



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 04:00 PM UTC

PDB ID : 7YX8 / pdb_00007yx8
Title : Crystal structure of the AM0627 (E326A) inactive mutant in complex with PSGL-1-like bis-T glycopeptide and Zn²⁺
Authors : Taleb, V.; Liao, Q.; Narimatsu, Y.; Garcia-Garcia, A.; Companon, I.; Borges, R.J.; Gonzalez-Ramirez, A.M.; Corzana, F.; Clausen, H.; Rovira, C.; Hurtado-Guerrero, R.
Deposited on : 2022-02-15
Resolution : 1.50 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

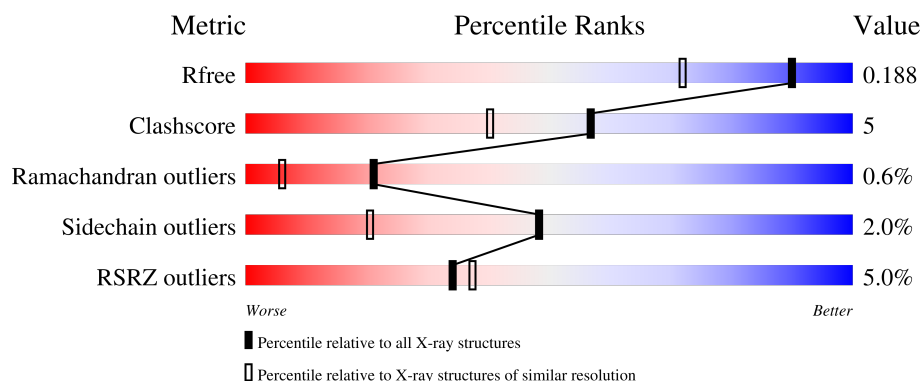
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.50 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.



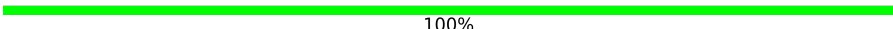
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	4037 (1.50-1.50)
Clashscore	190562	4235 (1.50-1.50)
Ramachandran outliers	187476	4153 (1.50-1.50)
Sidechain outliers	187428	4150 (1.50-1.50)
RSRZ outliers	180081	4039 (1.50-1.50)

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	441	2% 91% 9%
1	B	441	5% 91% 8%
2	F	10	70% 10% 40% 30% 20%
2	H	10	80% 20% 20% 30% 20% 10%

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Mol	Chain	Length	Quality of chain
3	C	2	 50% 50%
3	D	2	 50% 50%
3	E	2	 50% 50%
3	G	2	 100%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 8088 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 Peptidase M60 domain-containing protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	440	Total	C	N	O	S	0	1	0
			3521	2254	594	657	16			
1	B	438	Total	C	N	O	S	0	3	0
			3527	2261	596	653	17			

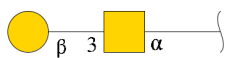
There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-4	GLY	-	expression tag	UNP B2UPI7
A	-3	GLY	-	expression tag	UNP B2UPI7
A	-2	GLY	-	expression tag	UNP B2UPI7
A	-1	GLY	-	expression tag	UNP B2UPI7
A	0	GLY	-	expression tag	UNP B2UPI7
A	326	ALA	GLU	engineered mutation	UNP B2UPI7
B	-4	GLY	-	expression tag	UNP B2UPI7
B	-3	GLY	-	expression tag	UNP B2UPI7
B	-2	GLY	-	expression tag	UNP B2UPI7
B	-1	GLY	-	expression tag	UNP B2UPI7
B	0	GLY	-	expression tag	UNP B2UPI7
B	326	ALA	GLU	engineered mutation	UNP B2UPI7

- Molecule 2 is a protein called PSGL-1-like bis-T glycopeptide.

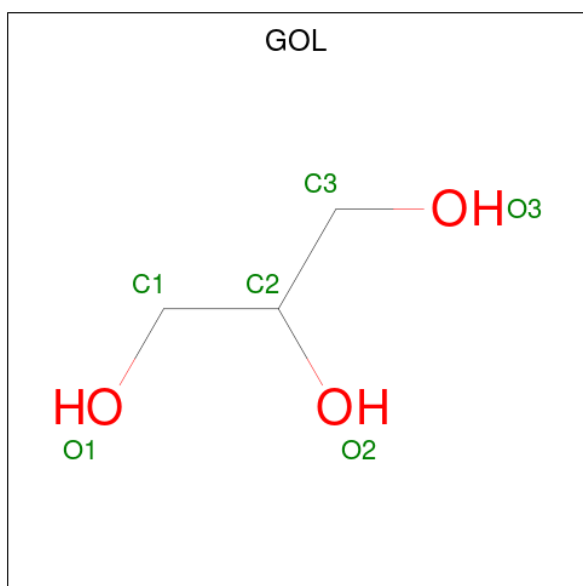
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	F	8	Total	C	N	O	0	0	1
			52	30	9	13			
2	H	9	Total	C	N	O	0	0	1
			59	35	10	14			

- Molecule 3 is an oligosaccharide called beta-D-galactopyranose-(1-3)-2-acetamido-2-deoxy-alpha-D-galactopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	D	2	Total	C	N	O	0	0	0
			25	14	1	10			
3	C	2	Total	C	N	O	0	0	0
			25	14	1	10			
3	G	2	Total	C	N	O	0	0	0
			25	14	1	10			
3	E	2	Total	C	N	O	0	0	0
			25	14	1	10			

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



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

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

- Molecule 5 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Zn	0	0
			1	1		
5	B	1	Total	Zn	0	0
			1	1		

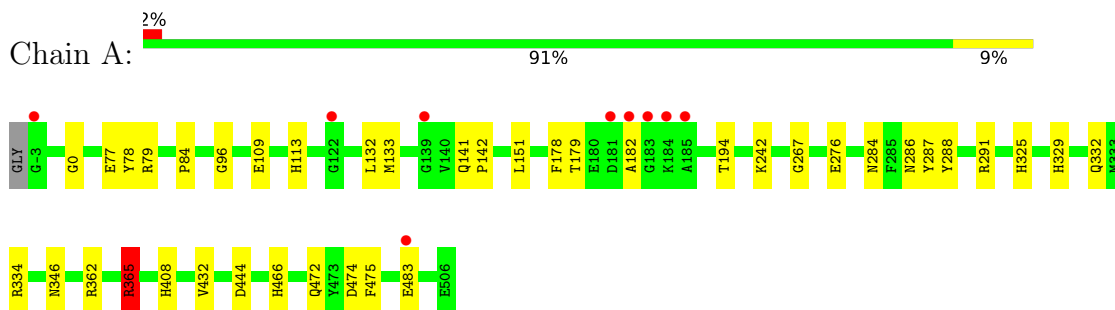
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	425	Total	O	0	0
			425	425		
6	B	325	Total	O	0	0
			325	325		
6	F	6	Total	O	0	0
			6	6		
6	H	11	Total	O	0	0
			11	11		

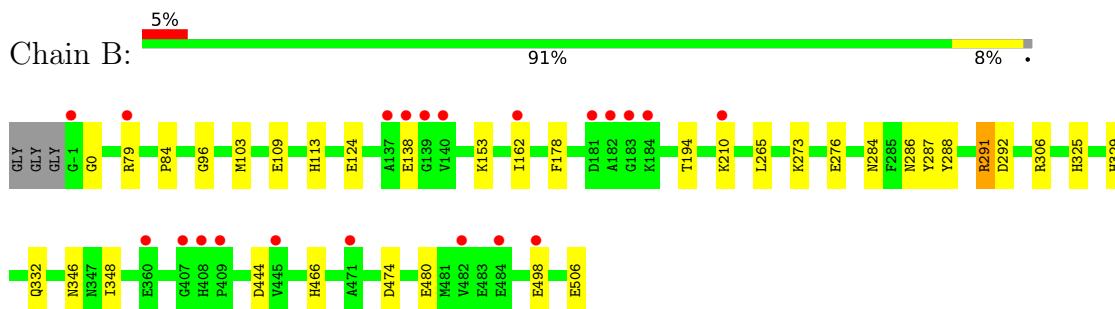
3 Residue-property plots

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.

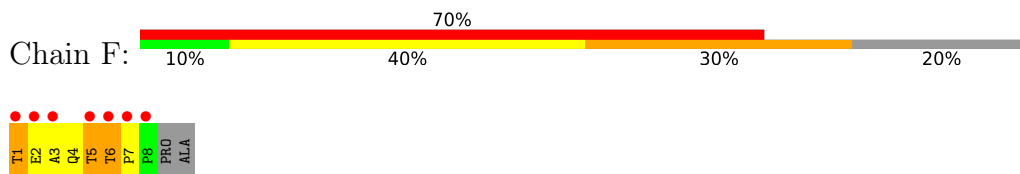
- Molecule 1: Peptidase M60 domain-containing protein



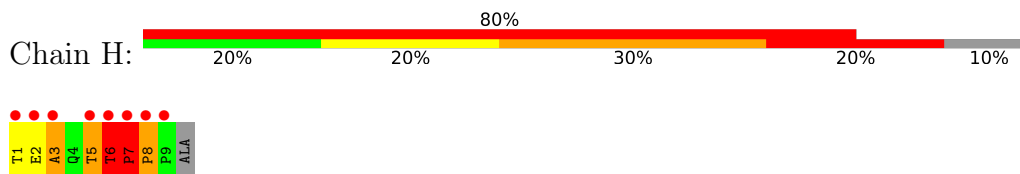
- Molecule 1: Peptidase M60 domain-containing protein



- Molecule 2: PSGL-1-like bis-T glycopeptide



- Molecule 2: PSGL-1-like bis-T glycopeptide



- Molecule 3: beta-D-galactopyranose-(1-3)-2-acetamido-2-deoxy-alpha-D-galactopyranose

Chain D:  50% 50%



- Molecule 3: beta-D-galactopyranose-(1-3)-2-acetamido-2-deoxy-alpha-D-galactopyranose

Chain C:  50% 50%



- Molecule 3: beta-D-galactopyranose-(1-3)-2-acetamido-2-deoxy-alpha-D-galactopyranose

Chain G:  100%



- Molecule 3: beta-D-galactopyranose-(1-3)-2-acetamido-2-deoxy-alpha-D-galactopyranose

Chain E:  50% 50%



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	73.14Å 82.69Å 172.61Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	86.30 – 1.50 86.30 – 1.50	Depositor EDS
% Data completeness (in resolution range)	100.0 (86.30-1.50) 100.0 (86.30-1.50)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.58 (at 1.50Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.167 , 0.182 0.175 , 0.188	Depositor DCC
R_{free} test set	6722 reflections (4.01%)	wwPDB-VP
Wilson B-factor (Å ²)	22.6	Xtriage
Anisotropy	0.354	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 29.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	8088	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.08% 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: ZN, GOL, A2G, GAL

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	0.89	1/3615 (0.0%)	1.08	2/4887 (0.0%)
1	B	0.90	1/3627 (0.0%)	1.11	4/4901 (0.1%)
2	F	1.59	1/52 (1.9%)	2.11	3/72 (4.2%)
2	H	2.26	3/60 (5.0%)	2.82	11/84 (13.1%)
All	All	0.92	6/7354 (0.1%)	1.13	20/9944 (0.2%)

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	0	GLY	C-N	10.79	1.46	1.33
2	H	7	PRO	CA-C	-9.81	1.43	1.52
1	A	0	GLY	C-N	9.61	1.46	1.33
2	H	6	THR	CA-C	5.71	1.60	1.52
2	H	8	PRO	CA-C	-5.46	1.41	1.52
2	F	6	THR	CA-C	5.08	1.59	1.52

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	0	GLY	O-C-N	8.63	130.40	121.77
1	A	0	GLY	O-C-N	8.56	130.33	121.77
2	H	7	PRO	N-CD-CG	-7.33	92.20	103.20
2	H	7	PRO	CA-N-CD	-7.20	101.92	112.00
2	H	7	PRO	N-CA-C	6.75	118.94	110.70
2	H	5	THR	N-CA-C	6.43	118.35	109.29
1	B	506	GLU	CA-C-O	-6.31	110.08	120.80
1	A	365	ARG	CG-CD-NE	6.23	125.71	112.00
2	H	8	PRO	CA-N-CD	-5.93	103.70	112.00
2	H	3	ALA	N-CA-C	5.63	117.86	109.59
2	F	5	THR	CA-C-N	5.45	135.09	121.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	5	THR	C-N-CA	5.45	135.09	121.80
2	F	7	PRO	CA-N-CD	-5.43	104.40	112.00
2	H	5	THR	N-CA-CB	-5.42	102.29	108.96
1	B	0	GLY	CA-C-N	-5.30	114.78	120.03
1	B	0	GLY	C-N-CA	-5.30	114.78	120.03
2	H	5	THR	CA-C-O	5.21	124.91	119.91
2	H	6	THR	CA-C-N	5.15	125.69	120.38
2	H	6	THR	C-N-CA	5.15	125.69	120.38
2	H	6	THR	CB-CA-C	5.12	120.27	110.17

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	3521	0	3442	31	0
1	B	3527	0	3467	20	0
2	F	52	0	47	7	0
2	H	59	0	54	9	0
3	C	25	0	21	2	0
3	D	25	0	21	0	0
3	E	25	0	21	1	0
3	G	25	0	21	0	0
4	A	48	0	64	8	0
4	B	12	0	16	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
6	A	425	0	0	5	0
6	B	325	0	0	4	0
6	F	6	0	0	7	0
6	H	11	0	0	6	0
All	All	8088	0	7174	66	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 5.

All (66) 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)
2:F:6:THR:HA	6:F:102:HOH:O	1.74	0.87
1:A:362:ARG:HH21	4:A:606:GOL:H2	1.45	0.82
1:B:284:ASN:HD21	1:B:287:TYR:H	1.29	0.80
1:A:284:ASN:HD21	1:A:287:TYR:H	1.28	0.79
6:F:102:HOH:O	3:C:1:A2G:H8A	1.85	0.75
2:H:7:PRO:HD3	6:H:109:HOH:O	1.86	0.75
1:A:365:ARG:HG2	1:A:365:ARG:HH11	1.53	0.73
2:F:6:THR:CA	6:F:102:HOH:O	2.35	0.73
1:A:329:HIS:HD1	1:A:332:GLN:HE22	1.38	0.71
1:A:133:MET:HG2	4:A:605:GOL:H11	1.73	0.70
1:B:210:LYS:HE3	6:B:918:HOH:O	1.92	0.68
1:B:329:HIS:HD1	1:B:332:GLN:HE22	1.40	0.67
2:F:1:THR:HG21	6:F:104:HOH:O	1.97	0.63
1:A:329:HIS:HD1	1:A:332:GLN:NE2	1.97	0.63
1:B:329:HIS:HD1	1:B:332:GLN:NE2	1.98	0.62
2:H:6:THR:HA	6:H:101:HOH:O	2.00	0.61
1:A:109:GLU:O	1:A:113:HIS:HE1	1.83	0.60
1:A:267:GLY:HA2	6:A:709:HOH:O	1.99	0.60
1:A:179:THR:CG2	1:A:182:ALA:HA	2.32	0.60
1:A:408:HIS:HD2	6:A:884:HOH:O	1.84	0.59
1:B:109:GLU:O	1:B:113:HIS:HE1	1.84	0.59
1:A:284:ASN:ND2	1:A:286:ASN:H	2.01	0.59
1:A:78:TYR:CE2	4:A:602:GOL:H2	2.41	0.56
1:B:284:ASN:ND2	1:B:286:ASN:H	2.04	0.56
6:H:101:HOH:O	3:E:1:A2G:H8A	2.04	0.56
1:A:79:ARG:NH2	1:A:276:GLU:OE2	2.40	0.55
1:B:292:ASP:HB2	2:F:2:GLU:HG2	1.89	0.54
2:H:6:THR:C	2:H:8:PRO:HD3	2.33	0.54
1:B:113:HIS:HD2	1:B:194:THR:OG1	1.92	0.53
6:F:102:HOH:O	3:C:1:A2G:C8	2.51	0.52
2:H:6:THR:CA	6:H:101:HOH:O	2.55	0.51
1:A:113:HIS:HD2	1:A:194:THR:OG1	1.93	0.51
1:B:79:ARG:NH2	1:B:276:GLU:OE2	2.42	0.51
1:A:291:ARG:O	2:H:3:ALA:HA	2.11	0.50
1:B:291:ARG:O	2:F:3:ALA:HA	2.12	0.50
1:A:78:TYR:CD2	4:A:602:GOL:H2	2.47	0.49
1:B:103[A]:MET:HE3	6:B:890:HOH:O	2.12	0.49
1:A:334:ARG:NH1	6:A:707:HOH:O	2.46	0.47
1:A:113:HIS:CD2	1:A:194:THR:OG1	2.68	0.47
1:B:113:HIS:CD2	1:B:194:THR:OG1	2.68	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:5:THR:C	6:F:102:HOH:O	2.59	0.46
1:B:466:HIS:HD2	1:B:474:ASP:OD1	1.99	0.46
1:A:466:HIS:HD2	1:A:474:ASP:OD1	1.99	0.46
1:B:306:ARG:HD2	6:B:721:HOH:O	2.16	0.45
1:A:287:TYR:OH	2:H:7:PRO:HA	2.17	0.45
4:A:602:GOL:H32	6:A:791:HOH:O	2.16	0.45
1:B:273:LYS:NZ	6:B:705:HOH:O	2.49	0.43
2:F:4:GLN:OE1	6:F:101:HOH:O	2.21	0.43
1:A:84:PRO:HD3	1:A:178:PHE:CD1	2.54	0.43
1:A:284:ASN:ND2	1:A:287:TYR:H	2.06	0.43
1:B:84:PRO:HD3	1:B:178:PHE:CD1	2.54	0.42
2:H:5:THR:HB	2:H:6:THR:H	1.61	0.42
1:A:284:ASN:HD22	1:A:286:ASN:H	1.64	0.42
1:A:472:GLN:NE2	1:B:138:GLU:HB2	2.34	0.42
1:B:284:ASN:ND2	1:B:287:TYR:H	2.06	0.42
1:B:325:HIS:CE1	1:B:346:ASN:HD21	2.38	0.42
2:H:7:PRO:CD	6:H:109:HOH:O	2.54	0.41
2:H:5:THR:C	6:H:101:HOH:O	2.63	0.41
1:A:362:ARG:NH2	4:A:606:GOL:H2	2.25	0.41
1:B:265:LEU:HD21	1:B:348:ILE:HG22	2.02	0.41
1:A:77:GLU:H	4:A:601:GOL:C3	2.33	0.41
1:A:132:LEU:HB2	4:A:605:GOL:H31	2.02	0.41
1:A:141:GLN:HA	1:A:142:PRO:HD3	1.97	0.41
1:A:242:LYS:HD3	6:A:764:HOH:O	2.21	0.41
1:A:325:HIS:CE1	1:A:346:ASN:HD21	2.39	0.41
1:A:432:VAL:HB	1:A:475:PHE:CD1	2.57	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	439/441 (100%)	429 (98%)	8 (2%)	2 (0%)	24	8
1	B	439/441 (100%)	427 (97%)	10 (2%)	2 (0%)	24	8
2	F	6/10 (60%)	2 (33%)	4 (67%)	0	100	100
2	H	7/10 (70%)	3 (43%)	3 (43%)	1 (14%)	0	0
All	All	891/902 (99%)	861 (97%)	25 (3%)	5 (1%)	21	6

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	96	GLY
1	A	288	TYR
1	B	96	GLY
1	B	288	TYR
2	H	7	PRO

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	371/370 (100%)	367 (99%)	4 (1%)	65	41
1	B	373/370 (101%)	365 (98%)	8 (2%)	47	19
2	F	6/8 (75%)	5 (83%)	1 (17%)	2	0
2	H	7/8 (88%)	4 (57%)	3 (43%)	0	0
All	All	757/756 (100%)	741 (98%)	16 (2%)	48	19

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	151	LEU
1	A	365	ARG
1	A	444	ASP
1	A	483	GLU
1	B	124	GLU
1	B	153[A]	LYS

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Mol	Chain	Res	Type
1	B	153[B]	LYS
1	B	162	ILE
1	B	291	ARG
1	B	444	ASP
1	B	480	GLU
1	B	498	GLU
2	F	1	THR
2	H	1	THR
2	H	2	GLU
2	H	6	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	86	GLN
1	A	113	HIS
1	A	284	ASN
1	A	332	GLN
1	A	366	GLN
1	A	391	ASN
1	A	408	HIS
1	A	422	ASN
1	A	466	HIS
1	B	113	HIS
1	B	141	GLN
1	B	284	ASN
1	B	332	GLN
1	B	366	GLN
1	B	391	ASN
1	B	422	ASN
1	B	466	HIS

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
3	A2G	C	1	3,2	14,14,15	1.73	4 (28%)	17,19,21	1.89	4 (23%)
3	GAL	C	2	3	11,11,12	0.96	0	15,15,17	1.07	1 (6%)
3	A2G	D	1	3,2	14,14,15	1.07	1 (7%)	17,19,21	0.58	0
3	GAL	D	2	3	11,11,12	0.92	0	15,15,17	0.81	0
3	A2G	E	1	3,2	14,14,15	1.08	1 (7%)	17,19,21	0.88	0
3	GAL	E	2	3	11,11,12	0.73	0	15,15,17	1.00	1 (6%)
3	A2G	G	1	3,2	14,14,15	0.83	0	17,19,21	0.87	0
3	GAL	G	2	3	11,11,12	0.78	0	15,15,17	0.67	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	A2G	C	1	3,2	-	1/6/23/26	0/1/1/1
3	GAL	C	2	3	-	1/2/19/22	0/1/1/1
3	A2G	D	1	3,2	-	1/6/23/26	0/1/1/1
3	GAL	D	2	3	-	0/2/19/22	0/1/1/1
3	A2G	E	1	3,2	-	0/6/23/26	0/1/1/1
3	GAL	E	2	3	-	2/2/19/22	0/1/1/1
3	A2G	G	1	3,2	-	1/6/23/26	0/1/1/1
3	GAL	G	2	3	-	0/2/19/22	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	1	A2G	C1-C2	3.52	1.57	1.52
3	C	1	A2G	O5-C5	3.04	1.49	1.43
3	E	1	A2G	C1-C2	2.71	1.56	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	1	A2G	C2-N2	2.50	1.50	1.46
3	D	1	A2G	O3-C3	2.29	1.48	1.43
3	C	1	A2G	O5-C1	2.14	1.47	1.43

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	1	A2G	O5-C5-C6	5.59	118.54	107.66
3	C	2	GAL	C1-O5-C5	2.94	116.13	112.19
3	C	1	A2G	C1-C2-N2	2.59	114.52	110.43
3	E	2	GAL	C1-O5-C5	2.30	115.27	112.19
3	C	1	A2G	O7-C7-C8	-2.28	118.00	122.05
3	C	1	A2G	O5-C5-C4	-2.16	105.56	110.83

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	E	2	GAL	C4-C5-C6-O6
3	E	2	GAL	O5-C5-C6-O6
3	D	1	A2G	O5-C5-C6-O6
3	G	1	A2G	O5-C5-C6-O6
3	C	1	A2G	C4-C5-C6-O6
3	C	2	GAL	C4-C5-C6-O6

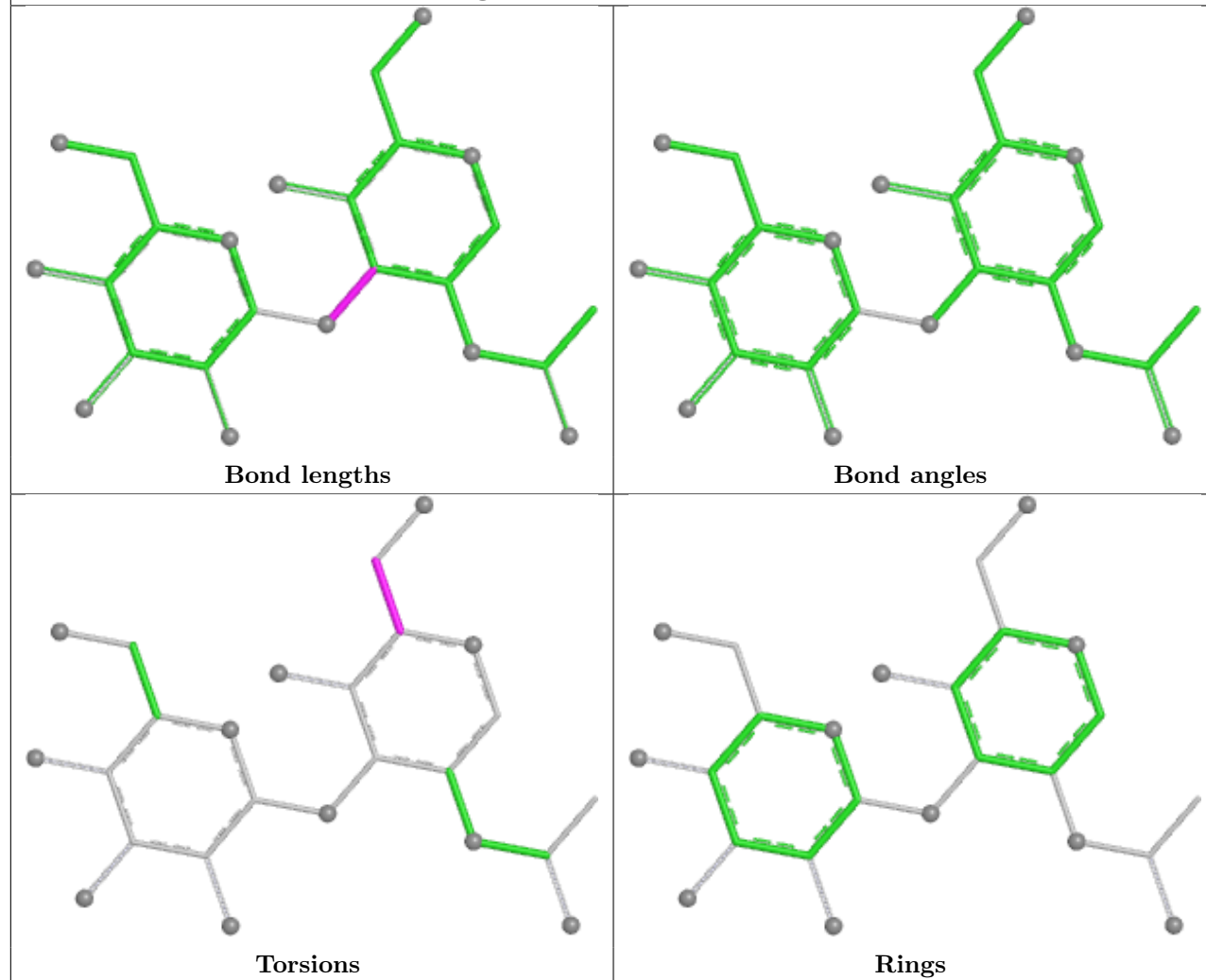
There are no ring outliers.

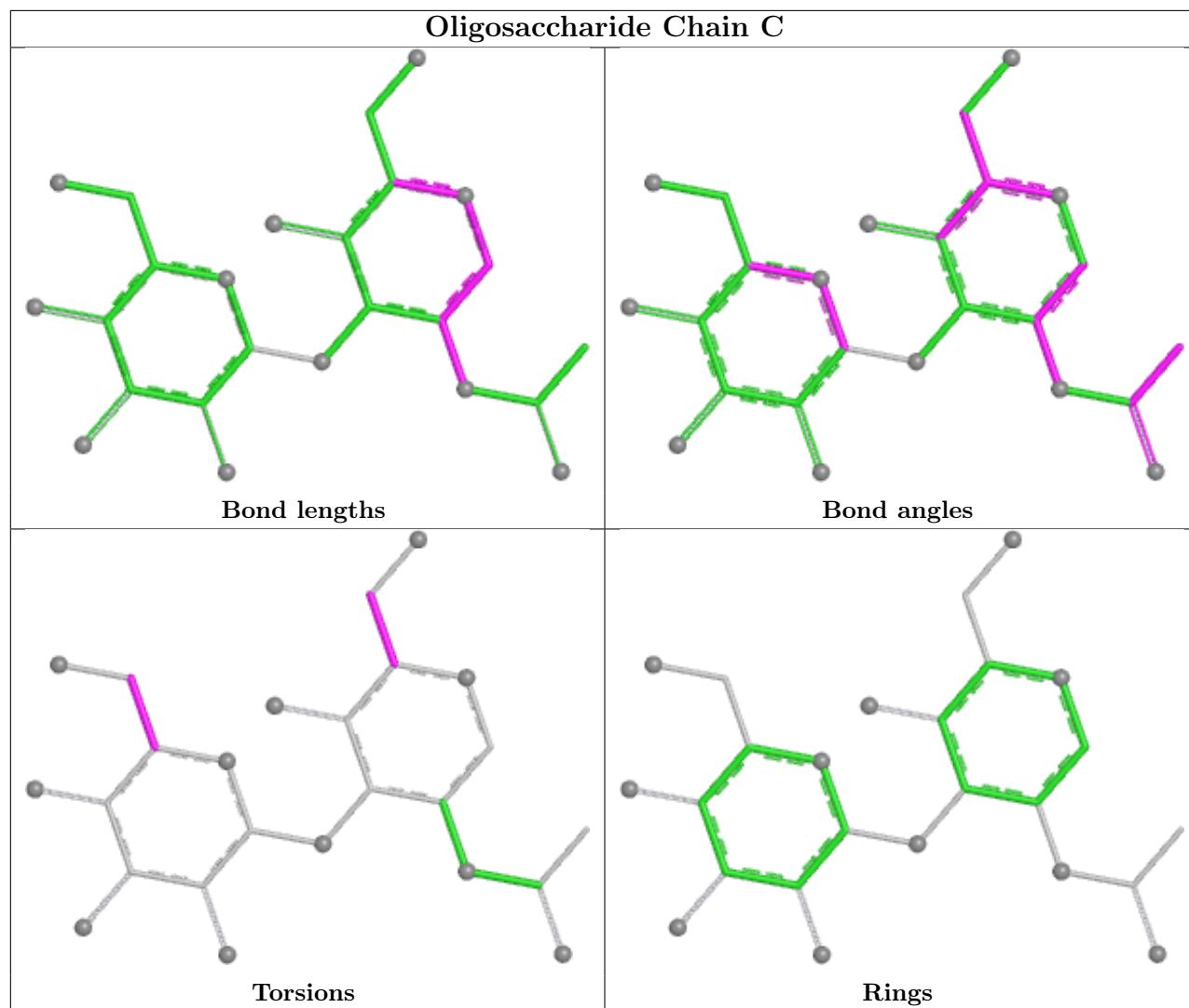
2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	1	A2G	2	0
3	E	1	A2G	1	0

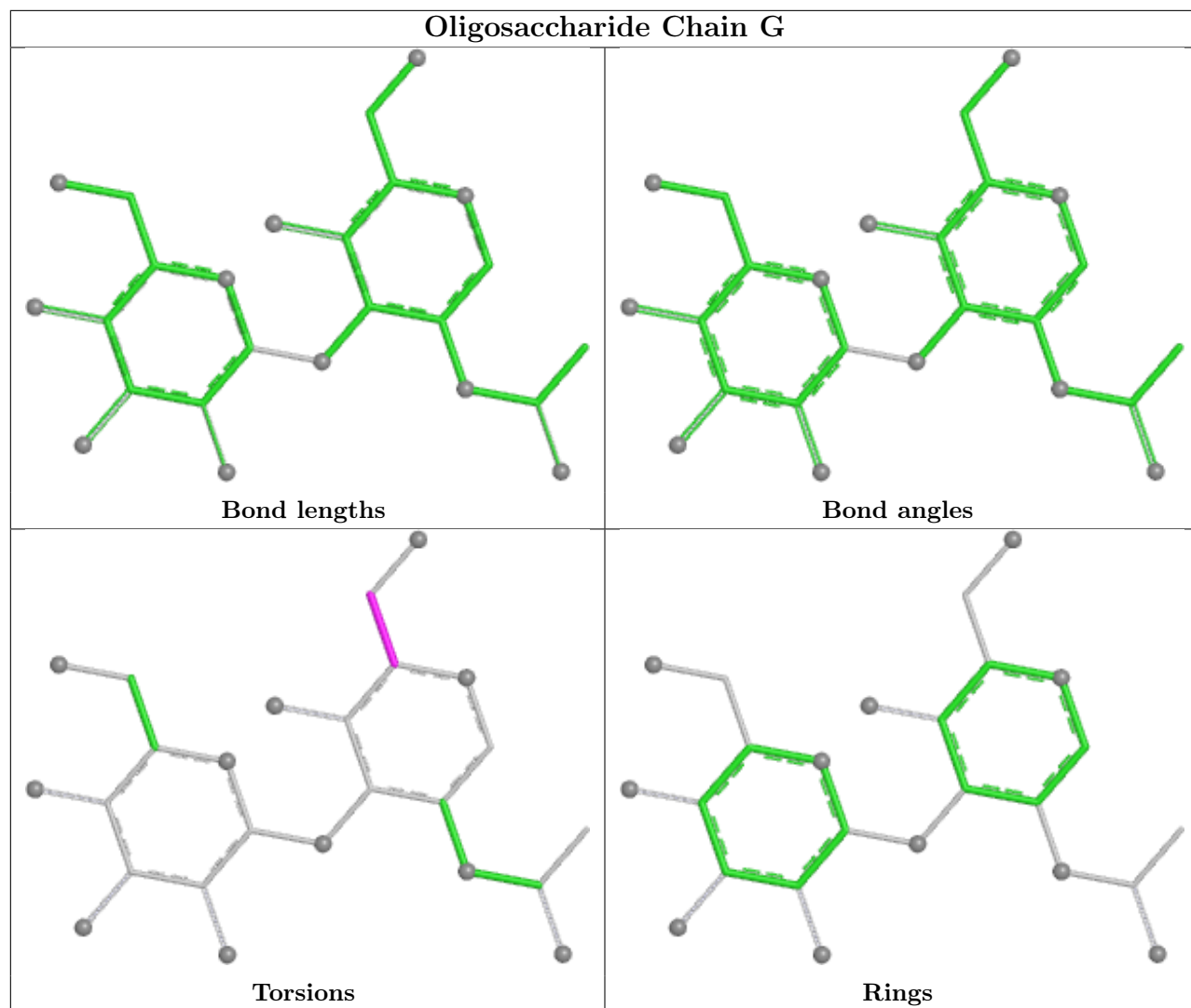
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

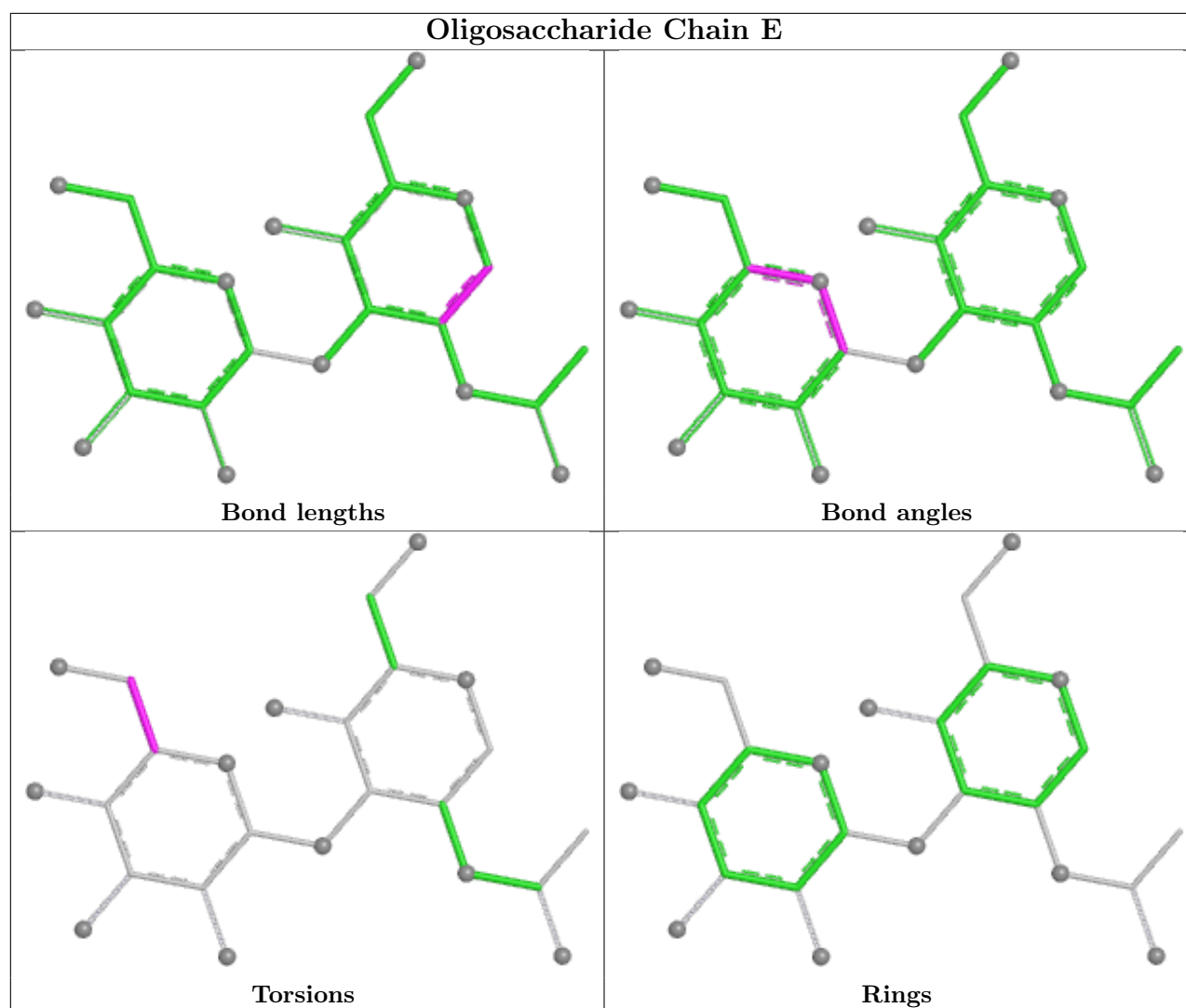
Oligosaccharide Chain D





Oligosaccharide Chain G





5.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 2 are monoatomic - leaving 10 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	$\# Z > 2$
4	GOL	A	602	-	5,5,5	0.08	0	5,5,5	0.34	0
4	GOL	B	601	-	5,5,5	0.09	0	5,5,5	0.28	0
4	GOL	A	604	-	5,5,5	0.13	0	5,5,5	0.44	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	GOL	A	608	-	5,5,5	0.09	0	5,5,5	0.25	0
4	GOL	A	607	-	5,5,5	0.10	0	5,5,5	0.24	0
4	GOL	A	603	-	5,5,5	0.17	0	5,5,5	0.92	0
4	GOL	B	602	-	5,5,5	0.10	0	5,5,5	0.41	0
4	GOL	A	606	-	5,5,5	0.07	0	5,5,5	0.38	0
4	GOL	A	601	-	5,5,5	0.10	0	5,5,5	0.25	0
4	GOL	A	605	-	5,5,5	0.16	0	5,5,5	0.24	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
4	GOL	A	602	-	-	3/4/4/4	-
4	GOL	B	601	-	-	2/4/4/4	-
4	GOL	A	604	-	-	4/4/4/4	-
4	GOL	A	608	-	-	4/4/4/4	-
4	GOL	A	607	-	-	2/4/4/4	-
4	GOL	A	603	-	-	3/4/4/4	-
4	GOL	B	602	-	-	4/4/4/4	-
4	GOL	A	606	-	-	2/4/4/4	-
4	GOL	A	601	-	-	1/4/4/4	-
4	GOL	A	605	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (27) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	604	GOL	O1-C1-C2-C3
4	A	605	GOL	O2-C2-C3-O3
4	A	606	GOL	C1-C2-C3-O3
4	A	607	GOL	O1-C1-C2-C3
4	B	601	GOL	O1-C1-C2-O2
4	B	601	GOL	O1-C1-C2-C3
4	B	602	GOL	C1-C2-C3-O3
4	A	606	GOL	O2-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
4	B	602	GOL	O2-C2-C3-O3
4	A	602	GOL	O1-C1-C2-C3
4	A	602	GOL	C1-C2-C3-O3
4	A	603	GOL	C1-C2-C3-O3
4	A	604	GOL	C1-C2-C3-O3
4	A	605	GOL	C1-C2-C3-O3
4	A	608	GOL	O1-C1-C2-C3
4	A	608	GOL	C1-C2-C3-O3
4	B	602	GOL	O1-C1-C2-C3
4	A	604	GOL	O1-C1-C2-O2
4	A	607	GOL	O1-C1-C2-O2
4	A	608	GOL	O1-C1-C2-O2
4	A	608	GOL	O2-C2-C3-O3
4	B	602	GOL	O1-C1-C2-O2
4	A	603	GOL	O2-C2-C3-O3
4	A	604	GOL	O2-C2-C3-O3
4	A	602	GOL	O2-C2-C3-O3
4	A	601	GOL	O1-C1-C2-C3
4	A	603	GOL	O1-C1-C2-O2

There are no ring outliers.

4 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	602	GOL	3	0
4	A	606	GOL	2	0
4	A	601	GOL	1	0
4	A	605	GOL	2	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	440/441 (99%)	0.03	9 (2%) 65 68	14, 23, 39, 69	1 (0%)
1	B	438/441 (99%)	0.45	21 (4%) 35 39	14, 29, 46, 69	3 (0%)
2	F	8/10 (80%)	3.97	7 (87%) 0 0	37, 46, 68, 69	0
2	H	9/10 (90%)	4.33	8 (88%) 0 0	36, 49, 71, 77	0
All	All	895/902 (99%)	0.31	45 (5%) 34 37	14, 26, 46, 77	4 (0%)

All (45) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	F	8	PRO	7.6
1	A	182	ALA	7.0
2	H	8	PRO	6.5
2	H	1	THR	6.3
2	F	7	PRO	6.1
2	F	1	THR	5.4
1	B	182	ALA	5.2
1	B	139	GLY	5.0
2	H	3	ALA	4.8
2	H	7	PRO	4.7
2	H	5	THR	4.1
2	H	9	PRO	4.1
1	B	183	GLY	3.9
1	B	140	VAL	3.9
1	B	184	LYS	3.5
2	H	6	THR	3.5
1	B	138	GLU	3.4
2	F	5	THR	3.2
1	A	181	ASP	3.0
2	F	3	ALA	2.9
1	B	408	HIS	2.9

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Mol	Chain	Res	Type	RSRZ
2	H	2	GLU	2.9
1	B	407	GLY	2.9
2	F	2	GLU	2.8
2	F	6	THR	2.7
1	B	482	VAL	2.7
1	B	498	GLU	2.7
1	A	483	GLU	2.5
1	B	137	ALA	2.4
1	A	185	ALA	2.4
1	B	471	ALA	2.4
1	B	360	GLU	2.4
1	A	184	LYS	2.4
1	B	409	PRO	2.3
1	A	183	GLY	2.3
1	A	139	GLY	2.2
1	B	79	ARG	2.2
1	B	181	ASP	2.2
1	B	162	ILE	2.1
1	B	210	LYS	2.1
1	A	122	GLY	2.1
1	B	-1	GLY	2.1
1	B	484	GLU	2.0
1	A	-3	GLY	2.0
1	B	445	VAL	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
3	A2G	D	1	14/15	-	-	30,36,41,47	0
3	GAL	D	2	11/12	-	-	53,59,63,64	0
3	A2G	C	1	14/15	-	-	47,52,56,56	0
3	GAL	C	2	11/12	-	-	59,61,62,64	0

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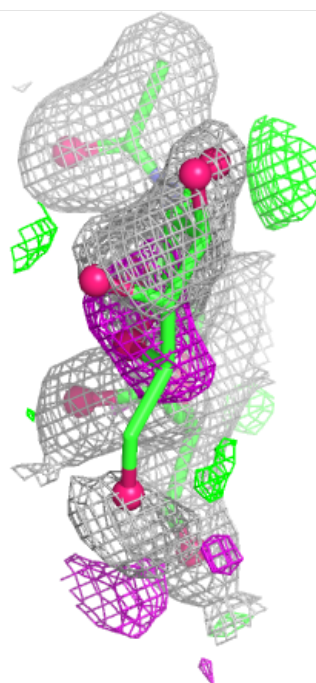
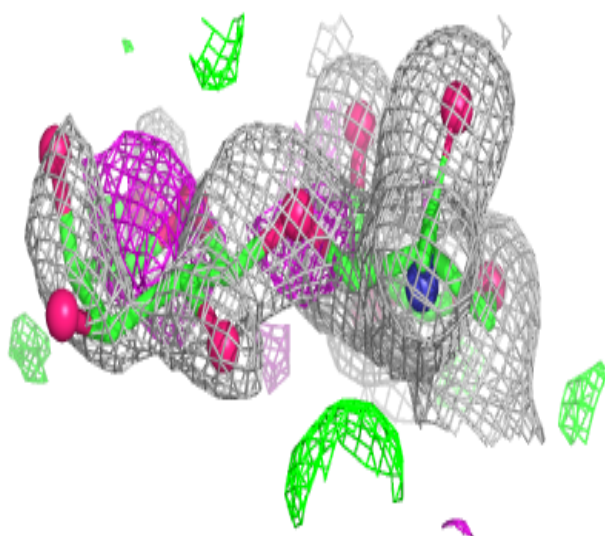
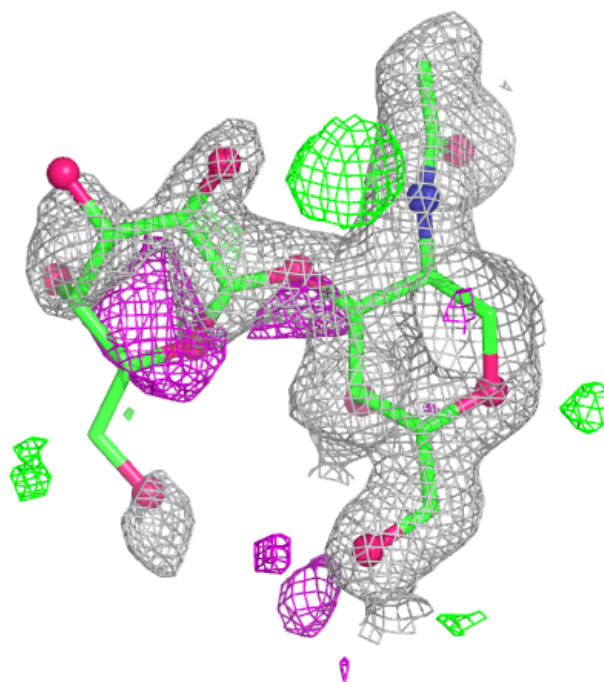
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	GAL	E	2	11/12	0.53	0.18	66,68,70,72	0
3	GAL	G	2	11/12	0.62	0.18	46,56,60,60	0
3	A2G	E	1	14/15	0.86	0.11	54,59,64,68	0
3	A2G	G	1	14/15	0.94	0.08	22,26,29,36	0

The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

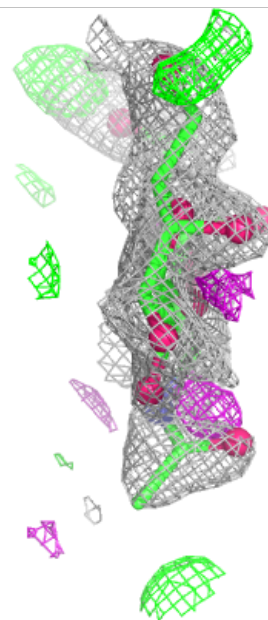
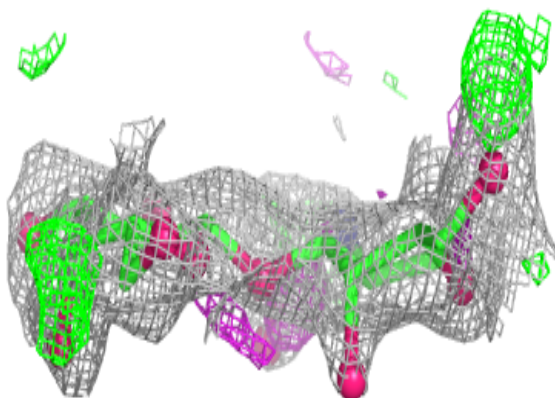
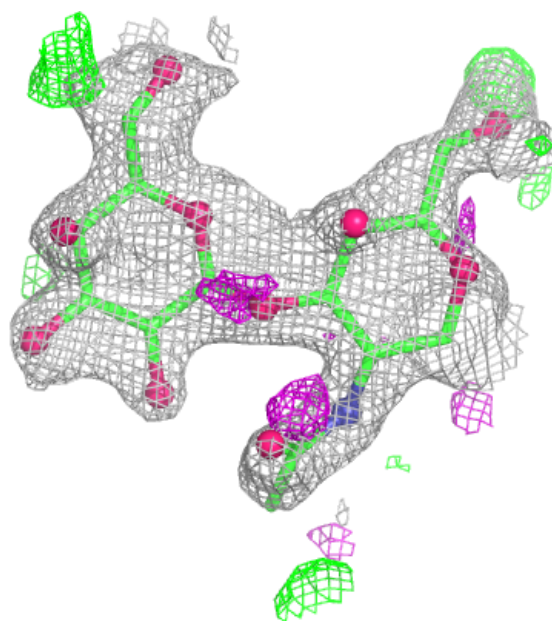
Electron density around Chain D:

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



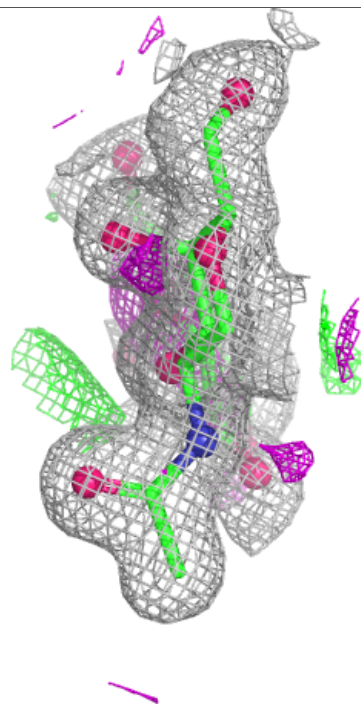
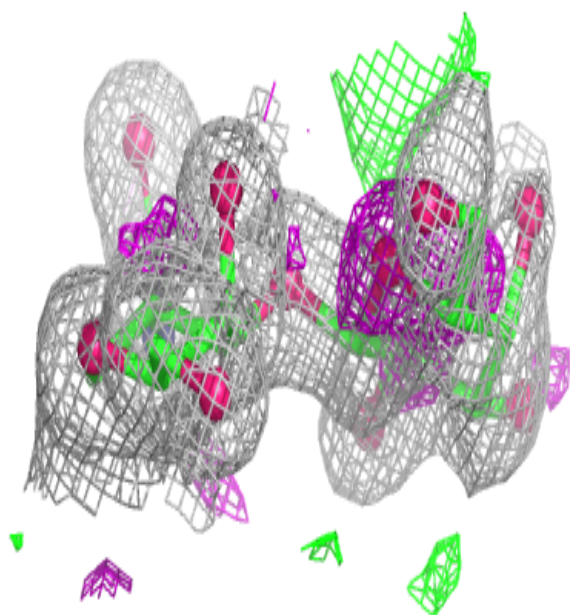
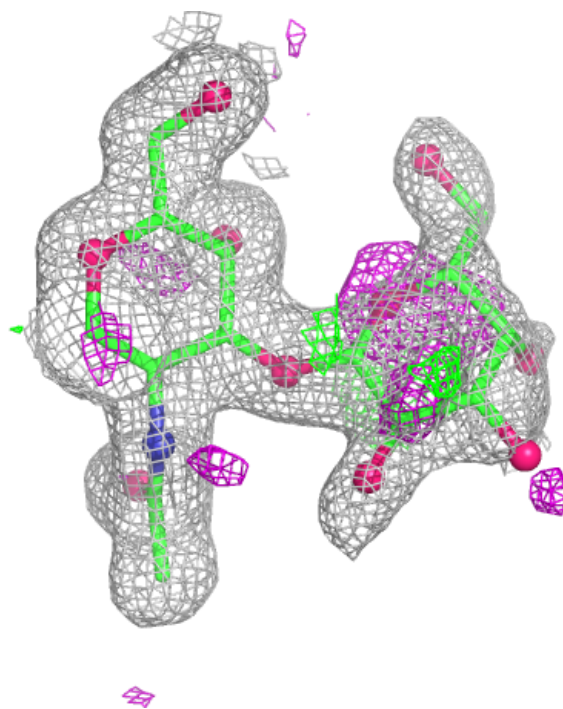
Electron density around Chain C:

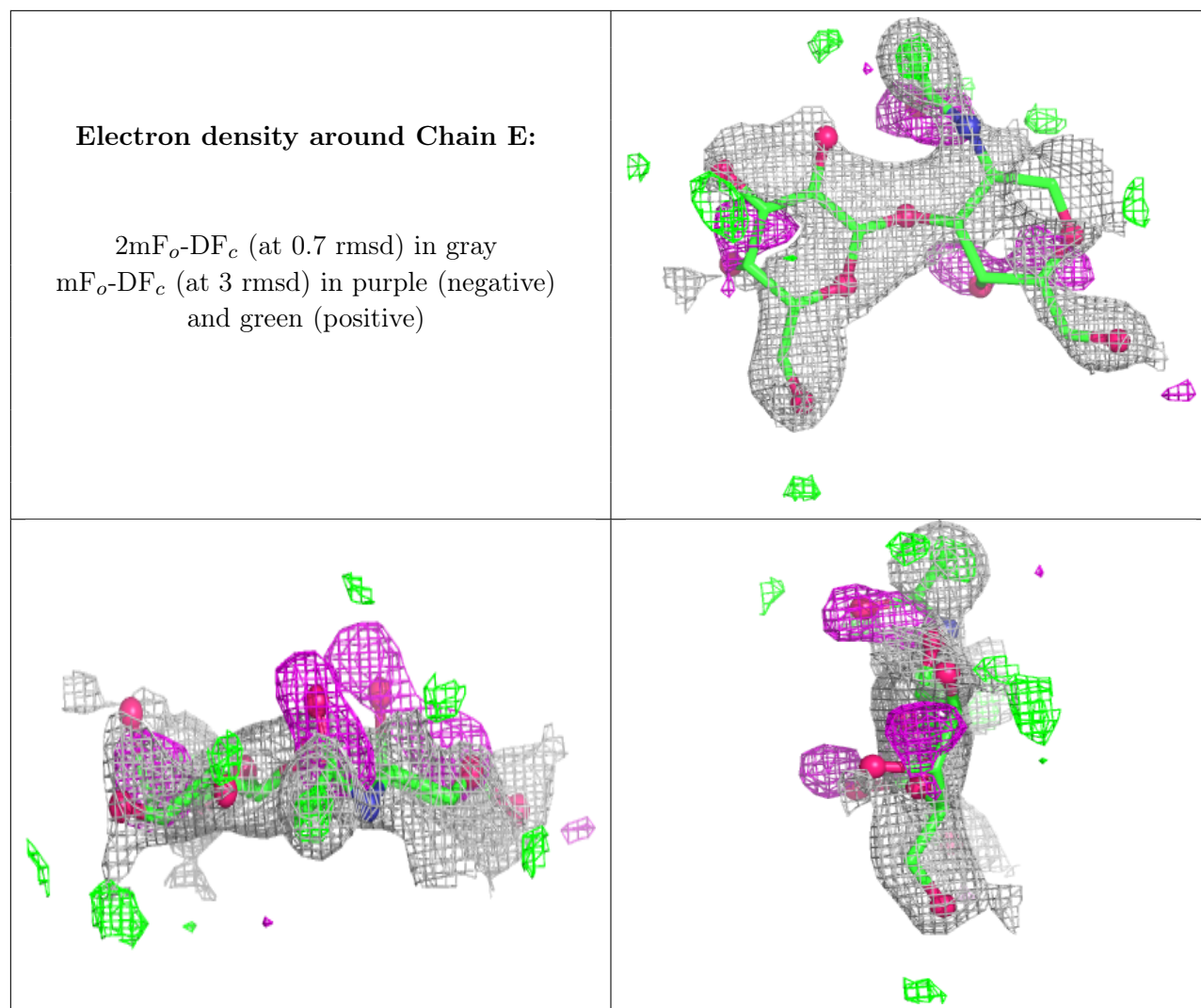
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around Chain G:

$2mF_o-DF_c$ (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($\text{\AA}^2$)	Q<0.9
4	GOL	B	601	6/6	0.77	0.23	67,69,71,72	0
4	GOL	A	607	6/6	0.78	0.19	61,63,64,67	0
4	GOL	B	602	6/6	0.79	0.16	39,48,50,53	0
4	GOL	A	604	6/6	0.82	0.15	41,45,48,49	0
4	GOL	A	601	6/6	0.83	0.16	39,45,46,48	0
4	GOL	A	606	6/6	0.84	0.13	50,52,52,54	0
4	GOL	A	605	6/6	0.87	0.17	30,37,38,46	0
4	GOL	A	608	6/6	0.88	0.13	44,53,56,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	GOL	A	602	6/6	0.90	0.13	32,41,43,47	0
4	GOL	A	603	6/6	0.93	0.09	26,29,34,35	0
5	ZN	B	603	1/1	0.99	0.02	22,22,22,22	0
5	ZN	A	609	1/1	1.00	0.01	19,19,19,19	0

6.5 Other polymers [i](#)

There are no such residues in this entry.