



# Full wwPDB X-ray Structure Validation Report ⓘ

Apr 5, 2026 – 02:14 AM UTC

PDB ID : 9NJ0 / pdb\_00009nj0  
Title : GlfT2 from Nocardia brasiliensis Bound to Galf Trisaccharide  
Authors : Carter, A.W.; Dodge, G.J.; Kiessling, L.L.  
Deposited on : 2025-02-26  
Resolution : 3.20 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](mailto: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

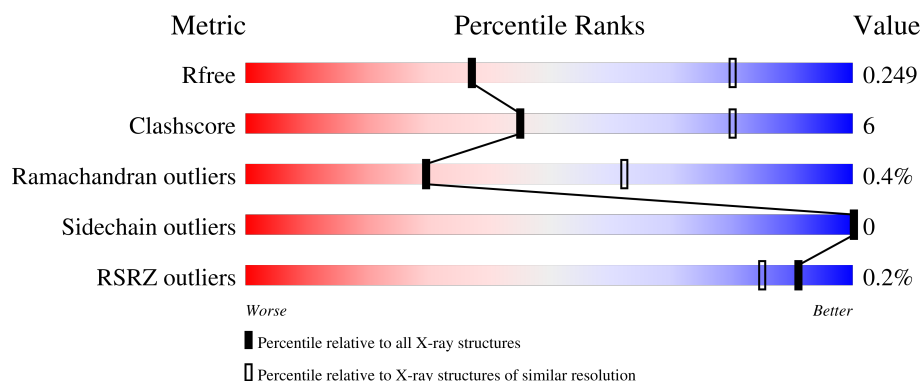
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.20 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	1466 (3.20-3.20)
Clashscore	190562	1573 (3.20-3.20)
Ramachandran outliers	187476	1548 (3.20-3.20)
Sidechain outliers	187428	1547 (3.20-3.20)
RSRZ outliers	180081	1466 (3.20-3.20)

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  $\geq 3$ , 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	666	<div><div></div><div>79%</div><div>14%</div><div>6%</div></div>
1	B	666	<div><div></div><div>79%</div><div>15%</div><div>6%</div></div>
1	C	666	<div><div></div><div>79%</div><div>15%</div><div>6%</div></div>
1	D	666	<div><div></div><div>80%</div><div>14%</div><div>6%</div></div>
1	E	666	<div><div></div><div>78%</div><div>16%</div><div>6%</div></div>

*Continued on next page...*

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	666	<div><div></div><div>80%14%6%</div></div>
1	G	666	<div><div></div><div>79%15%6%</div></div>
1	H	666	<div><div></div><div>79%15%6%</div></div>
2	I	3	<div><div></div><div>67%33%</div></div>
2	J	3	<div><div></div><div>33%67%</div></div>
2	K	3	<div><div></div><div>100%</div></div>
2	L	3	<div><div></div><div>100%</div></div>
2	M	3	<div><div></div><div>33%67%</div></div>
2	N	3	<div><div></div><div>67%33%</div></div>
2	O	3	<div><div></div><div>100%</div></div>
2	P	3	<div><div></div><div>100%</div></div>

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 39667 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 Galactofuranosyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	626	Total	C	N	O	S	0	1	0
			4901	3113	881	892	15			
1	B	626	Total	C	N	O	S	0	1	0
			4901	3113	881	892	15			
1	C	626	Total	C	N	O	S	0	1	0
			4901	3113	881	892	15			
1	D	626	Total	C	N	O	S	0	1	0
			4901	3113	881	892	15			
1	E	626	Total	C	N	O	S	0	1	0
			4901	3113	881	892	15			
1	F	626	Total	C	N	O	S	0	1	0
			4901	3113	881	892	15			
1	G	626	Total	C	N	O	S	0	1	0
			4901	3113	881	892	15			
1	H	626	Total	C	N	O	S	0	1	0
			4901	3113	881	892	15			

There are 216 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	expression tag	UNP K0EQQ2
A	-18	GLY	-	expression tag	UNP K0EQQ2
A	-17	SER	-	expression tag	UNP K0EQQ2
A	-16	SER	-	expression tag	UNP K0EQQ2
A	-15	HIS	-	expression tag	UNP K0EQQ2
A	-14	HIS	-	expression tag	UNP K0EQQ2
A	-13	HIS	-	expression tag	UNP K0EQQ2
A	-12	HIS	-	expression tag	UNP K0EQQ2
A	-11	HIS	-	expression tag	UNP K0EQQ2
A	-10	HIS	-	expression tag	UNP K0EQQ2
A	-9	SER	-	expression tag	UNP K0EQQ2
A	-8	SER	-	expression tag	UNP K0EQQ2
A	-7	GLY	-	expression tag	UNP K0EQQ2

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
A	-6	LEU	-	expression tag	UNP K0EQQ2
A	-5	VAL	-	expression tag	UNP K0EQQ2
A	-4	PRO	-	expression tag	UNP K0EQQ2
A	-3	ARG	-	expression tag	UNP K0EQQ2
A	-2	GLY	-	expression tag	UNP K0EQQ2
A	-1	SER	-	expression tag	UNP K0EQQ2
A	0	HIS	-	expression tag	UNP K0EQQ2
A	1	MET	-	expression tag	UNP K0EQQ2
A	2	THR	-	expression tag	UNP K0EQQ2
A	3	SER	-	expression tag	UNP K0EQQ2
A	4	GLN	-	expression tag	UNP K0EQQ2
A	5	SER	-	expression tag	UNP K0EQQ2
A	6	LEU	-	expression tag	UNP K0EQQ2
A	7	LEU	-	expression tag	UNP K0EQQ2
B	-19	MET	-	expression tag	UNP K0EQQ2
B	-18	GLY	-	expression tag	UNP K0EQQ2
B	-17	SER	-	expression tag	UNP K0EQQ2
B	-16	SER	-	expression tag	UNP K0EQQ2
B	-15	HIS	-	expression tag	UNP K0EQQ2
B	-14	HIS	-	expression tag	UNP K0EQQ2
B	-13	HIS	-	expression tag	UNP K0EQQ2
B	-12	HIS	-	expression tag	UNP K0EQQ2
B	-11	HIS	-	expression tag	UNP K0EQQ2
B	-10	HIS	-	expression tag	UNP K0EQQ2
B	-9	SER	-	expression tag	UNP K0EQQ2
B	-8	SER	-	expression tag	UNP K0EQQ2
B	-7	GLY	-	expression tag	UNP K0EQQ2
B	-6	LEU	-	expression tag	UNP K0EQQ2
B	-5	VAL	-	expression tag	UNP K0EQQ2
B	-4	PRO	-	expression tag	UNP K0EQQ2
B	-3	ARG	-	expression tag	UNP K0EQQ2
B	-2	GLY	-	expression tag	UNP K0EQQ2
B	-1	SER	-	expression tag	UNP K0EQQ2
B	0	HIS	-	expression tag	UNP K0EQQ2
B	1	MET	-	expression tag	UNP K0EQQ2
B	2	THR	-	expression tag	UNP K0EQQ2
B	3	SER	-	expression tag	UNP K0EQQ2
B	4	GLN	-	expression tag	UNP K0EQQ2
B	5	SER	-	expression tag	UNP K0EQQ2
B	6	LEU	-	expression tag	UNP K0EQQ2
B	7	LEU	-	expression tag	UNP K0EQQ2
C	-19	MET	-	expression tag	UNP K0EQQ2

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
C	-18	GLY	-	expression tag	UNP K0EQQ2
C	-17	SER	-	expression tag	UNP K0EQQ2
C	-16	SER	-	expression tag	UNP K0EQQ2
C	-15	HIS	-	expression tag	UNP K0EQQ2
C	-14	HIS	-	expression tag	UNP K0EQQ2
C	-13	HIS	-	expression tag	UNP K0EQQ2
C	-12	HIS	-	expression tag	UNP K0EQQ2
C	-11	HIS	-	expression tag	UNP K0EQQ2
C	-10	HIS	-	expression tag	UNP K0EQQ2
C	-9	SER	-	expression tag	UNP K0EQQ2
C	-8	SER	-	expression tag	UNP K0EQQ2
C	-7	GLY	-	expression tag	UNP K0EQQ2
C	-6	LEU	-	expression tag	UNP K0EQQ2
C	-5	VAL	-	expression tag	UNP K0EQQ2
C	-4	PRO	-	expression tag	UNP K0EQQ2
C	-3	ARG	-	expression tag	UNP K0EQQ2
C	-2	GLY	-	expression tag	UNP K0EQQ2
C	-1	SER	-	expression tag	UNP K0EQQ2
C	0	HIS	-	expression tag	UNP K0EQQ2
C	1	MET	-	expression tag	UNP K0EQQ2
C	2	THR	-	expression tag	UNP K0EQQ2
C	3	SER	-	expression tag	UNP K0EQQ2
C	4	GLN	-	expression tag	UNP K0EQQ2
C	5	SER	-	expression tag	UNP K0EQQ2
C	6	LEU	-	expression tag	UNP K0EQQ2
C	7	LEU	-	expression tag	UNP K0EQQ2
D	-19	MET	-	expression tag	UNP K0EQQ2
D	-18	GLY	-	expression tag	UNP K0EQQ2
D	-17	SER	-	expression tag	UNP K0EQQ2
D	-16	SER	-	expression tag	UNP K0EQQ2
D	-15	HIS	-	expression tag	UNP K0EQQ2
D	-14	HIS	-	expression tag	UNP K0EQQ2
D	-13	HIS	-	expression tag	UNP K0EQQ2
D	-12	HIS	-	expression tag	UNP K0EQQ2
D	-11	HIS	-	expression tag	UNP K0EQQ2
D	-10	HIS	-	expression tag	UNP K0EQQ2
D	-9	SER	-	expression tag	UNP K0EQQ2
D	-8	SER	-	expression tag	UNP K0EQQ2
D	-7	GLY	-	expression tag	UNP K0EQQ2
D	-6	LEU	-	expression tag	UNP K0EQQ2
D	-5	VAL	-	expression tag	UNP K0EQQ2
D	-4	PRO	-	expression tag	UNP K0EQQ2

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
D	-3	ARG	-	expression tag	UNP K0EQQ2
D	-2	GLY	-	expression tag	UNP K0EQQ2
D	-1	SER	-	expression tag	UNP K0EQQ2
D	0	HIS	-	expression tag	UNP K0EQQ2
D	1	MET	-	expression tag	UNP K0EQQ2
D	2	THR	-	expression tag	UNP K0EQQ2
D	3	SER	-	expression tag	UNP K0EQQ2
D	4	GLN	-	expression tag	UNP K0EQQ2
D	5	SER	-	expression tag	UNP K0EQQ2
D	6	LEU	-	expression tag	UNP K0EQQ2
D	7	LEU	-	expression tag	UNP K0EQQ2
E	-19	MET	-	expression tag	UNP K0EQQ2
E	-18	GLY	-	expression tag	UNP K0EQQ2
E	-17	SER	-	expression tag	UNP K0EQQ2
E	-16	SER	-	expression tag	UNP K0EQQ2
E	-15	HIS	-	expression tag	UNP K0EQQ2
E	-14	HIS	-	expression tag	UNP K0EQQ2
E	-13	HIS	-	expression tag	UNP K0EQQ2
E	-12	HIS	-	expression tag	UNP K0EQQ2
E	-11	HIS	-	expression tag	UNP K0EQQ2
E	-10	HIS	-	expression tag	UNP K0EQQ2
E	-9	SER	-	expression tag	UNP K0EQQ2
E	-8	SER	-	expression tag	UNP K0EQQ2
E	-7	GLY	-	expression tag	UNP K0EQQ2
E	-6	LEU	-	expression tag	UNP K0EQQ2
E	-5	VAL	-	expression tag	UNP K0EQQ2
E	-4	PRO	-	expression tag	UNP K0EQQ2
E	-3	ARG	-	expression tag	UNP K0EQQ2
E	-2	GLY	-	expression tag	UNP K0EQQ2
E	-1	SER	-	expression tag	UNP K0EQQ2
E	0	HIS	-	expression tag	UNP K0EQQ2
E	1	MET	-	expression tag	UNP K0EQQ2
E	2	THR	-	expression tag	UNP K0EQQ2
E	3	SER	-	expression tag	UNP K0EQQ2
E	4	GLN	-	expression tag	UNP K0EQQ2
E	5	SER	-	expression tag	UNP K0EQQ2
E	6	LEU	-	expression tag	UNP K0EQQ2
E	7	LEU	-	expression tag	UNP K0EQQ2
F	-19	MET	-	expression tag	UNP K0EQQ2
F	-18	GLY	-	expression tag	UNP K0EQQ2
F	-17	SER	-	expression tag	UNP K0EQQ2
F	-16	SER	-	expression tag	UNP K0EQQ2

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
F	-15	HIS	-	expression tag	UNP K0EQQ2
F	-14	HIS	-	expression tag	UNP K0EQQ2
F	-13	HIS	-	expression tag	UNP K0EQQ2
F	-12	HIS	-	expression tag	UNP K0EQQ2
F	-11	HIS	-	expression tag	UNP K0EQQ2
F	-10	HIS	-	expression tag	UNP K0EQQ2
F	-9	SER	-	expression tag	UNP K0EQQ2
F	-8	SER	-	expression tag	UNP K0EQQ2
F	-7	GLY	-	expression tag	UNP K0EQQ2
F	-6	LEU	-	expression tag	UNP K0EQQ2
F	-5	VAL	-	expression tag	UNP K0EQQ2
F	-4	PRO	-	expression tag	UNP K0EQQ2
F	-3	ARG	-	expression tag	UNP K0EQQ2
F	-2	GLY	-	expression tag	UNP K0EQQ2
F	-1	SER	-	expression tag	UNP K0EQQ2
F	0	HIS	-	expression tag	UNP K0EQQ2
F	1	MET	-	expression tag	UNP K0EQQ2
F	2	THR	-	expression tag	UNP K0EQQ2
F	3	SER	-	expression tag	UNP K0EQQ2
F	4	GLN	-	expression tag	UNP K0EQQ2
F	5	SER	-	expression tag	UNP K0EQQ2
F	6	LEU	-	expression tag	UNP K0EQQ2
F	7	LEU	-	expression tag	UNP K0EQQ2
G	-19	MET	-	expression tag	UNP K0EQQ2
G	-18	GLY	-	expression tag	UNP K0EQQ2
G	-17	SER	-	expression tag	UNP K0EQQ2
G	-16	SER	-	expression tag	UNP K0EQQ2
G	-15	HIS	-	expression tag	UNP K0EQQ2
G	-14	HIS	-	expression tag	UNP K0EQQ2
G	-13	HIS	-	expression tag	UNP K0EQQ2
G	-12	HIS	-	expression tag	UNP K0EQQ2
G	-11	HIS	-	expression tag	UNP K0EQQ2
G	-10	HIS	-	expression tag	UNP K0EQQ2
G	-9	SER	-	expression tag	UNP K0EQQ2
G	-8	SER	-	expression tag	UNP K0EQQ2
G	-7	GLY	-	expression tag	UNP K0EQQ2
G	-6	LEU	-	expression tag	UNP K0EQQ2
G	-5	VAL	-	expression tag	UNP K0EQQ2
G	-4	PRO	-	expression tag	UNP K0EQQ2
G	-3	ARG	-	expression tag	UNP K0EQQ2
G	-2	GLY	-	expression tag	UNP K0EQQ2
G	-1	SER	-	expression tag	UNP K0EQQ2

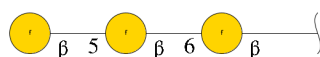
*Continued on next page...*



Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
G	0	HIS	-	expression tag	UNP K0EQQ2
G	1	MET	-	expression tag	UNP K0EQQ2
G	2	THR	-	expression tag	UNP K0EQQ2
G	3	SER	-	expression tag	UNP K0EQQ2
G	4	GLN	-	expression tag	UNP K0EQQ2
G	5	SER	-	expression tag	UNP K0EQQ2
G	6	LEU	-	expression tag	UNP K0EQQ2
G	7	LEU	-	expression tag	UNP K0EQQ2
H	-19	MET	-	expression tag	UNP K0EQQ2
H	-18	GLY	-	expression tag	UNP K0EQQ2
H	-17	SER	-	expression tag	UNP K0EQQ2
H	-16	SER	-	expression tag	UNP K0EQQ2
H	-15	HIS	-	expression tag	UNP K0EQQ2
H	-14	HIS	-	expression tag	UNP K0EQQ2
H	-13	HIS	-	expression tag	UNP K0EQQ2
H	-12	HIS	-	expression tag	UNP K0EQQ2
H	-11	HIS	-	expression tag	UNP K0EQQ2
H	-10	HIS	-	expression tag	UNP K0EQQ2
H	-9	SER	-	expression tag	UNP K0EQQ2
H	-8	SER	-	expression tag	UNP K0EQQ2
H	-7	GLY	-	expression tag	UNP K0EQQ2
H	-6	LEU	-	expression tag	UNP K0EQQ2
H	-5	VAL	-	expression tag	UNP K0EQQ2
H	-4	PRO	-	expression tag	UNP K0EQQ2
H	-3	ARG	-	expression tag	UNP K0EQQ2
H	-2	GLY	-	expression tag	UNP K0EQQ2
H	-1	SER	-	expression tag	UNP K0EQQ2
H	0	HIS	-	expression tag	UNP K0EQQ2
H	1	MET	-	expression tag	UNP K0EQQ2
H	2	THR	-	expression tag	UNP K0EQQ2
H	3	SER	-	expression tag	UNP K0EQQ2
H	4	GLN	-	expression tag	UNP K0EQQ2
H	5	SER	-	expression tag	UNP K0EQQ2
H	6	LEU	-	expression tag	UNP K0EQQ2
H	7	LEU	-	expression tag	UNP K0EQQ2

- Molecule 2 is an oligosaccharide called beta-D-galactofuranose-(1-5)-beta-D-galactofuranose-(1-6)-beta-D-galactofuranose.

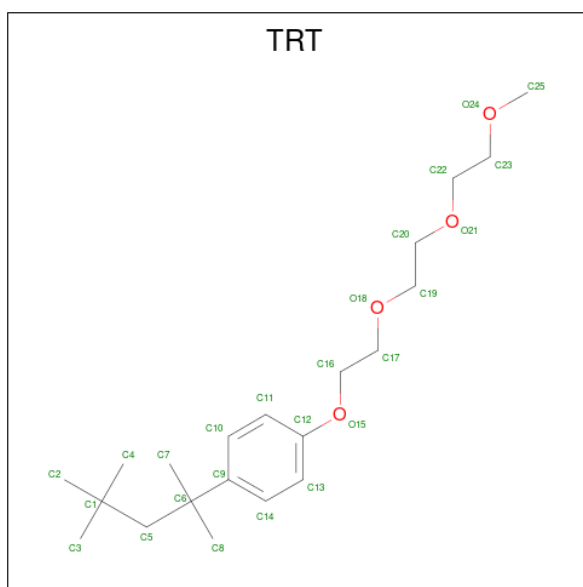


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
2	I	3	Total C O 33 18 15	0	0	0
2	J	3	Total C O 33 18 15	0	0	0
2	K	3	Total C O 33 18 15	0	0	0
2	L	3	Total C O 33 18 15	0	0	0
2	M	3	Total C O 33 18 15	0	0	0
2	N	3	Total C O 33 18 15	0	0	0
2	O	3	Total C O 33 18 15	0	0	0
2	P	3	Total C O 33 18 15	0	0	0

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

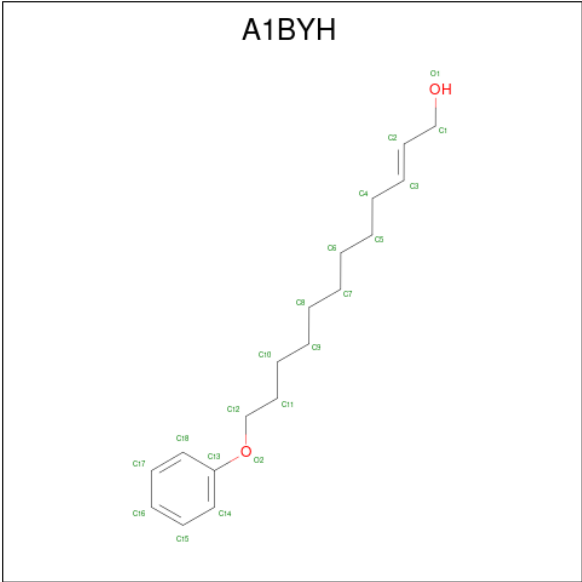
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Mg 1 1	0	0
3	B	1	Total Mg 1 1	0	0
3	C	1	Total Mg 1 1	0	0
3	D	1	Total Mg 1 1	0	0
3	E	1	Total Mg 1 1	0	0
3	F	1	Total Mg 1 1	0	0
3	G	1	Total Mg 1 1	0	0
3	H	1	Total Mg 1 1	0	0

- Molecule 4 is FRAGMENT OF TRITON X-100 (CCD ID: TRT) (formula: C<sub>21</sub>H<sub>36</sub>O<sub>4</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			20	18	2		
4	B	1	Total	C	O	0	0
			20	18	2		
4	C	1	Total	C	O	0	0
			20	18	2		
4	D	1	Total	C	O	0	0
			20	18	2		
4	E	1	Total	C	O	0	0
			20	18	2		
4	F	1	Total	C	O	0	0
			20	18	2		
4	G	1	Total	C	O	0	0
			20	18	2		
4	H	1	Total	C	O	0	0
			20	18	2		

- Molecule 5 is (2E)-12-phenoxydodec-2-en-1-ol (CCD ID: A1BYH) (formula:  $C_{18}H_{28}O_2$ ) (labeled as "Ligand of Interest" by depositor).




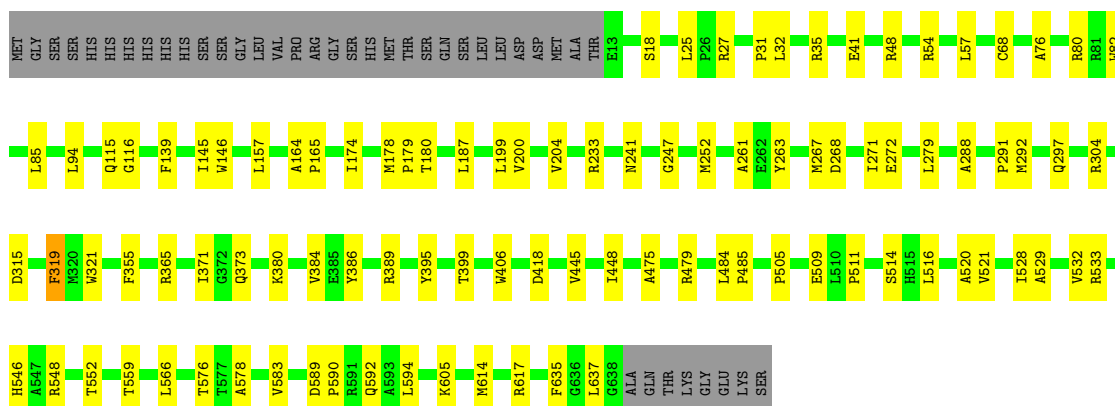
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			2	1	1		
5	B	1	Total	C	O	0	0
			4	3	1		
5	C	1	Total	C	O	0	0
			3	2	1		
5	D	1	Total	C	O	0	0
			3	2	1		
5	E	1	Total	C	O	0	0
			3	2	1		
5	F	1	Total	C	O	0	0
			5	4	1		
5	G	1	Total	C	O	0	0
			4	3	1		
5	H	1	Total	C	O	0	0
			3	2	1		

### 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.

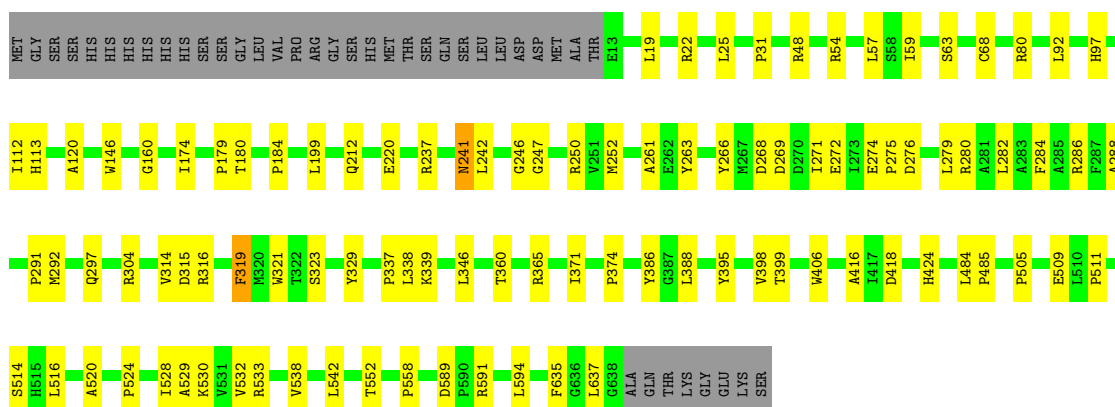
#### • Molecule 1: Galactofuranosyltransferase

Chain A: 




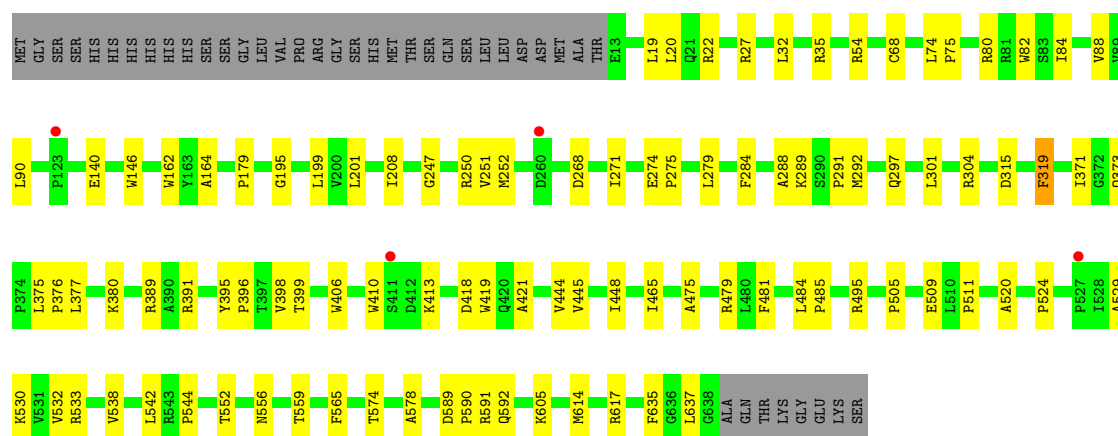
#### • Molecule 1: Galactofuranosyltransferase

Chain B: 



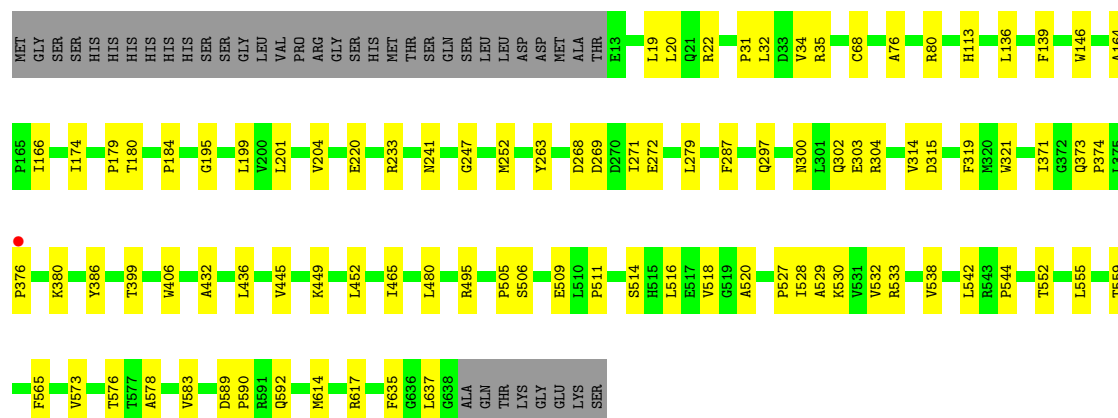
#### • Molecule 1: Galactofuranosyltransferase

Chain C: 



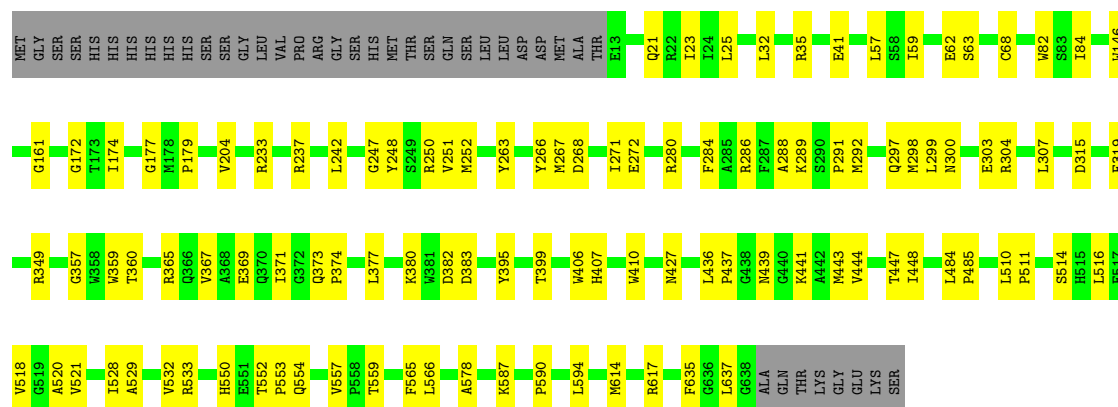
• Molecule 1: Galactofuranosyltransferase

Chain D: 80% 14% 6%



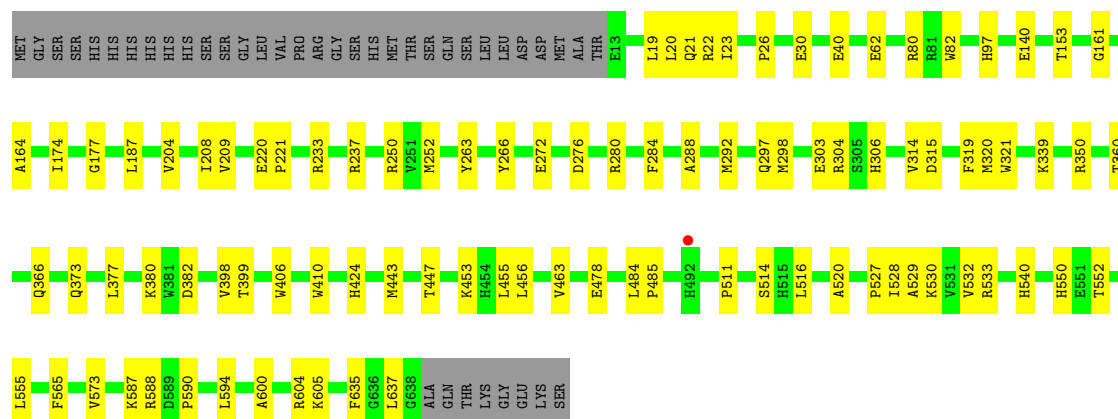
• Molecule 1: Galactofuranosyltransferase

Chain E: 78% 16% 6%



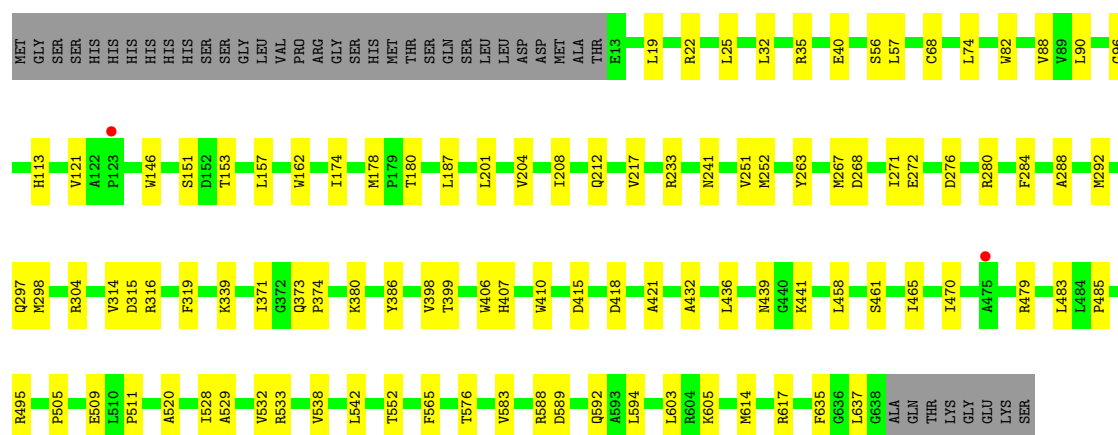
• Molecule 1: Galactofuranosyltransferase

Chain F: 80% 14% 6%



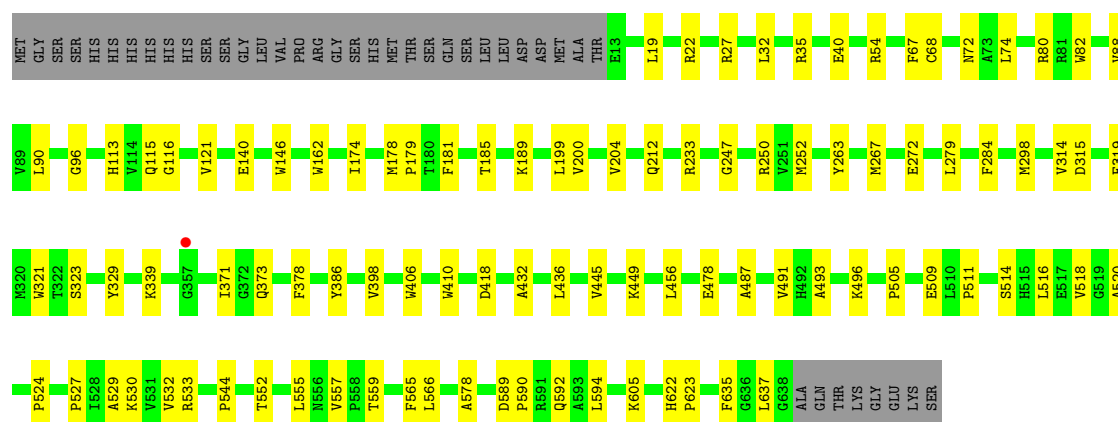
• Molecule 1: Galactofuranosyltransferase

Chain G: 79% 15% 6%



• Molecule 1: Galactofuranosyltransferase

Chain H: 79% 15% 6%



• Molecule 2: beta-D-galactofuranose-(1-5)-beta-D-galactofuranose-(1-6)-beta-D-galactofuranos  
e

Chain I:  67% 33%

GZL1  
GZL2  
GZL3

- Molecule 2: beta-D-galactofuranose-(1-5)-beta-D-galactofuranose-(1-6)-beta-D-galactofuranose

Chain J:  33% 67%

GZL1  
GZL2  
GZL3

- Molecule 2: beta-D-galactofuranose-(1-5)-beta-D-galactofuranose-(1-6)-beta-D-galactofuranose

Chain K:  100%

GZL1  
GZL2  
GZL3

- Molecule 2: beta-D-galactofuranose-(1-5)-beta-D-galactofuranose-(1-6)-beta-D-galactofuranose

Chain L:  100%


GZL1  
GZL2  
GZL3

- Molecule 2: beta-D-galactofuranose-(1-5)-beta-D-galactofuranose-(1-6)-beta-D-galactofuranose

Chain M:  33% 67%

GZL1  
GZL2  
GZL3

- Molecule 2: beta-D-galactofuranose-(1-5)-beta-D-galactofuranose-(1-6)-beta-D-galactofuranose

Chain N:  67% 33%

GZL1  
GZL2  
GZL3

- Molecule 2: beta-D-galactofuranose-(1-5)-beta-D-galactofuranose-(1-6)-beta-D-galactofuranose

Chain O:  100%

GZL1  
GZL2  
GZL3



- Molecule 2: beta-D-galactofuranose-(1-5)-beta-D-galactofuranose-(1-6)-beta-D-galactofuranose

Chain P:

100%

GZL1  
GZL2  
GZL3

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	106.78Å 204.97Å 294.13Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	34.61 – 3.20 34.61 – 3.20	Depositor EDS
% Data completeness (in resolution range)	92.1 (34.61-3.20) 91.5 (34.61-3.20)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.29 (at 3.18Å)	Xtrriage
Refinement program	PHENIX 1.21.2_5419	Depositor
R, $R_{free}$	0.200 , 0.248 0.200 , 0.249	Depositor DCC
$R_{free}$ test set	1947 reflections (1.81%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	56.9	Xtrriage
Anisotropy	0.166	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.28 , 39.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.43$ , $\langle L^2 \rangle = 0.25$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	39667	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	51.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 32.48 % 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 9.3336e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: TRT, MG, GZL, A1BYH

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	0.13	0/5022	0.32	0/6838
1	B	0.13	0/5022	0.31	0/6838
1	C	0.13	0/5022	0.31	0/6838
1	D	0.13	0/5022	0.32	0/6838
1	E	0.13	0/5022	0.32	0/6838
1	F	0.15	0/5022	0.32	0/6838
1	G	0.13	0/5022	0.32	0/6838
1	H	0.13	0/5022	0.32	0/6838
All	All	0.13	0/40176	0.32	0/54704

There are no bond length outliers.

There are no bond angle outliers.

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	4901	0	4866	59	0
1	B	4901	0	4866	57	0
1	C	4901	0	4866	59	0
1	D	4901	0	4866	57	0
1	E	4901	0	4866	66	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	4901	0	4866	56	0
1	G	4901	0	4866	57	0
1	H	4901	0	4866	61	0
2	I	33	0	21	2	0
2	J	33	0	21	2	0
2	K	33	0	22	0	0
2	L	33	0	21	0	0
2	M	33	0	21	0	0
2	N	33	0	21	2	0
2	O	33	0	21	0	0
2	P	33	0	21	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
3	G	1	0	0	0	0
3	H	1	0	0	0	0
4	A	20	0	27	3	0
4	B	20	0	27	2	0
4	C	20	0	27	2	0
4	D	20	0	27	1	0
4	E	20	0	27	4	0
4	F	20	0	27	4	0
4	G	20	0	27	2	0
4	H	20	0	27	4	0
5	A	2	0	0	0	0
5	B	4	0	0	0	0
5	C	3	0	0	0	0
5	D	3	0	0	0	0
5	E	3	0	0	0	0
5	F	5	0	0	1	0
5	G	4	0	0	0	0
5	H	3	0	0	0	0
All	All	39667	0	39313	468	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 6.

All (468) 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:199:LEU:HD22	1:A:279:LEU:HD13	1.22	1.11
1:A:199:LEU:HD22	1:A:279:LEU:CD1	1.88	1.03
1:C:199:LEU:HD22	1:C:279:LEU:HD13	1.55	0.88
1:H:493:ALA:HA	1:H:496:LYS:HE3	1.54	0.87
1:C:199:LEU:HD22	1:C:279:LEU:CD1	2.07	0.84
1:D:315:ASP:O	1:D:319:PHE:HA	1.85	0.76
1:D:520:ALA:HB1	1:D:533:ARG:HH21	1.55	0.71
1:B:315:ASP:O	1:B:319:PHE:HA	1.92	0.70
1:D:505:PRO:HD2	1:D:509:GLU:HG3	1.73	0.69
1:E:174:ILE:HG22	1:E:263:TYR:HB2	1.76	0.68
1:D:272:GLU:HB3	1:D:406:TRP:HB2	1.76	0.68
1:A:199:LEU:CD2	1:A:279:LEU:HD13	2.13	0.67
1:E:594:LEU:HD13	4:E:702:TRT:H11	1.77	0.67
1:G:594:LEU:HD13	4:G:702:TRT:H11	1.77	0.67
1:H:199:LEU:HD22	1:H:279:LEU:HD22	1.77	0.66
1:C:589:ASP:HB3	1:C:592:GLN:HB2	1.78	0.66
1:D:32:LEU:HD23	1:D:35[A]:ARG:HH11	1.62	0.64
1:B:514:SER:HB2	1:B:516:LEU:HD13	1.79	0.64
1:F:19:LEU:HD21	1:F:22:ARG:HG3	1.77	0.64
1:F:520:ALA:HB1	1:F:533:ARG:HH21	1.62	0.64
1:H:511:PRO:HG2	1:H:552:THR:HA	1.80	0.64
1:H:32:LEU:HD23	1:H:35[A]:ARG:HH11	1.63	0.64
1:H:174:ILE:HG22	1:H:263:TYR:HB2	1.80	0.63
1:D:514:SER:HB2	1:D:516:LEU:HD13	1.80	0.62
1:B:505:PRO:HD2	1:B:509:GLU:HG3	1.81	0.62
1:C:635:PHE:HB2	1:C:637:LEU:HD22	1.82	0.61
1:D:614:MET:HE1	1:D:617:ARG:NH1	2.15	0.61
1:C:511:PRO:HG2	1:C:552:THR:HA	1.82	0.61
1:C:505:PRO:HD2	1:C:509:GLU:HG3	1.81	0.61
1:H:80:ARG:HH12	1:H:140:GLU:HG2	1.66	0.61
1:C:80:ARG:HH12	1:C:140:GLU:HG2	1.66	0.61
1:A:321:TRP:CD1	2:I:3:GZL:O3	2.54	0.61
1:F:304:ARG:HG3	1:F:304:ARG:HH11	1.65	0.61
1:H:514:SER:HB2	1:H:516:LEU:HD13	1.82	0.61
1:D:544:PRO:HA	1:D:590:PRO:HG2	1.83	0.60
1:E:529:ALA:HA	1:E:532:VAL:HG22	1.84	0.60
1:F:514:SER:HB2	1:F:516:LEU:HD13	1.81	0.60
1:A:514:SER:HB2	1:A:516:LEU:HD13	1.83	0.60
1:C:559:THR:HG21	1:C:578:ALA:HA	1.84	0.60
1:G:272:GLU:HB3	1:G:406:TRP:HB2	1.83	0.60
1:D:174:ILE:HG22	1:D:263:TYR:HB2	1.83	0.60
1:E:511:PRO:HG2	1:E:552:THR:HA	1.84	0.60

Continued on next page...

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:68:CYS:HB2	1:B:146:TRP:CD1	2.37	0.60
1:H:505:PRO:HD2	1:H:509:GLU:HG3	1.84	0.60
1:D:614:MET:HE1	1:D:617:ARG:HH11	1.67	0.59
1:D:511:PRO:HG2	1:D:552:THR:HA	1.84	0.59
1:C:614:MET:HE1	1:C:617:ARG:NH1	2.17	0.59
1:A:635:PHE:HB2	1:A:637:LEU:HD22	1.85	0.59
1:B:19:LEU:HD21	1:B:22:ARG:HG3	1.84	0.59
1:G:511:PRO:HG2	1:G:552:THR:HA	1.84	0.59
1:A:546:HIS:HB3	1:A:548:ARG:NH1	2.17	0.59
1:A:614:MET:HE1	1:A:617:ARG:NH1	2.18	0.59
1:C:80:ARG:NH1	1:C:140:GLU:HG2	2.17	0.59
1:G:288:ALA:HB1	1:G:292:MET:HE3	1.84	0.59
1:D:80:ARG:HB2	1:D:136:LEU:HB3	1.84	0.58
1:E:520:ALA:HB1	1:E:533:ARG:HH21	1.68	0.58
1:H:199:LEU:HD22	1:H:279:LEU:HD13	1.86	0.57
1:E:514:SER:HB2	1:E:516:LEU:HD13	1.86	0.57
1:B:179:PRO:HB3	1:B:247:GLY:HA3	1.87	0.57
1:H:80:ARG:NH1	1:H:140:GLU:HG2	2.19	0.57
1:H:252:MET:HE3	1:H:373:GLN:HA	1.87	0.56
1:F:456:LEU:HD12	4:F:702:TRT:H8C1	1.88	0.56
1:D:589:ASP:HB3	1:D:592:GLN:HB2	1.87	0.56
1:E:252:MET:HE3	1:E:373:GLN:HA	1.88	0.56
1:B:174:ILE:HG22	1:B:263:TYR:HB2	1.87	0.55
1:D:268:ASP:HB3	1:D:271:ILE:HG23	1.88	0.55
1:D:533:ARG:NH1	1:D:565:PHE:HB2	2.21	0.55
1:B:48:ARG:HD2	1:E:62:GLU:HG3	1.87	0.55
1:C:74:LEU:HD12	1:C:75:PRO:HD2	1.87	0.55
1:C:304:ARG:HH12	1:H:113:HIS:CG	2.24	0.55
1:A:272:GLU:HB3	1:A:406:TRP:HB2	1.87	0.55
1:G:96:GLY:H	1:G:121:VAL:HG23	1.72	0.55
1:C:250:ARG:HH21	1:C:635:PHE:HB3	1.71	0.55
1:H:524:PRO:HG2	1:H:530:LYS:HD3	1.89	0.54
1:H:559:THR:HG21	1:H:578:ALA:HA	1.89	0.54
1:D:19:LEU:HD21	1:D:22:ARG:HG3	1.88	0.54
1:E:315:ASP:O	1:E:319:PHE:HA	2.08	0.54
1:H:19:LEU:HD21	1:H:22:ARG:HG3	1.88	0.54
1:A:590:PRO:HB3	4:A:702:TRT:H162	1.90	0.54
1:G:533:ARG:NH1	1:G:565:PHE:HB2	2.23	0.54
1:G:32:LEU:HD23	1:G:35[A]:ARG:HH11	1.72	0.54
1:A:80:ARG:HD2	1:A:139:PHE:HB2	1.88	0.54
1:E:377:LEU:HD12	1:E:382:ASP:HA	1.90	0.54

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:511:PRO:HG2	1:F:552:THR:HA	1.90	0.54
1:H:529:ALA:HA	1:H:532:VAL:HG22	1.90	0.54
1:E:550:HIS:CE1	1:E:587:LYS:HB3	2.43	0.54
1:C:288:ALA:HB1	1:C:292:MET:HE3	1.89	0.53
1:G:297:GLN:HG2	1:G:399:THR:HG22	1.90	0.53
1:A:179:PRO:HB3	1:A:247:GLY:HA3	1.90	0.53
1:B:242:LEU:HB2	1:B:246:GLY:HA3	1.90	0.53
1:E:237:ARG:HD2	1:E:250:ARG:HH12	1.72	0.53
1:G:520:ALA:HB1	1:G:533:ARG:HH21	1.73	0.53
1:H:179:PRO:HB3	1:H:247:GLY:HA3	1.91	0.53
1:C:421:ALA:HB3	1:C:465:ILE:HD11	1.90	0.53
1:E:439:ASN:HB2	1:E:441:LYS:HE2	1.89	0.53
1:G:304:ARG:HG3	1:G:304:ARG:HH11	1.72	0.53
1:D:204:VAL:HG12	1:D:233:ARG:HD3	1.91	0.53
1:E:271:ILE:HG22	1:E:407:HIS:HB2	1.89	0.53
1:C:199:LEU:HD23	1:C:199:LEU:O	2.09	0.53
1:F:529:ALA:HA	1:F:532:VAL:HG22	1.90	0.53
1:H:445:VAL:HG12	1:H:449:LYS:HE3	1.90	0.53
1:A:268:ASP:HB3	1:A:271:ILE:HG23	1.91	0.53
1:B:268:ASP:HB3	1:B:271:ILE:HG23	1.91	0.53
1:A:475:ALA:HB1	1:A:479:ARG:HG3	1.90	0.53
1:C:590:PRO:HB2	4:C:702:TRT:H191	1.89	0.53
1:A:321:TRP:CG	2:I:3:GZL:O3	2.62	0.53
1:B:371:ILE:HD11	1:B:386:TYR:CZ	2.43	0.53
1:A:511:PRO:HG2	1:A:552:THR:HA	1.90	0.53
1:F:555:LEU:H	1:F:573:VAL:HG12	1.74	0.53
1:C:32:LEU:HD23	1:C:35[A]:ARG:HH11	1.74	0.52
1:G:529:ALA:HA	1:G:532:VAL:HG22	1.91	0.52
1:H:272:GLU:HB3	1:H:406:TRP:HB2	1.90	0.52
1:F:82:TRP:HB3	1:F:292:MET:HE1	1.91	0.52
1:A:204:VAL:HG12	1:A:233:ARG:HD3	1.91	0.52
1:F:252:MET:HE3	1:F:373:GLN:HA	1.91	0.52
1:G:204:VAL:HG12	1:G:233:ARG:HD3	1.91	0.52
1:G:614:MET:HE1	1:G:617:ARG:NH1	2.25	0.52
1:D:529:ALA:HA	1:D:532:VAL:HG22	1.92	0.52
1:A:614:MET:HE1	1:A:617:ARG:HH11	1.75	0.52
1:E:179:PRO:HB3	1:E:247:GLY:HA3	1.92	0.52
1:E:518:VAL:HG12	1:E:554:GLN:HE21	1.75	0.52
1:H:250:ARG:HH21	1:H:635:PHE:HB3	1.75	0.52
1:A:484:LEU:HB3	1:A:485:PRO:HD3	1.92	0.51
1:D:376:PRO:HG2	1:D:480:LEU:HB3	1.92	0.51

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:178:MET:HE3	1:H:267:MET:HB2	1.92	0.51
1:B:524:PRO:HG2	1:B:530:LYS:HG2	1.91	0.51
1:C:195:GLY:HA2	1:C:201:LEU:HG	1.92	0.51
1:C:520:ALA:HB1	1:C:533:ARG:HH21	1.76	0.51
1:D:180:THR:HA	1:D:269:ASP:OD2	2.10	0.51
1:E:172:GLY:HA3	1:E:286:ARG:NH1	2.25	0.51
1:D:635:PHE:HB2	1:D:637:LEU:HD22	1.92	0.51
1:A:48:ARG:HD2	1:F:62:GLU:HG3	1.92	0.51
1:G:461:SER:HB2	1:G:495:ARG:HG2	1.92	0.51
1:B:594:LEU:HD13	4:B:702:TRT:H11	1.93	0.51
1:F:550:HIS:CE1	1:F:587:LYS:HB3	2.46	0.51
1:C:274:GLU:OE2	1:C:275:PRO:HD2	2.11	0.51
1:D:371:ILE:HD11	1:D:386:TYR:CZ	2.46	0.51
1:D:538:VAL:O	1:D:542:LEU:HG	2.10	0.51
1:G:19:LEU:HD21	1:G:22:ARG:HG3	1.93	0.51
1:A:315:ASP:O	1:A:319:PHE:HA	2.10	0.50
1:A:594:LEU:HD13	4:A:702:TRT:H11	1.93	0.50
1:A:18:SER:HB2	1:A:164:ALA:HB3	1.93	0.50
1:C:252:MET:HE3	1:C:373:GLN:HA	1.92	0.50
1:D:80:ARG:HD2	1:D:139:PHE:HB2	1.92	0.50
1:E:533:ARG:NH1	1:E:565:PHE:HB2	2.26	0.50
1:D:179:PRO:HB3	1:D:247:GLY:HA3	1.93	0.50
1:F:272:GLU:HB3	1:F:406:TRP:HB2	1.94	0.50
1:D:252:MET:HE3	1:D:373:GLN:HA	1.93	0.50
1:C:410:TRP:HA	1:C:413:LYS:HD2	1.94	0.50
1:H:432:ALA:O	1:H:436:LEU:HB3	2.11	0.50
1:A:115:GLN:HG2	1:A:116:GLY:H	1.77	0.50
1:A:200:VAL:HA	1:A:279:LEU:HD21	1.93	0.50
1:G:589:ASP:HB3	1:G:592:GLN:HB2	1.94	0.50
1:A:25:LEU:HD22	1:A:57:LEU:HD13	1.93	0.49
1:F:635:PHE:HB2	1:F:637:LEU:HD22	1.94	0.49
1:H:520:ALA:HB1	1:H:533:ARG:HH21	1.77	0.49
1:B:284:PHE:HE2	1:B:398:VAL:HG21	1.77	0.49
1:E:32:LEU:HD23	1:E:35[A]:ARG:HH11	1.78	0.49
1:F:284:PHE:HE2	1:F:398:VAL:HG21	1.76	0.49
1:A:174:ILE:HG22	1:A:263:TYR:HB2	1.94	0.49
1:F:590:PRO:HB3	4:F:702:TRT:H162	1.93	0.49
1:G:470:ILE:HG21	1:G:603:LEU:HB3	1.94	0.49
1:B:276:ASP:O	1:B:280:ARG:HG3	2.12	0.49
1:B:416:ALA:HB2	2:J:2:GZL:H21	1.95	0.49
1:D:314:VAL:HA	1:D:321:TRP:HA	1.95	0.49

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:432:ALA:O	1:D:436:LEU:HB3	2.12	0.49
1:C:297:GLN:HG2	1:C:399:THR:HG22	1.93	0.49
1:A:68:CYS:HB2	1:A:146:TRP:CD1	2.48	0.49
1:A:589:ASP:HB3	1:A:592:GLN:HB2	1.94	0.49
1:B:297:GLN:HG2	1:B:399:THR:HG22	1.95	0.49
1:B:511:PRO:HG2	1:B:552:THR:HA	1.92	0.49
1:C:524:PRO:HG2	1:C:530:LYS:HG2	1.93	0.49
1:E:272:GLU:HB3	1:E:406:TRP:HB2	1.94	0.49
1:H:90:LEU:HB2	1:H:162:TRP:CZ3	2.48	0.49
1:C:268:ASP:HB3	1:C:271:ILE:HG23	1.95	0.49
1:F:174:ILE:HG22	1:F:263:TYR:HB2	1.95	0.49
1:H:200:VAL:HG22	1:H:279:LEU:HD21	1.95	0.49
1:H:635:PHE:HB2	1:H:637:LEU:HD22	1.94	0.49
1:B:212:GLN:HB3	1:B:241:ASN:HA	1.95	0.48
1:E:291:PRO:HB2	1:E:395:TYR:CD1	2.48	0.48
1:G:96:GLY:H	1:G:121:VAL:CG2	2.26	0.48
1:B:635:PHE:HB2	1:B:637:LEU:HD22	1.95	0.48
1:G:538:VAL:O	1:G:542:LEU:HG	2.13	0.48
1:D:465:ILE:HG21	1:D:495:ARG:HG3	1.96	0.48
1:D:527:PRO:HA	1:D:530:LYS:HG3	1.95	0.48
1:C:74:LEU:HD21	1:C:88:VAL:HG11	1.94	0.48
1:C:199:LEU:HD22	1:C:279:LEU:HD11	1.95	0.48
1:A:31:PRO:HG2	1:A:304:ARG:HH21	1.78	0.48
1:B:274:GLU:OE2	1:B:275:PRO:HD2	2.14	0.48
1:B:529:ALA:HA	1:B:532:VAL:HG22	1.94	0.48
1:F:40:GLU:HG2	1:F:339:LYS:HE3	1.94	0.48
1:E:23:ILE:HG12	1:E:161:GLY:HA2	1.94	0.48
1:E:533:ARG:HH12	1:E:565:PHE:HB2	1.79	0.48
1:E:635:PHE:HB2	1:E:637:LEU:HD22	1.96	0.48
1:B:31:PRO:HG2	1:B:304:ARG:HH21	1.79	0.48
1:B:288:ALA:HB1	1:B:292:MET:HE3	1.95	0.48
1:C:27:ARG:HG3	1:C:54:ARG:NH1	2.29	0.48
1:C:544:PRO:HA	1:C:590:PRO:HG2	1.96	0.48
1:F:527:PRO:HA	1:F:530:LYS:HG3	1.96	0.48
1:G:151:SER:HB2	1:G:153:THR:O	2.14	0.48
1:G:201:LEU:HD22	1:G:233:ARG:NH1	2.28	0.48
1:F:484:LEU:HB3	1:F:485:PRO:HD3	1.96	0.48
1:C:20:LEU:HD21	1:C:164:ALA:HB2	1.96	0.47
4:F:702:TRT:H13	4:F:702:TRT:H161	1.60	0.47
1:G:187:LEU:HD23	1:G:217:VAL:HG21	1.95	0.47
1:G:576:THR:HA	1:G:583:VAL:HG12	1.96	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:520:ALA:HB1	1:A:533:ARG:HH21	1.79	0.47
1:C:90:LEU:HB2	1:C:162:TRP:CZ3	2.49	0.47
1:G:314:VAL:HG13	1:G:316:ARG:NH1	2.30	0.47
1:D:113:HIS:CG	1:G:304:ARG:NH1	2.82	0.47
1:A:32:LEU:HD23	1:A:35[A]:ARG:HH11	1.79	0.47
1:G:74:LEU:HD21	1:G:88:VAL:HG11	1.97	0.47
1:B:80:ARG:HH12	1:D:506:SER:HB2	1.78	0.47
1:C:475:ALA:HB1	1:C:479:ARG:HG3	1.95	0.47
1:D:68:CYS:HB2	1:D:146:TRP:CD1	2.50	0.47
1:E:288:ALA:HB1	1:E:292:MET:HE3	1.97	0.47
1:B:180:THR:HA	1:B:269:ASP:OD2	2.14	0.47
1:A:27:ARG:HG3	1:A:54:ARG:NH1	2.30	0.47
1:A:288:ALA:HB1	1:A:292:MET:HE3	1.95	0.47
1:B:25:LEU:O	1:B:54:ARG:HD2	2.14	0.47
1:E:614:MET:HE1	1:E:617:ARG:NH1	2.30	0.47
1:F:288:ALA:HB1	1:F:292:MET:HE3	1.95	0.47
1:D:518:VAL:HG11	1:D:555:LEU:HD13	1.96	0.47
1:G:90:LEU:HB2	1:G:162:TRP:CZ3	2.49	0.47
1:F:97:HIS:HB3	1:F:153:THR:HG23	1.97	0.46
1:A:529:ALA:HA	1:A:532:VAL:HG22	1.97	0.46
1:D:199:LEU:HD22	1:D:279:LEU:HD13	1.96	0.46
1:F:237:ARG:HD2	1:F:250:ARG:HH12	1.80	0.46
1:A:261:ALA:O	1:A:365:ARG:HD2	2.16	0.46
1:E:521:VAL:HB	1:E:566:LEU:HD12	1.98	0.46
1:H:533:ARG:NH1	1:H:565:PHE:HB2	2.30	0.46
1:H:622:HIS:HB3	1:H:623:PRO:HD3	1.96	0.46
1:B:31:PRO:HG2	1:B:304:ARG:NH2	2.30	0.46
1:B:589:ASP:OD2	1:B:591:ARG:HB2	2.16	0.46
1:E:614:MET:HE1	1:E:617:ARG:HH11	1.81	0.46
1:F:23:ILE:HG12	1:F:161:GLY:HA2	1.97	0.46
1:H:67:PHE:HD2	1:H:72:ASN:HD22	1.63	0.46
1:G:40:GLU:HG2	1:G:339:LYS:HE3	1.97	0.46
1:B:252:MET:CE	1:B:374:PRO:HD3	2.45	0.46
1:F:204:VAL:HG12	1:F:233:ARG:HD3	1.96	0.46
1:F:276:ASP:O	1:F:280:ARG:HG3	2.16	0.46
1:A:85:LEU:HD22	1:A:165:PRO:HD2	1.97	0.46
1:E:84:ILE:HG22	1:E:289:LYS:HG2	1.98	0.46
1:F:315:ASP:O	1:F:319:PHE:HA	2.15	0.46
1:H:533:ARG:HH12	1:H:565:PHE:HB2	1.81	0.46
1:H:590:PRO:HB3	4:H:702:TRT:H162	1.98	0.46
1:A:178:MET:HE3	1:A:267:MET:HB2	1.98	0.46

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:323:SER:HB3	1:B:329:TYR:CE2	2.51	0.46
1:C:284:PHE:CE1	1:C:398:VAL:HG21	2.51	0.46
1:E:557:VAL:HG21	1:E:566:LEU:HD21	1.97	0.46
1:F:20:LEU:HD21	1:F:164:ALA:HB2	1.98	0.46
1:A:31:PRO:HG2	1:A:304:ARG:NH2	2.30	0.45
1:C:82:TRP:HB3	1:C:292:MET:HE1	1.97	0.45
1:D:297:GLN:HG2	1:D:399:THR:HG22	1.98	0.45
1:E:32:LEU:HD23	1:E:35[B]:ARG:HD2	1.98	0.45
1:B:337:PRO:HG2	1:B:339:LYS:HG2	1.98	0.45
1:D:559:THR:HG21	1:D:578:ALA:HA	1.99	0.45
1:E:268:ASP:HB3	1:E:271:ILE:HG23	1.98	0.45
1:G:439:ASN:HB2	1:G:441:LYS:HE2	1.98	0.45
1:G:505:PRO:HD2	1:G:509:GLU:HG3	1.99	0.45
1:H:594:LEU:HD13	4:H:702:TRT:H11	1.99	0.45
1:B:424:HIS:HB3	2:J:1:GZL:H51	1.98	0.45
1:B:528:ILE:O	1:B:532:VAL:HG13	2.17	0.45
1:F:533:ARG:NH1	1:F:565:PHE:HB2	2.32	0.45
1:A:528:ILE:O	1:A:532:VAL:HG13	2.16	0.45
1:G:635:PHE:HB2	1:G:637:LEU:HD22	1.98	0.45
1:H:518:VAL:HG11	1:H:555:LEU:HD13	1.99	0.45
1:C:391:ARG:NH1	1:C:396:PRO:HB3	2.32	0.45
1:C:529:ALA:HA	1:C:532:VAL:HG22	1.98	0.45
1:F:443:MET:O	1:F:447:THR:HG23	2.16	0.45
1:H:199:LEU:HD23	1:H:199:LEU:O	2.16	0.45
1:E:237:ARG:HD2	1:E:250:ARG:NH1	2.32	0.45
1:F:453:LYS:HD3	5:F:703:A1BYH:C3	2.46	0.45
1:F:528:ILE:O	1:F:532:VAL:HG13	2.17	0.45
1:C:444:VAL:O	1:C:448:ILE:HG13	2.16	0.45
1:E:82:TRP:HB3	1:E:292:MET:HE1	1.99	0.45
1:H:204:VAL:HG12	1:H:233:ARG:HD3	1.99	0.45
1:A:199:LEU:HD22	1:A:279:LEU:HD11	1.90	0.45
1:B:284:PHE:CE2	1:B:398:VAL:HG21	2.52	0.45
1:C:84:ILE:HG22	1:C:289:LYS:HG2	1.98	0.45
1:C:419:TRP:HA	1:C:495:ARG:HD2	1.99	0.45
1:C:533:ARG:NH1	1:C:565:PHE:HB2	2.31	0.45
1:D:76:ALA:HB1	1:D:136:LEU:HD22	1.98	0.45
1:G:82:TRP:HB3	1:G:292:MET:HE1	1.98	0.45
1:B:520:ALA:HB1	1:B:533:ARG:HH21	1.81	0.44
1:E:68:CYS:HB2	1:E:146:TRP:CD1	2.52	0.44
1:E:266:TYR:O	1:E:360:THR:HA	2.16	0.44
1:F:21:GLN:HG3	1:F:280:ARG:CZ	2.47	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:320:MET:HE1	2:N:1:GZL:H61	1.99	0.44
1:G:410:TRP:HD1	1:G:415:ASP:OD2	2.00	0.44
1:H:487:ALA:O	1:H:491:VAL:HG23	2.17	0.44
1:A:576:THR:HA	1:A:583:VAL:HG12	1.99	0.44
1:B:25:LEU:HD22	1:B:57:LEU:HD13	1.98	0.44
1:C:445:VAL:HA	1:C:448:ILE:HD12	2.00	0.44
1:E:35[B]:ARG:NH1	1:E:41:GLU:OE2	2.49	0.44
1:E:377:LEU:HB3	1:E:427:ASN:ND2	2.33	0.44
1:G:298:MET:HG3	1:G:407:HIS:HB3	1.98	0.44
1:A:180:THR:HG21	1:A:187:LEU:HD22	1.99	0.44
1:E:204:VAL:HG12	1:E:233:ARG:HD3	1.99	0.44
1:G:212:GLN:HB3	1:G:241:ASN:HA	1.99	0.44
1:A:35[B]:ARG:NH1	1:A:41:GLU:OE2	2.50	0.44
1:G:174:ILE:HG22	1:G:263:TYR:HB2	1.99	0.44
1:H:181:PHE:HD1	1:H:212:GLN:HB2	1.82	0.44
1:A:297:GLN:HG2	1:A:399:THR:HG22	1.99	0.44
1:D:20:LEU:HD21	1:D:164:ALA:HB2	1.99	0.44
1:F:594:LEU:HD13	4:F:702:TRT:H11	2.00	0.44
1:H:185:THR:HG22	1:H:189:LYS:HE3	2.00	0.44
1:A:605:LYS:HA	1:A:605:LYS:HD3	1.68	0.44
1:E:590:PRO:HB3	4:E:702:TRT:H162	1.98	0.44
1:F:187:LEU:HD21	1:F:209:VAL:HG11	1.99	0.44
1:H:68:CYS:HB2	1:H:146:TRP:CD1	2.52	0.44
1:A:521:VAL:HB	1:A:566:LEU:HD12	1.99	0.44
1:E:357:GLY:HA2	1:E:383:ASP:OD2	2.18	0.44
1:F:80:ARG:NH1	1:F:140:GLU:HG2	2.33	0.44
1:F:424:HIS:HB3	2:N:1:GZL:H51	2.00	0.44
1:G:252:MET:HE3	1:G:373:GLN:HA	2.00	0.44
1:A:82:TRP:HB3	1:A:292:MET:HE1	2.00	0.44
4:C:702:TRT:H13	4:C:702:TRT:H161	1.63	0.44
1:D:252:MET:HE3	1:D:374:PRO:HD3	1.98	0.44
1:G:421:ALA:HB3	1:G:465:ILE:HD11	1.98	0.44
1:G:439:ASN:CG	1:G:441:LYS:HG2	2.43	0.44
1:B:59:ILE:HG22	1:B:63:SER:HB2	1.99	0.44
1:G:605:LYS:HD3	1:G:605:LYS:HA	1.80	0.44
1:H:298:MET:HE1	1:H:410:TRP:CZ3	2.52	0.44
1:H:323:SER:HB3	1:H:329:TYR:CE2	2.53	0.44
4:B:702:TRT:H13	4:B:702:TRT:H161	1.74	0.43
1:C:208:ILE:HG21	1:C:251:VAL:HA	2.00	0.43
1:D:304:ARG:HG3	1:D:304:ARG:HH11	1.82	0.43
1:G:208:ILE:HG21	1:G:251:VAL:HA	2.00	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:179:PRO:HB3	1:C:247:GLY:HA3	2.00	0.43
1:D:166:ILE:HG13	1:D:287:PHE:HE1	1.83	0.43
1:F:266:TYR:O	1:F:360:THR:HA	2.18	0.43
1:F:314:VAL:HA	1:F:321:TRP:HA	1.99	0.43
1:G:432:ALA:O	1:G:436:LEU:HB3	2.18	0.43
1:C:19:LEU:HD21	1:C:22:ARG:HG3	1.98	0.43
1:C:376:PRO:HG3	1:C:481:PHE:CE2	2.54	0.43
1:D:576:THR:HA	1:D:583:VAL:HG12	2.00	0.43
1:E:444:VAL:O	1:E:448:ILE:HG13	2.18	0.43
1:G:315:ASP:O	1:G:319:PHE:HA	2.17	0.43
1:A:199:LEU:HD23	1:A:199:LEU:O	2.19	0.43
1:B:558:PRO:HG2	1:E:349:ARG:NH1	2.34	0.43
1:G:458:LEU:HD21	1:G:588:ARG:HB2	2.00	0.43
1:B:261:ALA:O	1:B:365:ARG:HD2	2.18	0.43
1:E:252:MET:HE3	1:E:374:PRO:HD3	2.00	0.43
1:F:478:GLU:H	1:F:478:GLU:CD	2.27	0.43
1:G:479:ARG:HH21	1:G:483:LEU:HD21	1.83	0.43
1:H:115:GLN:HG2	1:H:116:GLY:H	1.82	0.43
1:H:478:GLU:H	1:H:478:GLU:CD	2.27	0.43
1:E:297:GLN:HG2	1:E:399:THR:HG22	2.01	0.43
1:A:371:ILE:HD11	1:A:386:TYR:CZ	2.53	0.43
1:A:559:THR:HG21	1:A:578:ALA:HA	2.00	0.43
1:C:301:LEU:HD13	1:C:406:TRP:HB3	1.99	0.43
1:C:304:ARG:NH1	1:H:113:HIS:CG	2.87	0.43
1:H:314:VAL:HA	1:H:321:TRP:HA	2.00	0.43
1:E:21:GLN:HG3	1:E:280:ARG:NE	2.34	0.43
1:G:284:PHE:HE2	1:G:398:VAL:HG21	1.83	0.43
1:A:505:PRO:HD2	1:A:509:GLU:HG3	1.99	0.43
1:E:25:LEU:HD22	1:E:57:LEU:HD13	2.00	0.43
1:E:267:MET:HA	1:E:359:TRP:O	2.18	0.43
1:A:94:LEU:HD23	1:A:157:LEU:HA	2.01	0.43
1:C:68:CYS:HB2	1:C:146:TRP:CD1	2.54	0.43
1:D:300:ASN:HB3	1:D:303:GLU:O	2.19	0.43
1:H:527:PRO:HA	1:H:530:LYS:HG3	2.01	0.43
1:E:528:ILE:O	1:E:532:VAL:HG13	2.19	0.42
1:G:178:MET:HE3	1:G:267:MET:HB2	2.00	0.42
1:G:276:ASP:O	1:G:280:ARG:HG3	2.18	0.42
1:B:92:LEU:HD23	1:B:160:GLY:HA3	2.01	0.42
1:C:371:ILE:HD12	1:C:389:ARG:HD2	2.01	0.42
1:F:298:MET:HE1	1:F:410:TRP:CZ3	2.54	0.42
1:A:291:PRO:HB2	1:A:395:TYR:CD1	2.54	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:199:LEU:HD22	1:H:279:LEU:CD2	2.48	0.42
1:E:248:TYR:HB3	1:E:266:TYR:CZ	2.54	0.42
1:F:600:ALA:HB1	1:F:604:ARG:NH1	2.34	0.42
1:D:184:PRO:HB2	1:D:220:GLU:HB2	2.01	0.42
1:D:555:LEU:H	1:D:573:VAL:HG12	1.85	0.42
1:G:528:ILE:O	1:G:532:VAL:HG13	2.19	0.42
4:A:702:TRT:H161	4:A:702:TRT:H13	1.72	0.42
1:C:538:VAL:O	1:C:542:LEU:HG	2.19	0.42
4:D:702:TRT:H13	4:D:702:TRT:H161	1.63	0.42
1:H:589:ASP:HB3	1:H:592:GLN:HB2	2.02	0.42
1:F:303:GLU:HB3	1:F:306:HIS:ND1	2.35	0.42
1:F:377:LEU:HD12	1:F:382:ASP:HA	2.02	0.42
1:B:113:HIS:CG	1:D:304:ARG:NH1	2.88	0.42
1:B:272:GLU:HB3	1:B:406:TRP:HB2	2.02	0.42
1:C:556:ASN:HA	1:C:574:THR:OG1	2.20	0.42
1:E:298:MET:HE1	1:E:410:TRP:CZ3	2.55	0.42
1:E:304:ARG:NH1	1:G:113:HIS:CG	2.88	0.42
1:E:443:MET:O	1:E:447:THR:HG23	2.20	0.42
1:E:559:THR:HG21	1:E:578:ALA:HA	2.02	0.42
1:G:252:MET:CE	1:G:374:PRO:HD3	2.50	0.42
1:H:40:GLU:HG2	1:H:339:LYS:HE3	2.02	0.42
1:E:299:LEU:HD23	1:E:307:LEU:HA	2.02	0.42
1:E:590:PRO:HB2	4:E:702:TRT:H191	2.01	0.42
1:F:304:ARG:HG3	1:F:304:ARG:NH1	2.33	0.42
1:H:74:LEU:HD21	1:H:88:VAL:HG11	2.01	0.42
1:B:184:PRO:HB2	1:B:220:GLU:HB2	2.01	0.41
1:C:591:ARG:HG2	1:F:366:GLN:HE22	1.84	0.41
1:D:445:VAL:O	1:D:449:LYS:HG3	2.20	0.41
1:E:367:VAL:O	1:E:371:ILE:HG12	2.20	0.41
4:E:702:TRT:H13	4:E:702:TRT:H161	1.69	0.41
1:F:140:GLU:O	1:F:350:ARG:NH1	2.53	0.41
1:G:268:ASP:HB3	1:G:271:ILE:HG23	2.01	0.41
1:B:314:VAL:HA	1:B:321:TRP:HA	2.02	0.41
1:E:82:TRP:HB2	1:E:284:PHE:CZ	2.54	0.41
1:E:300:ASN:HB3	1:E:303:GLU:O	2.20	0.41
1:E:484:LEU:HB3	1:E:485:PRO:HD3	2.01	0.41
1:F:297:GLN:HE21	1:F:399:THR:HG22	1.85	0.41
1:F:540:HIS:CD2	1:F:588:ARG:NH1	2.88	0.41
1:F:605:LYS:HD3	1:F:605:LYS:HA	1.62	0.41
1:H:544:PRO:HA	1:H:590:PRO:HG2	2.01	0.41
1:H:605:LYS:HA	1:H:605:LYS:HD3	1.74	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:371:ILE:HD12	1:A:389:ARG:HD2	2.01	0.41
1:C:375:LEU:HB2	1:C:377:LEU:HG	2.03	0.41
1:G:25:LEU:HD22	1:G:57:LEU:HD13	2.02	0.41
1:H:371:ILE:HD11	1:H:386:TYR:CZ	2.54	0.41
1:B:97:HIS:HD2	1:B:120:ALA:HB2	1.85	0.41
1:D:452:LEU:HD23	1:D:452:LEU:HA	1.92	0.41
1:F:26:PRO:HB3	1:F:30:GLU:HG2	2.02	0.41
1:G:56:SER:HA	1:G:157:LEU:O	2.20	0.41
4:G:702:TRT:H161	4:G:702:TRT:H13	1.65	0.41
1:C:484:LEU:HB3	1:C:485:PRO:HD3	2.02	0.41
1:C:605:LYS:HA	1:C:605:LYS:HD3	1.75	0.41
1:E:436:LEU:HD12	1:E:437:PRO:HD2	2.03	0.41
1:H:557:VAL:HG21	1:H:566:LEU:HD21	2.03	0.41
1:B:266:TYR:O	1:B:360:THR:HA	2.21	0.41
1:E:177:GLY:HA3	1:E:251:VAL:HG11	2.01	0.41
1:G:180:THR:HG21	1:G:187:LEU:HD22	2.02	0.41
1:H:27:ARG:HG3	1:H:54:ARG:NH1	2.36	0.41
1:H:82:TRP:HB2	1:H:284:PHE:CZ	2.55	0.41
1:H:456:LEU:HD12	4:H:702:TRT:H8C1	2.02	0.41
1:A:76:ALA:HB2	1:A:145:ILE:HG13	2.02	0.41
1:B:112:ILE:HG23	1:D:302:GLN:HB3	2.03	0.41
1:B:199:LEU:HD22	1:B:279:LEU:HD13	2.02	0.41
1:B:538:VAL:O	1:B:542:LEU:HG	2.20	0.41
1:B:237:ARG:HD2	1:B:250:ARG:HH12	1.85	0.41
1:C:315:ASP:O	1:C:319:PHE:HA	2.20	0.41
1:E:365:ARG:O	1:E:369:GLU:HG2	2.21	0.41
1:F:177:GLY:HA2	1:F:208:ILE:O	2.21	0.41
1:A:355:PHE:CD1	1:A:384:VAL:HG13	2.56	0.41
1:B:291:PRO:HB2	1:B:395:TYR:CE1	2.55	0.41
1:C:614:MET:HE1	1:C:617:ARG:HH11	1.84	0.41
1:D:315:ASP:O	1:D:319:PHE:CA	2.63	0.41
1:D:520:ALA:HB1	1:D:533:ARG:NH2	2.29	0.41
1:E:510:LEU:HD23	1:E:553:PRO:HG3	2.02	0.41
1:F:455:LEU:HG	1:F:463:VAL:HG21	2.01	0.41
1:G:371:ILE:HD11	1:G:386:TYR:CZ	2.55	0.41
1:B:282:LEU:O	1:B:286:ARG:HG3	2.21	0.41
1:B:338:LEU:HD12	1:B:338:LEU:HA	1.93	0.41
1:D:31:PRO:HB2	1:D:34:VAL:HG23	2.03	0.41
1:D:195:GLY:HA2	1:D:201:LEU:HG	2.03	0.41
1:D:528:ILE:O	1:D:532:VAL:HG13	2.21	0.41
1:B:346:LEU:HD23	1:B:346:LEU:HA	1.93	0.40

*Continued on next page...*



Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:291:PRO:HB2	1:C:395:TYR:CE1	2.56	0.40
1:E:242:LEU:HD22	1:E:484:LEU:HD23	2.03	0.40
1:H:284:PHE:CE2	1:H:398:VAL:HG21	2.56	0.40
1:A:445:VAL:HA	1:A:448:ILE:HD12	2.03	0.40
1:D:319:PHE:CD2	1:D:436:LEU:HB2	2.56	0.40
1:E:59:ILE:HG22	1:E:63:SER:HB2	2.04	0.40
1:F:284:PHE:CE2	1:F:398:VAL:HG21	2.56	0.40
1:H:315:ASP:O	1:H:319:PHE:HA	2.21	0.40
1:H:590:PRO:HB2	4:H:702:TRT:H191	2.03	0.40
1:B:316:ARG:HH22	1:B:388:LEU:HD22	1.86	0.40
1:B:484:LEU:HB3	1:B:485:PRO:HD3	2.03	0.40
1:H:96:GLY:H	1:H:121:VAL:HG23	1.87	0.40
1:A:252:MET:HE3	1:A:373:GLN:HA	2.02	0.40
1:D:533:ARG:HH11	1:D:565:PHE:HB2	1.85	0.40
1:F:220:GLU:CD	1:F:221:PRO:HD2	2.46	0.40
1:G:68:CYS:HB2	1:G:146:TRP:CD1	2.57	0.40

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	625/666 (94%)	597 (96%)	24 (4%)	4 (1%)	21	56
1	B	625/666 (94%)	595 (95%)	27 (4%)	3 (0%)	24	59
1	C	625/666 (94%)	595 (95%)	27 (4%)	3 (0%)	24	59
1	D	625/666 (94%)	599 (96%)	24 (4%)	2 (0%)	36	68
1	E	625/666 (94%)	599 (96%)	25 (4%)	1 (0%)	43	73
1	F	625/666 (94%)	598 (96%)	26 (4%)	1 (0%)	43	73
1	G	625/666 (94%)	601 (96%)	21 (3%)	3 (0%)	24	59

Continued on next page...



*Continued from previous page...*

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	H	625/666 (94%)	595 (95%)	28 (4%)	2 (0%)	36	68
All	All	5000/5328 (94%)	4779 (96%)	202 (4%)	19 (0%)	30	62

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	319	PHE
1	B	241	ASN
1	C	418	ASP
1	H	378	PHE
1	A	418	ASP
1	B	319	PHE
1	B	418	ASP
1	C	319	PHE
1	C	380	LYS
1	D	241	ASN
1	D	380	LYS
1	G	418	ASP
1	H	418	ASP
1	A	241	ASN
1	A	380	LYS
1	F	380	LYS
1	G	380	LYS
1	E	380	LYS
1	G	485	PRO

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	510/543 (94%)	510 (100%)	0	100	100
1	B	510/543 (94%)	510 (100%)	0	100	100
1	C	510/543 (94%)	510 (100%)	0	100	100
1	D	510/543 (94%)	510 (100%)	0	100	100

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	510/543 (94%)	510 (100%)	0	100	100
1	F	510/543 (94%)	510 (100%)	0	100	100
1	G	510/543 (94%)	510 (100%)	0	100	100
1	H	510/543 (94%)	510 (100%)	0	100	100
All	All	4080/4344 (94%)	4080 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	435	HIS
1	A	546	HIS
1	B	97	HIS
1	B	326	ASN
1	B	407	HIS
1	C	97	HIS
1	C	239	GLN
1	C	297	GLN
1	C	373	GLN
1	C	515	HIS
1	D	239	GLN
1	D	343	ASN
1	D	435	HIS
1	D	550	HIS
1	E	241	ASN
1	E	435	HIS
1	E	556	ASN
1	F	239	GLN
1	F	297	GLN
1	F	308	HIS
1	F	343	ASN
1	F	435	HIS
1	F	466	GLN
1	F	515	HIS
1	G	331	HIS
1	G	541	ASN
1	G	546	HIS
1	H	50	HIS
1	H	72	ASN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	H	343	ASN
1	H	435	HIS
1	H	466	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 ⓘ

24 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	GZL	I	1	5,2	11,11,12	0.52	0	13,15,17	1.33	2 (15%)
2	GZL	I	2	2	11,11,12	0.73	1 (9%)	13,15,17	1.25	2 (15%)
2	GZL	I	3	2	11,11,12	0.51	0	13,15,17	1.29	2 (15%)
2	GZL	J	1	5,2	11,11,12	0.41	0	13,15,17	1.46	3 (23%)
2	GZL	J	2	2	11,11,12	0.56	0	13,15,17	1.35	1 (7%)
2	GZL	J	3	2	11,11,12	0.35	0	13,15,17	1.27	2 (15%)
2	GZL	K	1	5,2	11,11,12	0.37	0	13,15,17	1.30	2 (15%)
2	GZL	K	2	2	11,11,12	0.51	0	13,15,17	1.48	2 (15%)
2	GZL	K	3	2	11,11,12	0.33	0	13,15,17	1.12	2 (15%)
2	GZL	L	1	5,2	11,11,12	0.40	0	13,15,17	1.36	2 (15%)
2	GZL	L	2	2	11,11,12	0.54	0	13,15,17	1.57	3 (23%)
2	GZL	L	3	2	11,11,12	0.40	0	13,15,17	1.17	2 (15%)
2	GZL	M	1	5,2	11,11,12	0.40	0	13,15,17	1.29	2 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	GZL	M	2	2	11,11,12	0.46	0	13,15,17	1.01	0
2	GZL	M	3	2	11,11,12	0.36	0	13,15,17	1.04	1 (7%)
2	GZL	N	1	5,2	11,11,12	0.41	0	13,15,17	1.22	2 (15%)
2	GZL	N	2	2	11,11,12	0.51	0	13,15,17	1.23	1 (7%)
2	GZL	N	3	2	11,11,12	0.37	0	13,15,17	1.23	2 (15%)
2	GZL	O	1	5,2	11,11,12	0.43	0	13,15,17	1.29	2 (15%)
2	GZL	O	2	2	11,11,12	0.49	0	13,15,17	1.27	1 (7%)
2	GZL	O	3	2	11,11,12	0.37	0	13,15,17	1.25	2 (15%)
2	GZL	P	1	5,2	11,11,12	0.41	0	13,15,17	1.13	2 (15%)
2	GZL	P	2	2	11,11,12	0.55	0	13,15,17	1.07	1 (7%)
2	GZL	P	3	2	11,11,12	0.38	0	13,15,17	1.05	1 (7%)

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	GZL	I	1	5,2	-	4/6/19/22	0/1/1/1
2	GZL	I	2	2	-	0/6/19/22	0/1/1/1
2	GZL	I	3	2	-	2/6/19/22	0/1/1/1
2	GZL	J	1	5,2	-	4/6/19/22	0/1/1/1
2	GZL	J	2	2	-	3/6/19/22	0/1/1/1
2	GZL	J	3	2	-	0/6/19/22	0/1/1/1
2	GZL	K	1	5,2	-	4/6/19/22	0/1/1/1
2	GZL	K	2	2	-	0/6/19/22	0/1/1/1
2	GZL	K	3	2	-	6/6/19/22	0/1/1/1
2	GZL	L	1	5,2	-	4/6/19/22	0/1/1/1
2	GZL	L	2	2	-	4/6/19/22	0/1/1/1
2	GZL	L	3	2	-	6/6/19/22	0/1/1/1
2	GZL	M	1	5,2	-	4/6/19/22	0/1/1/1
2	GZL	M	2	2	-	0/6/19/22	0/1/1/1
2	GZL	M	3	2	-	0/6/19/22	0/1/1/1
2	GZL	N	1	5,2	-	4/6/19/22	0/1/1/1
2	GZL	N	2	2	-	1/6/19/22	0/1/1/1
2	GZL	N	3	2	-	0/6/19/22	0/1/1/1
2	GZL	O	1	5,2	-	6/6/19/22	0/1/1/1

Continued on next page...

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GZL	O	2	2	-	3/6/19/22	0/1/1/1
2	GZL	O	3	2	-	2/6/19/22	0/1/1/1
2	GZL	P	1	5,2	-	4/6/19/22	0/1/1/1
2	GZL	P	2	2	-	0/6/19/22	0/1/1/1
2	GZL	P	3	2	-	0/6/19/22	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	I	2	GZL	C2-C3	-2.06	1.50	1.53

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	2	GZL	C5-C4-C3	-3.68	110.67	115.95
2	L	1	GZL	C5-C4-C3	-3.52	110.90	115.95
2	K	2	GZL	C5-C4-C3	-3.50	110.92	115.95
2	J	2	GZL	C5-C4-C3	-3.48	110.95	115.95
2	N	2	GZL	C5-C4-C3	-3.43	111.02	115.95
2	J	1	GZL	C5-C4-C3	-3.40	111.06	115.95
2	O	2	GZL	C5-C4-C3	-3.32	111.19	115.95
2	I	2	GZL	C5-C4-C3	-3.30	111.21	115.95
2	O	1	GZL	C5-C4-C3	-3.29	111.23	115.95
2	I	3	GZL	C5-C4-C3	-3.10	111.49	115.95
2	M	1	GZL	C5-C4-C3	-3.00	111.64	115.95
2	I	1	GZL	C5-C4-C3	-2.99	111.66	115.95
2	K	1	GZL	C5-C4-C3	-2.92	111.76	115.95
2	O	3	GZL	C1-C2-C3	2.84	106.17	101.63
2	J	3	GZL	C5-C4-C3	-2.81	111.91	115.95
2	K	1	GZL	C1-C2-C3	2.73	106.00	101.63
2	N	1	GZL	C5-C4-C3	-2.72	112.04	115.95
2	N	3	GZL	C5-C4-C3	-2.71	112.06	115.95
2	L	3	GZL	C5-C4-C3	-2.63	112.17	115.95
2	J	3	GZL	C1-C2-C3	2.59	105.77	101.63
2	I	3	GZL	C1-C2-C3	2.59	105.77	101.63
2	P	1	GZL	C5-C4-C3	-2.57	112.26	115.95
2	I	1	GZL	C1-C2-C3	2.56	105.72	101.63
2	P	2	GZL	C5-C4-C3	-2.54	112.31	115.95
2	N	1	GZL	C1-C2-C3	2.53	105.67	101.63
2	L	1	GZL	C1-C2-C3	2.49	105.61	101.63
2	M	1	GZL	C1-C2-C3	2.47	105.57	101.63

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	1	GZL	O6-C6-C5	2.43	116.26	111.16
2	K	3	GZL	C5-C4-C3	-2.43	112.46	115.95
2	O	3	GZL	C5-C4-C3	-2.40	112.51	115.95
2	P	1	GZL	C1-C2-C3	2.40	105.46	101.63
2	K	2	GZL	C1-C2-C3	2.37	105.41	101.63
2	N	3	GZL	C1-C2-C3	2.32	105.34	101.63
2	O	1	GZL	C1-C2-C3	2.27	105.26	101.63
2	P	3	GZL	C1-C2-C3	2.23	105.20	101.63
2	J	1	GZL	C1-C2-C3	2.22	105.17	101.63
2	L	3	GZL	C1-C2-C3	2.18	105.11	101.63
2	K	3	GZL	C1-C2-C3	2.17	105.10	101.63
2	I	2	GZL	C1-C2-C3	2.15	105.06	101.63
2	L	2	GZL	C1-C2-C3	2.10	104.99	101.63
2	L	2	GZL	C6-C5-C4	-2.07	107.94	112.05
2	M	3	GZL	C1-C2-C3	2.05	104.91	101.63

There are no chirality outliers.

All (61) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	J	1	GZL	C3-C4-C5-C6
2	J	1	GZL	O4-C4-C5-C6
2	J	1	GZL	C3-C4-C5-O5
2	J	2	GZL	C3-C4-C5-O5
2	K	3	GZL	O5-C5-C6-O6
2	K	3	GZL	O4-C4-C5-C6
2	K	3	GZL	C3-C4-C5-O5
2	L	1	GZL	C3-C4-C5-C6
2	L	1	GZL	O4-C4-C5-C6
2	L	1	GZL	C3-C4-C5-O5
2	L	1	GZL	O4-C4-C5-O5
2	L	2	GZL	O4-C4-C5-C6
2	L	3	GZL	O4-C4-C5-O5
2	M	1	GZL	C3-C4-C5-C6
2	M	1	GZL	O4-C4-C5-C6
2	M	1	GZL	C3-C4-C5-O5
2	M	1	GZL	O4-C4-C5-O5
2	N	1	GZL	C4-C5-C6-O6
2	N	1	GZL	O5-C5-C6-O6
2	N	1	GZL	O4-C4-C5-C6
2	O	1	GZL	O5-C5-C6-O6
2	O	1	GZL	C3-C4-C5-C6

*Continued on next page...*

*Continued from previous page...*

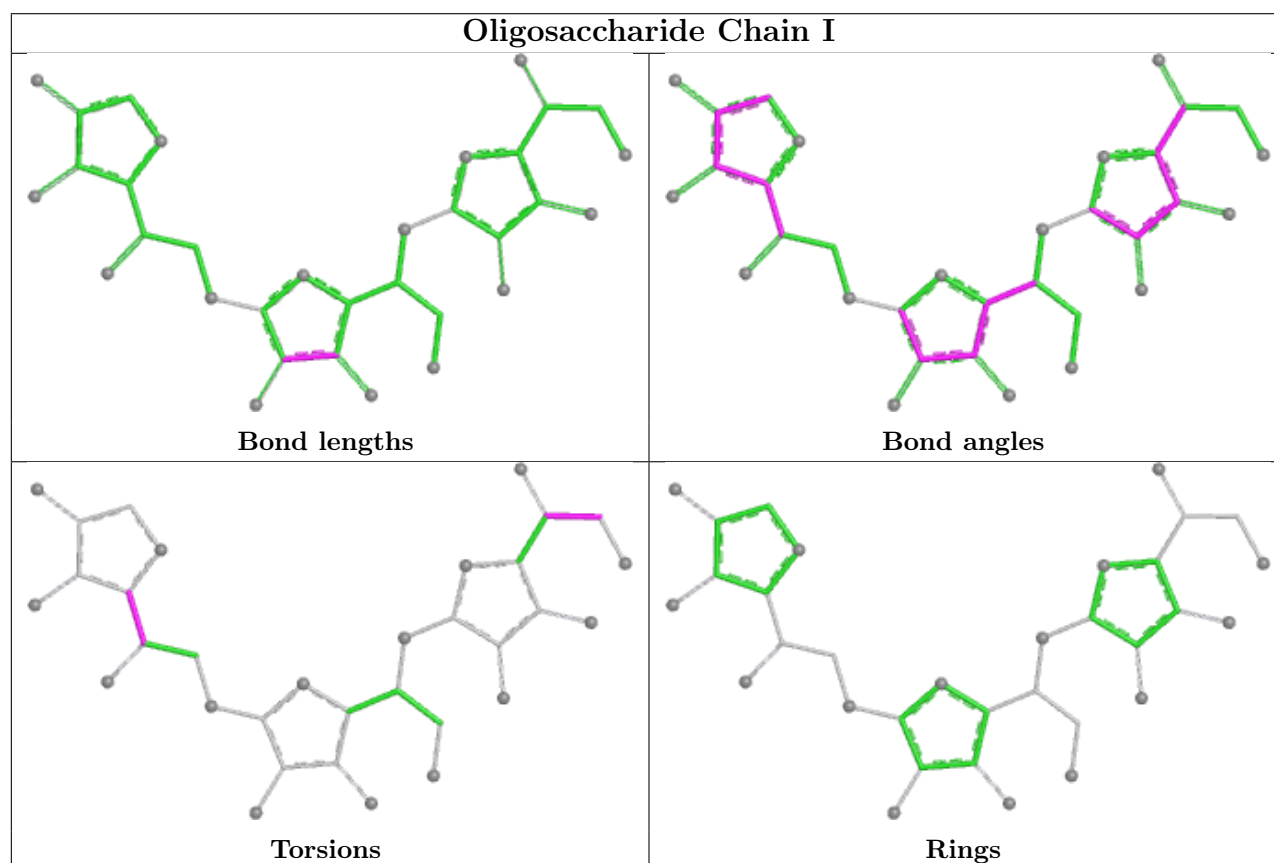
Mol	Chain	Res	Type	Atoms
2	O	1	GZL	O4-C4-C5-C6
2	O	1	GZL	C3-C4-C5-O5
2	O	2	GZL	C3-C4-C5-O5
2	P	1	GZL	C3-C4-C5-C6
2	P	1	GZL	O4-C4-C5-C6
2	P	1	GZL	C3-C4-C5-O5
2	K	1	GZL	C4-C5-C6-O6
2	K	3	GZL	C4-C5-C6-O6
2	O	1	GZL	C4-C5-C6-O6
2	K	1	GZL	O5-C5-C6-O6
2	L	3	GZL	O5-C5-C6-O6
2	O	3	GZL	O5-C5-C6-O6
2	I	1	GZL	C3-C4-C5-O5
2	L	2	GZL	C3-C4-C5-O5
2	L	3	GZL	C3-C4-C5-O5
2	I	1	GZL	O4-C4-C5-O5
2	J	1	GZL	O4-C4-C5-O5
2	J	2	GZL	O4-C4-C5-O5
2	K	1	GZL	O4-C4-C5-O5
2	L	2	GZL	O4-C4-C5-O5
2	N	1	GZL	O4-C4-C5-O5
2	O	1	GZL	O4-C4-C5-O5
2	O	2	GZL	O4-C4-C5-O5
2	P	1	GZL	O4-C4-C5-O5
2	I	3	GZL	O5-C5-C6-O6
2	I	1	GZL	C3-C4-C5-C6
2	L	2	GZL	C3-C4-C5-C6
2	L	3	GZL	C3-C4-C5-C6
2	I	1	GZL	O4-C4-C5-C6
2	L	3	GZL	O4-C4-C5-C6
2	K	3	GZL	O4-C4-C5-O5
2	O	3	GZL	C4-C5-C6-O6
2	L	3	GZL	C4-C5-C6-O6
2	K	3	GZL	C3-C4-C5-C6
2	I	3	GZL	C4-C5-C6-O6
2	J	2	GZL	C3-C4-C5-C6
2	N	2	GZL	C3-C4-C5-C6
2	O	2	GZL	C3-C4-C5-C6
2	K	1	GZL	O4-C4-C5-C6

There are no ring outliers.

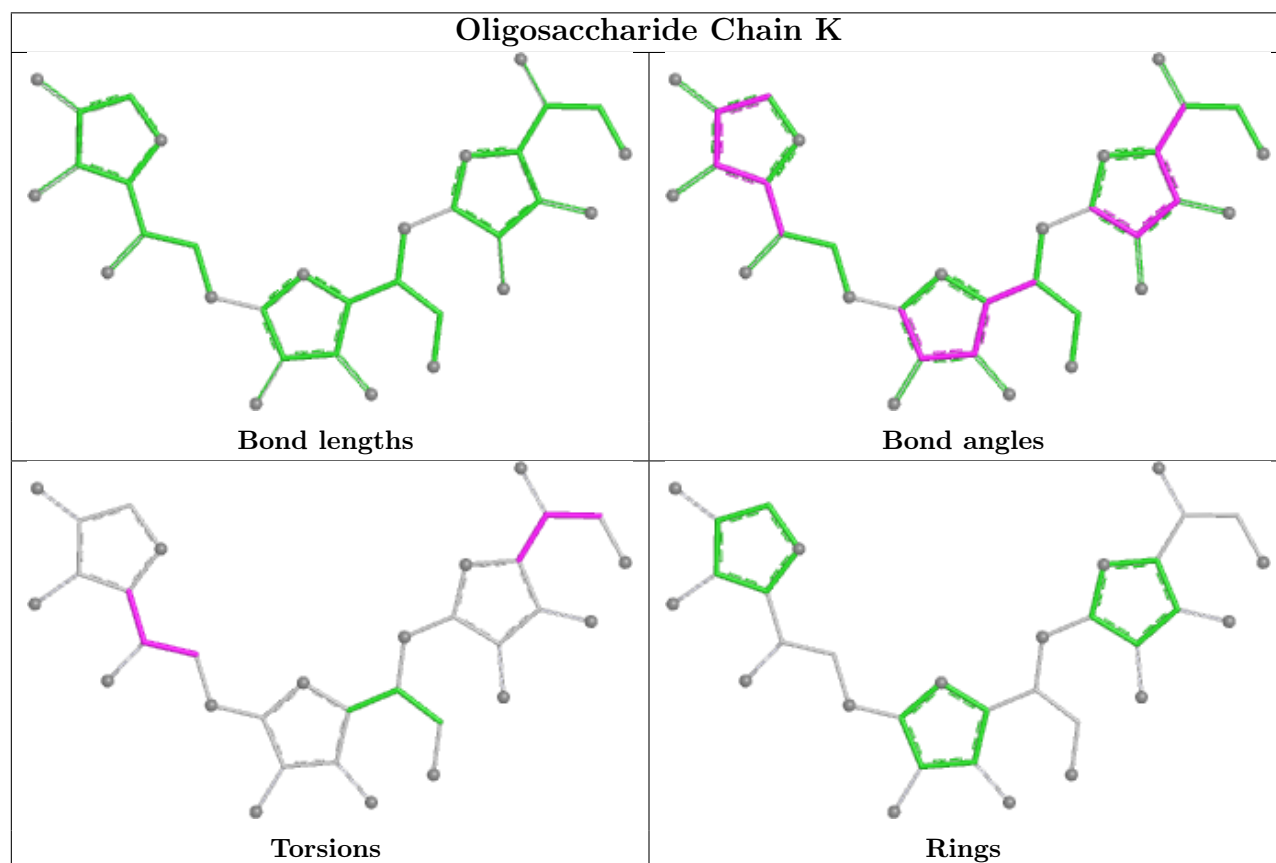
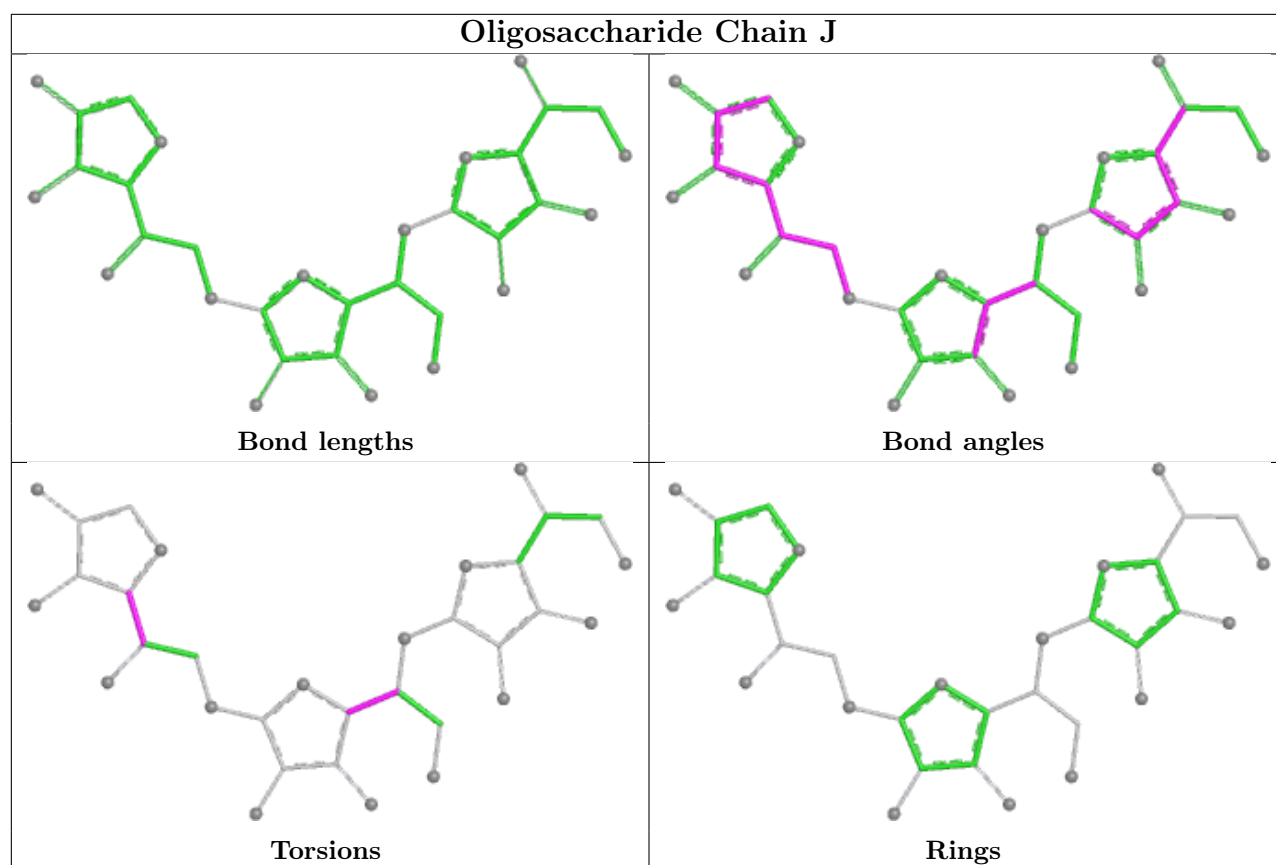
4 monomers are involved in 6 short contacts:

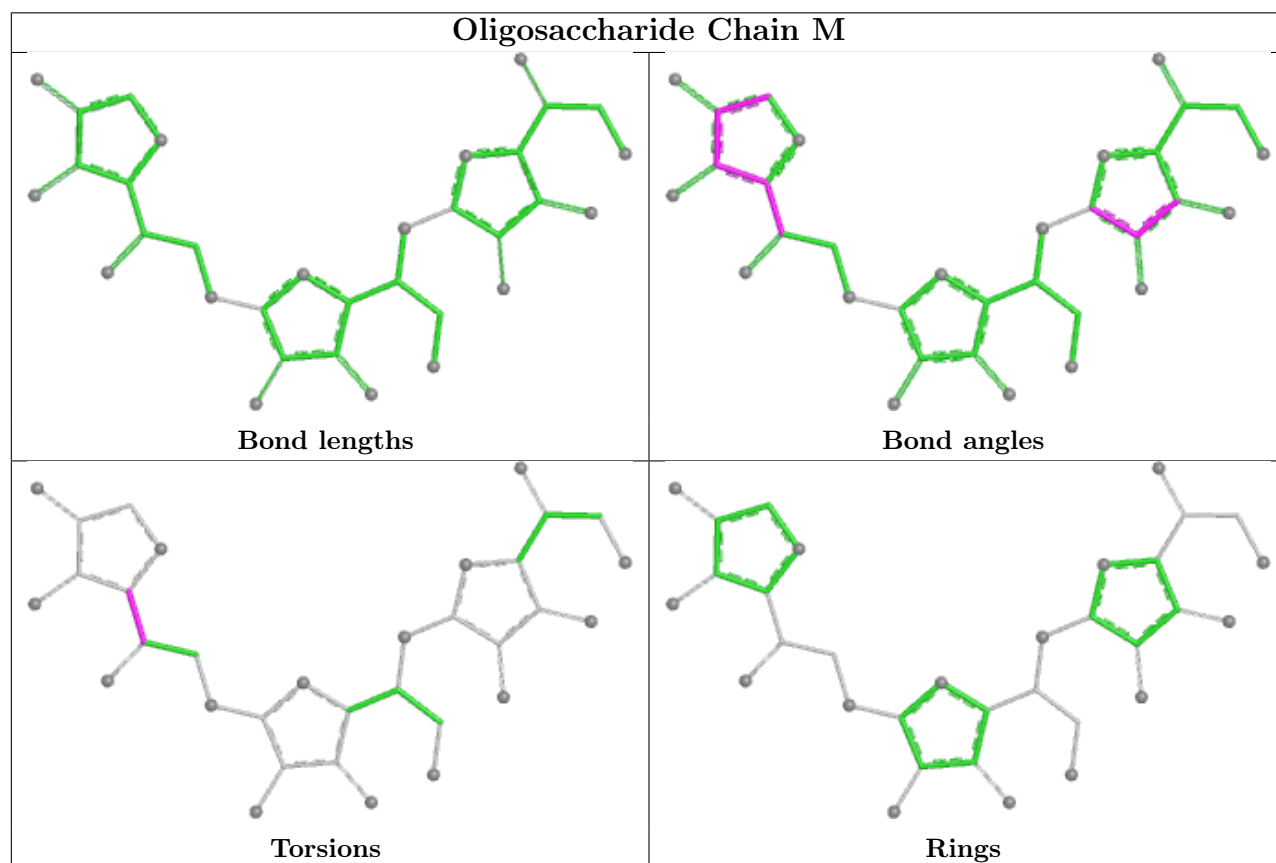
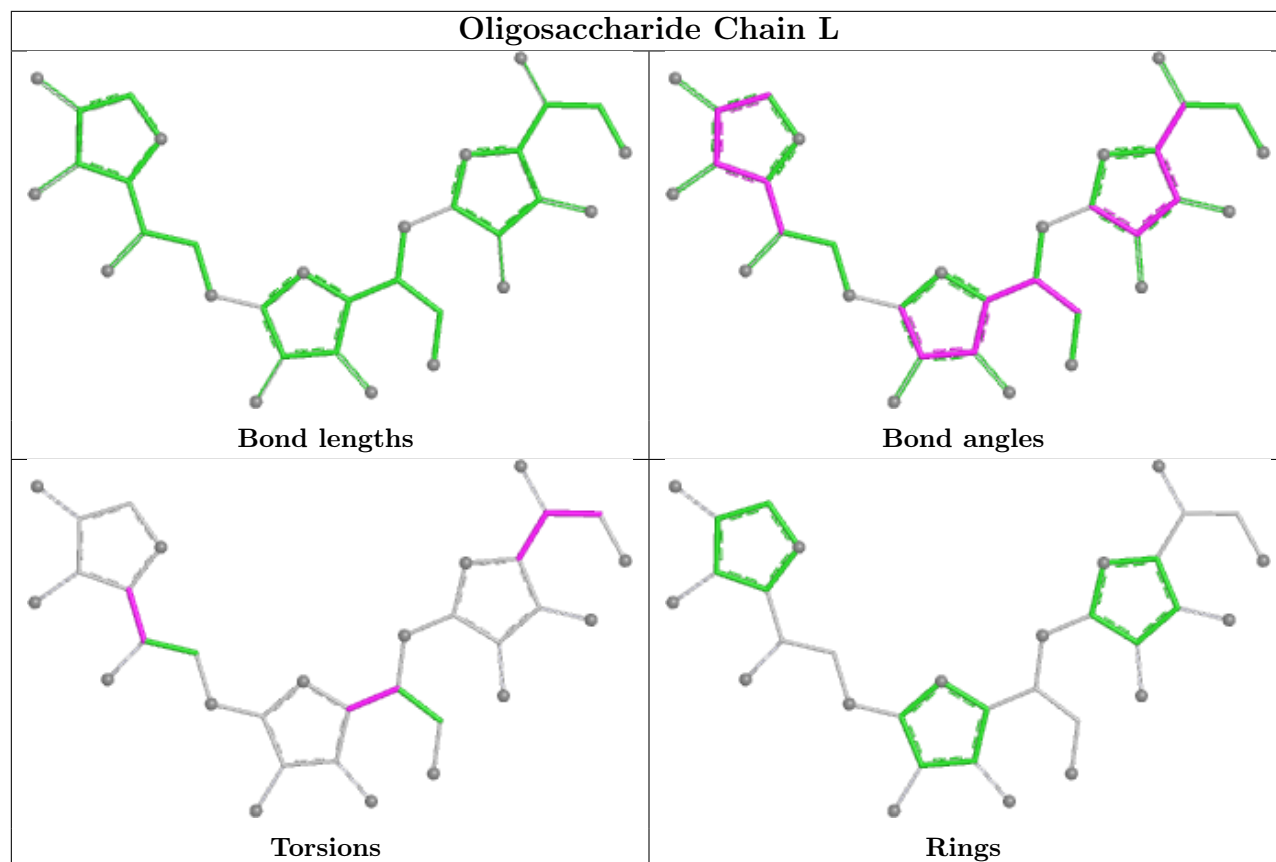
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	I	3	GZL	2	0
2	J	2	GZL	1	0
2	N	1	GZL	2	0
2	J	1	GZL	1	0

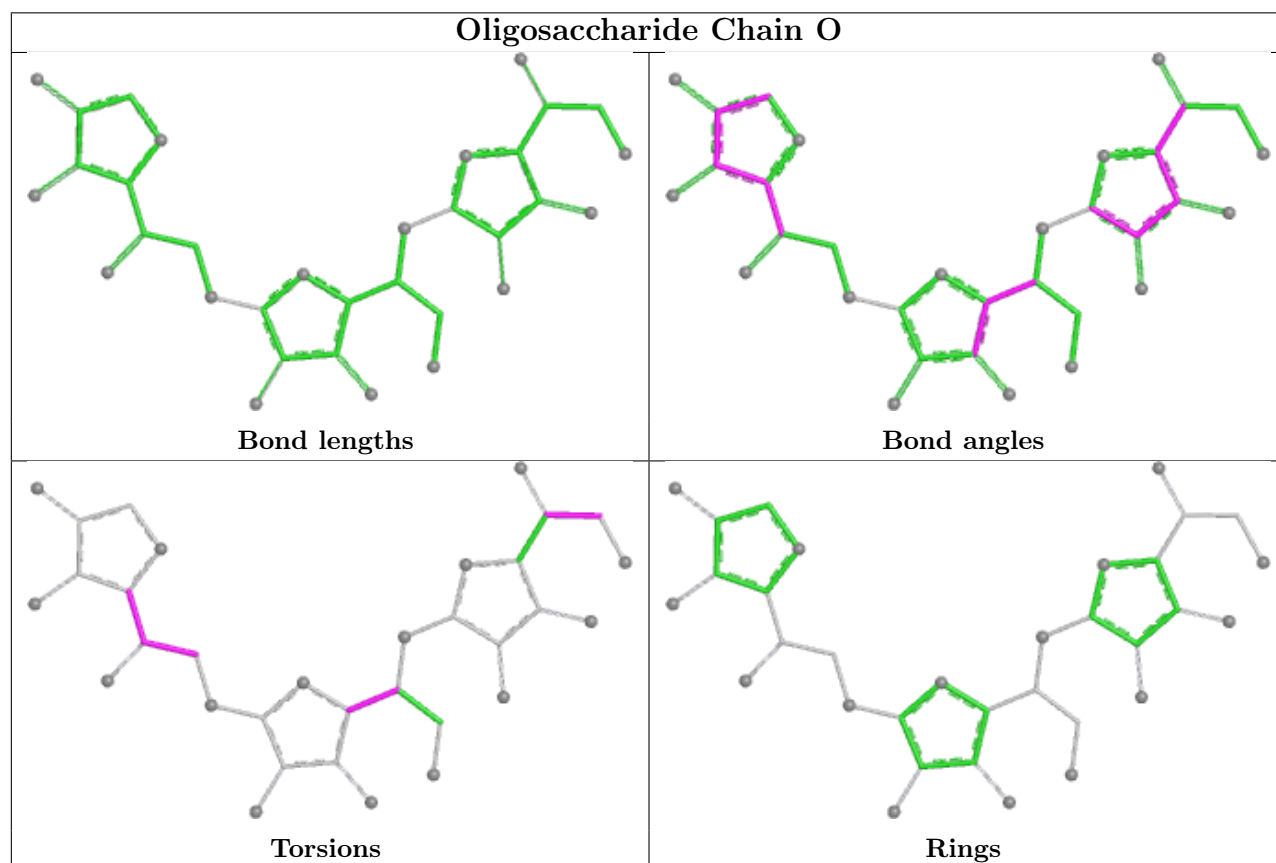
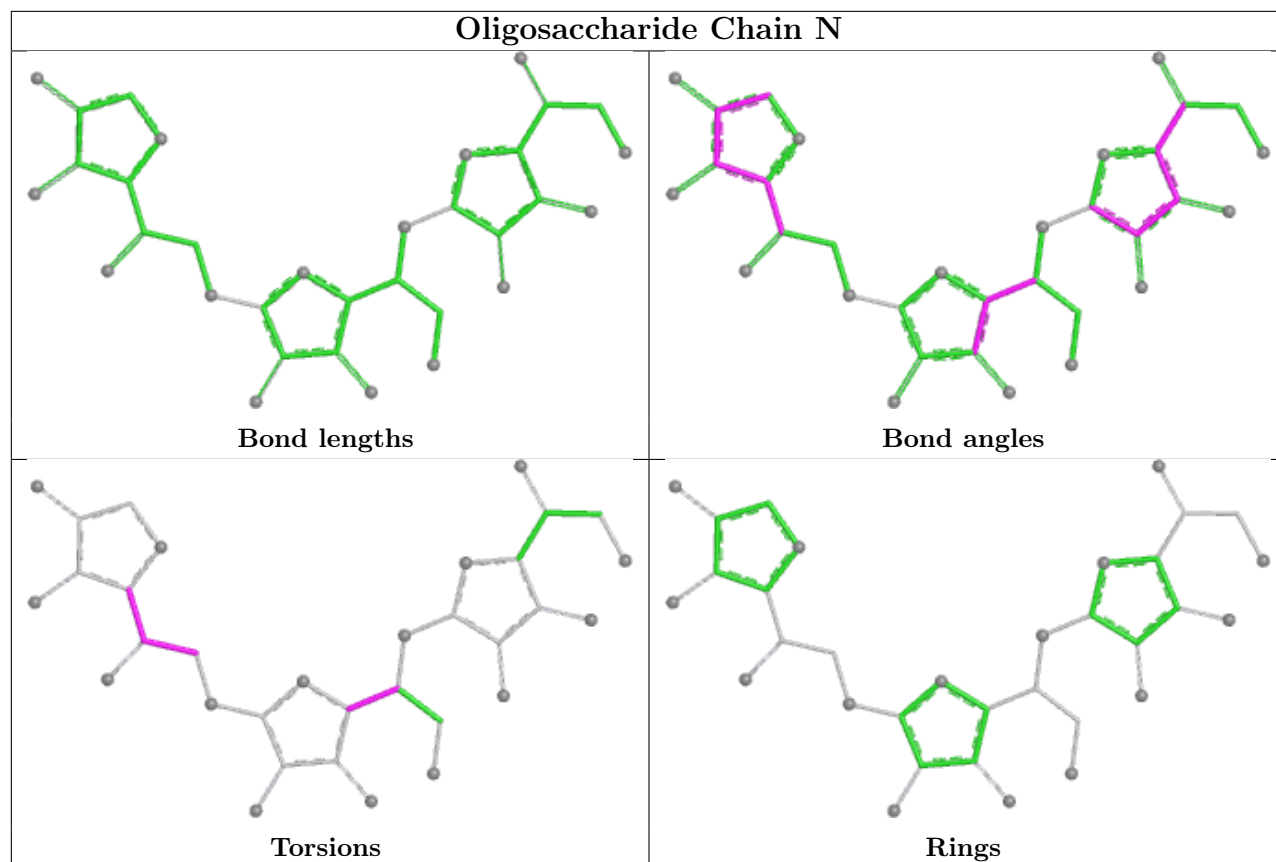
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

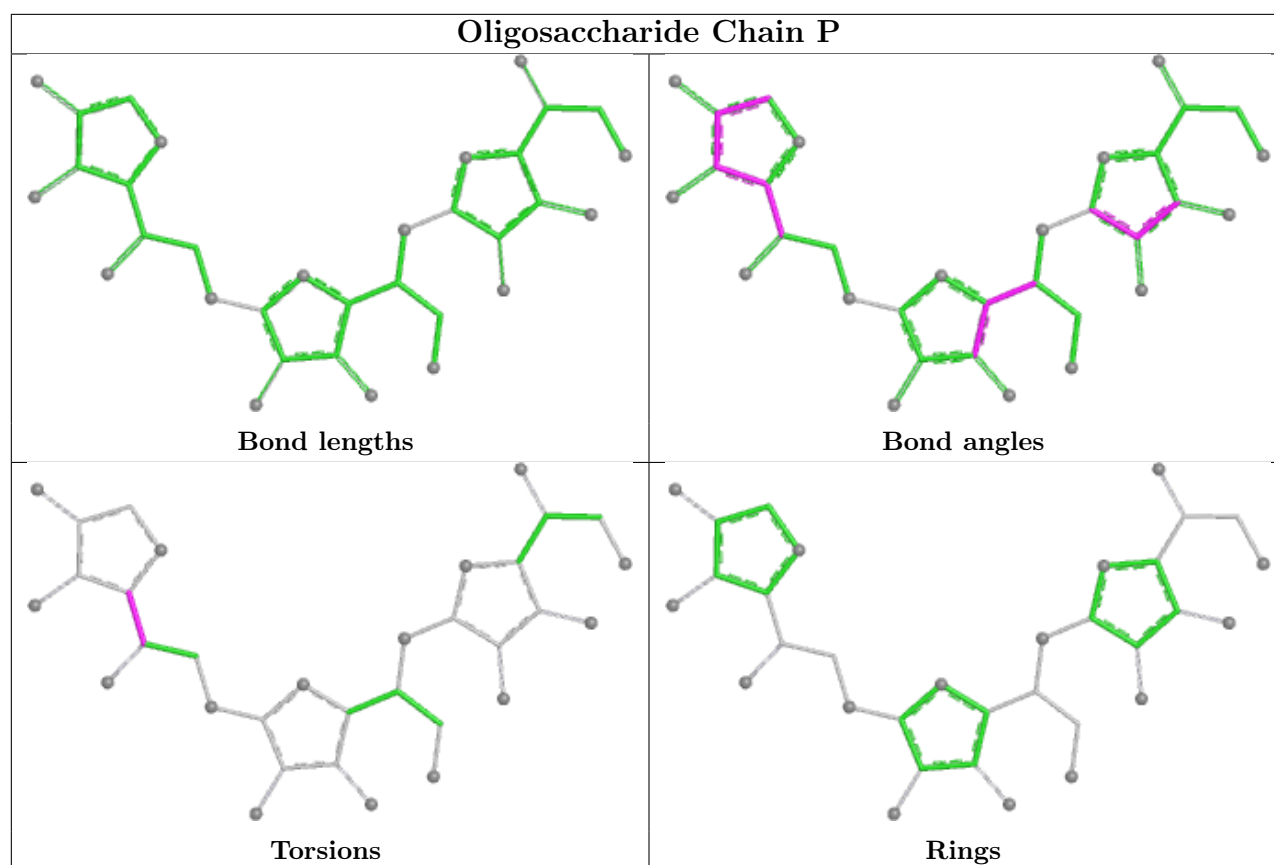












## 5.6 Ligand geometry [i](#)

Of 24 ligands modelled in this entry, 8 are monoatomic - leaving 16 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	TRT	F	702	-	20,20,25	0.43	0	28,28,33	0.90	0
4	TRT	C	702	-	20,20,25	0.45	0	28,28,33	0.92	0
4	TRT	H	702	-	20,20,25	0.46	0	28,28,33	0.94	0
4	TRT	A	702	-	20,20,25	0.45	0	28,28,33	0.93	0
5	A1BYH	C	703	2	2,2,20	0.31	0	1,1,21	0.37	0
5	A1BYH	E	703	2	2,2,20	0.32	0	1,1,21	0.36	0
5	A1BYH	A	703	2	1,1,20	0.08	0	-		
5	A1BYH	F	703	2	4,4,20	0.31	0	2,3,21	0.56	0
5	A1BYH	G	703	2	3,3,20	0.37	0	2,2,21	0.33	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	A1BYH	H	703	2	2,2,20	0.32	0	1,1,21	0.35	0
4	TRT	G	702	-	20,20,25	0.44	0	28,28,33	0.87	0
4	TRT	D	702	-	20,20,25	0.44	0	28,28,33	0.91	0
5	A1BYH	B	703	2	3,3,20	0.37	0	2,2,21	0.39	0
5	A1BYH	D	703	2	2,2,20	0.31	0	1,1,21	0.34	0
4	TRT	B	702	-	20,20,25	0.43	0	28,28,33	0.88	0
4	TRT	E	702	-	20,20,25	0.45	0	28,28,33	0.90	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	TRT	F	702	-	-	5/18/18/23	0/1/1/1
4	TRT	C	702	-	-	4/18/18/23	0/1/1/1
4	TRT	H	702	-	-	4/18/18/23	0/1/1/1
4	TRT	A	702	-	-	5/18/18/23	0/1/1/1
5	A1BYH	F	703	2	-	0/2/2/14	-
5	A1BYH	G	703	2	-	0/0/1/14	-
4	TRT	G	702	-	-	4/18/18/23	0/1/1/1
4	TRT	D	702	-	-	6/18/18/23	0/1/1/1
5	A1BYH	B	703	2	-	0/0/1/14	-
4	TRT	B	702	-	-	7/18/18/23	0/1/1/1
4	TRT	E	702	-	-	4/18/18/23	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (39) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	702	TRT	C2-C1-C5-C6
4	D	702	TRT	C2-C1-C5-C6
4	A	702	TRT	C2-C1-C5-C6
4	C	702	TRT	C2-C1-C5-C6
4	H	702	TRT	C2-C1-C5-C6
4	B	702	TRT	C3-C1-C5-C6
4	E	702	TRT	C2-C1-C5-C6

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
4	D	702	TRT	C3-C1-C5-C6
4	F	702	TRT	C2-C1-C5-C6
4	G	702	TRT	C2-C1-C5-C6
4	B	702	TRT	C4-C1-C5-C6
4	D	702	TRT	C4-C1-C5-C6
4	A	702	TRT	C3-C1-C5-C6
4	A	702	TRT	C4-C1-C5-C6
4	H	702	TRT	C3-C1-C5-C6
4	C	702	TRT	C4-C1-C5-C6
4	H	702	TRT	C4-C1-C5-C6
4	E	702	TRT	C4-C1-C5-C6
4	B	702	TRT	C11-C12-O15-C16
4	C	702	TRT	C3-C1-C5-C6
4	E	702	TRT	C3-C1-C5-C6
4	F	702	TRT	C4-C1-C5-C6
4	B	702	TRT	C13-C12-O15-C16
4	F	702	TRT	C3-C1-C5-C6
4	E	702	TRT	C20-C19-O18-C17
4	G	702	TRT	C4-C1-C5-C6
4	D	702	TRT	C17-C16-O15-C12
4	C	702	TRT	C20-C19-O18-C17
4	A	702	TRT	C20-C19-O18-C17
4	F	702	TRT	C20-C19-O18-C17
4	G	702	TRT	C3-C1-C5-C6
4	F	702	TRT	C17-C16-O15-C12
4	D	702	TRT	O15-C16-C17-O18
4	B	702	TRT	C20-C19-O18-C17
4	G	702	TRT	C20-C19-O18-C17
4	H	702	TRT	C20-C19-O18-C17
4	D	702	TRT	C20-C19-O18-C17
4	A	702	TRT	C16-C17-O18-C19
4	B	702	TRT	C16-C17-O18-C19

There are no ring outliers.

9 monomers are involved in 23 short contacts:

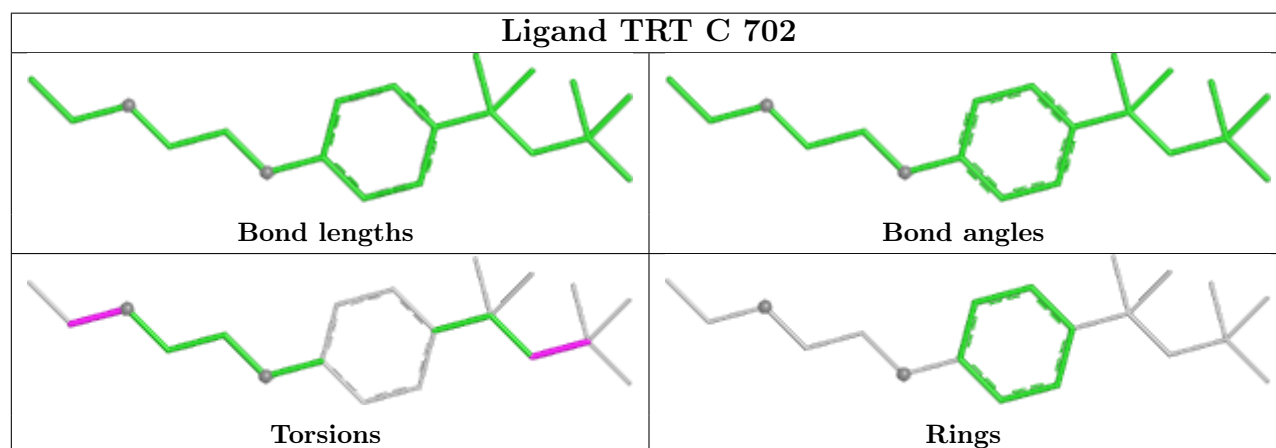
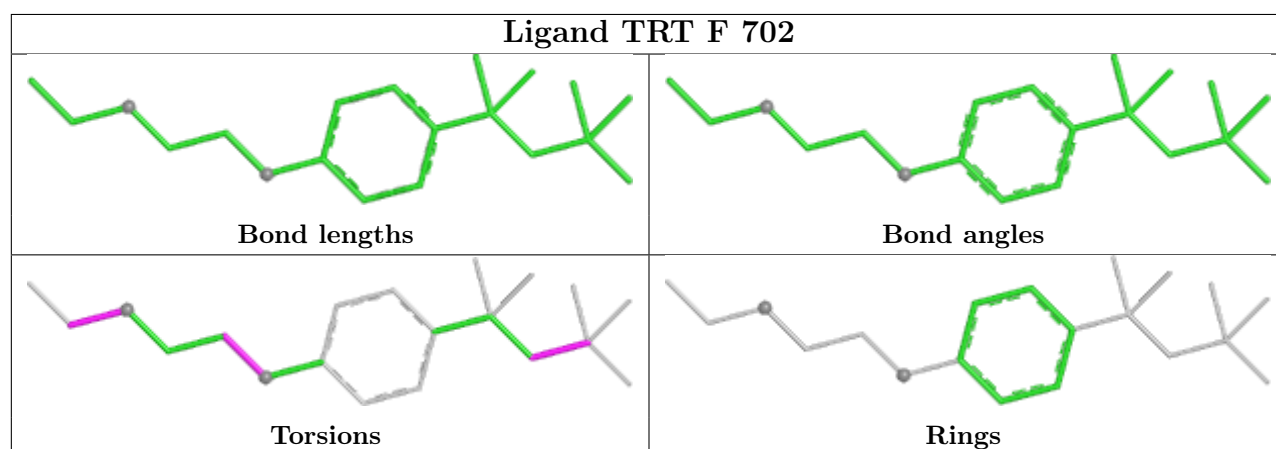
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	F	702	TRT	4	0
4	C	702	TRT	2	0
4	H	702	TRT	4	0
4	A	702	TRT	3	0
5	F	703	A1BYH	1	0

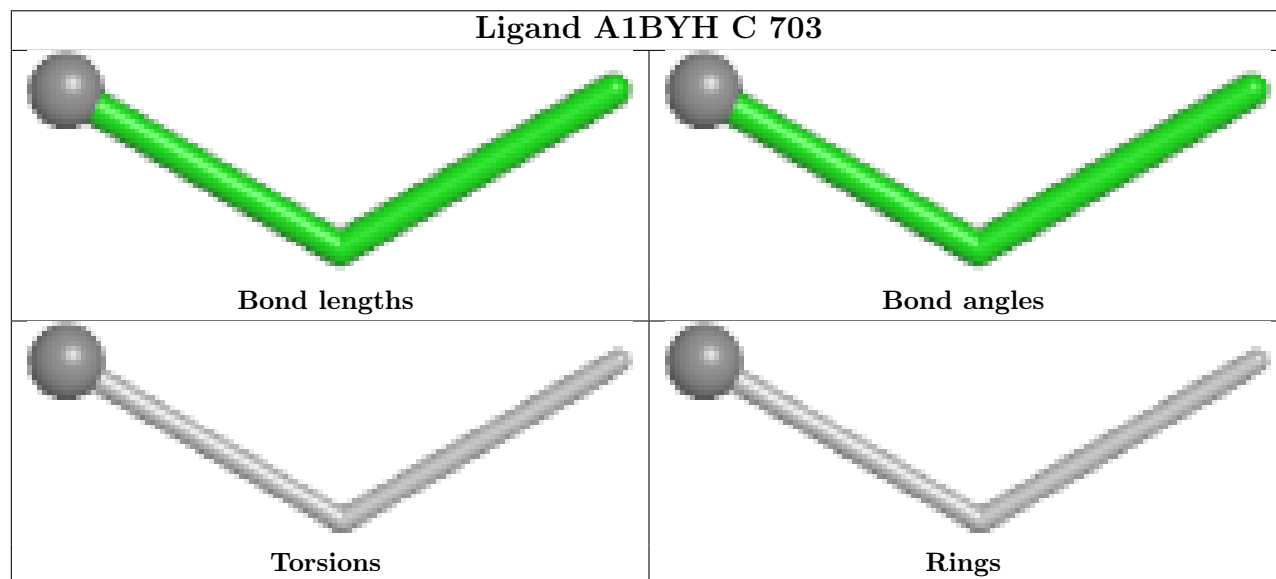
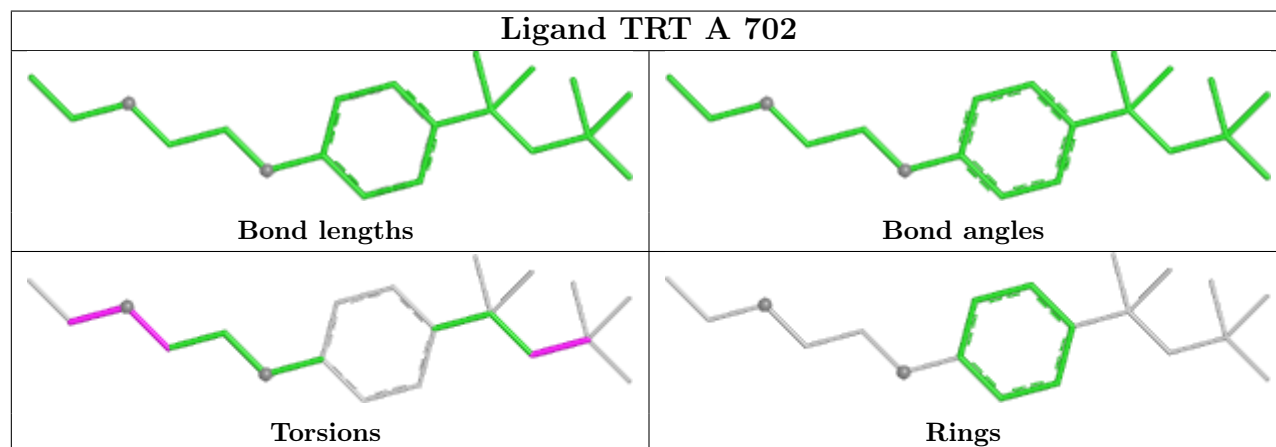
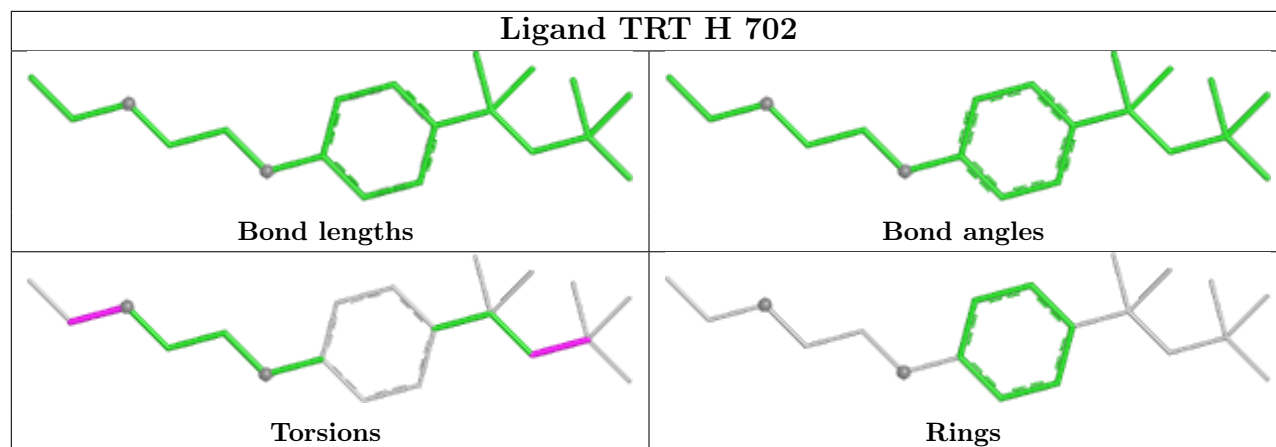
*Continued on next page...*

Continued from previous page...

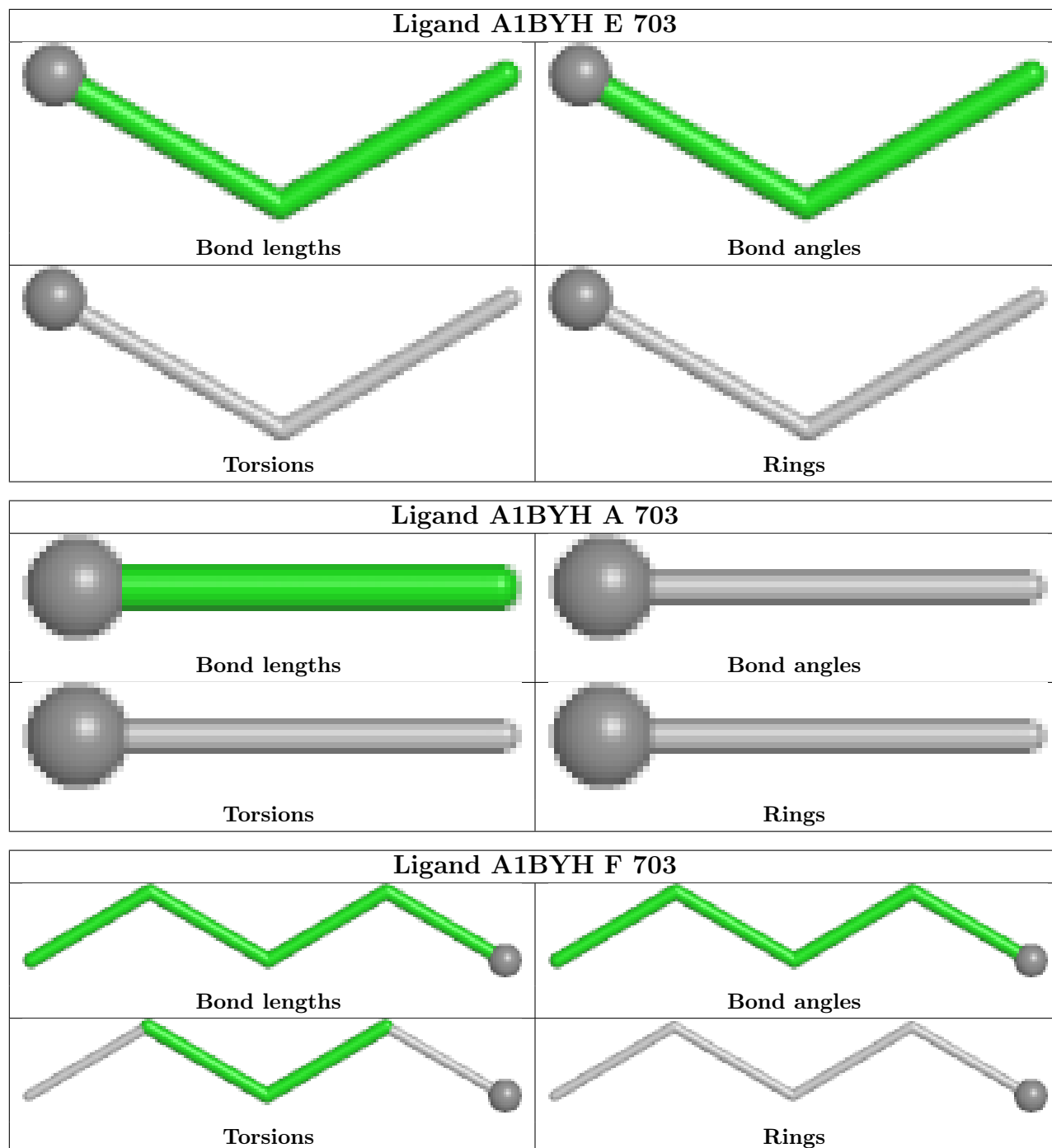
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	G	702	TRT	2	0
4	D	702	TRT	1	0
4	B	702	TRT	2	0
4	E	702	TRT	4	0

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.

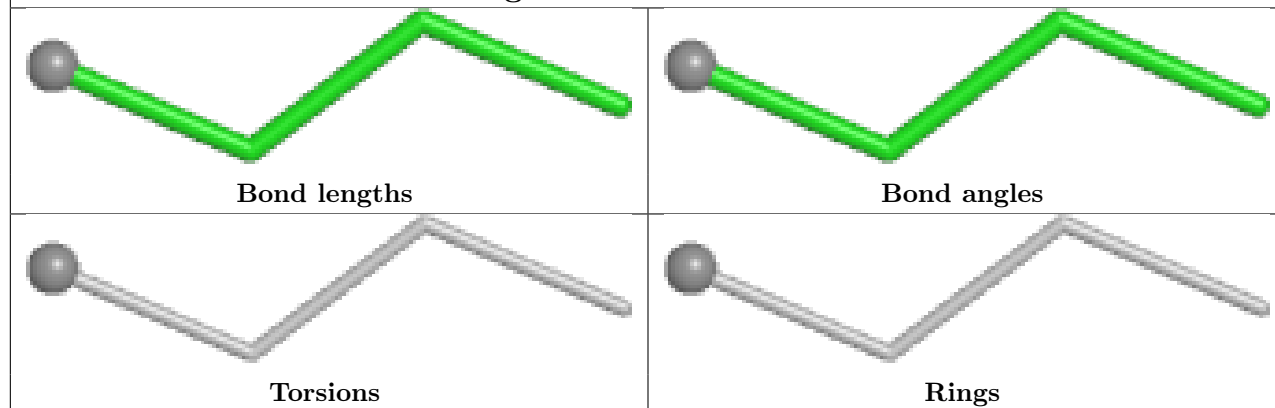




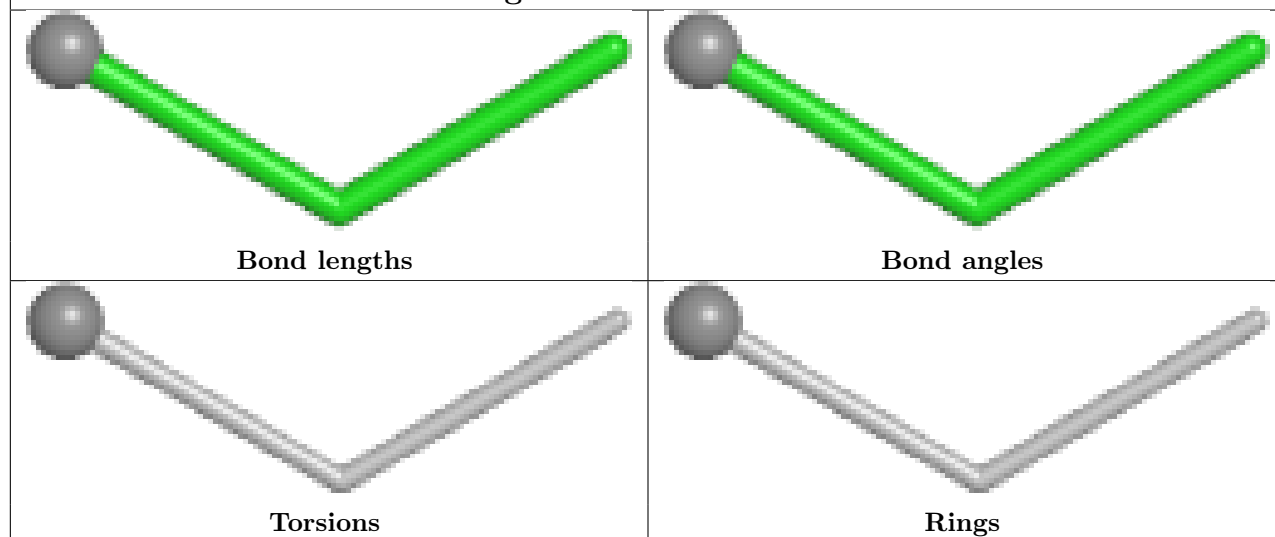




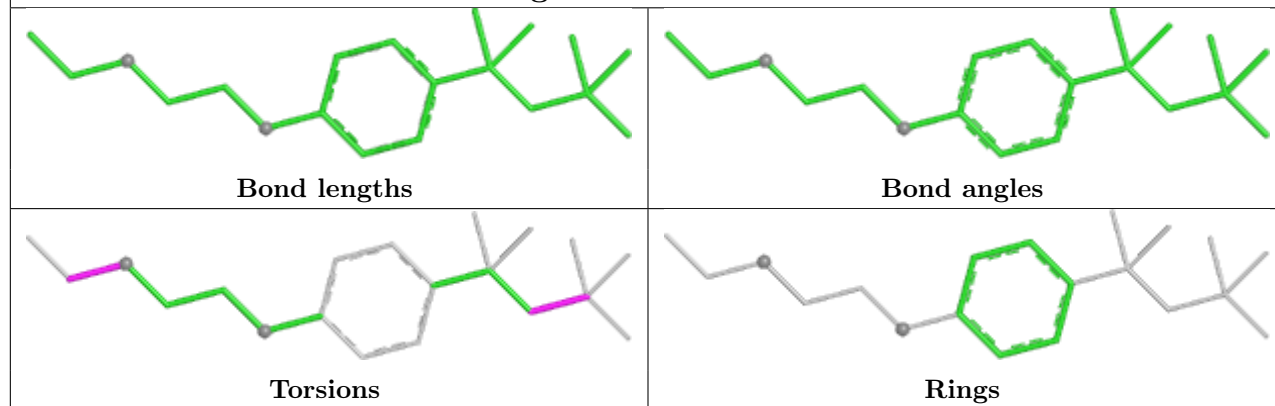
## Ligand A1BYH G 703

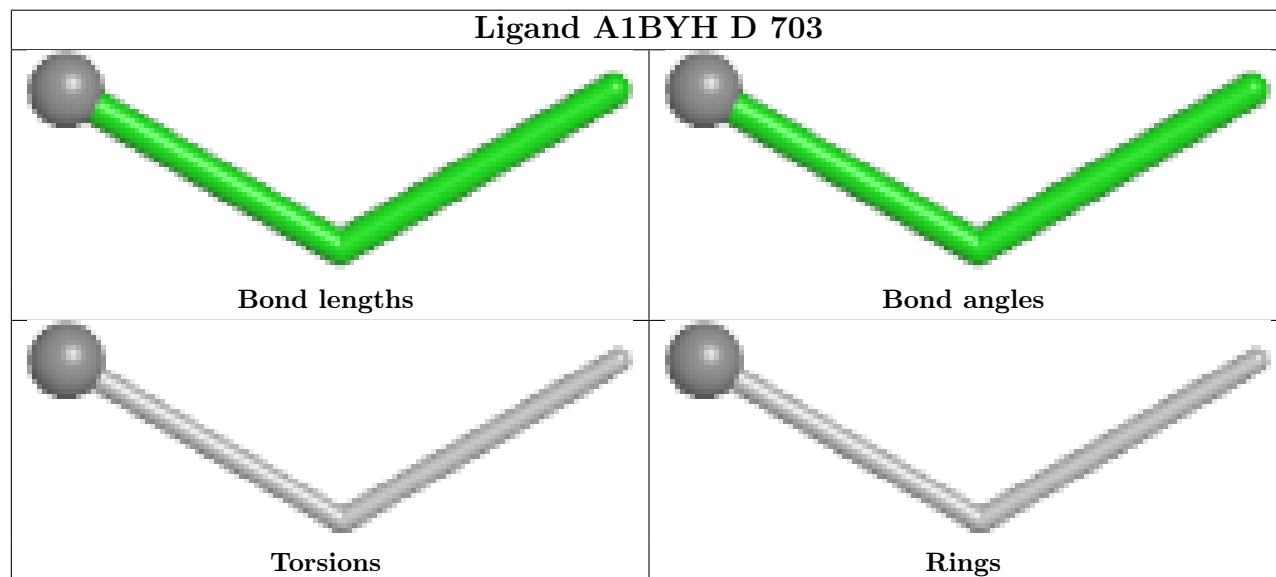
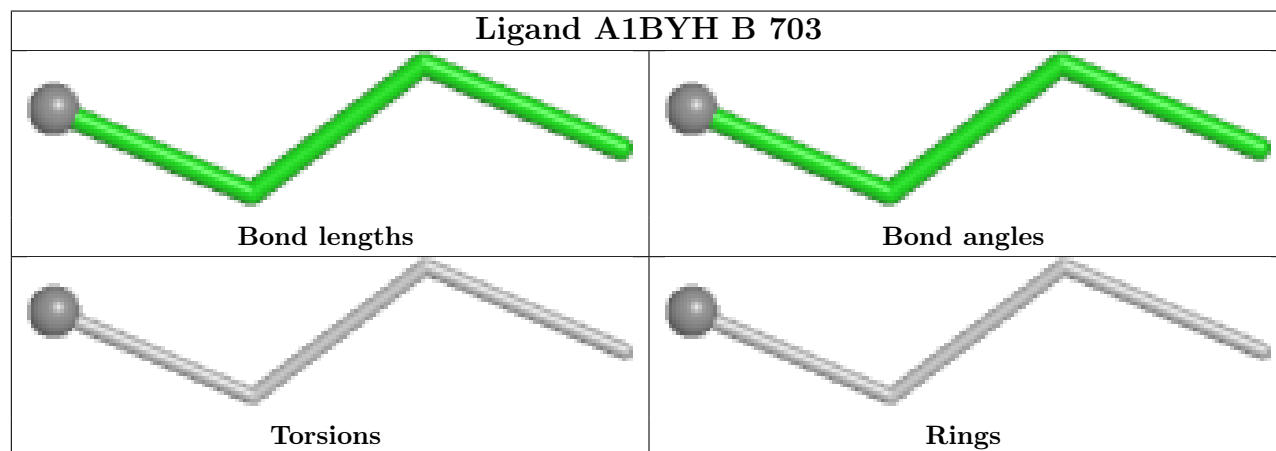
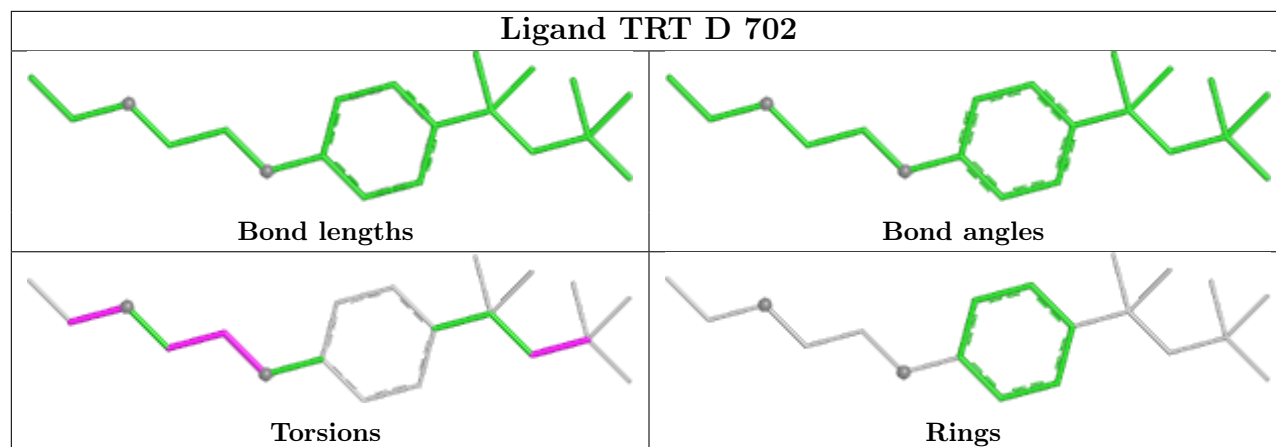


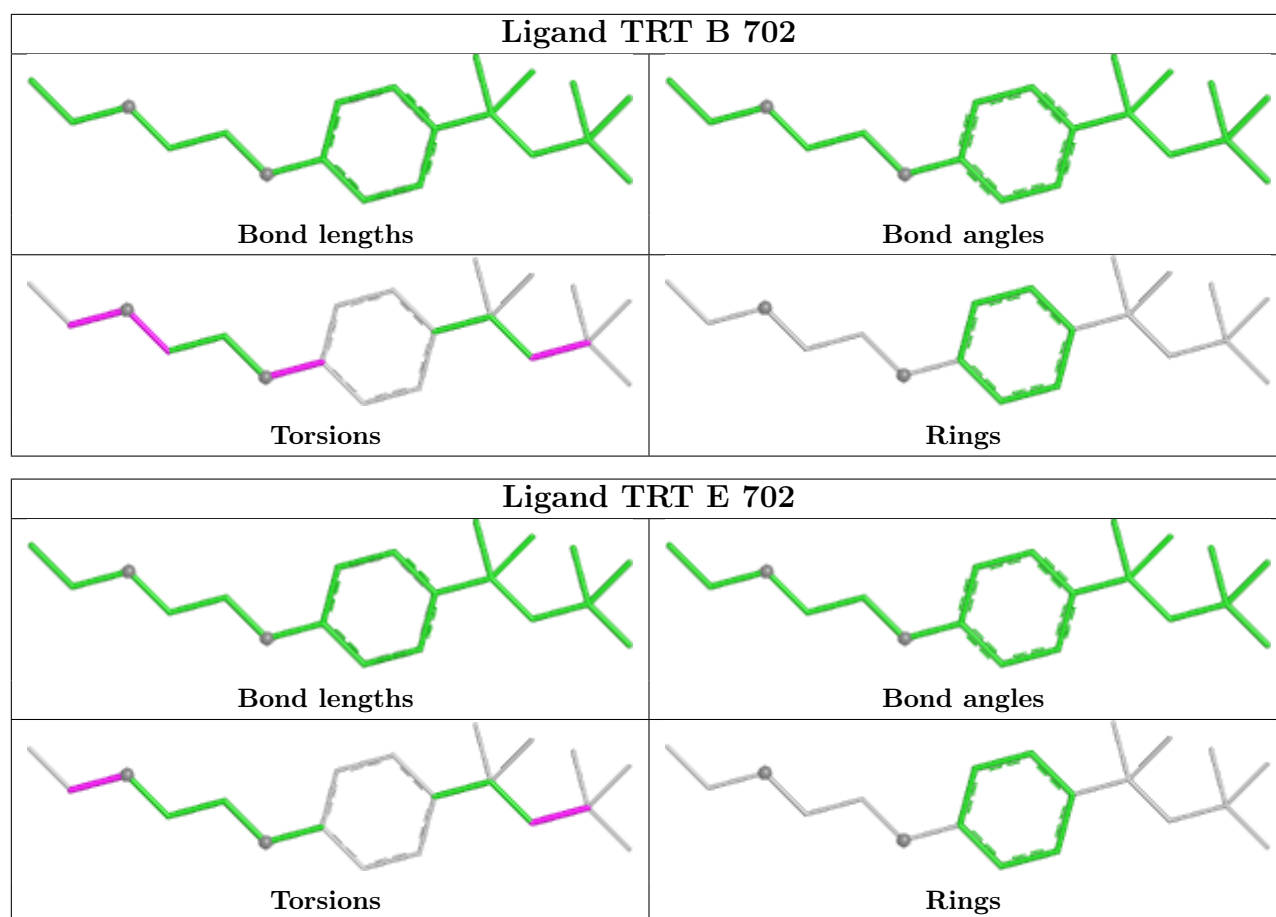
## Ligand A1BYH H 703



## Ligand TRT G 702







## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	626/666 (93%)	-0.32	0	100	100	20, 47, 74, 106	1 (0%)
1	B	626/666 (93%)	-0.27	0	100	100	23, 48, 74, 118	1 (0%)
1	C	626/666 (93%)	-0.23	4 (0%)	85	73	20, 50, 79, 116	1 (0%)
1	D	626/666 (93%)	-0.29	1 (0%)	91	85	18, 48, 72, 101	1 (0%)
1	E	626/666 (93%)	-0.34	0	100	100	20, 45, 72, 111	1 (0%)
1	F	626/666 (93%)	-0.36	1 (0%)	91	85	19, 42, 71, 112	1 (0%)
1	G	626/666 (93%)	-0.15	2 (0%)	90	81	19, 56, 82, 118	1 (0%)
1	H	626/666 (93%)	-0.15	1 (0%)	91	85	20, 59, 86, 104	1 (0%)
All	All	5008/5328 (93%)	-0.26	9 (0%)	91	85	18, 49, 78, 118	8 (0%)

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	123	PRO	3.6
1	C	123	PRO	2.8
1	H	357	GLY	2.6
1	G	475	ALA	2.5
1	C	260	ASP	2.3
1	C	527	PRO	2.2
1	F	492	HIS	2.2
1	D	376	PRO	2.0
1	C	411	SER	2.0

### 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

### 6.3 Carbohydrates

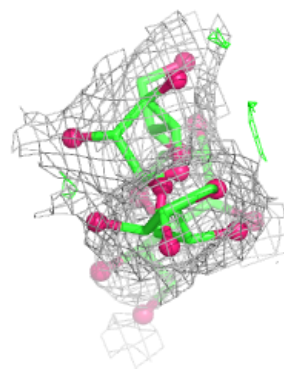
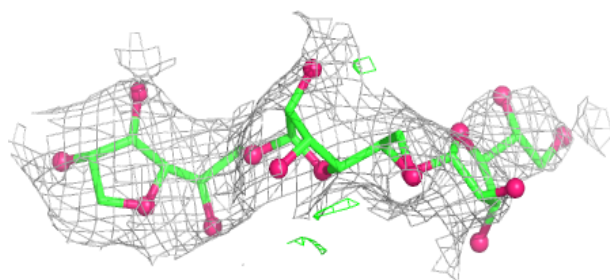
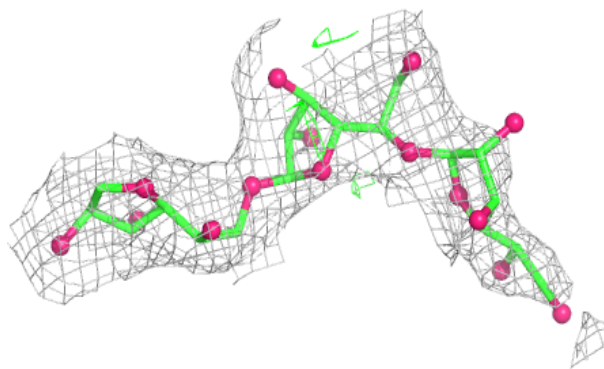
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	GZL	P	3	11/12	0.75	0.15	56,80,103,107	0
2	GZL	I	2	11/12	0.76	0.12	45,74,91,95	0
2	GZL	K	2	11/12	0.80	0.12	68,78,92,93	0
2	GZL	M	3	11/12	0.83	0.13	47,71,101,102	0
2	GZL	N	2	11/12	0.83	0.14	51,74,93,98	0
2	GZL	M	2	11/12	0.83	0.15	55,70,98,100	0
2	GZL	J	3	11/12	0.84	0.15	63,73,90,105	0
2	GZL	N	3	11/12	0.84	0.14	66,75,98,102	0
2	GZL	P	2	11/12	0.84	0.14	68,85,101,108	0
2	GZL	J	2	11/12	0.84	0.12	62,78,93,96	0
2	GZL	O	2	11/12	0.85	0.10	68,78,92,105	0
2	GZL	O	3	11/12	0.85	0.17	80,86,102,108	0
2	GZL	K	3	11/12	0.87	0.15	58,73,96,100	0
2	GZL	L	3	11/12	0.89	0.11	57,77,87,89	0
2	GZL	M	1	11/12	0.89	0.11	33,41,57,59	0
2	GZL	N	1	11/12	0.89	0.09	32,49,59,64	0
2	GZL	L	2	11/12	0.91	0.13	61,72,87,91	0
2	GZL	P	1	11/12	0.91	0.08	66,76,81,81	0
2	GZL	I	3	11/12	0.92	0.12	52,75,94,98	0
2	GZL	I	1	11/12	0.93	0.09	33,53,64,75	0
2	GZL	O	1	11/12	0.94	0.08	50,63,70,74	0
2	GZL	K	1	11/12	0.94	0.07	43,50,66,68	0
2	GZL	J	1	11/12	0.95	0.07	37,47,66,68	0
2	GZL	L	1	11/12	0.95	0.08	46,50,61,64	0

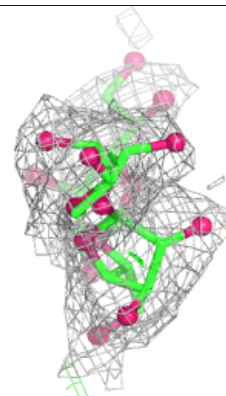
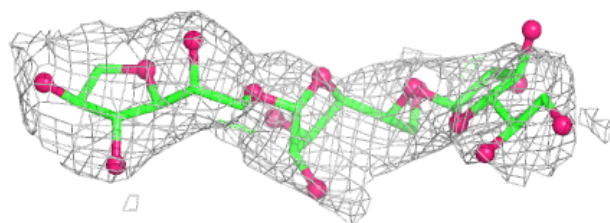
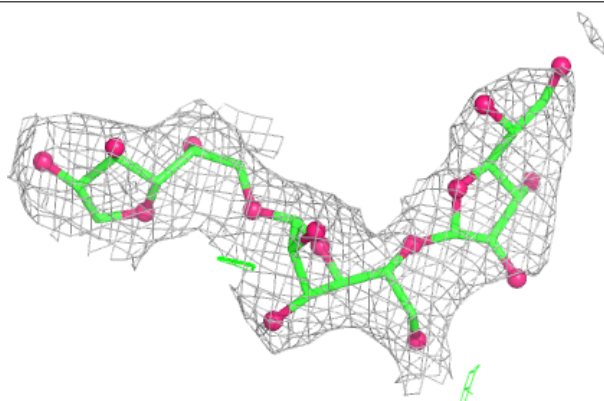
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

**Electron density around Chain I:**

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

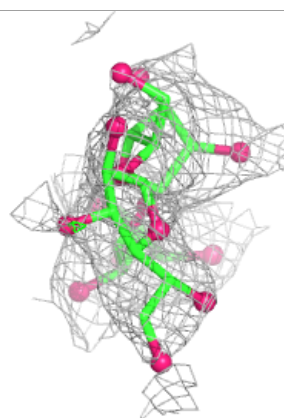
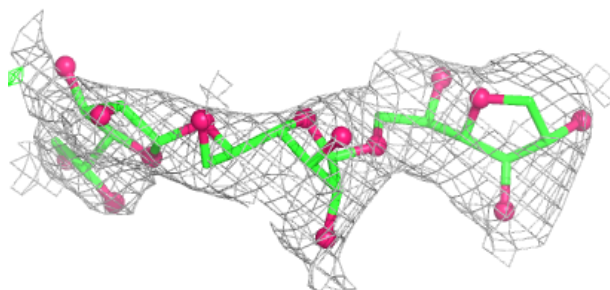
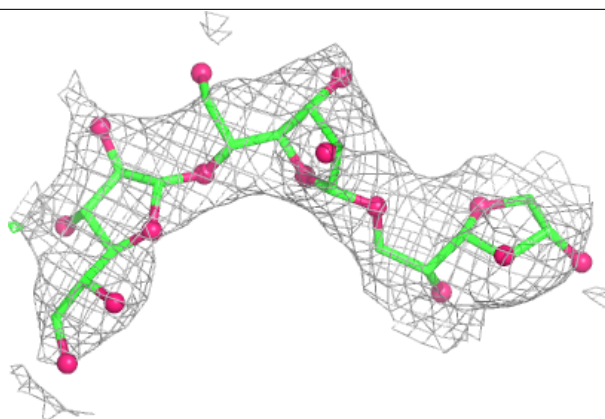
**Electron density around Chain J:**

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

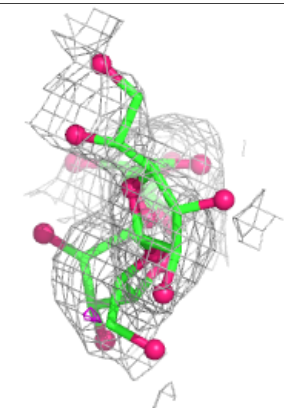
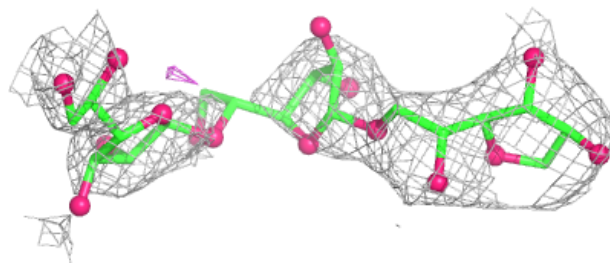
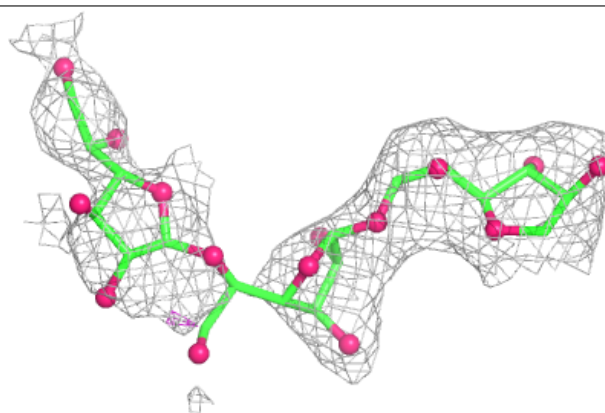


**Electron density around Chain K:**

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

**Electron density around Chain L:**

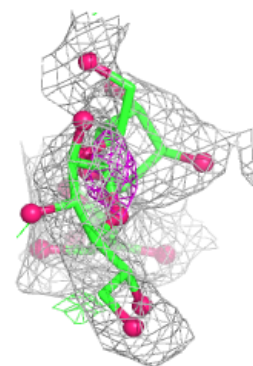
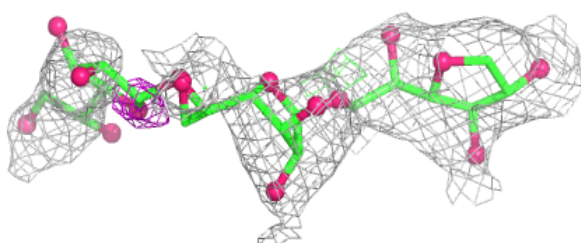
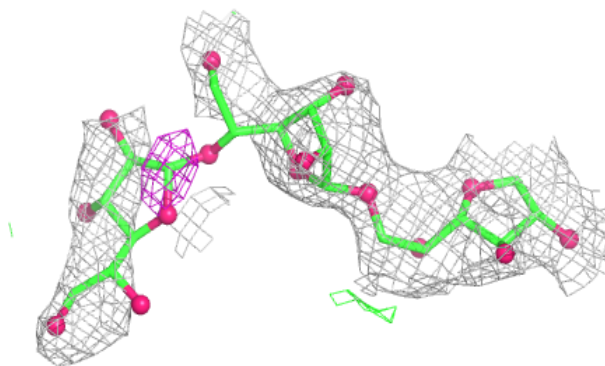
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



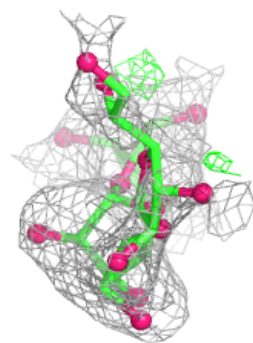
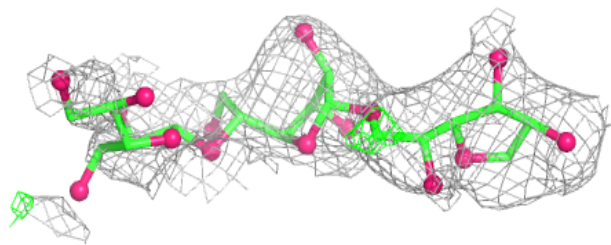
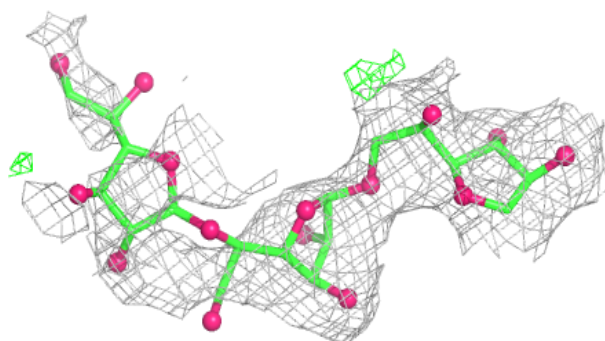


**Electron density around Chain M:**

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

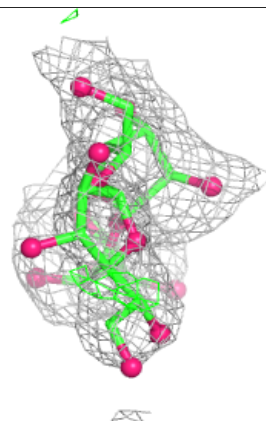
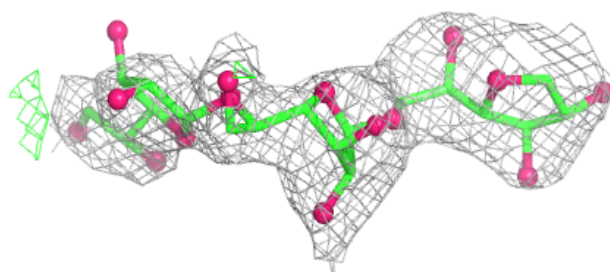
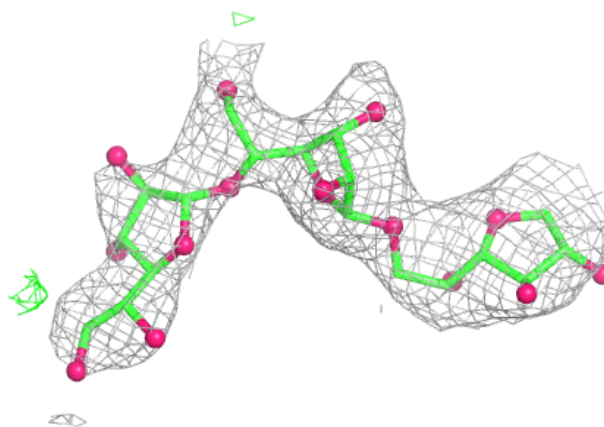
**Electron density around Chain N:**

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

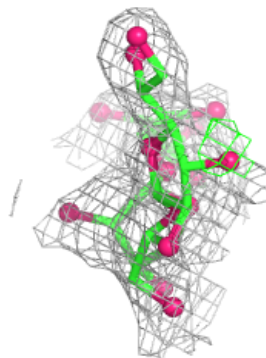
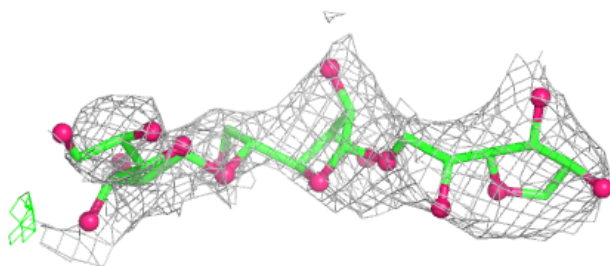
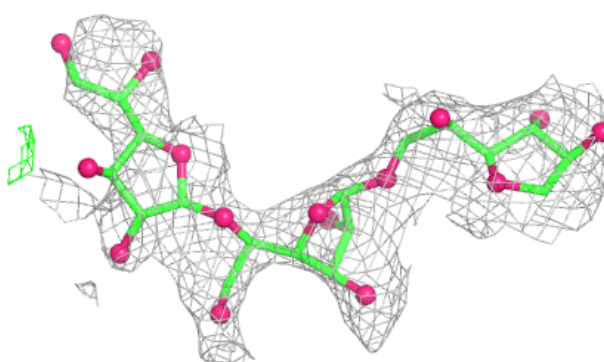


**Electron density around Chain O:**

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

**Electron density around Chain P:**

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



## 6.4 Ligands ⓘ

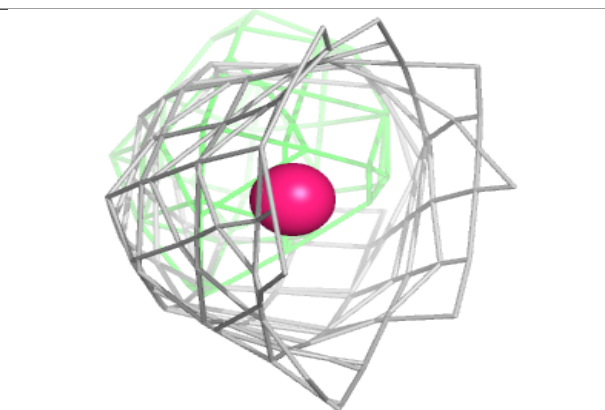
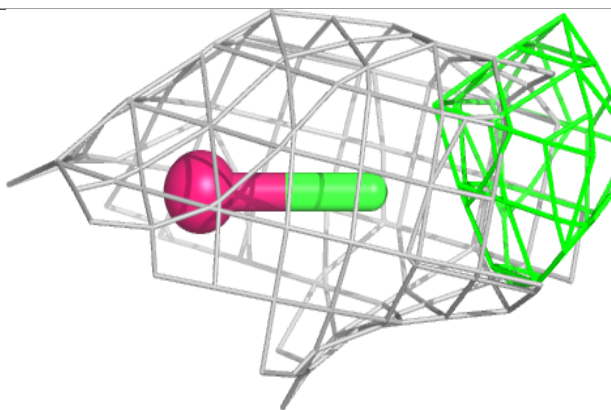
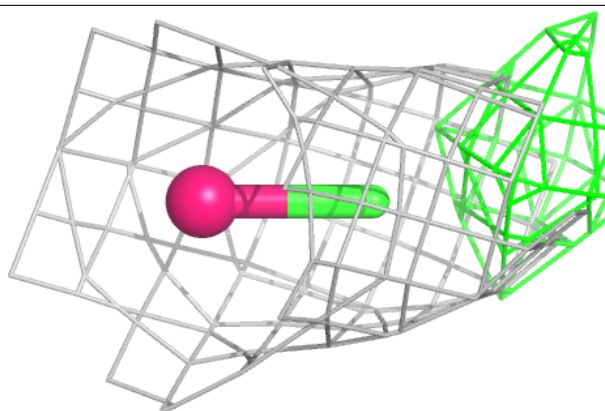
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
5	A1BYH	A	703	2/20	0.60	0.18	41,41,41,70	0
3	MG	G	701	1/1	0.63	0.13	51,51,51,51	0
4	TRT	G	702	20/25	0.72	0.25	80,89,107,119	0
3	MG	H	701	1/1	0.74	0.12	52,52,52,52	0
4	TRT	C	702	20/25	0.75	0.23	66,90,105,109	0
4	TRT	H	702	20/25	0.78	0.23	88,102,116,125	0
4	TRT	E	702	20/25	0.79	0.20	59,84,97,97	0
3	MG	A	701	1/1	0.80	0.10	56,56,56,56	0
4	TRT	F	702	20/25	0.81	0.21	72,84,95,95	0
4	TRT	D	702	20/25	0.82	0.19	62,89,100,100	0
4	TRT	A	702	20/25	0.82	0.19	55,96,108,110	0
5	A1BYH	E	703	3/20	0.82	0.18	39,39,43,47	0
5	A1BYH	H	703	3/20	0.82	0.16	36,36,63,71	0
4	TRT	B	702	20/25	0.83	0.20	61,100,105,106	0
3	MG	E	701	1/1	0.86	0.06	55,55,55,55	0
5	A1BYH	D	703	3/20	0.86	0.18	44,44,62,65	0
5	A1BYH	G	703	4/20	0.87	0.13	43,49,71,75	0
3	MG	B	701	1/1	0.87	0.08	48,48,48,48	0
5	A1BYH	F	703	5/20	0.88	0.13	17,30,49,58	0
5	A1BYH	B	703	4/20	0.89	0.11	27,44,48,49	0
5	A1BYH	C	703	3/20	0.90	0.11	48,48,48,59	0
3	MG	C	701	1/1	0.92	0.07	48,48,48,48	0
3	MG	D	701	1/1	0.93	0.05	40,40,40,40	0
3	MG	F	701	1/1	0.94	0.05	43,43,43,43	0

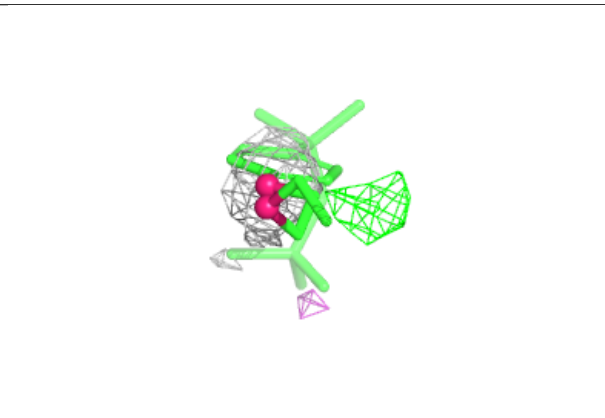
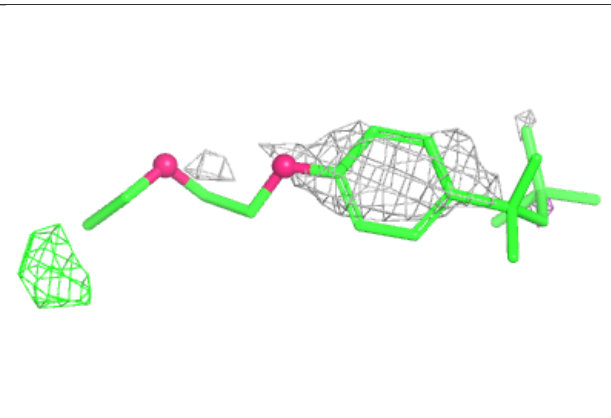
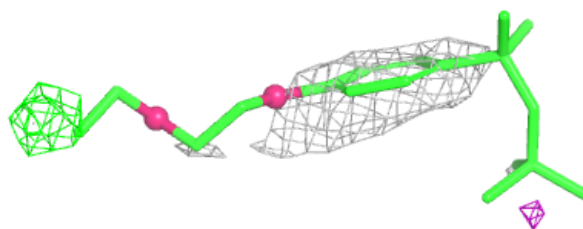
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around A1BYH A 703:**

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

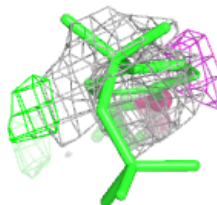
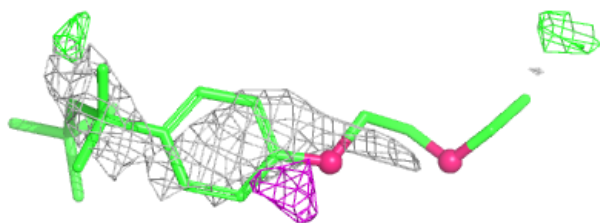
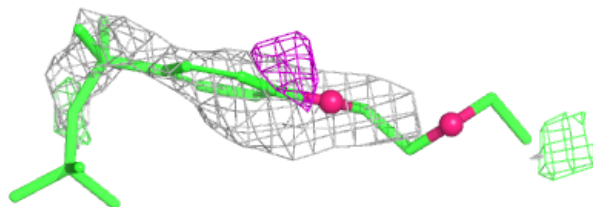
**Electron density around TRT G 702:**

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

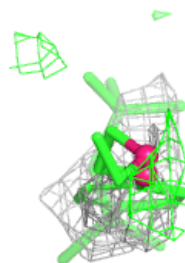
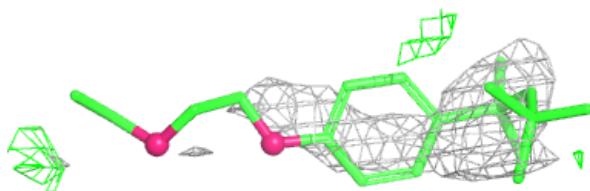
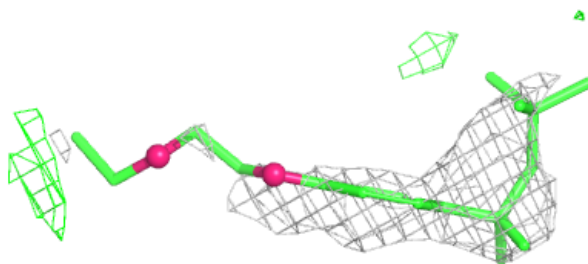


**Electron density around TRT C 702:**

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

**Electron density around TRT H 702:**

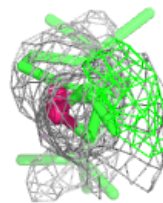
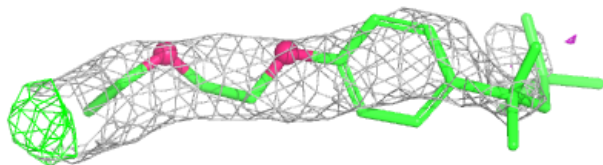
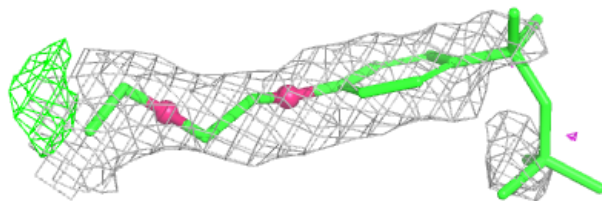
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



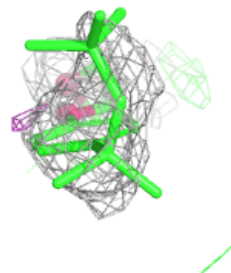
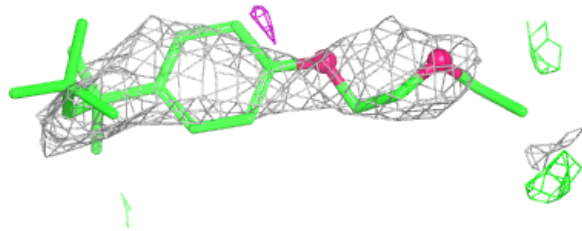
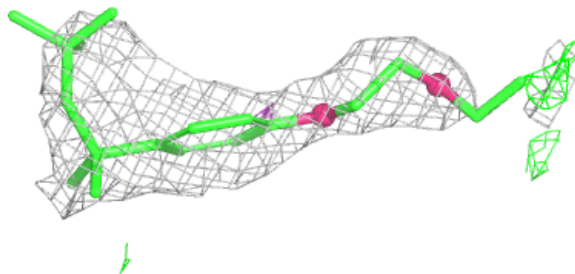


**Electron density around TRT E 702:**

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

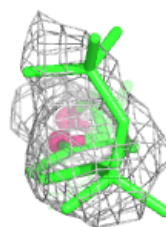
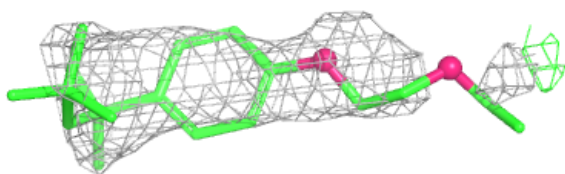
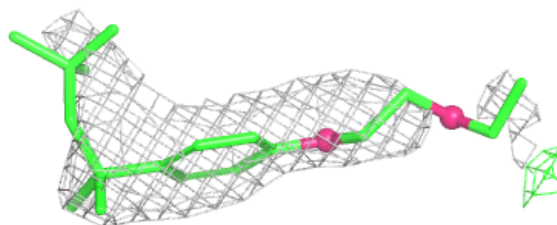
**Electron density around TRT F 702:**

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

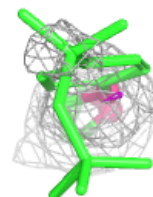
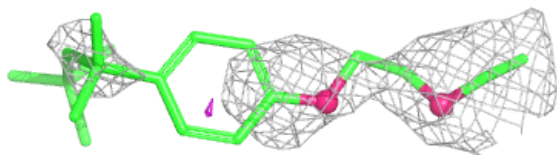
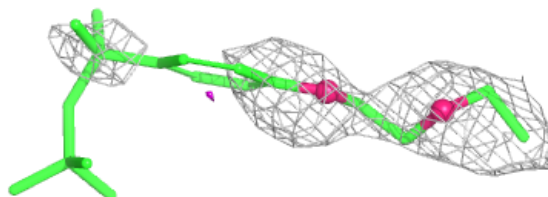


**Electron density around TRT D 702:**

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

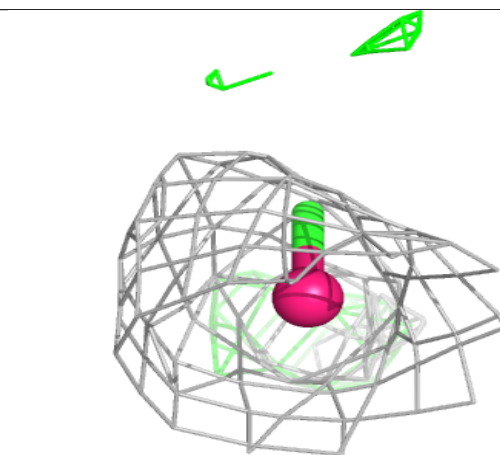
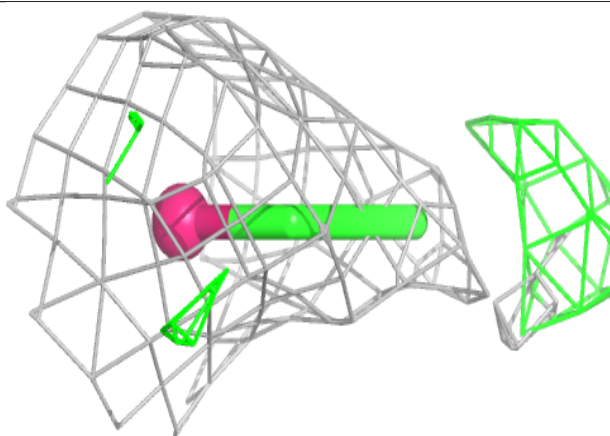
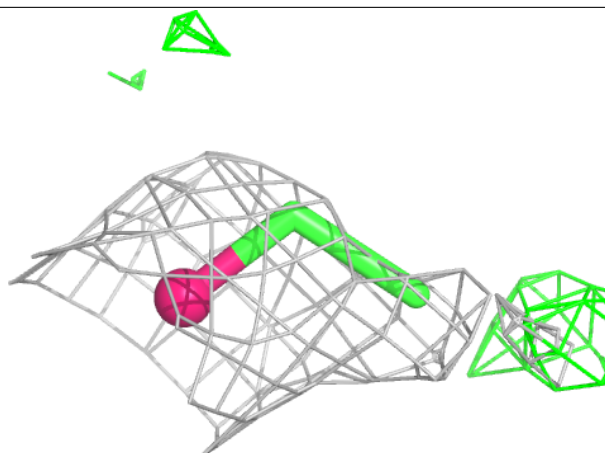
**Electron density around TRT A 702:**

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



**Electron density around A1BYH E 703:**

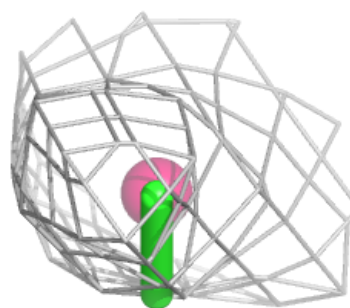
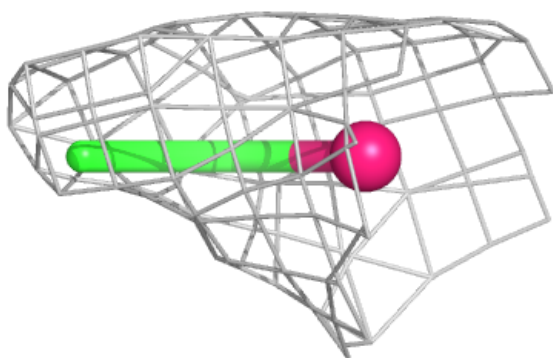
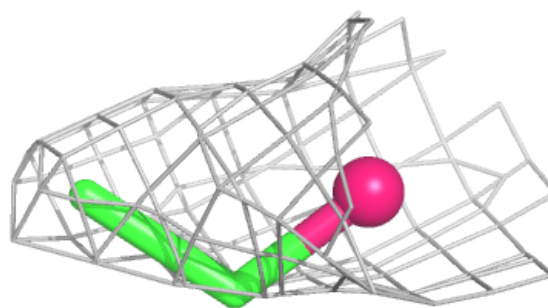
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



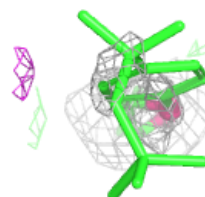
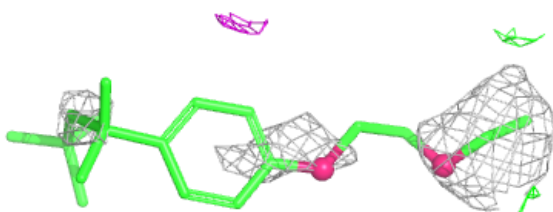
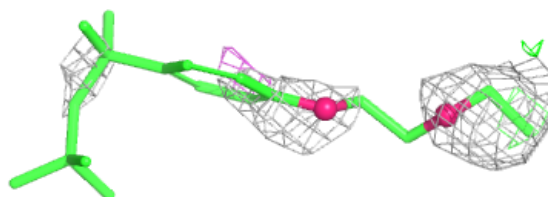


**Electron density around A1BYH H 703:**

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

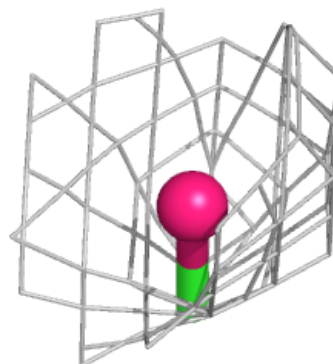
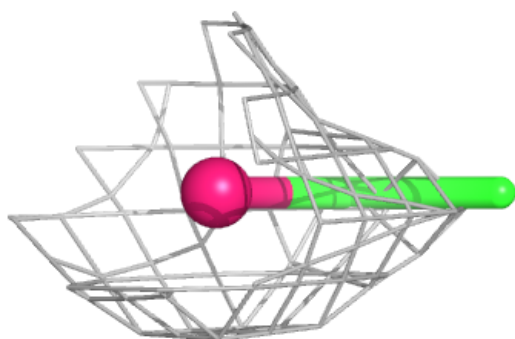
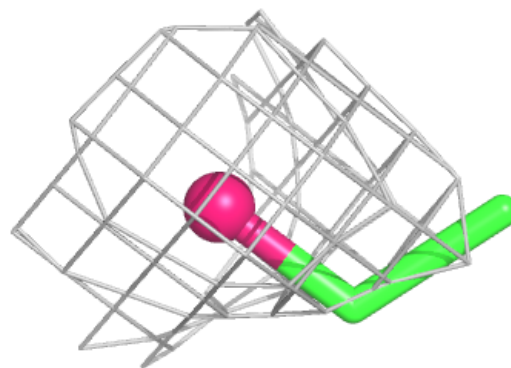
**Electron density around TRT B 702:**

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

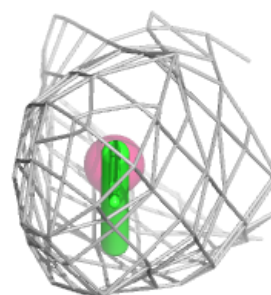
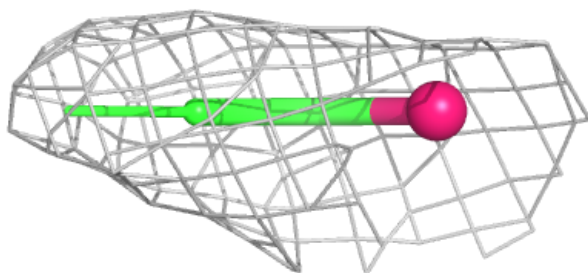
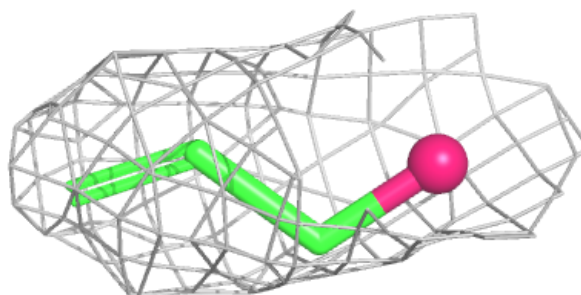


**Electron density around A1BYH D 703:**

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

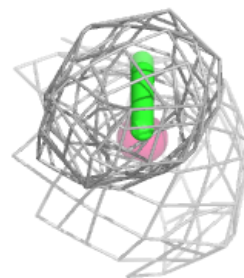
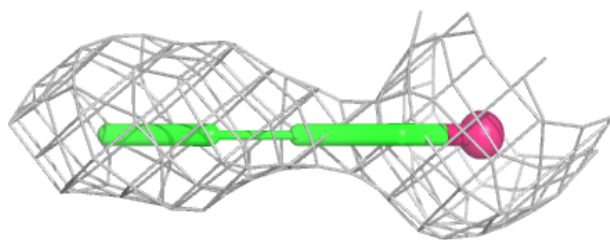
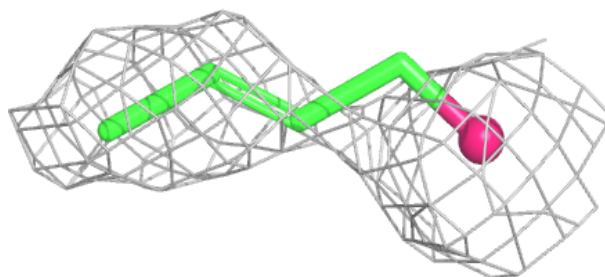
**Electron density around A1BYH G 703:**

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

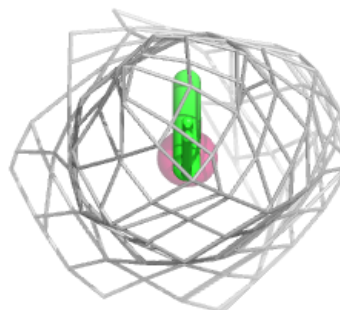
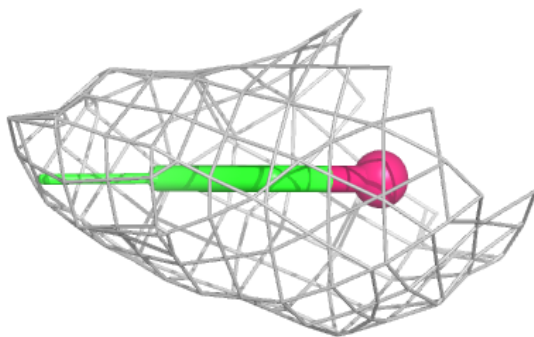
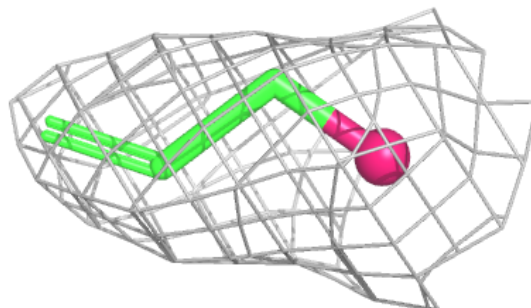


**Electron density around A1BYH F 703:**

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

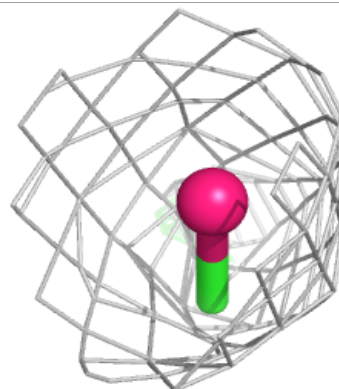
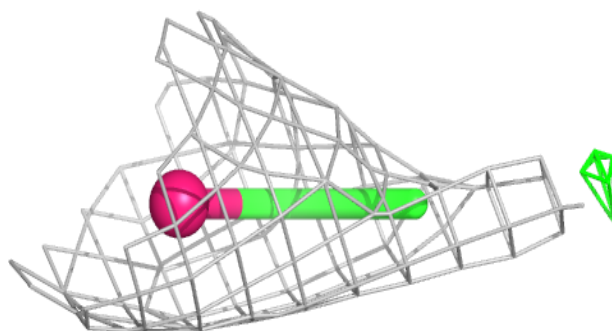
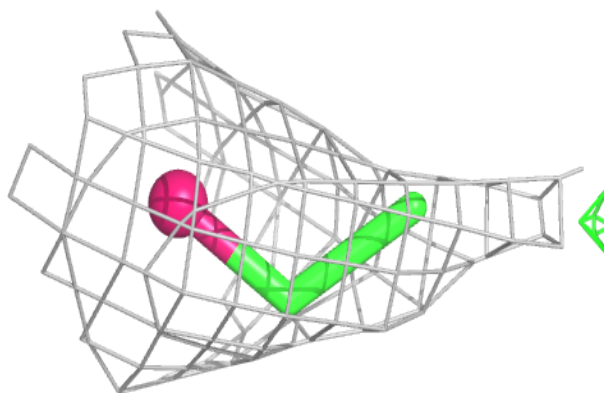
**Electron density around A1BYH B 703:**

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



**Electron density around A1BYH C 703:**

$2mF_o-DF_c$  (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.