



# Full wwPDB X-ray Structure Validation Report ⓘ

Sep 29, 2025 – 01:02 PM EDT

PDB ID : 9DTP / pdb\_00009dtp  
Title : GlfT2 from Nocardia brasiliensis  
Authors : Carter, A.W.; Dodge, G.J.; Kiessling, L.L.  
Deposited on : 2024-10-01  
Resolution : 3.11 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>.

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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 : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
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) : 2.46

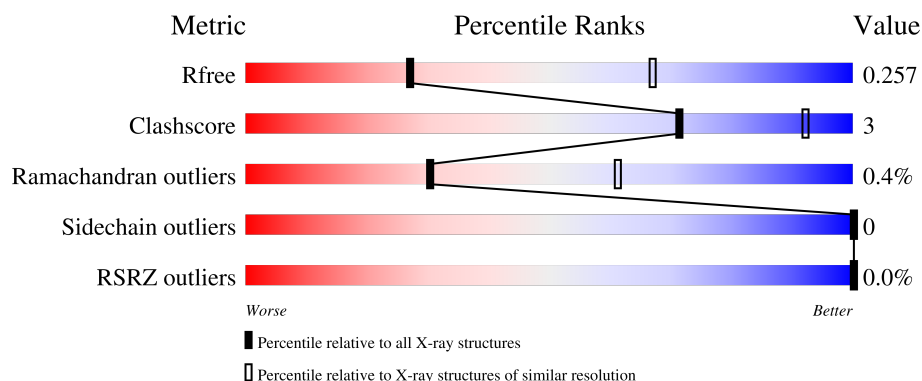
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*




The reported resolution of this entry is 3.11 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))
$R_{free}$	164625	1668 (3.14-3.10)
Clashscore	180529	1788 (3.14-3.10)
Ramachandran outliers	177936	1696 (3.14-3.10)
Sidechain outliers	177891	1696 (3.14-3.10)
RSRZ outliers	164620	1668 (3.14-3.10)

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	
1	B	666	
1	C	666	
1	D	666	
1	E	666	

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Mol	Chain	Length	Quality of chain
1	F	666	 84% 9% 6%
1	G	666	 84% 9% 6%
1	H	666	 84% 9% 6%

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 39330 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	624	Total	C	N	O	S	0	1	0
			4885	3105	876	889	15			
1	B	624	Total	C	N	O	S	0	1	0
			4885	3105	876	889	15			
1	C	623	Total	C	N	O	S	0	1	0
			4881	3103	875	888	15			
1	D	624	Total	C	N	O	S	0	1	0
			4885	3105	876	889	15			
1	E	624	Total	C	N	O	S	0	1	0
			4885	3105	876	889	15			
1	F	623	Total	C	N	O	S	0	1	0
			4881	3103	875	888	15			
1	G	623	Total	C	N	O	S	0	1	0
			4881	3103	875	888	15			
1	H	624	Total	C	N	O	S	0	1	0
			4885	3105	876	889	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

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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

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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

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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

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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

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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 MAGNESIUM ION (CCD ID: MG) (formula: Mg).

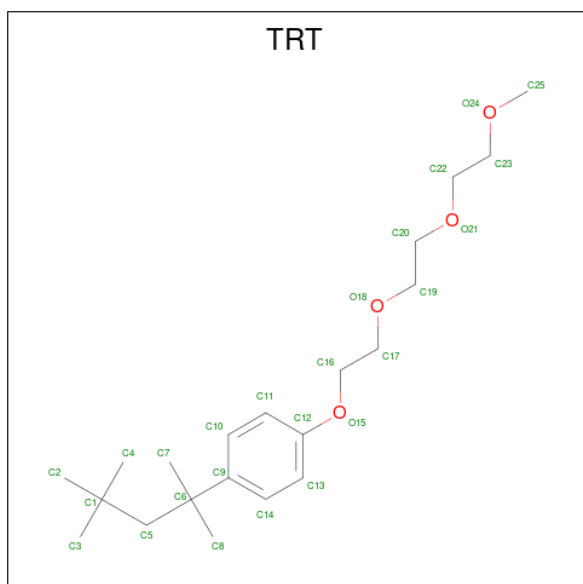
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Mg 1 1	0	0
2	B	1	Total Mg 1 1	0	0

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

- Molecule 3 is FRAGMENT OF TRITON X-100 (CCD ID: TRT) (formula:  $C_{21}H_{36}O_4$ ).



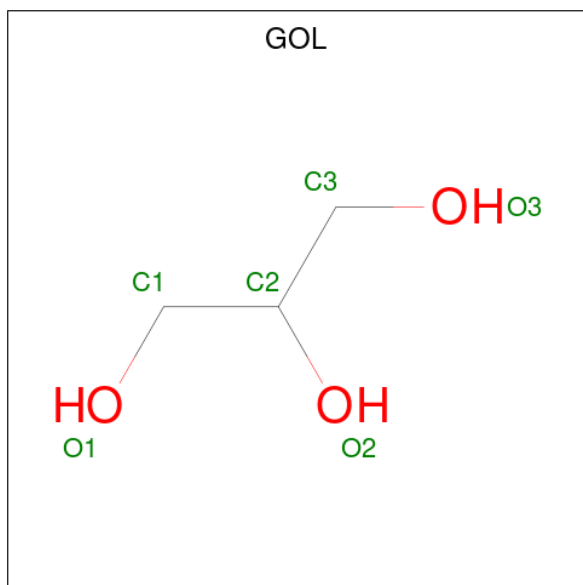
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			23	20	3		
3	B	1	Total	C	O	0	0
			23	20	3		
3	C	1	Total	C	O	0	0
			20	18	2		
3	D	1	Total	C	O	0	0
			21	18	3		
3	E	1	Total	C	O	0	0
			19	17	2		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	F	1	Total	C	O	0	0
			18	16	2		
3	G	1	Total	C	O	0	0
			17	16	1		
3	H	1	Total	C	O	0	0
			23	20	3		

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula:  $C_3H_8O_3$ ).



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

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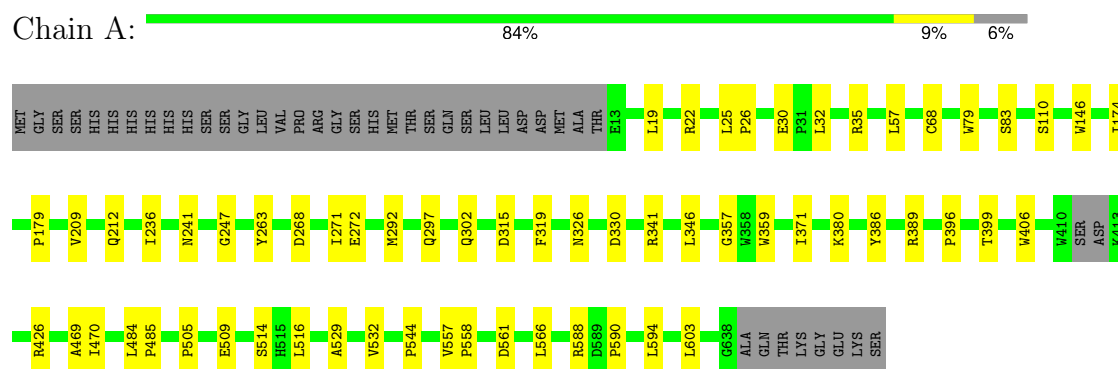
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	E	1	Total	C	O	0	0
			6	3	3		
4	E	1	Total	C	O	0	0
			6	3	3		
4	F	1	Total	C	O	0	0
			6	3	3		
4	F	1	Total	C	O	0	0
			6	3	3		
4	G	1	Total	C	O	0	0
			6	3	3		
4	H	1	Total	C	O	0	0
			6	3	3		
4	H	1	Total	C	O	0	0
			6	3	3		

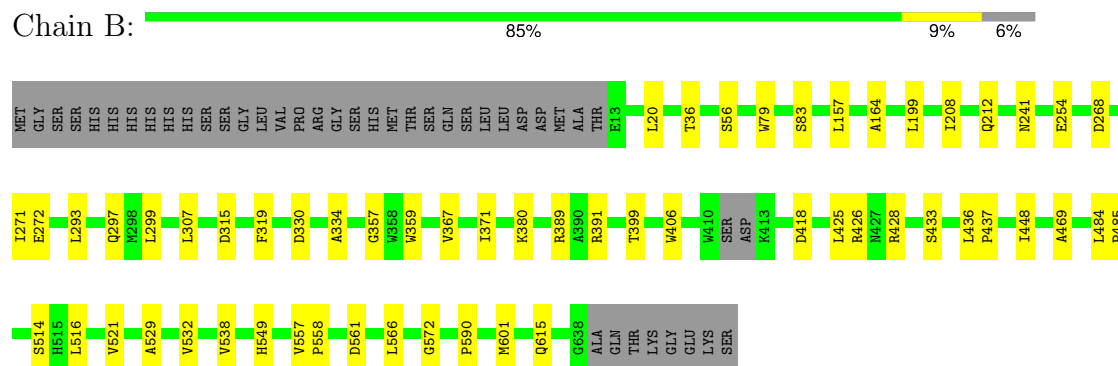
### 3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

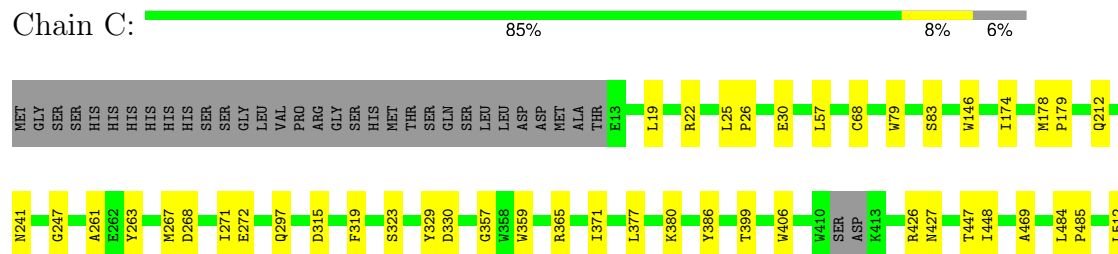
#### • Molecule 1: Galactofuranosyltransferase

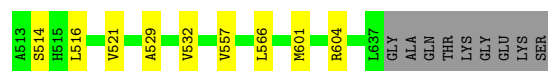


#### • Molecule 1: Galactofuranosyltransferase



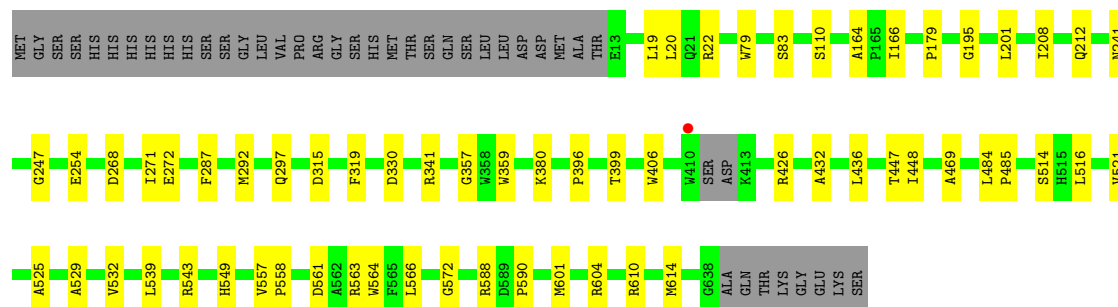
#### • Molecule 1: Galactofuranosyltransferase





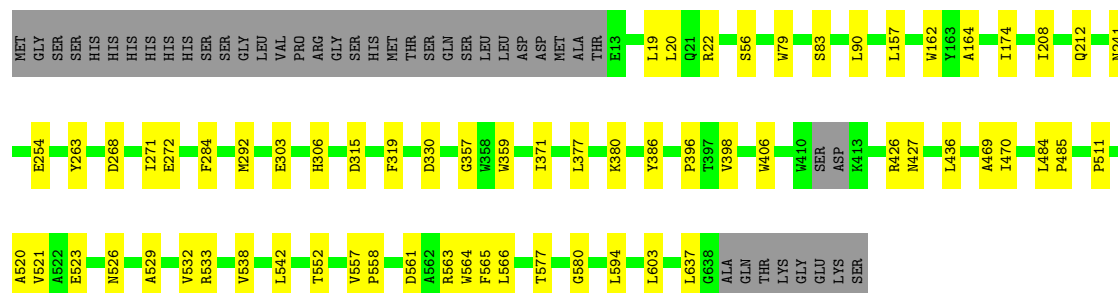
• Molecule 1: Galactofuranosyltransferase

Chain D: 84% 9% 6%



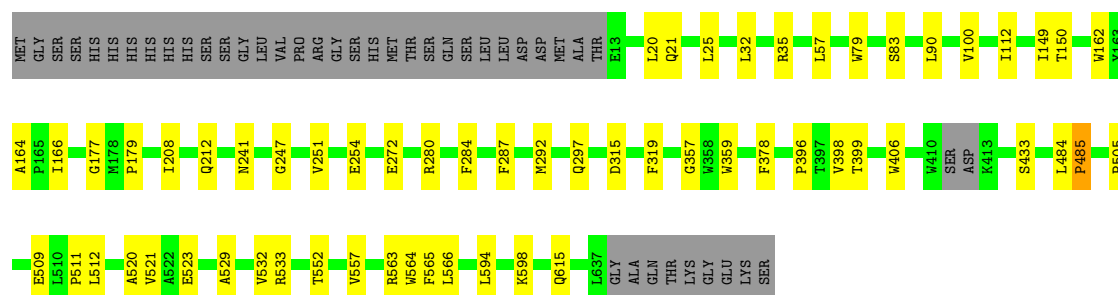
• Molecule 1: Galactofuranosyltransferase

Chain E: 84% 10% 6%



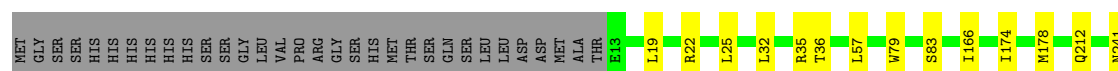
• Molecule 1: Galactofuranosyltransferase

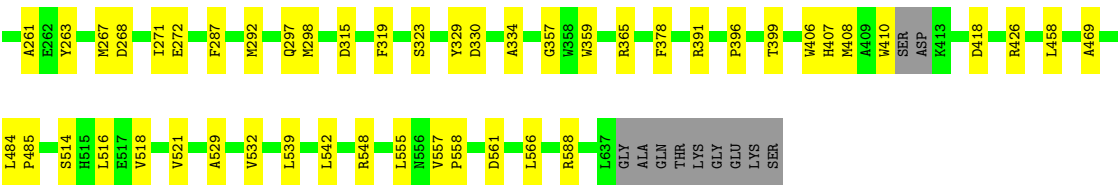
Chain F: 84% 9% 6%



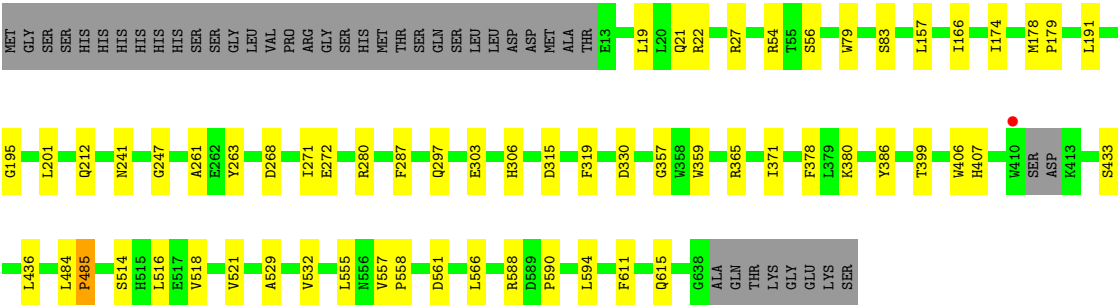
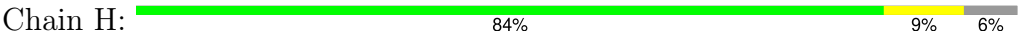
• Molecule 1: Galactofuranosyltransferase

Chain G: 84% 9% 6%





• Molecule 1: Galactofuranosyltransferase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	107.03Å 205.04Å 295.32Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.05 – 3.11 20.05 – 3.11	Depositor EDS
% Data completeness (in resolution range)	94.9 (20.05-3.11) 94.3 (20.05-3.11)	Depositor EDS
$R_{merge}$	0.26	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.12 (at 3.09Å)	Xtrriage
Refinement program	PHENIX 1.21.2_5419	Depositor
R, $R_{free}$	0.221 , 0.258 0.221 , 0.257	Depositor DCC
$R_{free}$ test set	1977 reflections (1.69%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	66.5	Xtrriage
Anisotropy	0.274	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 38.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.44$ , $\langle L^2 \rangle = 0.26$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	39330	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	64.0	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 35.03 % 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 6.2164e-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: GOL, TRT, MG

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	0.08	0/5005	0.23	0/6814
1	B	0.08	0/5005	0.24	0/6814
1	C	0.08	0/5001	0.23	0/6809
1	D	0.08	0/5005	0.24	0/6814
1	E	0.08	0/5005	0.24	0/6814
1	F	0.08	0/5001	0.24	0/6809
1	G	0.08	0/5001	0.23	0/6809
1	H	0.08	0/5005	0.23	0/6814
All	All	0.08	0/40028	0.23	0/54497

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	4885	0	4849	34	0
1	B	4885	0	4849	31	0
1	C	4881	0	4846	27	0
1	D	4885	0	4849	31	0
1	E	4885	0	4849	34	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	4881	0	4846	33	0
1	G	4881	0	4846	32	0
1	H	4885	0	4849	32	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
2	G	1	0	0	0	0
2	H	1	0	0	0	0
3	A	23	0	31	1	0
3	B	23	0	31	2	0
3	C	20	0	27	0	0
3	D	21	0	29	0	0
3	E	19	0	25	1	0
3	F	18	0	25	2	0
3	G	17	0	23	0	0
3	H	23	0	31	1	0
4	A	12	0	16	0	0
4	B	12	0	16	0	0
4	C	12	0	16	0	0
4	D	12	0	16	0	0
4	E	12	0	16	0	0
4	F	12	0	16	0	0
4	G	6	0	8	0	0
4	H	12	0	16	0	0
All	All	39330	0	39125	251	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 3.

All (251) 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:B:315:ASP:O	1:B:319:PHE:HA	1.90	0.70
1:F:315:ASP:O	1:F:319:PHE:HA	1.92	0.69
1:E:315:ASP:O	1:E:319:PHE:HA	1.92	0.68
1:H:315:ASP:O	1:H:319:PHE:HA	1.93	0.68
1:C:315:ASP:O	1:C:319:PHE:HA	1.94	0.67
1:G:557:VAL:HG21	1:G:566:LEU:HD21	1.78	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:315:ASP:O	1:A:319:PHE:HA	1.95	0.66
1:C:272:GLU:HB3	1:C:406:TRP:HB2	1.76	0.65
1:F:557:VAL:HG21	1:F:566:LEU:HD21	1.79	0.64
1:E:557:VAL:HG21	1:E:566:LEU:HD21	1.78	0.64
1:A:557:VAL:HG21	1:A:566:LEU:HD21	1.80	0.62
1:A:174:ILE:HG22	1:A:263:TYR:HB2	1.81	0.62
1:H:272:GLU:HB3	1:H:406:TRP:HB2	1.81	0.62
1:D:272:GLU:HB3	1:D:406:TRP:HB2	1.80	0.62
1:H:557:VAL:HG21	1:H:566:LEU:HD21	1.81	0.61
1:D:315:ASP:O	1:D:319:PHE:HA	2.01	0.61
1:G:212:GLN:HB3	1:G:241:ASN:HA	1.83	0.61
1:C:514:SER:HB2	1:C:516:LEU:HD23	1.83	0.60
1:G:315:ASP:O	1:G:319:PHE:HA	2.02	0.60
1:H:514:SER:HB2	1:H:516:LEU:HD23	1.83	0.59
1:B:557:VAL:HG21	1:B:566:LEU:HD21	1.82	0.59
1:E:174:ILE:HG22	1:E:263:TYR:HB2	1.83	0.59
1:A:272:GLU:HB3	1:A:406:TRP:HB2	1.84	0.58
1:E:292:MET:HE3	1:E:396:PRO:HG2	1.85	0.58
1:C:557:VAL:HG21	1:C:566:LEU:HD21	1.85	0.58
1:A:212:GLN:HB3	1:A:241:ASN:HA	1.86	0.58
1:E:272:GLU:HB3	1:E:406:TRP:HB2	1.86	0.58
1:E:594:LEU:HD22	3:E:702:TRT:H161	1.86	0.58
1:E:212:GLN:HB3	1:E:241:ASN:HA	1.86	0.57
1:G:272:GLU:HB3	1:G:406:TRP:HB2	1.86	0.57
1:F:272:GLU:HB3	1:F:406:TRP:HB2	1.86	0.56
1:D:292:MET:HE3	1:D:396:PRO:HG2	1.86	0.56
1:E:529:ALA:HA	1:E:532:VAL:HG22	1.88	0.56
1:F:529:ALA:HA	1:F:532:VAL:HG22	1.88	0.56
1:E:521:VAL:HB	1:E:566:LEU:HD12	1.88	0.55
1:D:588:ARG:HH12	1:D:590:PRO:HG3	1.71	0.55
1:B:425:LEU:O	1:B:428:ARG:HB3	2.06	0.55
1:G:514:SER:HB2	1:G:516:LEU:HD23	1.87	0.54
1:C:212:GLN:HB3	1:C:241:ASN:HA	1.89	0.54
1:D:212:GLN:HB3	1:D:241:ASN:HA	1.89	0.53
1:B:297:GLN:HG2	1:B:399:THR:HG22	1.89	0.53
1:A:19:LEU:HD21	1:A:22:ARG:HG3	1.91	0.53
1:E:19:LEU:HD21	1:E:22:ARG:HG3	1.90	0.53
1:A:505:PRO:HD2	1:A:509:GLU:HG3	1.90	0.53
1:F:297:GLN:HG2	1:F:399:THR:HG22	1.92	0.51
1:H:521:VAL:HB	1:H:566:LEU:HD12	1.92	0.51
1:B:529:ALA:HA	1:B:532:VAL:HG22	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:529:ALA:HA	1:D:532:VAL:HG22	1.91	0.51
1:B:590:PRO:HB2	3:B:702:TRT:H192	1.92	0.51
1:F:563:ARG:HE	1:F:564:TRP:H	1.57	0.51
1:A:558:PRO:HD2	1:A:561:ASP:HB2	1.92	0.51
1:G:292:MET:HE3	1:G:396:PRO:HG2	1.93	0.51
1:C:529:ALA:HA	1:C:532:VAL:HG22	1.94	0.50
1:C:174:ILE:HG22	1:C:263:TYR:HB2	1.93	0.50
1:A:79:TRP:O	1:A:83:SER:HB3	2.11	0.50
1:B:371:ILE:HB	1:B:389:ARG:HD2	1.93	0.50
1:C:268:ASP:HB3	1:C:271:ILE:HG23	1.94	0.50
1:B:391:ARG:HH21	1:C:512:LEU:HD21	1.77	0.50
1:G:529:ALA:HA	1:G:532:VAL:HG22	1.94	0.49
1:A:297:GLN:HG2	1:A:399:THR:HG22	1.94	0.49
1:A:514:SER:HB2	1:A:516:LEU:HD23	1.94	0.49
1:H:79:TRP:O	1:H:83:SER:HB3	2.11	0.49
1:B:79:TRP:O	1:B:83:SER:HB3	2.12	0.49
1:A:529:ALA:HA	1:A:532:VAL:HG22	1.94	0.49
1:C:179:PRO:HB3	1:C:247:GLY:HA3	1.93	0.49
1:D:179:PRO:HB3	1:D:247:GLY:HA3	1.93	0.49
1:E:208:ILE:HD13	1:E:254:GLU:HB2	1.95	0.49
1:D:19:LEU:HD21	1:D:22:ARG:HG3	1.94	0.49
1:D:20:LEU:HD11	1:D:164:ALA:HB2	1.94	0.49
1:G:558:PRO:HD2	1:G:561:ASP:HB2	1.95	0.49
1:F:505:PRO:HD2	1:F:509:GLU:HG3	1.94	0.49
1:H:518:VAL:HG11	1:H:555:LEU:HD21	1.95	0.49
1:B:514:SER:HB2	1:B:516:LEU:HD23	1.95	0.49
1:C:448:ILE:HG12	1:C:601:MET:HE1	1.95	0.49
1:F:212:GLN:HB3	1:F:241:ASN:HA	1.95	0.49
1:H:174:ILE:HG22	1:H:263:TYR:HB2	1.94	0.49
1:G:521:VAL:HB	1:G:566:LEU:HD12	1.94	0.48
1:D:558:PRO:HD2	1:D:561:ASP:HB2	1.95	0.48
1:E:357:GLY:HA3	1:E:359:TRP:CZ3	2.48	0.48
1:B:448:ILE:HG12	1:B:601:MET:HE1	1.95	0.48
1:B:521:VAL:HB	1:B:566:LEU:HD12	1.96	0.48
1:F:79:TRP:O	1:F:83:SER:HB3	2.14	0.48
1:C:426:ARG:HB2	1:C:469:ALA:HB1	1.96	0.48
1:D:268:ASP:HB3	1:D:271:ILE:HG23	1.94	0.48
1:F:521:VAL:HB	1:F:566:LEU:HD12	1.94	0.48
1:B:272:GLU:HB3	1:B:406:TRP:HB2	1.95	0.48
1:D:79:TRP:O	1:D:83:SER:HB3	2.14	0.47
1:G:79:TRP:O	1:G:83:SER:HB3	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:594:LEU:HD22	3:A:702:TRT:H161	1.96	0.47
1:E:511:PRO:HB2	1:E:552:THR:HG23	1.95	0.47
1:A:110:SER:HA	1:A:341:ARG:HH21	1.79	0.47
1:F:511:PRO:HB2	1:F:552:THR:HG23	1.97	0.47
1:F:208:ILE:HD13	1:F:254:GLU:HB2	1.96	0.47
1:A:179:PRO:HB3	1:A:247:GLY:HA3	1.96	0.47
1:A:588:ARG:HH12	1:A:590:PRO:HG3	1.79	0.47
1:F:100:VAL:HG22	1:F:149:ILE:HG12	1.95	0.47
1:F:292:MET:HE3	1:F:396:PRO:HG2	1.96	0.47
1:G:268:ASP:HB3	1:G:271:ILE:HG23	1.97	0.47
1:E:577:THR:HG23	1:E:580:GLY:H	1.80	0.47
1:H:212:GLN:HB3	1:H:241:ASN:HA	1.97	0.47
1:B:357:GLY:HA3	1:B:359:TRP:CZ3	2.50	0.46
1:B:36:THR:HG21	1:B:334:ALA:HA	1.96	0.46
1:D:447:THR:HB	1:D:604:ARG:HH21	1.81	0.46
1:G:518:VAL:HG11	1:G:555:LEU:HD21	1.97	0.46
1:H:178:MET:HE1	1:H:191:LEU:HD21	1.96	0.46
1:F:284:PHE:HE2	1:F:398:VAL:HG21	1.81	0.46
1:E:470:ILE:HG21	1:E:603:LEU:HB3	1.98	0.46
1:D:297:GLN:HG2	1:D:399:THR:HG22	1.98	0.46
1:H:297:GLN:HG2	1:H:399:THR:HG22	1.98	0.46
1:D:563:ARG:HE	1:D:564:TRP:H	1.62	0.46
1:G:25:LEU:HD22	1:G:57:LEU:HD13	1.98	0.46
1:E:371:ILE:HD11	1:E:386:TYR:CZ	2.51	0.46
1:E:319:PHE:HB2	1:E:436:LEU:HD13	1.96	0.46
1:G:32:LEU:HD23	1:G:35:ARG:HH11	1.81	0.46
1:A:544:PRO:HA	1:A:590:PRO:HG2	1.98	0.45
1:H:19:LEU:HD21	1:H:22:ARG:HG3	1.98	0.45
1:A:426:ARG:HB2	1:A:469:ALA:HB1	1.98	0.45
1:E:90:LEU:HB2	1:E:162:TRP:CZ3	2.51	0.45
1:G:166:ILE:HG13	1:G:287:PHE:HE1	1.81	0.45
1:A:25:LEU:HD22	1:A:57:LEU:HD13	1.99	0.45
1:H:484:LEU:HB3	1:H:485:PRO:HD3	1.99	0.45
1:B:212:GLN:HB3	1:B:241:ASN:HA	1.98	0.45
1:F:21:GLN:HG3	1:F:280:ARG:NE	2.31	0.45
1:F:520:ALA:HB1	1:F:533:ARG:NH2	2.31	0.45
1:D:588:ARG:NH1	1:D:590:PRO:HG3	2.32	0.45
1:E:377:LEU:HD13	1:E:427:ASN:HB3	1.98	0.45
1:A:302:GLN:HG2	1:F:112:ILE:HG23	1.98	0.45
1:C:25:LEU:HD22	1:C:57:LEU:HD13	1.99	0.45
1:C:357:GLY:HA3	1:C:359:TRP:CZ3	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:166:ILE:HG13	1:D:287:PHE:HE1	1.82	0.45
1:B:484:LEU:HB3	1:B:485:PRO:HD3	1.99	0.44
1:A:357:GLY:HA3	1:A:359:TRP:CZ3	2.52	0.44
1:H:268:ASP:HB3	1:H:271:ILE:HG23	1.99	0.44
1:D:514:SER:HB2	1:D:516:LEU:HD23	1.99	0.44
1:E:20:LEU:HD11	1:E:164:ALA:HB2	1.98	0.44
1:F:484:LEU:HB3	1:F:485:PRO:HD3	1.98	0.44
1:G:174:ILE:HG22	1:G:263:TYR:HB2	1.99	0.44
1:B:558:PRO:HD2	1:B:561:ASP:HB2	2.00	0.44
1:C:26:PRO:HB3	1:C:30:GLU:HG2	1.99	0.44
1:C:178:MET:HG2	1:C:267:MET:HB2	2.00	0.44
1:D:357:GLY:HA3	1:D:359:TRP:CZ3	2.52	0.44
1:E:268:ASP:HB3	1:E:271:ILE:HG23	1.98	0.44
1:E:538:VAL:O	1:E:542:LEU:HG	2.17	0.44
1:A:268:ASP:HB3	1:A:271:ILE:HG23	1.99	0.44
1:C:447:THR:HB	1:C:604:ARG:HH21	1.81	0.44
1:C:484:LEU:HB3	1:C:485:PRO:HD3	2.00	0.44
1:H:357:GLY:HA3	1:H:359:TRP:CZ3	2.53	0.44
1:B:426:ARG:HB2	1:B:469:ALA:HB1	1.98	0.44
1:C:521:VAL:HB	1:C:566:LEU:HD12	2.00	0.44
1:D:484:LEU:HB3	1:D:485:PRO:HD3	2.00	0.43
1:F:523:GLU:HB3	1:F:565:PHE:CE2	2.53	0.43
1:B:208:ILE:HD13	1:B:254:GLU:HB2	1.99	0.43
1:B:433:SER:HA	1:B:615:GLN:HG2	2.00	0.43
1:C:377:LEU:HB3	1:C:427:ASN:ND2	2.33	0.43
1:G:36:THR:HG21	1:G:334:ALA:HA	1.98	0.43
1:F:433:SER:HB3	1:F:615:GLN:HA	2.00	0.43
1:D:557:VAL:HG21	1:D:566:LEU:HD21	2.01	0.43
1:A:292:MET:HE3	1:A:396:PRO:HG2	2.00	0.43
1:A:588:ARG:NH1	1:A:590:PRO:HG3	2.33	0.43
1:D:521:VAL:HB	1:D:566:LEU:HD12	2.00	0.43
1:H:195:GLY:HA2	1:H:201:LEU:HG	1.99	0.43
1:H:433:SER:HB3	1:H:615:GLN:HA	2.01	0.43
1:G:458:LEU:HD21	1:G:588:ARG:HB2	2.01	0.43
1:G:323:SER:HB3	1:G:329:TYR:CE2	2.53	0.43
1:H:558:PRO:HD2	1:H:561:ASP:HB2	2.01	0.43
1:H:588:ARG:HH12	1:H:590:PRO:HG3	1.82	0.43
1:H:594:LEU:HD22	3:H:702:TRT:H162	2.01	0.43
1:A:32:LEU:HD23	1:A:35:ARG:HH11	1.84	0.43
1:G:271:ILE:HG22	1:G:407:HIS:HB2	2.01	0.43
1:A:371:ILE:HB	1:A:389:ARG:HD2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:549:HIS:O	1:B:572:GLY:HA3	2.19	0.43
1:E:523:GLU:HB3	1:E:565:PHE:CZ	2.53	0.43
1:A:470:ILE:HG21	1:A:603:LEU:HB3	2.01	0.42
1:F:20:LEU:HD11	1:F:164:ALA:HB2	2.00	0.42
1:F:179:PRO:HB3	1:F:247:GLY:HA3	2.00	0.42
1:H:56:SER:HA	1:H:157:LEU:O	2.19	0.42
1:H:371:ILE:HD11	1:H:386:TYR:CZ	2.54	0.42
1:A:484:LEU:HB3	1:A:485:PRO:HD3	2.01	0.42
1:G:178:MET:HG2	1:G:267:MET:HB2	2.01	0.42
1:G:261:ALA:O	1:G:365:ARG:HD2	2.20	0.42
1:H:271:ILE:HG22	1:H:407:HIS:HB2	2.01	0.42
1:B:268:ASP:HB3	1:B:271:ILE:HG23	2.00	0.42
1:D:208:ILE:HD13	1:D:254:GLU:HB2	2.00	0.42
1:G:297:GLN:HG2	1:G:399:THR:HG22	2.01	0.42
1:F:357:GLY:HA3	1:F:359:TRP:CZ3	2.55	0.42
1:G:484:LEU:HB3	1:G:485:PRO:HD3	2.01	0.42
1:H:179:PRO:HB3	1:H:247:GLY:HA3	2.01	0.42
1:B:56:SER:HA	1:B:157:LEU:O	2.20	0.42
1:C:371:ILE:HD11	1:C:386:TYR:CZ	2.55	0.42
1:E:284:PHE:HE2	1:E:398:VAL:HG21	1.85	0.42
1:F:32:LEU:HD23	1:F:35:ARG:HH11	1.83	0.42
1:B:199:LEU:HD23	1:B:199:LEU:HA	1.94	0.42
1:E:79:TRP:O	1:E:83:SER:HB3	2.19	0.42
1:C:297:GLN:HG2	1:C:399:THR:HG22	2.01	0.42
1:F:594:LEU:HG	1:F:598:LYS:HE3	2.00	0.42
1:G:298:MET:HE1	1:G:410:TRP:HZ3	1.84	0.42
1:A:68:CYS:HB2	1:A:146:TRP:CD1	2.55	0.42
1:B:538:VAL:HG13	3:B:702:TRT:H3C1	2.02	0.42
1:E:426:ARG:HB2	1:E:469:ALA:HB1	2.01	0.42
1:G:357:GLY:HA3	1:G:359:TRP:CZ3	2.55	0.42
1:G:408:MET:HE2	1:G:408:MET:HB3	1.94	0.42
1:G:539:LEU:HD13	1:G:542:LEU:HD12	2.02	0.42
1:B:436:LEU:HD12	1:B:437:PRO:HD2	2.02	0.42
1:F:90:LEU:HB2	1:F:162:TRP:CZ3	2.54	0.42
1:H:529:ALA:HA	1:H:532:VAL:HG22	2.02	0.42
1:A:326:ASN:HB3	1:A:346:LEU:HD22	2.02	0.41
1:B:299:LEU:HD23	1:B:307:LEU:HA	2.02	0.41
1:A:30:GLU:O	1:F:150:THR:HG21	2.20	0.41
1:E:558:PRO:HD2	1:E:561:ASP:HB2	2.01	0.41
1:F:166:ILE:HG13	1:F:287:PHE:HE1	1.85	0.41
1:E:56:SER:HA	1:E:157:LEU:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:702:TRT:H14	3:F:702:TRT:H7C3	1.82	0.41
1:G:426:ARG:HB2	1:G:469:ALA:HB1	2.02	0.41
1:G:548:ARG:HE	1:G:548:ARG:HB2	1.63	0.41
1:B:293:LEU:HD11	1:B:367:VAL:HG11	2.03	0.41
1:C:68:CYS:HB2	1:C:146:TRP:CD1	2.56	0.41
1:C:79:TRP:O	1:C:83:SER:HB3	2.20	0.41
1:D:110:SER:HA	1:D:341:ARG:HH21	1.86	0.41
1:D:610:ARG:O	1:D:614:MET:HG2	2.21	0.41
1:F:25:LEU:HD22	1:F:57:LEU:HD13	2.03	0.41
1:H:27:ARG:HG3	1:H:54:ARG:NH1	2.35	0.41
1:D:432:ALA:O	1:D:436:LEU:HB3	2.21	0.41
1:H:315:ASP:O	1:H:319:PHE:CA	2.66	0.41
1:H:261:ALA:O	1:H:365:ARG:HD2	2.21	0.41
1:C:261:ALA:O	1:C:365:ARG:HD2	2.21	0.41
1:C:323:SER:HB3	1:C:329:TYR:CE2	2.56	0.41
1:D:426:ARG:HB2	1:D:469:ALA:HB1	2.03	0.41
1:E:484:LEU:HB3	1:E:485:PRO:HD3	2.02	0.41
1:F:594:LEU:HD22	3:F:702:TRT:H161	2.02	0.41
1:H:166:ILE:HG13	1:H:287:PHE:HE1	1.86	0.41
1:H:21:GLN:HG3	1:H:280:ARG:NE	2.36	0.41
1:C:19:LEU:HD21	1:C:22:ARG:HG3	2.02	0.40
1:D:448:ILE:HG12	1:D:601:MET:HE1	2.02	0.40
1:E:303:GLU:HB3	1:E:306:HIS:ND1	2.37	0.40
1:E:526:ASN:H	1:E:526:ASN:ND2	2.20	0.40
1:H:303:GLU:HB3	1:H:306:HIS:ND1	2.36	0.40
1:D:195:GLY:HA2	1:D:201:LEU:HG	2.03	0.40
1:E:520:ALA:HB1	1:E:533:ARG:NH2	2.36	0.40
1:A:371:ILE:HD11	1:A:386:TYR:CZ	2.57	0.40
1:B:367:VAL:O	1:B:371:ILE:HG12	2.21	0.40
1:E:563:ARG:HG3	1:E:564:TRP:H	1.86	0.40
1:F:177:GLY:HA3	1:F:251:VAL:HG11	2.03	0.40
1:H:436:LEU:HD23	1:H:611:PHE:CZ	2.57	0.40
1:B:20:LEU:HD11	1:B:164:ALA:HB2	2.02	0.40
1:E:315:ASP:O	1:E:319:PHE:CA	2.67	0.40
1:F:512:LEU:HD21	1:G:391:ARG:HH21	1.86	0.40
1:A:26:PRO:HB3	1:A:30:GLU:HG2	2.04	0.40
1:A:209:VAL:HB	1:A:236:ILE:HG12	2.03	0.40
1:D:539:LEU:O	1:D:543:ARG:HG3	2.21	0.40
1:D:549:HIS:O	1:D:572:GLY:HA3	2.22	0.40
1:G:19:LEU:HD21	1:G:22:ARG:HG3	2.03	0.40

There are no symmetry-related clashes.



## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	621/666 (93%)	591 (95%)	28 (4%)	2 (0%)	37	67
1	B	621/666 (93%)	592 (95%)	26 (4%)	3 (0%)	25	56
1	C	620/666 (93%)	592 (96%)	26 (4%)	2 (0%)	37	67
1	D	621/666 (93%)	595 (96%)	23 (4%)	3 (0%)	25	56
1	E	621/666 (93%)	590 (95%)	28 (4%)	3 (0%)	25	56
1	F	620/666 (93%)	591 (95%)	27 (4%)	2 (0%)	37	67
1	G	620/666 (93%)	591 (95%)	26 (4%)	3 (0%)	25	56
1	H	621/666 (93%)	594 (96%)	23 (4%)	4 (1%)	22	52
All	All	4965/5328 (93%)	4736 (95%)	207 (4%)	22 (0%)	30	61

All (22) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	330	ASP
1	B	380	LYS
1	C	330	ASP
1	D	330	ASP
1	D	525	ALA
1	E	330	ASP
1	F	378	PHE
1	H	330	ASP
1	H	378	PHE
1	A	330	ASP
1	A	380	LYS
1	C	380	LYS
1	D	380	LYS
1	E	380	LYS
1	E	637	LEU
1	G	378	PHE
1	G	418	ASP

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Mol	Chain	Res	Type
1	H	380	LYS
1	B	418	ASP
1	G	330	ASP
1	H	485	PRO
1	F	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	508/543 (94%)	508 (100%)	0	100	100
1	B	508/543 (94%)	508 (100%)	0	100	100
1	C	508/543 (94%)	508 (100%)	0	100	100
1	D	508/543 (94%)	508 (100%)	0	100	100
1	E	508/543 (94%)	508 (100%)	0	100	100
1	F	508/543 (94%)	508 (100%)	0	100	100
1	G	508/543 (94%)	508 (100%)	0	100	100
1	H	508/543 (94%)	508 (100%)	0	100	100
All	All	4064/4344 (94%)	4064 (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 (35) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	212	GLN
1	A	239	GLN
1	A	258	ASN
1	A	343	ASN
1	A	515	HIS
1	A	554	GLN
1	A	616	GLN
1	B	343	ASN

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Mol	Chain	Res	Type
1	B	515	HIS
1	B	546	HIS
1	C	212	GLN
1	C	239	GLN
1	C	336	HIS
1	D	212	GLN
1	D	239	GLN
1	D	554	GLN
1	D	556	ASN
1	E	326	ASN
1	E	343	ASN
1	E	407	HIS
1	E	549	HIS
1	F	336	HIS
1	F	549	HIS
1	G	258	ASN
1	G	326	ASN
1	G	343	ASN
1	G	373	GLN
1	G	446	ASN
1	G	546	HIS
1	H	50	HIS
1	H	203	GLN
1	H	258	ASN
1	H	454	HIS
1	H	482	GLN
1	H	546	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry

Of 31 ligands modelled in this entry, 8 are monoatomic - leaving 23 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z  > 2$	Counts	RMSZ	# $ Z  > 2$
4	GOL	D	703	-	5,5,5	0.35	0	5,5,5	0.43	0
4	GOL	C	704	-	5,5,5	0.34	0	5,5,5	0.40	0
4	GOL	A	703	-	5,5,5	0.34	0	5,5,5	0.43	0
4	GOL	A	704	-	5,5,5	0.34	0	5,5,5	0.42	0
3	TRT	H	702	-	23,23,25	0.45	0	31,31,33	0.86	0
4	GOL	F	703	-	5,5,5	0.34	0	5,5,5	0.42	0
4	GOL	G	703	-	5,5,5	0.34	0	5,5,5	0.41	0
4	GOL	B	703	-	5,5,5	0.34	0	5,5,5	0.44	0
4	GOL	B	704	-	5,5,5	0.35	0	5,5,5	0.42	0
4	GOL	E	704	-	5,5,5	0.34	0	5,5,5	0.42	0
3	TRT	G	702	-	17,17,25	0.48	0	25,25,33	0.96	0
4	GOL	H	704	-	5,5,5	0.34	0	5,5,5	0.40	0
4	GOL	F	704	-	5,5,5	0.34	0	5,5,5	0.43	0
3	TRT	C	702	-	20,20,25	0.46	0	28,28,33	0.91	0
4	GOL	D	704	-	5,5,5	0.34	0	5,5,5	0.43	0
3	TRT	D	702	-	21,21,25	0.43	0	29,29,33	0.90	1 (3%)
3	TRT	E	702	-	19,19,25	0.44	0	27,27,33	0.91	0
4	GOL	C	703	-	5,5,5	0.34	0	5,5,5	0.41	0
4	GOL	E	703	-	5,5,5	0.34	0	5,5,5	0.42	0
3	TRT	F	702	-	18,18,25	0.46	0	26,26,33	0.94	0
4	GOL	H	703	-	5,5,5	0.34	0	5,5,5	0.42	0
3	TRT	B	702	-	23,23,25	0.43	0	31,31,33	0.86	1 (3%)
3	TRT	A	702	-	23,23,25	0.43	0	31,31,33	0.87	1 (3%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GOL	D	703	-	-	0/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GOL	C	704	-	-	2/4/4/4	-
4	GOL	A	703	-	-	2/4/4/4	-
4	GOL	A	704	-	-	0/4/4/4	-
3	TRT	H	702	-	-	14/21/21/23	0/1/1/1
4	GOL	F	703	-	-	0/4/4/4	-
4	GOL	G	703	-	-	2/4/4/4	-
4	GOL	B	703	-	-	0/4/4/4	-
4	GOL	B	704	-	-	0/4/4/4	-
4	GOL	E	704	-	-	0/4/4/4	-
3	TRT	G	702	-	-	7/15/15/23	0/1/1/1
4	GOL	H	704	-	-	0/4/4/4	-
4	GOL	F	704	-	-	0/4/4/4	-
3	TRT	C	702	-	-	12/18/18/23	0/1/1/1
4	GOL	D	704	-	-	2/4/4/4	-
3	TRT	D	702	-	-	8/19/19/23	0/1/1/1
3	TRT	E	702	-	-	4/17/17/23	0/1/1/1
4	GOL	C	703	-	-	0/4/4/4	-
4	GOL	E	703	-	-	0/4/4/4	-
3	TRT	F	702	-	-	12/16/16/23	0/1/1/1
4	GOL	H	703	-	-	0/4/4/4	-
3	TRT	B	702	-	-	5/21/21/23	0/1/1/1
3	TRT	A	702	-	-	6/21/21/23	0/1/1/1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	702	TRT	C7-C6-C9	-2.10	104.87	110.18
3	A	702	TRT	C7-C6-C9	-2.07	104.94	110.18
3	B	702	TRT	C7-C6-C9	-2.02	105.08	110.18

There are no chirality outliers.

All (76) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	702	TRT	O15-C16-C17-O18
3	B	702	TRT	O18-C19-C20-O21
3	H	702	TRT	C11-C12-O15-C16

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Mol	Chain	Res	Type	Atoms
3	H	702	TRT	C13-C12-O15-C16
3	A	702	TRT	C11-C12-O15-C16
3	E	702	TRT	C11-C12-O15-C16
3	A	702	TRT	C13-C12-O15-C16
3	G	702	TRT	C1-C5-C6-C7
3	D	702	TRT	C11-C12-O15-C16
3	D	702	TRT	O15-C16-C17-O18
3	E	702	TRT	C13-C12-O15-C16
3	H	702	TRT	O15-C16-C17-O18
3	B	702	TRT	C20-C19-O18-C17
3	D	702	TRT	C13-C12-O15-C16
4	A	703	GOL	C1-C2-C3-O3
4	C	704	GOL	C1-C2-C3-O3
4	D	704	GOL	O1-C1-C2-C3
4	G	703	GOL	C1-C2-C3-O3
4	D	704	GOL	O1-C1-C2-O2
3	C	702	TRT	C1-C5-C6-C7
3	F	702	TRT	C1-C5-C6-C7
3	H	702	TRT	C1-C5-C6-C7
3	C	702	TRT	C1-C5-C6-C9
3	F	702	TRT	C1-C5-C6-C9
3	G	702	TRT	C1-C5-C6-C9
3	H	702	TRT	C1-C5-C6-C9
3	F	702	TRT	C11-C12-O15-C16
3	F	702	TRT	C13-C12-O15-C16
4	C	704	GOL	O2-C2-C3-O3
4	G	703	GOL	O2-C2-C3-O3
3	C	702	TRT	C11-C12-O15-C16
3	C	702	TRT	C13-C12-O15-C16
3	A	702	TRT	C2-C1-C5-C6
3	A	702	TRT	C20-C19-O18-C17
3	C	702	TRT	C1-C5-C6-C8
3	F	702	TRT	C1-C5-C6-C8
3	G	702	TRT	C1-C5-C6-C8
3	A	702	TRT	C17-C16-O15-C12
3	H	702	TRT	O18-C19-C20-O21
3	D	702	TRT	C17-C16-O15-C12
3	E	702	TRT	C17-C16-O15-C12
3	F	702	TRT	C17-C16-O15-C12
3	E	702	TRT	C2-C1-C5-C6
4	A	703	GOL	O2-C2-C3-O3
3	H	702	TRT	C1-C5-C6-C8

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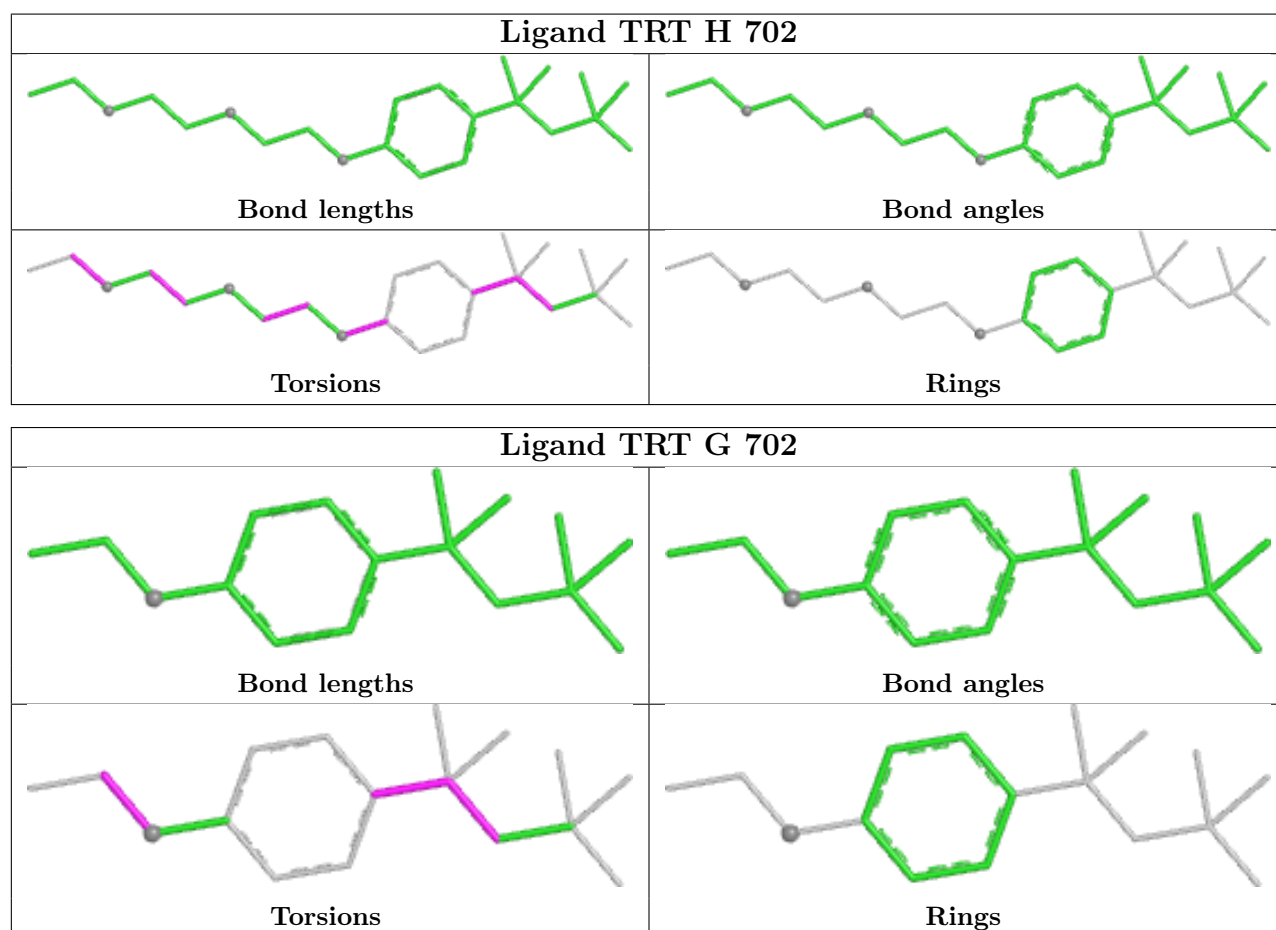
Mol	Chain	Res	Type	Atoms
3	B	702	TRT	C16-C17-O18-C19
3	D	702	TRT	C2-C1-C5-C6
3	B	702	TRT	C2-C1-C5-C6
3	G	702	TRT	C17-C16-O15-C12
3	D	702	TRT	O18-C19-C20-O21
3	D	702	TRT	C16-C17-O18-C19
3	H	702	TRT	C23-C22-O21-C20
3	B	702	TRT	C17-C16-O15-C12
3	A	702	TRT	C23-C22-O21-C20
3	H	702	TRT	C8-C6-C9-C14
3	C	702	TRT	C8-C6-C9-C14
3	F	702	TRT	C7-C6-C9-C10
3	F	702	TRT	C8-C6-C9-C14
3	C	702	TRT	C7-C6-C9-C10
3	H	702	TRT	C7-C6-C9-C10
3	G	702	TRT	C7-C6-C9-C14
3	C	702	TRT	C5-C6-C9-C10
3	F	702	TRT	C5-C6-C9-C10
3	H	702	TRT	C5-C6-C9-C10
3	C	702	TRT	C8-C6-C9-C10
3	H	702	TRT	C8-C6-C9-C10
3	F	702	TRT	C8-C6-C9-C10
3	F	702	TRT	C7-C6-C9-C14
3	C	702	TRT	C5-C6-C9-C14
3	H	702	TRT	C5-C6-C9-C14
3	H	702	TRT	C7-C6-C9-C14
3	G	702	TRT	C7-C6-C9-C10
3	F	702	TRT	C5-C6-C9-C14
3	C	702	TRT	C7-C6-C9-C14
3	G	702	TRT	C8-C6-C9-C14
3	D	702	TRT	C20-C19-O18-C17

There are no ring outliers.

5 monomers are involved in 7 short contacts:

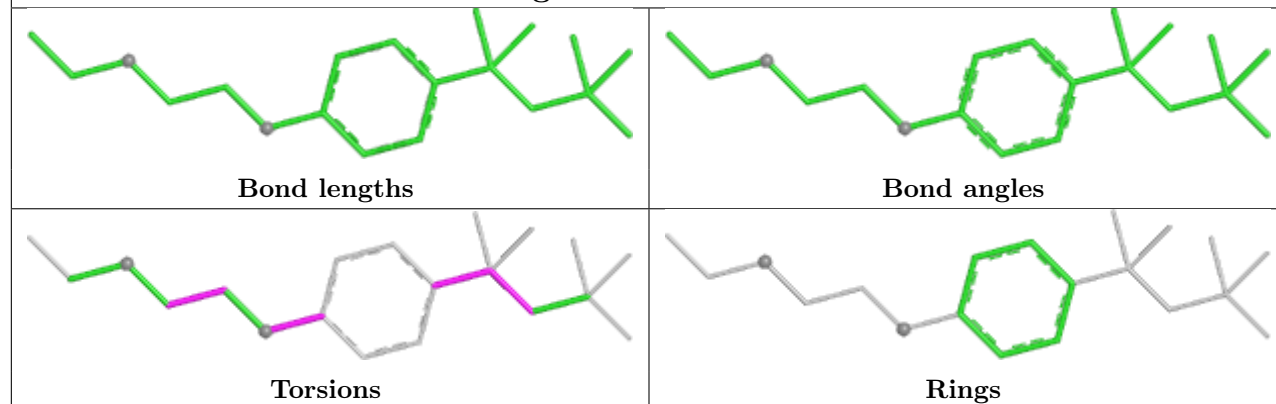
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	H	702	TRT	1	0
3	E	702	TRT	1	0
3	F	702	TRT	2	0
3	B	702	TRT	2	0
3	A	702	TRT	1	0

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

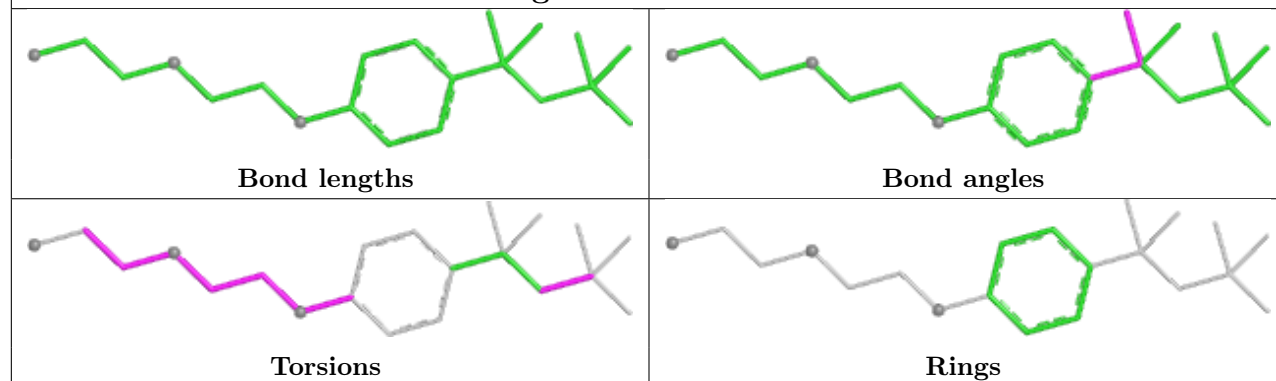




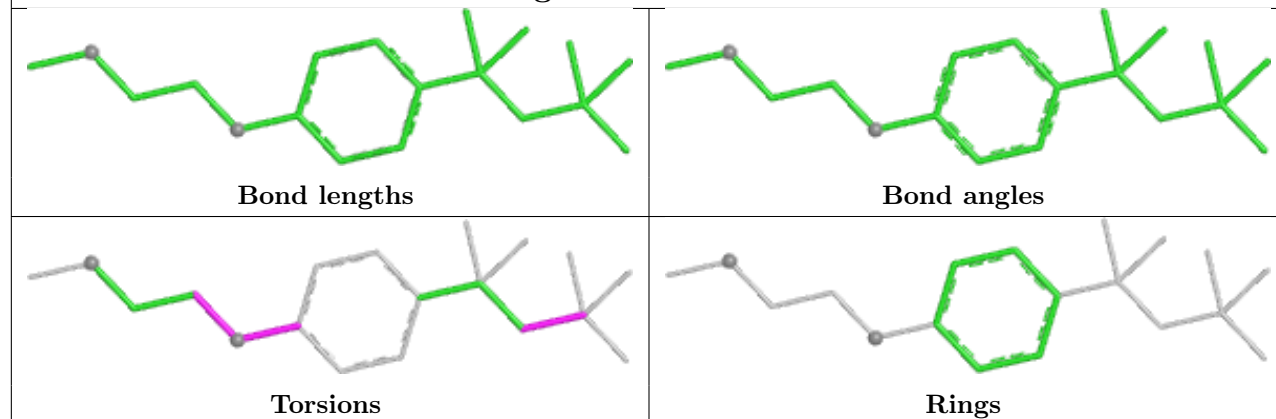
## Ligand TRT C 702

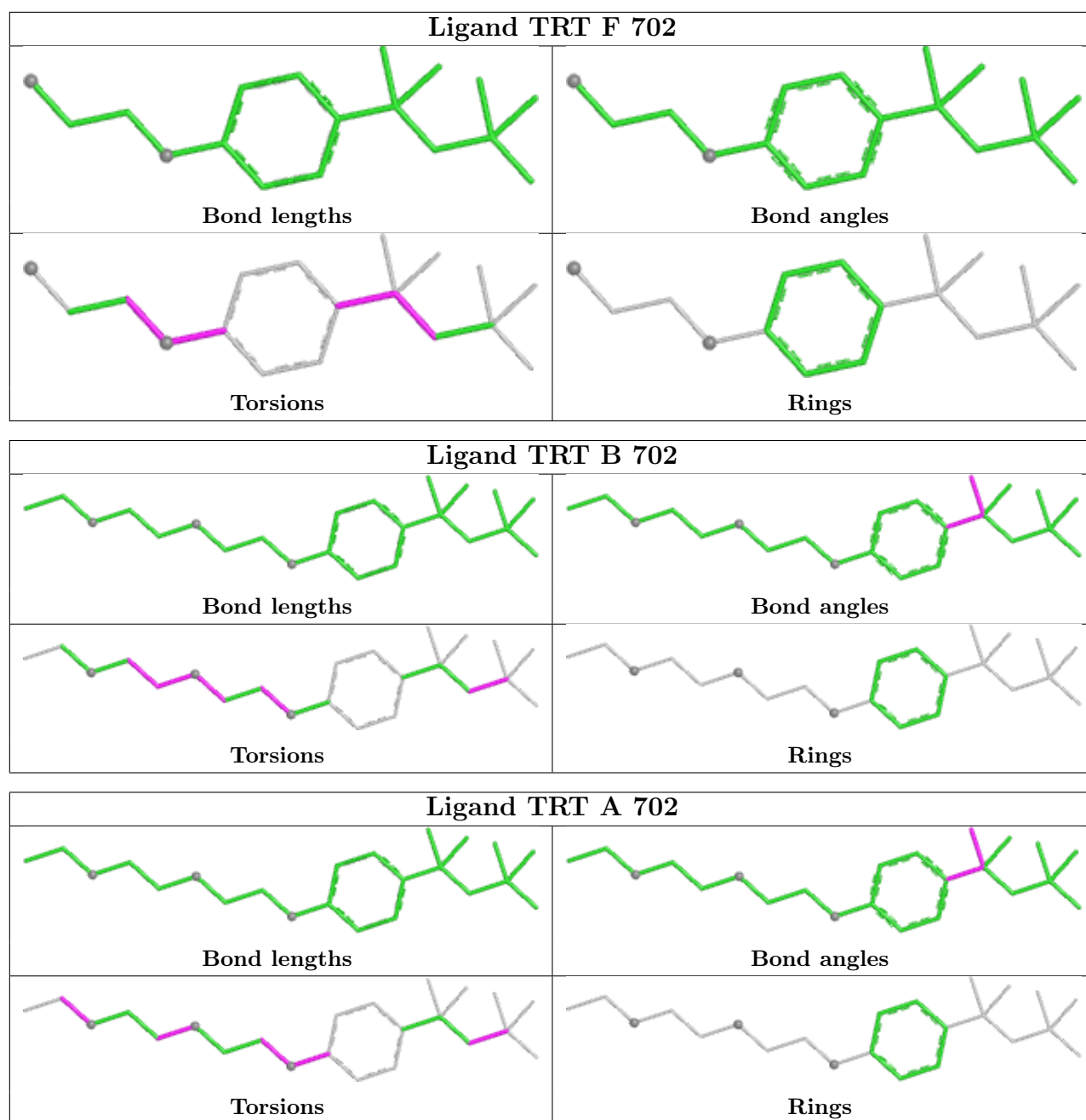


## Ligand TRT D 702



## Ligand TRT E 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 [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, 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	624/666 (93%)	-0.50	0 <a href="#">100</a> <a href="#">100</a>	28, 55, 77, 108	1 (0%)
1	B	624/666 (93%)	-0.42	0 <a href="#">100</a> <a href="#">100</a>	29, 57, 83, 107	1 (0%)
1	C	623/666 (93%)	-0.39	0 <a href="#">100</a> <a href="#">100</a>	27, 61, 81, 112	1 (0%)
1	D	624/666 (93%)	-0.43	1 (0%) <a href="#">92</a> <a href="#">84</a>	32, 58, 81, 112	1 (0%)
1	E	624/666 (93%)	-0.26	0 <a href="#">100</a> <a href="#">100</a>	30, 70, 94, 110	1 (0%)
1	F	623/666 (93%)	-0.23	0 <a href="#">100</a> <a href="#">100</a>	32, 69, 92, 117	1 (0%)
1	G	623/666 (93%)	-0.29	0 <a href="#">100</a> <a href="#">100</a>	28, 72, 93, 111	1 (0%)
1	H	624/666 (93%)	-0.39	1 (0%) <a href="#">92</a> <a href="#">84</a>	30, 65, 85, 113	1 (0%)
All	All	4989/5328 (93%)	-0.36	2 (0%) <a href="#">100</a> <a href="#">100</a>	27, 62, 88, 117	8 (0%)

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	410	TRP	2.6
1	H	410	TRP	2.2

### 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](#)

There are no oligosaccharides in this entry.

## 6.4 Ligands ⓘ

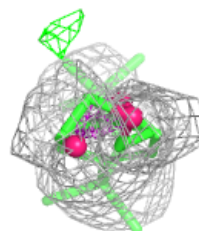
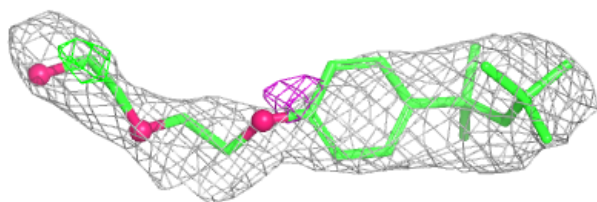
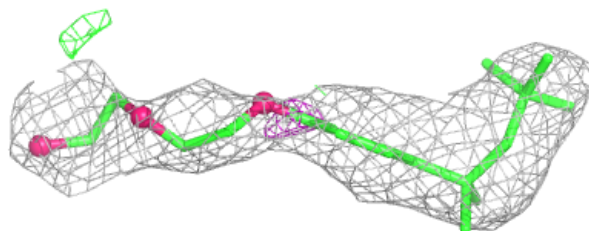
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 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
2	MG	G	701	1/1	0.72	0.14	65,65,65,65	0
4	GOL	A	704	6/6	0.74	0.20	53,63,67,70	0
4	GOL	H	704	6/6	0.75	0.17	78,89,89,90	0
4	GOL	F	704	6/6	0.78	0.21	67,81,91,109	0
4	GOL	C	704	6/6	0.81	0.13	58,78,81,89	0
3	TRT	D	702	21/25	0.81	0.15	52,77,91,93	0
4	GOL	B	704	6/6	0.81	0.15	58,66,79,88	0
4	GOL	C	703	6/6	0.82	0.16	50,64,67,71	0
4	GOL	E	703	6/6	0.82	0.16	58,69,76,77	0
4	GOL	D	704	6/6	0.83	0.25	56,83,87,91	0
3	TRT	G	702	17/25	0.83	0.17	69,87,96,97	0
3	TRT	H	702	23/25	0.83	0.14	67,83,97,99	0
3	TRT	E	702	19/25	0.83	0.14	44,73,92,97	0
4	GOL	F	703	6/6	0.84	0.18	64,75,81,84	0
3	TRT	A	702	23/25	0.84	0.15	54,70,84,88	0
3	TRT	B	702	23/25	0.84	0.14	54,72,87,90	0
3	TRT	C	702	20/25	0.85	0.15	60,77,91,94	0
4	GOL	E	704	6/6	0.86	0.19	71,91,96,99	0
4	GOL	D	703	6/6	0.86	0.12	57,63,67,70	0
4	GOL	B	703	6/6	0.88	0.12	45,61,69,73	0
2	MG	F	701	1/1	0.89	0.17	67,67,67,67	0
3	TRT	F	702	18/25	0.89	0.14	74,86,94,99	0
4	GOL	A	703	6/6	0.91	0.10	47,64,70,74	0
2	MG	H	701	1/1	0.92	0.10	54,54,54,54	0
4	GOL	G	703	6/6	0.92	0.16	73,78,82,96	0
2	MG	D	701	1/1	0.92	0.09	55,55,55,55	0
4	GOL	H	703	6/6	0.93	0.08	49,54,68,70	0
2	MG	E	701	1/1	0.95	0.10	55,55,55,55	0
2	MG	A	701	1/1	0.97	0.07	50,50,50,50	0
2	MG	B	701	1/1	0.97	0.07	48,48,48,48	0
2	MG	C	701	1/1	0.99	0.04	60,60,60,60	0

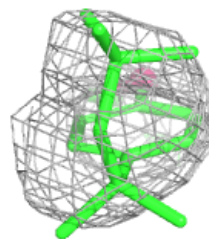
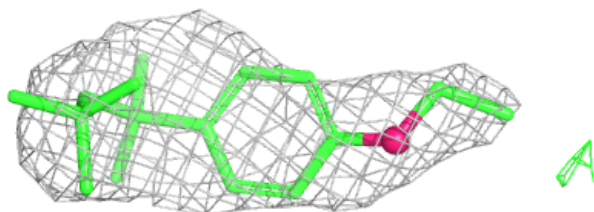
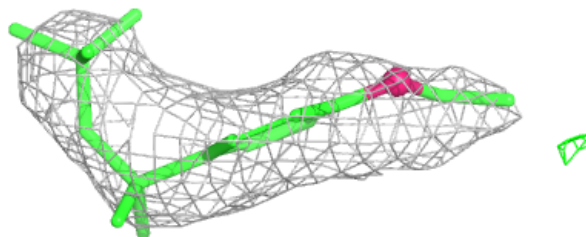
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around 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)

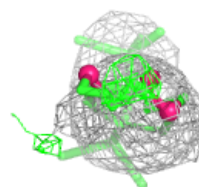
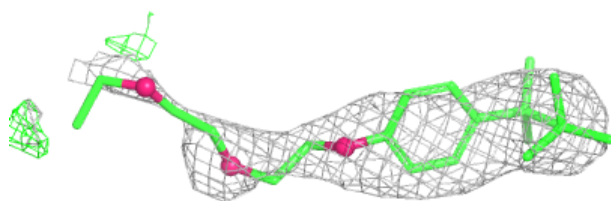
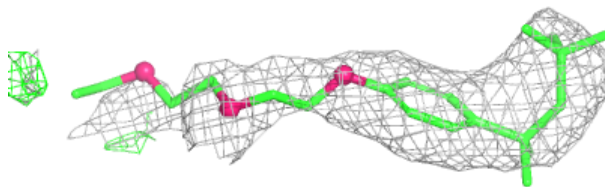
**Electron density around TRT G 702:**

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

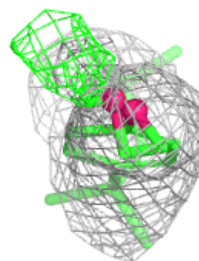
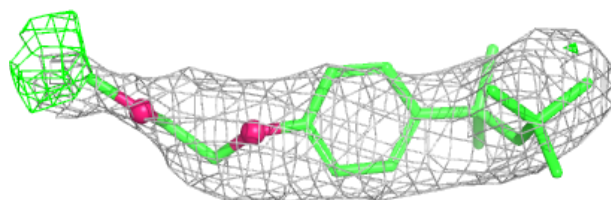
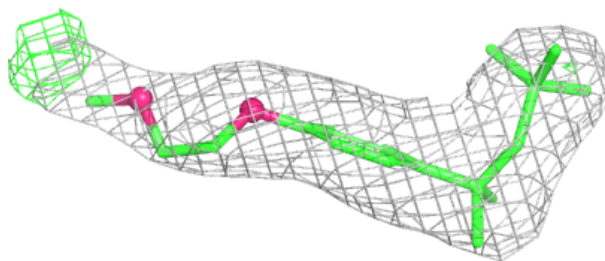


**Electron density around TRT H 702:**

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

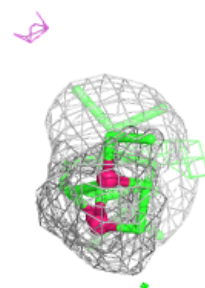
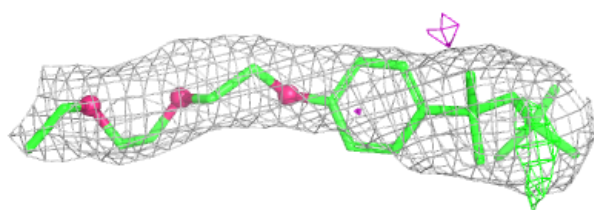
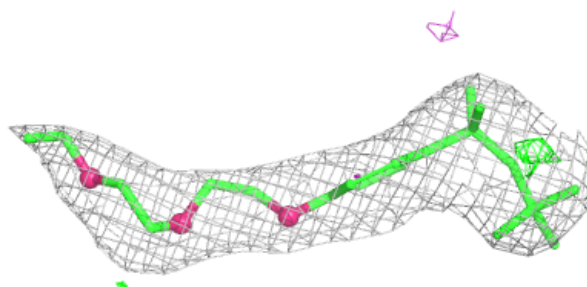
**Electron density around TRT E 702:**

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

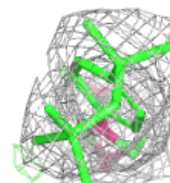
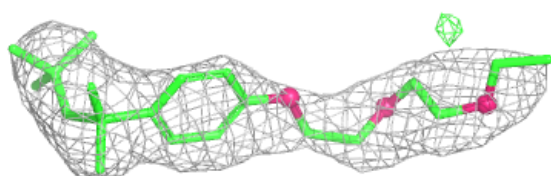
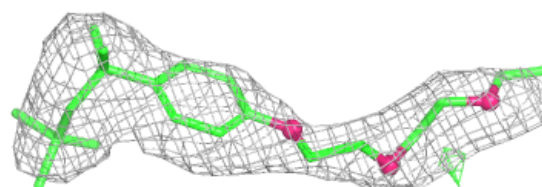


**Electron density around TRT A 702:**

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

**Electron density around TRT B 702:**

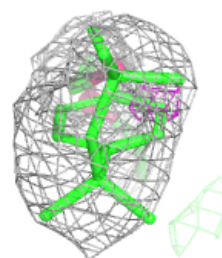
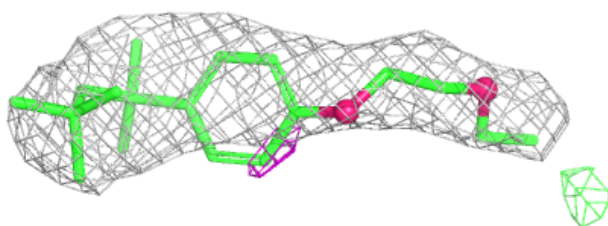
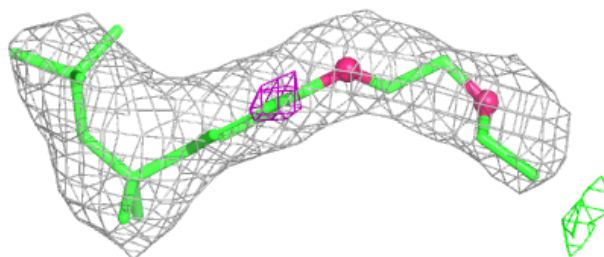
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



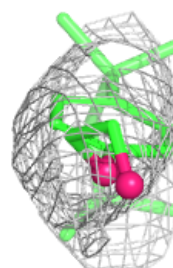
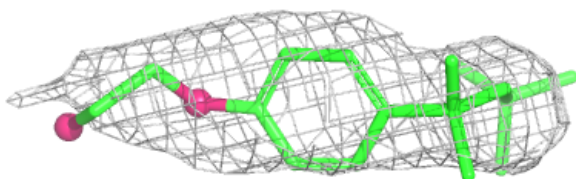
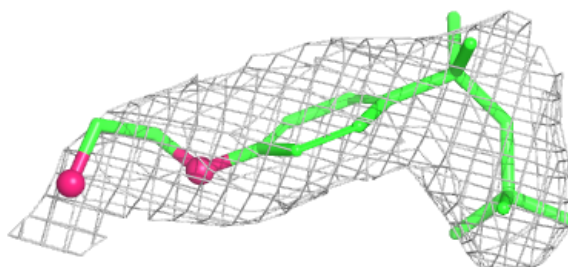


**Electron density around TRT C 702:**

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

**Electron density around TRT 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)





## 6.5 Other polymers [i](#)

There are no such residues in this entry.