



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 18, 2024 – 12:17 PM JST

PDB ID : 5ZKW
Title : Crystal structure of DFA-IIIase from *Arthrobacter chlorophenicus* A6 in complex with GF2
Authors : Yu, S.H.; Shen, H.; Li, X.; Mu, W.M.
Deposited on : 2018-03-26
Resolution : 1.86 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:

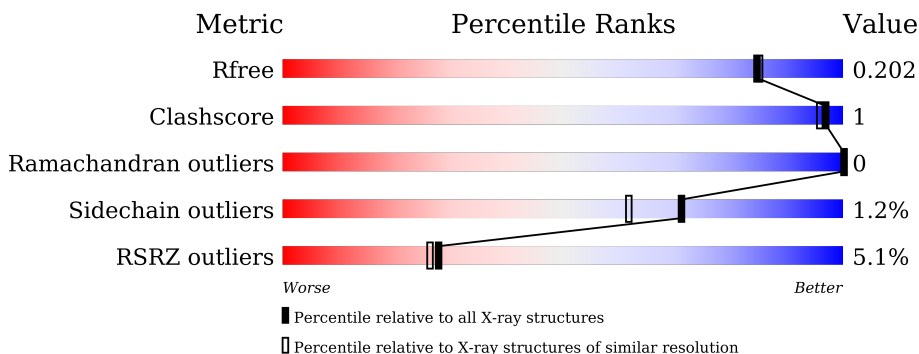
MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.36
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

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 1.86 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.






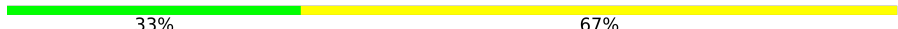
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2469 (1.86-1.86)
Clashscore	141614	2625 (1.86-1.86)
Ramachandran outliers	138981	2592 (1.86-1.86)
Sidechain outliers	138945	2592 (1.86-1.86)
RSRZ outliers	127900	2436 (1.86-1.86)

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	445	 3% 90% 6%
1	B	445	 2% 91% 5%
1	C	445	 6% 91% 7%
1	D	445	 4% 95%
1	E	445	 7% 95%
1	F	445	 8% 90% 6%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	G	3	 67% 33%
2	H	3	 67% 33%
2	I	3	 67% 33%
2	J	3	 33% 67%

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 20591 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 DFA-IIIase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	417	Total 3139	C 1956	N 563	O 614	S 6	0	0	0
1	B	422	Total 3163	C 1972	N 565	O 620	S 6	0	0	0
1	D	438	Total 3283	C 2041	N 585	O 650	S 7	0	0	0
1	C	412	Total 3107	C 1938	N 555	O 608	S 6	0	0	0
1	E	436	Total 3271	C 2035	N 583	O 646	S 7	0	0	0
1	F	420	Total 3157	C 1966	N 566	O 619	S 6	0	0	0

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



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
			Total	C	O			
2	G	3	Total 34	C 18	O 16	0	0	0
2	H	3	Total 34	C 18	O 16	0	0	0
2	I	3	Total 34	C 18	O 16	0	0	0
2	J	3	Total 34	C 18	O 16	0	0	0

- Molecule 3 is water.

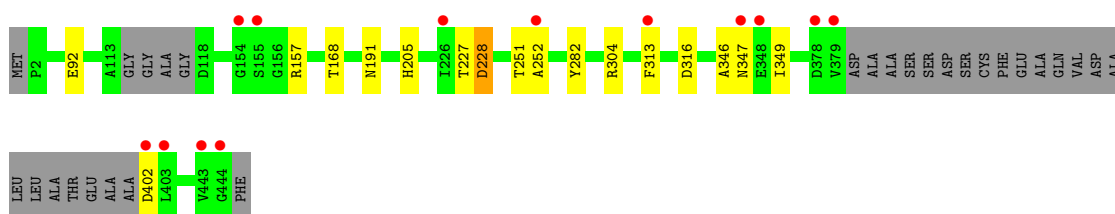
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	281	Total O 281 281	0	0
3	B	260	Total O 260 260	0	0
3	D	285	Total O 285 285	0	0
3	C	138	Total O 138 138	0	0
3	E	165	Total O 165 165	0	0
3	F	206	Total O 206 206	0	0

3 Residue-property plots

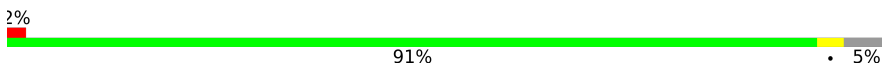
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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.

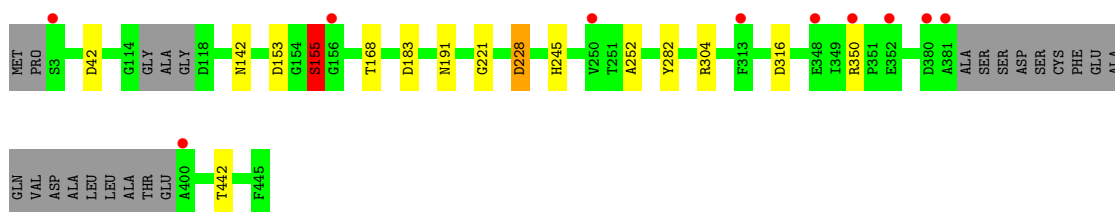
- Molecule 1: DFA-IIIase

Chain A: 



- Molecule 1: DFA-IIIase

Chain B: 

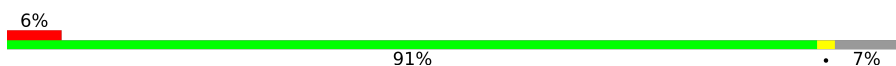


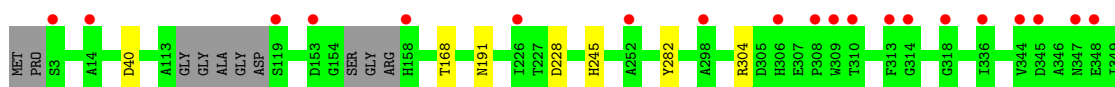
- Molecule 1: DFA-IIIase

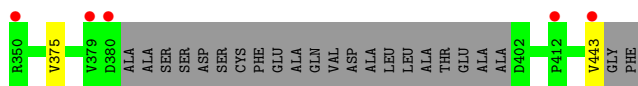
Chain D: 



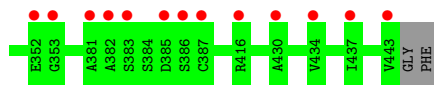
- Molecule 1: DFA-IIIase

Chain C: 

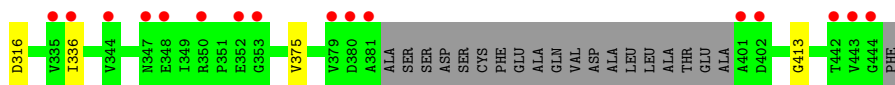
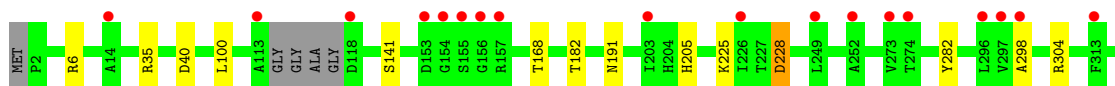
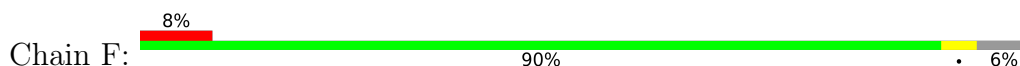




- Molecule 1: DFA-IIIase



- Molecule 1: DFA-IIIase



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



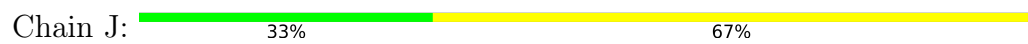
- Molecule 2: alpha-D-glucopyranose-(1-2)-beta-D-fructofuranose-(2-1)-beta-D-fructofuranos e



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



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



FRU1
FRU2
GLC3

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	116.12Å 79.23Å 140.57Å 90.00° 100.38° 90.00°	Depositor
Resolution (Å)	50.00 – 1.86 39.84 – 1.86	Depositor EDS
% Data completeness (in resolution range)	99.1 (50.00-1.86) 99.1 (39.84-1.86)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.75 (at 1.85Å)	Xtrriage
Refinement program	REFMAC 5.8.0189	Depositor
R, R_{free}	0.166 , 0.194 0.176 , 0.202	Depositor DCC
R_{free} test set	10583 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	24.8	Xtrriage
Anisotropy	0.147	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 41.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	20591	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.44% 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: GLC, FRU

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	0.42	0/3209	0.69	0/4373
1	B	0.45	0/3233	0.71	2/4407 (0.0%)
1	C	0.41	0/3175	0.65	0/4327
1	D	0.46	0/3354	0.75	4/4573 (0.1%)
1	E	0.40	0/3342	0.68	6/4557 (0.1%)
1	F	0.41	0/3227	0.69	2/4398 (0.0%)
All	All	0.43	0/19540	0.70	14/26635 (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	B	0	1

There are no bond length outliers.

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	180	ARG	NE-CZ-NH2	-8.73	115.94	120.30
1	D	180	ARG	NE-CZ-NH1	8.63	124.61	120.30
1	B	155	SER	C-N-CA	-8.48	104.50	122.30
1	D	35	ARG	NE-CZ-NH1	7.50	124.05	120.30
1	E	35	ARG	NE-CZ-NH1	7.47	124.03	120.30
1	D	35	ARG	NE-CZ-NH2	-7.40	116.60	120.30
1	E	180	ARG	NE-CZ-NH1	7.37	123.98	120.30
1	E	35	ARG	NE-CZ-NH2	-6.76	116.92	120.30
1	B	155	SER	N-CA-C	-6.74	92.79	111.00
1	E	180	ARG	NE-CZ-NH2	-6.12	117.24	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	35	ARG	NE-CZ-NH1	5.67	123.14	120.30
1	E	106	ARG	NE-CZ-NH1	5.15	122.87	120.30
1	E	6	ARG	NE-CZ-NH2	5.12	122.86	120.30
1	F	35	ARG	NE-CZ-NH2	-5.03	117.79	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	155	SER	Peptide

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	3139	0	3005	6	0
1	B	3163	0	3014	8	0
1	C	3107	0	2972	2	0
1	D	3283	0	3132	7	0
1	E	3271	0	3125	5	0
1	F	3157	0	3019	8	0
2	G	34	0	31	0	0
2	H	34	0	31	0	0
2	I	34	0	31	0	0
2	J	34	0	31	0	0
3	A	281	0	0	0	0
3	B	260	0	0	1	0
3	C	138	0	0	0	0
3	D	285	0	0	1	0
3	E	165	0	0	0	0
3	F	206	0	0	0	0
All	All	20591	0	18391	33	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 1.

All (33) 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:D:379:VAL:HG12	1:D:400:ALA:HB2	1.70	0.73
1:D:382:ALA:HB1	1:F:413:GLY:O	2.01	0.60
1:D:180:ARG:HD3	3:D:735:HOH:O	2.03	0.58
1:E:168:THR:HA	1:E:191:ASN:O	2.08	0.53
1:A:168:THR:HA	1:A:191:ASN:O	2.09	0.52
1:D:168:THR:HA	1:D:191:ASN:O	2.11	0.51
1:C:40:ASP:HB2	1:F:100:LEU:HD12	1.94	0.49
1:F:168:THR:HA	1:F:191:ASN:O	2.13	0.49
1:C:168:THR:HA	1:C:191:ASN:O	2.13	0.48
1:D:343:VAL:HG12	1:D:379:VAL:HG21	1.96	0.47
1:E:100:LEU:HD12	1:F:40:ASP:HB2	1.96	0.47
1:B:228:ASP:HA	1:B:252:ALA:O	2.15	0.46
1:B:168:THR:HA	1:B:191:ASN:O	2.15	0.46
1:B:153:ASP:OD1	1:B:155:SER:O	2.33	0.46
1:B:153:ASP:OD1	1:B:155:SER:C	2.55	0.46
1:E:282:TYR:CE1	1:E:316:ASP:HA	2.51	0.46
1:A:282:TYR:CE1	1:A:316:ASP:HA	2.52	0.45
1:F:282:TYR:CE1	1:F:316:ASP:HA	2.52	0.43
1:D:282:TYR:CE1	1:D:316:ASP:HA	2.53	0.43
1:E:205:HIS:HA	1:E:228:ASP:O	2.18	0.43
1:F:205:HIS:HA	1:F:228:ASP:O	2.20	0.42
1:D:142:ASN:HA	1:D:183:ASP:O	2.19	0.42
1:A:346:ALA:HA	1:A:349:ILE:HD12	2.01	0.42
1:A:205:HIS:HA	1:A:228:ASP:O	2.19	0.42
1:B:442:THR:HG23	3:B:638:HOH:O	2.20	0.41
1:A:228:ASP:HA	1:A:252:ALA:O	2.20	0.41
1:B:282:TYR:CE1	1:B:316:ASP:HA	2.55	0.41
1:A:227:THR:HA	1:A:251:THR:O	2.21	0.41
1:F:141:SER:HA	1:F:182:THR:O	2.20	0.41
1:F:298:ALA:HA	1:F:336:ILE:O	2.21	0.41
1:B:221:GLY:HA3	1:B:245:HIS:CE1	2.56	0.40
1:E:298:ALA:HA	1:E:336:ILE:O	2.21	0.40
1:B:142:ASN:HA	1:B:183:ASP:O	2.21	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	411/445 (92%)	392 (95%)	19 (5%)	0	100	100
1	B	416/445 (94%)	397 (95%)	19 (5%)	0	100	100
1	C	404/445 (91%)	386 (96%)	18 (4%)	0	100	100
1	D	434/445 (98%)	414 (95%)	20 (5%)	0	100	100
1	E	432/445 (97%)	411 (95%)	21 (5%)	0	100	100
1	F	414/445 (93%)	396 (96%)	18 (4%)	0	100	100
All	All	2511/2670 (94%)	2396 (95%)	115 (5%)	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	336/353 (95%)	329 (98%)	7 (2%)	53	38
1	B	335/353 (95%)	331 (99%)	4 (1%)	71	62
1	C	333/353 (94%)	327 (98%)	6 (2%)	59	45
1	D	350/353 (99%)	348 (99%)	2 (1%)	86	83
1	E	349/353 (99%)	348 (100%)	1 (0%)	92	91
1	F	337/353 (96%)	332 (98%)	5 (2%)	65	53
All	All	2040/2118 (96%)	2015 (99%)	25 (1%)	71	62

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	92	GLU
1	A	157	ARG
1	A	228	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	304	ARG
1	A	313	PHE
1	A	347	ASN
1	A	402	ASP
1	B	42	ASP
1	B	228	ASP
1	B	304	ARG
1	B	350	ARG
1	D	228	ASP
1	D	304	ARG
1	C	228	ASP
1	C	245	HIS
1	C	282	TYR
1	C	304	ARG
1	C	375	VAL
1	C	443	VAL
1	E	228	ASP
1	F	6	ARG
1	F	225	LYS
1	F	228	ASP
1	F	304	ARG
1	F	375	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	171	HIS
1	C	149	HIS

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](#)

12 monosaccharides are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	FRU	G	1	2	11,11,12	0.52	0	15,15,18	0.74	0
2	FRU	G	2	2	11,12,12	0.73	0	10,18,18	0.53	0
2	GLC	G	3	2	11,11,12	0.32	0	15,15,17	1.74	2 (13%)
2	FRU	H	1	2	11,11,12	0.50	0	15,15,18	0.93	0
2	FRU	H	2	2	11,12,12	0.85	0	10,18,18	0.73	0
2	GLC	H	3	2	11,11,12	0.48	0	15,15,17	0.80	1 (6%)
2	FRU	I	1	2	11,11,12	0.46	0	15,15,18	0.64	0
2	FRU	I	2	2	11,12,12	0.70	0	10,18,18	0.86	0
2	GLC	I	3	2	11,11,12	0.36	0	15,15,17	0.88	1 (6%)
2	FRU	J	1	2	11,11,12	0.36	0	15,15,18	0.78	0
2	FRU	J	2	2	11,12,12	0.78	1 (9%)	10,18,18	0.67	0
2	GLC	J	3	2	11,11,12	0.42	0	15,15,17	2.40	3 (20%)

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	FRU	G	1	2	-	0/4/20/24	0/1/1/1
2	FRU	G	2	2	-	0/5/24/24	0/1/1/1
2	GLC	G	3	2	-	2/2/19/22	0/1/1/1
2	FRU	H	1	2	-	0/4/20/24	0/1/1/1
2	FRU	H	2	2	-	0/5/24/24	0/1/1/1
2	GLC	H	3	2	-	0/2/19/22	0/1/1/1
2	FRU	I	1	2	-	0/4/20/24	0/1/1/1
2	FRU	I	2	2	-	0/5/24/24	0/1/1/1
2	GLC	I	3	2	-	0/2/19/22	0/1/1/1
2	FRU	J	1	2	-	0/4/20/24	0/1/1/1
2	FRU	J	2	2	-	0/5/24/24	0/1/1/1
2	GLC	J	3	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	J	2	FRU	O2-C2	2.05	1.44	1.40

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	3	GLC	C1-O5-C5	7.57	122.45	112.19
2	G	3	GLC	C1-O5-C5	4.80	118.69	112.19
2	J	3	GLC	C3-C4-C5	3.16	115.88	110.24
2	J	3	GLC	O5-C5-C4	2.95	118.00	110.83
2	G	3	GLC	C6-C5-C4	-2.31	107.59	113.00
2	H	3	GLC	O5-C5-C6	2.13	110.55	107.20
2	I	3	GLC	O5-C5-C6	2.12	110.53	107.20

There are no chirality outliers.

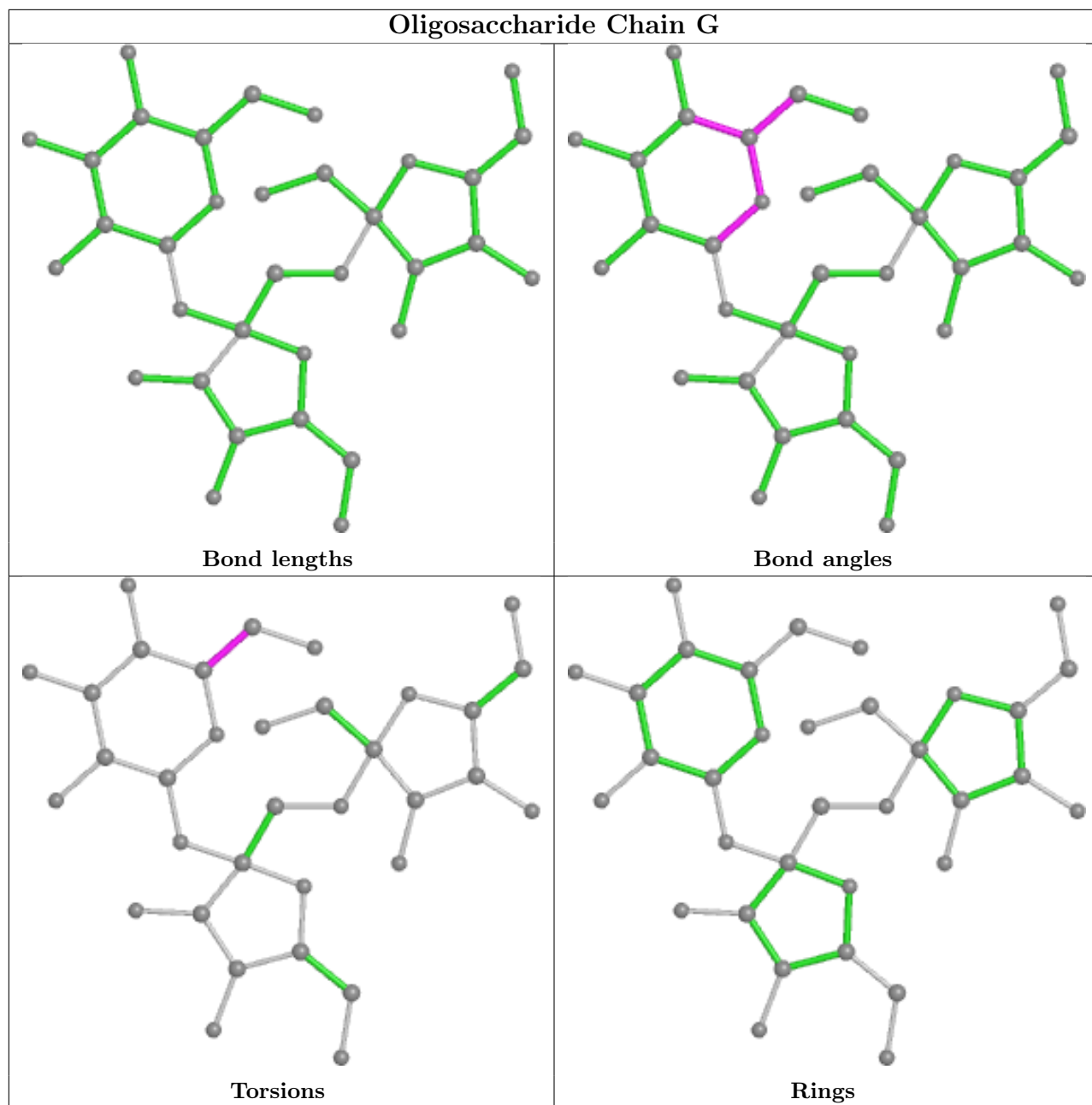
All (4) torsion outliers are listed below:

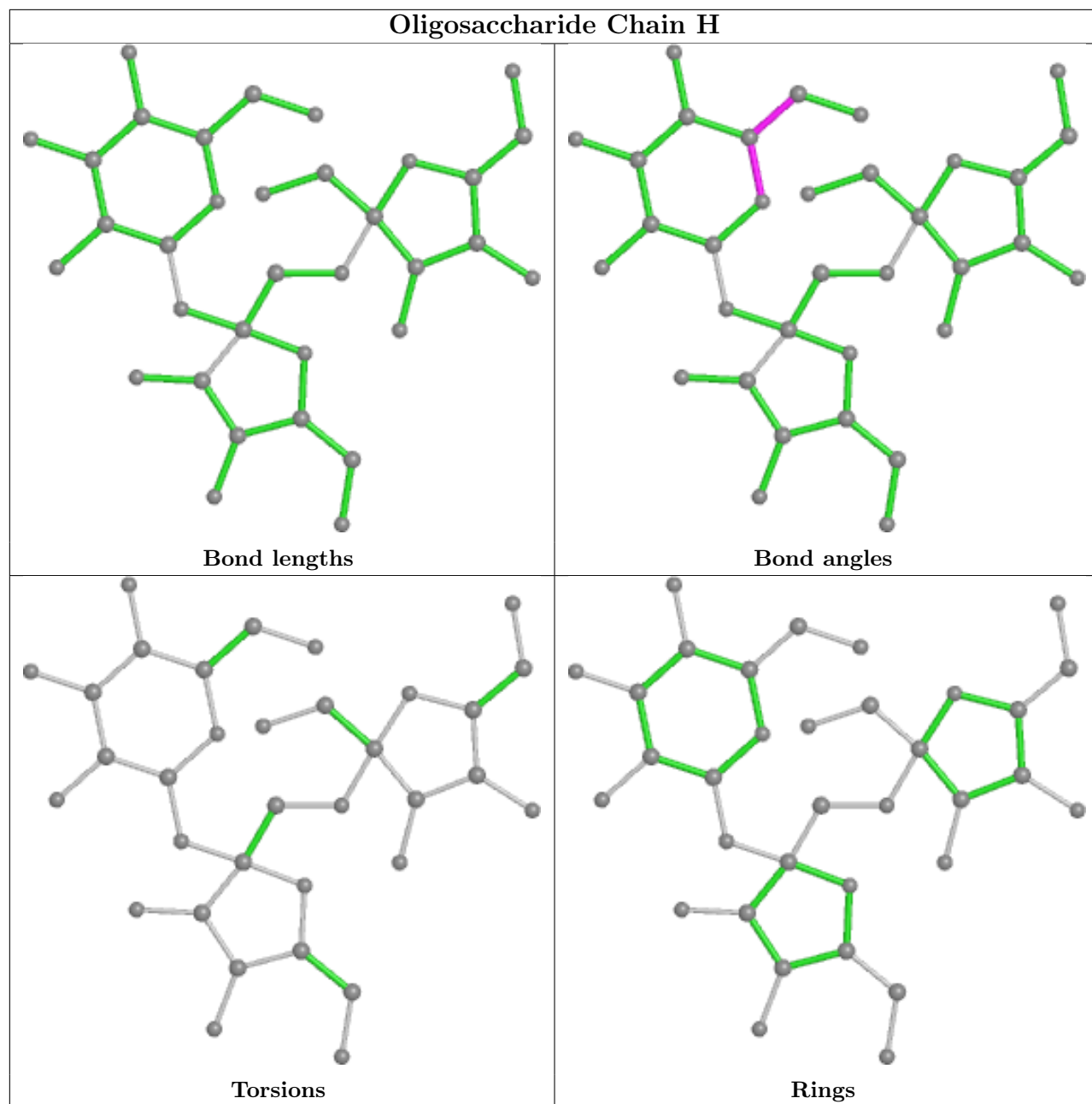
Mol	Chain	Res	Type	Atoms
2	G	3	GLC	O5-C5-C6-O6
2	G	3	GLC	C4-C5-C6-O6
2	J	3	GLC	C4-C5-C6-O6
2	J	3	GLC	O5-C5-C6-O6

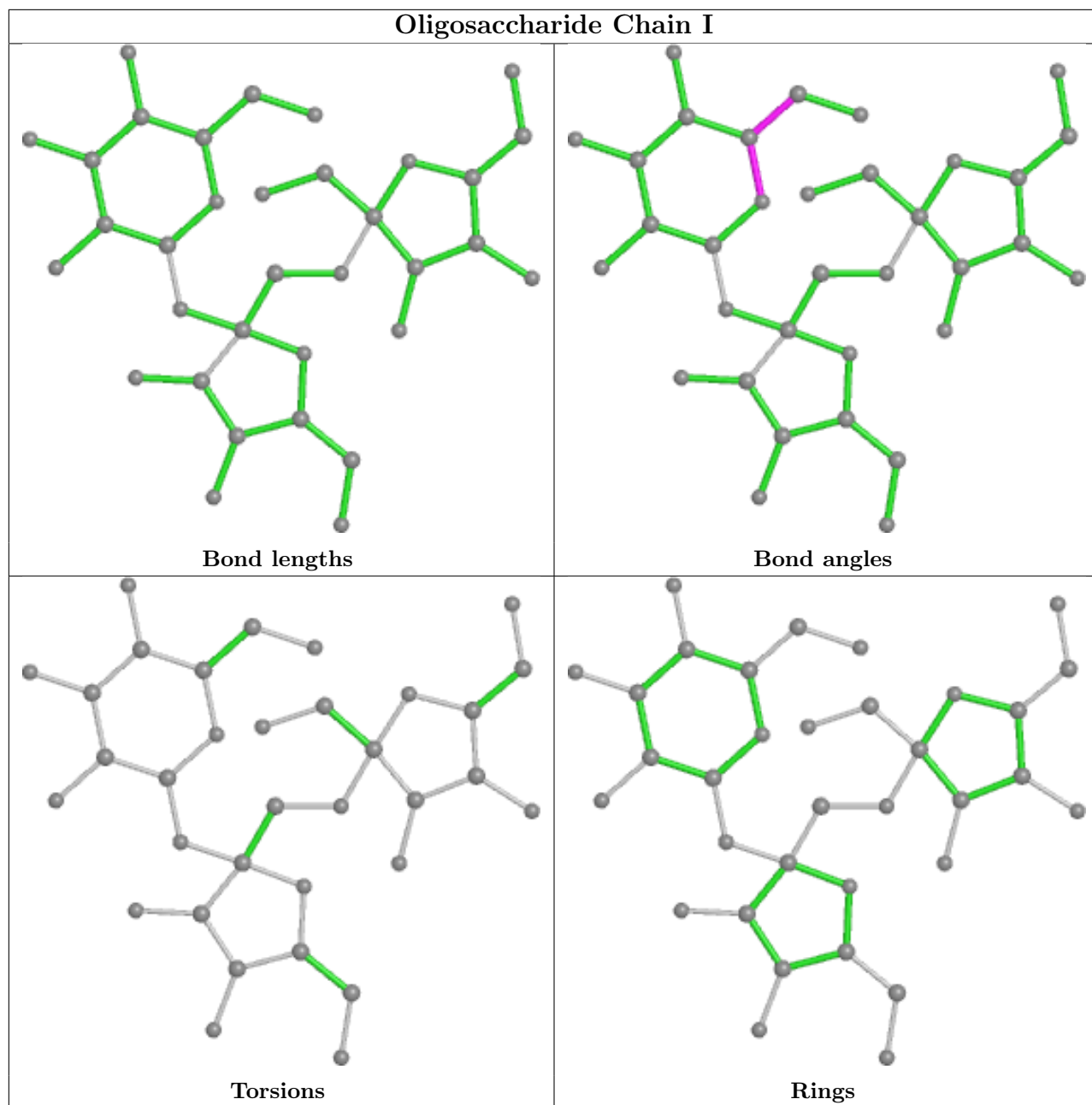
There are no ring outliers.

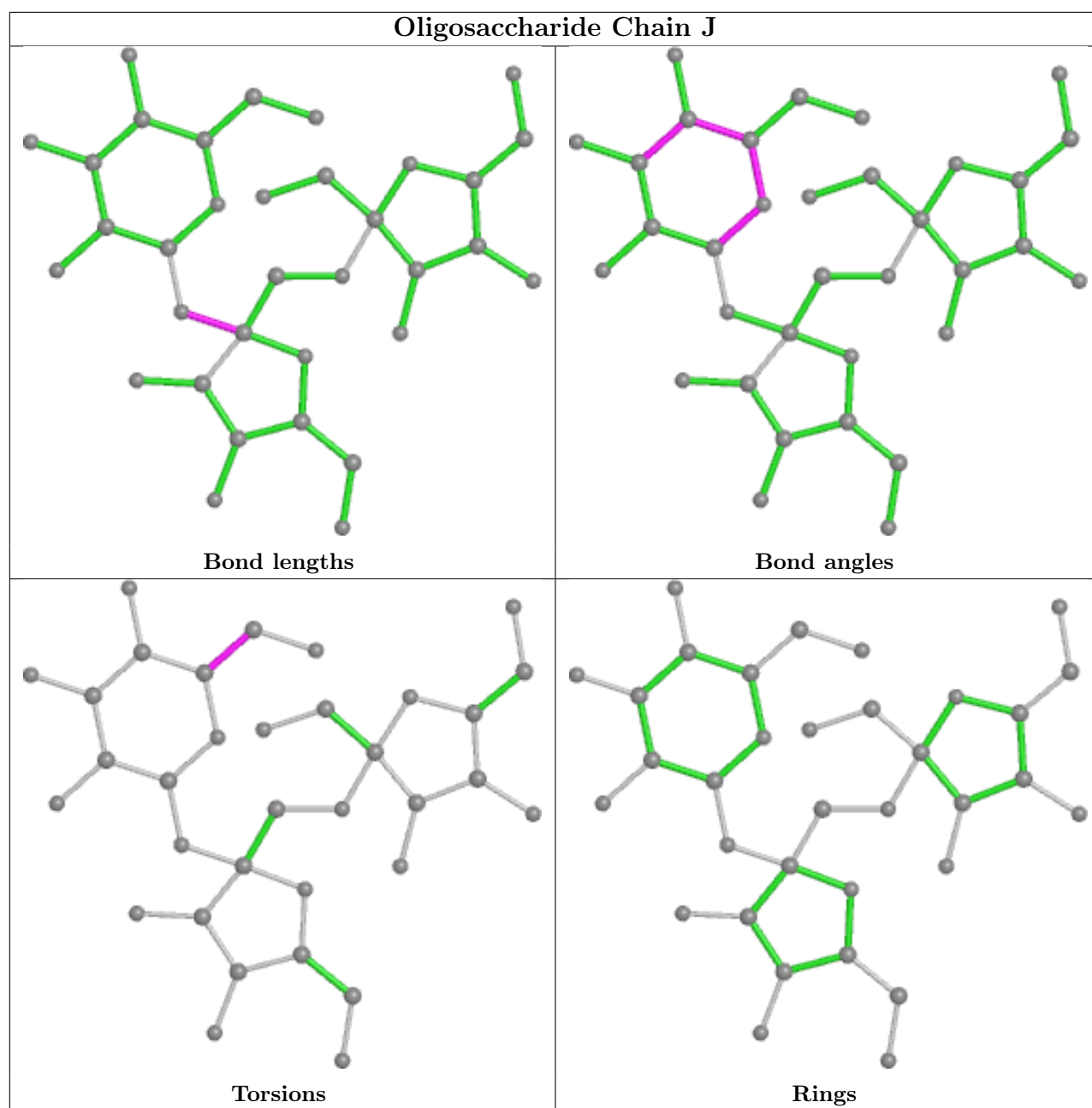
No monomer is involved in short contacts.

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](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

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	417/445 (93%)	-0.14	13 (3%) 49 47	14, 20, 41, 69	0
1	B	422/445 (94%)	-0.18	10 (2%) 59 57	15, 22, 41, 65	0
1	C	412/445 (92%)	0.31	25 (6%) 21 20	20, 31, 57, 76	0
1	D	438/445 (98%)	-0.09	19 (4%) 35 33	15, 22, 47, 69	0
1	E	436/445 (97%)	0.31	29 (6%) 17 17	19, 32, 58, 83	0
1	F	420/445 (94%)	0.05	34 (8%) 12 12	17, 24, 50, 75	0
All	All	2545/2670 (95%)	0.05	130 (5%) 28 26	14, 25, 51, 83	0

All (130) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	444	GLY	8.0
1	E	387	CYS	6.8
1	D	381	ALA	6.0
1	C	313	PHE	5.5
1	F	381	ALA	5.2
1	C	443	VAL	4.9
1	B	156	GLY	4.9
1	D	118	ASP	4.8
1	F	402	ASP	4.8
1	E	385	ASP	4.7
1	F	380	ASP	4.6
1	E	156	GLY	4.5
1	F	379	VAL	4.5
1	E	381	ALA	4.5
1	F	347	ASN	4.2
1	D	398	THR	4.1
1	F	156	GLY	4.0
1	E	154	GLY	4.0
1	D	154	GLY	4.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	347	ASN	3.9
1	C	380	ASP	3.9
1	B	400	ALA	3.7
1	B	380	ASP	3.7
1	F	401	ALA	3.7
1	A	379	VAL	3.7
1	A	402	ASP	3.7
1	D	392	VAL	3.6
1	E	434	VAL	3.6
1	C	348	GLU	3.5
1	A	154	GLY	3.4
1	E	352	GLU	3.4
1	E	382	ALA	3.4
1	D	155	SER	3.3
1	D	156	GLY	3.3
1	C	379	VAL	3.3
1	E	155	SER	3.3
1	D	400	ALA	3.2
1	C	318	GLY	3.2
1	C	119	SER	3.2
1	F	444	GLY	3.2
1	A	313	PHE	3.2
1	E	383	SER	3.2
1	F	313	PHE	3.2
1	E	318	GLY	3.1
1	F	443	VAL	3.1
1	C	306	HIS	3.1
1	C	14	ALA	3.1
1	E	313	PHE	3.0
1	E	40	ASP	3.0
1	F	348	GLU	3.0
1	C	350	ARG	2.9
1	F	118	ASP	2.9
1	D	3	SER	2.9
1	F	273	VAL	2.9
1	B	3	SER	2.9
1	C	347	ASN	2.9
1	F	157	ARG	2.9
1	F	442	THR	2.9
1	F	226	ILE	2.9
1	F	14	ALA	2.9
1	E	443	VAL	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	314	GLY	2.8
1	C	3	SER	2.8
1	A	347	ASN	2.8
1	C	336	ILE	2.8
1	D	113	ALA	2.7
1	B	348	GLU	2.7
1	F	336	ILE	2.7
1	C	309	TRP	2.7
1	E	353	GLY	2.7
1	D	402	ASP	2.7
1	F	203	ILE	2.6
1	F	154	GLY	2.6
1	D	401	ALA	2.6
1	C	310	THR	2.6
1	E	3	SER	2.5
1	D	152	ALA	2.5
1	F	252	ALA	2.5
1	A	348	GLU	2.5
1	A	226	ILE	2.5
1	D	220	TRP	2.4
1	E	252	ALA	2.4
1	F	298	ALA	2.4
1	E	249	LEU	2.4
1	E	236	ARG	2.4
1	B	381	ALA	2.4
1	E	430	ALA	2.4
1	C	153	ASP	2.4
1	C	308	PRO	2.4
1	A	252	ALA	2.4
1	A	378	ASP	2.3
1	B	313	PHE	2.3
1	A	155	SER	2.3
1	D	394	ALA	2.3
1	B	350	ARG	2.3
1	B	250	VAL	2.3
1	F	249	LEU	2.3
1	E	310	THR	2.3
1	E	153	ASP	2.3
1	A	443	VAL	2.3
1	F	335	VAL	2.3
1	C	298	ALA	2.3
1	C	158	HIS	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	412	PRO	2.2
1	F	113	ALA	2.2
1	E	416	ARG	2.2
1	F	296	LEU	2.2
1	F	353	GLY	2.2
1	F	274	THR	2.2
1	D	114	GLY	2.2
1	E	314	GLY	2.2
1	F	153	ASP	2.2
1	E	386	SER	2.2
1	D	181	VAL	2.2
1	C	345	ASP	2.1
1	F	155	SER	2.1
1	C	226	ILE	2.1
1	B	352	GLU	2.1
1	D	252	ALA	2.1
1	F	350	ARG	2.1
1	D	397	ALA	2.1
1	E	298	ALA	2.1
1	E	437	ILE	2.1
1	E	39	ALA	2.1
1	F	352	GLU	2.0
1	C	344	VAL	2.0
1	F	344	VAL	2.0
1	A	403	LEU	2.0
1	F	297	VAL	2.0
1	C	252	ALA	2.0

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

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

6.3 Carbohydrates [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists the number of atoms with occupancy less than 0.9.

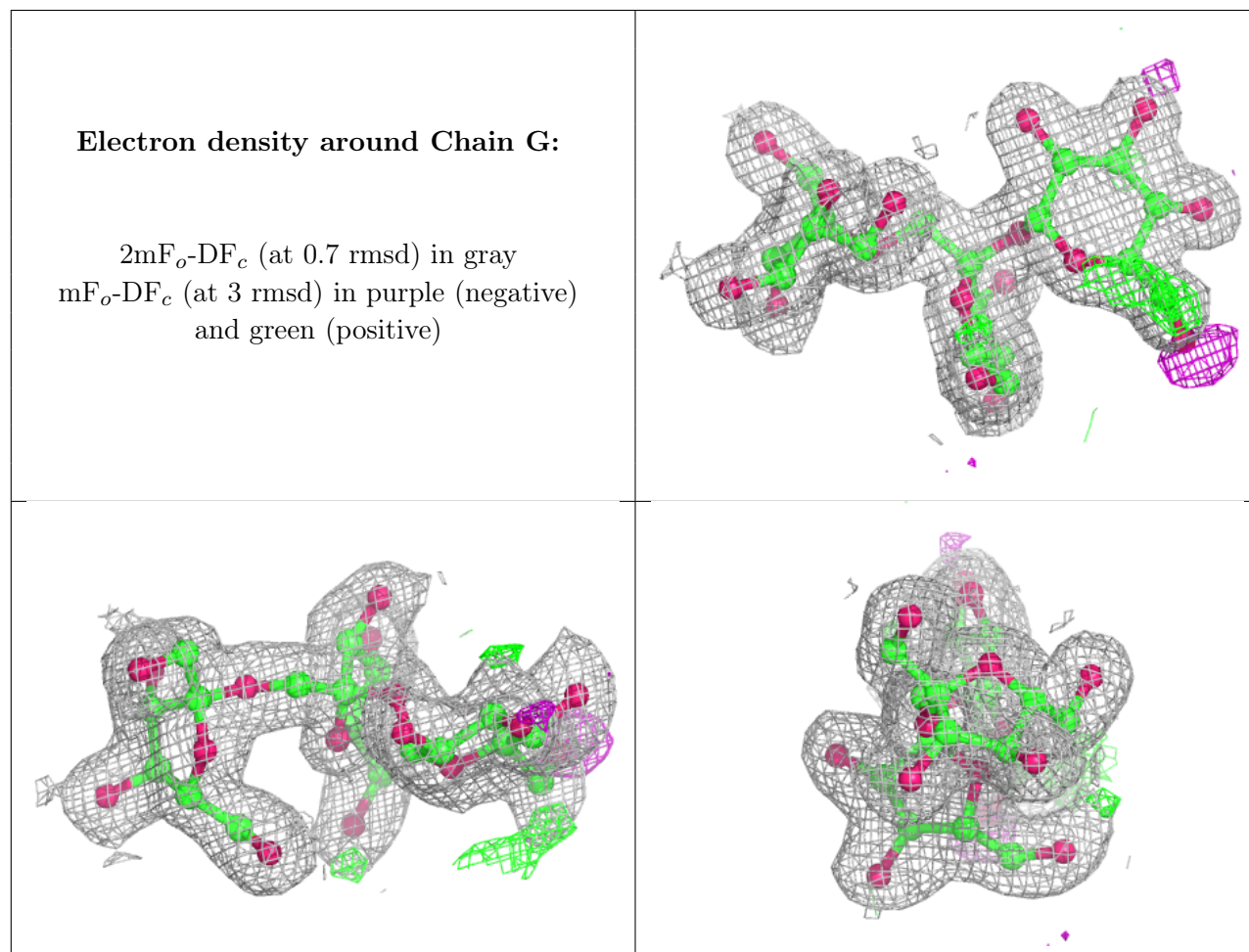
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	GLC	H	3	11/12	0.79	0.22	42,44,46,46	0

Continued on next page...

Continued from previous page...

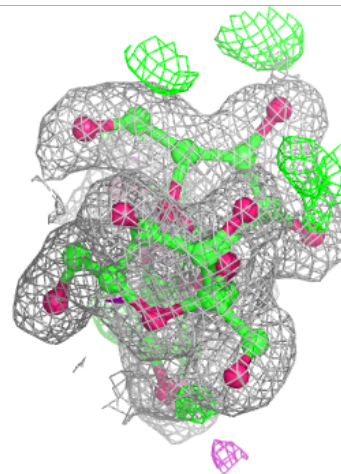
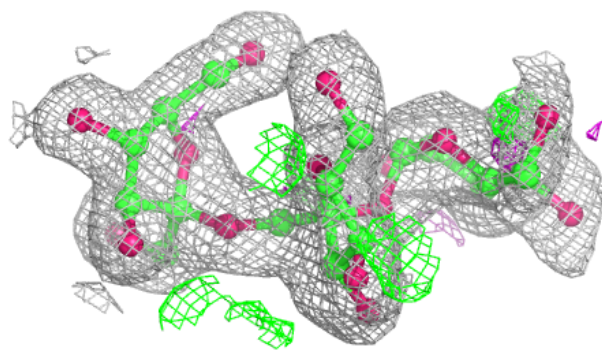
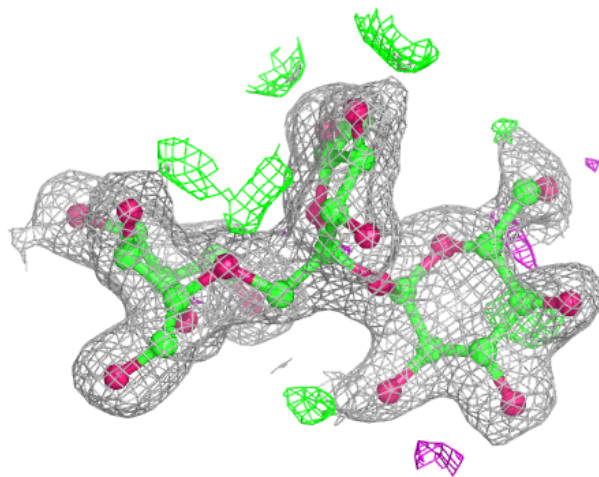
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	GLC	I	3	11/12	0.80	0.22	55,58,59,60	0
2	FRU	H	2	12/12	0.82	0.14	33,41,43,47	0
2	GLC	J	3	11/12	0.85	0.18	42,45,49,49	0
2	FRU	I	2	12/12	0.86	0.16	43,51,54,55	0
2	FRU	I	1	11/12	0.87	0.10	34,39,41,41	0
2	GLC	G	3	11/12	0.88	0.11	25,27,32,38	0
2	FRU	J	2	12/12	0.89	0.11	31,39,43,45	0
2	FRU	H	1	11/12	0.93	0.10	26,28,29,29	0
2	FRU	J	1	11/12	0.95	0.07	26,27,28,28	0
2	FRU	G	2	12/12	0.96	0.07	20,24,25,26	0
2	FRU	G	1	11/12	0.97	0.06	18,19,20,20	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.



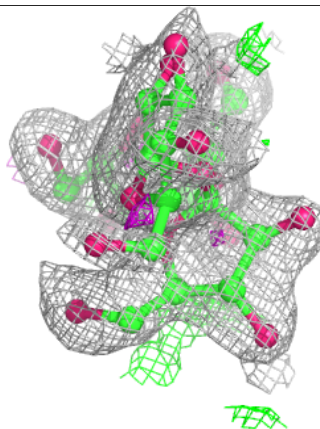
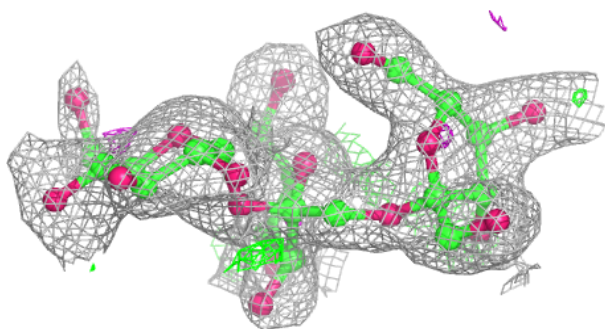
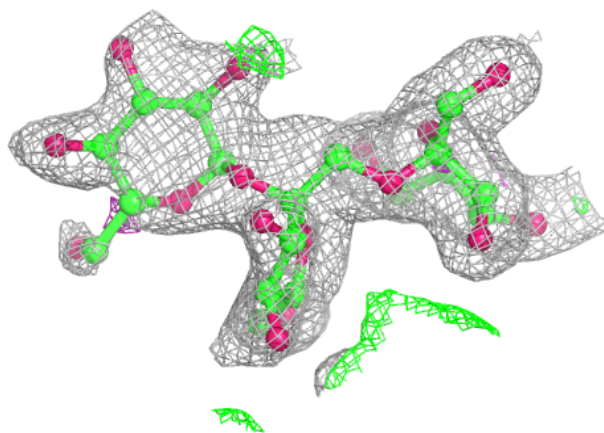
Electron density around Chain H:

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

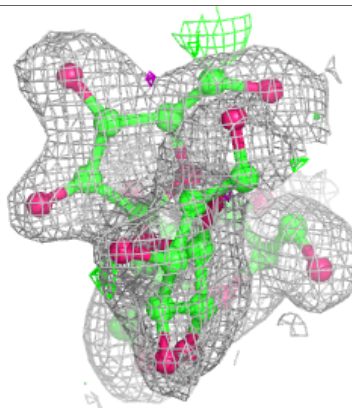
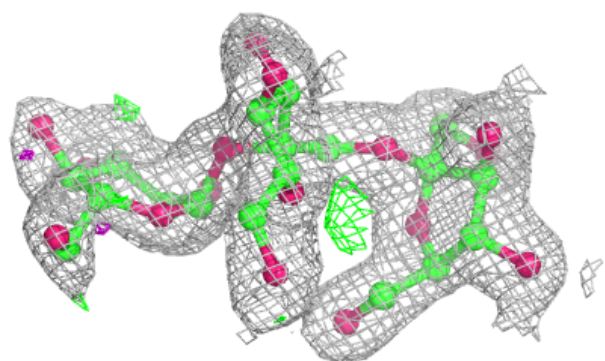
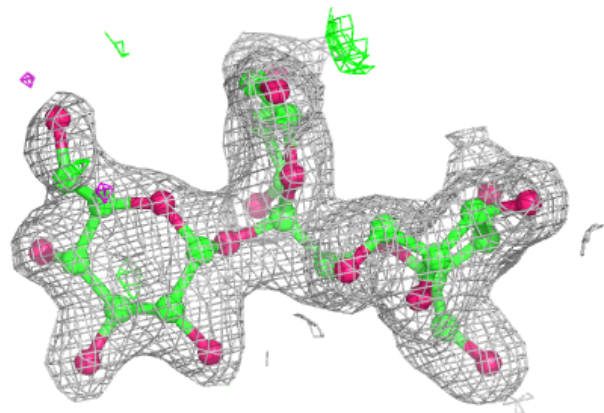


Electron density around Chain I:

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

**Electron density around Chain J:**

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



6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.