



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 12:26 PM UTC

PDB ID : 1W2T / pdb_00001w2t
Title : beta-fructosidase from *Thermotoga maritima* in complex with raffinose
Authors : Alberto, F.; Henrissat, B.; Czjzek, M.
Deposited on : 2004-07-08
Resolution : 1.87 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

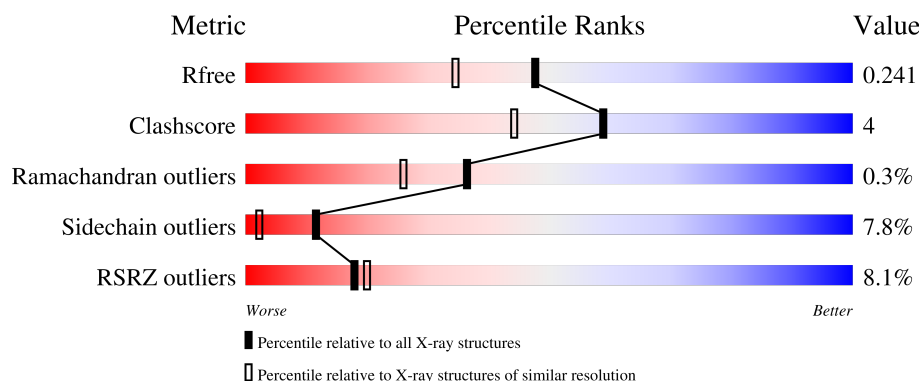
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.87 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



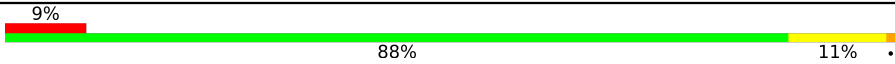
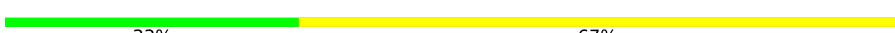
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1220 (1.88-1.88)
Clashscore	190562	1234 (1.88-1.88)
Ramachandran outliers	187476	1222 (1.88-1.88)
Sidechain outliers	187428	1222 (1.88-1.88)
RSRZ outliers	180081	1220 (1.88-1.88)

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	432	7% 87% 12% .
1	B	432	8% 84% 14% .
1	C	432	8% 87% 11% .
1	D	432	8% 86% 13% .
1	E	432	8% 88% 12% .

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Mol	Chain	Length	Quality of chain
1	F	432	
2	G	3	
2	H	3	
2	I	3	
2	J	3	
2	K	3	
2	L	3	

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	CIT	A	1433	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 23234 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 FRUCTOSIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	432	Total	C	N	O	S	0	0	0
			3517	2250	589	665	13			
1	B	432	Total	C	N	O	S	0	0	0
			3519	2252	589	665	13			
1	C	432	Total	C	N	O	S	0	0	0
			3519	2252	589	665	13			
1	D	432	Total	C	N	O	S	0	0	0
			3518	2251	589	665	13			
1	E	432	Total	C	N	O	S	0	0	0
			3518	2251	589	665	13			
1	F	432	Total	C	N	O	S	0	0	0
			3518	2252	588	665	13			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	190	ASP	GLU	engineered mutation	UNP O33833
A	108	VAL	ALA	cloning artifact	UNP O33833
A	179	ALA	VAL	cloning artifact	UNP O33833
B	190	ASP	GLU	engineered mutation	UNP O33833
B	108	VAL	ALA	cloning artifact	UNP O33833
B	179	ALA	VAL	cloning artifact	UNP O33833
C	190	ASP	GLU	engineered mutation	UNP O33833
C	108	VAL	ALA	cloning artifact	UNP O33833
C	179	ALA	VAL	cloning artifact	UNP O33833
D	190	ASP	GLU	engineered mutation	UNP O33833
D	108	VAL	ALA	cloning artifact	UNP O33833
D	179	ALA	VAL	cloning artifact	UNP O33833
E	190	ASP	GLU	engineered mutation	UNP O33833
E	108	VAL	ALA	cloning artifact	UNP O33833
E	179	ALA	VAL	cloning artifact	UNP O33833
F	190	ASP	GLU	engineered mutation	UNP O33833
F	108	VAL	ALA	cloning artifact	UNP O33833

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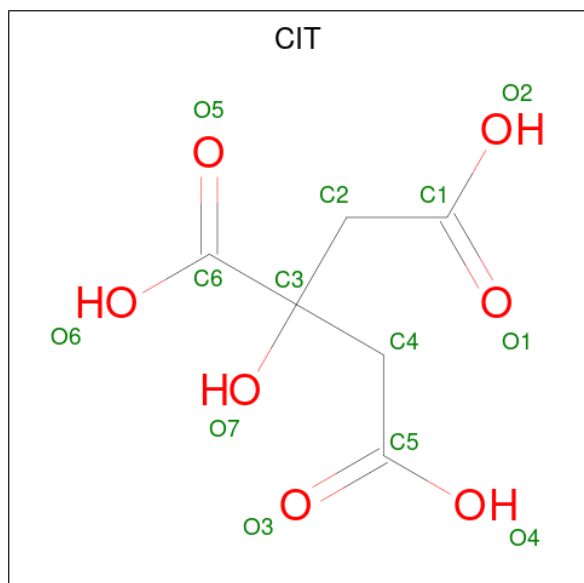
Chain	Residue	Modelled	Actual	Comment	Reference
F	179	ALA	VAL	cloning artifact	UNP O33833

- Molecule 2 is an oligosaccharide called beta-D-fructofuranose-(2-1)-[alpha-D-galactopyranose-(1-6)]alpha-D-glucopyranose.



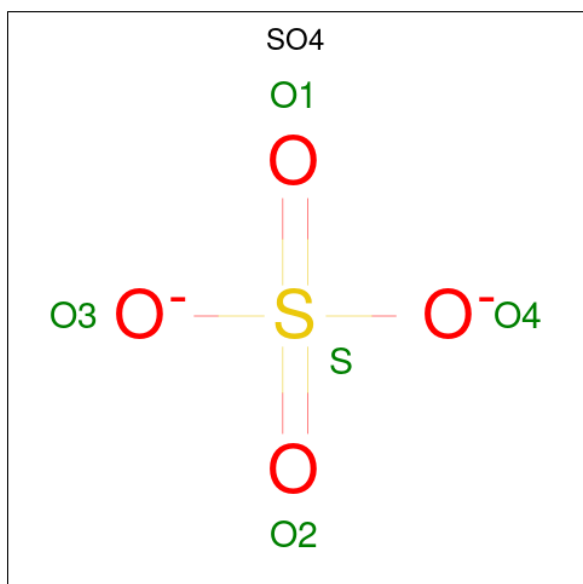
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
2	G	3	Total	C	O	0	0	0
			34	18	16			
2	H	3	Total	C	O	0	0	0
			34	18	16			
2	I	3	Total	C	O	0	0	0
			34	18	16			
2	J	3	Total	C	O	0	0	0
			34	18	16			
2	K	3	Total	C	O	0	0	0
			34	18	16			
2	L	3	Total	C	O	0	0	0
			34	18	16			

- Molecule 3 is CITRIC ACID (CCD ID: CIT) (formula: C₆H₈O₇).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			13	6	7		

- Molecule 4 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	O	S	0	0
			5	4	1		
4	C	1	Total	O	S	0	0
			5	4	1		
4	C	1	Total	O	S	0	0
			5	4	1		
4	E	1	Total	O	S	0	0
			5	4	1		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	339	Total	O	0	0
			339	339		
5	B	259	Total	O	0	0
			259	259		
5	C	316	Total	O	0	0
			316	316		
5	D	364	Total	O	0	0
			364	364		
5	E	296	Total	O	0	0
			296	296		

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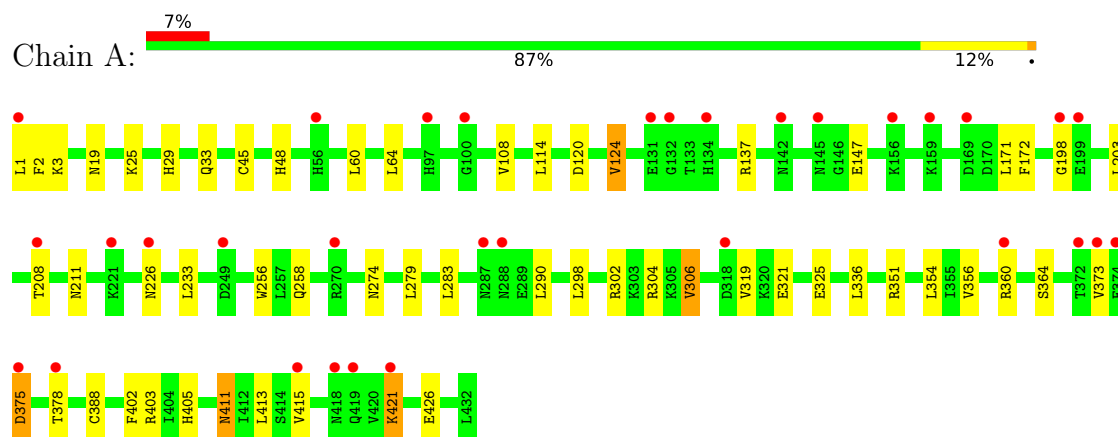
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	F	314	Total 314	O 314	0	0

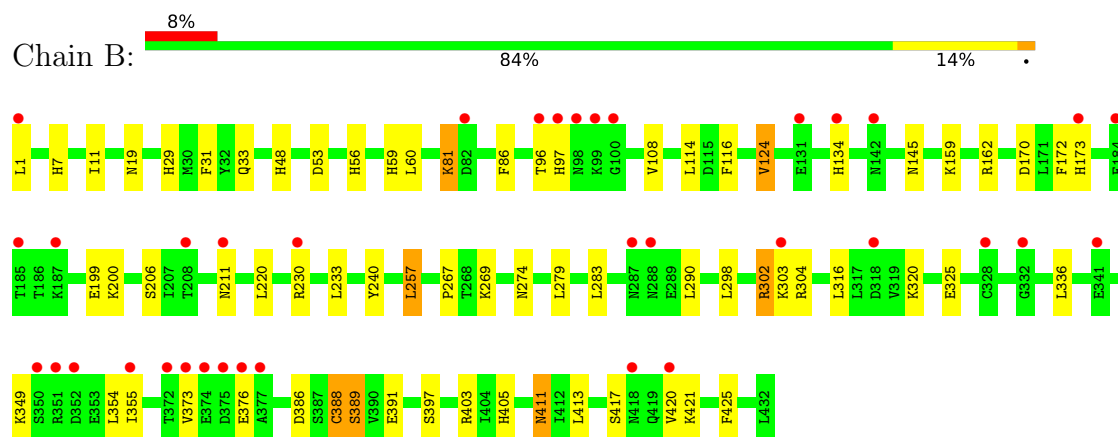
3 Residue-property plots [i](#)

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.

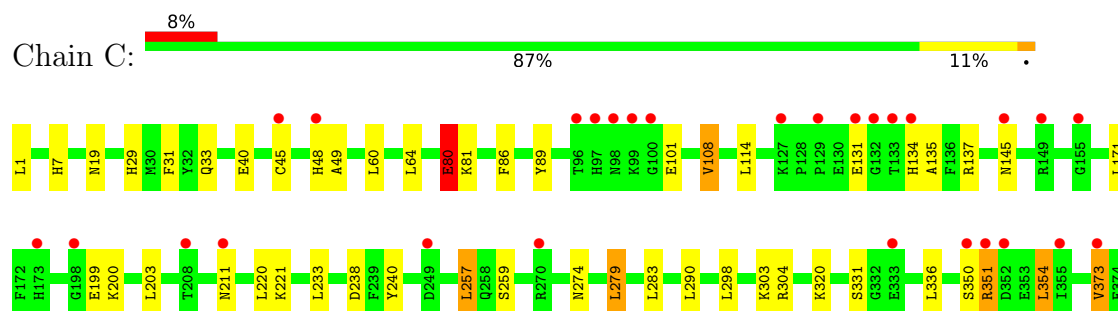
• Molecule 1: BETA FRUCTOSIDASE



• Molecule 1: BETA FRUCTOSIDASE

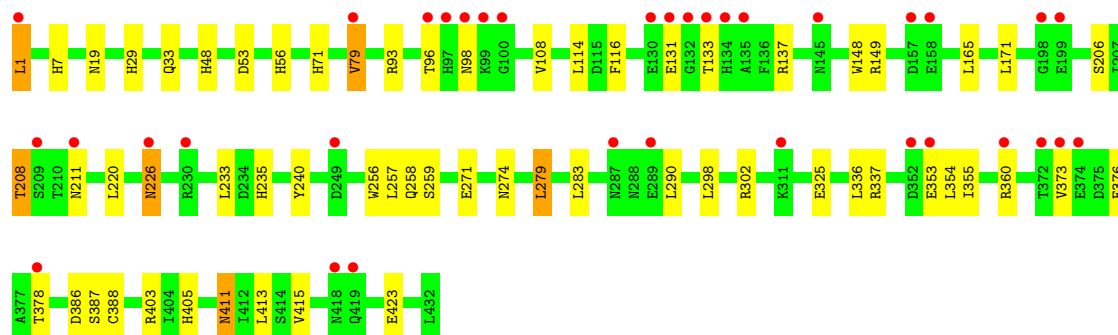
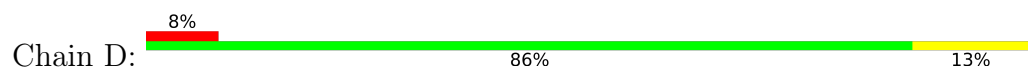


• Molecule 1: BETA FRUCTOSIDASE

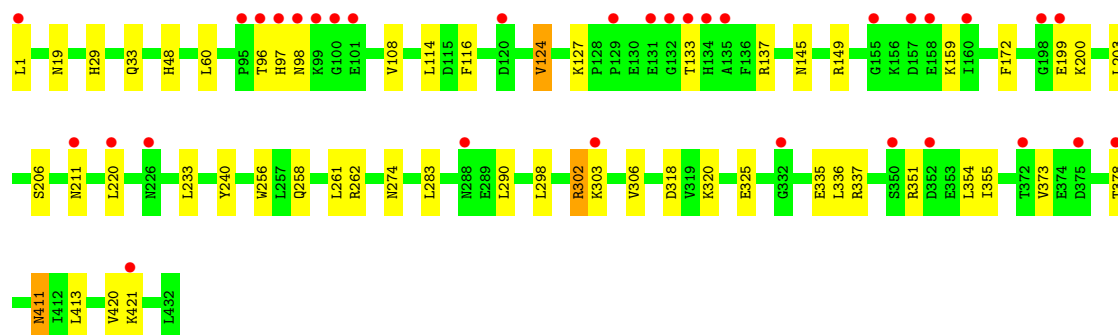
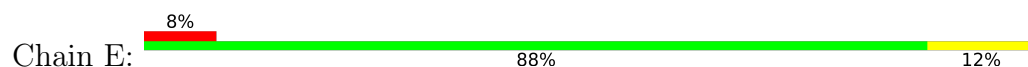




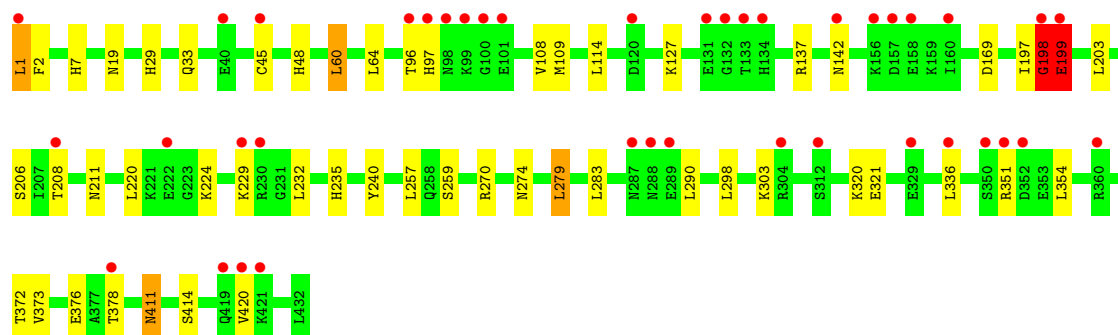
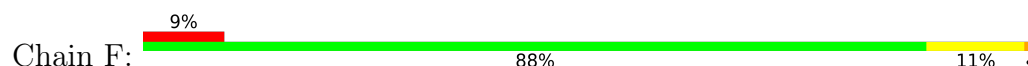
• Molecule 1: BETA FRUCTOSIDASE



• Molecule 1: BETA FRUCTOSIDASE



• Molecule 1: BETA FRUCTOSIDASE



• Molecule 2: beta-D-fructofuranose-(2-1)-[alpha-D-galactopyranose-(1-6)]alpha-D-glucopyranos e



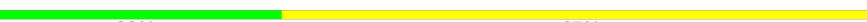


- Molecule 2: beta-D-fructofuranose-(2-1)-[alpha-D-galactopyranose-(1-6)]alpha-D-glucopyranose

Chain H:  67% 33%

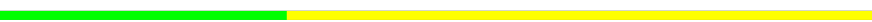


- Molecule 2: beta-D-fructofuranose-(2-1)-[alpha-D-galactopyranose-(1-6)]alpha-D-glucopyranose

Chain I:  33% 67%

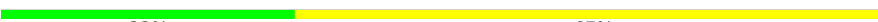


- Molecule 2: beta-D-fructofuranose-(2-1)-[alpha-D-galactopyranose-(1-6)]alpha-D-glucopyranose

Chain J:  33% 67%



- Molecule 2: beta-D-fructofuranose-(2-1)-[alpha-D-galactopyranose-(1-6)]alpha-D-glucopyranose

Chain K:  33% 67%



- Molecule 2: beta-D-fructofuranose-(2-1)-[alpha-D-galactopyranose-(1-6)]alpha-D-glucopyranose

Chain L:  33% 67%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	94.50Å 114.70Å 130.00Å 90.00° 98.90° 90.00°	Depositor
Resolution (Å)	40.00 – 1.87 40.00 – 1.87	Depositor EDS
% Data completeness (in resolution range)	97.7 (40.00-1.87) 97.7 (40.00-1.87)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.97 (at 1.87Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.198 , 0.229 0.213 , 0.241	Depositor DCC
R_{free} test set	11055 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	17.7	Xtriage
Anisotropy	0.198	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 42.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	23234	wwPDB-VP
Average B, all atoms (Å ²)	18.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.89% 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: CIT, FRU, SO4, GLC, GLA

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	0.46	1/3607 (0.0%)	0.74	3/4881 (0.1%)
1	B	0.44	0/3610	0.73	0/4885
1	C	0.58	1/3610 (0.0%)	0.72	1/4885 (0.0%)
1	D	0.43	0/3608	0.70	1/4883 (0.0%)
1	E	0.43	0/3609	0.71	1/4883 (0.0%)
1	F	0.46	1/3609 (0.0%)	0.75	4/4884 (0.1%)
All	All	0.47	3/21653 (0.0%)	0.73	10/29301 (0.0%)

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
1	C	0	1
1	F	0	2
All	All	0	4

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	80	GLU	C-N	22.95	1.63	1.33
1	A	2	PHE	C-N	-6.35	1.21	1.33
1	F	198	GLY	C-O	5.48	1.31	1.23

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	198	GLY	O-C-N	-9.73	110.04	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2	PHE	O-C-N	-9.45	110.21	122.39
1	F	198	GLY	CA-C-O	-8.81	105.24	120.57
1	F	199	GLU	N-CA-C	7.33	126.41	110.80
1	D	137	ARG	N-CA-C	6.32	117.83	108.60
1	A	1	LEU	CB-CA-C	-5.94	98.82	110.10
1	E	137	ARG	N-CA-C	5.74	116.98	108.60
1	A	137	ARG	N-CA-C	5.73	116.97	108.60
1	F	137	ARG	N-CA-C	5.23	116.24	108.60
1	C	137	ARG	N-CA-C	5.02	115.93	108.60

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	388	CYS	Mainchain
1	C	80	GLU	Mainchain
1	F	198	GLY	Peptide,Mainchain

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	3517	0	3399	33	0
1	B	3519	0	3411	33	0
1	C	3519	0	3411	42	0
1	D	3518	0	3404	31	0
1	E	3518	0	3407	27	0
1	F	3518	0	3406	21	0
2	G	34	0	29	0	0
2	H	34	0	29	0	0
2	I	34	0	29	0	0
2	J	34	0	29	0	0
2	K	34	0	29	0	0
2	L	34	0	29	0	0
3	A	13	0	5	6	0
4	B	5	0	0	0	0
4	C	10	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	E	5	0	0	0	0
5	A	339	0	0	16	0
5	B	259	0	0	1	0
5	C	316	0	0	5	0
5	D	364	0	0	4	0
5	E	296	0	0	4	0
5	F	314	0	0	6	0
All	All	23234	0	20617	185	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 4.

All (185) 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:211:ASN:OD1	5:A:2179:HOH:O	1.56	1.20
1:F:270:ARG:CZ	5:F:2203:HOH:O	1.88	1.18
1:B:267:PRO:HD2	1:B:405:HIS:CD2	1.87	1.08
3:A:1433:CIT:O2	5:A:2332:HOH:O	1.75	1.03
1:C:211:ASN:HD21	1:C:259:SER:HA	1.19	1.02
1:E:211:ASN:ND2	1:E:261:LEU:HG	1.89	0.88
1:C:31:PHE:CZ	1:C:48:HIS:CE1	2.65	0.85
1:F:270:ARG:NE	5:F:2203:HOH:O	2.04	0.83
3:A:1433:CIT:O3	5:A:2331:HOH:O	1.95	0.83
3:A:1433:CIT:C6	5:A:2336:HOH:O	2.27	0.82
3:A:1433:CIT:O5	5:A:2336:HOH:O	1.97	0.81
1:C:211:ASN:HD21	1:C:259:SER:CA	1.93	0.81
1:C:211:ASN:ND2	1:C:259:SER:HA	1.95	0.80
1:C:31:PHE:CE2	1:C:48:HIS:ND1	2.51	0.79
1:C:211:ASN:ND2	1:C:259:SER:CB	2.47	0.77
1:B:11:ILE:HG23	1:B:59:HIS:CE1	2.20	0.77
1:F:45:CYS:HB2	1:F:64:LEU:O	1.89	0.73
3:A:1433:CIT:O6	5:A:2333:HOH:O	2.06	0.73
1:C:211:ASN:CG	5:C:2163:HOH:O	2.31	0.73
1:E:262:ARG:NH2	5:E:2184:HOH:O	2.22	0.71
1:B:267:PRO:CD	1:B:405:HIS:CD2	2.70	0.71
1:F:48:HIS:CE1	1:F:60:LEU:HD23	2.26	0.70
1:A:3:LYS:NZ	5:A:2002:HOH:O	2.04	0.70
1:A:360:ARG:NE	5:A:2281:HOH:O	2.25	0.70
1:D:7:HIS:CE1	1:D:279:LEU:HD13	2.27	0.69
1:E:19:ASN:HD21	1:E:33:GLN:HE21	1.39	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:211:ASN:ND2	1:C:259:SER:CA	2.55	0.68
1:B:145:ASN:OD1	1:C:81:LYS:HA	1.94	0.68
1:F:7:HIS:CE1	1:F:279:LEU:HD13	2.29	0.68
1:C:45:CYS:HB2	1:C:64:LEU:O	1.94	0.67
1:D:208:THR:O	1:D:211:ASN:ND2	2.28	0.67
1:E:211:ASN:HD21	1:E:261:LEU:HG	1.58	0.67
1:B:267:PRO:HD2	1:B:405:HIS:HD2	1.60	0.65
1:D:19:ASN:HD21	1:D:33:GLN:HE21	1.45	0.65
1:F:19:ASN:HD21	1:F:33:GLN:HE21	1.45	0.65
1:E:336:LEU:HD11	1:E:413:LEU:HD11	1.77	0.65
1:D:79:VAL:HG11	1:D:148:TRP:CZ3	2.31	0.64
1:A:19:ASN:HD21	1:A:33:GLN:HE21	1.46	0.63
1:D:1:LEU:N	1:D:1:LEU:HD12	2.15	0.62
1:C:211:ASN:ND2	1:C:259:SER:OG	2.32	0.61
1:A:360:ARG:CD	5:A:2281:HOH:O	2.48	0.60
1:A:360:ARG:CG	5:A:2280:HOH:O	2.50	0.60
1:F:1:LEU:CD1	1:F:2:PHE:CD1	2.86	0.59
1:C:211:ASN:ND2	5:C:2163:HOH:O	2.35	0.58
1:C:351:ARG:NH2	5:C:2258:HOH:O	2.36	0.58
1:E:335:GLU:OE1	1:E:337:ARG:NE	2.37	0.58
1:B:19:ASN:HD21	1:B:33:GLN:HE21	1.52	0.58
1:D:1:LEU:HD12	1:D:1:LEU:H3	1.67	0.58
1:E:211:ASN:HD21	1:E:261:LEU:H	1.52	0.57
1:F:320:LYS:NZ	5:F:2244:HOH:O	2.37	0.57
1:C:211:ASN:HD22	1:C:259:SER:CB	2.13	0.57
1:E:302:ARG:HD3	1:E:325:GLU:OE1	2.04	0.57
1:C:411:ASN:HD22	1:C:411:ASN:H	1.53	0.57
1:E:19:ASN:ND2	1:E:33:GLN:HE21	2.02	0.57
1:B:31:PHE:CE2	1:B:48:HIS:CE1	2.92	0.57
1:B:31:PHE:CZ	1:B:48:HIS:CE1	2.93	0.56
1:D:302:ARG:HD3	1:D:325:GLU:OE1	2.06	0.56
1:B:7:HIS:HD2	1:B:386:ASP:OD2	1.88	0.56
1:A:336:LEU:HD11	1:A:413:LEU:HD11	1.88	0.56
1:D:29:HIS:HD2	1:D:48:HIS:NE2	2.04	0.56
1:E:1:LEU:HD23	5:E:2002:HOH:O	2.06	0.55
1:E:29:HIS:HD2	1:E:48:HIS:NE2	2.04	0.55
1:C:31:PHE:CZ	1:C:48:HIS:HE1	2.20	0.55
1:D:235:HIS:HD2	5:D:2308:HOH:O	1.90	0.55
1:D:19:ASN:ND2	1:D:33:GLN:HE21	2.05	0.55
1:F:411:ASN:H	1:F:411:ASN:HD22	1.54	0.55
1:C:31:PHE:CE2	1:C:48:HIS:CE1	2.94	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:134:HIS:CD2	1:C:135:ALA:H	2.25	0.54
1:B:11:ILE:HG23	1:B:59:HIS:ND1	2.22	0.54
1:C:19:ASN:HD21	1:C:33:GLN:HE21	1.53	0.54
1:A:421:LYS:HZ3	1:E:318:ASP:HB3	1.72	0.54
1:C:29:HIS:HD2	1:C:48:HIS:NE2	2.06	0.54
1:A:360:ARG:HD3	5:A:2281:HOH:O	2.05	0.54
1:F:232:LEU:HB2	1:F:235:HIS:CE1	2.42	0.54
1:B:29:HIS:HD2	1:B:48:HIS:NE2	2.06	0.54
1:D:388:CYS:HB2	1:D:405:HIS:CE1	2.43	0.54
1:A:302:ARG:HD3	1:A:325:GLU:OE1	2.08	0.54
1:D:149:ARG:HD2	5:D:2130:HOH:O	2.08	0.54
1:A:360:ARG:HG2	5:A:2280:HOH:O	2.07	0.53
1:F:1:LEU:HD12	1:F:2:PHE:N	2.24	0.53
1:B:7:HIS:HE1	1:B:391:GLU:OE1	1.92	0.53
1:A:208:THR:HG22	5:A:2165:HOH:O	2.08	0.53
1:C:101:GLU:CD	1:C:134:HIS:CE1	2.87	0.52
1:F:7:HIS:ND1	1:F:279:LEU:HD13	2.25	0.52
1:F:19:ASN:ND2	1:F:33:GLN:HE21	2.07	0.52
1:A:304:ARG:NE	5:A:2319:HOH:O	2.42	0.52
1:B:411:ASN:H	1:B:411:ASN:HD22	1.57	0.52
1:A:426:GLU:CD	5:A:2319:HOH:O	2.53	0.52
1:B:145:ASN:HA	1:C:80:GLU:O	2.10	0.51
1:A:351:ARG:NH2	1:C:220:LEU:O	2.42	0.51
1:B:336:LEU:HD11	1:B:413:LEU:HD11	1.92	0.51
1:E:411:ASN:H	1:E:411:ASN:HD22	1.58	0.51
1:B:81:LYS:NZ	1:B:86:PHE:CZ	2.80	0.50
1:D:7:HIS:HD2	1:D:386:ASP:OD2	1.93	0.50
1:E:211:ASN:ND2	1:E:261:LEU:H	2.10	0.50
1:F:270:ARG:NH2	5:F:2203:HOH:O	2.21	0.50
1:A:403:ARG:HH21	1:A:405:HIS:HE1	1.58	0.50
1:F:1:LEU:HD22	5:F:2287:HOH:O	2.11	0.50
1:C:81:LYS:HB3	1:C:86:PHE:CE1	2.46	0.49
1:C:134:HIS:CD2	1:C:135:ALA:N	2.80	0.49
1:A:19:ASN:ND2	1:A:33:GLN:HE21	2.08	0.49
1:B:302:ARG:HD2	1:B:425:PHE:CG	2.47	0.49
1:D:336:LEU:HD11	1:D:413:LEU:HD11	1.94	0.49
1:B:11:ILE:CG2	1:B:59:HIS:CE1	2.95	0.49
1:F:29:HIS:HD2	1:F:48:HIS:NE2	2.11	0.49
1:C:19:ASN:ND2	1:C:33:GLN:HE21	2.12	0.48
1:C:336:LEU:HD11	1:C:413:LEU:HD11	1.94	0.48
1:A:375:ASP:OD2	1:C:200:LYS:NZ	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:1:LEU:HB3	5:E:2002:HOH:O	2.13	0.48
1:D:337:ARG:O	1:D:413:LEU:HD12	2.14	0.48
1:E:206:SER:HB3	1:E:240:TYR:CE1	2.49	0.48
1:B:29:HIS:HE1	5:B:2015:HOH:O	1.97	0.48
1:B:108:VAL:HG11	1:B:116:PHE:HB3	1.96	0.48
1:E:108:VAL:HG11	1:E:116:PHE:HB3	1.94	0.48
1:B:19:ASN:ND2	1:B:33:GLN:HE21	2.11	0.48
1:B:124:VAL:HG22	1:B:172:PHE:O	2.13	0.48
1:D:108:VAL:HG11	1:D:116:PHE:HB3	1.96	0.48
1:E:211:ASN:ND2	1:E:261:LEU:CG	2.70	0.47
1:C:7:HIS:NE2	1:C:279:LEU:HD13	2.29	0.47
1:D:7:HIS:CD2	1:D:386:ASP:OD2	2.68	0.47
1:D:53:ASP:OD2	1:D:56:HIS:HD2	1.98	0.47
1:C:29:HIS:HE1	5:C:2020:HOH:O	1.98	0.47
1:F:1:LEU:HD13	1:F:2:PHE:CD1	2.49	0.47
1:E:108:VAL:CG1	1:E:116:PHE:HB3	2.45	0.47
1:C:350:SER:O	1:C:351:ARG:C	2.58	0.47
1:A:421:LYS:HG2	1:E:306:VAL:HA	1.97	0.46
1:B:53:ASP:OD2	1:B:56:HIS:HD2	1.98	0.46
1:C:351:ARG:CZ	5:C:2258:HOH:O	2.62	0.46
1:A:421:LYS:NZ	1:E:318:ASP:HB3	2.29	0.46
1:E:19:ASN:HD21	1:E:33:GLN:NE2	2.11	0.46
1:D:411:ASN:HD22	1:D:411:ASN:H	1.63	0.46
1:B:388:CYS:O	1:B:389:SER:HB3	2.15	0.46
1:C:238:ASP:O	1:C:257:LEU:HD23	2.16	0.46
1:C:354:LEU:HB2	1:C:373:VAL:HG21	1.98	0.46
1:D:7:HIS:ND1	1:D:279:LEU:HD13	2.31	0.46
1:F:270:ARG:NH2	5:F:2204:HOH:O	2.49	0.46
1:B:302:ARG:HD3	1:B:325:GLU:OE1	2.16	0.45
1:F:1:LEU:HD12	1:F:2:PHE:H	1.81	0.45
1:B:267:PRO:HD2	1:B:405:HIS:NE2	2.25	0.45
1:A:29:HIS:HD2	1:A:48:HIS:NE2	2.15	0.45
1:C:211:ASN:OD1	1:C:240:TYR:HB2	2.16	0.45
1:A:388:CYS:HB2	1:A:405:HIS:CE1	2.52	0.45
1:D:1:LEU:HD13	1:D:271:GLU:OE1	2.16	0.45
1:D:108:VAL:CG1	1:D:116:PHE:HB3	2.46	0.45
1:C:48:HIS:CD2	1:C:49:ALA:N	2.85	0.44
1:A:306:VAL:HG12	1:A:426:GLU:HG3	2.00	0.44
1:A:45:CYS:HB3	1:A:64:LEU:O	2.18	0.44
1:C:48:HIS:CD2	1:C:60:LEU:HD12	2.53	0.44
1:E:124:VAL:HG22	1:E:172:PHE:O	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:336:LEU:CD1	1:E:413:LEU:HD11	2.47	0.43
1:F:197:ILE:C	1:F:198:GLY:O	2.60	0.43
1:D:149:ARG:CG	1:D:165:LEU:HD11	2.48	0.43
1:A:306:VAL:HG21	1:A:319:VAL:HG13	2.00	0.43
1:A:356:VAL:HG11	1:A:402:PHE:CE2	2.54	0.43
1:A:120:ASP:CG	3:A:1433:CIT:H41	2.43	0.43
1:B:108:VAL:CG1	1:B:116:PHE:HB3	2.48	0.43
1:B:257:LEU:HD23	1:B:403:ARG:HG2	1.99	0.43
1:D:1:LEU:O	1:D:387:SER:HB3	2.18	0.43
1:D:360:ARG:HG2	5:D:2293:HOH:O	2.18	0.43
1:D:226:ASN:HD22	1:D:226:ASN:N	2.17	0.43
1:D:256:TRP:CE2	1:D:258:GLN:HB3	2.53	0.43
1:A:124:VAL:HG22	1:A:172:PHE:O	2.18	0.42
1:C:7:HIS:CD2	1:C:279:LEU:HD13	2.54	0.42
1:C:101:GLU:CD	1:C:134:HIS:HE1	2.28	0.42
1:F:206:SER:HB3	1:F:240:TYR:CE1	2.53	0.42
1:B:170:ASP:OD2	1:B:173:HIS:HD2	2.01	0.42
1:C:373:VAL:HG11	1:C:394:PHE:CD2	2.55	0.42
1:E:256:TRP:CE2	1:E:258:GLN:HB3	2.54	0.42
1:C:101:GLU:OE2	1:C:134:HIS:CE1	2.72	0.42
1:E:29:HIS:CD2	1:E:48:HIS:NE2	2.87	0.42
1:A:360:ARG:HG3	5:A:2280:HOH:O	2.15	0.42
1:A:411:ASN:H	1:A:411:ASN:HD22	1.66	0.42
1:A:124:VAL:CG2	1:A:172:PHE:HA	2.49	0.42
1:B:206:SER:HB3	1:B:240:TYR:CE1	2.55	0.42
1:D:206:SER:HB3	1:D:240:TYR:CE1	2.55	0.41
1:B:19:ASN:HD21	1:B:33:GLN:NE2	2.16	0.41
1:B:11:ILE:CG2	1:B:59:HIS:ND1	2.83	0.41
1:B:417:SER:HB3	1:B:420:VAL:CG1	2.50	0.41
1:E:145:ASN:ND2	5:E:2128:HOH:O	2.48	0.41
1:A:364:SER:OG	1:A:405:HIS:HD2	2.04	0.41
1:C:89:TYR:HE1	1:C:108:VAL:HG22	1.85	0.41
1:D:29:HIS:HE1	5:D:2018:HOH:O	2.04	0.41
1:D:403:ARG:HH21	1:D:405:HIS:HE1	1.68	0.40
1:A:256:TRP:CE2	1:A:258:GLN:HB3	2.56	0.40
1:D:71:HIS:ND1	1:D:93:ARG:HA	2.37	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	430/432 (100%)	411 (96%)	18 (4%)	1 (0%)	43	34
1	B	430/432 (100%)	412 (96%)	17 (4%)	1 (0%)	43	34
1	C	430/432 (100%)	414 (96%)	15 (4%)	1 (0%)	43	34
1	D	430/432 (100%)	414 (96%)	15 (4%)	1 (0%)	43	34
1	E	430/432 (100%)	414 (96%)	15 (4%)	1 (0%)	43	34
1	F	430/432 (100%)	412 (96%)	16 (4%)	2 (0%)	24	13
All	All	2580/2592 (100%)	2477 (96%)	96 (4%)	7 (0%)	36	26

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	351	ARG
1	F	199	GLU
1	D	98	ASN
1	E	98	ASN
1	B	389	SER
1	A	198	GLY
1	F	198	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	385/387 (100%)	361 (94%)	24 (6%)	16 4

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	387/387 (100%)	351 (91%)	36 (9%)	8	1
1	C	387/387 (100%)	359 (93%)	28 (7%)	13	3
1	D	386/387 (100%)	359 (93%)	27 (7%)	14	3
1	E	387/387 (100%)	358 (92%)	29 (8%)	12	2
1	F	386/387 (100%)	350 (91%)	36 (9%)	8	1
All	All	2318/2322 (100%)	2138 (92%)	180 (8%)	11	2

All (180) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	25	LYS
1	A	60	LEU
1	A	108	VAL
1	A	114	LEU
1	A	124	VAL
1	A	147	GLU
1	A	171	LEU
1	A	203	LEU
1	A	226	ASN
1	A	233	LEU
1	A	274	ASN
1	A	279	LEU
1	A	283	LEU
1	A	290	LEU
1	A	298	LEU
1	A	306	VAL
1	A	321	GLU
1	A	354	LEU
1	A	373	VAL
1	A	375	ASP
1	A	378	THR
1	A	411	ASN
1	A	415	VAL
1	A	421	LYS
1	B	1	LEU
1	B	60	LEU
1	B	81	LYS
1	B	96	THR
1	B	97	HIS
1	B	114	LEU

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Mol	Chain	Res	Type
1	B	124	VAL
1	B	134	HIS
1	B	159	LYS
1	B	162	ARG
1	B	199	GLU
1	B	200	LYS
1	B	211	ASN
1	B	220	LEU
1	B	230	ARG
1	B	233	LEU
1	B	257	LEU
1	B	269	LYS
1	B	274	ASN
1	B	279	LEU
1	B	283	LEU
1	B	290	LEU
1	B	298	LEU
1	B	302	ARG
1	B	303	LYS
1	B	304	ARG
1	B	316	LEU
1	B	320	LYS
1	B	349	LYS
1	B	354	LEU
1	B	355	ILE
1	B	373	VAL
1	B	376	GLU
1	B	397	SER
1	B	411	ASN
1	B	421	LYS
1	C	1	LEU
1	C	40	GLU
1	C	108	VAL
1	C	114	LEU
1	C	131	GLU
1	C	145	ASN
1	C	171	LEU
1	C	199	GLU
1	C	203	LEU
1	C	221	LYS
1	C	233	LEU
1	C	257	LEU

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Mol	Chain	Res	Type
1	C	274	ASN
1	C	279	LEU
1	C	283	LEU
1	C	290	LEU
1	C	298	LEU
1	C	303	LYS
1	C	304	ARG
1	C	320	LYS
1	C	331	SER
1	C	354	LEU
1	C	373	VAL
1	C	376	GLU
1	C	411	ASN
1	C	419	GLN
1	C	420	VAL
1	C	421	LYS
1	D	1	LEU
1	D	79	VAL
1	D	96	THR
1	D	114	LEU
1	D	131	GLU
1	D	133	THR
1	D	171	LEU
1	D	208	THR
1	D	220	LEU
1	D	226	ASN
1	D	233	LEU
1	D	257	LEU
1	D	259	SER
1	D	274	ASN
1	D	279	LEU
1	D	283	LEU
1	D	290	LEU
1	D	298	LEU
1	D	353	GLU
1	D	354	LEU
1	D	355	ILE
1	D	373	VAL
1	D	376	GLU
1	D	378	THR
1	D	411	ASN
1	D	415	VAL

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Mol	Chain	Res	Type
1	D	423	GLU
1	E	60	LEU
1	E	96	THR
1	E	97	HIS
1	E	114	LEU
1	E	124	VAL
1	E	127	LYS
1	E	133	THR
1	E	149	ARG
1	E	159	LYS
1	E	199	GLU
1	E	200	LYS
1	E	203	LEU
1	E	220	LEU
1	E	233	LEU
1	E	274	ASN
1	E	283	LEU
1	E	290	LEU
1	E	298	LEU
1	E	302	ARG
1	E	303	LYS
1	E	320	LYS
1	E	351	ARG
1	E	354	LEU
1	E	355	ILE
1	E	373	VAL
1	E	378	THR
1	E	411	ASN
1	E	420	VAL
1	E	421	LYS
1	F	1	LEU
1	F	60	LEU
1	F	96	THR
1	F	97	HIS
1	F	108	VAL
1	F	109	MET
1	F	114	LEU
1	F	127	LYS
1	F	142	ASN
1	F	169	ASP
1	F	199	GLU
1	F	203	LEU

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Mol	Chain	Res	Type
1	F	208	THR
1	F	211	ASN
1	F	220	LEU
1	F	224	LYS
1	F	229	LYS
1	F	257	LEU
1	F	259	SER
1	F	274	ASN
1	F	279	LEU
1	F	283	LEU
1	F	290	LEU
1	F	298	LEU
1	F	303	LYS
1	F	321	GLU
1	F	336	LEU
1	F	351	ARG
1	F	354	LEU
1	F	372	THR
1	F	373	VAL
1	F	376	GLU
1	F	378	THR
1	F	411	ASN
1	F	414	SER
1	F	420	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (55) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	19	ASN
1	A	29	HIS
1	A	43	ASN
1	A	98	ASN
1	A	211	ASN
1	A	235	HIS
1	A	405	HIS
1	A	411	ASN
1	B	7	HIS
1	B	19	ASN
1	B	29	HIS
1	B	56	HIS
1	B	59	HIS
1	B	173	HIS

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Mol	Chain	Res	Type
1	B	211	ASN
1	B	274	ASN
1	B	411	ASN
1	C	19	ASN
1	C	29	HIS
1	C	56	HIS
1	C	134	HIS
1	C	145	ASN
1	C	211	ASN
1	C	235	HIS
1	C	274	ASN
1	C	411	ASN
1	D	7	HIS
1	D	19	ASN
1	D	29	HIS
1	D	56	HIS
1	D	98	ASN
1	D	226	ASN
1	D	235	HIS
1	D	274	ASN
1	D	405	HIS
1	D	411	ASN
1	E	19	ASN
1	E	29	HIS
1	E	56	HIS
1	E	59	HIS
1	E	211	ASN
1	E	235	HIS
1	E	274	ASN
1	E	405	HIS
1	E	411	ASN
1	E	419	GLN
1	F	7	HIS
1	F	19	ASN
1	F	29	HIS
1	F	59	HIS
1	F	71	HIS
1	F	142	ASN
1	F	235	HIS
1	F	405	HIS
1	F	411	ASN

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 ⓘ

18 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	G	1	2	11,11,12	0.80	0	15,15,17	1.46	2 (13%)
2	FRU	G	2	2	11,12,12	2.01	1 (9%)	10,18,18	0.72	0
2	GLA	G	3	2	11,11,12	0.61	0	15,15,17	0.52	0
2	GLC	H	1	2	11,11,12	0.65	0	15,15,17	0.78	0
2	FRU	H	2	2	11,12,12	2.03	1 (9%)	10,18,18	0.47	0
2	GLA	H	3	2	11,11,12	0.54	0	15,15,17	0.59	0
2	GLC	I	1	2	11,11,12	0.62	0	15,15,17	0.84	1 (6%)
2	FRU	I	2	2	11,12,12	2.04	1 (9%)	10,18,18	0.62	0
2	GLA	I	3	2	11,11,12	0.56	0	15,15,17	0.52	0
2	GLC	J	1	2	11,11,12	0.97	1 (9%)	15,15,17	1.87	3 (20%)
2	FRU	J	2	2	11,12,12	1.96	1 (9%)	10,18,18	0.59	0
2	GLA	J	3	2	11,11,12	0.60	0	15,15,17	0.48	0
2	GLC	K	1	2	11,11,12	0.81	0	15,15,17	1.20	2 (13%)
2	FRU	K	2	2	11,12,12	2.02	1 (9%)	10,18,18	0.68	0
2	GLA	K	3	2	11,11,12	0.54	0	15,15,17	0.45	0
2	GLC	L	1	2	11,11,12	0.67	0	15,15,17	1.17	2 (13%)
2	FRU	L	2	2	11,12,12	2.02	1 (9%)	10,18,18	0.47	0
2	GLA	L	3	2	11,11,12	0.54	0	15,15,17	0.55	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	G	1	2	-	0/2/19/22	0/1/1/1
2	FRU	G	2	2	-	3/5/24/24	0/1/1/1
2	GLA	G	3	2	-	2/2/19/22	0/1/1/1
2	GLC	H	1	2	-	0/2/19/22	0/1/1/1
2	FRU	H	2	2	-	3/5/24/24	0/1/1/1
2	GLA	H	3	2	-	2/2/19/22	0/1/1/1
2	GLC	I	1	2	-	0/2/19/22	0/1/1/1
2	FRU	I	2	2	-	3/5/24/24	0/1/1/1
2	GLA	I	3	2	-	1/2/19/22	0/1/1/1
2	GLC	J	1	2	-	0/2/19/22	0/1/1/1
2	FRU	J	2	2	-	3/5/24/24	0/1/1/1
2	GLA	J	3	2	-	2/2/19/22	0/1/1/1
2	GLC	K	1	2	-	0/2/19/22	0/1/1/1
2	FRU	K	2	2	-	3/5/24/24	0/1/1/1
2	GLA	K	3	2	-	0/2/19/22	0/1/1/1
2	GLC	L	1	2	-	0/2/19/22	0/1/1/1
2	FRU	L	2	2	-	3/5/24/24	0/1/1/1
2	GLA	L	3	2	-	1/2/19/22	0/1/1/1

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	K	2	FRU	O6-C6	-6.56	1.14	1.42
2	I	2	FRU	O6-C6	-6.52	1.15	1.42
2	H	2	FRU	O6-C6	-6.45	1.15	1.42
2	G	2	FRU	O6-C6	-6.43	1.15	1.42
2	L	2	FRU	O6-C6	-6.40	1.15	1.42
2	J	2	FRU	O6-C6	-6.28	1.16	1.42
2	J	1	GLC	C4-C5	2.02	1.57	1.53

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	1	GLC	C1-O5-C5	-4.75	105.82	112.19
2	G	1	GLC	C1-O5-C5	-3.74	107.17	112.19
2	J	1	GLC	C1-C2-C3	-3.45	104.62	109.64
2	L	1	GLC	O5-C1-C2	-2.94	103.77	110.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	K	1	GLC	C1-O5-C5	-2.82	108.41	112.19
2	G	1	GLC	C1-C2-C3	-2.74	105.66	109.64
2	J	1	GLC	O5-C1-C2	2.65	117.11	110.79
2	I	1	GLC	C1-O5-C5	2.56	115.62	112.19
2	K	1	GLC	C1-C2-C3	-2.28	106.33	109.64
2	L	1	GLC	C1-O5-C5	2.21	115.14	112.19

There are no chirality outliers.

All (26) torsion outliers are listed below:

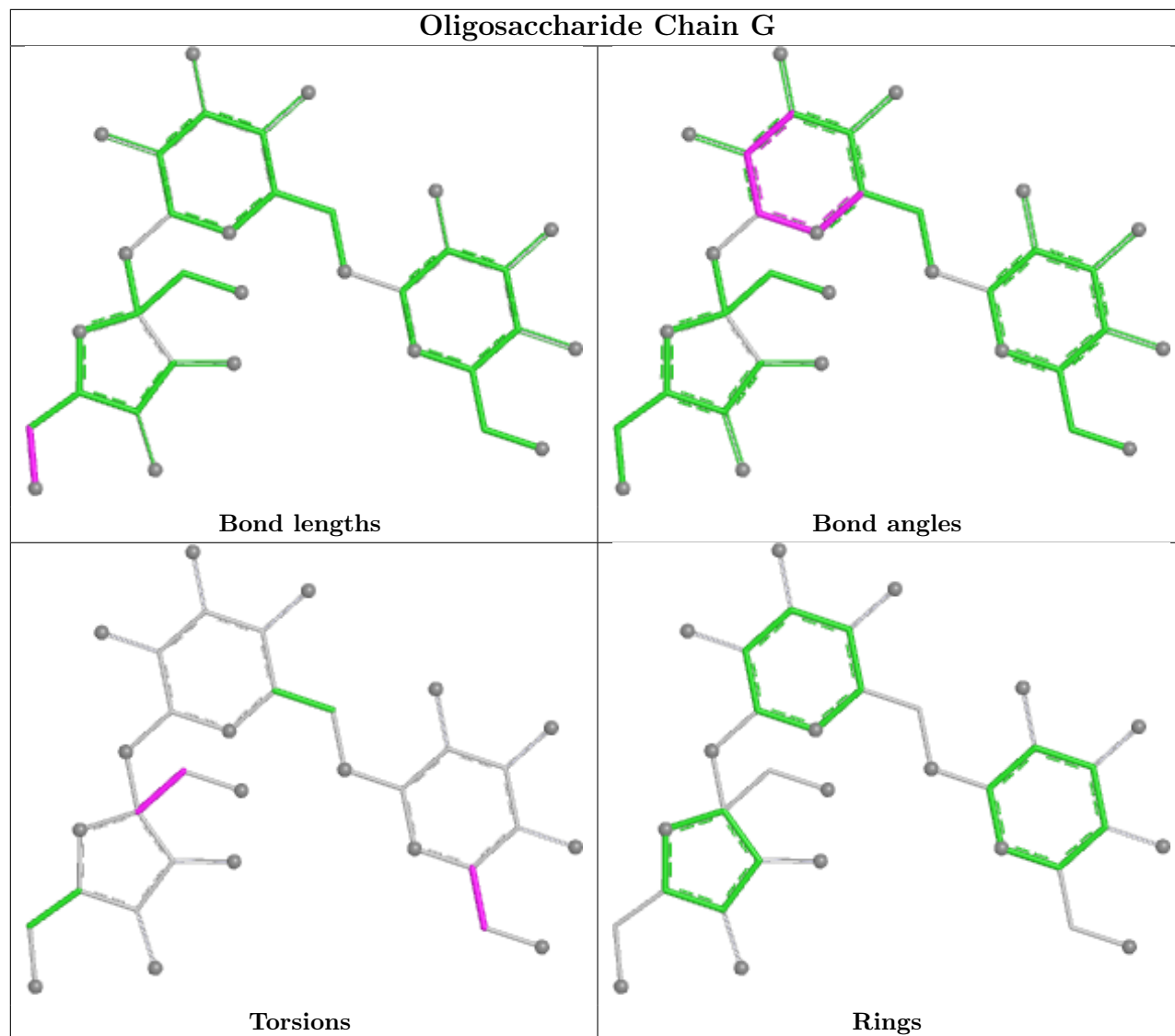
Mol	Chain	Res	Type	Atoms
2	G	2	FRU	O1-C1-C2-O2
2	H	2	FRU	O1-C1-C2-O2
2	I	2	FRU	O1-C1-C2-O2
2	J	2	FRU	O1-C1-C2-O2
2	K	2	FRU	O1-C1-C2-O2
2	L	2	FRU	O1-C1-C2-C3
2	L	2	FRU	O1-C1-C2-O2
2	G	3	GLA	O5-C5-C6-O6
2	L	2	FRU	O1-C1-C2-O5
2	J	3	GLA	O5-C5-C6-O6
2	H	3	GLA	O5-C5-C6-O6
2	H	2	FRU	O1-C1-C2-C3
2	I	2	FRU	O1-C1-C2-C3
2	H	2	FRU	O1-C1-C2-O5
2	I	2	FRU	O1-C1-C2-O5
2	J	2	FRU	O1-C1-C2-O5
2	K	2	FRU	O1-C1-C2-O5
2	L	3	GLA	O5-C5-C6-O6
2	G	2	FRU	O1-C1-C2-O5
2	G	2	FRU	O1-C1-C2-C3
2	J	2	FRU	O1-C1-C2-C3
2	K	2	FRU	O1-C1-C2-C3
2	I	3	GLA	C4-C5-C6-O6
2	G	3	GLA	C4-C5-C6-O6
2	H	3	GLA	C4-C5-C6-O6
2	J	3	GLA	C4-C5-C6-O6

There are no ring outliers.

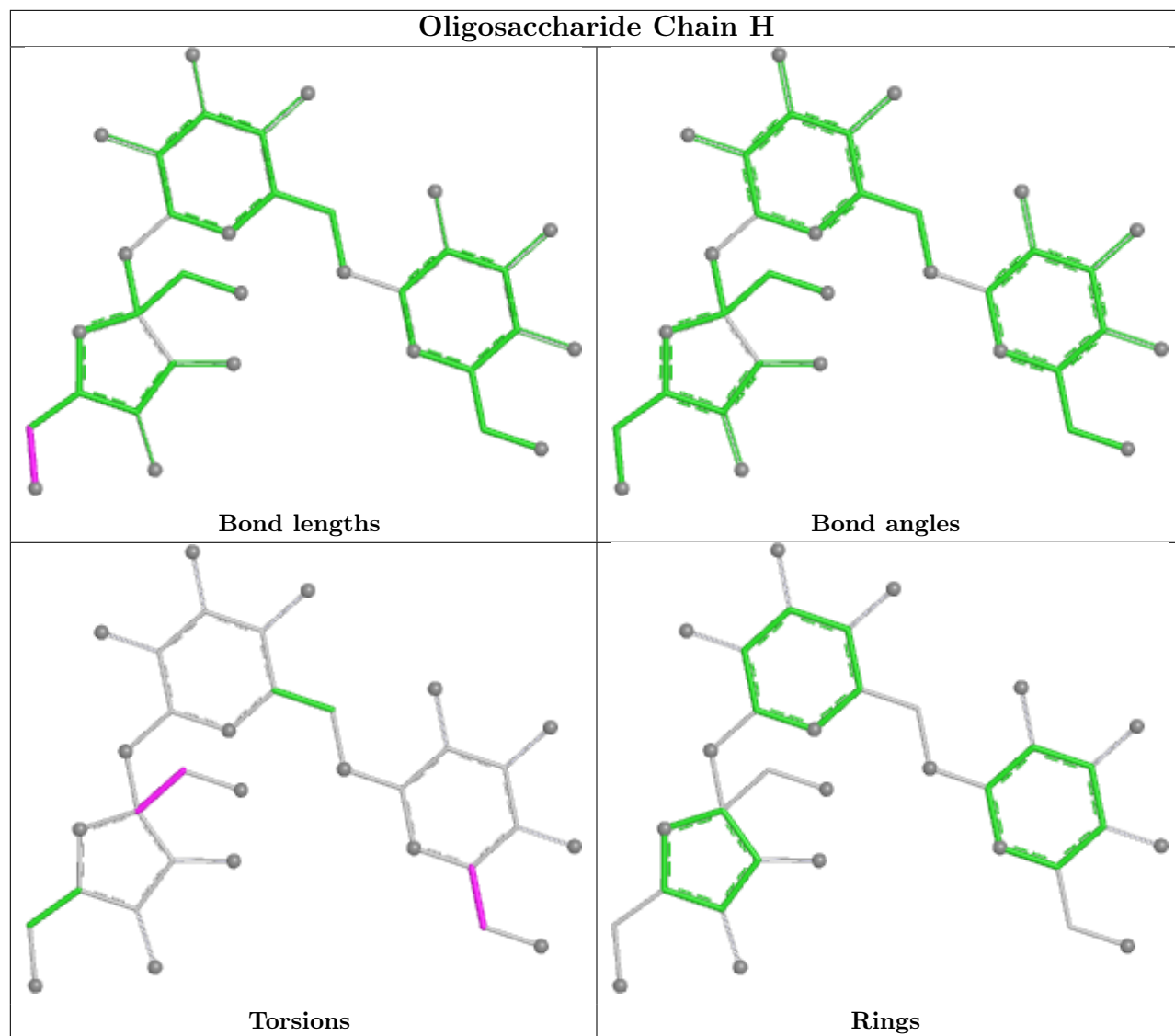
No monomer is involved in short contacts.

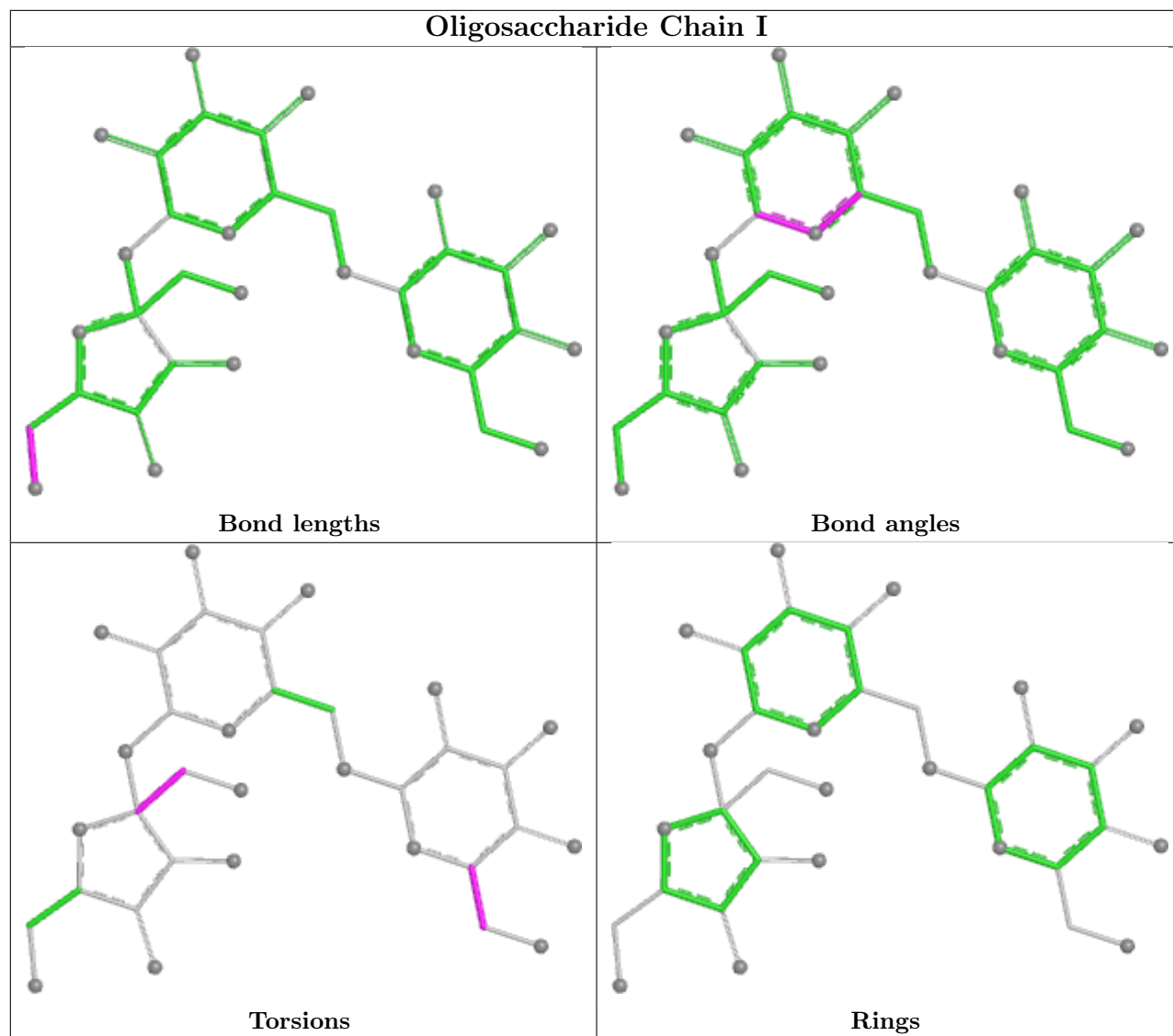
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

bond angles, torsion angles, and ring geometry for oligosaccharide.

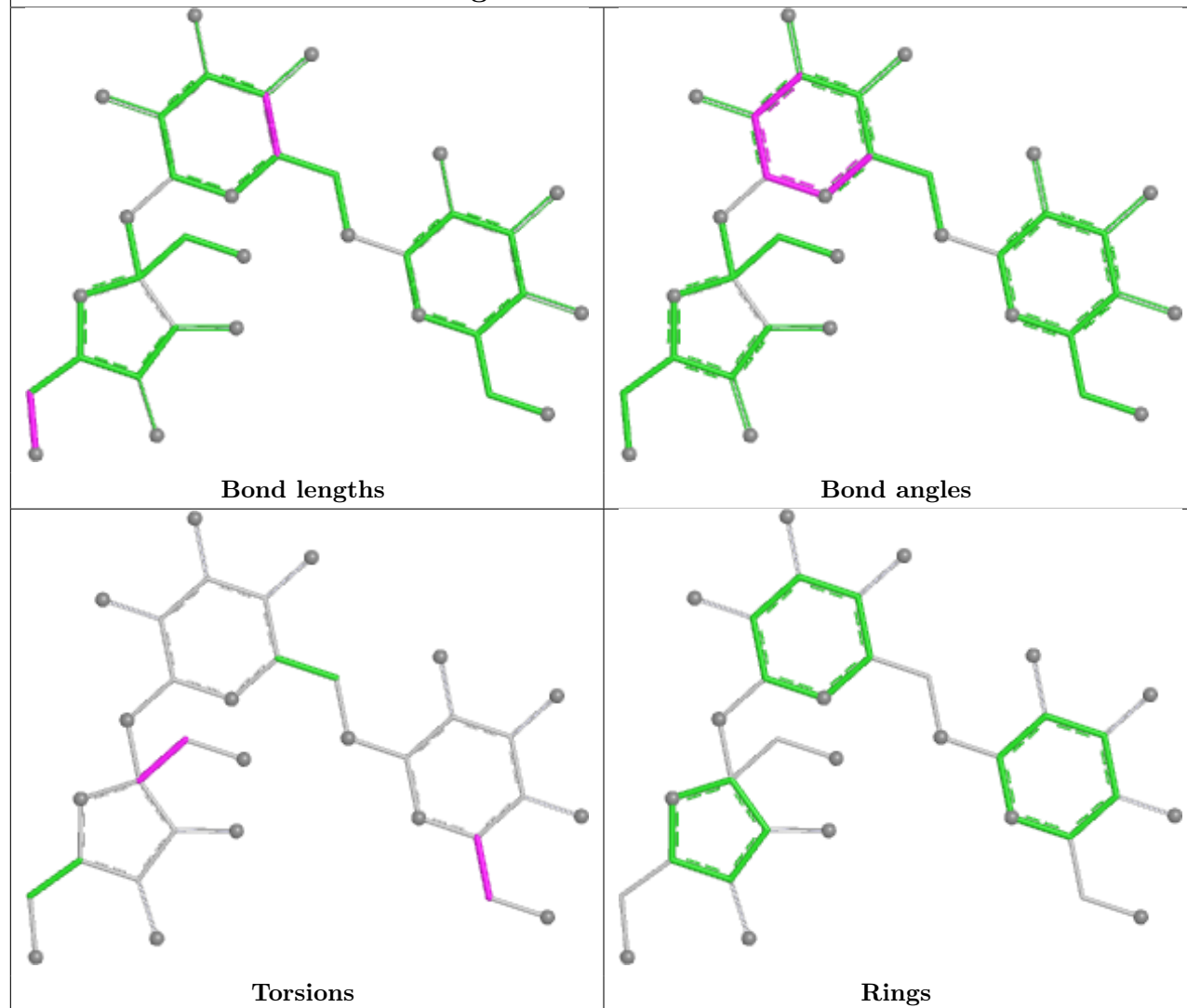


Oligosaccharide Chain H

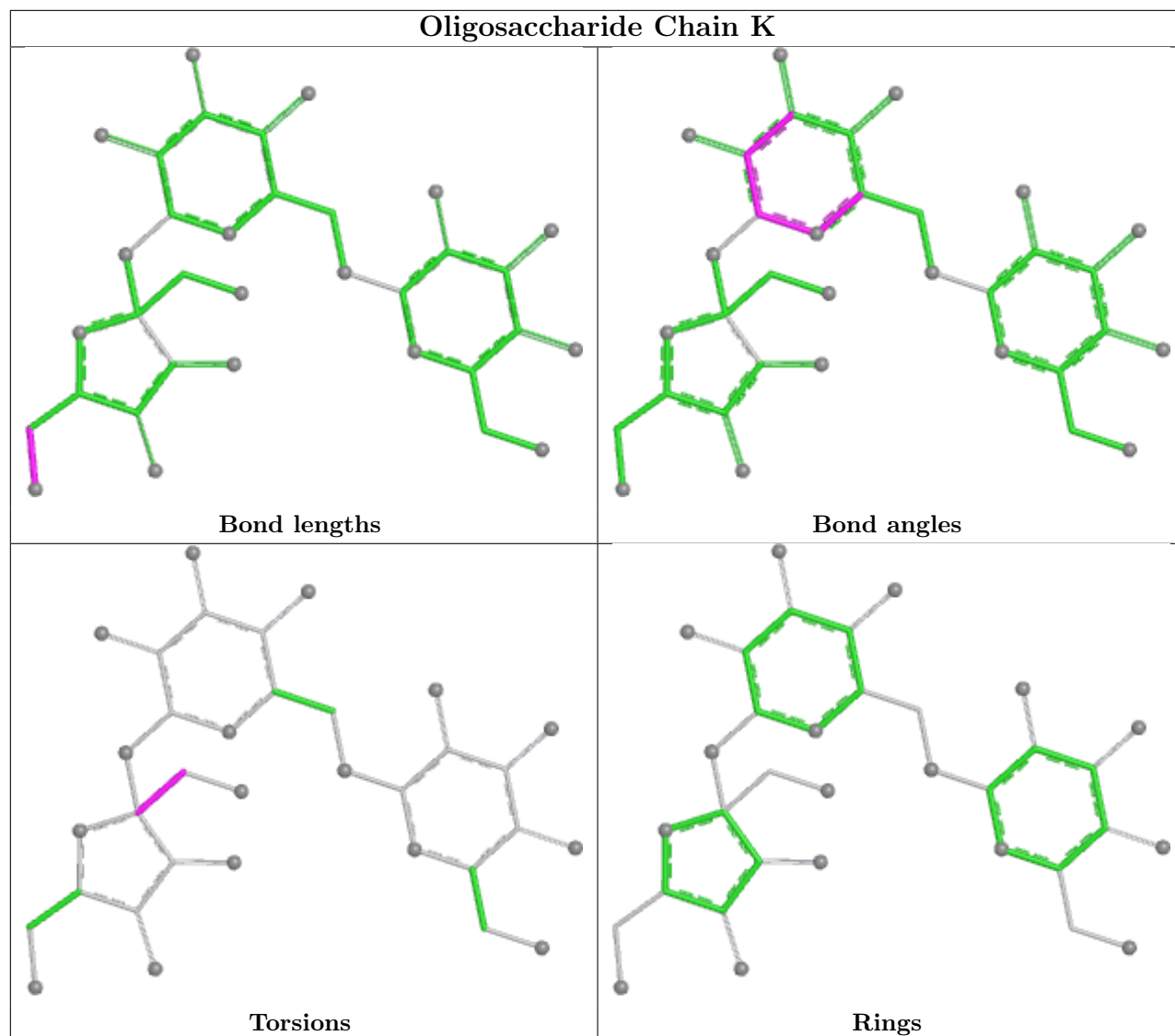


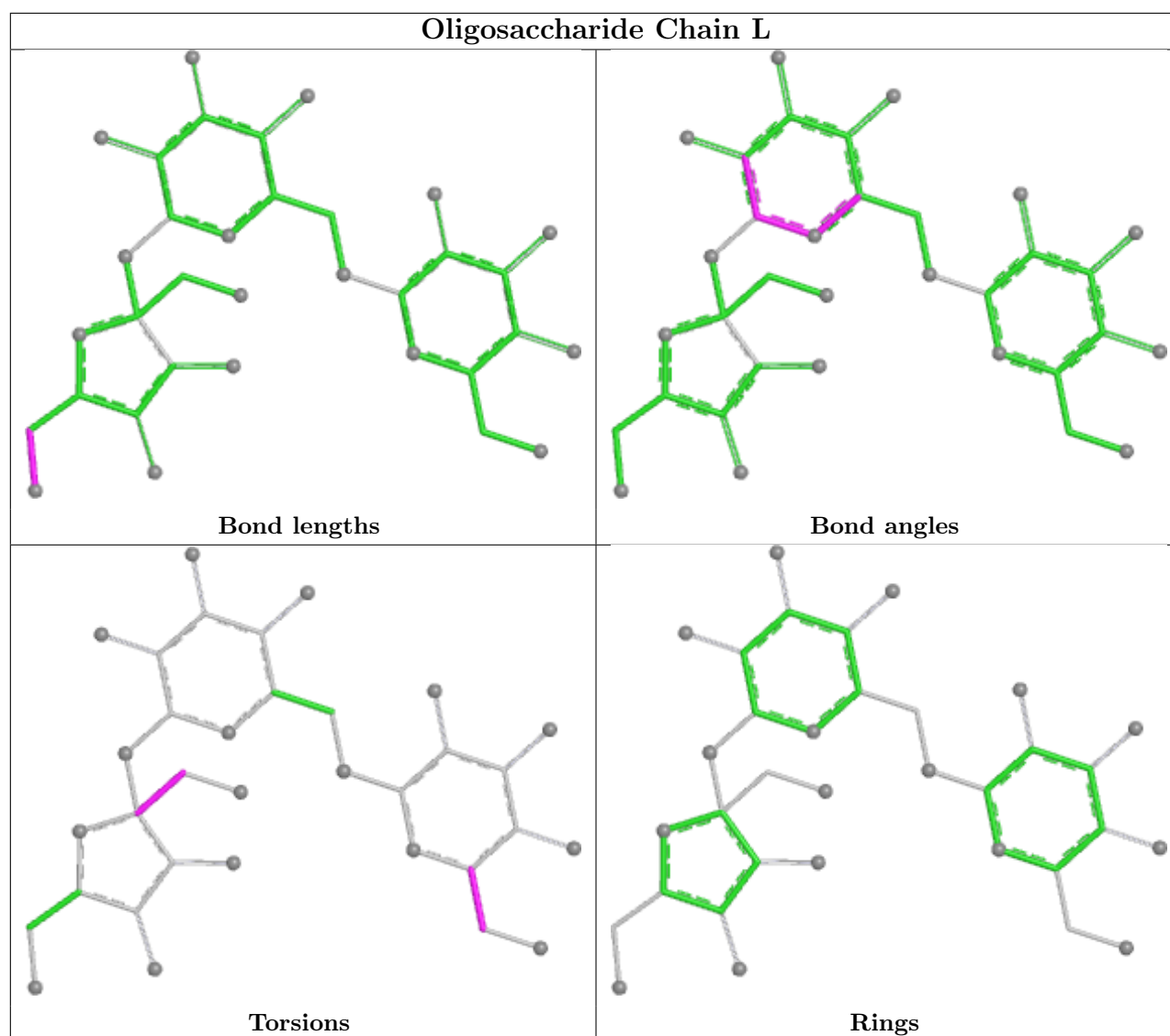


Oligosaccharide Chain J



Oligosaccharide Chain K





5.6 Ligand geometry [i](#)

5 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	SO4	C	1434	-	4,4,4	0.24	0	6,6,6	0.09	0
3	CIT	A	1433	-	12,12,12	1.10	0	17,17,17	1.69	5 (29%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	SO4	C	1433	-	4,4,4	0.23	0	6,6,6	0.34	0
4	SO4	B	1433	-	4,4,4	0.25	0	6,6,6	0.19	0
4	SO4	E	1433	-	4,4,4	0.42	0	6,6,6	0.87	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	CIT	A	1433	-	-	4/16/16/16	-

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1433	CIT	O6-C6-C3	3.24	119.35	113.14
3	A	1433	CIT	C4-C3-C2	3.17	117.45	109.31
3	A	1433	CIT	C2-C3-C6	-2.62	104.23	110.03
3	A	1433	CIT	C4-C3-C6	-2.05	105.50	110.03
3	A	1433	CIT	O4-C5-C4	2.01	120.72	114.35

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1433	CIT	C1-C2-C3-C6
3	A	1433	CIT	C1-C2-C3-O7
3	A	1433	CIT	C1-C2-C3-C4
3	A	1433	CIT	C2-C3-C4-C5

There are no ring outliers.

1 monomer is involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1433	CIT	6	0

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	C	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	C	80:GLU	C	81:LYS	N	1.63

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	432/432 (100%)	0.31	32 (7%)	20 23	7, 16, 28, 33	4 (0%)
1	B	432/432 (100%)	0.56	36 (8%)	17 19	8, 17, 28, 34	6 (1%)
1	C	432/432 (100%)	0.47	33 (7%)	20 22	7, 16, 27, 34	8 (1%)
1	D	432/432 (100%)	0.39	35 (8%)	18 20	8, 16, 27, 34	8 (1%)
1	E	432/432 (100%)	0.34	33 (7%)	20 22	8, 16, 28, 34	9 (2%)
1	F	432/432 (100%)	0.41	40 (9%)	14 16	7, 16, 27, 34	10 (2%)
All	All	2592/2592 (100%)	0.41	209 (8%)	18 20	7, 16, 28, 34	45 (1%)

All (209) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	100	GLY	6.9
1	D	96	THR	6.5
1	C	96	THR	6.2
1	C	97	HIS	5.9
1	D	98	ASN	5.8
1	D	100	GLY	5.7
1	E	97	HIS	5.5
1	A	418	ASN	5.4
1	D	134	HIS	5.3
1	B	96	THR	5.3
1	E	96	THR	5.2
1	F	96	THR	5.2
1	F	97	HIS	5.2
1	D	99	LYS	5.1
1	E	100	GLY	5.0
1	F	352	ASP	5.0
1	C	98	ASN	4.9
1	C	270	ARG	4.8
1	D	199	GLU	4.7

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Mol	Chain	Res	Type	RSRZ
1	D	1	LEU	4.7
1	E	98	ASN	4.7
1	C	99	LYS	4.7
1	F	1	LEU	4.6
1	C	352	ASP	4.5
1	F	287	ASN	4.5
1	B	100	GLY	4.4
1	D	418	ASN	4.4
1	B	97	HIS	4.3
1	E	99	LYS	4.3
1	C	351	ARG	4.3
1	B	350	SER	4.2
1	A	419	GLN	4.2
1	B	372	THR	4.2
1	C	134	HIS	4.1
1	A	134	HIS	4.1
1	E	134	HIS	4.1
1	C	132	GLY	4.0
1	D	419	GLN	4.0
1	F	100	GLY	4.0
1	B	99	LYS	4.0
1	B	352	ASP	3.9
1	B	287	ASN	3.8
1	F	134	HIS	3.7
1	E	198	GLY	3.7
1	B	173	HIS	3.7
1	B	230	ARG	3.7
1	D	352	ASP	3.7
1	F	98	ASN	3.7
1	F	99	LYS	3.6
1	D	97	HIS	3.6
1	D	360	ARG	3.6
1	B	134	HIS	3.5
1	F	208	THR	3.5
1	D	145	ASN	3.5
1	F	289	GLU	3.4
1	D	249	ASP	3.3
1	B	98	ASN	3.3
1	F	288	ASN	3.3
1	E	131	GLU	3.3
1	E	155	GLY	3.3
1	D	353	GLU	3.2

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Mol	Chain	Res	Type	RSRZ
1	C	173	HIS	3.2
1	F	360	ARG	3.2
1	C	350	SER	3.2
1	A	249	ASP	3.2
1	B	351	ARG	3.2
1	A	372	THR	3.1
1	C	377	ALA	3.1
1	E	378	THR	3.1
1	A	373	VAL	3.1
1	B	82	ASP	3.1
1	D	209	SER	3.1
1	A	198	GLY	3.1
1	E	352	ASP	3.1
1	B	375	ASP	3.0
1	F	142	ASN	3.0
1	C	133	THR	3.0
1	B	131	GLU	3.0
1	C	155	GLY	3.0
1	E	95	PRO	3.0
1	D	311	LYS	3.0
1	A	208	THR	3.0
1	F	158	GLU	3.0
1	F	133	THR	2.9
1	E	303	LYS	2.9
1	E	101	GLU	2.9
1	D	287	ASN	2.9
1	A	318	ASP	2.9
1	A	374	GLU	2.8
1	C	333	GLU	2.8
1	B	332	GLY	2.8
1	A	1	LEU	2.8
1	C	355	ILE	2.8
1	D	230	ARG	2.8
1	F	419	GLN	2.8
1	F	378	THR	2.8
1	C	376	GLU	2.7
1	F	222	GLU	2.7
1	D	157	ASP	2.7
1	C	45	CYS	2.7
1	C	375	ASP	2.7
1	F	312	SER	2.7
1	A	375	ASP	2.7

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Mol	Chain	Res	Type	RSRZ
1	F	120	ASP	2.7
1	D	374	GLU	2.7
1	A	156	LYS	2.7
1	A	287	ASN	2.7
1	B	355	ILE	2.7
1	B	373	VAL	2.7
1	A	100	GLY	2.6
1	A	169	ASP	2.6
1	E	158	GLU	2.6
1	B	185	THR	2.6
1	B	328	CYS	2.6
1	C	419	GLN	2.6
1	B	184	GLU	2.6
1	A	56	HIS	2.6
1	E	1	LEU	2.6
1	B	341	GLU	2.6
1	E	375	ASP	2.6
1	C	373	VAL	2.6
1	B	208	THR	2.6
1	D	372	THR	2.6
1	D	133	THR	2.5
1	B	1	LEU	2.5
1	D	132	GLY	2.5
1	F	198	GLY	2.5
1	B	418	ASN	2.5
1	E	211	ASN	2.5
1	C	48	HIS	2.5
1	F	45	CYS	2.5
1	A	132	GLY	2.5
1	E	288	ASN	2.5
1	C	131	GLU	2.5
1	F	229	LYS	2.4
1	F	199	GLU	2.4
1	B	303	LYS	2.4
1	C	249	ASP	2.3
1	F	336	LEU	2.3
1	F	40	GLU	2.3
1	E	135	ALA	2.3
1	B	142	ASN	2.3
1	D	158	GLU	2.3
1	C	208	THR	2.3
1	E	132	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	289	GLU	2.3
1	F	101	GLU	2.3
1	E	220	LEU	2.3
1	A	142	ASN	2.3
1	A	288	ASN	2.3
1	A	221	LYS	2.3
1	E	332	GLY	2.3
1	A	415	VAL	2.3
1	D	378	THR	2.3
1	C	129	PRO	2.2
1	F	131	GLU	2.2
1	F	350	SER	2.2
1	F	157	ASP	2.2
1	A	145	ASN	2.2
1	C	145	ASN	2.2
1	D	135	ALA	2.2
1	A	97	HIS	2.2
1	E	226	ASN	2.2
1	F	156	LYS	2.2
1	D	131	GLU	2.2
1	C	378	THR	2.2
1	E	120	ASP	2.2
1	E	421	LYS	2.2
1	B	374	GLU	2.2
1	A	378	THR	2.2
1	B	377	ALA	2.2
1	A	421	LYS	2.2
1	B	187	LYS	2.2
1	C	127	LYS	2.2
1	B	288	ASN	2.1
1	A	199	GLU	2.1
1	B	420	VAL	2.1
1	D	373	VAL	2.1
1	D	198	GLY	2.1
1	E	199	GLU	2.1
1	D	226	ASN	2.1
1	B	318	ASP	2.1
1	E	157	ASP	2.1
1	E	350	SER	2.1
1	D	79	VAL	2.1
1	F	421	LYS	2.1
1	E	129	PRO	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	226	ASN	2.1
1	E	160	ILE	2.1
1	A	270	ARG	2.1
1	A	131	GLU	2.1
1	E	133	THR	2.1
1	E	372	THR	2.1
1	C	198	GLY	2.1
1	D	211	ASN	2.1
1	F	420	VAL	2.1
1	C	149	ARG	2.1
1	F	230	ARG	2.1
1	A	159	LYS	2.0
1	F	132	GLY	2.0
1	A	360	ARG	2.0
1	F	351	ARG	2.0
1	B	376	GLU	2.0
1	D	130	GLU	2.0
1	F	329	GLU	2.0
1	F	160	ILE	2.0
1	B	211	ASN	2.0
1	C	211	ASN	2.0
1	F	304	ARG	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.

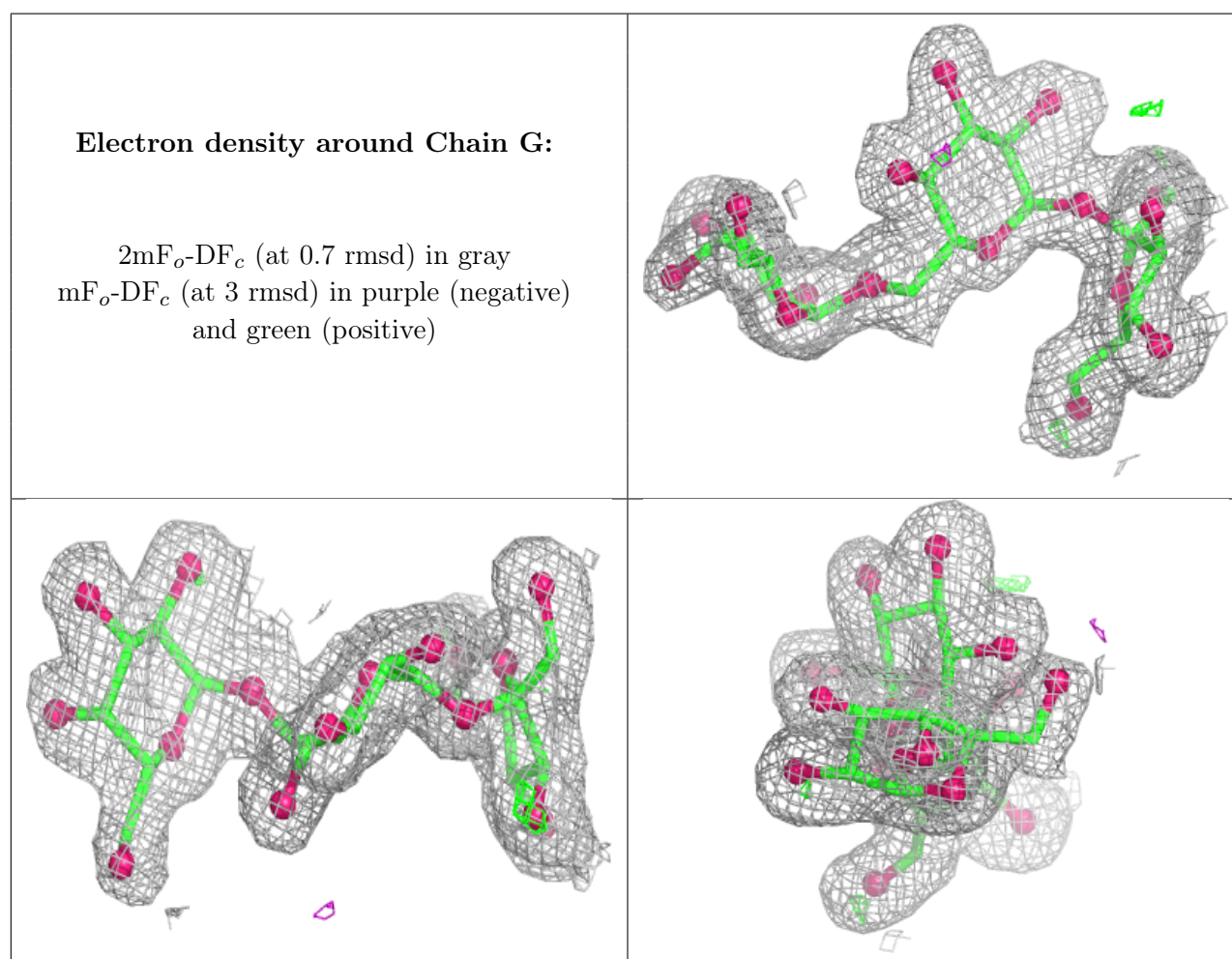
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	FRU	I	2	12/12	0.68	0.18	24,28,29,31	0
2	GLA	I	3	11/12	0.71	0.14	43,44,45,45	0
2	GLA	H	3	11/12	0.77	0.13	41,42,42,43	0
2	GLC	H	1	11/12	0.78	0.14	31,33,34,36	0
2	GLA	L	3	11/12	0.78	0.12	33,35,36,36	0
2	FRU	H	2	12/12	0.79	0.13	25,27,27,29	0

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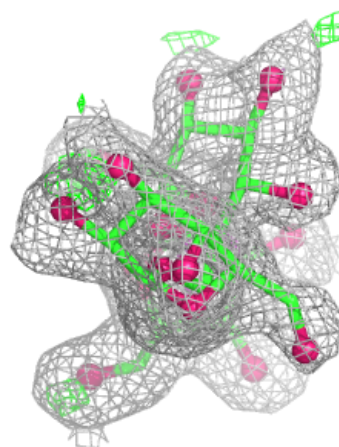
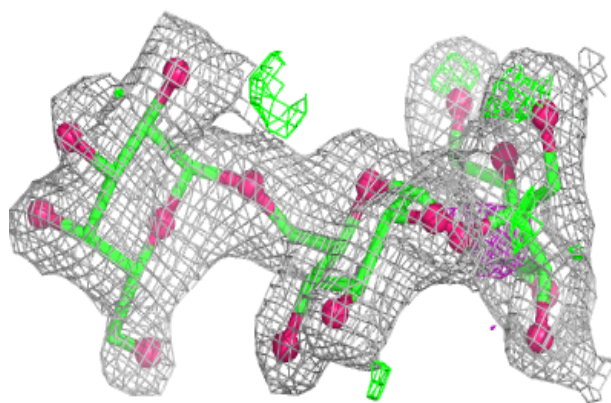
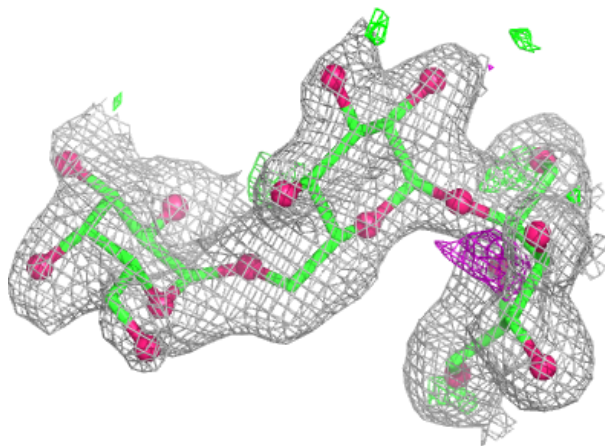
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	GLC	I	1	11/12	0.80	0.13	33,34,36,37	0
2	FRU	K	2	12/12	0.81	0.13	21,23,25,25	0
2	GLA	G	3	11/12	0.83	0.12	29,30,31,31	0
2	GLA	J	3	11/12	0.84	0.11	29,31,32,32	0
2	GLA	K	3	11/12	0.86	0.11	35,36,37,38	0
2	GLC	K	1	11/12	0.87	0.10	27,28,29,30	0
2	GLC	L	1	11/12	0.88	0.09	23,24,25,26	0
2	FRU	L	2	12/12	0.88	0.10	18,19,20,21	0
2	FRU	J	2	12/12	0.88	0.10	16,17,18,19	0
2	GLC	J	1	11/12	0.90	0.10	20,21,22,24	0
2	FRU	G	2	12/12	0.90	0.09	17,19,20,21	0
2	GLC	G	1	11/12	0.90	0.08	23,24,25,27	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.



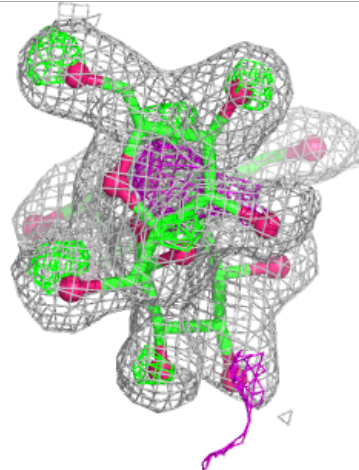
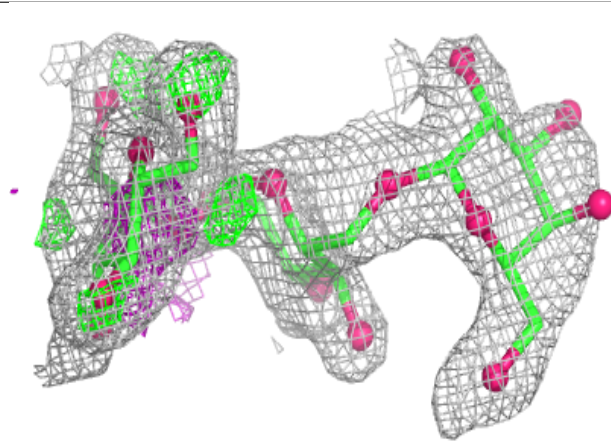
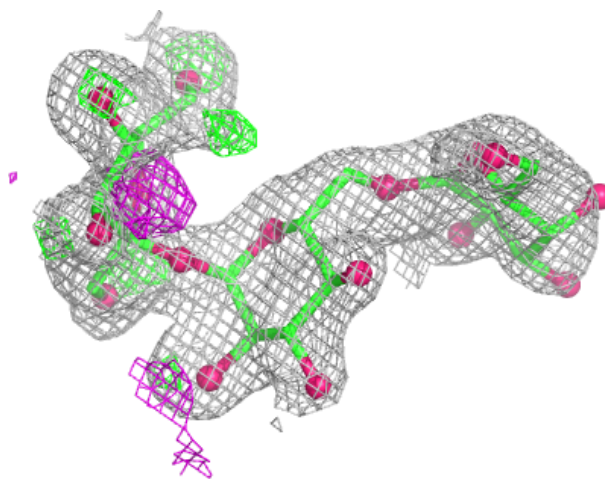
Electron density around Chain H:

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



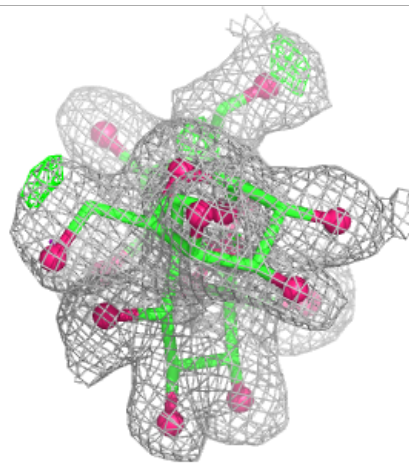
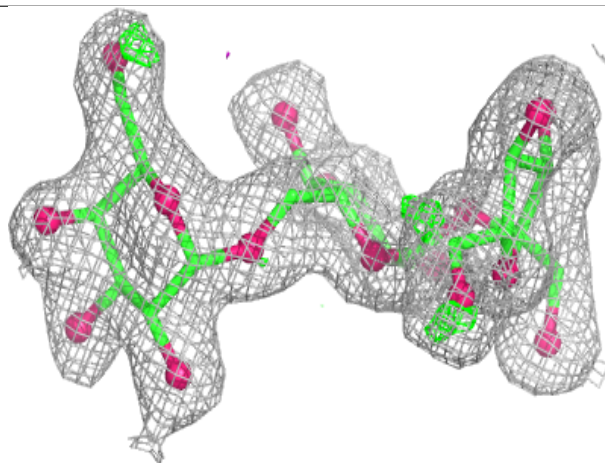
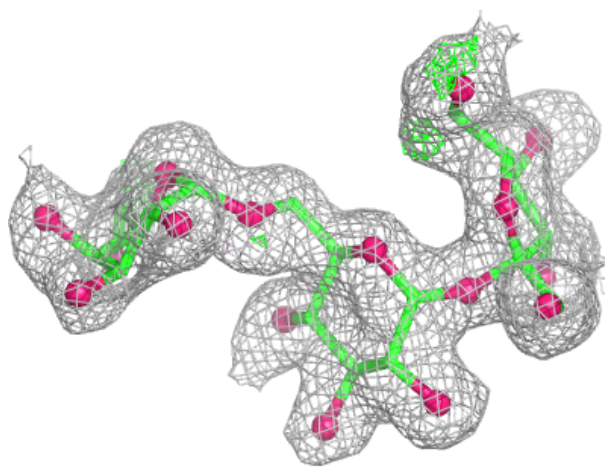
Electron density around Chain I:

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



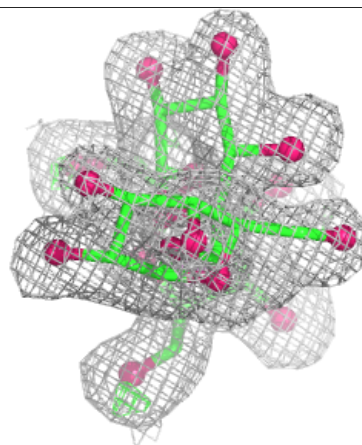
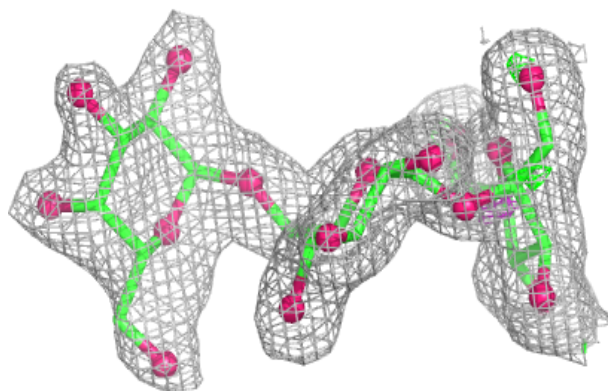
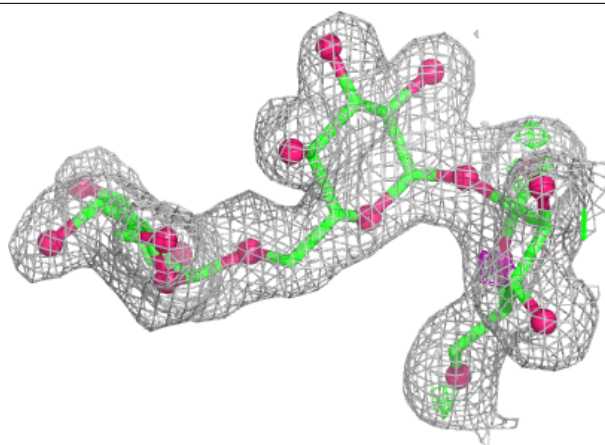
Electron density around Chain J:

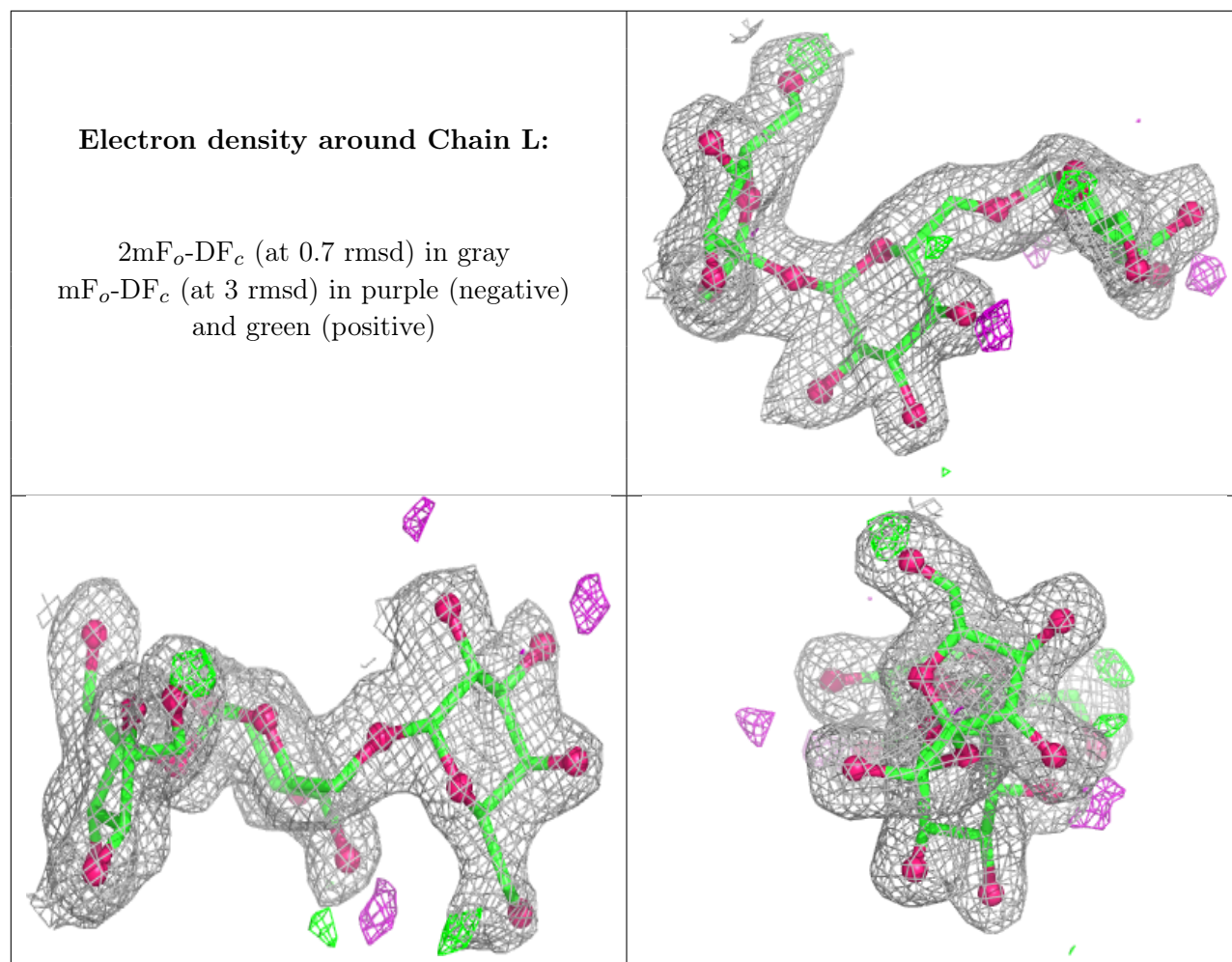
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around Chain K:

$2mF_o - DF_c$ (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
3	CIT	A	1433	13/13	0.72	0.21	50,51,51,52	0
4	SO4	B	1433	5/5	0.77	0.18	43,44,44,45	0
4	SO4	C	1434	5/5	0.78	0.21	44,45,45,46	0
4	SO4	C	1433	5/5	0.84	0.36	2,2,13,14	0
4	SO4	E	1433	5/5	0.92	0.35	2,2,2,2	0

6.5 Other polymers [i](#)

There are no such residues in this entry.