



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 9, 2026 – 08:39 PM UTC

PDB ID : 8EL1 / pdb_00008el1
Title : Structure of MBP-Mcl-1 in complex with ABBV-467
Authors : Judge, R.A.; Judd, A.S.; Souers, A.J.
Deposited on : 2022-09-22
Resolution : 2.41 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
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

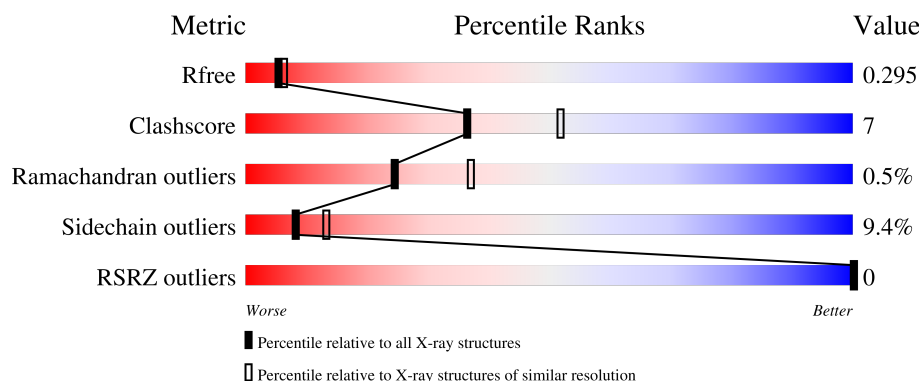
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.41 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	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

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	532	70% 25% • •
1	B	532	73% 22% • •
1	C	532	68% 24% • 6%
1	D	532	73% 20% • 7%
2	E	2	50% 50%

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Mol	Chain	Length	Quality of chain
2	F	2	 50% 50%
2	G	2	 50% 50%
2	H	2	 50% 50%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 16036 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 Maltose/maltodextrin-binding periplasmic protein, Induced myeloid leukemia cell differentiation protein Mcl-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	512	Total	C	N	O	S	0	0	0
			3936	2512	660	754	10			
1	B	515	Total	C	N	O	S	0	0	0
			3938	2511	659	758	10			
1	C	499	Total	C	N	O	S	0	0	0
			3808	2424	640	734	10			
1	D	497	Total	C	N	O	S	0	0	0
			3792	2418	635	729	10			

There are 80 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-210	MET	-	initiating methionine	UNP P0AEX9
A	-209	ALA	-	expression tag	UNP P0AEX9
A	-208	HIS	-	expression tag	UNP P0AEX9
A	-207	HIS	-	expression tag	UNP P0AEX9
A	-206	HIS	-	expression tag	UNP P0AEX9
A	-205	HIS	-	expression tag	UNP P0AEX9
A	-204	HIS	-	expression tag	UNP P0AEX9
A	-203	HIS	-	expression tag	UNP P0AEX9
A	-202	GLU	-	expression tag	UNP P0AEX9
A	-201	ASN	-	expression tag	UNP P0AEX9
A	-200	LEU	-	expression tag	UNP P0AEX9
A	-199	TYR	-	expression tag	UNP P0AEX9
A	-198	PHE	-	expression tag	UNP P0AEX9
A	-197	GLN	-	expression tag	UNP P0AEX9
A	-196	GLY	-	expression tag	UNP P0AEX9
A	171	GLY	-	linker	UNP P0AEX9
A	172	SER	-	linker	UNP P0AEX9
A	194	ALA	LYS	engineered mutation	UNP Q07820
A	197	ALA	LYS	engineered mutation	UNP Q07820
A	201	ALA	ARG	engineered mutation	UNP Q07820

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-210	MET	-	initiating methionine	UNP P0AEX9
B	-209	ALA	-	expression tag	UNP P0AEX9
B	-208	HIS	-	expression tag	UNP P0AEX9
B	-207	HIS	-	expression tag	UNP P0AEX9
B	-206	HIS	-	expression tag	UNP P0AEX9
B	-205	HIS	-	expression tag	UNP P0AEX9
B	-204	HIS	-	expression tag	UNP P0AEX9
B	-203	HIS	-	expression tag	UNP P0AEX9
B	-202	GLU	-	expression tag	UNP P0AEX9
B	-201	ASN	-	expression tag	UNP P0AEX9
B	-200	LEU	-	expression tag	UNP P0AEX9
B	-199	TYR	-	expression tag	UNP P0AEX9
B	-198	PHE	-	expression tag	UNP P0AEX9
B	-197	GLN	-	expression tag	UNP P0AEX9
B	-196	GLY	-	expression tag	UNP P0AEX9
B	171	GLY	-	linker	UNP P0AEX9
B	172	SER	-	linker	UNP P0AEX9
B	194	ALA	LYS	engineered mutation	UNP Q07820
B	197	ALA	LYS	engineered mutation	UNP Q07820
B	201	ALA	ARG	engineered mutation	UNP Q07820
C	-210	MET	-	initiating methionine	UNP P0AEX9
C	-209	ALA	-	expression tag	UNP P0AEX9
C	-208	HIS	-	expression tag	UNP P0AEX9
C	-207	HIS	-	expression tag	UNP P0AEX9
C	-206	HIS	-	expression tag	UNP P0AEX9
C	-205	HIS	-	expression tag	UNP P0AEX9
C	-204	HIS	-	expression tag	UNP P0AEX9
C	-203	HIS	-	expression tag	UNP P0AEX9
C	-202	GLU	-	expression tag	UNP P0AEX9
C	-201	ASN	-	expression tag	UNP P0AEX9
C	-200	LEU	-	expression tag	UNP P0AEX9
C	-199	TYR	-	expression tag	UNP P0AEX9
C	-198	PHE	-	expression tag	UNP P0AEX9
C	-197	GLN	-	expression tag	UNP P0AEX9
C	-196	GLY	-	expression tag	UNP P0AEX9
C	171	GLY	-	linker	UNP P0AEX9
C	172	SER	-	linker	UNP P0AEX9
C	194	ALA	LYS	engineered mutation	UNP Q07820
C	197	ALA	LYS	engineered mutation	UNP Q07820
C	201	ALA	ARG	engineered mutation	UNP Q07820
D	-210	MET	-	initiating methionine	UNP P0AEX9
D	-209	ALA	-	expression tag	UNP P0AEX9

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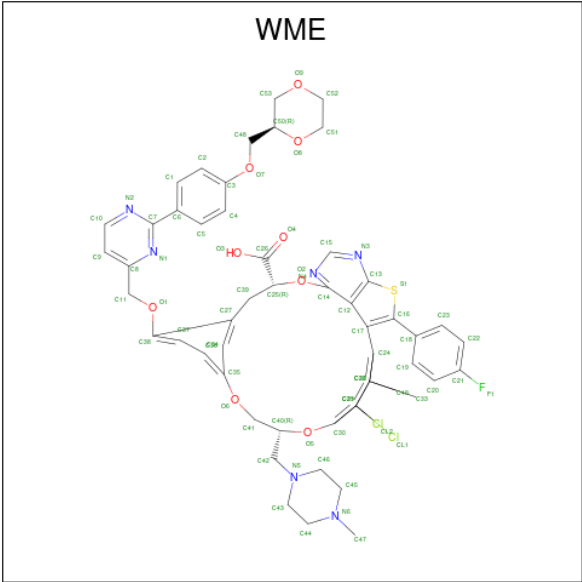
Chain	Residue	Modelled	Actual	Comment	Reference
D	-208	HIS	-	expression tag	UNP P0AEX9
D	-207	HIS	-	expression tag	UNP P0AEX9
D	-206	HIS	-	expression tag	UNP P0AEX9
D	-205	HIS	-	expression tag	UNP P0AEX9
D	-204	HIS	-	expression tag	UNP P0AEX9
D	-203	HIS	-	expression tag	UNP P0AEX9
D	-202	GLU	-	expression tag	UNP P0AEX9
D	-201	ASN	-	expression tag	UNP P0AEX9
D	-200	LEU	-	expression tag	UNP P0AEX9
D	-199	TYR	-	expression tag	UNP P0AEX9
D	-198	PHE	-	expression tag	UNP P0AEX9
D	-197	GLN	-	expression tag	UNP P0AEX9
D	-196	GLY	-	expression tag	UNP P0AEX9
D	171	GLY	-	linker	UNP P0AEX9
D	172	SER	-	linker	UNP P0AEX9
D	194	ALA	LYS	engineered mutation	UNP Q07820
D	197	ALA	LYS	engineered mutation	UNP Q07820
D	201	ALA	ARG	engineered mutation	UNP Q07820

- Molecule 2 is an oligosaccharide called alpha-D-glucopyranose-(1-4)-alpha-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 (7R,16R)-19,23-dichloro-10-{{[2-(4-{{[(2R)-1,4-dioxan-2-yl]methoxy}phenyl]pyrimidin-4-yl]methoxy}-1-(4-fluorophenyl)-20,22-dimethyl-16-[(4-methylpiperazin-1-yl)methyl]-7,8,15,16-tetrahydro-18,21-etheno-13,9-(metheno)-6,14,17-trioxa-2-thia-3,5-diazacyclononadeca[1,2,3-cd]indene-7-carboxylic acid (CCD ID: WME) (formula: C₅₃H₅₁Cl₂FN₆O₉S) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms							ZeroOcc	AltConf
3	A	1	Total	C	Cl	F	N	O	S	0	0
			72	53	2	1	6	9	1		
3	B	1	Total	C	Cl	F	N	O	S	0	0
			72	53	2	1	6	9	1		
3	C	1	Total	C	Cl	F	N	O	S	0	0
			72	53	2	1	6	9	1		
3	D	1	Total	C	Cl	F	N	O	S	0	0
			72	53	2	1	6	9	1		

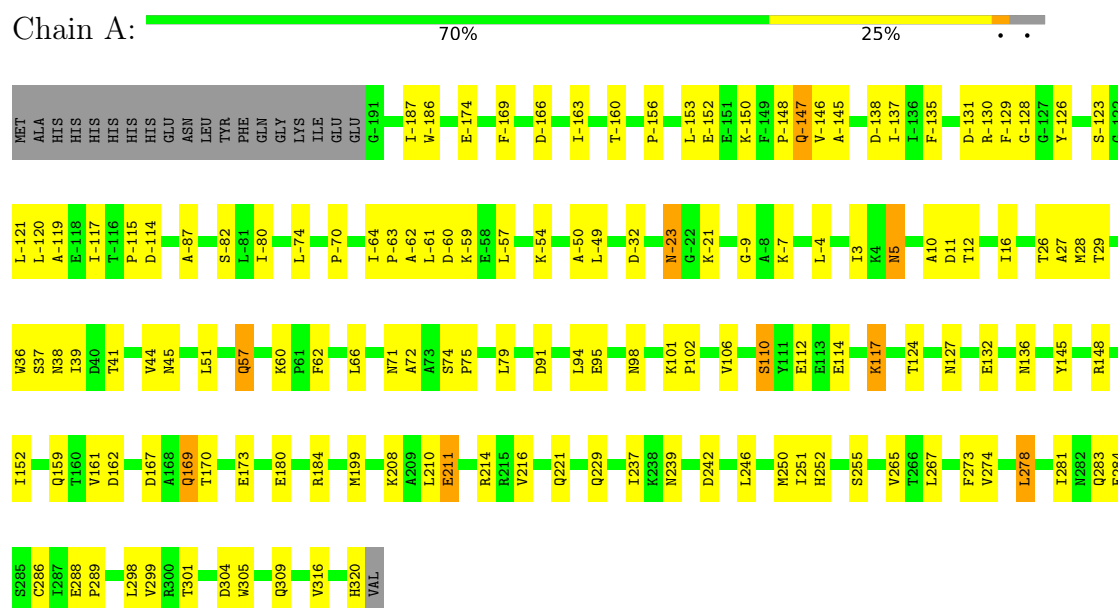
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	52	Total	O	0	0
			52	52		
4	B	42	Total	O	0	0
			42	42		
4	C	44	Total	O	0	0
			44	44		
4	D	44	Total	O	0	0
			44	44		

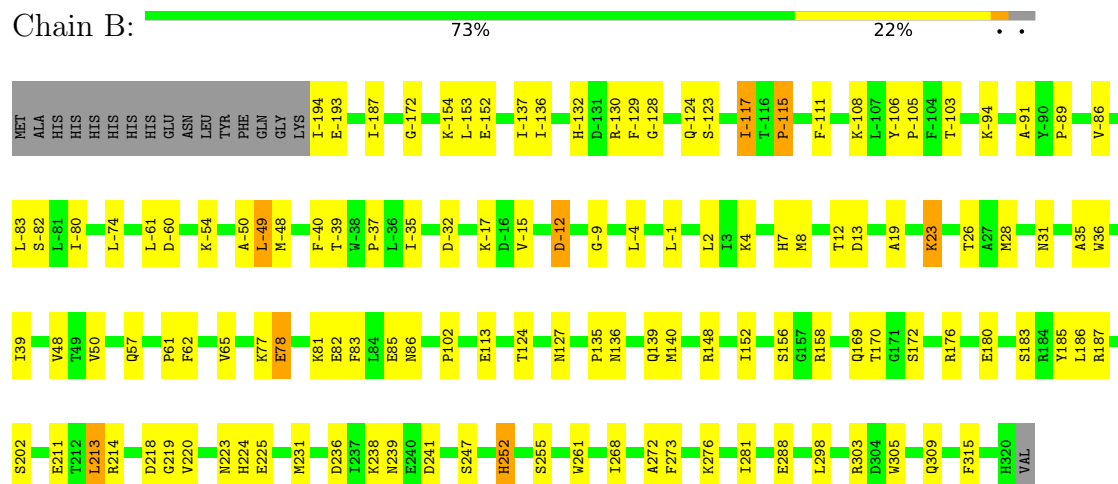
3 Residue-property plots

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: Maltose/maltodextrin-binding periplasmic protein, Induced myeloid leukemia cell differentiation protein Mcl-1

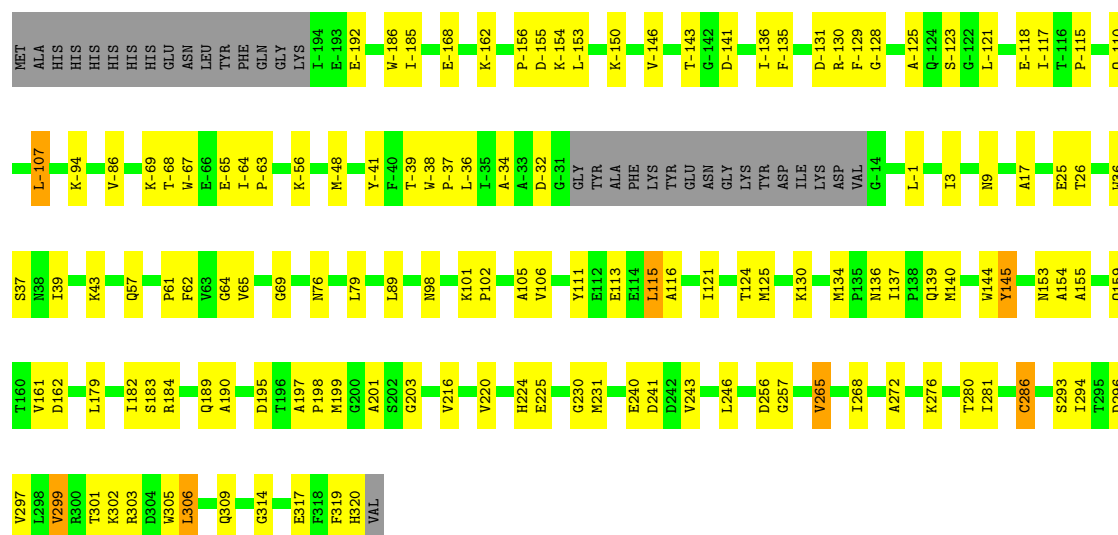


- Molecule 1: Maltose/maltodextrin-binding periplasmic protein, Induced myeloid leukemia cell differentiation protein Mcl-1



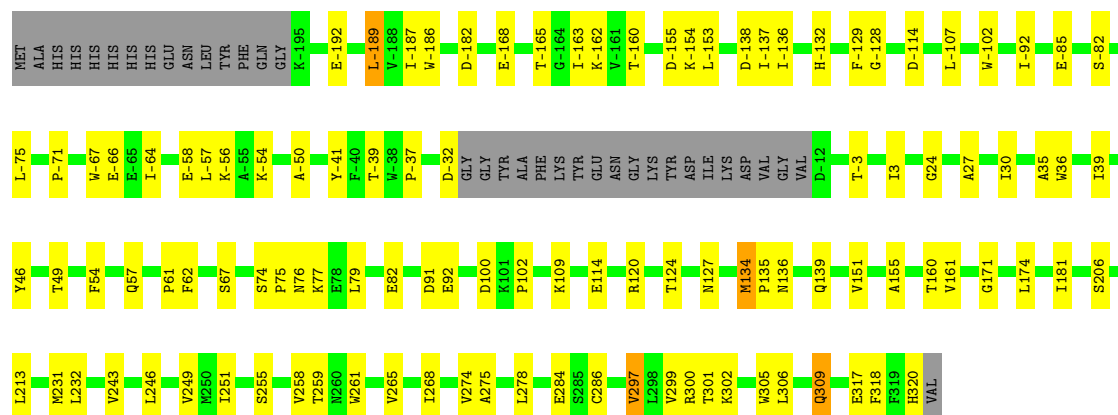
- Molecule 1: Maltose/maltodextrin-binding periplasmic protein, Induced myeloid leukemia cell differentiation protein Mcl-1

Chain C: 



- Molecule 1: Maltose/maltodextrin-binding periplasmic protein, Induced myeloid leukemia cell differentiation protein Mcl-1

Chain D: 



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

Chain E: 



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

Chain F: 



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

Chain G:  50% 50%



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

Chain H:  50% 50%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	111.38Å 79.62Å 137.85Å 90.00° 90.22° 90.00°	Depositor
Resolution (Å)	45.63 – 2.41 45.63 – 2.41	Depositor EDS
% Data completeness (in resolution range)	47.3 (45.63-2.41) 47.5 (45.63-2.41)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.51 (at 2.39Å)	Xtriage
Refinement program	BUSTER 2.11.8	Depositor
R, R_{free}	0.197 , 0.291 0.200 , 0.295	Depositor DCC
R_{free} test set	2162 reflections (4.86%)	wwPDB-VP
Wilson B-factor (Å ²)	52.2	Xtriage
Anisotropy	0.088	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 60.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	0.120 for h,-k,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	16036	wwPDB-VP
Average B, all atoms (Å ²)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.65% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: WME, GLC

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	0.81	1/4026 (0.0%)	1.21	11/5472 (0.2%)
1	B	0.80	0/4028	1.23	6/5482 (0.1%)
1	C	0.77	0/3893	1.24	15/5298 (0.3%)
1	D	0.80	2/3877 (0.1%)	1.23	14/5279 (0.3%)
All	All	0.80	3/15824 (0.0%)	1.23	46/21531 (0.2%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	-131	ASP	CA-C	5.16	1.59	1.52
1	D	-165	THR	CA-C	5.05	1.58	1.52
1	D	-64	ILE	CA-C	5.04	1.56	1.52

The worst 5 of 46 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	265	VAL	N-CA-CB	7.48	119.30	110.55
1	B	13	ASP	CA-CB-CG	7.21	119.81	112.60
1	A	-23	ASN	CA-CB-CG	7.15	119.75	112.60
1	C	230	GLY	CA-C-N	6.88	129.79	120.44
1	C	230	GLY	C-N-CA	6.88	129.79	120.44

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3936	0	3822	64	0
1	B	3938	0	3788	52	0
1	C	3808	0	3670	66	0
1	D	3792	0	3651	39	0
2	E	23	0	21	0	0
2	F	23	0	21	1	0
2	G	23	0	21	1	0
2	H	23	0	21	1	0
3	A	72	0	0	0	0
3	B	72	0	0	0	0
3	C	72	0	0	0	0
3	D	72	0	0	1	0
4	A	52	0	0	0	0
4	B	42	0	0	0	0
4	C	44	0	0	0	0
4	D	44	0	0	0	0
All	All	16036	0	15015	222	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 7.

The worst 5 of 222 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:-62:ALA:HA	1:A:-59:LYS:HD2	1.42	1.00
1:D:-187:ILE:HG12	1:D:-137:ILE:HB	1.52	0.89
1:B:-111:PHE:HA	1:B:-108:LYS:HE3	1.55	0.87
1:A:114:GLU:HA	1:A:117:LYS:HE3	1.59	0.84
1:C:37:SER:HB3	1:C:101:LYS:NZ	1.93	0.82

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	510/532 (96%)	482 (94%)	25 (5%)	3 (1%)	21	32
1	B	513/532 (96%)	478 (93%)	32 (6%)	3 (1%)	21	32
1	C	495/532 (93%)	463 (94%)	31 (6%)	1 (0%)	43	58
1	D	493/532 (93%)	456 (92%)	34 (7%)	3 (1%)	21	32
All	All	2011/2128 (94%)	1879 (93%)	122 (6%)	10 (0%)	24	37

5 of 10 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	-163	ILE
1	A	-114	ASP
1	B	-132	HIS
1	B	-115	PRO
1	C	201	ALA

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	401/434 (92%)	360 (90%)	41 (10%)	7	11
1	B	398/434 (92%)	362 (91%)	36 (9%)	9	15
1	C	386/434 (89%)	350 (91%)	36 (9%)	8	14
1	D	383/434 (88%)	348 (91%)	35 (9%)	9	14
All	All	1568/1736 (90%)	1420 (91%)	148 (9%)	8	13

5 of 148 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	-155	ASP
1	D	301	THR
1	D	-58	GLU

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Mol	Chain	Res	Type
1	D	92	GLU
1	B	4	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 27 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	239	ASN
1	C	-46	ASN
1	D	221	GLN
1	C	-178	ASN
1	C	57	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

8 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	GLC	E	1	2	12,12,12	0.26	0	17,17,17	0.61	0
2	GLC	E	2	2	11,11,12	0.30	0	15,15,17	0.86	1 (6%)
2	GLC	F	1	2	12,12,12	0.26	0	17,17,17	0.61	0
2	GLC	F	2	2	11,11,12	0.37	0	15,15,17	0.88	1 (6%)
2	GLC	G	1	2	12,12,12	0.32	0	17,17,17	0.66	0
2	GLC	G	2	2	11,11,12	0.33	0	15,15,17	0.67	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	GLC	H	1	2	12,12,12	0.41	0	17,17,17	0.92	0
2	GLC	H	2	2	11,11,12	0.34	0	15,15,17	0.94	1 (6%)

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	E	1	2	-	0/2/22/22	0/1/1/1
2	GLC	E	2	2	-	0/2/19/22	0/1/1/1
2	GLC	F	1	2	-	0/2/22/22	0/1/1/1
2	GLC	F	2	2	-	0/2/19/22	0/1/1/1
2	GLC	G	1	2	-	0/2/22/22	0/1/1/1
2	GLC	G	2	2	-	0/2/19/22	0/1/1/1
2	GLC	H	1	2	-	0/2/22/22	0/1/1/1
2	GLC	H	2	2	-	0/2/19/22	0/1/1/1

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	2	GLC	C1-O5-C5	2.71	115.82	112.19
2	G	2	GLC	C1-O5-C5	2.17	115.10	112.19
2	H	2	GLC	C1-O5-C5	2.14	115.05	112.19
2	F	2	GLC	C1-O5-C5	2.12	115.03	112.19

There are no chirality outliers.

There are no torsion outliers.

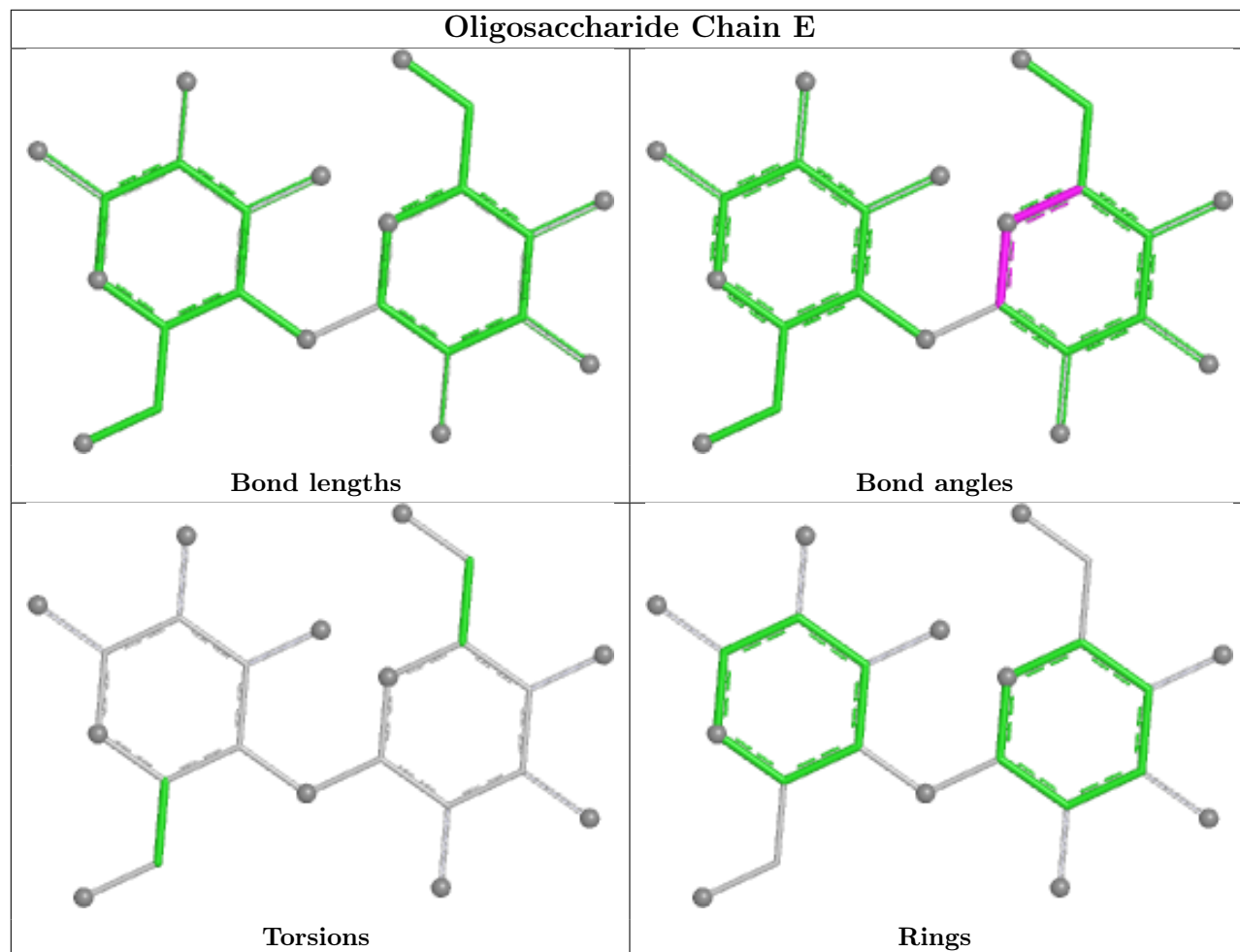
There are no ring outliers.

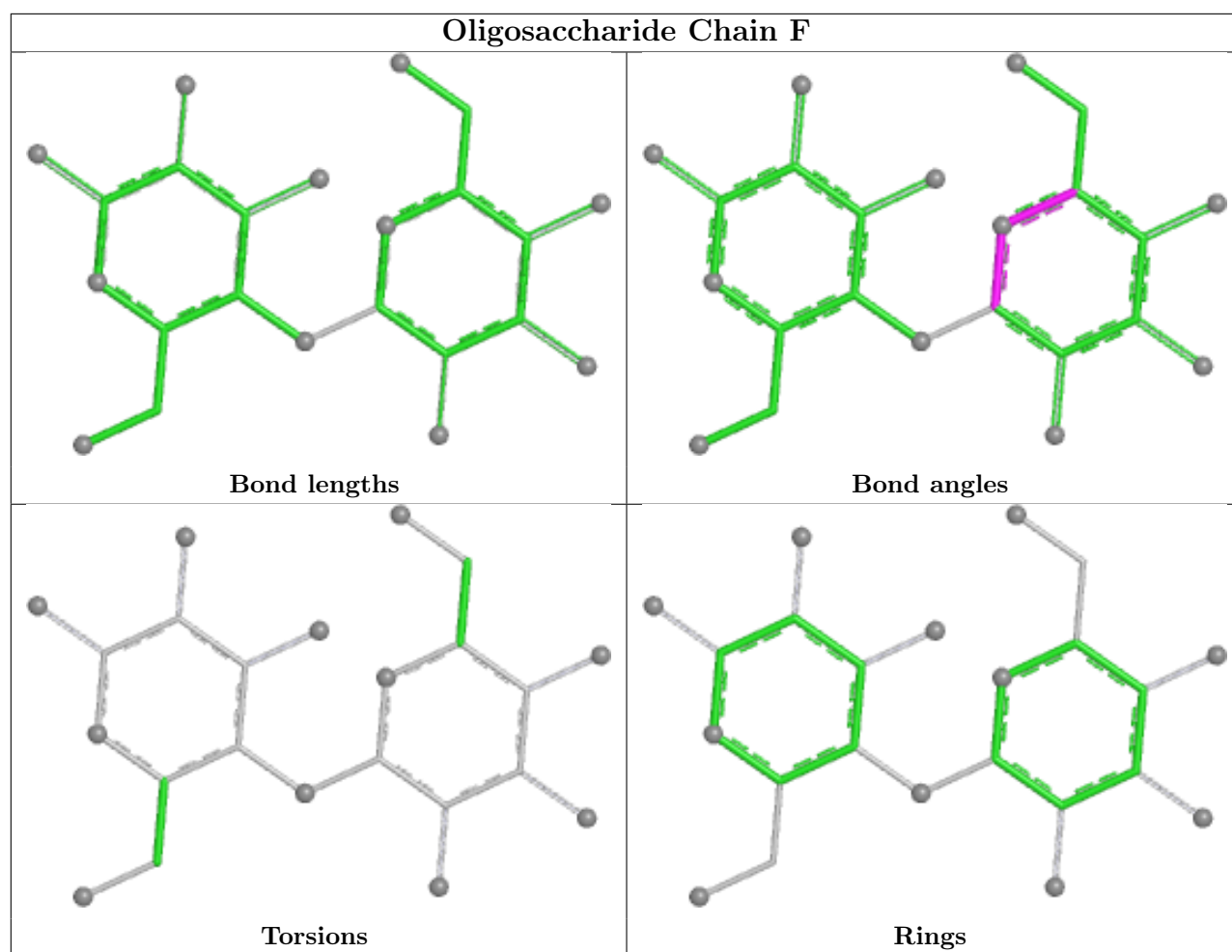
5 monomers are involved in 3 short contacts:

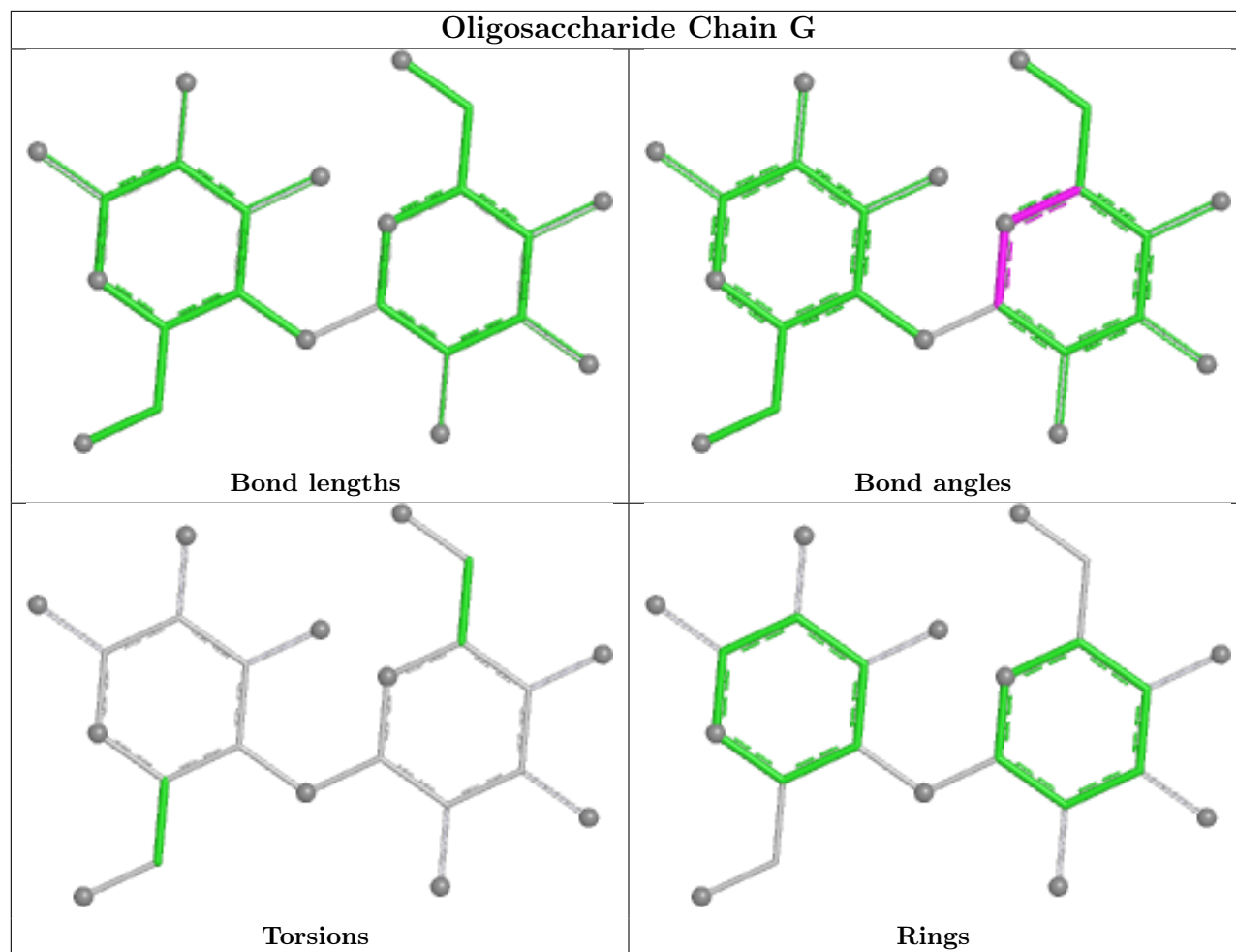
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	1	GLC	1	0
2	G	2	GLC	1	0
2	F	2	GLC	1	0
2	H	2	GLC	1	0
2	H	1	GLC	1	0

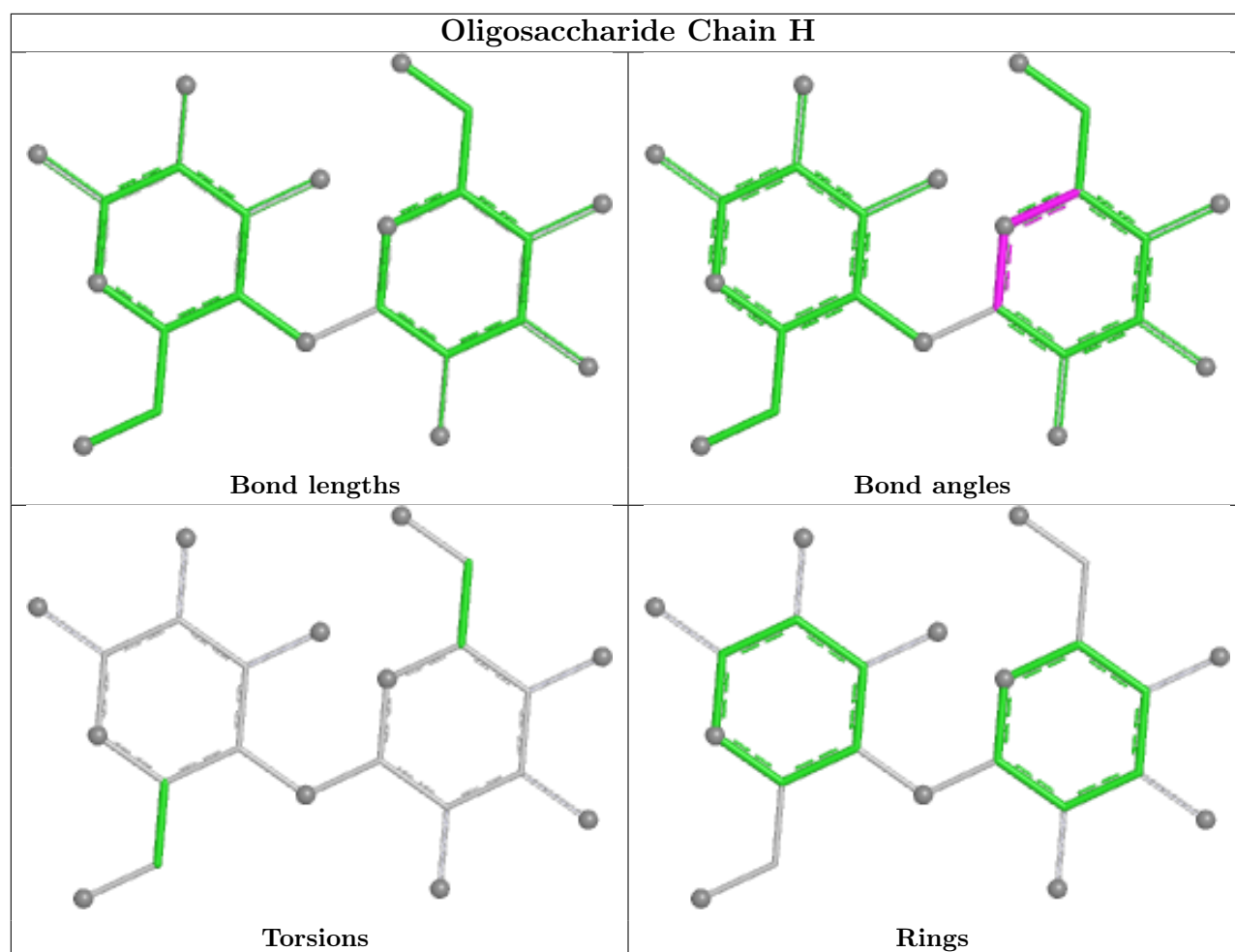
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

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









5.6 Ligand geometry [i](#)

4 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	$\# Z > 2$
3	WME	A	4000	-	81,81,81	0.69	3 (3%)	104,116,116	0.89	5 (4%)
3	WME	D	4000	-	81,81,81	0.76	3 (3%)	104,116,116	1.04	6 (5%)
3	WME	C	4000	-	81,81,81	0.62	2 (2%)	104,116,116	0.84	4 (3%)
3	WME	B	4000	-	81,81,81	0.69	3 (3%)	104,116,116	1.02	6 (5%)

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	WME	A	4000	-	-	9/47/65/65	0/9/10/10
3	WME	D	4000	-	-	7/47/65/65	0/9/10/10
3	WME	C	4000	-	-	8/47/65/65	0/9/10/10
3	WME	B	4000	-	-	8/47/65/65	0/9/10/10

The worst 5 of 11 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	4000	WME	C17-C16	4.46	1.40	1.36
3	A	4000	WME	O4-C26	3.80	1.33	1.22
3	B	4000	WME	O4-C26	3.34	1.32	1.22
3	C	4000	WME	O4-C26	3.28	1.31	1.22
3	D	4000	WME	O4-C26	3.18	1.31	1.22

The worst 5 of 21 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	4000	WME	C28-C24-C17	-4.57	114.24	120.23
3	B	4000	WME	O4-C26-C25	-4.39	113.37	122.85
3	A	4000	WME	C28-C24-C17	-4.26	114.65	120.23
3	B	4000	WME	O5-C40-C42	4.25	114.54	107.05
3	D	4000	WME	C14-O2-C25	4.21	123.14	117.01

There are no chirality outliers.

5 of 32 torsion outliers are listed below:

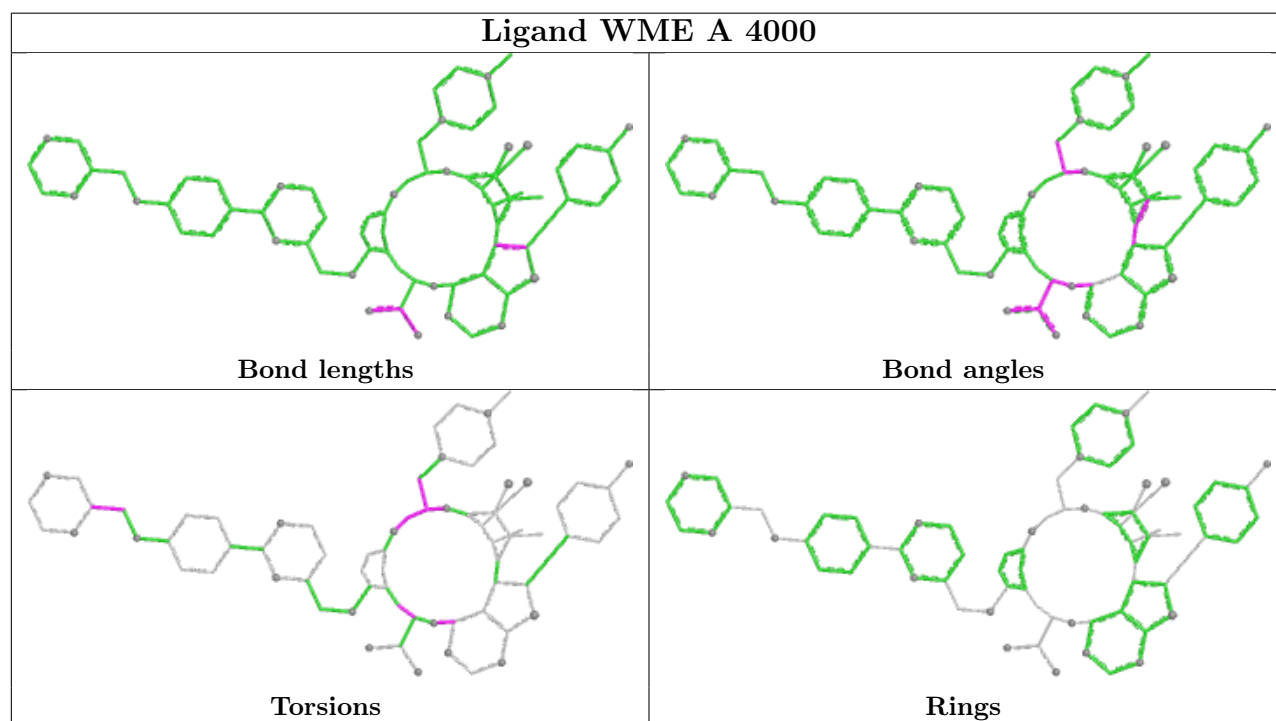
Mol	Chain	Res	Type	Atoms
3	A	4000	WME	O7-C48-C50-O8
3	A	4000	WME	O7-C48-C50-C53
3	B	4000	WME	O7-C48-C50-O8
3	C	4000	WME	C41-C40-O5-C30
3	D	4000	WME	C41-C40-O5-C30

There are no ring outliers.

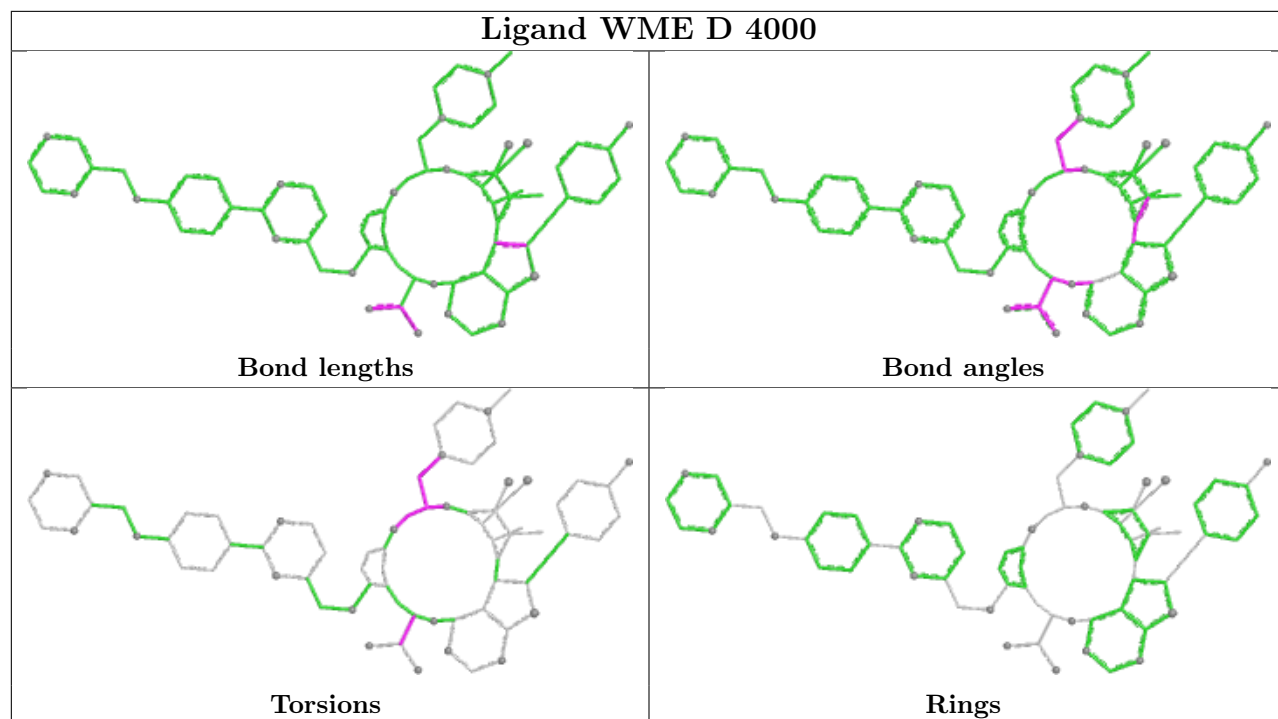
1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	4000	WME	1	0

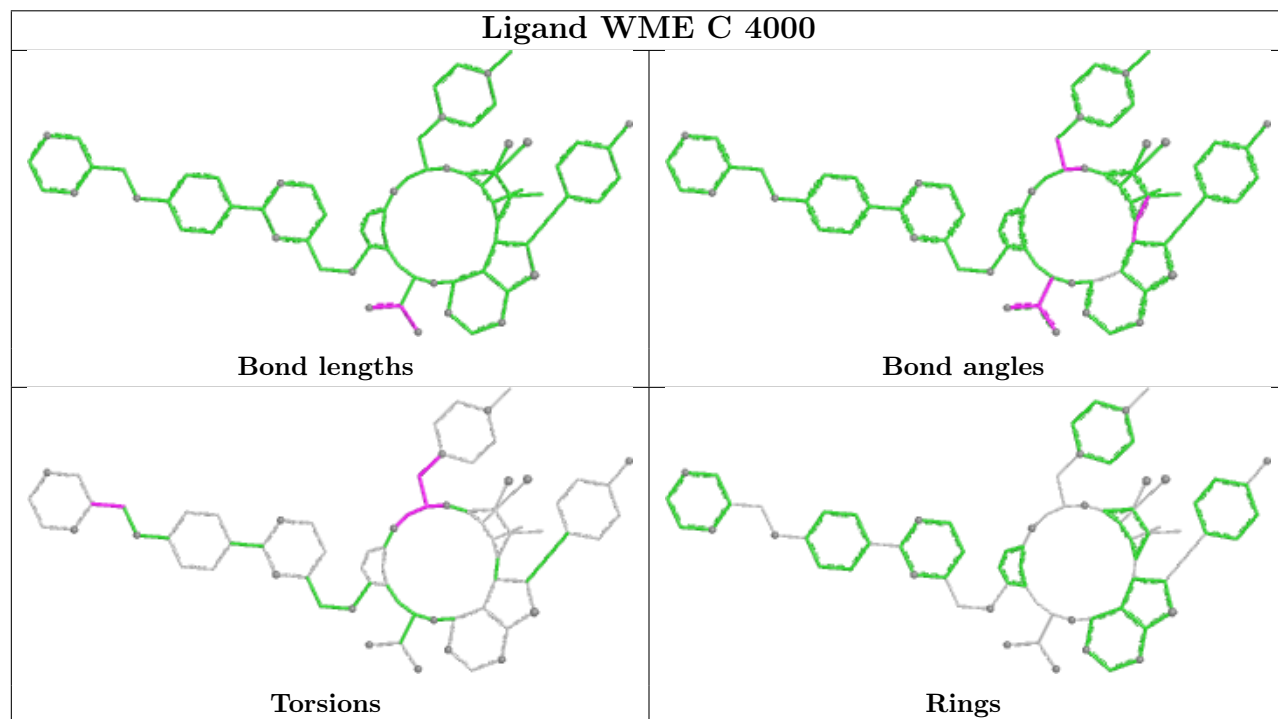
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

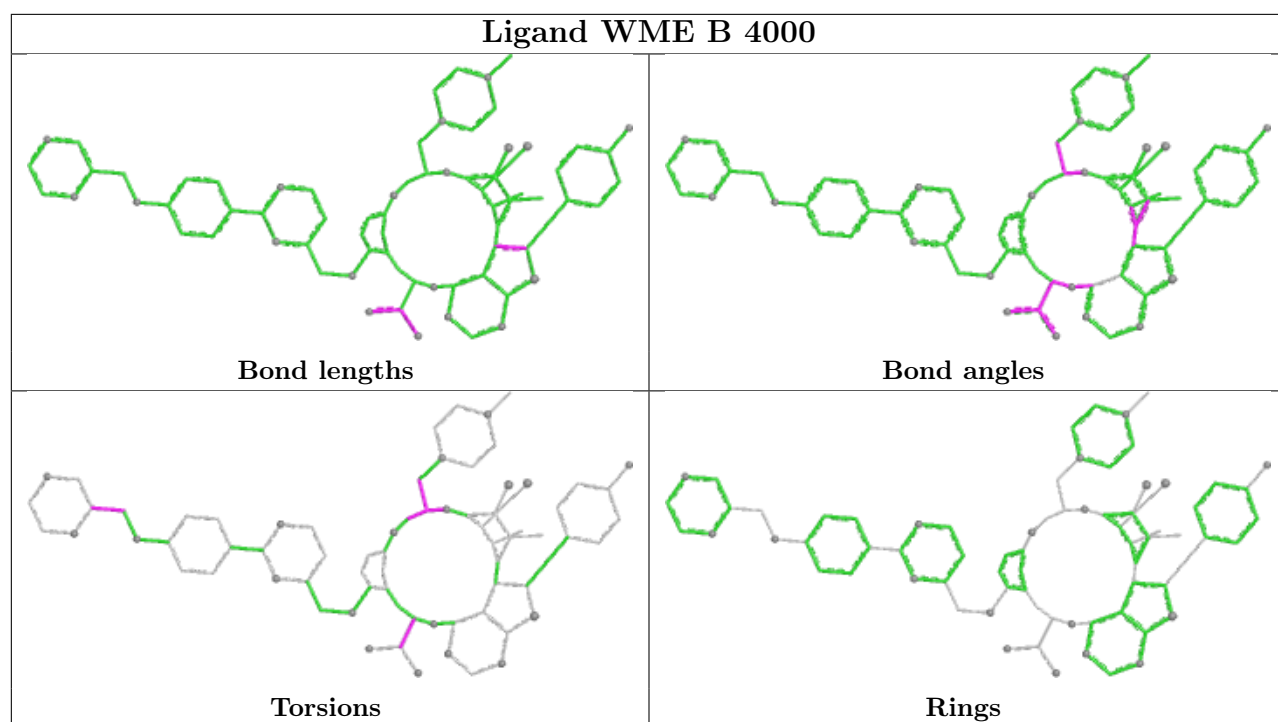


Ligand WME D 4000



Ligand WME C 4000





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	512/532 (96%)	-1.54	0 100 100	26, 46, 63, 81	0
1	B	515/532 (96%)	-1.51	0 100 100	29, 51, 71, 84	0
1	C	499/532 (93%)	-1.48	0 100 100	33, 54, 77, 96	0
1	D	497/532 (93%)	-1.46	0 100 100	32, 54, 77, 86	0
All	All	2023/2128 (95%)	-1.50	0 100 100	26, 51, 74, 96	0

There are no RSRZ outliers to report.

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

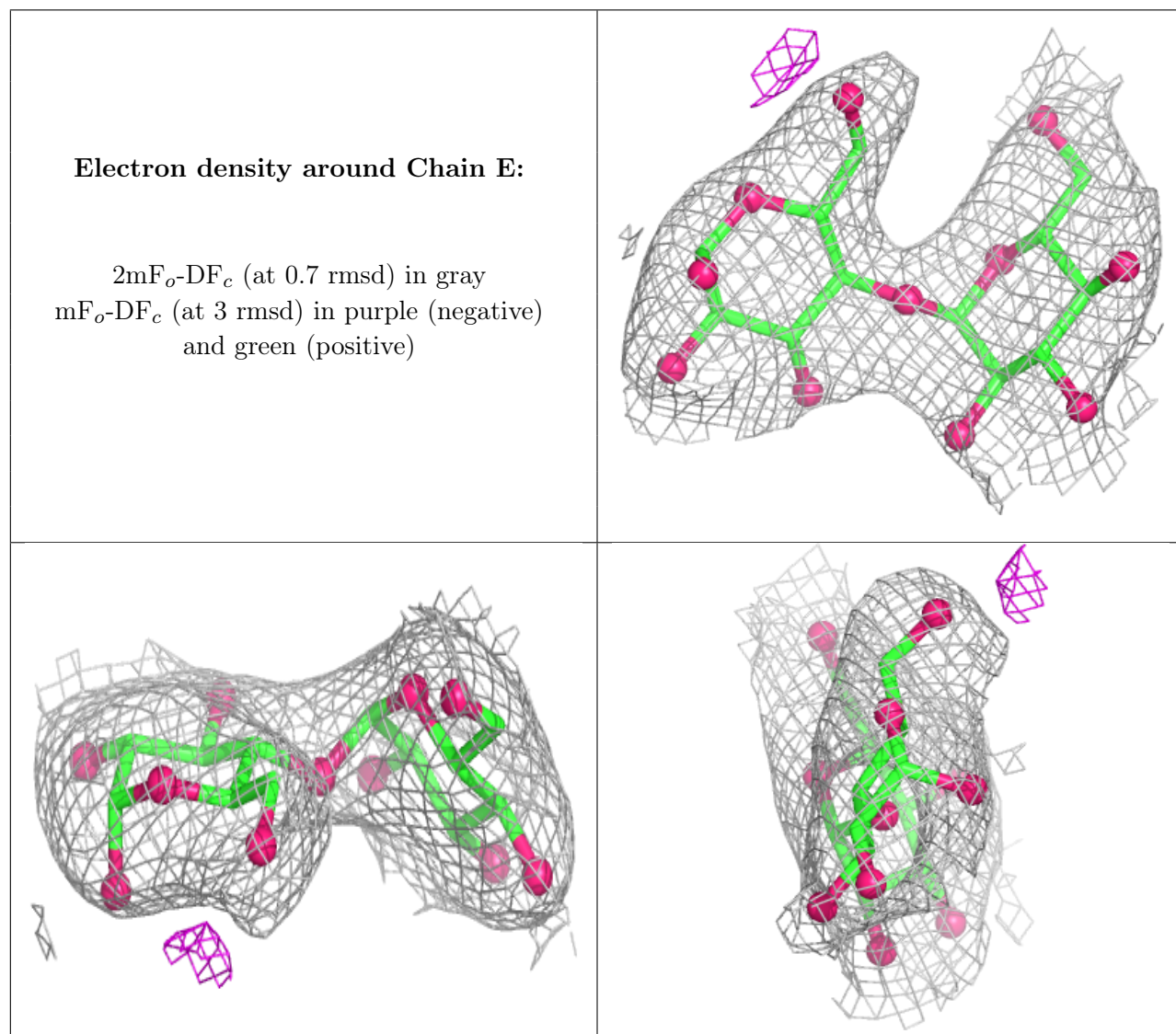
There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

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

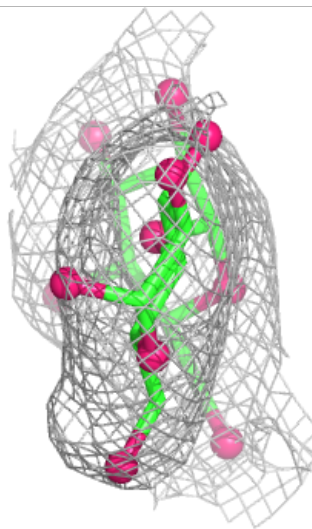
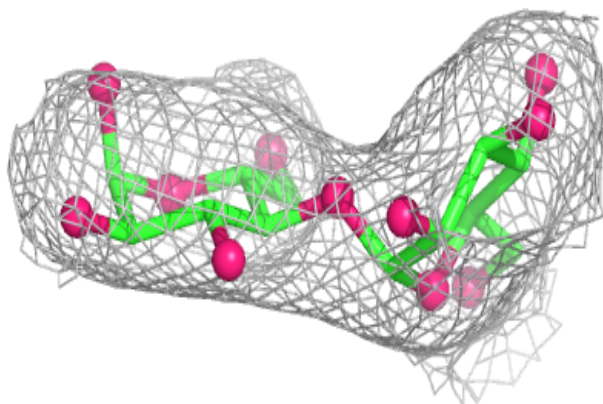
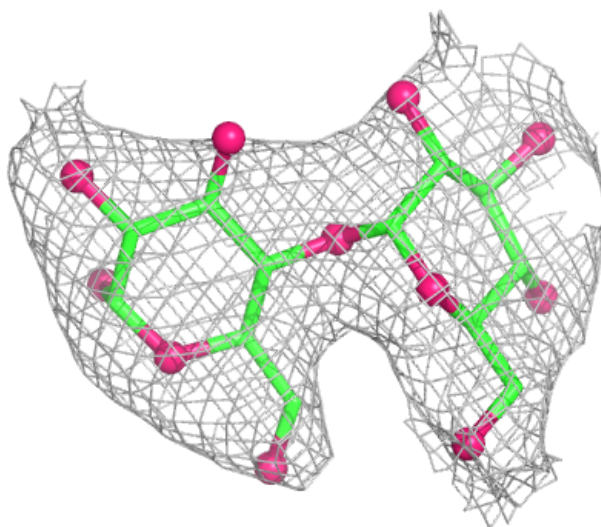
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	GLC	E	1	12/12	0.99	0.02	38,41,41,41	0
2	GLC	E	2	11/12	0.99	0.02	34,35,37,37	0
2	GLC	G	1	12/12	0.99	0.02	38,39,39,39	0
2	GLC	G	2	11/12	0.99	0.02	36,38,39,40	0
2	GLC	H	1	12/12	0.99	0.03	44,46,46,47	0
2	GLC	H	2	11/12	0.99	0.03	45,45,45,46	0
2	GLC	F	1	12/12	1.00	0.02	41,42,43,43	0
2	GLC	F	2	11/12	1.00	0.02	41,42,43,44	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.



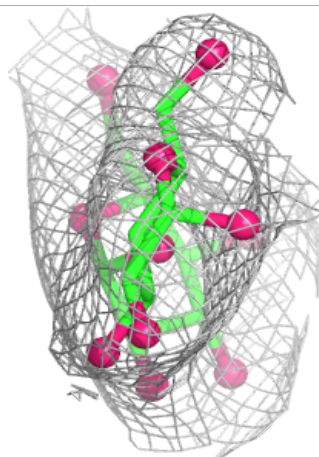
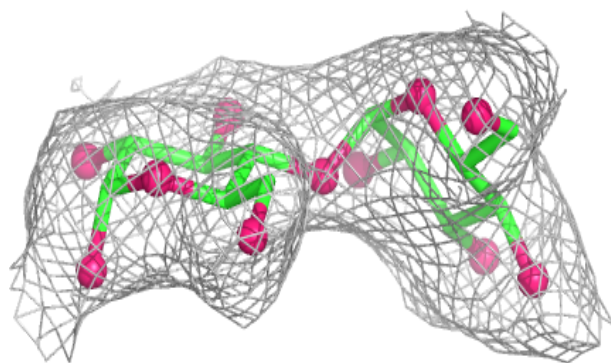
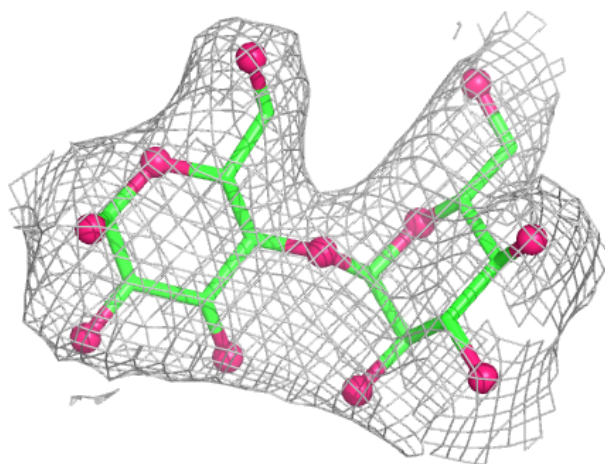
Electron density around Chain F:

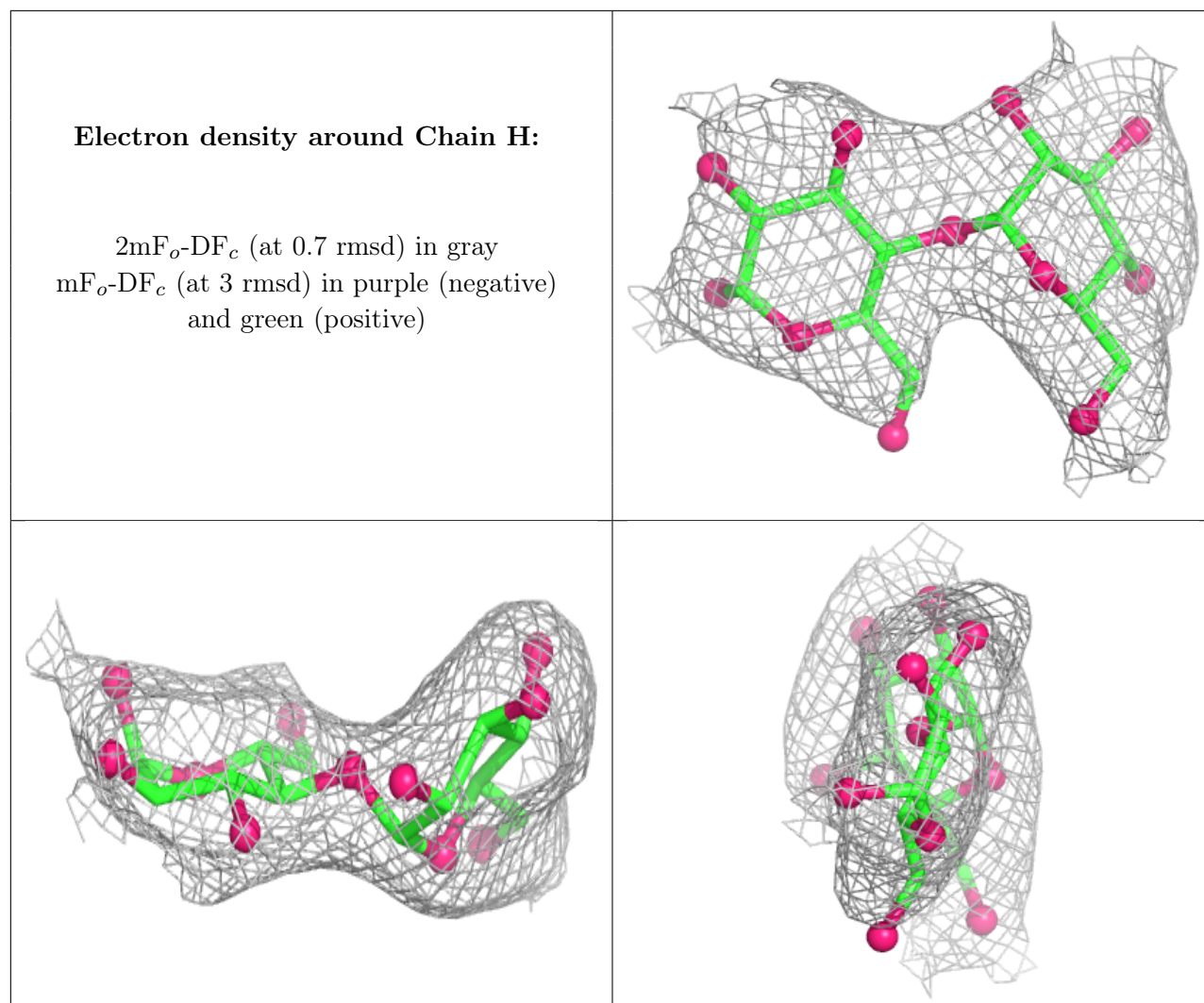
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



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](#)

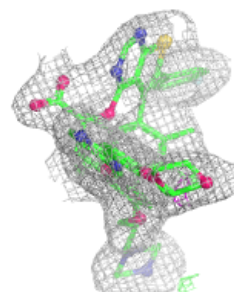
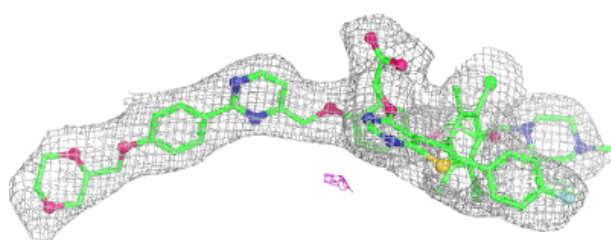
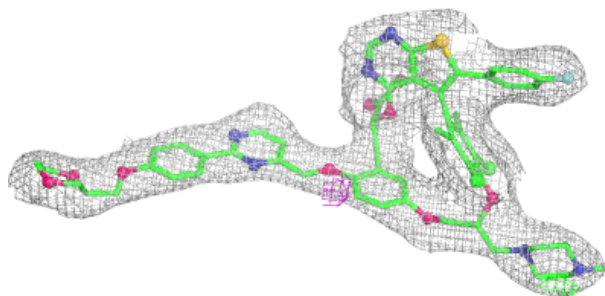
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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
3	WME	A	4000	72/72	0.99	0.02	37,42,46,46	0
3	WME	B	4000	72/72	0.99	0.03	46,50,52,53	0
3	WME	C	4000	72/72	0.99	0.03	60,62,67,68	0
3	WME	D	4000	72/72	0.99	0.02	46,50,65,65	0

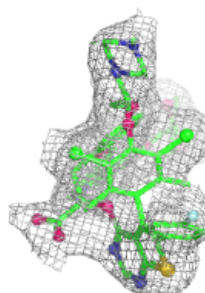
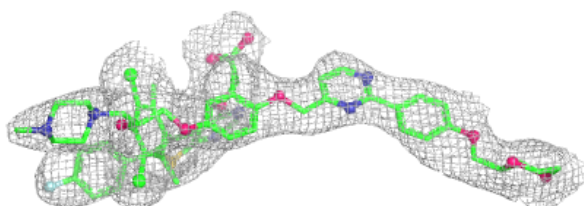
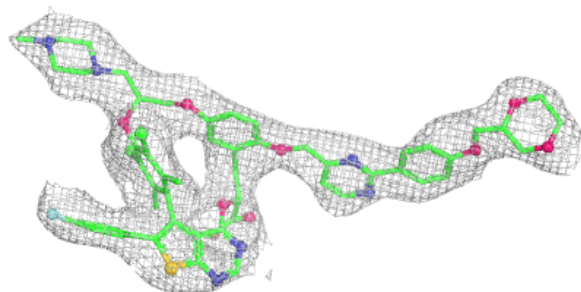
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around WME A 4000:

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

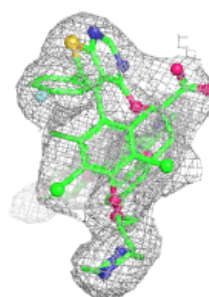
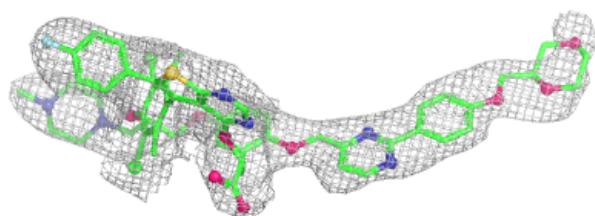
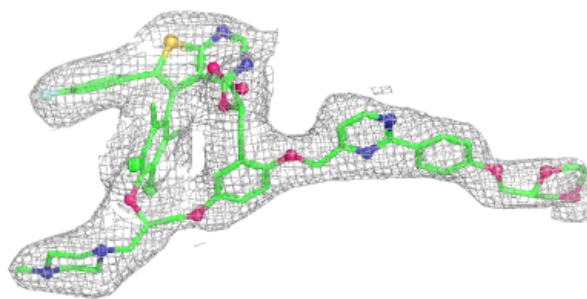
**Electron density around WME B 4000:**

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

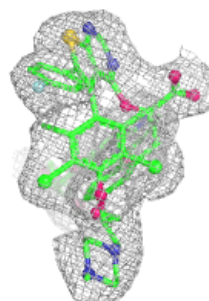
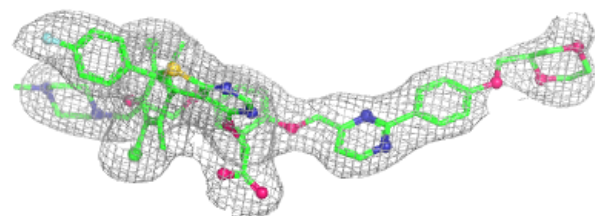
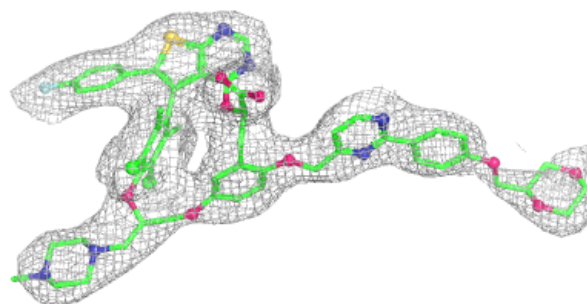


Electron density around WME C 4000:

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

**Electron density around WME D 4000:**

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



6.5 Other polymers [i](#)

There are no such residues in this entry.