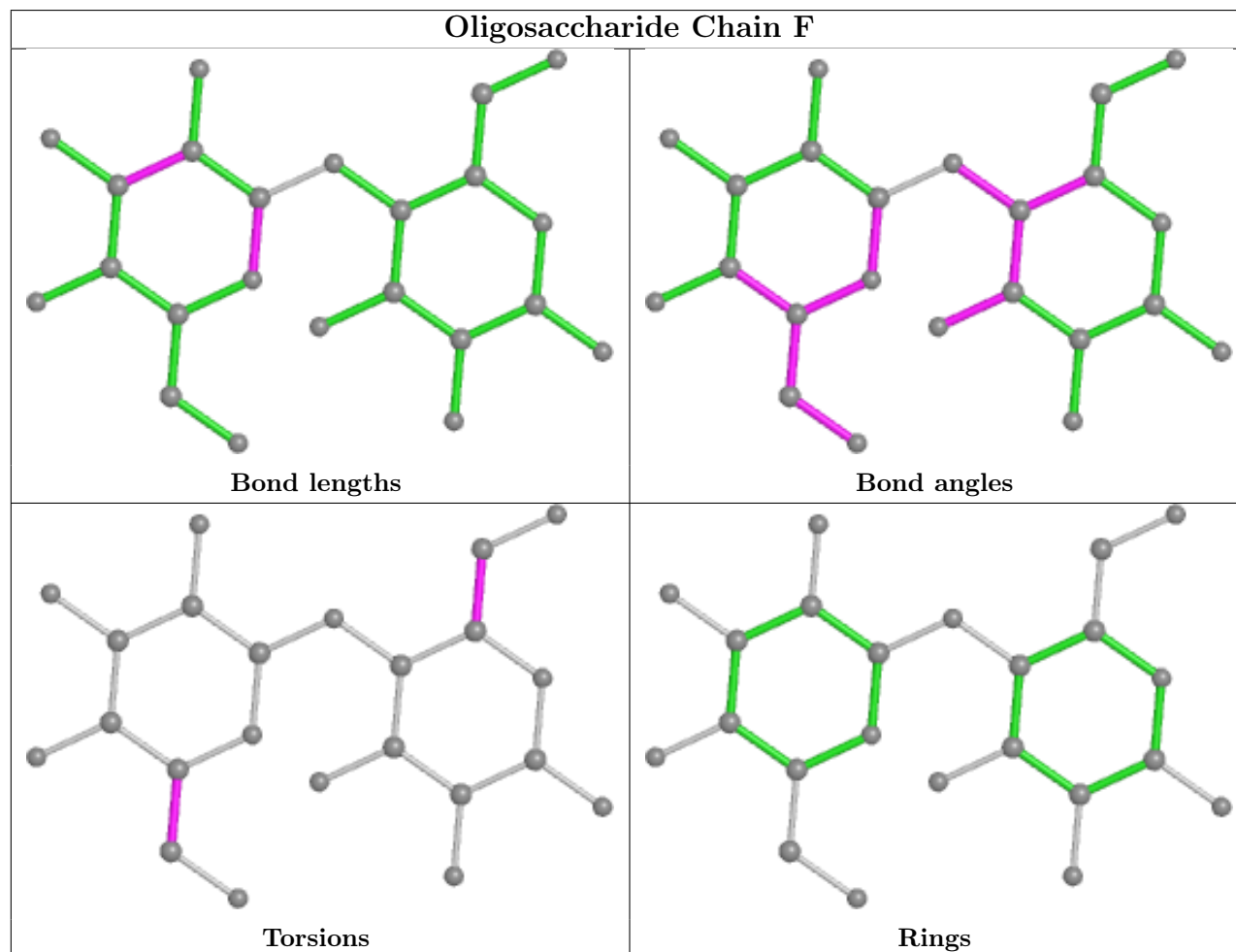
Mol	Chain	Res	Type	Atoms
2	G	2	GUP	C4-C5-C6-O6
2	I	1	Z2D	C4-C5-C6-O6
2	I	2	GUP	C4-C5-C6-O6
2	F	2	GUP	C4-C5-C6-O6
2	H	1	Z2D	C4-C5-C6-O6

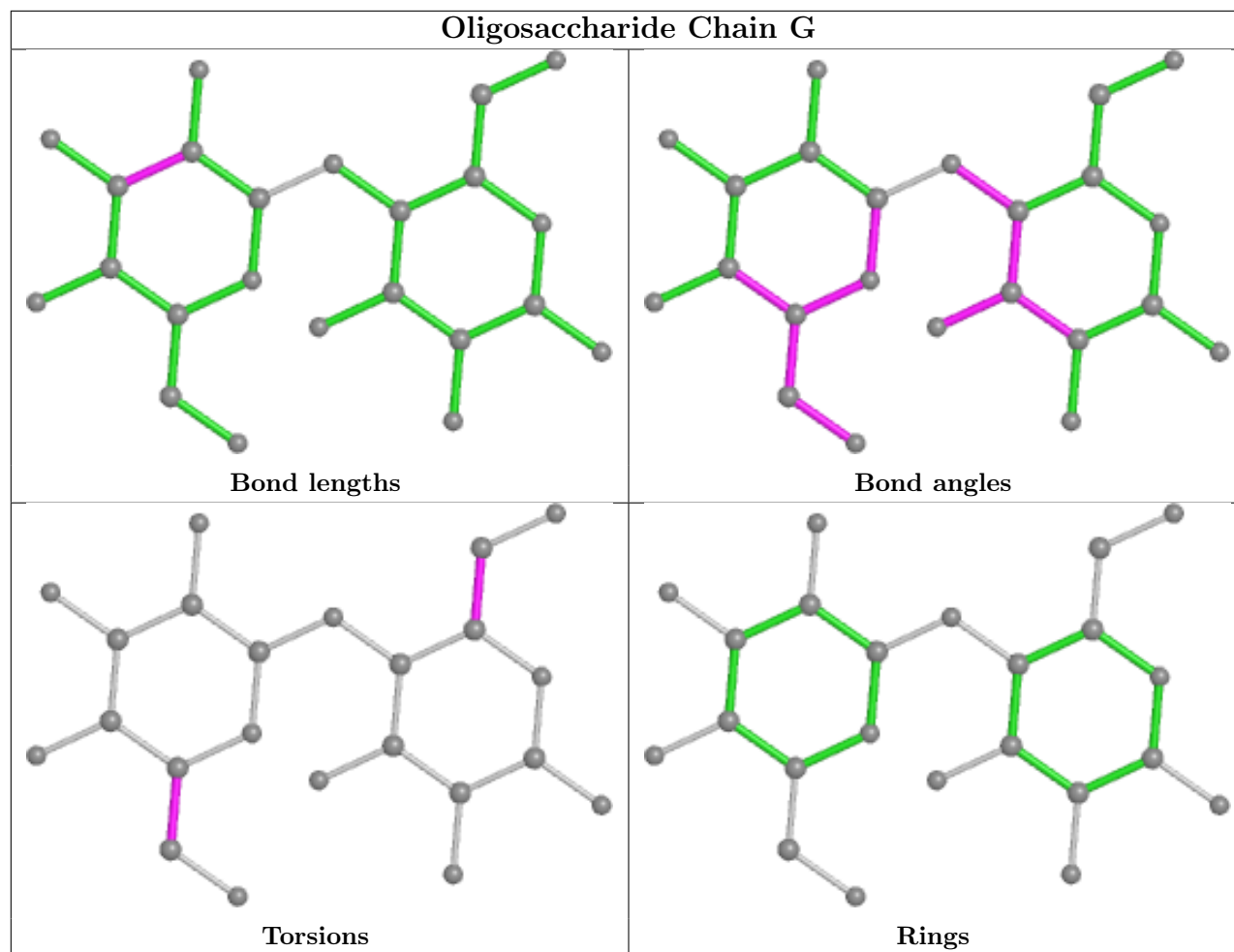
There are no ring outliers.

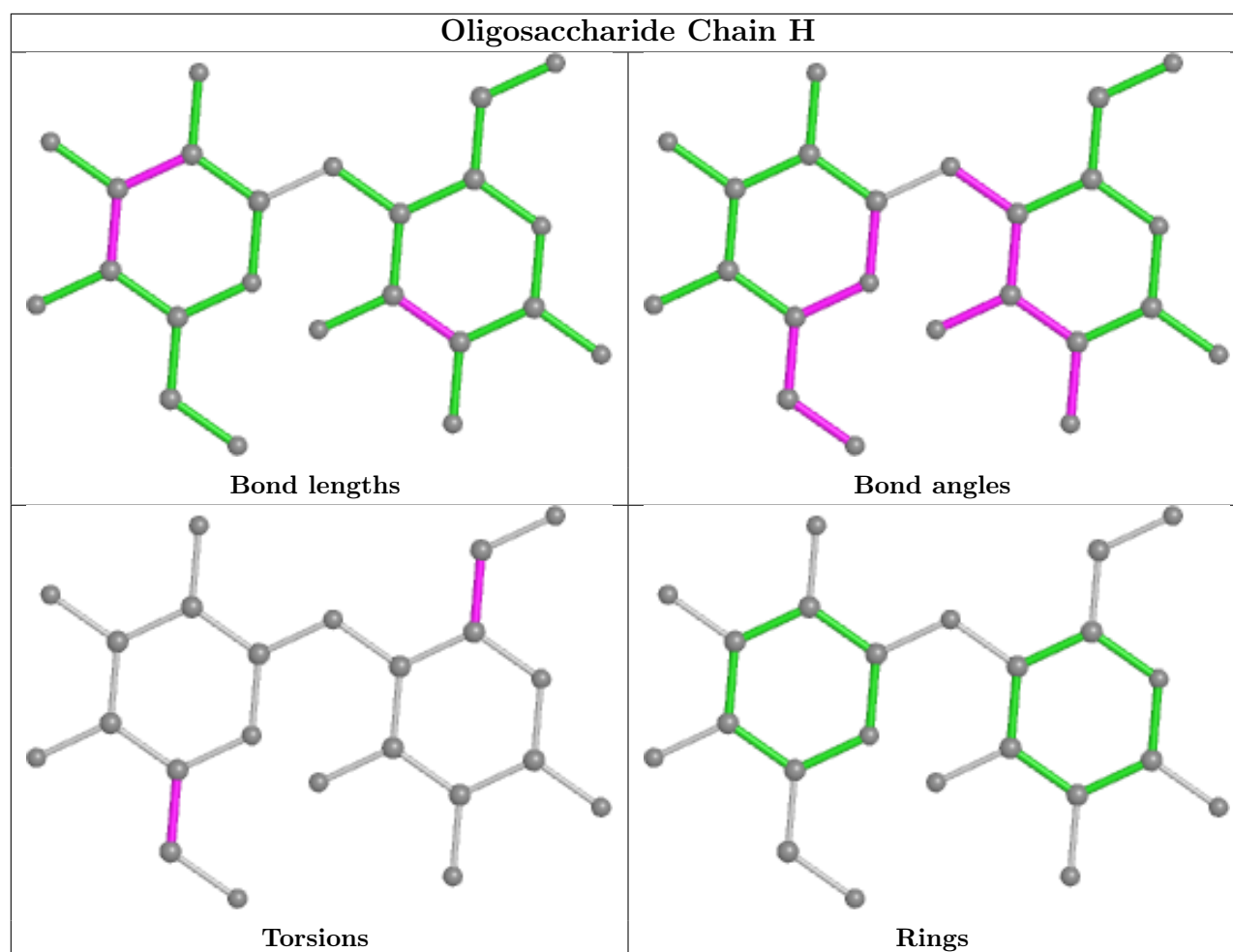
3 monomers are involved in 4 short contacts:

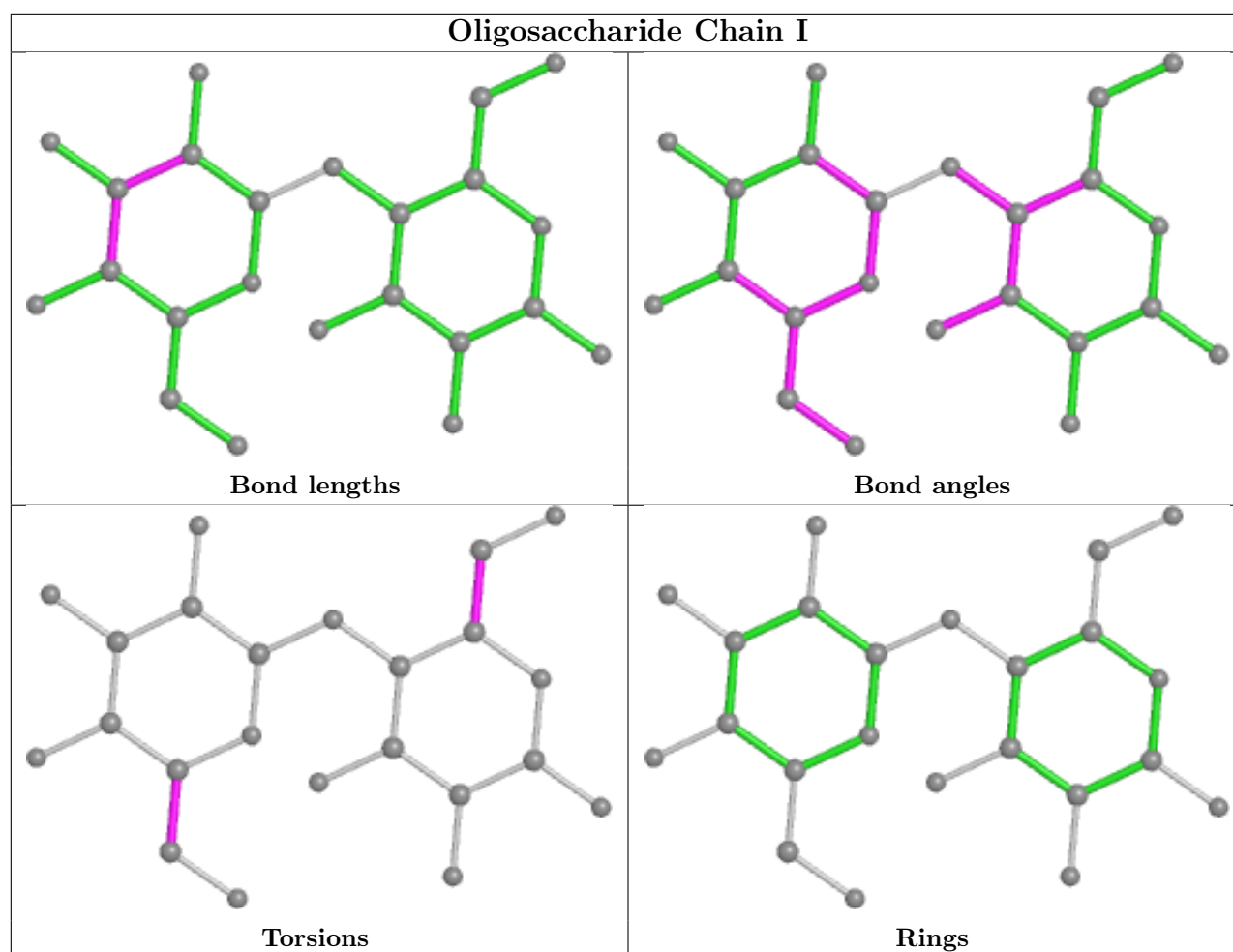
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	I	2	GUP	1	0
2	G	2	GUP	1	0
2	H	2	GUP	2	0

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 19 ligands modelled in this entry, 17 are monoatomic - leaving 2 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	PGE	A	501	-	9,9,9	0.54	0	8,8,8	0.34	0
5	1PE	C	501	-	15,15,15	0.49	0	14,14,14	0.40	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	PGE	A	501	-	-	4/7/7/7	-
5	1PE	C	501	-	-	7/13/13/13	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	501	PGE	O2-C3-C4-O3
5	C	501	1PE	OH5-C14-C24-OH4
5	C	501	1PE	OH4-C13-C23-OH3
5	C	501	1PE	C23-C13-OH4-C24
3	A	501	PGE	C4-C3-O2-C2
5	C	501	1PE	C12-C22-OH3-C23
3	A	501	PGE	O1-C1-C2-O2
5	C	501	1PE	C25-C15-OH6-C26
5	C	501	1PE	C13-C23-OH3-C22
3	A	501	PGE	C1-C2-O2-C3
5	C	501	1PE	C14-C24-OH4-C13

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	501	1PE	1	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	302/313 (96%)	-0.53	0 100 100	15, 20, 33, 48	0
1	B	302/313 (96%)	-0.58	1 (0%) 94 93	17, 24, 38, 58	0
1	C	304/313 (97%)	-0.36	1 (0%) 94 93	16, 23, 39, 72	0
1	D	301/313 (96%)	-0.25	2 (0%) 87 86	18, 29, 49, 61	0
All	All	1209/1252 (96%)	-0.43	4 (0%) 94 93	15, 24, 43, 72	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	-1	ALA	4.0
1	B	1	MET	2.8
1	D	270	CYS	2.5
1	D	36	ASN	2.2

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.

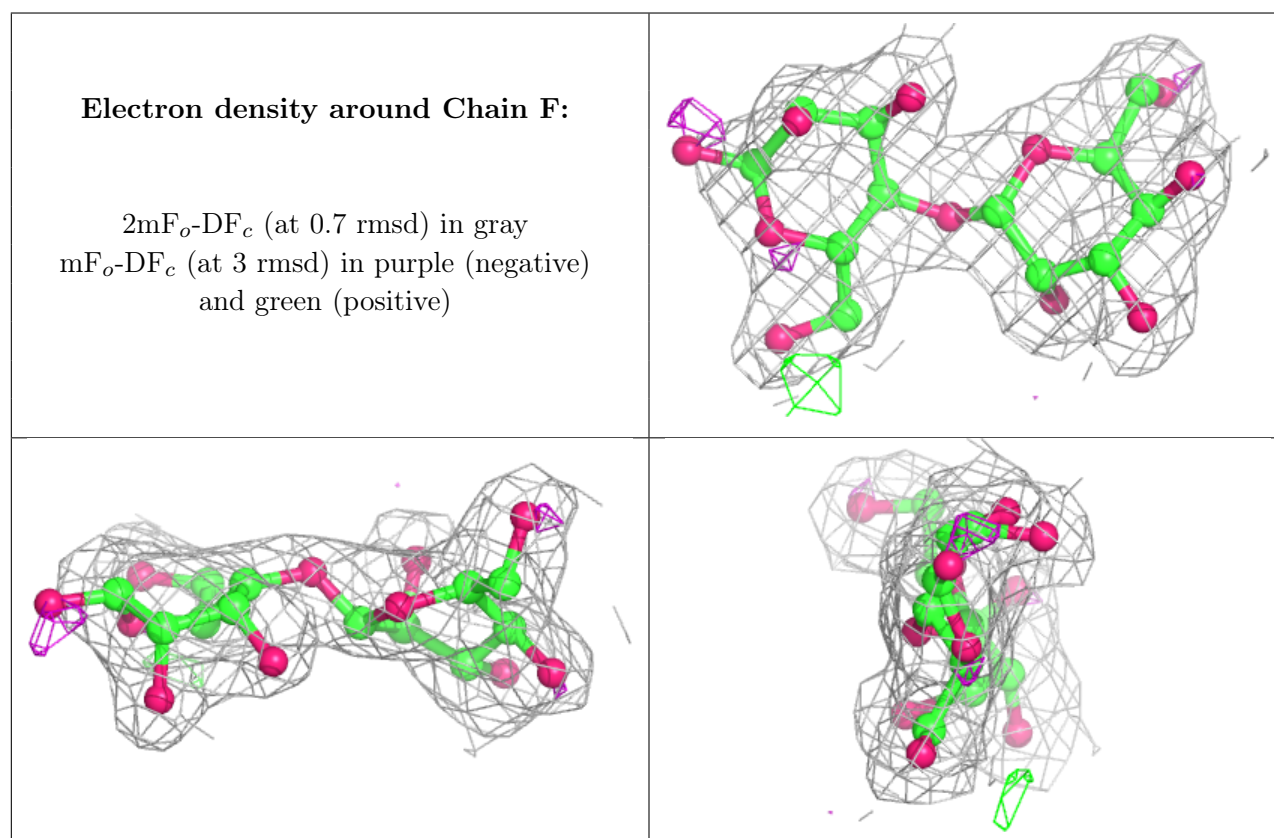
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	Z2D	G	1	12/12	0.83	0.23	35,43,48,62	0
2	Z2D	H	1	12/12	0.88	0.15	38,42,52,54	0
2	Z2D	I	1	12/12	0.88	0.15	39,44,52,62	0

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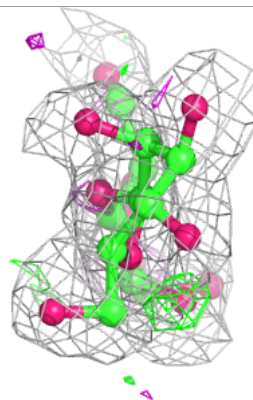
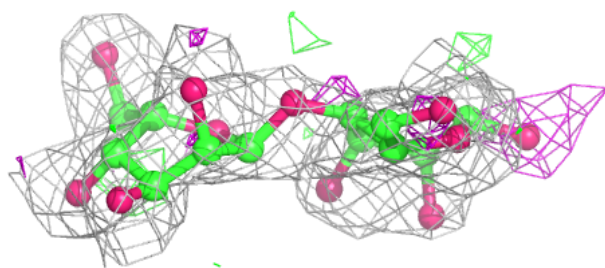
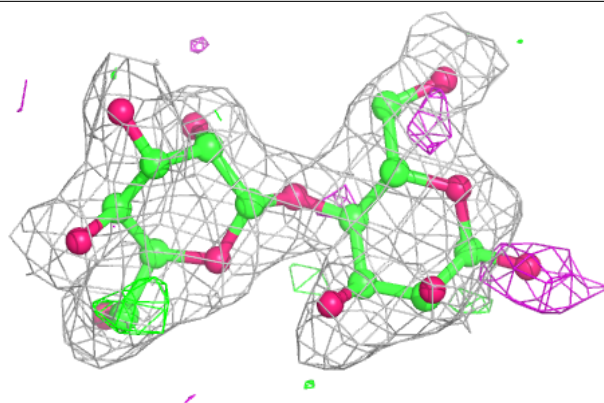
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	Z2D	F	1	12/12	0.91	0.14	31,36,40,56	0
2	GUP	G	2	11/12	0.91	0.12	21,30,35,38	0
2	GUP	H	2	11/12	0.93	0.12	21,27,32,35	0
2	GUP	I	2	11/12	0.93	0.12	25,30,35,36	0
2	GUP	F	2	11/12	0.94	0.10	19,24,27,29	0

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.

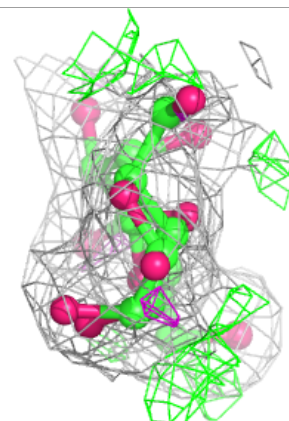
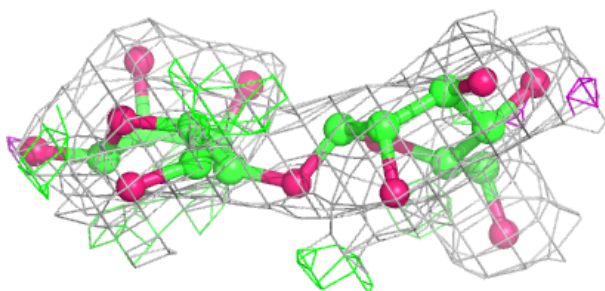
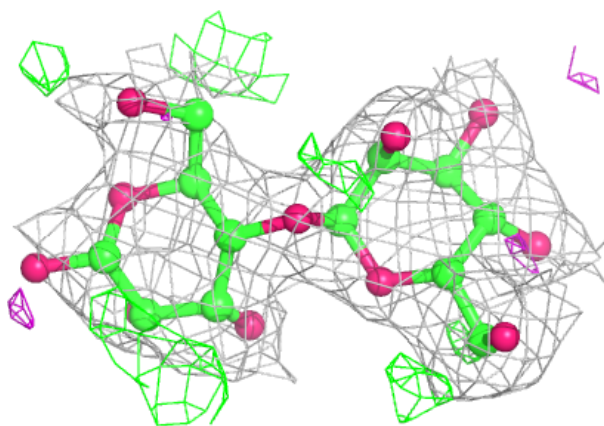


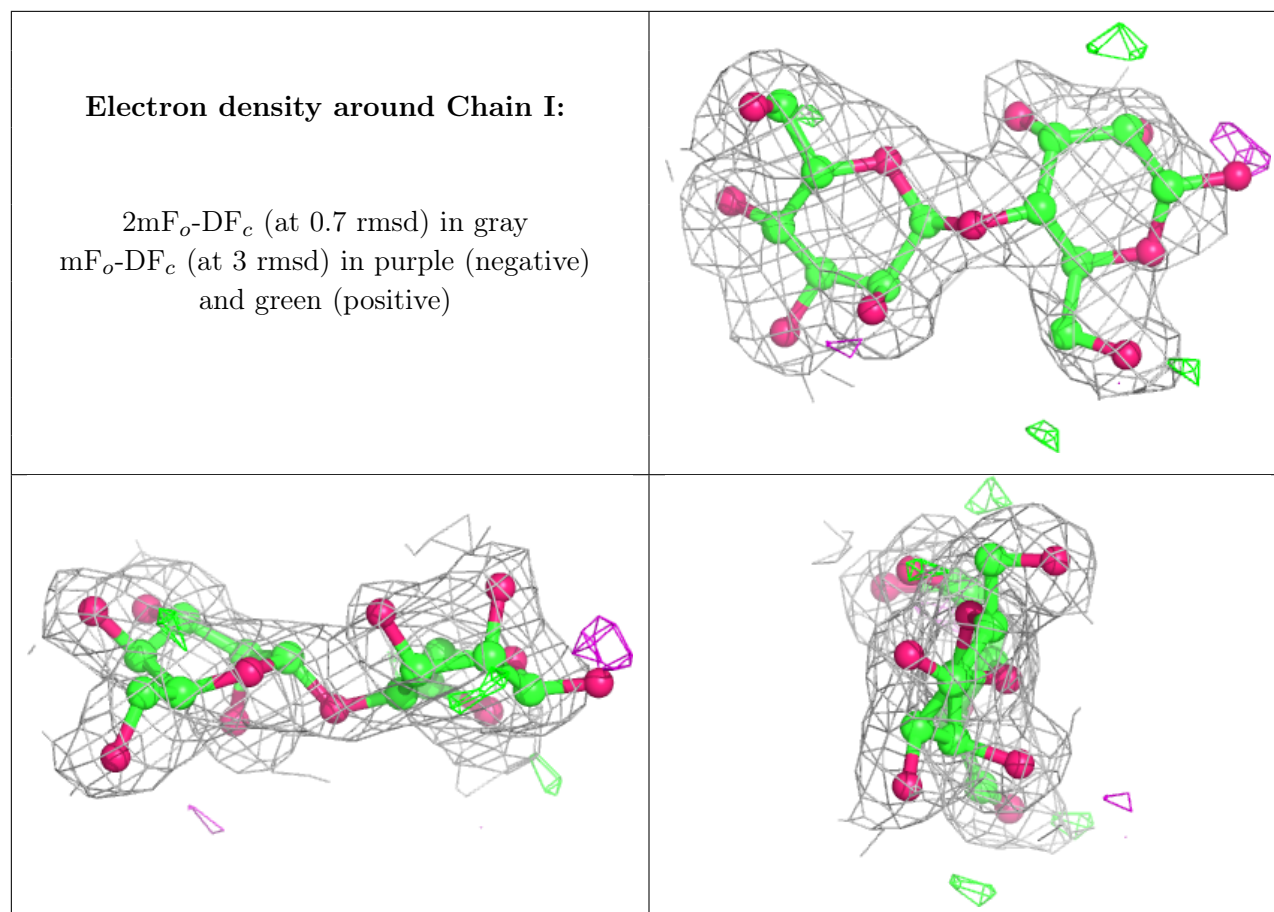
Electron density around Chain G:

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

**Electron density around Chain H:**

$2mF_o-DF_c$ (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, 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
4	ZN	A	506	1/1	0.85	0.20	83,83,83,83	0
4	ZN	D	401	1/1	0.85	0.09	73,73,73,73	0
4	ZN	B	404	1/1	0.87	0.06	66,66,66,66	0
3	PGE	A	501	10/10	0.88	0.14	22,32,44,49	0
5	1PE	C	501	16/16	0.89	0.18	28,38,44,46	0
4	ZN	C	505	1/1	0.91	0.04	72,72,72,72	0
4	ZN	B	401	1/1	0.92	0.05	39,39,39,39	0
4	ZN	C	504	1/1	0.93	0.05	61,61,61,61	0
4	ZN	D	403	1/1	0.97	0.06	44,44,44,44	0
4	ZN	A	507	1/1	0.99	0.04	31,31,31,31	0
4	ZN	A	503	1/1	0.99	0.07	23,23,23,23	0
4	ZN	B	402	1/1	0.99	0.02	33,33,33,33	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	ZN	A	502	1/1	0.99	0.02	33,33,33,33	0
4	ZN	C	502	1/1	0.99	0.09	24,24,24,24	0
4	ZN	A	504	1/1	1.00	0.02	30,30,30,30	0
4	ZN	A	505	1/1	1.00	0.03	25,25,25,25	0
4	ZN	D	402	1/1	1.00	0.08	28,28,28,28	0
4	ZN	C	503	1/1	1.00	0.05	25,25,25,25	0
4	ZN	B	403	1/1	1.00	0.06	24,24,24,24	0

6.5 Other polymers [i](#)

There are no such residues in this entry.