



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 24, 2024 – 10:56 PM EDT

PDB ID : 6TER  
Title : Crystal structure of a galactokinase from Bifidobacterium infantis in complex with Galactose  
Authors : Keenan, T.; Parmeggiani, F.; Fontenelle, C.Q.; Malassis, J.; Vendeville, J.; Offen, W.A.; Both, P.; Huang, K.; Marchesi, A.; Heyam, A.; Young, C.; Charnock, S.; Davies, G.J.; Linclau, B.; Flitsch, S.L.; Fascione, M.A.  
Deposited on : 2019-11-12  
Resolution : 1.68 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](#) ①) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

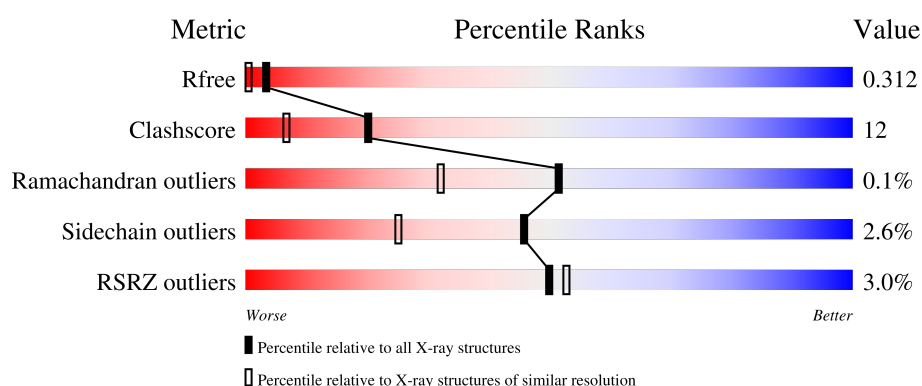
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.68 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))
$R_{free}$	130704	6780 (1.70-1.66)
Clashscore	141614	7310 (1.70-1.66)
Ramachandran outliers	138981	7173 (1.70-1.66)
Sidechain outliers	138945	7172 (1.70-1.66)
RSRZ outliers	127900	6661 (1.70-1.66)

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	429	<div> <div> <div>0%</div> <div>80%</div> <div>17%</div> <div>•</div> </div> </div>
1	B	429	<div> <div>2%</div> <div>80%</div> <div>16%</div> <div>••</div> </div>
1	C	429	<div> <div>2%</div> <div>85%</div> <div>12%</div> <div>•</div> </div>
1	D	429	<div> <div>7%</div> <div>78%</div> <div>19%</div> <div>•</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	GOL	A	911	-	-	X	-
2	GOL	B	701	-	-	X	-
2	GOL	B	710	-	-	X	-
2	GOL	C	606	-	-	X	-
3	PEG	A	903	-	-	X	-
3	PEG	A	904	-	-	X	-
3	PEG	A	907	-	-	X	-
3	PEG	A	912	-	-	X	-
3	PEG	A	918[A]	-	-	X	-
3	PEG	B	702	-	-	X	-
3	PEG	B	704	-	-	X	-
4	PGE	A	919	-	-	X	-
4	PGE	A	921	-	-	X	-
5	PG4	A	922	-	-	X	-

## 2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 14073 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 Galactokinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	418	Total	C	N	O	S	0	11	0
			3182	1982	559	629	12			
1	B	418	Total	C	N	O	S	0	12	0
			3212	1999	566	633	14			
1	C	416	Total	C	N	O	S	0	12	0
			3188	1983	563	629	13			
1	D	416	Total	C	N	O	S	0	15	0
			3207	2001	560	634	12			

There are 52 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	417	LYS	-	expression tag	UNP B7GUI0
A	418	LEU	-	expression tag	UNP B7GUI0
A	419	ALA	-	expression tag	UNP B7GUI0
A	420	ALA	-	expression tag	UNP B7GUI0
A	421	ALA	-	expression tag	UNP B7GUI0
A	422	LEU	-	expression tag	UNP B7GUI0
A	423	GLU	-	expression tag	UNP B7GUI0
A	424	HIS	-	expression tag	UNP B7GUI0
A	425	HIS	-	expression tag	UNP B7GUI0
A	426	HIS	-	expression tag	UNP B7GUI0
A	427	HIS	-	expression tag	UNP B7GUI0
A	428	HIS	-	expression tag	UNP B7GUI0
A	429	HIS	-	expression tag	UNP B7GUI0
B	417	LYS	-	expression tag	UNP B7GUI0
B	418	LEU	-	expression tag	UNP B7GUI0
B	419	ALA	-	expression tag	UNP B7GUI0
B	420	ALA	-	expression tag	UNP B7GUI0
B	421	ALA	-	expression tag	UNP B7GUI0
B	422	LEU	-	expression tag	UNP B7GUI0
B	423	GLU	-	expression tag	UNP B7GUI0
B	424	HIS	-	expression tag	UNP B7GUI0

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Chain	Residue	Modelled	Actual	Comment	Reference
B	425	HIS	-	expression tag	UNP B7GUI0
B	426	HIS	-	expression tag	UNP B7GUI0
B	427	HIS	-	expression tag	UNP B7GUI0
B	428	HIS	-	expression tag	UNP B7GUI0
B	429	HIS	-	expression tag	UNP B7GUI0
C	417	LYS	-	expression tag	UNP B7GUI0
C	418	LEU	-	expression tag	UNP B7GUI0
C	419	ALA	-	expression tag	UNP B7GUI0
C	420	ALA	-	expression tag	UNP B7GUI0
C	421	ALA	-	expression tag	UNP B7GUI0
C	422	LEU	-	expression tag	UNP B7GUI0
C	423	GLU	-	expression tag	UNP B7GUI0
C	424	HIS	-	expression tag	UNP B7GUI0
C	425	HIS	-	expression tag	UNP B7GUI0
C	426	HIS	-	expression tag	UNP B7GUI0
C	427	HIS	-	expression tag	UNP B7GUI0
C	428	HIS	-	expression tag	UNP B7GUI0
C	429	HIS	-	expression tag	UNP B7GUI0
D	417	LYS	-	expression tag	UNP B7GUI0
D	418	LEU	-	expression tag	UNP B7GUI0
D	419	ALA	-	expression tag	UNP B7GUI0
D	420	ALA	-	expression tag	UNP B7GUI0
D	421	ALA	-	expression tag	UNP B7GUI0
D	422	LEU	-	expression tag	UNP B7GUI0
D	423	GLU	-	expression tag	UNP B7GUI0
D	424	HIS	-	expression tag	UNP B7GUI0
D	425	HIS	-	expression tag	UNP B7GUI0
D	426	HIS	-	expression tag	UNP B7GUI0
D	427	HIS	-	expression tag	UNP B7GUI0
D	428	HIS	-	expression tag	UNP B7GUI0
D	429	HIS	-	expression tag	UNP B7GUI0

- Molecule 2 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



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

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

- Molecule 3 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: C<sub>4</sub>H<sub>10</sub>O<sub>3</sub>).





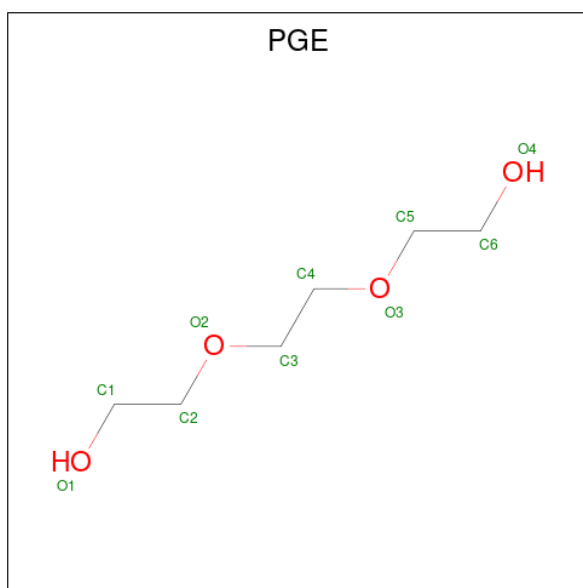
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			7	4	3		
3	A	1	Total	C	O	0	0
			7	4	3		
3	A	1	Total	C	O	0	0
			7	4	3		
3	A	1	Total	C	O	0	0
			7	4	3		
3	A	1	Total	C	O	0	1
			14	8	6		
3	A	1	Total	C	O	0	0
			7	4	3		
3	A	1	Total	C	O	0	0
			7	4	3		
3	A	1	Total	C	O	0	0
			7	4	3		
3	A	1	Total	C	O	0	1
			14	8	6		
3	A	1	Total	C	O	0	0
			7	4	3		
3	B	1	Total	C	O	0	0
			7	4	3		
3	B	1	Total	C	O	0	0
			7	4	3		

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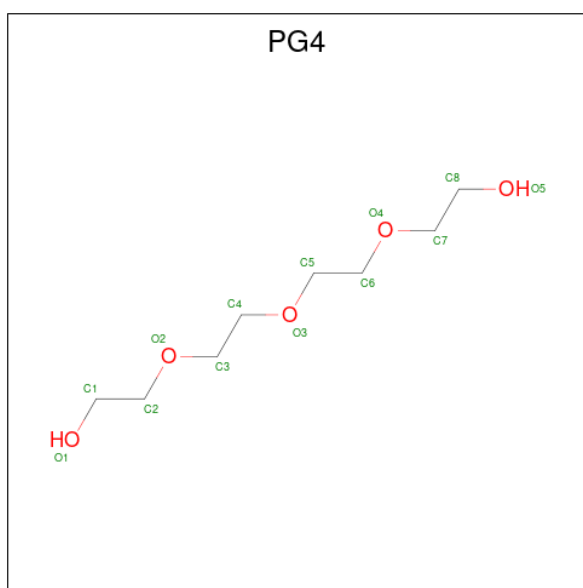
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total C O 7 4 3	0	0
3	B	1	Total C O 7 4 3	0	0
3	B	1	Total C O 7 4 3	0	0
3	B	1	Total C O 7 4 3	0	0
3	B	1	Total C O 7 4 3	0	0
3	B	1	Total C O 7 4 3	0	0
3	B	1	Total C O 7 4 3	0	0
3	C	1	Total C O 14 8 6	0	1
3	C	1	Total C O 7 4 3	0	0
3	C	1	Total C O 7 4 3	0	0
3	D	1	Total C O 7 4 3	0	0
3	D	1	Total C O 7 4 3	0	0

- Molecule 4 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula:  $C_6H_{14}O_4$ ).



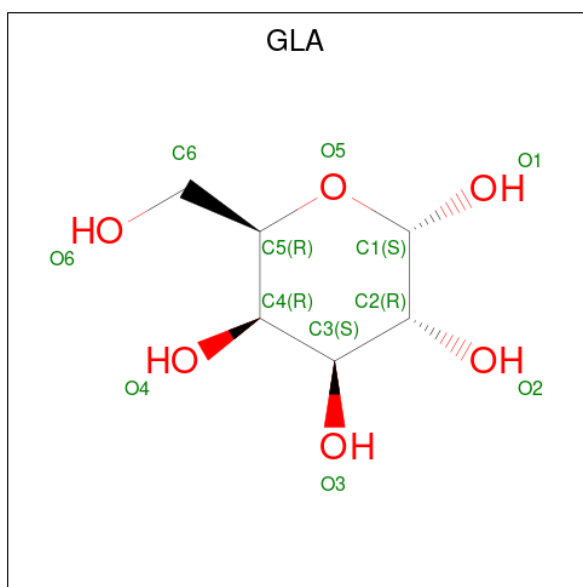
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			10	6	4		
4	A	1	Total	C	O	0	0
			10	6	4		
4	A	1	Total	C	O	0	0
			10	6	4		
4	B	1	Total	C	O	0	0
			10	6	4		

- Molecule 5 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula:  $C_8H_{18}O_5$ ).



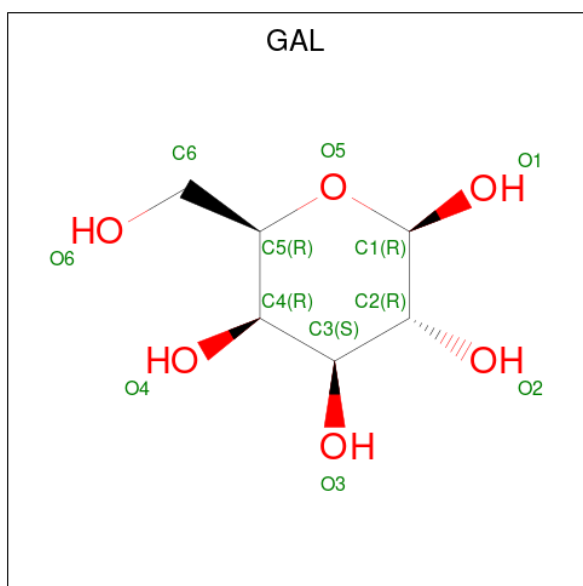
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			13	8	5		
5	A	1	Total	C	O	0	0
			13	8	5		

- Molecule 6 is alpha-D-galactopyranose (three-letter code: GLA) (formula:  $C_6H_{12}O_6$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	1
			12	6	6		
6	B	1	Total	C	O	0	1
			12	6	6		
6	C	1	Total	C	O	0	0
			12	6	6		
6	D	1	Total	C	O	0	0
			12	6	6		

- Molecule 7 is beta-D-galactopyranose (three-letter code: GAL) (formula: C<sub>6</sub>H<sub>12</sub>O<sub>6</sub>) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total C O 12 6 6	0	1
7	B	1	Total C O 12 6 6	0	1

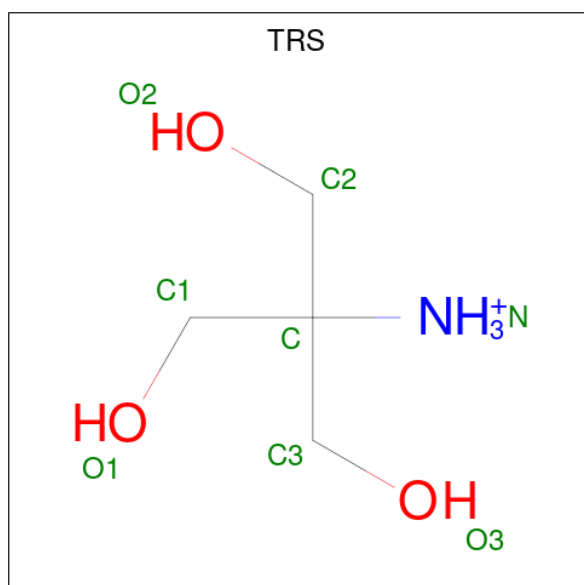
- Molecule 8 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	1	Total Cl 1 1	0	0
8	C	2	Total Cl 2 2	0	0

- Molecule 9 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	B	3	Total Na 3 3	0	0
9	C	1	Total Na 1 1	0	0
9	D	2	Total Na 2 2	0	0

- Molecule 10 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (three-letter code: TRS) (formula: C<sub>4</sub>H<sub>12</sub>NO<sub>3</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
10	D	1	Total	C	N	O	0	0
			8	4	1	3		

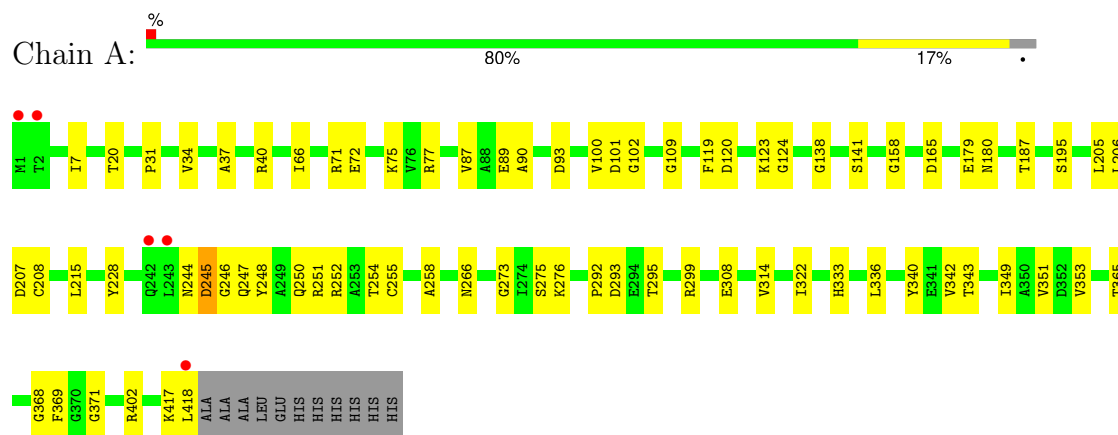
- Molecule 11 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	A	214	Total	O	0	0
			214	214		
11	B	209	Total	O	0	0
			209	209		
11	C	201	Total	O	0	0
			201	201		
11	D	140	Total	O	0	0
			140	140		

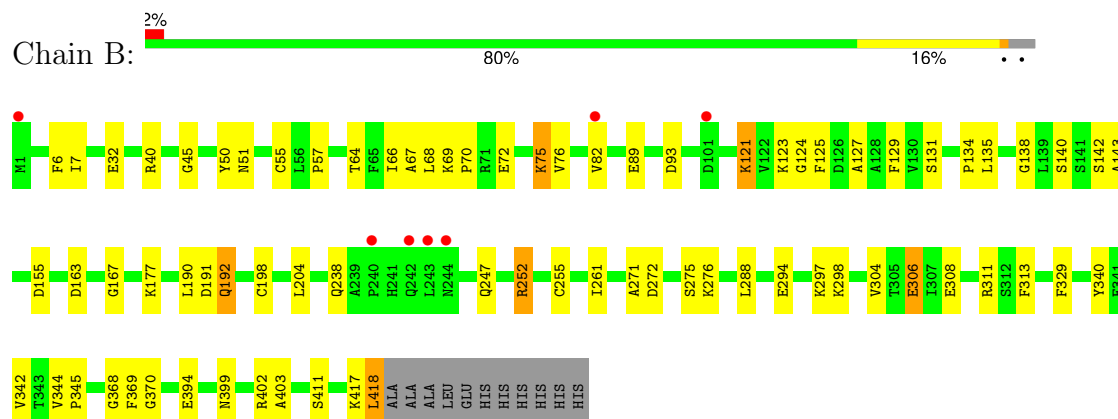
### 3 Residue-property plots

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.

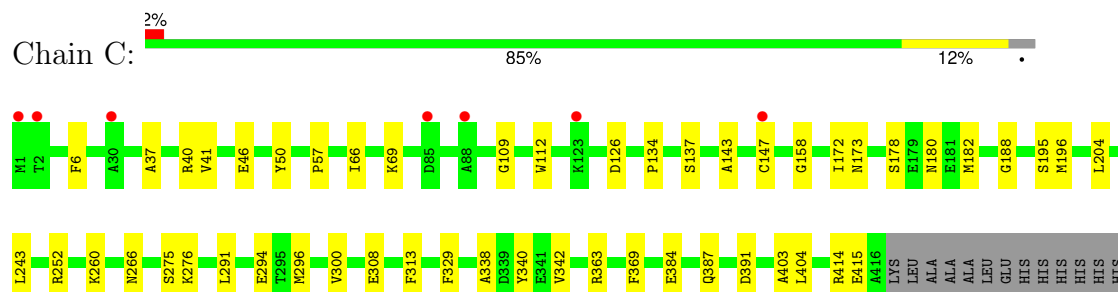
#### • Molecule 1: Galactokinase



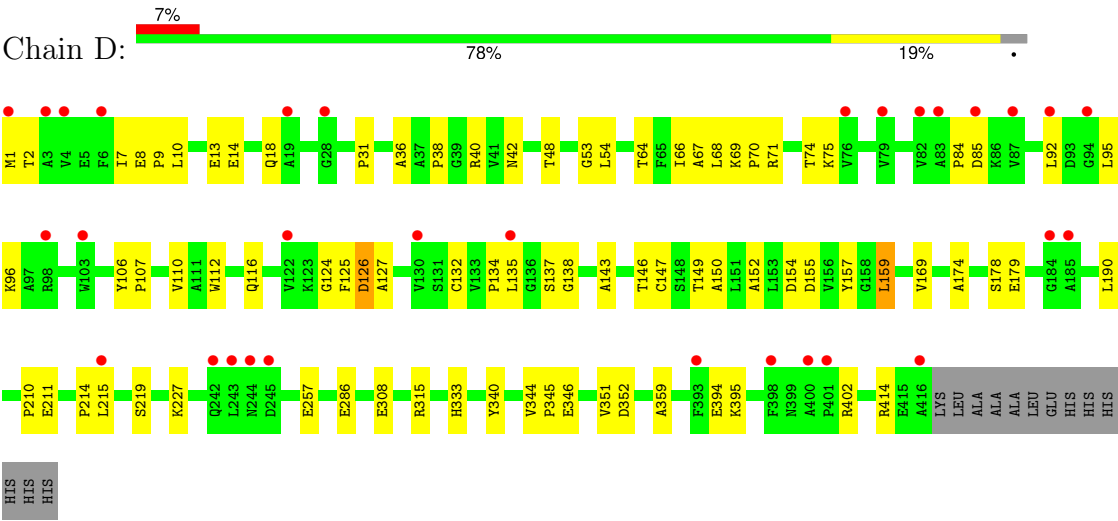
#### • Molecule 1: Galactokinase



#### • Molecule 1: Galactokinase



● Molecule 1: Galactokinase





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	52.32Å 164.93Å 113.63Å 90.00° 94.97° 90.00°	Depositor
Resolution (Å)	82.60 – 1.68 82.46 – 1.68	Depositor EDS
% Data completeness (in resolution range)	94.5 (82.60-1.68) 94.6 (82.46-1.68)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.69 (at 1.68Å)	Xtriage
Refinement program	REFMAC 5.8.0253	Depositor
R, $R_{free}$	0.224 , 0.308 0.231 , 0.312	Depositor DCC
$R_{free}$ test set	10249 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	19.5	Xtriage
Anisotropy	0.743	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 47.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	14073	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 18.34% of the height of the origin peak. No significant pseudotranslation is detected.*

<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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GLA, PGE, CL, NA, PEG, PG4, GOL, TRS, GAL

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	0.93	1/3236 (0.0%)	1.00	0/4392
1	B	0.94	2/3265 (0.1%)	1.01	3/4425 (0.1%)
1	C	0.90	2/3242 (0.1%)	1.00	2/4398 (0.0%)
1	D	0.85	1/3259 (0.0%)	1.01	0/4417
All	All	0.90	6/13002 (0.0%)	1.01	5/17632 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	D	0	1
All	All	0	2

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	306	GLU	CD-OE1	8.27	1.34	1.25
1	D	286	GLU	CD-OE2	-6.44	1.18	1.25
1	B	167	GLY	C-O	6.22	1.33	1.23
1	C	46	GLU	CD-OE2	5.55	1.31	1.25
1	A	109	GLY	C-O	5.36	1.32	1.23
1	C	188	GLY	C-O	5.16	1.31	1.23

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	252	ARG	NE-CZ-NH1	-9.18	115.71	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	363	ARG	NE-CZ-NH1	6.12	123.36	120.30
1	B	252	ARG	NE-CZ-NH2	5.98	123.29	120.30
1	B	121	LYS	CB-CA-C	-5.81	98.78	110.40
1	C	363	ARG	NE-CZ-NH2	-5.31	117.65	120.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	244	ASN	Peptide
1	D	38	PRO	Peptide

## 5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3182	0	3065	97	0
1	B	3212	0	3131	89	0
1	C	3188	0	3093	37	0
1	D	3207	0	3119	70	0
2	A	54	0	72	21	0
2	B	42	0	56	21	0
2	C	42	0	56	7	0
2	D	24	0	32	3	0
3	A	98	0	140	40	0
3	B	63	0	90	24	0
3	C	28	0	40	8	0
3	D	14	0	20	0	0
4	A	30	0	42	28	0
4	B	10	0	14	0	0
5	A	26	0	36	8	0
6	A	12	0	12	0	0
6	B	12	0	12	0	0
6	C	12	0	12	0	0
6	D	12	0	12	0	0
7	A	12	0	12	2	0
7	B	12	0	12	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	A	1	0	0	0	0
8	C	2	0	0	0	0
9	B	3	0	0	0	0
9	C	1	0	0	0	0
9	D	2	0	0	0	0
10	D	8	0	12	3	0
11	A	214	0	0	14	0
11	B	209	0	0	14	0
11	C	201	0	0	7	0
11	D	140	0	0	5	0
All	All	14073	0	13090	331	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 12.

All (331) 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:C:147[B]:CYS:HB3	11:C:889:HOH:O	1.42	1.14
3:A:918[A]:PEG:O4	3:A:918[A]:PEG:H22	1.58	1.04
1:B:64[A]:THR:HG21	11:B:844:HOH:O	1.58	1.01
1:D:159[B]:LEU:N	1:D:159[B]:LEU:HD22	1.76	0.99
1:D:71:ARG:HD2	1:D:126:ASP:OD1	1.65	0.96
1:B:125:PHE:CE1	11:B:1002:HOH:O	2.18	0.96
4:A:921:PGE:H4	11:A:1005:HOH:O	1.63	0.95
1:B:64[A]:THR:HG22	1:B:131:SER:OG	1.66	0.94
4:A:921:PGE:C4	11:A:1005:HOH:O	2.15	0.93
1:A:89:GLU:O	4:A:919:PGE:H32	1.70	0.91
3:C:607[A]:PEG:O4	11:C:701:HOH:O	1.81	0.91
1:A:89:GLU:H	4:A:919:PGE:H2	1.38	0.89
1:D:154:ASP:HA	1:D:159[A]:LEU:HD22	1.56	0.87
1:B:311[A]:ARG:NH1	2:B:701:GOL:O1	2.08	0.86
1:C:275:SER:OG	1:C:308:GLU:OE1	1.95	0.85
1:C:387:GLN:NE2	1:C:391:ASP:OD1	2.09	0.84
3:A:918[A]:PEG:O4	3:A:918[A]:PEG:C2	2.27	0.82
1:C:266:ASN:HB3	2:C:606:GOL:H11	1.62	0.81
1:A:206[B]:LEU:HD22	1:A:208:CYS:SG	2.20	0.81
1:A:93:ASP:O	11:A:1002:HOH:O	1.96	0.81
1:D:96[B]:LYS:H	1:D:96[B]:LYS:HD2	1.44	0.80
1:B:140[B]:SER:OG	1:B:143:ALA:HB3	1.82	0.80
1:B:163[B]:ASP:OD2	11:B:801:HOH:O	1.98	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:154:ASP:HA	1:D:159[B]:LEU:HD23	1.64	0.79
1:B:125:PHE:HE1	11:B:1002:HOH:O	1.61	0.79
1:B:271:ALA:HB1	2:B:701:GOL:H31	1.65	0.79
1:D:159[B]:LEU:HD22	1:D:159[B]:LEU:H	1.46	0.78
3:A:917:PEG:H41	11:A:1186:HOH:O	1.83	0.78
3:B:702:PEG:H12	3:B:702:PEG:H41	1.63	0.77
1:D:159[B]:LEU:N	1:D:159[B]:LEU:CD2	2.46	0.77
1:A:7:ILE:HD11	1:A:402:ARG:HD2	1.66	0.77
1:D:48[B]:THR:HG23	1:D:53:GLY:HA3	1.67	0.75
1:B:93:ASP:OD2	11:B:802:HOH:O	2.04	0.75
1:D:159[B]:LEU:H	1:D:159[B]:LEU:CD2	1.99	0.75
1:B:191:ASP:OD2	3:B:704:PEG:H41	1.87	0.74
1:A:77:ARG:NH1	5:A:922:PG4:H21	2.03	0.73
4:A:921:PGE:C1	4:A:921:PGE:H42	2.18	0.73
1:B:275:SER:HB2	2:B:701:GOL:H2	1.70	0.73
1:C:37:ALA:CB	1:C:147[B]:CYS:SG	2.76	0.73
1:C:291:LEU:HD22	1:C:296[B]:MET:HE2	1.71	0.73
3:A:918[A]:PEG:H22	3:A:918[A]:PEG:HO4	1.55	0.72
1:C:415:GLU:O	3:C:608:PEG:H32	1.90	0.72
5:A:922:PG4:C7	2:A:923:GOL:O3	2.37	0.71
1:A:368:GLY:H	3:A:912:PEG:H22	1.55	0.71
1:C:415:GLU:O	3:C:608:PEG:C3	2.39	0.70
1:A:365:THR:O	3:A:912:PEG:H11	1.91	0.70
1:B:50:TYR:CG	1:B:252:ARG:HD3	2.26	0.70
1:D:68[B]:LEU:HD13	1:D:127:ALA:HB2	1.74	0.70
1:B:89:GLU:O	3:B:716:PEG:H31	1.92	0.69
1:D:7:ILE:HD11	1:D:402:ARG:HD2	1.74	0.69
1:C:415:GLU:O	3:C:608:PEG:O2	2.10	0.69
1:D:31:PRO:HG2	2:D:606:GOL:O2	1.93	0.69
1:A:20:THR:HG21	3:A:906:PEG:H12	1.75	0.68
1:D:68[B]:LEU:HD11	1:D:125:PHE:CD2	2.29	0.68
1:B:191:ASP:OD2	3:B:704:PEG:H32	1.94	0.68
1:C:69[B]:LYS:CE	11:C:738:HOH:O	2.42	0.67
1:D:67:ALA:O	1:D:127:ALA:HA	1.94	0.67
1:A:275[A]:SER:O	3:A:918[A]:PEG:H21	1.94	0.67
1:B:140[B]:SER:OG	1:B:140[B]:SER:O	1.99	0.67
1:A:138:GLY:N	2:A:911:GOL:H2	2.10	0.67
1:B:311[A]:ARG:NH2	2:B:701:GOL:O1	2.28	0.67
1:C:291:LEU:HD22	1:C:296[B]:MET:CE	2.25	0.67
1:D:42:ASN:ND2	1:D:190:LEU:HD11	2.10	0.67
1:B:135:LEU:HD12	1:B:135:LEU:H	1.60	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:371:GLY:HA3	3:A:912:PEG:H12	1.77	0.66
5:A:922:PG4:H71	2:A:923:GOL:O3	1.96	0.66
1:A:250[B]:GLN:OE1	4:A:920:PGE:H3	1.96	0.66
1:D:68[B]:LEU:CD1	1:D:127:ALA:HB2	2.26	0.66
1:C:57:PRO:HD2	1:C:204:LEU:O	1.95	0.66
1:D:359:ALA:O	11:D:701:HOH:O	2.13	0.66
1:A:165:ASP:HB2	3:A:908[A]:PEG:H32	1.77	0.65
1:D:157:TYR:HB2	1:D:159[B]:LEU:HD21	1.77	0.65
1:A:342:VAL:HG12	1:A:369:PHE:CZ	2.32	0.65
1:A:266:ASN:HD22	3:A:907:PEG:H42	1.62	0.64
1:B:418:LEU:C	1:B:418:LEU:HD22	2.16	0.64
1:C:266:ASN:HD22	2:C:606:GOL:C1	2.10	0.64
3:A:926:PEG:H41	11:A:1189:HOH:O	1.96	0.64
1:D:8:GLU:HG3	1:D:9:PRO:HD2	1.80	0.64
5:A:922:PG4:C7	2:A:923:GOL:HO3	2.11	0.63
1:D:1:MET:N	1:D:394[B]:GLU:OE2	2.18	0.63
1:A:89:GLU:N	4:A:919:PGE:H2	2.12	0.62
1:A:250[B]:GLN:NE2	4:A:921:PGE:O3	2.32	0.62
1:B:76:VAL:CG2	11:B:1002:HOH:O	2.47	0.62
1:B:238:GLN:NE2	1:B:402:ARG:CZ	2.62	0.62
1:D:346:GLU:OE2	11:D:702:HOH:O	2.16	0.62
1:B:134:PRO:HB2	1:B:402:ARG:NH2	2.14	0.61
1:A:141:SER:H	2:A:911:GOL:H12	1.65	0.61
4:A:921:PGE:O3	11:A:1005:HOH:O	2.14	0.61
1:A:292:PRO:HD2	11:A:1157:HOH:O	2.00	0.61
1:D:96[B]:LYS:HD2	1:D:96[B]:LYS:N	2.15	0.61
1:A:365:THR:O	3:A:912:PEG:C1	2.48	0.60
1:A:228:TYR:OH	2:A:909:GOL:H31	2.01	0.60
1:D:257[A]:GLU:OE1	1:D:257[A]:GLU:HA	2.00	0.60
1:B:191:ASP:OD2	3:B:704:PEG:C4	2.49	0.59
1:D:146:THR:HG21	1:D:179:GLU:HG3	1.82	0.59
1:B:418:LEU:C	1:B:418:LEU:CD2	2.71	0.59
3:A:903:PEG:H11	11:A:1010:HOH:O	2.01	0.59
1:B:89:GLU:HB3	3:B:713:PEG:H12	1.85	0.59
1:B:76:VAL:HG21	11:B:1002:HOH:O	2.02	0.59
1:B:191:ASP:OD2	3:B:704:PEG:C3	2.49	0.59
1:B:304:VAL:O	2:B:701:GOL:O3	2.12	0.59
1:C:147[A]:CYS:SG	11:C:889:HOH:O	0.99	0.59
1:D:68[B]:LEU:HD23	1:D:152:ALA:HB1	1.85	0.58
1:A:141:SER:H	2:A:911:GOL:C1	2.16	0.58
1:B:311[A]:ARG:CZ	2:B:701:GOL:O1	2.51	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:37:ALA:HB1	1:C:147[B]:CYS:SG	2.44	0.58
1:B:72[B]:GLU:CD	11:B:808:HOH:O	2.42	0.58
1:B:32:GLU:OE2	11:B:806:HOH:O	2.16	0.58
1:A:120[A]:ASP:O	1:A:123[A]:LYS:NZ	2.35	0.58
1:D:13[A]:GLU:H	1:D:13[A]:GLU:CD	2.07	0.58
1:B:142:SER:OG	3:B:704:PEG:H31	2.04	0.58
1:C:50:TYR:CD2	1:C:252:ARG:HD3	2.38	0.58
1:B:138:GLY:HA3	2:B:710:GOL:O2	2.04	0.57
1:C:69[B]:LYS:HE2	11:C:738:HOH:O	2.02	0.57
1:B:66:ILE:HD12	1:B:129:PHE:CZ	2.39	0.57
1:C:266:ASN:HD22	2:C:606:GOL:H11	1.68	0.57
1:D:344:VAL:HB	1:D:345:PRO:HD2	1.85	0.57
1:A:90:ALA:HB2	4:A:919:PGE:O4	2.05	0.57
1:B:308:GLU:N	2:B:701:GOL:HO2	2.03	0.57
1:A:275[A]:SER:OG	3:A:914:PEG:H11	2.05	0.56
1:D:154:ASP:OD1	1:D:159[A]:LEU:HB2	2.04	0.56
1:A:293:ASP:OD1	2:A:905:GOL:H31	2.05	0.56
4:A:921:PGE:H42	4:A:921:PGE:H12	1.86	0.56
1:B:140[A]:SER:HA	3:B:704:PEG:H11	1.88	0.56
1:A:276:LYS:CG	3:A:918[A]:PEG:H32	2.36	0.56
1:B:368:GLY:HA2	2:B:710:GOL:H31	1.88	0.56
1:A:254:THR:HG21	1:A:299:ARG:HG3	1.88	0.56
1:B:140[A]:SER:HA	3:B:704:PEG:C1	2.36	0.56
1:D:174:ALA:HA	2:D:603:GOL:H12	1.88	0.56
1:D:96[B]:LYS:H	1:D:96[B]:LYS:CD	2.17	0.55
1:A:71:ARG:NH2	11:A:1011:HOH:O	2.39	0.55
1:D:14:GLU:O	1:D:18:GLN:HG3	2.07	0.55
1:C:173:ASN:OD1	11:C:702:HOH:O	2.18	0.54
3:A:904:PEG:H12	7:A:928[B]:GAL:O1	2.07	0.54
1:B:70:PRO:HG2	2:B:706:GOL:O3	2.07	0.54
1:B:271:ALA:HB1	2:B:701:GOL:C3	2.35	0.54
1:A:77:ARG:HH11	5:A:922:PG4:H21	1.72	0.54
1:D:48[B]:THR:HG21	1:D:54:LEU:O	2.07	0.54
1:A:250[B]:GLN:NE2	4:A:921:PGE:C5	2.71	0.54
1:B:192:GLN:H	1:B:192:GLN:NE2	2.06	0.54
1:A:206[B]:LEU:CD2	1:A:208:CYS:SG	2.96	0.54
1:A:250[B]:GLN:NE2	11:A:1005:HOH:O	2.21	0.53
1:A:322:ILE:H	2:A:925:GOL:H31	1.72	0.53
2:A:911:GOL:O2	11:A:1004:HOH:O	2.13	0.53
1:A:266:ASN:HD22	3:A:907:PEG:C4	2.22	0.53
1:C:338:ALA:HA	2:C:603:GOL:H11	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:155:ASP:OD1	3:B:705:PEG:H22	2.09	0.53
1:B:368:GLY:H	2:B:710:GOL:C3	2.22	0.52
1:D:68[B]:LEU:HD12	1:D:126:ASP:O	2.09	0.52
1:B:82:VAL:CG1	3:B:703:PEG:H11	2.40	0.52
1:A:187:THR:O	3:A:915:PEG:H21	2.09	0.52
1:D:169:VAL:HG21	1:D:214:PRO:HG3	1.90	0.52
5:A:922:PG4:H42	5:A:922:PG4:H72	1.92	0.52
1:D:66:ILE:HG23	1:D:66:ILE:O	2.09	0.52
1:A:138:GLY:H	2:A:911:GOL:H2	1.73	0.52
1:A:245:ASP:OD2	1:A:247[A]:GLN:HG2	2.09	0.52
1:D:333:HIS:CD2	1:D:351:VAL:HG11	2.45	0.52
1:A:228:TYR:HH	2:A:909:GOL:C3	2.23	0.51
1:A:276:LYS:HG2	3:A:918[A]:PEG:H32	1.91	0.51
1:B:271:ALA:C	2:B:701:GOL:H12	2.30	0.51
1:B:311[A]:ARG:HH12	2:B:701:GOL:C1	2.22	0.51
1:B:344:VAL:HB	1:B:345:PRO:CD	2.40	0.51
1:B:272:ASP:O	1:B:276:LYS:HD3	2.11	0.51
1:A:100:VAL:HG22	4:A:919:PGE:O4	2.11	0.51
1:B:308:GLU:N	2:B:701:GOL:O2	2.44	0.51
1:B:368:GLY:CA	2:B:710:GOL:H31	2.40	0.51
1:A:228:TYR:OH	2:A:909:GOL:C3	2.59	0.51
4:A:921:PGE:C4	4:A:921:PGE:C1	2.87	0.51
1:C:143:ALA:O	1:C:147[B]:CYS:SG	2.63	0.51
1:A:206[B]:LEU:C	1:A:206[B]:LEU:HD23	2.32	0.50
1:D:71:ARG:CD	1:D:126:ASP:OD1	2.51	0.50
1:B:7:ILE:HD11	1:B:402:ARG:HD2	1.93	0.50
3:A:903:PEG:C1	11:A:1010:HOH:O	2.60	0.50
1:B:247:GLN:HB3	1:B:369:PHE:CZ	2.47	0.49
1:A:417:LYS:O	1:A:418:LEU:HD23	2.12	0.49
1:B:76:VAL:HA	1:B:125:PHE:O	2.12	0.49
1:B:64[A]:THR:HG22	1:B:131:SER:CB	2.41	0.49
1:A:34:VAL:HA	1:A:66:ILE:O	2.13	0.49
2:A:913:GOL:H32	4:A:921:PGE:O4	2.12	0.49
1:A:273:GLY:O	3:A:926:PEG:C1	2.60	0.49
1:B:313:PHE:CE1	1:B:329:PHE:CE1	3.01	0.49
1:C:172:ILE:HD11	1:C:196:MET:HB2	1.95	0.49
1:D:143:ALA:O	1:D:147:CYS:HB2	2.13	0.49
1:A:158:GLY:HA3	5:A:924:PG4:H61	1.93	0.48
1:D:308[B]:GLU:OE2	1:D:308[B]:GLU:O	2.31	0.48
1:A:333[B]:HIS:CE1	1:A:351:VAL:HG21	2.48	0.48
1:D:68[B]:LEU:CD2	1:D:152:ALA:HB1	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:121:LYS:O	3:B:702:PEG:H21	2.14	0.48
1:B:67:ALA:O	1:B:127:ALA:HA	2.14	0.48
1:C:134:PRO:HB2	1:C:137[A]:SER:OG	2.13	0.48
1:D:48[B]:THR:CG2	1:D:53:GLY:HA3	2.42	0.48
1:D:344:VAL:HB	1:D:345:PRO:CD	2.43	0.48
1:B:140[B]:SER:HA	3:B:704:PEG:H11	1.97	0.47
1:C:66:ILE:HG23	1:C:66:ILE:O	2.13	0.47
1:B:123:LYS:HG3	3:B:702:PEG:H42	1.96	0.47
1:C:266:ASN:CB	2:C:606:GOL:H11	2.41	0.47
1:D:84:PRO:HD2	11:D:823:HOH:O	2.13	0.47
1:A:138:GLY:HA3	3:A:912:PEG:H21	1.97	0.47
1:B:394:GLU:OE2	2:B:717:GOL:O3	2.31	0.47
1:A:250[B]:GLN:HE21	4:A:921:PGE:C6	2.27	0.47
1:B:76:VAL:HG22	11:B:1002:HOH:O	2.12	0.47
1:D:75:LYS:O	1:D:124:GLY:HA3	2.14	0.47
1:A:119:PHE:HA	11:A:1119:HOH:O	2.14	0.47
1:B:75:LYS:O	1:B:124:GLY:HA3	2.15	0.47
1:A:77:ARG:HD2	5:A:922:PG4:H31	1.97	0.46
4:A:921:PGE:H42	4:A:921:PGE:H1	1.93	0.46
1:B:57:PRO:HD2	1:B:204:LEU:O	2.15	0.46
1:D:154:ASP:CA	1:D:159[B]:LEU:HD23	2.39	0.46
1:A:246:GLY:O	4:A:920:PGE:O4	2.33	0.46
1:A:266:ASN:ND2	3:A:907:PEG:H42	2.30	0.46
1:B:68:LEU:HD23	1:B:69:LYS:N	2.31	0.46
1:A:246:GLY:HA3	4:A:920:PGE:H6	1.96	0.46
1:B:238:GLN:NE2	1:B:402:ARG:NH2	2.62	0.46
1:D:112:TRP:HE1	1:D:116:GLN:HE21	1.63	0.46
1:B:55[B]:CYS:SG	1:B:190:LEU:HD13	2.56	0.46
1:B:370:GLY:O	2:B:710:GOL:H31	2.16	0.46
3:A:908[B]:PEG:H22	3:A:908[B]:PEG:H42	1.49	0.46
1:B:69:LYS:CE	2:B:706:GOL:H32	2.46	0.46
1:B:177:LYS:NZ	11:B:832:HOH:O	2.48	0.46
1:B:131:SER:HB3	3:B:703:PEG:H21	1.98	0.46
1:C:109:GLY:C	1:C:178:SER:HB2	2.35	0.46
3:C:607[A]:PEG:H32	3:C:607[A]:PEG:H11	1.45	0.46
2:A:913:GOL:C3	4:A:921:PGE:O4	2.64	0.46
1:B:344:VAL:HB	1:B:345:PRO:HD2	1.97	0.46
1:C:266:ASN:ND2	2:C:606:GOL:H11	2.30	0.46
3:C:610:PEG:H32	3:C:610:PEG:H12	1.65	0.46
1:A:180:ASN:ND2	1:A:187:THR:CG2	2.79	0.45
1:A:322:ILE:HB	2:A:925:GOL:H11	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:215[A]:LEU:CD1	1:D:215[A]:LEU:N	2.79	0.45
1:B:140[B]:SER:HA	3:B:704:PEG:C1	2.46	0.45
1:A:276:LYS:HA	3:A:918[A]:PEG:H21	1.98	0.45
2:A:913:GOL:O3	4:A:921:PGE:O4	2.31	0.45
1:A:215:LEU:N	1:A:215:LEU:CD1	2.79	0.45
1:B:294[B]:GLU:OE2	1:B:298:LYS:HE2	2.17	0.45
1:D:106:TYR:O	1:D:178:SER:OG	2.32	0.45
1:D:210:PRO:HD2	1:D:211:GLU:OE1	2.17	0.45
1:B:50:TYR:CD2	1:B:252:ARG:HD3	2.51	0.45
1:D:149:THR:O	1:D:152:ALA:HB3	2.17	0.45
1:A:206[B]:LEU:CD2	1:A:206[B]:LEU:C	2.85	0.45
1:D:215[A]:LEU:N	1:D:215[A]:LEU:HD12	2.31	0.45
1:A:87:VAL:O	4:A:919:PGE:H12	2.16	0.45
1:A:165:ASP:HB2	3:A:908[A]:PEG:C3	2.46	0.45
1:A:245:ASP:OD2	1:A:247[A]:GLN:CG	2.65	0.45
1:B:140[B]:SER:HB2	3:B:704:PEG:H32	1.99	0.45
1:D:138:GLY:N	10:D:601:TRS:H31	2.27	0.45
4:A:921:PGE:C4	4:A:921:PGE:H1	2.47	0.44
1:B:69:LYS:HE2	2:B:706:GOL:H32	1.98	0.44
3:B:702:PEG:H31	11:B:908:HOH:O	2.16	0.44
1:A:90:ALA:CB	4:A:919:PGE:O4	2.65	0.44
1:C:112:TRP:CD2	1:C:182:MET:HE3	2.53	0.44
1:A:276:LYS:HG3	3:A:918[A]:PEG:H32	1.99	0.44
1:B:121:LYS:CE	11:B:804:HOH:O	2.59	0.44
1:D:134:PRO:HB2	1:D:402:ARG:NH2	2.32	0.44
1:A:266:ASN:HB3	3:A:907:PEG:H31	1.98	0.44
3:C:607[A]:PEG:H11	11:C:773:HOH:O	2.18	0.44
1:D:36:ALA:HA	1:D:64:THR:O	2.18	0.44
1:D:190:LEU:HD23	1:D:190:LEU:C	2.37	0.44
1:A:138:GLY:H	2:A:911:GOL:H31	1.83	0.44
1:A:251:ARG:HH12	4:A:920:PGE:C1	2.30	0.44
1:D:106:TYR:HB2	1:D:107:PRO:HD3	1.99	0.44
1:A:273:GLY:O	3:A:926:PEG:H12	2.17	0.44
1:A:138:GLY:CA	2:A:911:GOL:H2	2.48	0.43
1:A:250[B]:GLN:HE21	4:A:921:PGE:H6	1.83	0.43
1:D:169:VAL:HG21	1:D:214:PRO:CG	2.47	0.43
1:C:134:PRO:HG3	1:C:404:LEU:HD21	1.99	0.43
1:A:179:GLU:OE2	3:A:904:PEG:H42	2.18	0.43
1:A:273:GLY:HA3	3:A:903:PEG:O1	2.18	0.43
3:A:914:PEG:H41	3:A:914:PEG:H21	1.79	0.43
1:D:154:ASP:HB3	11:D:712:HOH:O	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:155:ASP:OD2	1:D:414:ARG:HD3	2.18	0.43
1:A:90:ALA:HB2	4:A:919:PGE:HO4	1.82	0.43
1:D:10:LEU:HG	1:D:132:CYS:HB3	2.01	0.43
1:C:6:PHE:HA	1:C:403:ALA:O	2.18	0.43
1:A:180:ASN:ND2	1:A:187:THR:HG22	2.33	0.43
1:B:155:ASP:CG	3:B:705:PEG:H22	2.39	0.43
1:A:250[B]:GLN:HB2	4:A:920:PGE:H52	2.01	0.42
1:B:64[A]:THR:HG22	1:B:131:SER:HG	1.78	0.42
1:B:417:LYS:HA	11:B:978:HOH:O	2.18	0.42
1:A:37:ALA:HB1	1:A:195:SER:OG	2.18	0.42
1:A:255:CYS:O	1:A:258:ALA:HB3	2.19	0.42
1:C:291:LEU:HD11	1:C:300:VAL:HG21	2.01	0.42
1:A:333[A]:HIS:O	1:A:336:LEU:N	2.52	0.42
3:A:915:PEG:O4	3:A:915:PEG:H22	2.19	0.42
1:A:7:ILE:HD11	1:A:402:ARG:CD	2.42	0.42
1:A:187:THR:HB	3:A:904:PEG:H41	2.01	0.42
1:D:157:TYR:CB	1:D:159[B]:LEU:HD21	2.47	0.42
1:A:349:ILE:O	1:A:353:VAL:HG23	2.20	0.42
1:D:69:LYS:HG2	1:D:70:PRO:HD2	2.02	0.42
1:D:215[B]:LEU:HD12	11:D:744:HOH:O	2.19	0.42
1:A:138:GLY:CA	3:A:912:PEG:H31	2.49	0.42
1:A:322:ILE:HB	2:A:925:GOL:C1	2.50	0.42
1:D:95[A]:LEU:HD23	1:D:95[A]:LEU:HA	1.64	0.42
1:A:206[B]:LEU:HD23	1:A:207:ASP:N	2.34	0.42
1:A:275[A]:SER:HB2	1:A:308:GLU:OE1	2.20	0.42
1:B:72[B]:GLU:OE2	3:B:711:PEG:C1	2.68	0.42
1:B:140[A]:SER:HA	3:B:704:PEG:H12	2.01	0.42
1:C:37:ALA:HB1	1:C:195:SER:OG	2.20	0.42
1:C:180:ASN:O	2:C:609:GOL:O2	2.26	0.42
1:A:120[B]:ASP:OD1	2:A:901:GOL:O2	2.17	0.41
1:C:69[B]:LYS:NZ	1:C:126:ASP:OD2	2.53	0.41
1:D:174:ALA:CA	2:D:603:GOL:H12	2.49	0.41
1:A:101[A]:ASP:OD2	1:A:102:GLY:N	2.47	0.41
1:A:333[A]:HIS:NE2	1:A:343:THR:HG21	2.35	0.41
1:D:74:THR:O	1:D:92:LEU:HG	2.20	0.41
1:B:368:GLY:HA2	2:B:710:GOL:C3	2.50	0.41
1:A:180:ASN:HD21	1:A:187:THR:HG23	1.86	0.41
1:B:342:VAL:HG12	1:B:369:PHE:CZ	2.55	0.41
1:D:110:VAL:HG11	1:D:150:ALA:N	2.35	0.41
1:A:187:THR:HB	3:A:904:PEG:C4	2.51	0.41
3:A:903:PEG:H11	11:A:1023:HOH:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:157:TYR:C	1:D:159[B]:LEU:HD22	2.41	0.41
1:A:248:TYR:CE2	1:A:252:ARG:HD2	2.56	0.41
1:D:315:ARG:HG2	1:D:315:ARG:HH21	1.85	0.41
1:B:45:GLY:HA2	1:B:306:GLU:HG3	2.02	0.41
1:B:198:CYS:O	1:B:411:SER:HB3	2.21	0.41
3:B:704:PEG:H31	3:B:704:PEG:H11	1.77	0.41
1:C:313:PHE:CE1	1:C:329:PHE:CE1	3.09	0.41
1:D:1:MET:HB2	1:D:394[B]:GLU:OE2	2.20	0.41
3:A:904:PEG:C1	7:A:928[B]:GAL:O1	2.68	0.41
1:B:51:ASN:OD1	1:B:255:CYS:HB3	2.21	0.41
1:A:295:THR:O	1:A:299:ARG:HG2	2.21	0.40
1:B:6:PHE:HA	1:B:403:ALA:O	2.20	0.40
1:A:205:LEU:HD22	1:A:314:VAL:HG21	2.03	0.40
1:A:275[A]:SER:OG	3:A:914:PEG:C1	2.68	0.40
1:C:414:ARG:HB2	3:C:607[B]:PEG:O4	2.21	0.40
1:A:75:LYS:O	1:A:124:GLY:HA3	2.21	0.40
1:B:82:VAL:HG12	3:B:703:PEG:H32	2.03	0.40
1:B:288:LEU:O	1:B:297:LYS:NZ	2.49	0.40
1:C:342:VAL:HG12	1:C:369:PHE:CZ	2.57	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	427/429 (100%)	413 (97%)	14 (3%)	0	100	100
1	B	428/429 (100%)	413 (96%)	15 (4%)	0	100	100
1	C	426/429 (99%)	410 (96%)	15 (4%)	1 (0%)	47	29
1	D	427/429 (100%)	403 (94%)	24 (6%)	0	100	100
All	All	1708/1716 (100%)	1639 (96%)	68 (4%)	1 (0%)	51	32

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	158	GLY

### 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	317/326 (97%)	312 (98%)	5 (2%)	62	46
1	B	325/326 (100%)	317 (98%)	8 (2%)	47	26
1	C	322/326 (99%)	314 (98%)	8 (2%)	47	26
1	D	323/326 (99%)	309 (96%)	14 (4%)	29	10
All	All	1287/1304 (99%)	1252 (97%)	35 (3%)	46	24

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	31	PRO
1	A	40	ARG
1	A	72	GLU
1	A	245	ASP
1	A	340	TYR
1	B	40	ARG
1	B	75	LYS
1	B	192	GLN
1	B	261[A]	ILE
1	B	261[B]	ILE
1	B	340	TYR
1	B	399	ASN
1	B	418	LEU
1	C	40	ARG
1	C	41	VAL
1	C	243	LEU
1	C	260	LYS
1	C	276	LYS
1	C	294	GLU

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Mol	Chain	Res	Type
1	C	340	TYR
1	C	384	GLU
1	D	2	THR
1	D	40	ARG
1	D	85	ASP
1	D	126	ASP
1	D	135	LEU
1	D	137[A]	SER
1	D	137[B]	SER
1	D	159[A]	LEU
1	D	159[B]	LEU
1	D	219	SER
1	D	227	LYS
1	D	340	TYR
1	D	352	ASP
1	D	395	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	192	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 78 ligands modelled in this entry, 9 are monoatomic - leaving 69 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	$\# Z  > 2$
3	PEG	D	605	-	6,6,6	0.34	0	5,5,5	0.30	0
3	PEG	A	926	-	6,6,6	0.28	0	5,5,5	0.23	0
7	GAL	B	719[B]	-	12,12,12	0.45	0	17,17,17	0.69	0
3	PEG	A	912	-	6,6,6	0.39	0	5,5,5	0.27	0
3	PEG	A	914	-	6,6,6	0.46	0	5,5,5	0.25	0
3	PEG	B	703	-	6,6,6	0.43	0	5,5,5	0.30	0
2	GOL	B	712	-	5,5,5	0.15	0	5,5,5	0.40	0
2	GOL	C	604	-	5,5,5	0.11	0	5,5,5	0.27	0
3	PEG	A	906	-	6,6,6	0.27	0	5,5,5	0.19	0
3	PEG	A	918[B]	-	6,6,6	0.29	0	5,5,5	0.10	0
2	GOL	A	913	-	5,5,5	0.16	0	5,5,5	0.40	0
3	PEG	A	904	-	6,6,6	0.31	0	5,5,5	0.24	0
3	PEG	D	602	-	6,6,6	0.31	0	5,5,5	0.30	0
6	GLA	A	927[A]	-	12,12,12	1.23	1 (8%)	17,17,17	1.36	3 (17%)
2	GOL	B	701	-	5,5,5	0.21	0	5,5,5	0.41	0
2	GOL	A	923	-	5,5,5	0.14	0	5,5,5	0.30	0
2	GOL	D	607	-	5,5,5	0.16	0	5,5,5	0.44	0
3	PEG	B	715	-	6,6,6	0.39	0	5,5,5	0.24	0
2	GOL	C	606	-	5,5,5	0.17	0	5,5,5	0.41	0
3	PEG	C	610	-	6,6,6	0.24	0	5,5,5	0.33	0
5	PG4	A	924	-	12,12,12	0.21	0	11,11,11	0.26	0
3	PEG	B	713	-	6,6,6	0.27	0	5,5,5	0.43	0
2	GOL	B	709	-	5,5,5	0.09	0	5,5,5	0.28	0
2	GOL	A	902	-	5,5,5	0.24	0	5,5,5	0.55	0
2	GOL	A	909	-	5,5,5	0.08	0	5,5,5	0.30	0
6	GLA	C	611	-	12,12,12	1.13	0	17,17,17	1.44	3 (17%)
3	PEG	A	917	-	6,6,6	0.26	0	5,5,5	0.44	0
2	GOL	D	606	-	5,5,5	0.16	0	5,5,5	0.43	0
3	PEG	A	908[A]	-	6,6,6	0.20	0	5,5,5	0.21	0
3	PEG	A	903	-	6,6,6	0.29	0	5,5,5	0.29	0
3	PEG	A	908[B]	-	6,6,6	0.12	0	5,5,5	0.21	0
3	PEG	B	716	-	6,6,6	0.36	0	5,5,5	0.24	0
4	PGE	A	920	-	9,9,9	0.30	0	8,8,8	0.34	0
2	GOL	C	605	-	5,5,5	0.14	0	5,5,5	0.43	0
2	GOL	A	925	-	5,5,5	0.10	0	5,5,5	0.40	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	GOL	A	905	-	5,5,5	0.16	0	5,5,5	0.45	0
7	GAL	A	928[B]	-	12,12,12	0.48	0	17,17,17	0.91	0
6	GLA	D	608	-	12,12,12	0.90	0	17,17,17	1.28	2 (11%)
3	PEG	B	704	-	6,6,6	0.34	0	5,5,5	0.24	0
3	PEG	B	711	-	6,6,6	0.25	0	5,5,5	0.19	0
3	PEG	A	907	-	6,6,6	0.28	0	5,5,5	0.29	0
2	GOL	A	916	-	5,5,5	0.09	0	5,5,5	0.30	0
3	PEG	B	705	-	6,6,6	0.40	0	5,5,5	0.25	0
2	GOL	C	602	-	5,5,5	0.18	0	5,5,5	0.39	0
3	PEG	A	915	-	6,6,6	0.38	0	5,5,5	0.39	0
4	PGE	B	714	-	9,9,9	0.29	0	8,8,8	0.22	0
2	GOL	B	717	-	5,5,5	0.12	0	5,5,5	0.36	0
2	GOL	A	911	-	5,5,5	0.16	0	5,5,5	0.55	0
2	GOL	A	901	-	5,5,5	0.08	0	5,5,5	0.27	0
3	PEG	C	607[A]	-	6,6,6	0.42	0	5,5,5	0.37	0
2	GOL	B	710	-	5,5,5	0.21	0	5,5,5	0.54	0
2	GOL	C	603	-	5,5,5	0.13	0	5,5,5	0.32	0
3	PEG	B	702	-	6,6,6	0.45	0	5,5,5	0.38	0
2	GOL	B	706	-	5,5,5	0.11	0	5,5,5	0.31	0
3	PEG	A	910	-	6,6,6	0.17	0	5,5,5	0.18	0
3	PEG	C	607[B]	-	6,6,6	0.23	0	5,5,5	0.17	0
3	PEG	C	608	-	6,6,6	0.45	0	5,5,5	0.54	0
4	PGE	A	919	-	9,9,9	0.23	0	8,8,8	0.15	0
10	TRS	D	601	-	7,7,7	0.17	0	9,9,9	0.56	0
4	PGE	A	921	-	9,9,9	0.32	0	8,8,8	0.18	0
2	GOL	C	601	-	5,5,5	0.17	0	5,5,5	0.47	0
2	GOL	C	609	-	5,5,5	0.15	0	5,5,5	0.29	0
3	PEG	B	708	-	6,6,6	0.38	0	5,5,5	0.27	0
2	GOL	D	603	-	5,5,5	0.20	0	5,5,5	0.38	0
5	PG4	A	922	-	12,12,12	0.29	0	11,11,11	0.15	0
6	GLA	B	718[A]	-	12,12,12	0.90	0	17,17,17	1.00	0
3	PEG	A	918[A]	-	6,6,6	0.24	0	5,5,5	0.14	0
2	GOL	B	707	-	5,5,5	0.14	0	5,5,5	0.37	0
2	GOL	D	604	-	5,5,5	0.14	0	5,5,5	0.26	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
3	PEG	D	605	-	-	2/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PEG	A	926	-	-	3/4/4/4	-
7	GAL	B	719[B]	-	-	1/2/22/22	0/1/1/1
3	PEG	A	912	-	-	3/4/4/4	-
3	PEG	A	914	-	-	3/4/4/4	-
3	PEG	B	703	-	-	2/4/4/4	-
2	GOL	B	712	-	-	3/4/4/4	-
2	GOL	C	604	-	-	4/4/4/4	-
3	PEG	A	906	-	-	3/4/4/4	-
3	PEG	A	918[B]	-	-	3/4/4/4	-
2	GOL	A	913	-	-	0/4/4/4	-
3	PEG	A	904	-	-	2/4/4/4	-
3	PEG	D	602	-	-	4/4/4/4	-
6	GLA	A	927[A]	-	-	1/2/22/22	0/1/1/1
2	GOL	B	701	-	-	0/4/4/4	-
2	GOL	A	923	-	-	4/4/4/4	-
2	GOL	D	607	-	-	2/4/4/4	-
3	PEG	B	715	-	-	4/4/4/4	-
2	GOL	C	606	-	-	4/4/4/4	-
3	PEG	C	610	-	-	3/4/4/4	-
5	PG4	A	924	-	-	7/10/10/10	-
3	PEG	B	713	-	-	4/4/4/4	-
2	GOL	B	709	-	-	3/4/4/4	-
2	GOL	A	902	-	-	3/4/4/4	-
2	GOL	A	909	-	-	4/4/4/4	-
6	GLA	C	611	-	-	1/2/22/22	0/1/1/1
3	PEG	A	917	-	-	3/4/4/4	-
2	GOL	D	606	-	-	4/4/4/4	-
3	PEG	A	908[A]	-	-	3/4/4/4	-
3	PEG	A	903	-	-	4/4/4/4	-
3	PEG	A	908[B]	-	-	3/4/4/4	-
3	PEG	B	716	-	-	4/4/4/4	-
4	PGE	A	920	-	-	4/7/7/7	-
2	GOL	C	605	-	-	2/4/4/4	-
2	GOL	A	925	-	-	2/4/4/4	-
2	GOL	A	905	-	-	0/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	GAL	A	928[B]	-	-	2/2/22/22	0/1/1/1
6	GLA	D	608	-	-	2/2/22/22	0/1/1/1
3	PEG	B	704	-	-	3/4/4/4	-
3	PEG	B	711	-	-	1/4/4/4	-
3	PEG	A	907	-	-	3/4/4/4	-
2	GOL	A	916	-	-	3/4/4/4	-
3	PEG	B	705	-	-	3/4/4/4	-
2	GOL	C	602	-	-	1/4/4/4	-
3	PEG	A	915	-	-	2/4/4/4	-
4	PGE	B	714	-	-	4/7/7/7	-
2	GOL	B	717	-	-	4/4/4/4	-
2	GOL	A	911	-	-	4/4/4/4	-
2	GOL	A	901	-	-	2/4/4/4	-
3	PEG	C	607[A]	-	-	3/4/4/4	-
2	GOL	B	710	-	-	4/4/4/4	-
2	GOL	C	603	-	-	3/4/4/4	-
3	PEG	B	702	-	-	3/4/4/4	-
2	GOL	B	706	-	-	0/4/4/4	-
3	PEG	A	910	-	-	2/4/4/4	-
3	PEG	C	607[B]	-	-	3/4/4/4	-
3	PEG	C	608	-	-	4/4/4/4	-
4	PGE	A	919	-	-	4/7/7/7	-
10	TRS	D	601	-	-	2/9/9/9	-
4	PGE	A	921	-	-	4/7/7/7	-
2	GOL	C	601	-	-	2/4/4/4	-
2	GOL	C	609	-	-	2/4/4/4	-
3	PEG	B	708	-	-	3/4/4/4	-
2	GOL	D	603	-	-	2/4/4/4	-
5	PG4	A	922	-	-	5/10/10/10	-
6	GLA	B	718[A]	-	-	1/2/22/22	0/1/1/1
3	PEG	A	918[A]	-	-	2/4/4/4	-
2	GOL	B	707	-	-	4/4/4/4	-
2	GOL	D	604	-	-	0/4/4/4	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	927[A]	GLA	C4-C3	2.11	1.57	1.52

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	D	608	GLA	O3-C3-C4	3.11	117.70	110.38
6	C	611	GLA	O2-C2-C3	3.02	117.50	110.38
6	C	611	GLA	C1-O5-C5	2.92	119.30	113.65
6	A	927[A]	GLA	O5-C5-C6	2.82	113.42	106.44
6	A	927[A]	GLA	C1-O5-C5	2.55	118.58	113.65
6	C	611	GLA	C1-C2-C3	2.29	115.03	110.36
6	D	608	GLA	O5-C1-C2	-2.22	106.40	110.30
6	A	927[A]	GLA	O2-C2-C1	2.15	114.22	109.25

There are no chirality outliers.

All (189) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	901	GOL	O1-C1-C2-O2
2	A	901	GOL	O1-C1-C2-C3
2	A	902	GOL	O1-C1-C2-C3
2	A	909	GOL	O1-C1-C2-O2
2	A	909	GOL	O1-C1-C2-C3
2	A	911	GOL	O1-C1-C2-C3
2	A	911	GOL	C1-C2-C3-O3
2	A	923	GOL	C1-C2-C3-O3
2	A	925	GOL	O1-C1-C2-C3
2	B	707	GOL	O1-C1-C2-O2
2	B	707	GOL	O1-C1-C2-C3
2	B	709	GOL	C1-C2-C3-O3
2	B	710	GOL	O1-C1-C2-C3
2	B	717	GOL	O1-C1-C2-O2
2	B	717	GOL	C1-C2-C3-O3
2	C	601	GOL	C1-C2-C3-O3
2	C	603	GOL	C1-C2-C3-O3
2	C	604	GOL	O1-C1-C2-C3
2	C	606	GOL	O1-C1-C2-O2
2	C	606	GOL	O1-C1-C2-C3
2	C	609	GOL	C1-C2-C3-O3
2	C	609	GOL	O2-C2-C3-O3
2	D	606	GOL	O1-C1-C2-C3
2	D	607	GOL	O1-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
3	A	908[B]	PEG	C4-C3-O2-C2
3	A	918[A]	PEG	C4-C3-O2-C2
3	C	607[A]	PEG	C1-C2-O2-C3
3	B	702	PEG	C1-C2-O2-C3
3	A	914	PEG	C4-C3-O2-C2
3	C	610	PEG	C1-C2-O2-C3
3	C	608	PEG	C1-C2-O2-C3
3	B	705	PEG	O1-C1-C2-O2
4	B	714	PGE	O3-C5-C6-O4
4	A	919	PGE	O2-C3-C4-O3
6	A	927[A]	GLA	O5-C5-C6-O6
2	A	909	GOL	O2-C2-C3-O3
3	A	917	PEG	C4-C3-O2-C2
3	A	908[A]	PEG	O1-C1-C2-O2
3	A	908[B]	PEG	O1-C1-C2-O2
3	A	918[B]	PEG	O2-C3-C4-O4
3	A	926	PEG	O1-C1-C2-O2
3	B	703	PEG	O2-C3-C4-O4
3	B	708	PEG	O1-C1-C2-O2
3	B	711	PEG	O1-C1-C2-O2
3	B	716	PEG	O1-C1-C2-O2
3	C	607[B]	PEG	O2-C3-C4-O4
4	A	920	PGE	O1-C1-C2-O2
7	A	928[B]	GAL	O5-C5-C6-O6
3	A	910	PEG	O1-C1-C2-O2
3	A	912	PEG	O1-C1-C2-O2
3	B	713	PEG	O1-C1-C2-O2
3	C	610	PEG	O2-C3-C4-O4
3	D	602	PEG	O2-C3-C4-O4
4	A	919	PGE	O3-C5-C6-O4
4	A	920	PGE	O3-C5-C6-O4
4	A	921	PGE	O1-C1-C2-O2
4	A	921	PGE	O3-C5-C6-O4
5	A	922	PG4	O4-C7-C8-O5
6	D	608	GLA	O5-C5-C6-O6
2	A	909	GOL	C1-C2-C3-O3
2	A	916	GOL	C1-C2-C3-O3
2	A	923	GOL	O1-C1-C2-C3
2	B	707	GOL	C1-C2-C3-O3
2	B	710	GOL	C1-C2-C3-O3
2	B	712	GOL	C1-C2-C3-O3
2	B	717	GOL	O1-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
2	C	605	GOL	O1-C1-C2-C3
2	C	606	GOL	C1-C2-C3-O3
2	D	603	GOL	O1-C1-C2-C3
2	D	606	GOL	C1-C2-C3-O3
3	A	906	PEG	O2-C3-C4-O4
3	B	702	PEG	O1-C1-C2-O2
3	B	715	PEG	O1-C1-C2-O2
3	B	715	PEG	O2-C3-C4-O4
3	C	608	PEG	O2-C3-C4-O4
5	A	922	PG4	O1-C1-C2-O2
2	A	902	GOL	O1-C1-C2-O2
2	A	911	GOL	O1-C1-C2-O2
2	A	911	GOL	O2-C2-C3-O3
2	A	923	GOL	O2-C2-C3-O3
2	A	925	GOL	O1-C1-C2-O2
2	B	709	GOL	O2-C2-C3-O3
2	B	710	GOL	O1-C1-C2-O2
2	B	717	GOL	O2-C2-C3-O3
2	C	603	GOL	O2-C2-C3-O3
2	C	604	GOL	O1-C1-C2-O2
2	D	603	GOL	O1-C1-C2-O2
2	D	607	GOL	O1-C1-C2-O2
3	A	907	PEG	O2-C3-C4-O4
3	A	917	PEG	O2-C3-C4-O4
3	A	926	PEG	O2-C3-C4-O4
3	C	607[A]	PEG	O2-C3-C4-O4
5	A	924	PG4	O4-C7-C8-O5
3	D	602	PEG	C4-C3-O2-C2
5	A	924	PG4	O3-C5-C6-O4
6	B	718[A]	GLA	O5-C5-C6-O6
4	A	920	PGE	O2-C3-C4-O3
3	A	904	PEG	O1-C1-C2-O2
3	A	908[A]	PEG	O2-C3-C4-O4
3	B	713	PEG	O2-C3-C4-O4
3	C	610	PEG	O1-C1-C2-O2
3	D	605	PEG	O1-C1-C2-O2
6	C	611	GLA	O5-C5-C6-O6
2	A	916	GOL	O2-C2-C3-O3
2	B	710	GOL	O2-C2-C3-O3
2	D	606	GOL	O1-C1-C2-O2
3	D	602	PEG	O1-C1-C2-O2
3	A	903	PEG	C4-C3-O2-C2

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Mol	Chain	Res	Type	Atoms
7	B	719[B]	GAL	O5-C5-C6-O6
3	B	705	PEG	O2-C3-C4-O4
2	A	902	GOL	O2-C2-C3-O3
2	B	707	GOL	O2-C2-C3-O3
2	B	712	GOL	O2-C2-C3-O3
2	C	603	GOL	O1-C1-C2-O2
2	D	606	GOL	O2-C2-C3-O3
3	A	915	PEG	C4-C3-O2-C2
5	A	922	PG4	O2-C3-C4-O3
2	A	916	GOL	O1-C1-C2-O2
2	B	709	GOL	O1-C1-C2-O2
2	C	602	GOL	O2-C2-C3-O3
3	A	910	PEG	O2-C3-C4-O4
3	A	918[B]	PEG	O1-C1-C2-O2
3	B	703	PEG	C1-C2-O2-C3
3	A	918[B]	PEG	C1-C2-O2-C3
3	C	608	PEG	C4-C3-O2-C2
5	A	924	PG4	C4-C3-O2-C2
4	B	714	PGE	C6-C5-O3-C4
3	B	715	PEG	C4-C3-O2-C2
4	A	921	PGE	C3-C4-O3-C5
3	A	906	PEG	O1-C1-C2-O2
3	C	608	PEG	O1-C1-C2-O2
5	A	924	PG4	O1-C1-C2-O2
3	C	607[A]	PEG	C4-C3-O2-C2
3	B	704	PEG	C1-C2-O2-C3
3	B	708	PEG	C4-C3-O2-C2
5	A	924	PG4	C1-C2-O2-C3
3	A	907	PEG	C4-C3-O2-C2
5	A	922	PG4	C5-C6-O4-C7
4	B	714	PGE	O1-C1-C2-O2
3	D	602	PEG	C1-C2-O2-C3
2	A	923	GOL	O1-C1-C2-O2
2	C	601	GOL	O2-C2-C3-O3
2	C	606	GOL	O2-C2-C3-O3
3	B	713	PEG	C4-C3-O2-C2
4	B	714	PGE	C4-C3-O2-C2
3	A	903	PEG	O2-C3-C4-O4
3	A	914	PEG	O1-C1-C2-O2
3	A	918[A]	PEG	O1-C1-C2-O2
3	D	605	PEG	C1-C2-O2-C3
3	C	607[B]	PEG	C1-C2-O2-C3

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Mol	Chain	Res	Type	Atoms
3	B	704	PEG	C4-C3-O2-C2
3	B	705	PEG	C1-C2-O2-C3
3	A	906	PEG	C4-C3-O2-C2
3	A	907	PEG	C1-C2-O2-C3
3	B	708	PEG	C1-C2-O2-C3
5	A	924	PG4	C3-C4-O3-C5
3	B	704	PEG	O2-C3-C4-O4
2	C	605	GOL	O1-C1-C2-O2
3	A	912	PEG	C1-C2-O2-C3
5	A	924	PG4	C5-C6-O4-C7
3	A	903	PEG	O1-C1-C2-O2
3	A	915	PEG	O1-C1-C2-O2
3	A	908[A]	PEG	C4-C3-O2-C2
4	A	920	PGE	C6-C5-O3-C4
6	D	608	GLA	C4-C5-C6-O6
3	A	908[B]	PEG	C1-C2-O2-C3
3	B	716	PEG	C4-C3-O2-C2
3	A	917	PEG	C1-C2-O2-C3
3	B	716	PEG	O2-C3-C4-O4
3	C	607[B]	PEG	C4-C3-O2-C2
7	A	928[B]	GAL	C4-C5-C6-O6
10	D	601	TRS	C3-C-C1-O1
10	D	601	TRS	N-C-C1-O1
5	A	922	PG4	C6-C5-O3-C4
2	C	604	GOL	O2-C2-C3-O3
4	A	919	PGE	C3-C4-O3-C5
3	B	702	PEG	O2-C3-C4-O4
3	A	912	PEG	C4-C3-O2-C2
3	B	713	PEG	C1-C2-O2-C3
2	B	712	GOL	O1-C1-C2-O2
4	A	919	PGE	C6-C5-O3-C4
2	C	604	GOL	C1-C2-C3-O3
3	A	926	PEG	C4-C3-O2-C2
3	A	904	PEG	C1-C2-O2-C3
3	B	715	PEG	C1-C2-O2-C3
3	A	903	PEG	C1-C2-O2-C3
3	B	716	PEG	C1-C2-O2-C3
3	A	914	PEG	C1-C2-O2-C3
4	A	921	PGE	O2-C3-C4-O3

There are no ring outliers.

46 monomers are involved in 157 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	926	PEG	3	0
3	A	912	PEG	6	0
3	A	914	PEG	3	0
3	B	703	PEG	3	0
3	A	906	PEG	1	0
2	A	913	GOL	3	0
3	A	904	PEG	5	0
2	B	701	GOL	11	0
2	A	923	GOL	3	0
2	C	606	GOL	5	0
3	C	610	PEG	1	0
5	A	924	PG4	1	0
3	B	713	PEG	1	0
2	A	909	GOL	3	0
3	A	917	PEG	1	0
2	D	606	GOL	1	0
3	A	908[A]	PEG	2	0
3	A	903	PEG	4	0
3	A	908[B]	PEG	1	0
3	B	716	PEG	1	0
4	A	920	PGE	5	0
2	A	925	GOL	3	0
2	A	905	GOL	1	0
7	A	928[B]	GAL	2	0
3	B	704	PEG	12	0
3	B	711	PEG	1	0
3	A	907	PEG	4	0
3	B	705	PEG	2	0
3	A	915	PEG	2	0
2	B	717	GOL	1	0
2	A	911	GOL	7	0
2	A	901	GOL	1	0
3	C	607[A]	PEG	3	0
2	B	710	GOL	6	0
2	C	603	GOL	1	0
3	B	702	PEG	4	0
2	B	706	GOL	3	0
3	C	607[B]	PEG	1	0
3	C	608	PEG	3	0
4	A	919	PGE	8	0
10	D	601	TRS	3	0
4	A	921	PGE	15	0
2	C	609	GOL	1	0

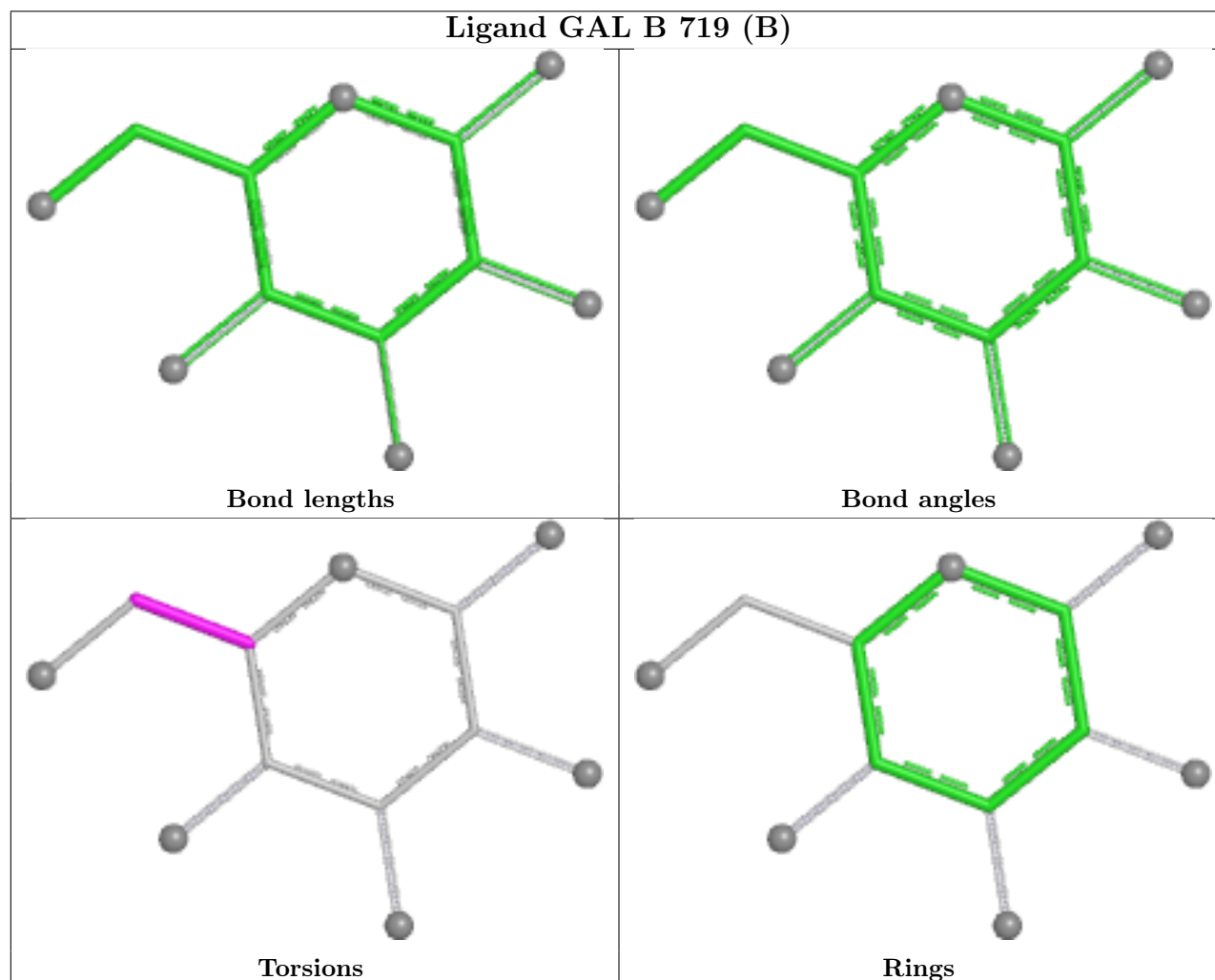
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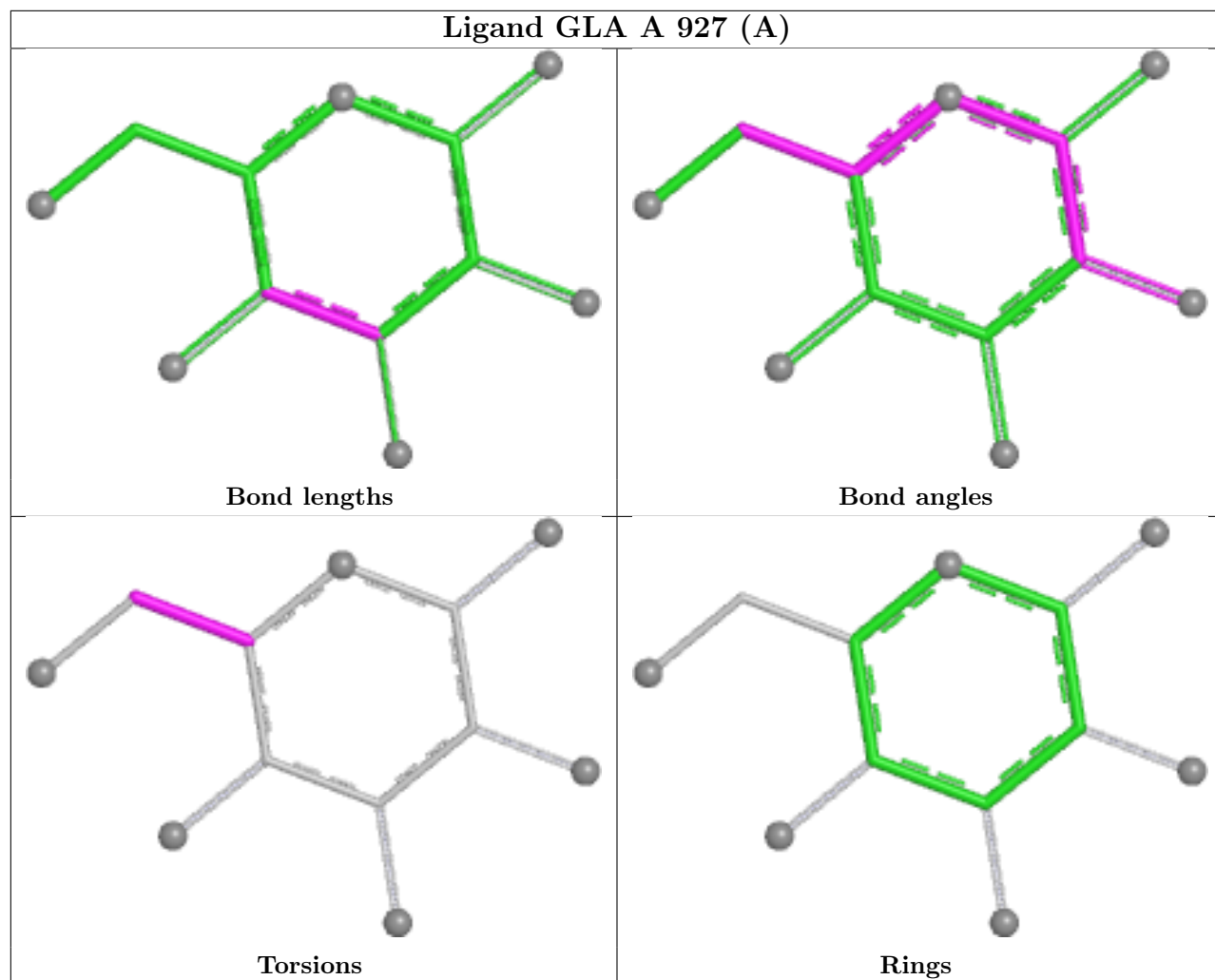
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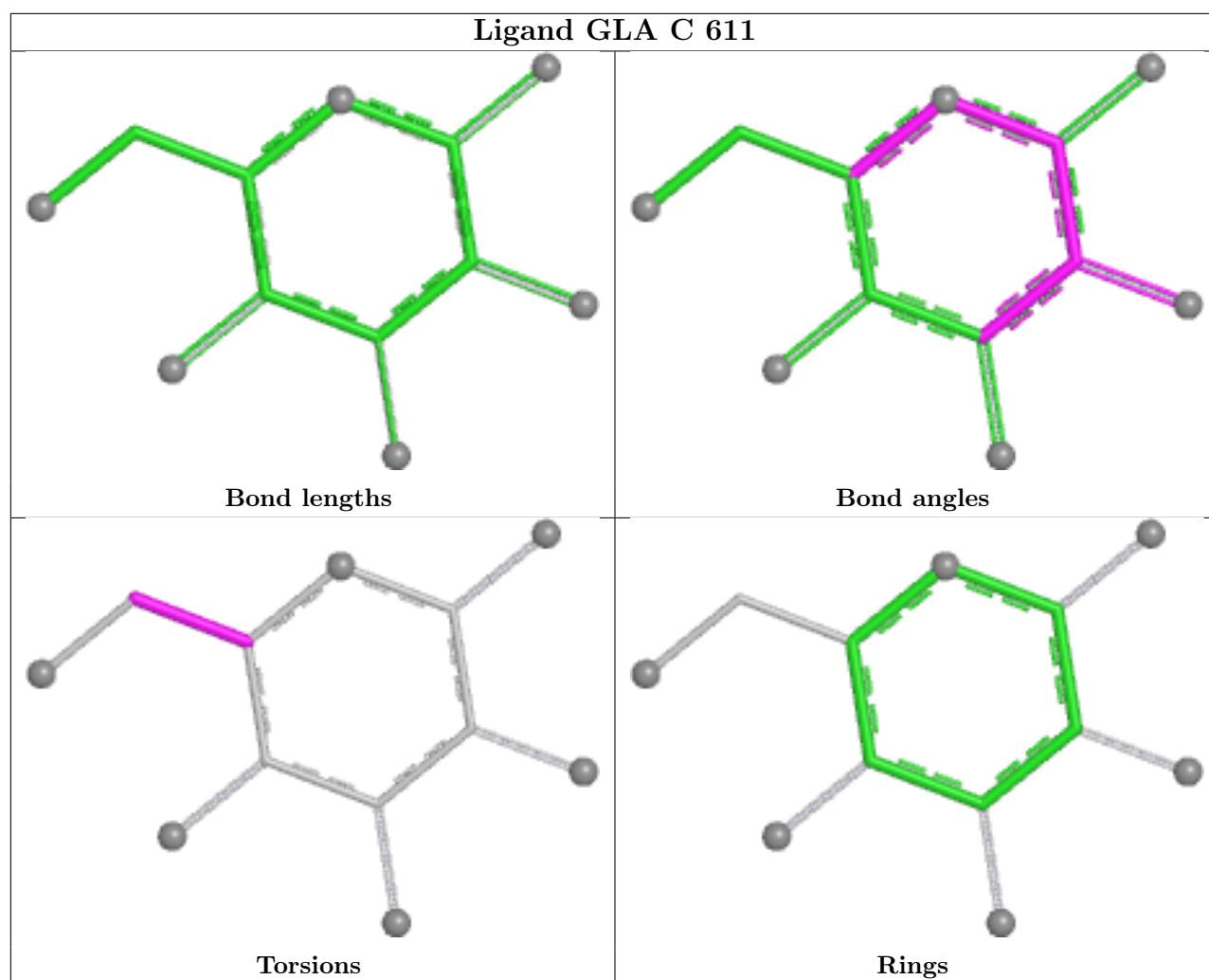
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	603	GOL	2	0
5	A	922	PG4	7	0
3	A	918[A]	PEG	8	0

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.

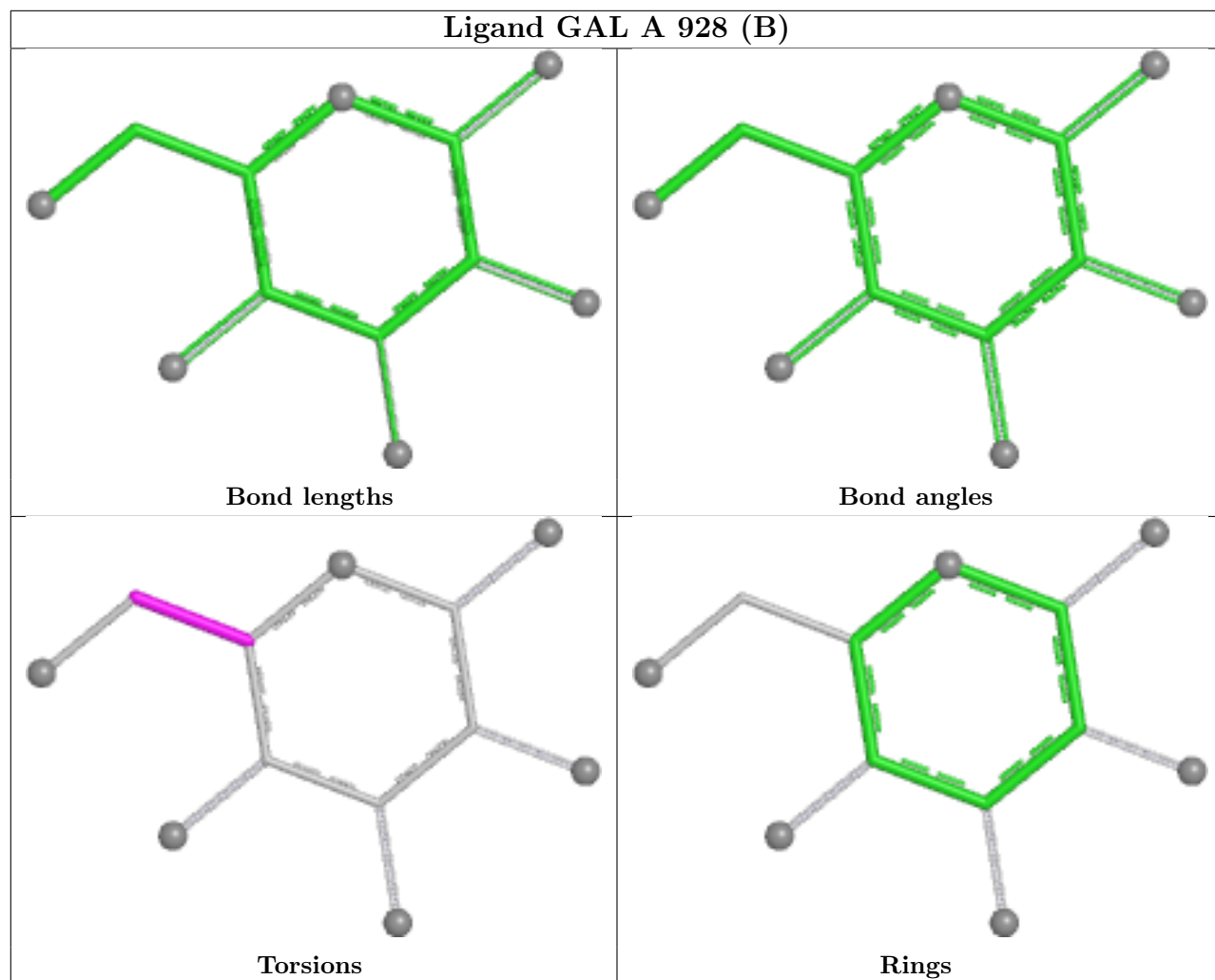


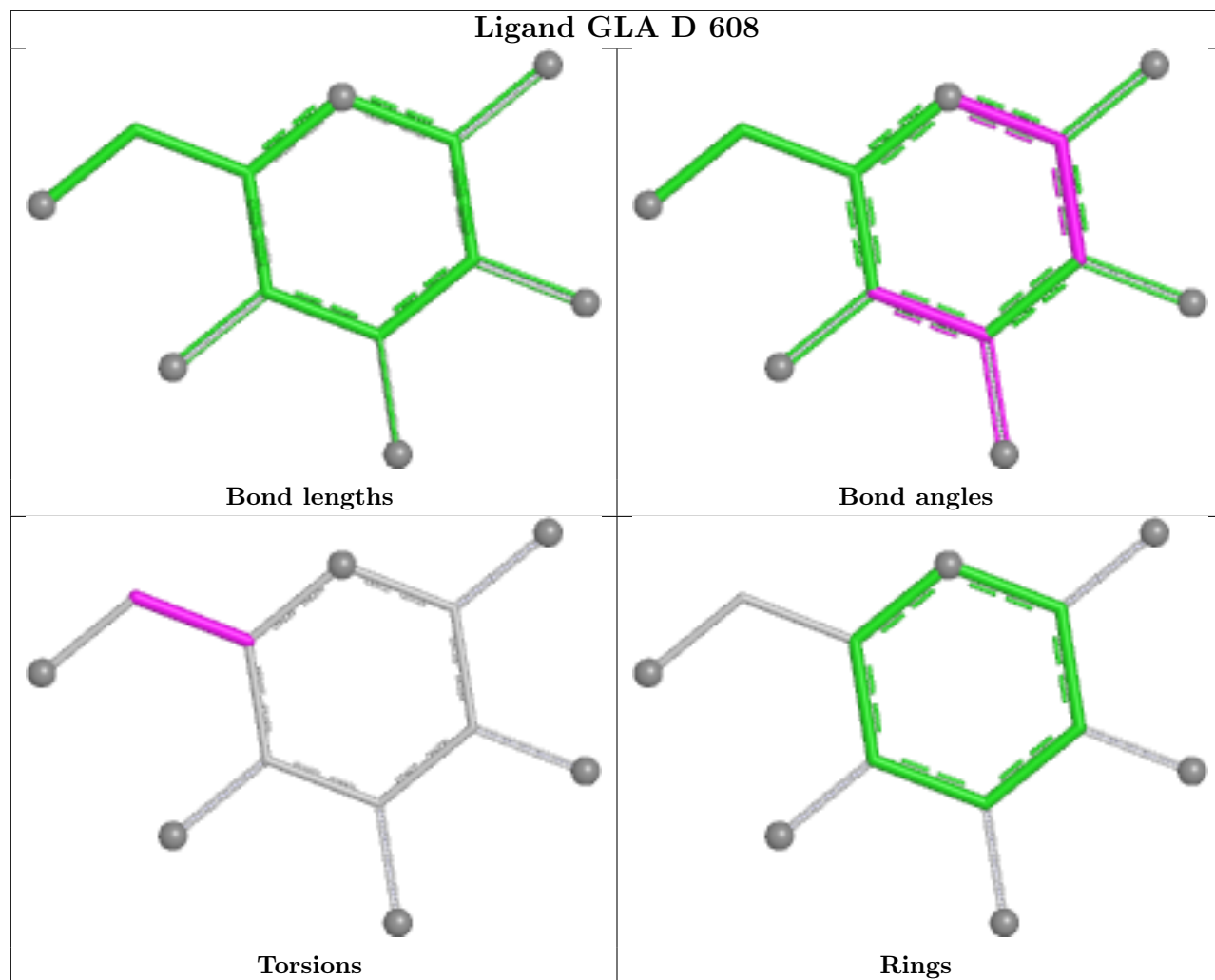
## Ligand GLA A 927 (A)

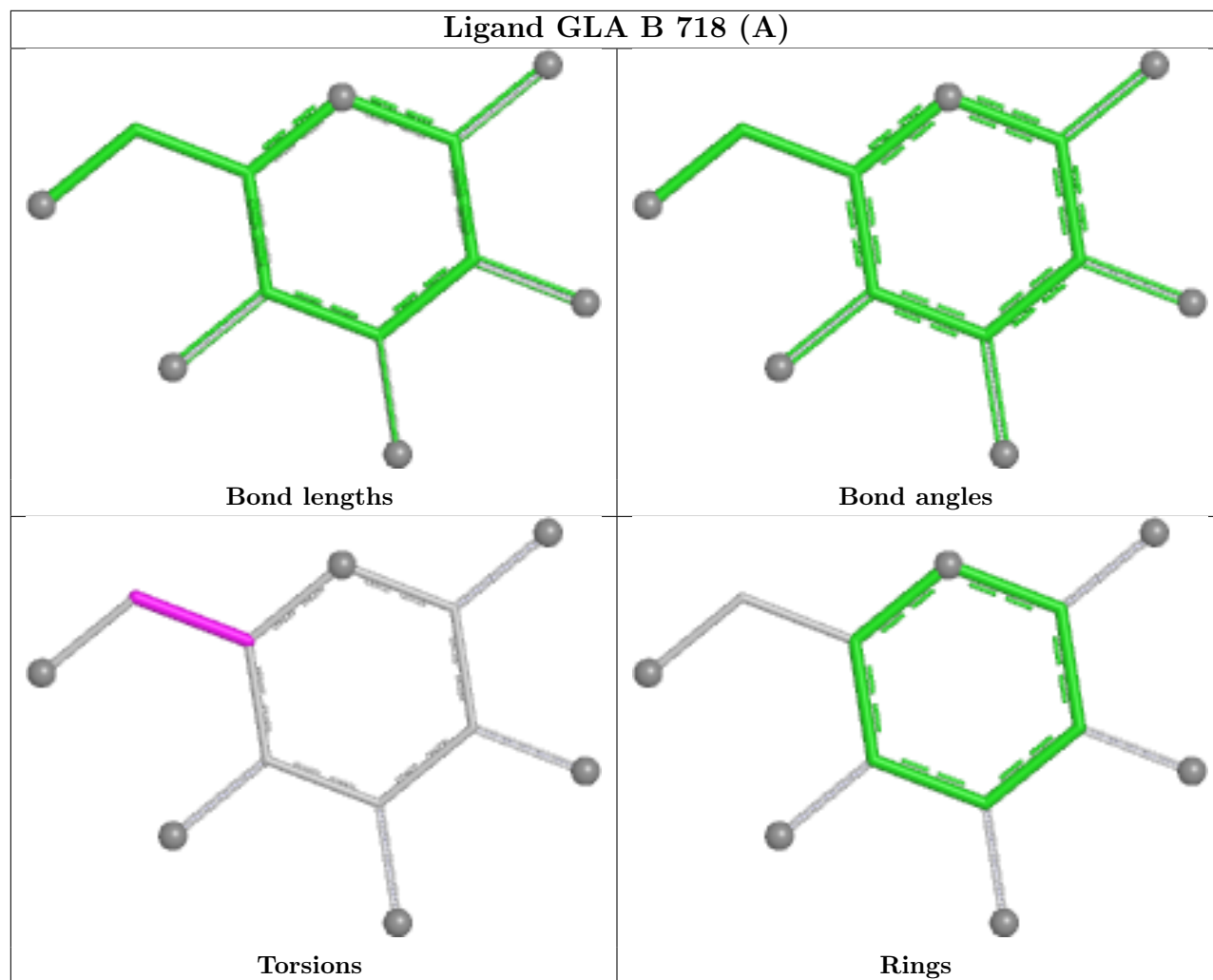




## Ligand GAL A 928 (B)







## 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	418/429 (97%)	0.14	5 (1%) 79 82	13, 22, 36, 66	6 (1%)
1	B	418/429 (97%)	0.20	7 (1%) 70 74	12, 21, 35, 65	5 (1%)
1	C	416/429 (96%)	0.22	7 (1%) 70 74	15, 24, 37, 71	6 (1%)
1	D	416/429 (96%)	0.56	31 (7%) 14 15	17, 31, 48, 69	3 (0%)
All	All	1668/1716 (97%)	0.28	50 (2%) 50 53	12, 24, 42, 71	20 (1%)

All (50) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	122	VAL	5.6
1	A	243	LEU	5.0
1	D	398	PHE	4.8
1	D	243	LEU	4.5
1	D	82	VAL	4.0
1	D	94	GLY	4.0
1	D	135	LEU	3.8
1	B	242	GLN	3.8
1	D	92	LEU	3.7
1	D	79	VAL	3.6
1	C	88	ALA	3.6
1	D	103	TRP	3.5
1	D	3	ALA	3.5
1	B	244	ASN	3.4
1	D	87	VAL	3.4
1	B	1	MET	3.2
1	D	83	ALA	3.1
1	D	4	VAL	3.1
1	D	416	ALA	3.0
1	C	2[A]	THR	3.0
1	B	243	LEU	3.0

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Mol	Chain	Res	Type	RSRZ
1	D	76	VAL	3.0
1	D	130	VAL	3.0
1	C	1	MET	2.9
1	D	19	ALA	2.8
1	A	242	GLN	2.8
1	D	245	ASP	2.7
1	D	400	ALA	2.6
1	D	393	PHE	2.6
1	D	98	ARG	2.5
1	D	244	ASN	2.5
1	D	6	PHE	2.5
1	D	215[A]	LEU	2.4
1	B	101	ASP	2.3
1	D	28	GLY	2.3
1	B	240	PRO	2.3
1	D	401	PRO	2.3
1	A	418	LEU	2.3
1	C	147[A]	CYS	2.2
1	B	82	VAL	2.2
1	D	184	GLY	2.2
1	D	242	GLN	2.2
1	A	1	MET	2.2
1	D	1	MET	2.1
1	C	30	ALA	2.1
1	D	185	ALA	2.1
1	C	85	ASP	2.1
1	D	85	ASP	2.1
1	C	123[A]	LYS	2.1
1	A	2	THR	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 ⓘ

There are no monosaccharides 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
3	PEG	A	915	7/7	0.70	0.29	34,40,51,79	0
2	GOL	C	603	6/6	0.71	0.26	45,49,58,58	0
2	GOL	A	911	6/6	0.75	0.20	18,22,24,29	6
2	GOL	A	913	6/6	0.78	0.22	30,36,47,51	0
2	GOL	B	701	6/6	0.78	0.29	17,18,21,29	6
3	PEG	B	705	7/7	0.78	0.18	28,39,47,47	0
3	PEG	A	908[B]	7/7	0.79	0.24	23,24,27,27	7
2	GOL	C	602	6/6	0.79	0.20	27,30,32,35	6
3	PEG	A	908[A]	7/7	0.79	0.24	14,19,23,28	7
2	GOL	B	710	6/6	0.82	0.36	31,35,42,53	0
3	PEG	A	918[B]	7/7	0.83	0.22	26,29,42,45	7
3	PEG	A	918[A]	7/7	0.83	0.22	21,23,26,27	7
3	PEG	C	608	7/7	0.83	0.11	40,41,46,49	0
4	PGE	B	714	10/10	0.83	0.16	36,46,52,60	0
9	NA	D	610	1/1	0.83	0.09	51,51,51,51	0
3	PEG	A	926	7/7	0.84	0.14	32,37,41,45	0
2	GOL	D	603	6/6	0.85	0.22	31,35,36,39	0
2	GOL	B	712	6/6	0.85	0.21	49,49,51,61	0
3	PEG	B	708	7/7	0.85	0.14	37,44,50,50	0
10	TRS	D	601	8/8	0.85	0.20	32,39,43,58	0
5	PG4	A	924	13/13	0.86	0.15	34,39,47,51	0
3	PEG	C	607[A]	7/7	0.86	0.22	13,14,17,17	7
3	PEG	C	607[B]	7/7	0.86	0.22	22,24,25,28	7
3	PEG	A	910	7/7	0.87	0.17	40,47,55,55	0
3	PEG	A	912	7/7	0.87	0.22	31,37,48,50	0
2	GOL	C	604	6/6	0.87	0.23	25,30,33,38	6
4	PGE	A	921	10/10	0.88	0.17	31,43,50,50	0
3	PEG	B	704	7/7	0.88	0.16	29,35,42,43	0
2	GOL	B	707	6/6	0.88	0.17	37,45,51,53	0
3	PEG	C	610	7/7	0.88	0.23	29,32,40,43	4
3	PEG	D	605	7/7	0.88	0.13	45,50,55,67	0
2	GOL	C	606	6/6	0.89	0.13	39,40,41,44	0
3	PEG	B	713	7/7	0.89	0.23	29,38,41,46	0
2	GOL	A	923	6/6	0.89	0.16	35,38,48,55	0
2	GOL	D	606	6/6	0.89	0.25	47,51,54,55	0
3	PEG	A	914	7/7	0.89	0.16	40,45,51,59	0
2	GOL	B	706	6/6	0.89	0.18	35,49,61,73	0

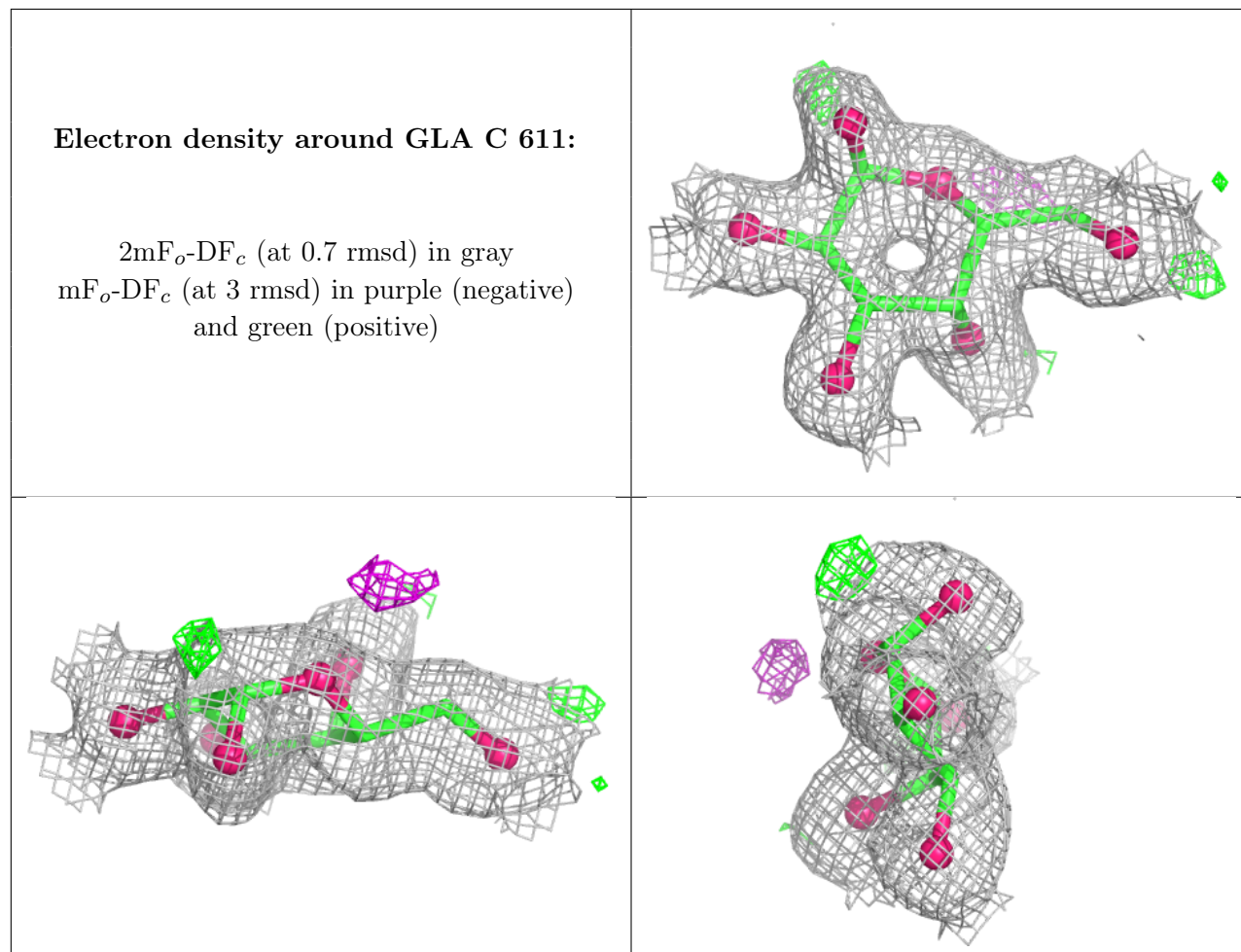
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	PGE	A	919	10/10	0.90	0.24	28,40,45,47	0
2	GOL	C	605	6/6	0.90	0.13	38,40,45,55	0
2	GOL	A	905	6/6	0.90	0.17	43,45,49,51	0
3	PEG	A	907	7/7	0.90	0.20	34,36,44,55	0
3	PEG	B	711	7/7	0.90	0.13	35,41,46,55	0
3	PEG	B	703	7/7	0.90	0.20	31,35,41,43	0
4	PGE	A	920	10/10	0.91	0.23	19,44,53,57	0
2	GOL	D	607	6/6	0.91	0.14	28,35,38,48	0
3	PEG	A	903	7/7	0.91	0.16	37,44,51,52	0
5	PG4	A	922	13/13	0.91	0.18	34,44,52,53	0
3	PEG	A	904	7/7	0.91	0.15	35,37,45,47	0
3	PEG	B	716	7/7	0.91	0.18	39,42,47,48	0
2	GOL	B	709	6/6	0.91	0.15	42,54,56,61	0
3	PEG	A	917	7/7	0.92	0.16	34,37,41,41	0
2	GOL	B	717	6/6	0.92	0.17	38,39,43,44	0
2	GOL	A	916	6/6	0.92	0.10	41,46,48,49	0
2	GOL	A	902	6/6	0.92	0.14	36,41,44,47	0
3	PEG	B	702	7/7	0.92	0.12	20,23,31,32	0
3	PEG	A	906	7/7	0.93	0.15	28,34,44,49	0
6	GLA	C	611	12/12	0.93	0.10	16,19,23,29	0
9	NA	B	720	1/1	0.93	0.09	50,50,50,50	0
2	GOL	A	901	6/6	0.93	0.16	23,27,31,35	6
2	GOL	D	604	6/6	0.93	0.12	40,41,42,45	0
3	PEG	D	602	7/7	0.94	0.13	28,35,43,44	0
2	GOL	A	909	6/6	0.94	0.15	31,33,36,40	0
2	GOL	A	925	6/6	0.94	0.22	23,23,26,31	4
2	GOL	C	601	6/6	0.95	0.19	35,43,47,49	0
6	GLA	D	608	12/12	0.95	0.07	18,23,25,26	0
7	GAL	A	928[B]	12/12	0.95	0.10	5,6,6,6	12
8	CL	A	929	1/1	0.95	0.06	49,49,49,49	0
3	PEG	B	715	7/7	0.95	0.11	36,37,50,52	0
9	NA	C	612	1/1	0.95	0.09	48,48,48,48	0
2	GOL	C	609	6/6	0.95	0.15	34,35,41,43	0
6	GLA	A	927[A]	12/12	0.95	0.09	16,19,21,22	0
7	GAL	B	719[B]	12/12	0.97	0.08	10,11,12,12	12
6	GLA	B	718[A]	12/12	0.97	0.07	16,21,23,23	0
8	CL	C	613	1/1	0.98	0.08	61,61,61,61	0
9	NA	D	609	1/1	0.98	0.08	42,42,42,42	0
9	NA	B	721	1/1	0.98	0.14	37,37,37,37	0
9	NA	B	722	1/1	0.98	0.07	40,40,40,40	0
8	CL	C	614	1/1	0.99	0.12	23,23,23,23	0

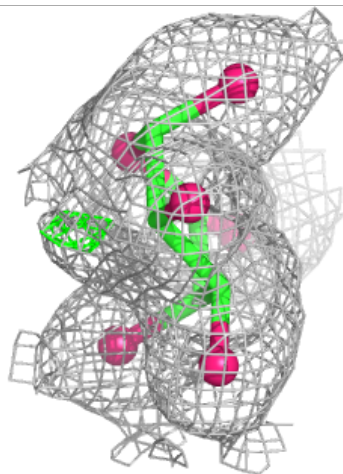
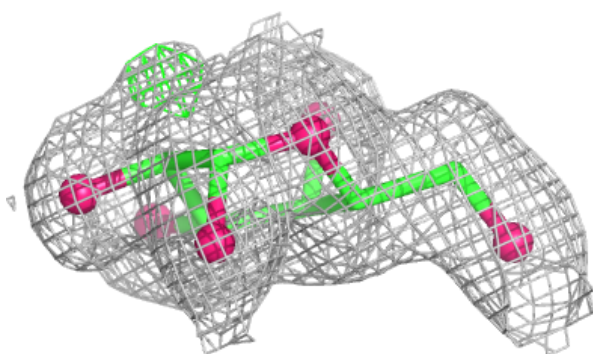
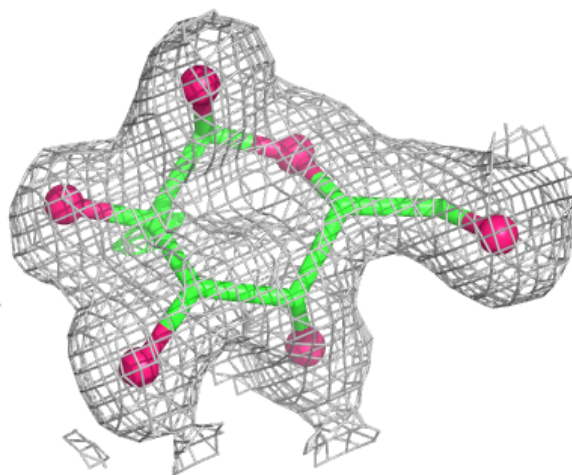
The following is a graphical depiction of the model fit to experimental electron density of all

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.



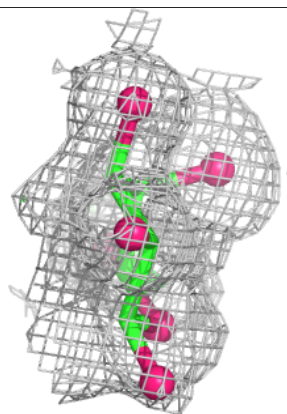
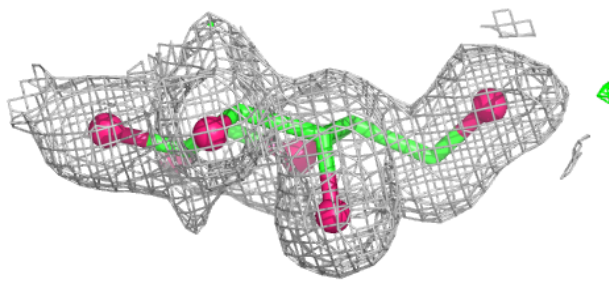
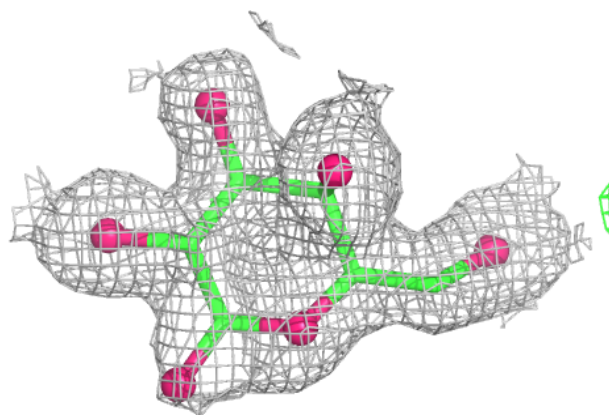
**Electron density around GLA D 608:**

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



**Electron density around GAL A 928 (B):**

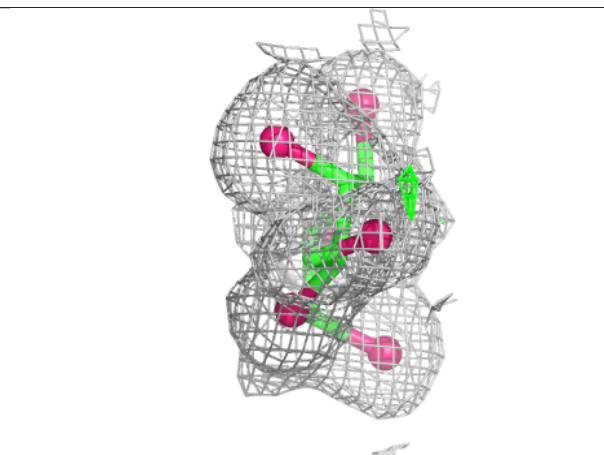
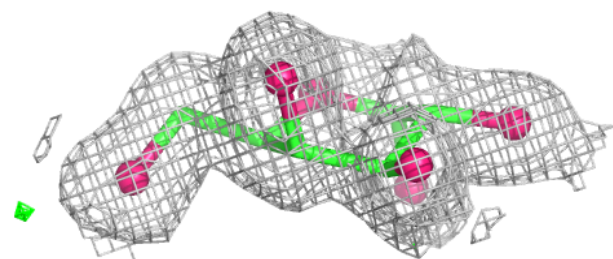
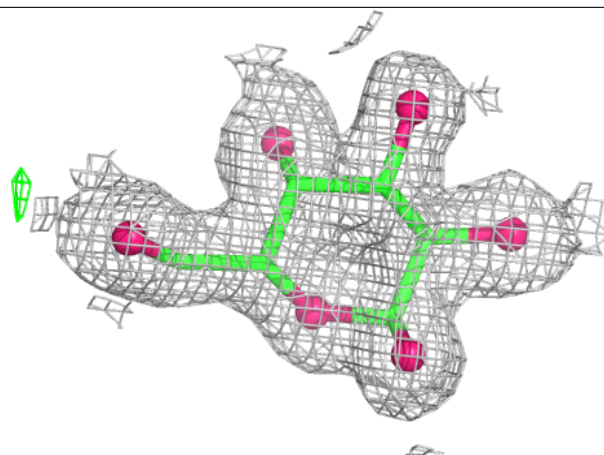
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



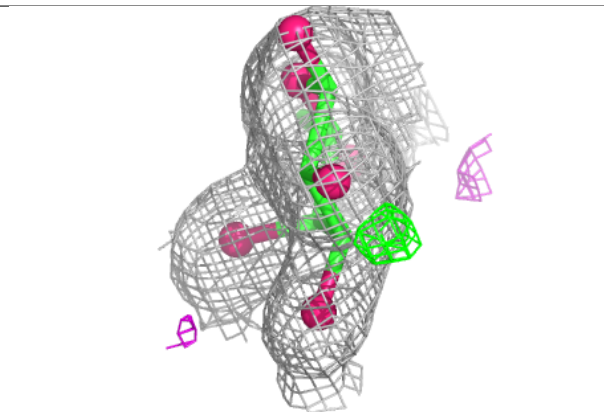
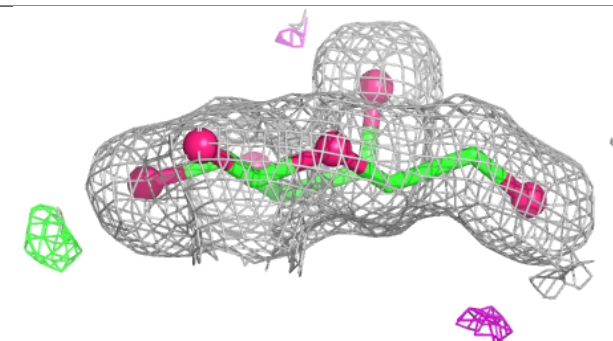
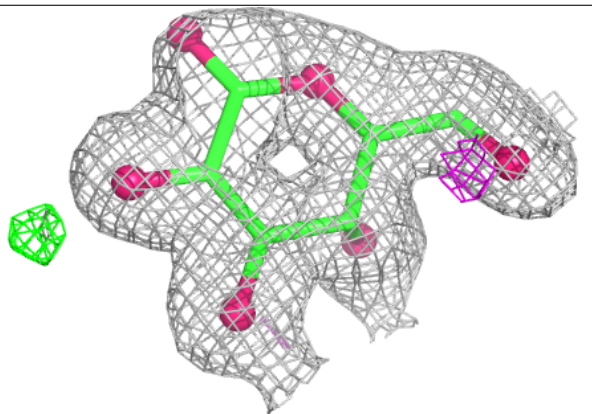


**Electron density around GLA A 927 (A):**

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

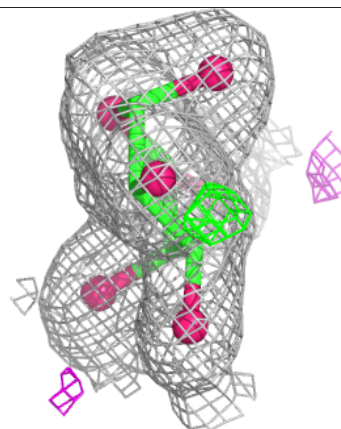
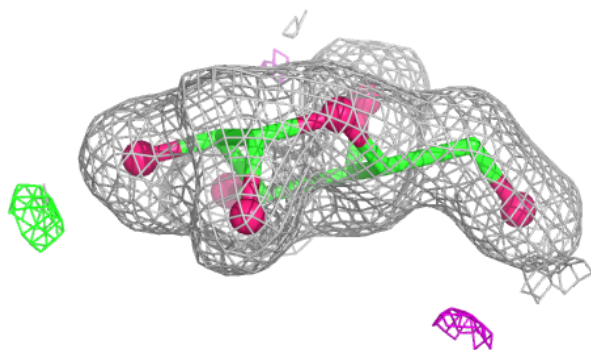
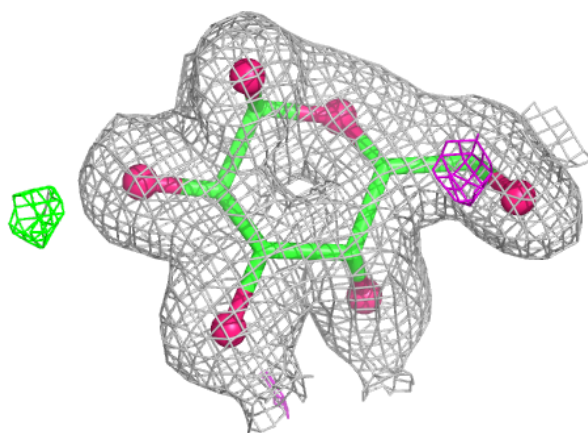
**Electron density around GAL B 719 (B):**

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



**Electron density around GLA B 718 (A):**

$2mF_o-DF_c$  (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.