



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 11:55 AM UTC

PDB ID : 6IDW / pdb_00006idw
Title : GH6 Orpinomyces sp. Y102 enzyme
Authors : Tsai, L.C.; Huang, H.C.
Deposited on : 2018-09-11
Resolution : 2.78 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

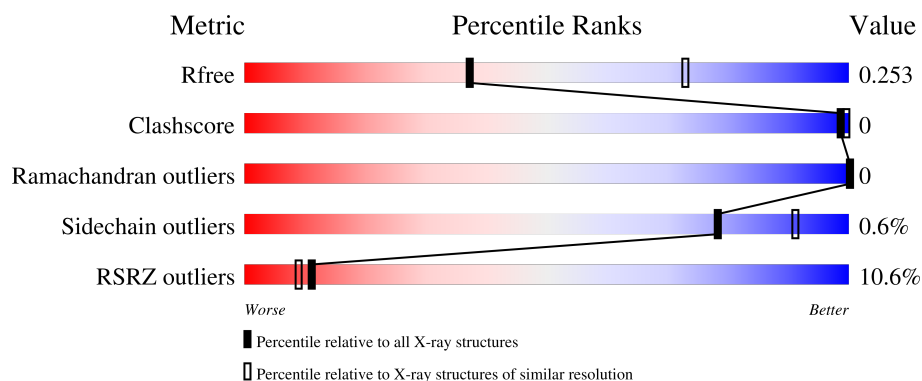
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.78 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	5248 (2.80-2.76)
Clashscore	190562	5693 (2.80-2.76)
Ramachandran outliers	187476	5590 (2.80-2.76)
Sidechain outliers	187428	5592 (2.80-2.76)
RSRZ outliers	180081	5251 (2.80-2.76)

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	322	11% 96% ..
1	B	322	11% 96% .
1	C	322	10% 95% ..
1	D	322	11% 93% 7%
2	E	2	100%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	F	2	 100%
2	G	2	 100%
2	H	2	 100%

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 10479 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 Glucanase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	322	Total	C	N	O	S	0	1	0
			2498	1557	445	485	11			
1	B	322	Total	C	N	O	S	0	0	0
			2494	1554	445	485	10			
1	C	322	Total	C	N	O	S	0	1	0
			2498	1557	445	485	11			
1	D	322	Total	C	N	O	S	0	0	0
			2494	1554	445	485	10			

- Molecule 2 is an oligosaccharide called beta-D-glucopyranose-(1-4)-beta-D-glucopyranose.



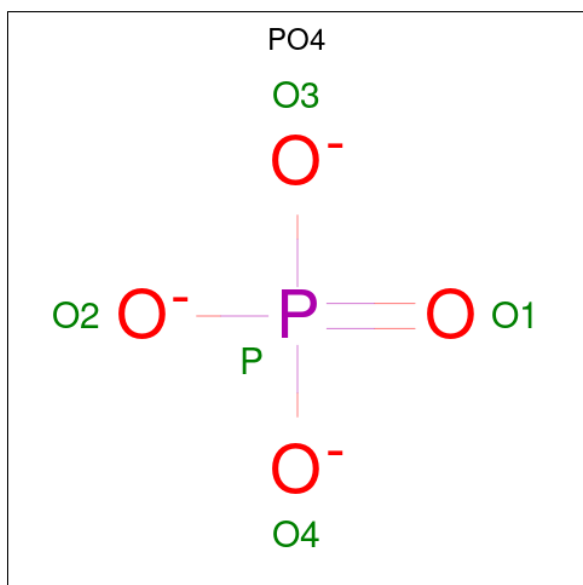
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
2	E	2	Total	C	O	0	0	0
			23	12	11			
2	F	2	Total	C	O	0	0	0
			23	12	11			
2	G	2	Total	C	O	0	0	0
			23	12	11			
2	H	2	Total	C	O	0	0	0
			23	12	11			

- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



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

- Molecule 4 is PHOSPHATE ION (CCD ID: PO4) (formula: O_4P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	P	0	0
			5	4	1		

- Molecule 5 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			4	2	2		
5	B	1	Total	C	O	0	0
			4	2	2		
5	B	1	Total	C	O	0	0
			4	2	2		
5	C	1	Total	C	O	0	0
			4	2	2		

- Molecule 6 is (4S)-2-METHYL-2,4-PENTANEDIOL (CCD ID: MPD) (formula: $C_6H_{14}O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total	C	O	0	0
			8	6	2		

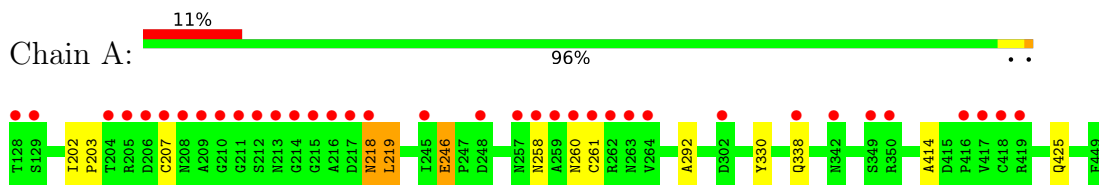
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	89	Total	O	0	0
			89	89		
7	B	102	Total	O	0	0
			102	102		
7	C	101	Total	O	0	0
			101	101		
7	D	58	Total	O	0	0
			58	58		

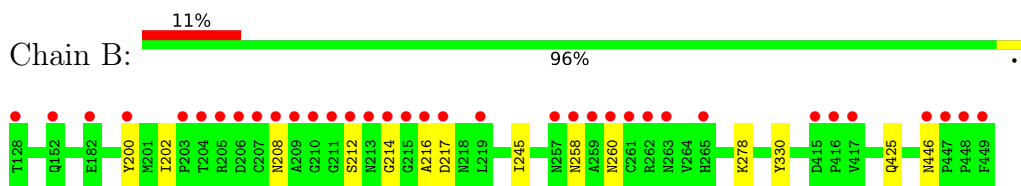
3 Residue-property plots [i](#)

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.

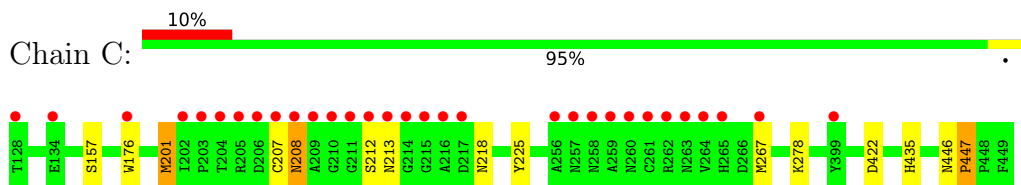
- Molecule 1: Glucanase



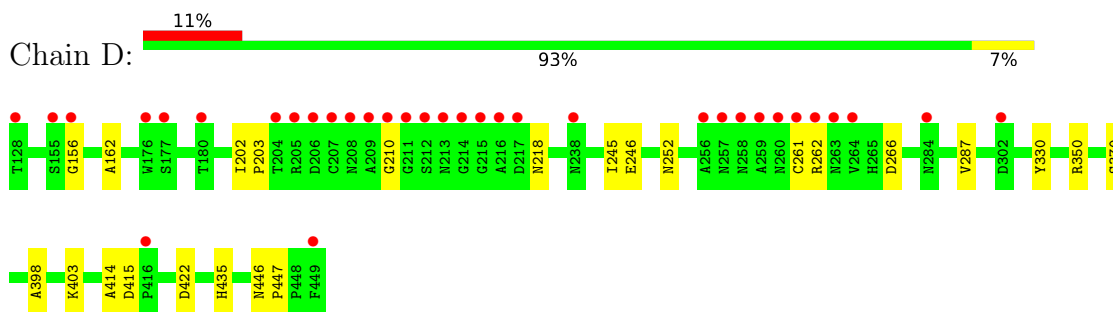
- Molecule 1: Glucanase



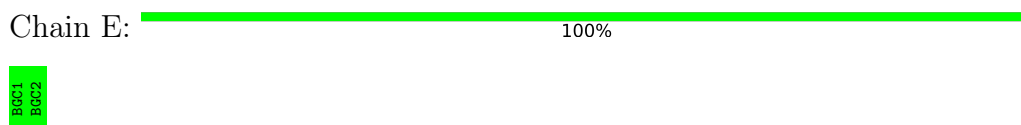
- Molecule 1: Glucanase



- Molecule 1: Glucanase



- Molecule 2: beta-D-glucopyranose-(1-4)-beta-D-glucopyranose



- Molecule 2: beta-D-glucopyranose-(1-4)-beta-D-glucopyranose

Chain F:  100%

BGC1
BGC2

- Molecule 2: beta-D-glucopyranose-(1-4)-beta-D-glucopyranose

Chain G:  100%

BGC1
BGC2

- Molecule 2: beta-D-glucopyranose-(1-4)-beta-D-glucopyranose

Chain H:  100%

BGC1
BGC2

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	310.37Å 86.59Å 82.31Å 90.00° 93.67° 90.00°	Depositor
Resolution (Å)	154.87 – 2.78 154.87 – 2.78	Depositor EDS
% Data completeness (in resolution range)	92.0 (154.87-2.78) 92.0 (154.87-2.78)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	6.11 (at 2.80Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, R_{free}	0.220 , 0.253 0.220 , 0.253	Depositor DCC
R_{free} test set	1934 reflections (3.52%)	wwPDB-VP
Wilson B-factor (Å ²)	27.5	Xtriage
Anisotropy	0.204	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 27.3	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	0.89	EDS
Total number of atoms	10479	wwPDB-VP
Average B, all atoms (Å ²)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.72% 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: MPD, BGC, PO4, GOL, EDO

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	1.03	5/2559 (0.2%)	1.17	13/3479 (0.4%)
1	B	1.13	5/2551 (0.2%)	1.24	11/3469 (0.3%)
1	C	1.14	8/2559 (0.3%)	1.19	7/3479 (0.2%)
1	D	1.04	5/2551 (0.2%)	1.12	13/3469 (0.4%)
All	All	1.09	23/10220 (0.2%)	1.18	44/13896 (0.3%)

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	217	ASP	CA-C	12.70	1.63	1.52
1	A	219	LEU	N-CA	-7.08	1.37	1.46
1	C	207	CYS	CA-C	6.67	1.61	1.52
1	D	162	ALA	C-N	-6.61	1.25	1.34
1	B	446	ASN	CA-C	6.53	1.58	1.52
1	D	203	PRO	CA-C	6.12	1.60	1.52
1	B	217	ASP	N-CA	6.07	1.53	1.46
1	C	201[A]	MET	N-CA	6.00	1.53	1.46
1	C	201[B]	MET	N-CA	6.00	1.53	1.46
1	C	157	SER	CA-C	5.64	1.59	1.52
1	C	208	ASN	CA-C	5.57	1.59	1.52
1	C	422	ASP	CA-C	5.31	1.60	1.52
1	A	258	ASN	CG-OD1	5.29	1.33	1.23
1	D	403	LYS	N-CA	-5.29	1.39	1.46
1	A	202	ILE	CA-C	5.28	1.58	1.52
1	C	212	SER	N-CA	5.23	1.52	1.46
1	B	260	ASN	CG-OD1	5.18	1.33	1.23
1	D	415	ASP	CA-C	-5.16	1.47	1.53
1	C	213	ASN	CG-OD1	5.14	1.33	1.23
1	A	260	ASN	CG-OD1	5.14	1.33	1.23
1	A	261	CYS	CA-C	-5.14	1.46	1.53
1	B	216	ALA	CA-C	5.03	1.58	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	218	ASN	N-CA	-5.02	1.40	1.46

All (44) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	208	ASN	N-CA-C	12.24	124.36	111.14
1	A	414	ALA	N-CA-C	10.61	122.84	111.28
1	B	245	ILE	N-CA-C	10.24	121.92	107.37
1	B	217	ASP	N-CA-C	8.54	123.83	112.13
1	D	414	ALA	N-CA-C	7.35	119.29	111.28
1	A	207	CYS	N-CA-C	-6.94	99.92	109.71
1	D	245	ILE	N-CA-C	6.88	118.75	108.23
1	B	258	ASN	N-CA-C	6.87	119.67	110.88
1	B	212	SER	N-CA-C	6.81	121.66	112.88
1	A	292	ALA	N-CA-C	6.80	118.64	108.31
1	B	245	ILE	CB-CA-C	-6.79	104.60	111.80
1	A	218	ASN	N-CA-C	6.78	117.45	107.88
1	A	246	GLU	N-CA-C	6.76	117.88	109.57
1	B	200	TYR	N-CA-C	6.59	118.56	109.54
1	D	246	GLU	N-CA-C	6.54	124.26	109.81
1	A	258	ASN	N-CA-C	6.39	120.70	112.26
1	B	278	LYS	N-CA-C	6.23	121.10	111.56
1	C	278	LYS	N-CA-C	6.23	119.28	111.24
1	D	287	VAL	N-CA-C	6.05	116.64	108.17
1	D	156	GLY	N-CA-C	6.03	122.42	110.77
1	A	203	PRO	N-CA-C	6.01	122.06	113.47
1	C	207	CYS	N-CA-C	5.95	117.63	111.03
1	D	203	PRO	N-CA-C	5.88	121.88	113.47
1	C	447	PRO	CA-C-N	5.83	126.29	120.52
1	C	447	PRO	C-N-CA	5.83	126.29	120.52
1	B	425	GLN	N-CA-C	5.59	118.09	110.55
1	C	208	ASN	N-CA-C	5.56	117.42	111.36
1	D	252	ASN	N-CA-C	5.55	117.33	111.28
1	B	214	GLY	N-CA-C	-5.51	104.91	111.36
1	C	435	HIS	N-CA-C	5.47	117.68	111.11
1	A	202	ILE	CA-C-N	5.45	124.63	118.97
1	A	202	ILE	C-N-CA	5.45	124.63	118.97
1	D	330	TYR	N-CA-CB	-5.41	102.28	111.20
1	A	330	TYR	N-CA-C	5.38	119.54	112.92
1	C	212	SER	N-CA-C	5.36	116.42	108.60
1	D	435	HIS	N-CA-C	5.33	117.51	111.11
1	D	210	GLY	N-CA-C	5.22	125.55	113.18

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	330	TYR	N-CA-C	5.18	119.56	112.88
1	A	218	ASN	CA-CB-CG	-5.17	107.43	112.60
1	D	245	ILE	CB-CA-C	-5.16	104.72	110.96
1	D	261	CYS	N-CA-C	-5.15	105.68	112.94
1	A	425	GLN	N-CA-C	5.14	117.50	110.55
1	D	398	ALA	N-CA-C	5.08	116.24	108.52
1	A	338	GLN	N-CA-C	-5.04	105.86	111.36

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	2498	0	2390	1	0
1	B	2494	0	2385	0	0
1	C	2498	0	2390	4	0
1	D	2494	0	2385	4	0
2	E	23	0	21	0	0
2	F	23	0	21	0	0
2	G	23	0	21	0	0
2	H	23	0	21	0	0
3	A	6	0	8	0	0
3	B	6	0	8	0	0
3	C	12	0	16	0	0
4	A	5	0	0	0	0
5	A	4	0	6	0	0
5	B	8	0	12	0	0
5	C	4	0	6	0	0
6	B	8	0	14	0	0
7	A	89	0	0	0	0
7	B	102	0	0	0	0
7	C	101	0	0	0	0
7	D	58	0	0	1	0
All	All	10479	0	9704	9	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 0.

All (9) 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:350:ARG:NH1	7:D:601:HOH:O	2.39	0.53
1:C:201[B]:MET:HE2	1:C:225:TYR:CE2	2.48	0.49
1:D:370:SER:OG	1:D:422:ASP:OD2	2.29	0.49
1:C:176:TRP:O	1:C:201[A]:MET:HE3	2.14	0.47
1:D:262:ARG:O	1:D:266:ASP:CG	2.60	0.44
1:A:218:ASN:O	1:A:219:LEU:C	2.61	0.43
1:C:446:ASN:HA	1:C:447:PRO:C	2.43	0.43
1:D:446:ASN:HA	1:D:447:PRO:C	2.44	0.42

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	321/322 (100%)	309 (96%)	12 (4%)	0	100	100
1	B	320/322 (99%)	308 (96%)	12 (4%)	0	100	100
1	C	321/322 (100%)	307 (96%)	14 (4%)	0	100	100
1	D	320/322 (99%)	309 (97%)	11 (3%)	0	100	100
All	All	1282/1288 (100%)	1233 (96%)	49 (4%)	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	267/266 (100%)	266 (100%)	1 (0%)	84	93
1	B	266/266 (100%)	265 (100%)	1 (0%)	84	93
1	C	267/266 (100%)	264 (99%)	3 (1%)	65	85
1	D	266/266 (100%)	265 (100%)	1 (0%)	84	93
All	All	1066/1064 (100%)	1060 (99%)	6 (1%)	78	91

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	246	GLU
1	B	202	ILE
1	C	208	ASN
1	C	218	ASN
1	C	267	MET
1	D	202	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	258	ASN
1	A	282	GLN
1	A	298	ASN
1	A	331	GLN
1	B	268	HIS
1	B	282	GLN
1	B	341	GLN
1	C	208	ASN
1	C	341	GLN
1	C	420	ASN
1	D	298	ASN
1	D	341	GLN
1	D	342	ASN

5.3.3 RNA ⓘ

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](#)

8 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	BGC	E	1	2	12,12,12	0.47	0	17,17,17	0.52	0
2	BGC	E	2	2	11,11,12	0.27	0	15,15,17	0.54	0
2	BGC	F	1	2	12,12,12	0.45	0	17,17,17	0.51	0
2	BGC	F	2	2	11,11,12	0.27	0	15,15,17	0.53	0
2	BGC	G	1	2	12,12,12	0.45	0	17,17,17	0.52	0
2	BGC	G	2	2	11,11,12	0.27	0	15,15,17	0.51	0
2	BGC	H	1	2	12,12,12	0.45	0	17,17,17	0.53	0
2	BGC	H	2	2	11,11,12	0.29	0	15,15,17	0.53	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	BGC	E	1	2	-	0/2/22/22	0/1/1/1
2	BGC	E	2	2	-	0/2/19/22	0/1/1/1
2	BGC	F	1	2	-	0/2/22/22	0/1/1/1
2	BGC	F	2	2	-	1/2/19/22	0/1/1/1
2	BGC	G	1	2	-	0/2/22/22	0/1/1/1
2	BGC	G	2	2	-	0/2/19/22	0/1/1/1
2	BGC	H	1	2	-	0/2/22/22	0/1/1/1
2	BGC	H	2	2	-	0/2/19/22	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

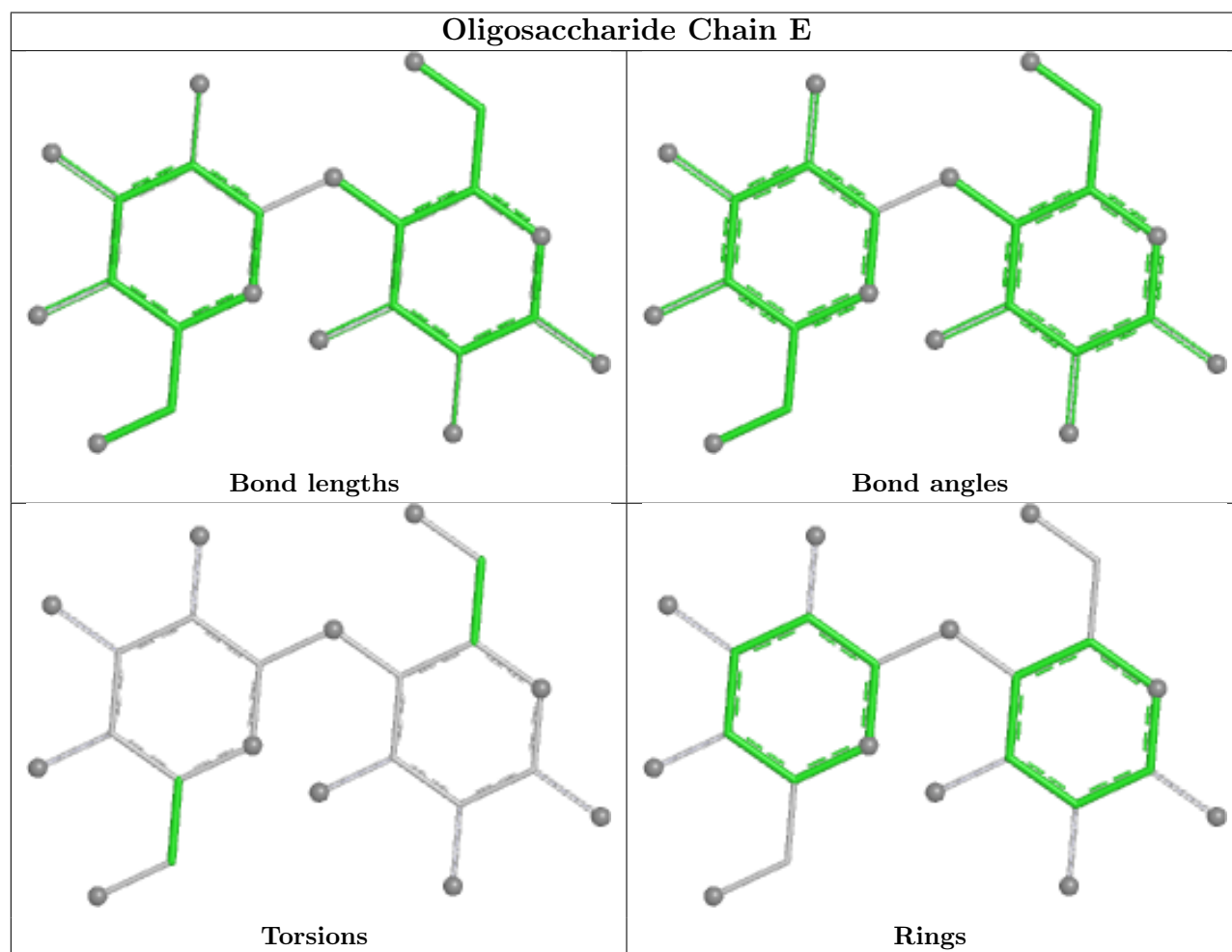
All (1) torsion outliers are listed below:

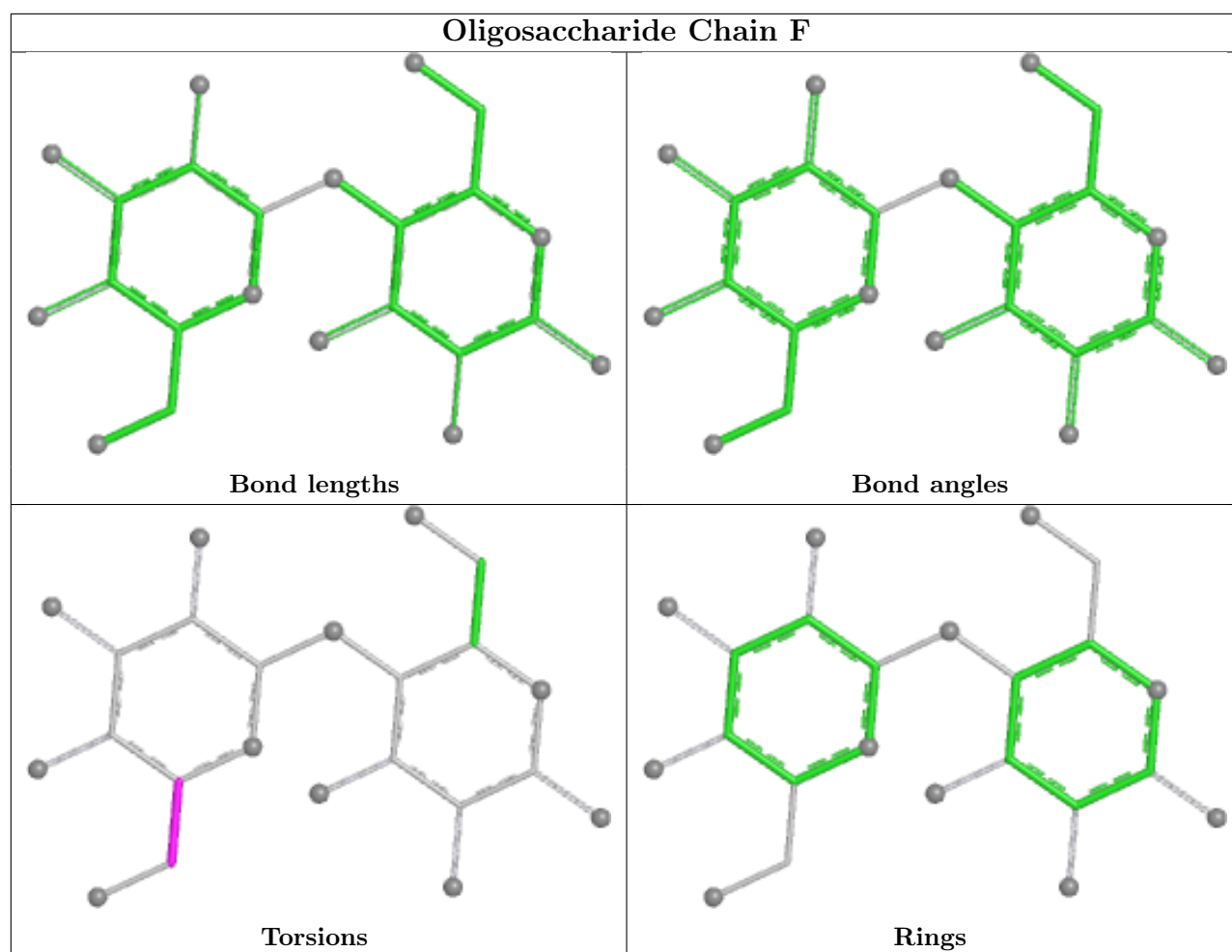
Mol	Chain	Res	Type	Atoms
2	F	2	BGC	C4-C5-C6-O6

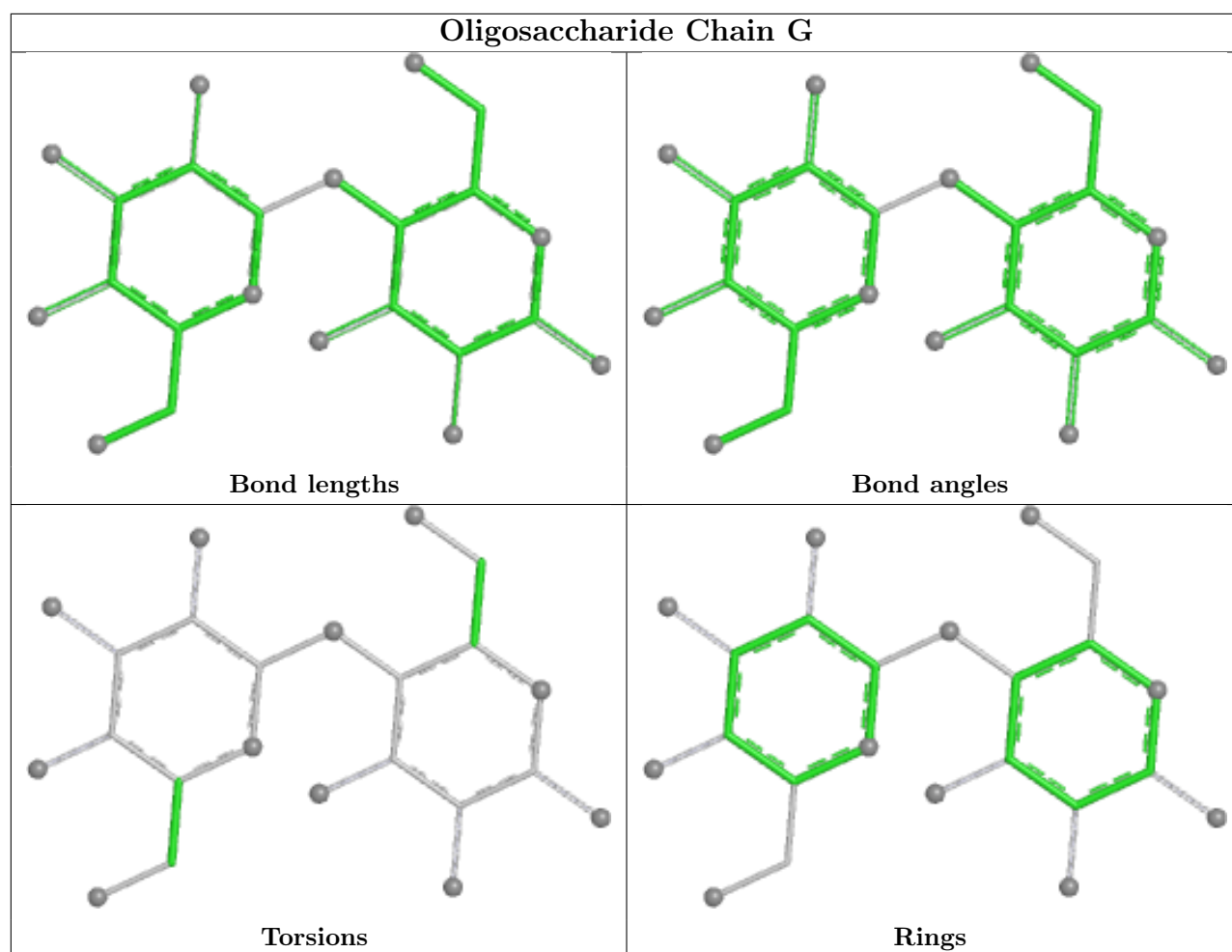
There are no ring outliers.

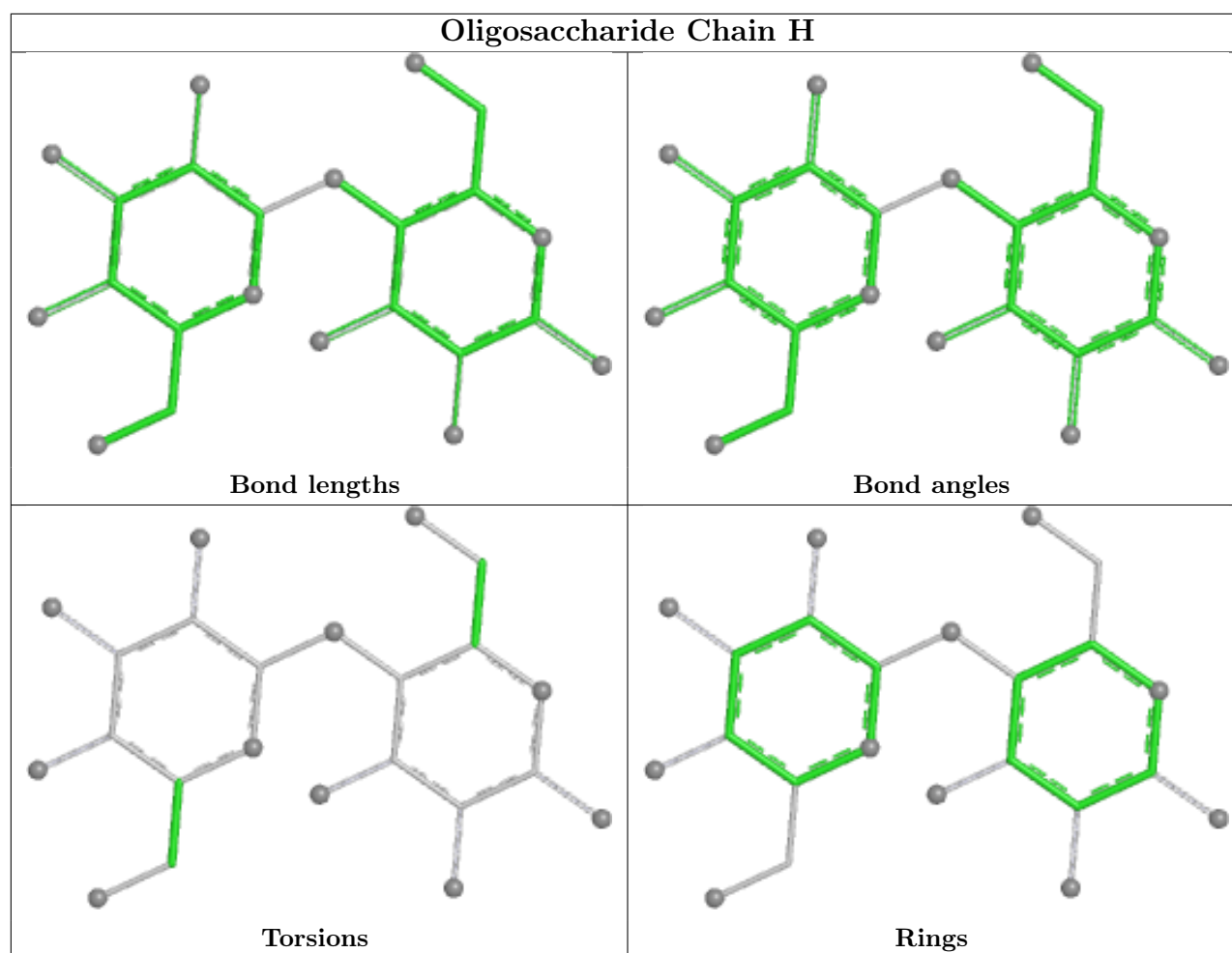
No monomer is involved in short contacts.

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









5.6 Ligand geometry [i](#)

10 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	$\# Z > 2$
5	EDO	B	503	-	3,3,3	0.29	0	2,2,2	0.86	0
3	GOL	B	502	-	5,5,5	0.44	0	5,5,5	0.67	0
5	EDO	B	505	-	3,3,3	0.30	0	2,2,2	0.07	0
5	EDO	C	504	-	3,3,3	0.27	0	2,2,2	0.46	0
4	PO4	A	503	-	4,4,4	0.90	0	6,6,6	0.47	0
5	EDO	A	504	-	3,3,3	0.42	0	2,2,2	0.39	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	GOL	A	502	-	5,5,5	0.27	0	5,5,5	0.32	0
3	GOL	C	503	-	5,5,5	0.27	0	5,5,5	0.32	0
3	GOL	C	502	-	5,5,5	0.36	0	5,5,5	0.88	0
6	MPD	B	504	-	7,7,7	0.29	0	9,10,10	0.20	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
5	EDO	B	503	-	-	1/1/1/1	-
3	GOL	B	502	-	-	4/4/4/4	-
5	EDO	B	505	-	-	0/1/1/1	-
5	EDO	C	504	-	-	1/1/1/1	-
5	EDO	A	504	-	-	0/1/1/1	-
3	GOL	A	502	-	-	0/4/4/4	-
3	GOL	C	503	-	-	0/4/4/4	-
3	GOL	C	502	-	-	2/4/4/4	-
6	MPD	B	504	-	-	0/5/5/5	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	502	GOL	O1-C1-C2-C3
3	B	502	GOL	C1-C2-C3-O3
3	C	502	GOL	C1-C2-C3-O3
3	B	502	GOL	O2-C2-C3-O3
5	B	503	EDO	O1-C1-C2-O2
3	C	502	GOL	O2-C2-C3-O3
3	B	502	GOL	O1-C1-C2-O2
5	C	504	EDO	O1-C1-C2-O2

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	322/322 (100%)	0.69	36 (11%)	10 8	16, 29, 50, 73	24 (7%)
1	B	322/322 (100%)	0.72	35 (10%)	10 8	11, 25, 48, 73	20 (6%)
1	C	322/322 (100%)	0.79	31 (9%)	13 11	9, 26, 48, 78	22 (6%)
1	D	322/322 (100%)	0.87	34 (10%)	11 9	20, 35, 57, 75	21 (6%)
All	All	1288/1288 (100%)	0.77	136 (10%)	11 9	9, 29, 52, 78	87 (6%)

All (136) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	214	GLY	16.4
1	C	215	GLY	13.4
1	B	215	GLY	13.3
1	B	214	GLY	13.0
1	C	209	ALA	12.3
1	C	213	ASN	11.7
1	B	204	THR	11.7
1	C	128	THR	11.4
1	C	259	ALA	11.3
1	A	128	THR	11.1
1	A	209	ALA	10.6
1	D	209	ALA	10.5
1	C	216	ALA	10.5
1	C	204	THR	10.4
1	D	215	GLY	10.2
1	B	259	ALA	10.1
1	D	128	THR	10.1
1	A	205	ARG	10.1
1	B	216	ALA	9.8
1	D	260	ASN	9.3
1	A	259	ALA	9.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	258	ASN	9.2
1	D	206	ASP	8.8
1	A	258	ASN	8.8
1	C	205	ARG	8.8
1	B	213	ASN	8.7
1	C	210	GLY	8.6
1	A	207	CYS	8.4
1	B	207	CYS	8.4
1	B	205	ARG	8.4
1	D	207	CYS	8.4
1	C	212	SER	8.2
1	A	261	CYS	8.1
1	C	260	ASN	8.1
1	B	210	GLY	8.0
1	B	217	ASP	8.0
1	A	206	ASP	8.0
1	B	212	SER	7.9
1	A	262	ARG	7.9
1	D	259	ALA	7.9
1	A	204	THR	7.8
1	C	208	ASN	7.8
1	A	213	ASN	7.7
1	A	257	ASN	7.7
1	C	217	ASP	7.7
1	A	217	ASP	7.6
1	B	257	ASN	7.6
1	D	212	SER	7.5
1	A	210	GLY	7.5
1	D	262	ARG	7.4
1	B	209	ALA	7.3
1	A	214	GLY	7.2
1	A	208	ASN	7.1
1	B	262	ARG	7.1
1	C	257	ASN	7.0
1	D	216	ALA	6.9
1	D	204	THR	6.9
1	C	206	ASP	6.8
1	D	205	ARG	6.7
1	D	258	ASN	6.6
1	B	261	CYS	6.5
1	B	211	GLY	6.4
1	C	211	GLY	6.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	208	ASN	6.2
1	A	215	GLY	6.1
1	D	210	GLY	6.1
1	D	208	ASN	6.0
1	A	260	ASN	5.9
1	B	206	ASP	5.8
1	B	260	ASN	5.8
1	C	262	ARG	5.7
1	A	211	GLY	5.7
1	C	261	CYS	5.6
1	D	257	ASN	5.6
1	D	261	CYS	5.5
1	C	256	ALA	5.4
1	B	258	ASN	5.3
1	C	207	CYS	5.3
1	D	214	GLY	5.3
1	A	216	ALA	5.2
1	D	155	SER	5.1
1	D	213	ASN	4.8
1	C	203	PRO	4.8
1	A	212	SER	4.7
1	D	211	GLY	4.6
1	B	417	VAL	3.8
1	D	256	ALA	3.8
1	C	263	ASN	3.6
1	A	248	ASP	3.5
1	D	302	ASP	3.4
1	A	263	ASN	3.4
1	C	264	VAL	3.4
1	A	349	SER	3.1
1	A	419	ARG	2.9
1	B	265	HIS	2.9
1	A	416	PRO	2.9
1	B	447	PRO	2.9
1	D	176	TRP	2.9
1	D	416	PRO	2.9
1	B	200	TYR	2.8
1	B	416	PRO	2.8
1	B	446	ASN	2.8
1	D	449	PHE	2.8
1	D	156	GLY	2.8
1	B	449	PHE	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	128	THR	2.7
1	D	264	VAL	2.7
1	B	263	ASN	2.6
1	D	263	ASN	2.6
1	D	217	ASP	2.6
1	D	177	SER	2.6
1	C	176	TRP	2.5
1	A	302	ASP	2.5
1	C	267	MET	2.5
1	C	202	ILE	2.4
1	B	182	GLU	2.4
1	B	203	PRO	2.4
1	B	152	GLN	2.4
1	A	342	ASN	2.3
1	A	350	ARG	2.3
1	A	417	VAL	2.3
1	B	219	LEU	2.3
1	C	134	GLU	2.3
1	D	284	ASN	2.3
1	C	265	HIS	2.2
1	D	238	ASN	2.2
1	A	264	VAL	2.2
1	B	415	ASP	2.2
1	B	448	PRO	2.2
1	A	218	ASN	2.1
1	A	129	SER	2.1
1	A	338	GLN	2.1
1	A	418	CYS	2.1
1	C	399	TYR	2.1
1	A	245	ILE	2.1
1	D	180	THR	2.0

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

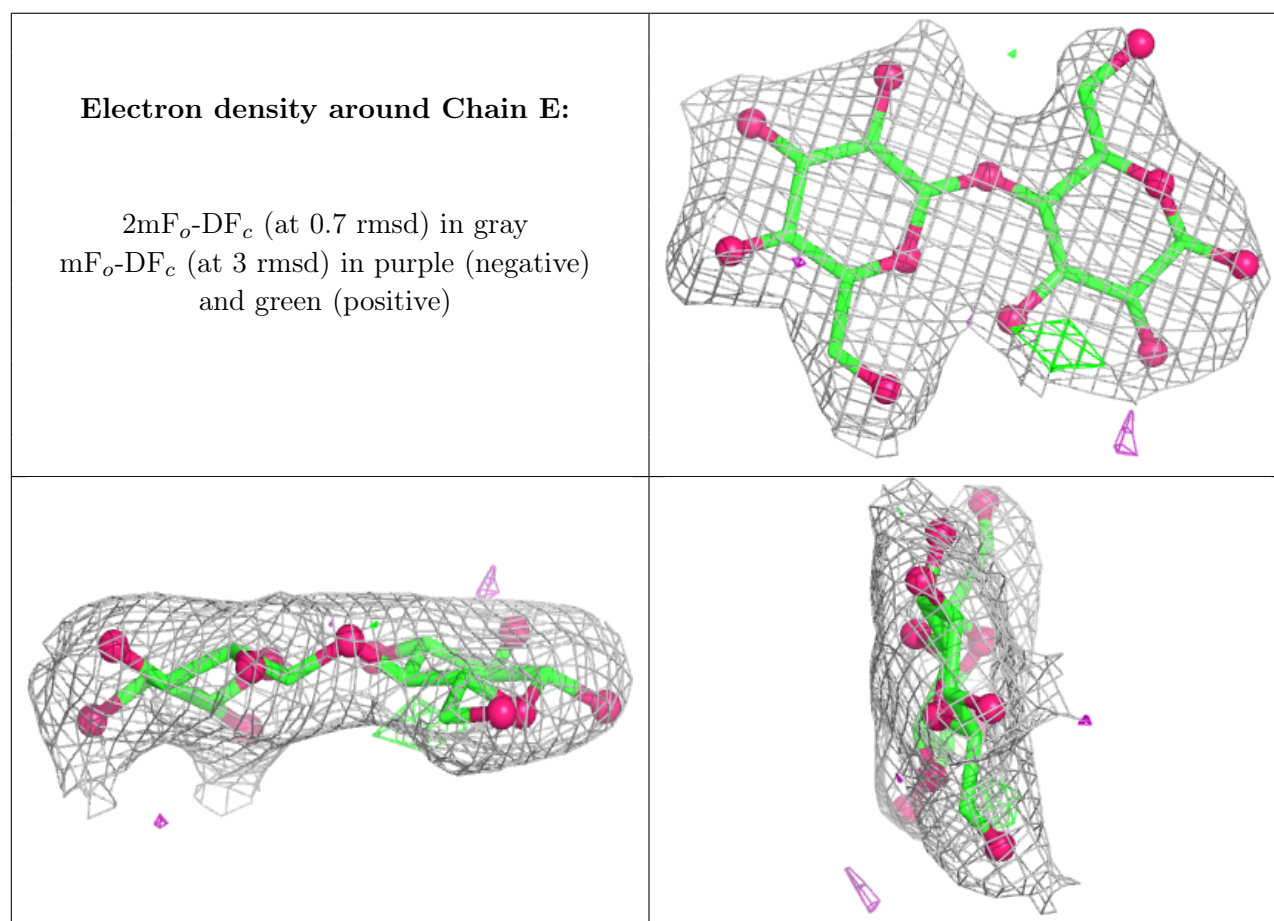
There are no non-standard protein/DNA/RNA residues in this entry.

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.

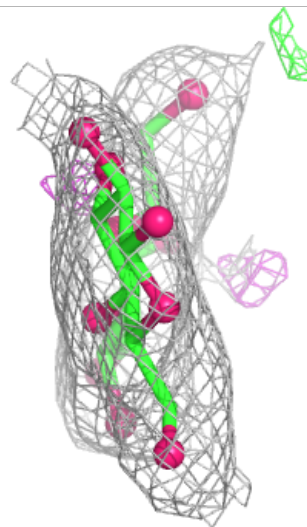
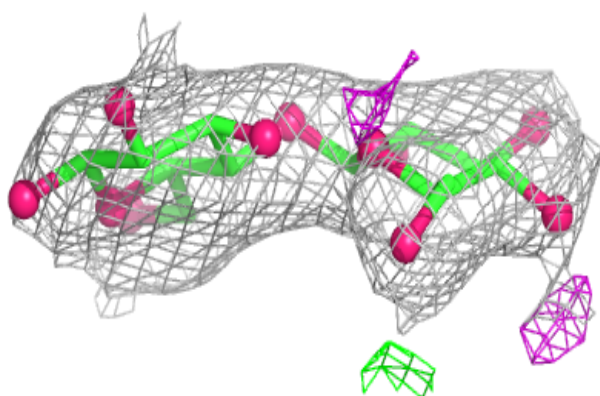
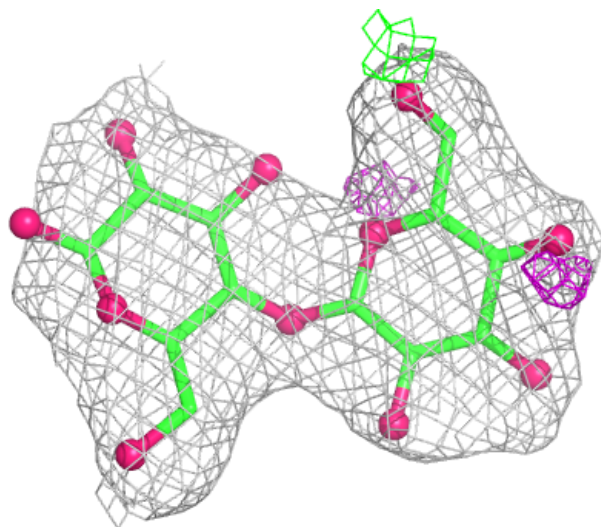
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	BGC	G	1	12/12	0.81	0.17	30,37,46,47	0
2	BGC	H	1	12/12	0.87	0.15	43,49,52,60	0
2	BGC	E	1	12/12	0.89	0.12	27,36,39,43	0
2	BGC	F	2	11/12	0.90	0.12	23,25,27,27	0
2	BGC	H	2	11/12	0.91	0.10	37,39,41,41	0
2	BGC	F	1	12/12	0.92	0.12	27,32,34,38	0
2	BGC	E	2	11/12	0.94	0.09	20,22,24,25	0
2	BGC	G	2	11/12	0.96	0.07	21,24,25,26	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.



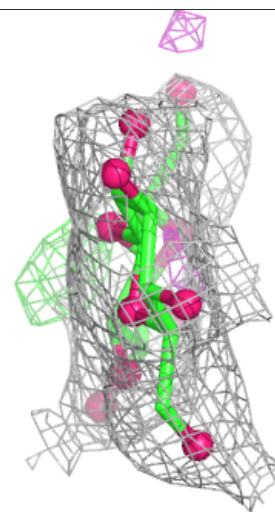
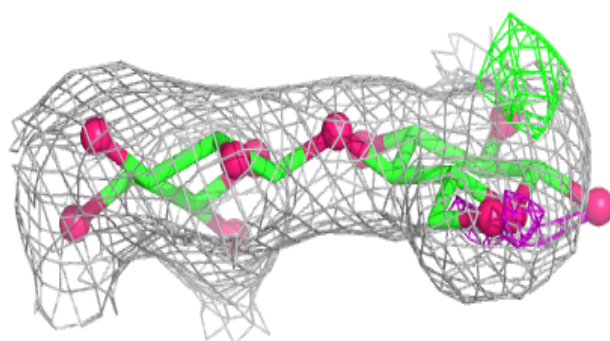
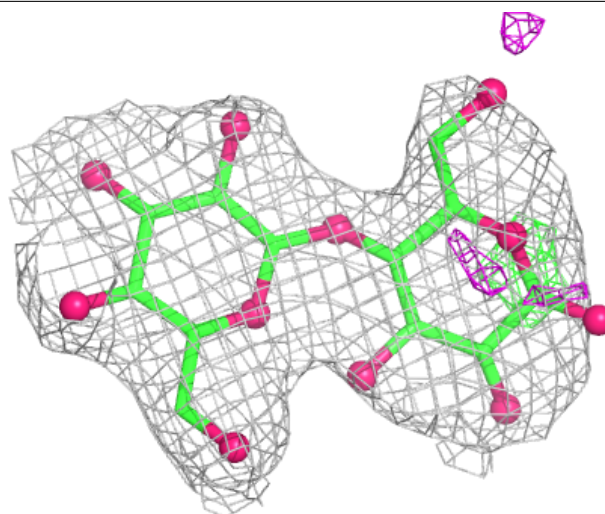
Electron density around Chain F:

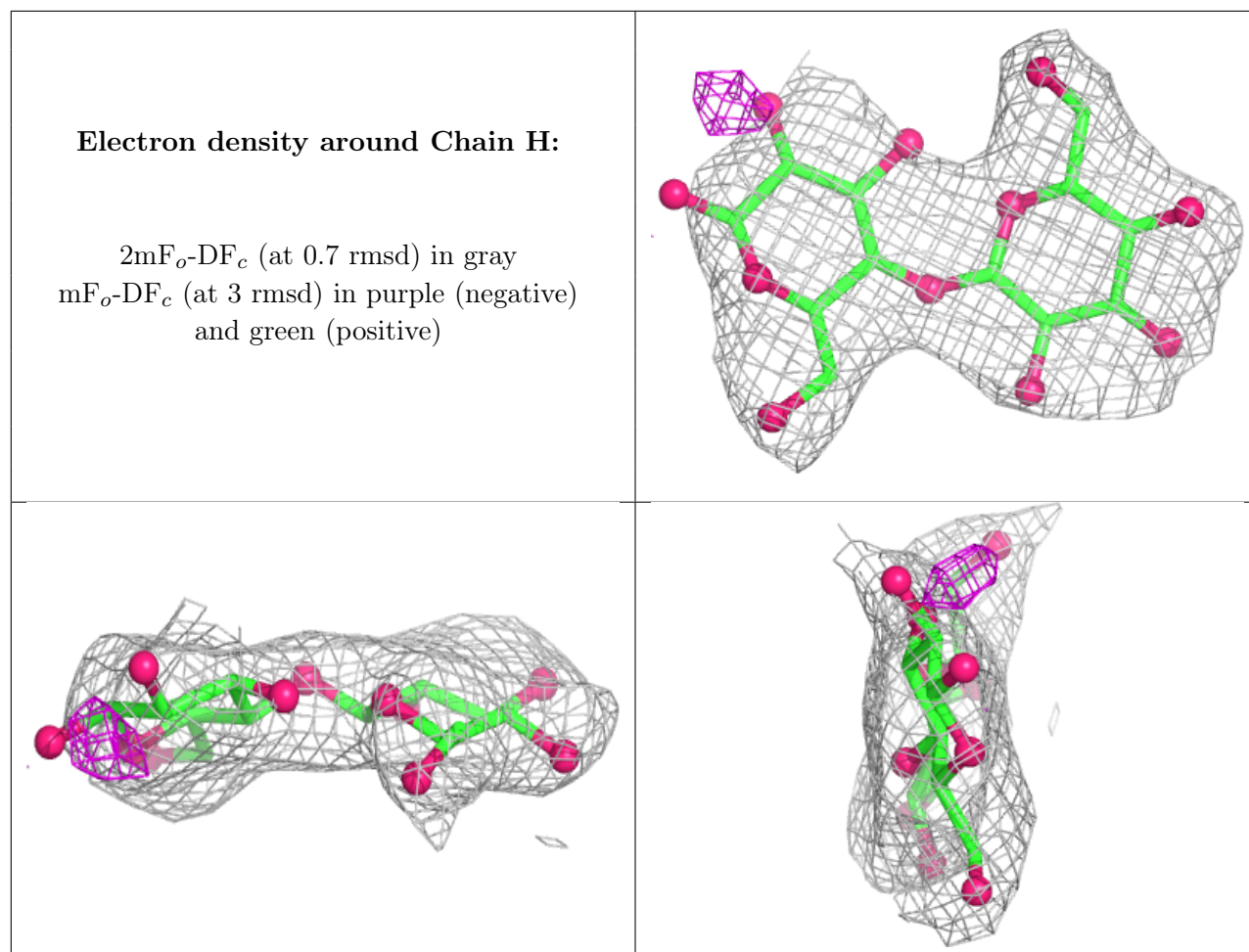
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



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
5	EDO	B	503	4/4	0.64	0.16	49,51,53,57	0
3	GOL	C	502	6/6	0.75	0.22	35,37,40,43	0
3	GOL	A	502	6/6	0.80	0.21	58,59,61,61	0
4	PO4	A	503	5/5	0.82	0.13	58,58,61,62	5
6	MPD	B	504	8/8	0.82	0.25	43,45,48,49	0
3	GOL	C	503	6/6	0.84	0.25	52,59,62,64	0
5	EDO	B	505	4/4	0.87	0.21	53,62,64,69	0
5	EDO	C	504	4/4	0.88	0.23	51,56,56,57	0
3	GOL	B	502	6/6	0.88	0.12	33,35,37,37	0
5	EDO	A	504	4/4	0.89	0.14	40,41,46,47	0

6.5 Other polymers ⓘ

There are no such residues in this entry.