



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 27, 2026 – 07:45 PM UTC

PDB ID : 6SGF / pdb_00006sgf
Title : Molecular insight into a new low affinity xylan binding module CBM86, from the xylanolytic gut symbiont *Roseburia intestinalis*.
Authors : Ejby, M.; Abou Hachem, M.; Leth, M.L.; Guskov, A.; Slotboom, D.
Deposited on : 2019-08-04
Resolution : 1.76 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

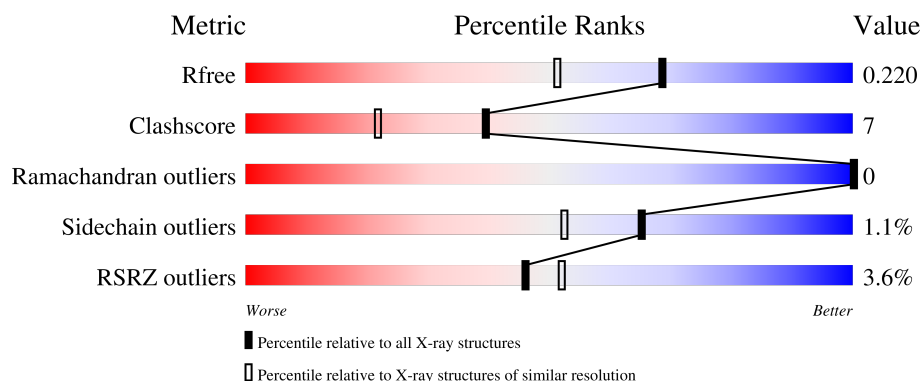
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.76 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	3183 (1.76-1.76)
Clashscore	190562	3299 (1.76-1.76)
Ramachandran outliers	187476	3274 (1.76-1.76)
Sidechain outliers	187428	3274 (1.76-1.76)
RSRZ outliers	180081	3183 (1.76-1.76)

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	141	 3% 84% 6% • 9%
1	B	141	 3% 86% 8% 6%
1	C	141	 3% 82% 11% • 7%
1	D	141	 2% 84% 9% 7%
1	E	141	 5% 83% 11% 6%

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Mol	Chain	Length	Quality of chain
1	F	141	
2	G	3	
3	H	4	
3	I	4	
3	J	4	
3	K	4	
3	L	4	

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
6	CL	A	208	-	-	X	-
6	CL	A	209	-	-	X	-
6	CL	B	207	-	-	X	-
6	CL	C	208	-	-	X	-
6	CL	C	209	-	-	X	-
6	CL	E	206	-	-	X	-
6	CL	F	205	-	-	X	-

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 12881 atoms, of which 6002 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-xylanase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	129	Total	C	H	N	O	S	0	0	0
			1940	623	957	157	201	2			
1	B	132	Total	C	H	N	O	S	0	0	0
			1964	630	968	160	204	2			
1	C	131	Total	C	H	N	O	S	0	0	0
			1957	628	965	159	203	2			
1	D	131	Total	C	H	N	O	S	0	0	0
			1964	630	969	159	203	3			
1	E	132	Total	C	H	N	O	S	0	1	0
			1976	634	974	161	205	2			
1	F	131	Total	C	H	N	O	S	0	0	0
			1957	628	965	159	203	2			

There are 18 discrepancies between the modelled and reference sequences:

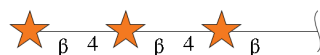
Chain	Residue	Modelled	Actual	Comment	Reference
A	25	GLY	-	expression tag	UNP C7G9B5
A	26	ALA	-	expression tag	UNP C7G9B5
A	27	MET	-	expression tag	UNP C7G9B5
B	25	GLY	-	expression tag	UNP C7G9B5
B	26	ALA	-	expression tag	UNP C7G9B5
B	27	MET	-	expression tag	UNP C7G9B5
C	25	GLY	-	expression tag	UNP C7G9B5
C	26	ALA	-	expression tag	UNP C7G9B5
C	27	MET	-	expression tag	UNP C7G9B5
D	25	GLY	-	expression tag	UNP C7G9B5
D	26	ALA	-	expression tag	UNP C7G9B5
D	27	MET	-	expression tag	UNP C7G9B5
E	25	GLY	-	expression tag	UNP C7G9B5
E	26	ALA	-	expression tag	UNP C7G9B5
E	27	MET	-	expression tag	UNP C7G9B5
F	25	GLY	-	expression tag	UNP C7G9B5
F	26	ALA	-	expression tag	UNP C7G9B5

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Chain	Residue	Modelled	Actual	Comment	Reference
F	27	MET	-	expression tag	UNP C7G9B5

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



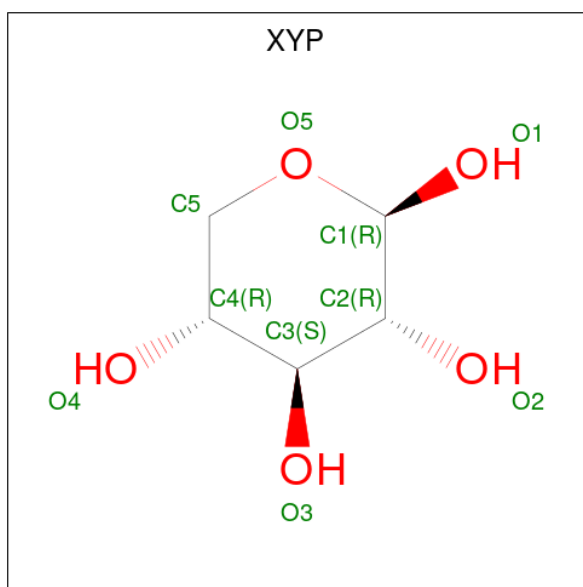
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	G	3	Total	C	H	O	0	0	0
			52	15	25	12			

- Molecule 3 is an oligosaccharide called beta-D-xylopyranose-(1-4)-beta-D-xylopyranose-(1-4)-beta-D-xylopyranose-(1-4)-beta-D-xylopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	H	4	Total	C	H	O	0	0	0
			71	20	34	17			
3	I	4	Total	C	H	O	0	0	0
			71	20	34	17			
3	J	4	Total	C	H	O	0	0	0
			71	20	34	17			
3	K	4	Total	C	H	O	0	0	0
			71	20	34	17			
3	L	4	Total	C	H	O	0	0	0
			71	20	34	17			

- Molecule 4 is beta-D-xylopyranose (CCD ID: XYP) (formula: C₅H₁₀O₅) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	H	O	0	0
			19	5	9	5		

- Molecule 5 is CADMIUM ION (CCD ID: CD) (formula: Cd).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	3	Total	Cd	0	0
			3	3		
5	B	2	Total	Cd	0	0
			2	2		
5	C	3	Total	Cd	0	0
			3	3		
5	D	1	Total	Cd	0	0
			1	1		
5	E	1	Total	Cd	0	0
			1	1		

- Molecule 6 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	2	Total	Cl	0	0
			2	2		
6	B	1	Total	Cl	0	0
			1	1		
6	C	3	Total	Cl	0	0
			3	3		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	E	1	Total 1	Cl 1	0	0
6	F	1	Total 1	Cl 1	0	0

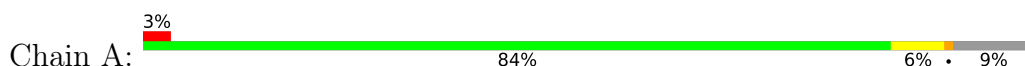
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	123	Total 123	O 123	0	0
7	B	128	Total 128	O 128	0	0
7	C	117	Total 117	O 117	0	0
7	D	108	Total 108	O 108	0	0
7	E	101	Total 101	O 101	0	0
7	F	102	Total 102	O 102	0	0

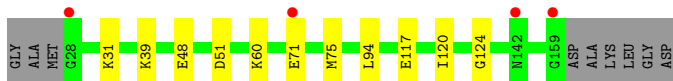
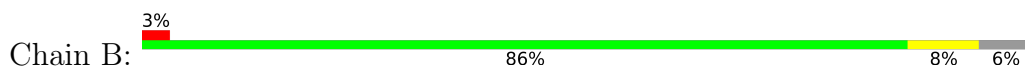
3 Residue-property plots [i](#)

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.

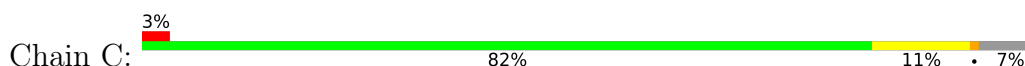
- Molecule 1: Beta-xylanase



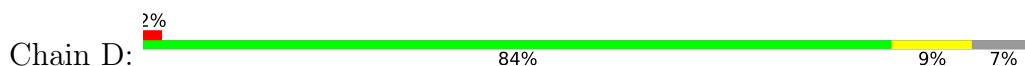
- Molecule 1: Beta-xylanase



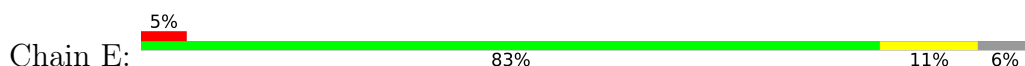
- Molecule 1: Beta-xylanase



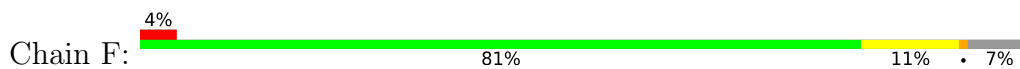
- Molecule 1: Beta-xylanase



- Molecule 1: Beta-xylanase



- Molecule 1: Beta-xylanase



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



- Molecule 3: beta-D-xylopyranose-(1-4)-beta-D-xylopyranose-(1-4)-beta-D-xylopyranose-(1-4)-beta-D-xylopyranose



- Molecule 3: beta-D-xylopyranose-(1-4)-beta-D-xylopyranose-(1-4)-beta-D-xylopyranose-(1-4)-beta-D-xylopyranose



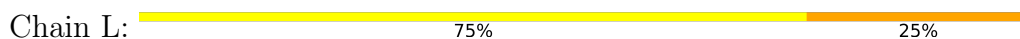
- Molecule 3: beta-D-xylopyranose-(1-4)-beta-D-xylopyranose-(1-4)-beta-D-xylopyranose-(1-4)-beta-D-xylopyranose



- Molecule 3: beta-D-xylopyranose-(1-4)-beta-D-xylopyranose-(1-4)-beta-D-xylopyranose-(1-4)-beta-D-xylopyranose



- Molecule 3: beta-D-xylopyranose-(1-4)-beta-D-xylopyranose-(1-4)-beta-D-xylopyranose-(1-4)-beta-D-xylopyranose



4 Data and refinement statistics

Property	Value	Source
Space group	P 65	Depositor
Cell constants a, b, c, α , β , γ	141.87Å 141.87Å 60.60Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	46.44 – 1.76 46.44 – 1.76	Depositor EDS
% Data completeness (in resolution range)	93.6 (46.44-1.76) 96.8 (46.44-1.76)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.21 (at 1.76Å)	Xtriage
Refinement program	PHENIX 1.14_3260	Depositor
R, R_{free}	0.179 , 0.224 0.184 , 0.220	Depositor DCC
R_{free} test set	2510 reflections (3.73%)	wwPDB-VP
Wilson B-factor (Å ²)	22.1	Xtriage
Anisotropy	0.066	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.41 , 41.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.032 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	12881	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 29.08 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.6474e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: CL, XYP, CD

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	0.56	0/1001	0.72	0/1362
1	B	0.52	0/1014	0.71	0/1379
1	C	0.49	0/1010	0.69	0/1374
1	D	0.55	0/1013	0.70	0/1377
1	E	0.65	2/1023 (0.2%)	0.75	0/1391
1	F	0.58	0/1010	0.82	1/1374 (0.1%)
All	All	0.56	2/6071 (0.0%)	0.73	1/8257 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	140	PRO	C-O	-6.08	1.16	1.23
1	E	70	PRO	C-O	-5.61	1.17	1.24

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	31	LYS	CG-CD-CE	5.37	123.65	111.30

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	983	957	957	10	0
1	B	996	968	968	10	1
1	C	992	965	965	14	0
1	D	995	969	969	11	0
1	E	1002	974	976	11	0
1	F	992	965	965	16	0
2	G	27	25	0	2	0
3	H	37	34	0	0	0
3	I	37	34	0	0	0
3	J	37	34	0	0	0
3	K	37	34	0	0	0
3	L	37	34	0	1	0
4	A	10	9	0	2	0
5	A	3	0	0	1	0
5	B	2	0	0	0	0
5	C	3	0	0	0	0
5	D	1	0	0	0	0
5	E	1	0	0	0	0
6	A	2	0	0	3	1
6	B	1	0	0	2	1
6	C	3	0	0	5	0
6	E	1	0	0	3	0
6	F	1	0	0	4	0
7	A	123	0	0	7	3
7	B	128	0	0	5	2
7	C	117	0	0	5	0
7	D	108	0	0	6	1
7	E	101	0	0	8	1
7	F	102	0	0	5	0
All	All	6879	6002	5800	80	5

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 80 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)
4:A:204:XYP:O4	2:G:1:XYP:C1	1.65	1.44
1:F:76:SER:OG	7:F:301:HOH:O	1.69	1.04
1:A:51:ASP:OD1	7:A:301:HOH:O	1.75	1.02
1:A:46:ASP:OD1	7:A:302:HOH:O	1.90	0.88
1:A:51:ASP:OD2	6:A:208:CL:CL	2.33	0.84

All (5) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:209:CL:CL	6:B:207:CL:CL[1_554]	0.23	1.97
1:B:51:ASP:OD1	7:A:302:HOH:O[6_655]	1.95	0.25
7:A:333:HOH:O	7:B:387:HOH:O[1_554]	2.07	0.13
7:A:306:HOH:O	7:B:313:HOH:O[1_554]	2.09	0.11
7:D:406:HOH:O	7:E:401:HOH:O[2_664]	2.17	0.03

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	127/141 (90%)	125 (98%)	2 (2%)	0	100	100
1	B	130/141 (92%)	129 (99%)	1 (1%)	0	100	100
1	C	129/141 (92%)	128 (99%)	1 (1%)	0	100	100
1	D	129/141 (92%)	126 (98%)	3 (2%)	0	100	100
1	E	131/141 (93%)	127 (97%)	4 (3%)	0	100	100
1	F	129/141 (92%)	126 (98%)	3 (2%)	0	100	100
All	All	775/846 (92%)	761 (98%)	14 (2%)	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	105/110 (96%)	104 (99%)	1 (1%)	68	56
1	B	105/110 (96%)	104 (99%)	1 (1%)	68	56
1	C	105/110 (96%)	104 (99%)	1 (1%)	68	56
1	D	106/110 (96%)	105 (99%)	1 (1%)	70	60
1	E	106/110 (96%)	104 (98%)	2 (2%)	50	31
1	F	105/110 (96%)	104 (99%)	1 (1%)	68	56
All	All	632/660 (96%)	625 (99%)	7 (1%)	65	52

5 of 7 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	60	LYS
1	E	139	LYS
1	F	39	LYS
1	E	141	GLU
1	C	60	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	53	GLN
1	D	84	GLN
1	D	109	GLN
1	F	63	ASN
1	F	77	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 ⓘ

23 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	XYP	G	1	2	9,9,10	1.71	3 (33%)	10,12,14	1.29	1 (10%)
2	XYP	G	2	2	9,9,10	2.07	2 (22%)	10,12,14	0.94	0
2	XYP	G	3	2	9,9,10	1.99	3 (33%)	10,12,14	2.23	3 (30%)
3	XYP	H	1	3	10,10,10	1.81	2 (20%)	14,14,14	1.90	4 (28%)
3	XYP	H	2	3	9,9,10	1.63	3 (33%)	10,12,14	1.37	2 (20%)
3	XYP	H	3	3	9,9,10	1.85	2 (22%)	10,12,14	1.70	3 (30%)
3	XYP	H	4	3	9,9,10	1.88	2 (22%)	10,12,14	0.92	0
3	XYP	I	1	3	10,10,10	1.87	3 (30%)	14,14,14	1.12	1 (7%)
3	XYP	I	2	3	9,9,10	1.85	2 (22%)	10,12,14	0.71	0
3	XYP	I	3	3	9,9,10	1.82	1 (11%)	10,12,14	1.61	3 (30%)
3	XYP	I	4	3	9,9,10	1.82	2 (22%)	10,12,14	1.89	2 (20%)
3	XYP	J	1	3	10,10,10	1.89	3 (30%)	14,14,14	1.51	2 (14%)
3	XYP	J	2	3	9,9,10	1.63	2 (22%)	10,12,14	1.67	2 (20%)
3	XYP	J	3	3	9,9,10	1.68	3 (33%)	10,12,14	1.12	0
3	XYP	J	4	3	9,9,10	1.71	2 (22%)	10,12,14	1.40	2 (20%)
3	XYP	K	1	3	10,10,10	2.01	2 (20%)	14,14,14	0.99	1 (7%)
3	XYP	K	2	3	9,9,10	1.82	2 (22%)	10,12,14	1.65	1 (10%)
3	XYP	K	3	3	9,9,10	1.85	2 (22%)	10,12,14	1.10	1 (10%)
3	XYP	K	4	3	9,9,10	1.99	3 (33%)	10,12,14	1.59	1 (10%)
3	XYP	L	1	3	10,10,10	1.93	3 (30%)	14,14,14	0.83	0
3	XYP	L	2	3	9,9,10	1.65	1 (11%)	10,12,14	1.34	2 (20%)
3	XYP	L	3	3	9,9,10	1.81	3 (33%)	10,12,14	1.64	2 (20%)
3	XYP	L	4	3	9,9,10	1.90	2 (22%)	10,12,14	0.99	1 (10%)

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	XYP	G	1	2	-	-	0/1/1/1
2	XYP	G	2	2	-	-	0/1/1/1
2	XYP	G	3	2	-	-	0/1/1/1
3	XYP	H	1	3	-	-	0/1/1/1
3	XYP	H	2	3	-	-	0/1/1/1
3	XYP	H	3	3	-	-	0/1/1/1
3	XYP	H	4	3	-	-	0/1/1/1
3	XYP	I	1	3	-	-	0/1/1/1
3	XYP	I	2	3	-	-	0/1/1/1
3	XYP	I	3	3	-	-	0/1/1/1
3	XYP	I	4	3	-	-	0/1/1/1
3	XYP	J	1	3	-	-	0/1/1/1
3	XYP	J	2	3	-	-	0/1/1/1
3	XYP	J	3	3	-	-	0/1/1/1
3	XYP	J	4	3	-	-	0/1/1/1
3	XYP	K	1	3	-	-	0/1/1/1
3	XYP	K	2	3	-	-	0/1/1/1
3	XYP	K	3	3	-	-	0/1/1/1
3	XYP	K	4	3	-	-	0/1/1/1
3	XYP	L	1	3	-	-	0/1/1/1
3	XYP	L	2	3	-	-	0/1/1/1
3	XYP	L	3	3	-	-	0/1/1/1
3	XYP	L	4	3	-	-	0/1/1/1

The worst 5 of 53 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	2	XYP	O5-C1	5.08	1.52	1.43
3	K	1	XYP	O5-C1	5.07	1.51	1.43
2	G	3	XYP	O5-C1	4.58	1.51	1.43
3	I	3	XYP	O5-C1	4.54	1.51	1.43
3	K	3	XYP	O5-C1	4.52	1.51	1.43

The worst 5 of 34 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	3	XYP	C4-C3-C2	-4.53	105.54	110.92
2	G	3	XYP	C5-C4-C3	4.50	116.19	109.64
3	H	1	XYP	C5-C4-C3	4.32	115.93	109.64
3	K	2	XYP	C4-C3-C2	4.09	115.77	110.92
3	K	4	XYP	C5-C4-C3	4.07	115.57	109.64

There are no chirality outliers.

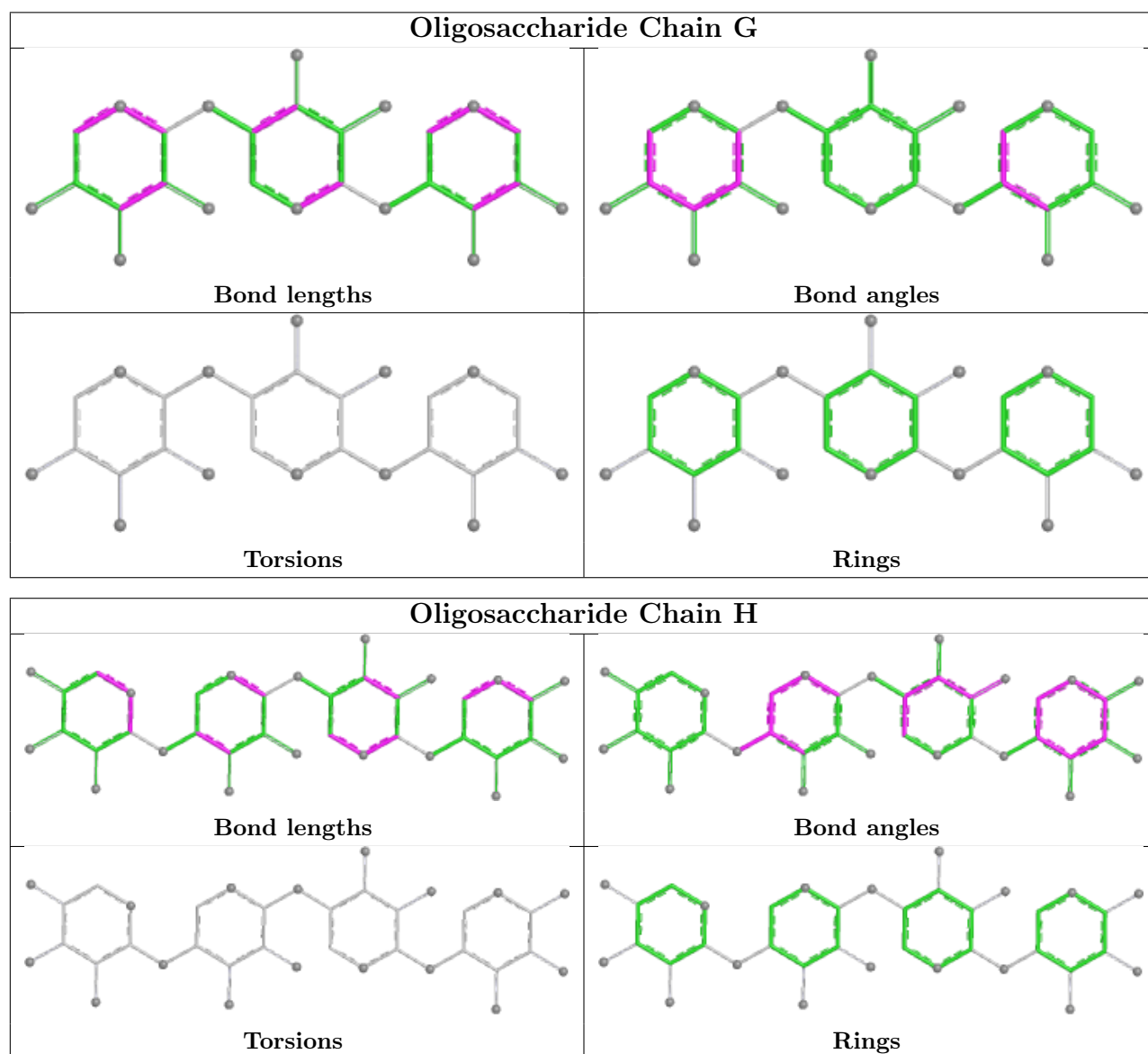
There are no torsion outliers.

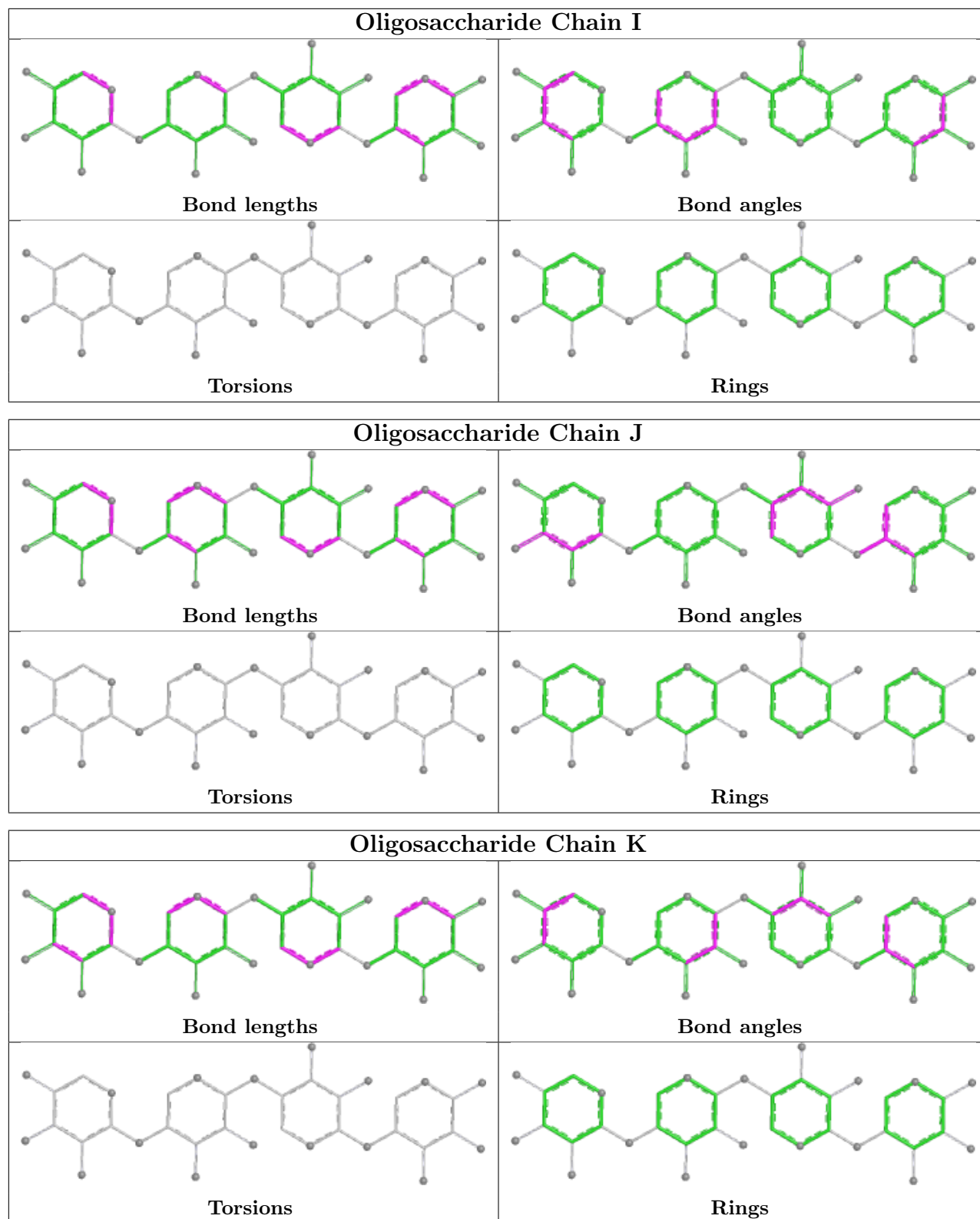
There are no ring outliers.

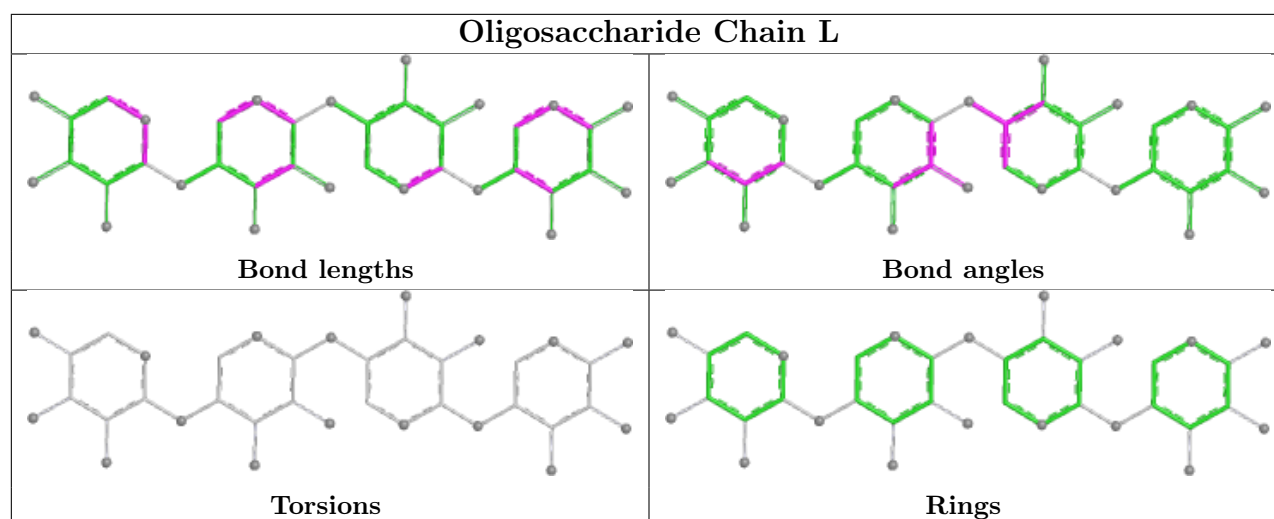
2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	L	1	XYP	1	0
2	G	1	XYP	2	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](#)

Of 19 ligands modelled in this entry, 18 are monoatomic - leaving 1 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	XYP	A	204	-	10,10,10	2.02	2 (20%)	14,14,14	0.58	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	XYP	A	204	-	-	-	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	204	XYP	O5-C1	5.04	1.51	1.43
4	A	204	XYP	O5-C5	3.24	1.49	1.43

There are no bond angle outliers.

There are no chirality outliers.

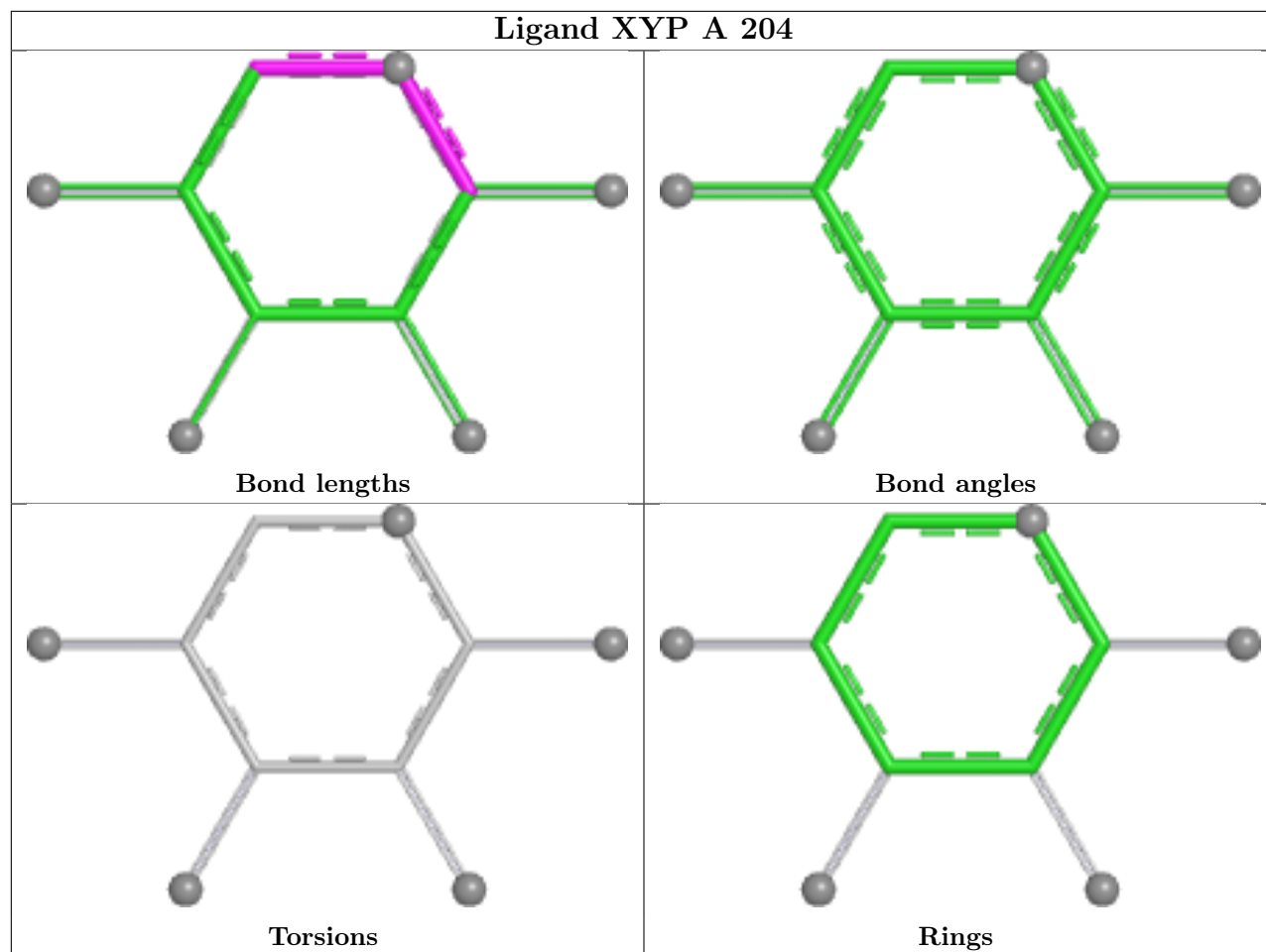
There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	204	XYP	2	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.



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	129/141 (91%)	0.08	4 (3%) 51 58	16, 23, 44, 56	0
1	B	132/141 (93%)	0.07	4 (3%) 52 59	13, 24, 43, 53	0
1	C	131/141 (92%)	0.14	4 (3%) 51 58	15, 25, 43, 55	0
1	D	131/141 (92%)	0.03	3 (2%) 61 67	16, 25, 45, 54	0
1	E	132/141 (93%)	0.19	7 (5%) 32 36	15, 27, 49, 68	1 (0%)
1	F	131/141 (92%)	0.30	6 (4%) 37 43	18, 29, 50, 60	0
All	All	786/846 (92%)	0.14	28 (3%) 46 52	13, 26, 47, 68	1 (0%)

The worst 5 of 28 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	156	ALA	5.7
1	D	156	ALA	5.3
1	F	156	ALA	4.5
1	F	28	GLY	4.0
1	F	158	ALA	3.8

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](#)

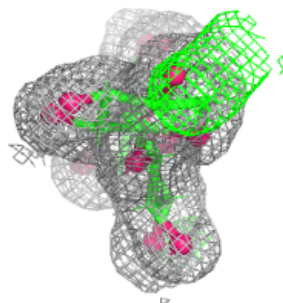
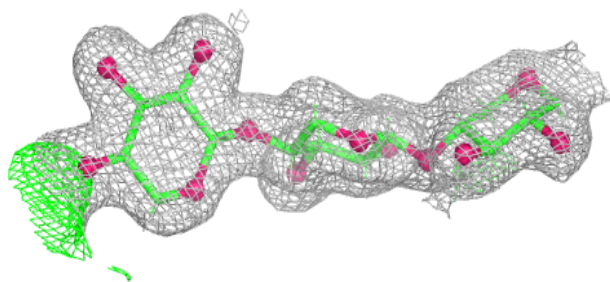
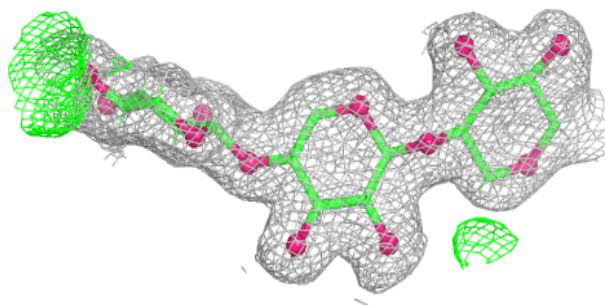
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists 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
3	XYP	I	4	9/10	0.81	0.11	32,44,60,69	0
3	XYP	K	4	9/10	0.83	0.10	32,44,63,75	0
3	XYP	L	4	9/10	0.86	0.10	28,42,50,54	0
3	XYP	H	1	10/10	0.88	0.10	25,48,61,73	0
3	XYP	L	1	10/10	0.88	0.11	28,43,53,56	0
3	XYP	J	1	10/10	0.88	0.11	24,44,62,64	0
3	XYP	K	1	10/10	0.89	0.09	28,38,54,59	0
3	XYP	K	3	9/10	0.92	0.08	20,24,29,30	0
2	XYP	G	3	9/10	0.92	0.06	16,20,25,28	0
3	XYP	H	4	9/10	0.92	0.08	26,34,46,50	0
3	XYP	I	1	10/10	0.92	0.08	25,34,51,52	0
3	XYP	L	2	9/10	0.93	0.07	19,26,35,35	0
3	XYP	J	4	9/10	0.93	0.08	29,41,50,58	0
3	XYP	J	3	9/10	0.94	0.07	20,23,28,30	0
2	XYP	G	1	9/10	0.94	0.07	20,29,44,44	0
3	XYP	K	2	9/10	0.95	0.07	17,26,34,36	0
3	XYP	I	3	9/10	0.95	0.07	15,22,29,30	0
3	XYP	L	3	9/10	0.95	0.06	24,27,31,31	0
2	XYP	G	2	9/10	0.95	0.06	14,22,28,29	0
3	XYP	H	3	9/10	0.96	0.05	20,24,28,30	0
3	XYP	I	2	9/10	0.96	0.06	14,25,31,32	0
3	XYP	H	2	9/10	0.96	0.06	17,21,26,28	0
3	XYP	J	2	9/10	0.97	0.04	16,22,30,30	0

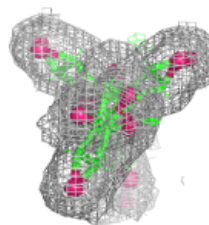
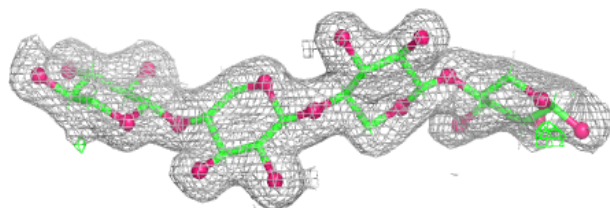
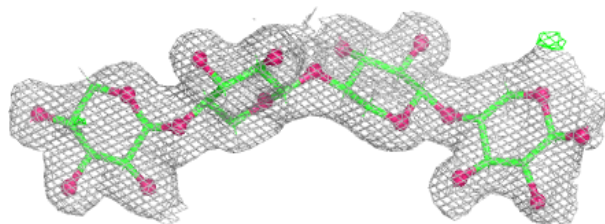
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain G:

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

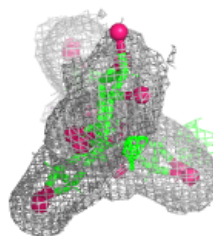
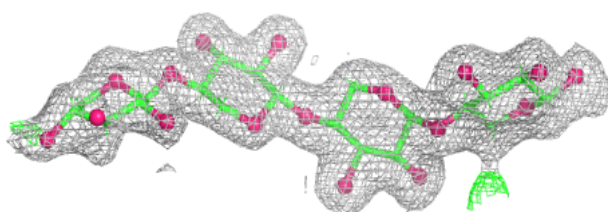
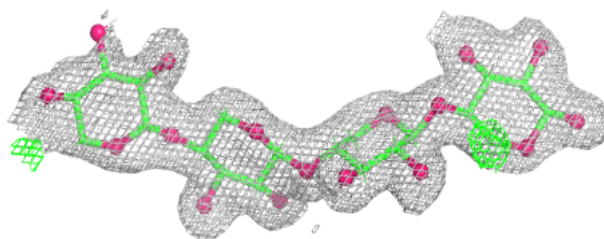
**Electron density around Chain H:**

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

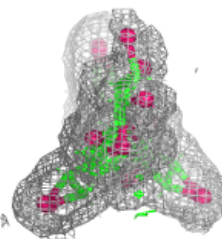
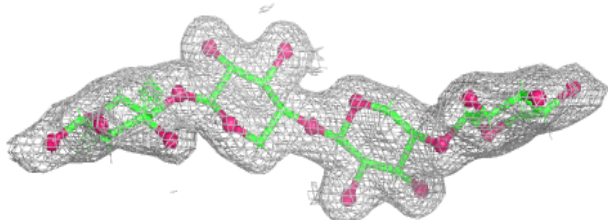
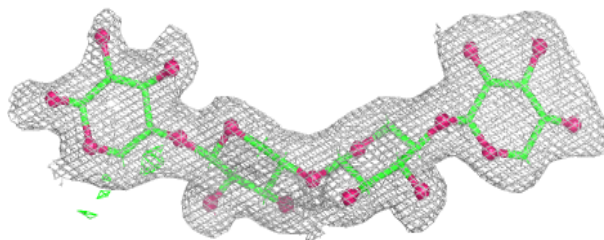


Electron density around Chain I:

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

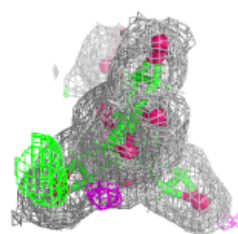
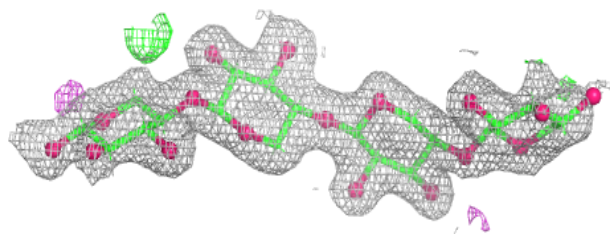
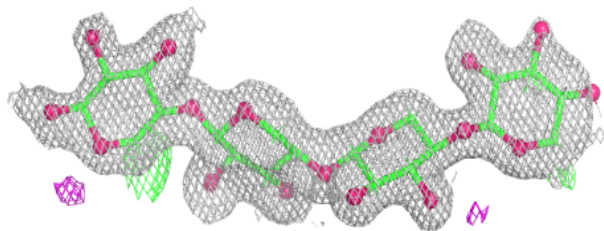
**Electron density around Chain J:**

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

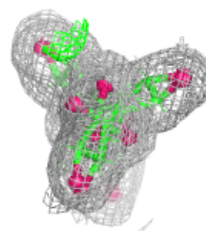
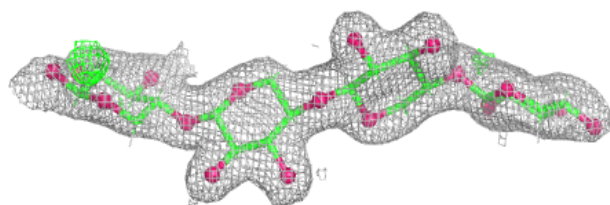
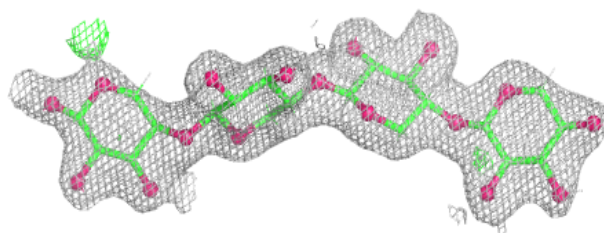


Electron density around Chain K:

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

**Electron density around Chain L:**

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



6.4 Ligands

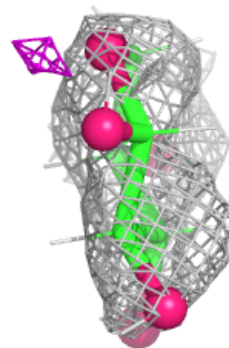
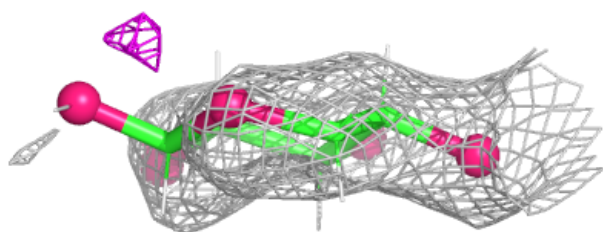
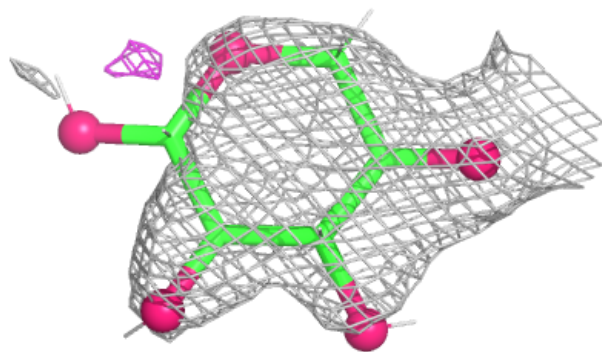
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
6	CL	C	210	1/1	0.35	0.23	30,30,30,30	0
4	XYP	A	204	10/10	0.75	0.11	38,51,70,73	0
5	CD	C	207	1/1	0.82	0.11	44,44,44,44	0
5	CD	A	207	1/1	0.85	0.31	30,30,30,30	0
5	CD	D	205	1/1	0.96	0.21	66,66,66,66	0
5	CD	E	205	1/1	0.96	0.05	35,35,35,35	0
6	CL	A	208	1/1	0.96	0.14	13,13,13,13	0
5	CD	B	206	1/1	0.96	0.20	101,101,101,101	0
6	CL	A	209	1/1	0.97	0.09	66,66,66,66	0
5	CD	C	205	1/1	0.97	0.04	31,31,31,31	0
5	CD	B	205	1/1	0.98	0.17	47,47,47,47	0
5	CD	A	206	1/1	0.98	0.04	27,27,27,27	0
5	CD	A	205	1/1	0.98	0.04	28,28,28,28	0
6	CL	E	206	1/1	0.98	0.15	5,5,5,5	0
6	CL	C	208	1/1	0.99	0.10	5,5,5,5	0
5	CD	C	206	1/1	0.99	0.02	27,27,27,27	0
6	CL	B	207	1/1	0.99	0.03	11,11,11,11	0
6	CL	F	205	1/1	0.99	0.13	12,12,12,12	0
6	CL	C	209	1/1	1.00	0.12	10,10,10,10	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 XYP A 204:

$2mF_o - DF_c$ (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.