



# wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 28, 2024 – 06:59 am GMT

PDB ID : 5H9O  
Title : Complex of Murine endoplasmic reticulum alpha-glucosidase II with D-Glucose  
Authors : Caputo, A.T.; Roversi, P.; Alonzi, D.S.; Kiappes, J.L.; Zitzmann, N.  
Deposited on : 2015-12-29  
Resolution : 2.37 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](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	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

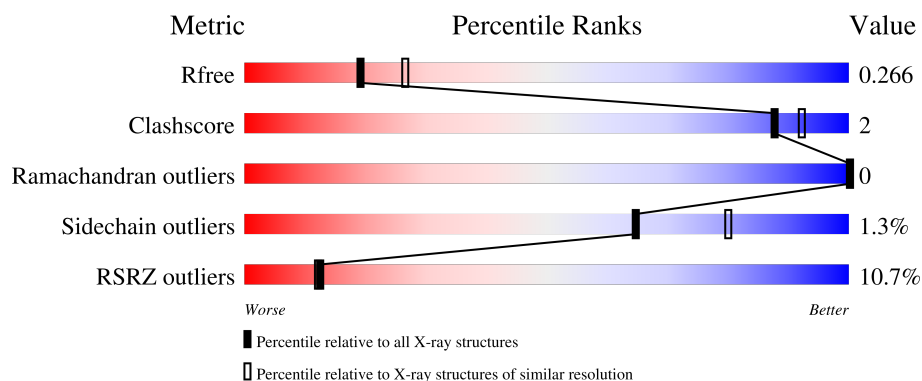
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.37 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	6699 (2.40-2.36)
Clashscore	180529	7414 (2.40-2.36)
Ramachandran outliers	177936	7337 (2.40-2.36)
Sidechain outliers	177891	7338 (2.40-2.36)
RSRZ outliers	164620	6699 (2.40-2.36)

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	857	<div> <div>7%</div> <div>96%</div> <div>.</div> </div>
1	C	857	<div> <div>9%</div> <div>96%</div> <div>.</div> </div>
2	B	88	<div> <div>36%</div> <div>100%</div> </div>
2	D	88	<div> <div>34%</div> <div>94%</div> <div>5%</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
3	NAG	A	1001	-	-	X	-
3	NAG	C	1001	-	-	X	-
4	EDO	C	1006	-	-	X	-
5	FMT	C	1009	-	-	-	X
6	PG4	B	201	-	-	-	X

## 2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 30841 atoms, of which 14798 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 Neutral alpha-glucosidase AB.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	857	Total	C	H	N	O	S	0	12	0
			13720	4471	6743	1206	1270	30			
1	C	857	Total	C	H	N	O	S	0	11	0
			13705	4467	6735	1205	1268	30			

There are 154 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	VAL	deletion	UNP Q8BHN3
A	?	-	PRO	deletion	UNP Q8BHN3
A	?	-	PHE	deletion	UNP Q8BHN3
A	?	-	SER	deletion	UNP Q8BHN3
A	?	-	ASP	deletion	UNP Q8BHN3
A	?	-	LYS	deletion	UNP Q8BHN3
A	?	-	VAL	deletion	UNP Q8BHN3
A	?	-	SER	deletion	UNP Q8BHN3
A	?	-	LEU	deletion	UNP Q8BHN3
A	?	-	ALA	deletion	UNP Q8BHN3
A	?	-	LEU	deletion	UNP Q8BHN3
A	?	-	GLY	deletion	UNP Q8BHN3
A	?	-	SER	deletion	UNP Q8BHN3
A	?	-	VAL	deletion	UNP Q8BHN3
A	?	-	TRP	deletion	UNP Q8BHN3
A	?	-	ASP	deletion	UNP Q8BHN3
A	?	-	LYS	deletion	UNP Q8BHN3
A	?	-	ILE	deletion	UNP Q8BHN3
A	?	-	LYS	deletion	UNP Q8BHN3
A	?	-	ASN	deletion	UNP Q8BHN3
A	?	-	LEU	deletion	UNP Q8BHN3
A	?	-	PHE	deletion	UNP Q8BHN3
A	?	-	SER	deletion	UNP Q8BHN3
A	?	-	ARG	deletion	UNP Q8BHN3
A	?	-	GLN	deletion	UNP Q8BHN3

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Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	GLU	deletion	UNP Q8BHN3
A	?	-	SER	deletion	UNP Q8BHN3
A	?	-	LYS	deletion	UNP Q8BHN3
A	?	-	ASP	deletion	UNP Q8BHN3
A	?	-	PRO	deletion	UNP Q8BHN3
A	?	-	ALA	deletion	UNP Q8BHN3
A	?	-	GLU	deletion	UNP Q8BHN3
A	?	-	GLY	deletion	UNP Q8BHN3
A	?	-	ASN	deletion	UNP Q8BHN3
A	?	-	GLY	deletion	UNP Q8BHN3
A	?	-	ALA	deletion	UNP Q8BHN3
A	?	-	GLN	deletion	UNP Q8BHN3
A	?	-	PRO	deletion	UNP Q8BHN3
A	?	-	GLU	deletion	UNP Q8BHN3
A	?	-	ALA	deletion	UNP Q8BHN3
A	?	-	THR	deletion	UNP Q8BHN3
A	?	-	PRO	deletion	UNP Q8BHN3
A	?	-	GLY	deletion	UNP Q8BHN3
A	?	-	ASP	deletion	UNP Q8BHN3
A	?	-	GLY	deletion	UNP Q8BHN3
A	?	-	ASP	deletion	UNP Q8BHN3
A	?	-	LYS	deletion	UNP Q8BHN3
A	?	-	PRO	deletion	UNP Q8BHN3
A	?	-	GLU	deletion	UNP Q8BHN3
A	?	-	GLU	deletion	UNP Q8BHN3
A	?	-	THR	deletion	UNP Q8BHN3
A	?	-	GLN	deletion	UNP Q8BHN3
A	?	-	GLU	deletion	UNP Q8BHN3
A	?	-	LYS	deletion	UNP Q8BHN3
A	?	-	ALA	deletion	UNP Q8BHN3
A	?	-	GLU	deletion	UNP Q8BHN3
A	?	-	LYS	deletion	UNP Q8BHN3
A	?	-	ASP	deletion	UNP Q8BHN3
A	?	-	THR	deletion	UNP Q8BHN3
A	?	-	ALA	deletion	UNP Q8BHN3
A	?	-	GLY	deletion	UNP Q8BHN3
A	?	-	LYS	deletion	UNP Q8BHN3
A	?	-	THR	deletion	UNP Q8BHN3
A	?	-	LEU	deletion	UNP Q8BHN3
A	?	-	PHE	deletion	UNP Q8BHN3
A	?	-	GLY	deletion	UNP Q8BHN3
A	?	-	LYS	deletion	UNP Q8BHN3

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Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	MET	deletion	UNP Q8BHN3
A	?	-	LEU	deletion	UNP Q8BHN3
A	?	-	ASP	deletion	UNP Q8BHN3
A	?	-	TYR	deletion	UNP Q8BHN3
A	?	-	LEU	deletion	UNP Q8BHN3
A	?	-	GLN	deletion	UNP Q8BHN3
A	?	-	GLY	deletion	UNP Q8BHN3
A	?	-	SER	deletion	UNP Q8BHN3
A	?	-	GLY	deletion	UNP Q8BHN3
A	?	-	GLU	deletion	UNP Q8BHN3
C	?	-	VAL	deletion	UNP Q8BHN3
C	?	-	PRO	deletion	UNP Q8BHN3
C	?	-	PHE	deletion	UNP Q8BHN3
C	?	-	SER	deletion	UNP Q8BHN3
C	?	-	ASP	deletion	UNP Q8BHN3
C	?	-	LYS	deletion	UNP Q8BHN3
C	?	-	VAL	deletion	UNP Q8BHN3
C	?	-	SER	deletion	UNP Q8BHN3
C	?	-	LEU	deletion	UNP Q8BHN3
C	?	-	ALA	deletion	UNP Q8BHN3
C	?	-	LEU	deletion	UNP Q8BHN3
C	?	-	GLY	deletion	UNP Q8BHN3
C	?	-	SER	deletion	UNP Q8BHN3
C	?	-	VAL	deletion	UNP Q8BHN3
C	?	-	TRP	deletion	UNP Q8BHN3
C	?	-	ASP	deletion	UNP Q8BHN3
C	?	-	LYS	deletion	UNP Q8BHN3
C	?	-	ILE	deletion	UNP Q8BHN3
C	?	-	LYS	deletion	UNP Q8BHN3
C	?	-	ASN	deletion	UNP Q8BHN3
C	?	-	LEU	deletion	UNP Q8BHN3
C	?	-	PHE	deletion	UNP Q8BHN3
C	?	-	SER	deletion	UNP Q8BHN3
C	?	-	ARG	deletion	UNP Q8BHN3
C	?	-	GLN	deletion	UNP Q8BHN3
C	?	-	GLU	deletion	UNP Q8BHN3
C	?	-	SER	deletion	UNP Q8BHN3
C	?	-	LYS	deletion	UNP Q8BHN3
C	?	-	ASP	deletion	UNP Q8BHN3
C	?	-	PRO	deletion	UNP Q8BHN3
C	?	-	ALA	deletion	UNP Q8BHN3
C	?	-	GLU	deletion	UNP Q8BHN3

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Chain	Residue	Modelled	Actual	Comment	Reference
C	?	-	GLY	deletion	UNP Q8BHN3
C	?	-	ASN	deletion	UNP Q8BHN3
C	?	-	GLY	deletion	UNP Q8BHN3
C	?	-	ALA	deletion	UNP Q8BHN3
C	?	-	GLN	deletion	UNP Q8BHN3
C	?	-	PRO	deletion	UNP Q8BHN3
C	?	-	GLU	deletion	UNP Q8BHN3
C	?	-	ALA	deletion	UNP Q8BHN3
C	?	-	THR	deletion	UNP Q8BHN3
C	?	-	PRO	deletion	UNP Q8BHN3
C	?	-	GLY	deletion	UNP Q8BHN3
C	?	-	ASP	deletion	UNP Q8BHN3
C	?	-	GLY	deletion	UNP Q8BHN3
C	?	-	ASP	deletion	UNP Q8BHN3
C	?	-	LYS	deletion	UNP Q8BHN3
C	?	-	PRO	deletion	UNP Q8BHN3
C	?	-	GLU	deletion	UNP Q8BHN3
C	?	-	GLU	deletion	UNP Q8BHN3
C	?	-	THR	deletion	UNP Q8BHN3
C	?	-	GLN	deletion	UNP Q8BHN3
C	?	-	GLU	deletion	UNP Q8BHN3
C	?	-	LYS	deletion	UNP Q8BHN3
C	?	-	ALA	deletion	UNP Q8BHN3
C	?	-	GLU	deletion	UNP Q8BHN3
C	?	-	LYS	deletion	UNP Q8BHN3
C	?	-	ASP	deletion	UNP Q8BHN3
C	?	-	THR	deletion	UNP Q8BHN3
C	?	-	ALA	deletion	UNP Q8BHN3
C	?	-	GLY	deletion	UNP Q8BHN3
C	?	-	LYS	deletion	UNP Q8BHN3
C	?	-	THR	deletion	UNP Q8BHN3
C	?	-	LEU	deletion	UNP Q8BHN3
C	?	-	PHE	deletion	UNP Q8BHN3
C	?	-	GLY	deletion	UNP Q8BHN3
C	?	-	LYS	deletion	UNP Q8BHN3
C	?	-	MET	deletion	UNP Q8BHN3
C	?	-	LEU	deletion	UNP Q8BHN3
C	?	-	ASP	deletion	UNP Q8BHN3
C	?	-	TYR	deletion	UNP Q8BHN3
C	?	-	LEU	deletion	UNP Q8BHN3
C	?	-	GLN	deletion	UNP Q8BHN3
C	?	-	GLY	deletion	UNP Q8BHN3

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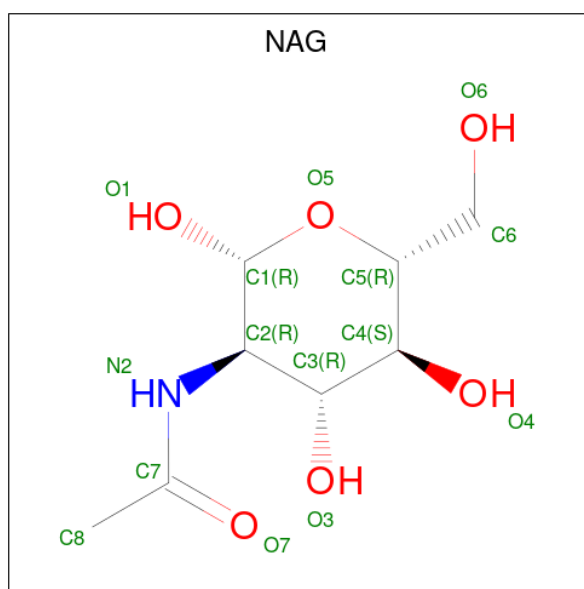
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Chain	Residue	Modelled	Actual	Comment	Reference
C	?	-	SER	deletion	UNP Q8BHN3
C	?	-	GLY	deletion	UNP Q8BHN3
C	?	-	GLU	deletion	UNP Q8BHN3

- Molecule 2 is a protein called Glucosidase 2 subunit beta.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	88	Total	C	H	N	O	S	0	0	0
			1201	399	538	106	148	10			
2	D	88	Total	C	H	N	O	S	0	0	0
			1218	399	555	106	148	10			

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	C	1	Total	C	N	O	0	0
			14	8	1	5		
3	C	1	Total	C	N	O	0	0
			14	8	1	5		

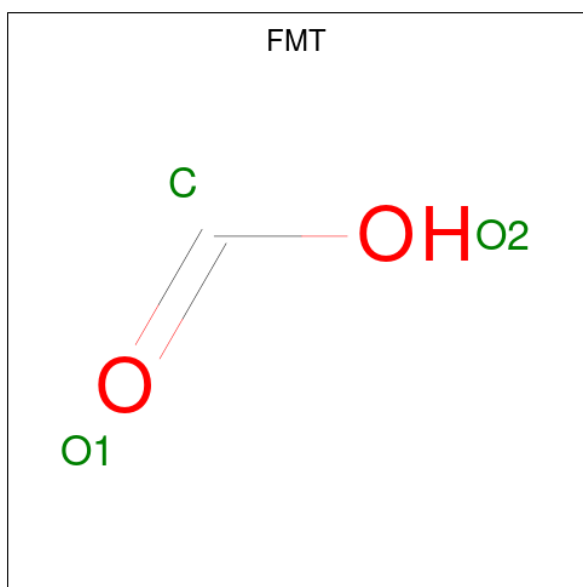
- Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).





Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	O		0	0
			4	2	2			
4	A	1	Total	C	O		0	0
			4	2	2			
4	A	1	Total	C	O		0	0
			4	2	2			
4	C	1	Total	C	O		0	0
			4	2	2			
4	C	1	Total	C	O		0	0
			4	2	2			
4	C	1	Total	C	O		0	0
			4	2	2			
4	C	1	Total	C	H	O	0	0
			10	2	6	2		

- Molecule 5 is FORMIC ACID (three-letter code: FMT) (formula: CH<sub>2</sub>O<sub>2</sub>).



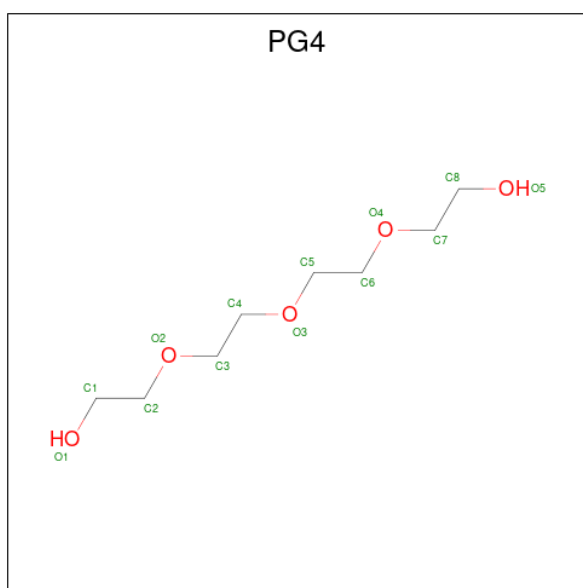
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	O		0	0
			3	1	2			
5	A	1	Total	C	O		0	0
			3	1	2			
5	A	1	Total	C	O		0	0
			3	1	2			
5	A	1	Total	C	O		0	0
			3	1	2			
5	A	1	Total	C	O		0	0
			3	1	2			
5	A	1	Total	C	O		0	0
			3	1	2			
5	A	1	Total	C	H	O	0	0
			5	1	2	2		
5	C	1	Total	C	O		0	0
			3	1	2			
5	C	1	Total	C	O		0	0
			3	1	2			
5	C	1	Total	C			0	0
			1	1				
5	C	1	Total	O			0	0
			2	2				

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	C	1	Total	C	O	0	0
			3	1	2		
5	C	1	Total	C	O	0	0
			3	1	2		
5	C	1	Total	C	O	0	0
			3	1	2		
5	C	1	Total	C	O	0	0
			3	1	2		
5	C	1	Total	C	O	0	0
			3	1	2		

- Molecule 6 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: C<sub>8</sub>H<sub>18</sub>O<sub>5</sub>).



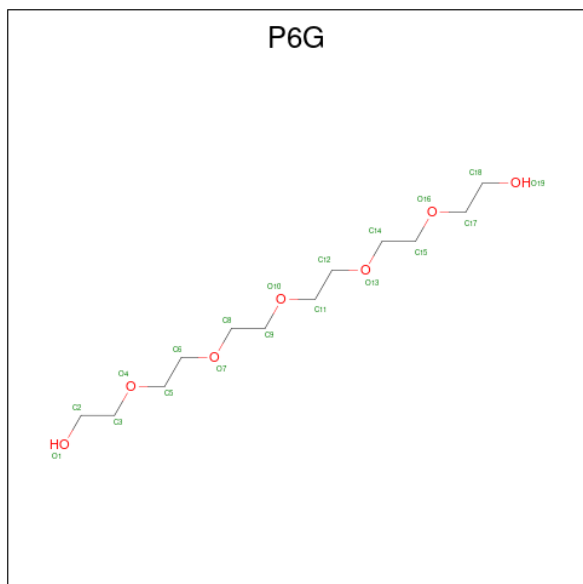
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	H	O	0	0
			17	5	9	3		
6	A	1	Total	C	H	O	0	0
			20	6	11	3		
6	B	1	Total	C	H	O	0	0
			24	7	13	4		
6	B	1	Total	C	H	O	0	0
			17	6	8	3		
6	C	1	Total	C	H	O	0	0
			17	5	9	3		
6	C	1	Total	C	H	O	0	0
			20	6	11	3		

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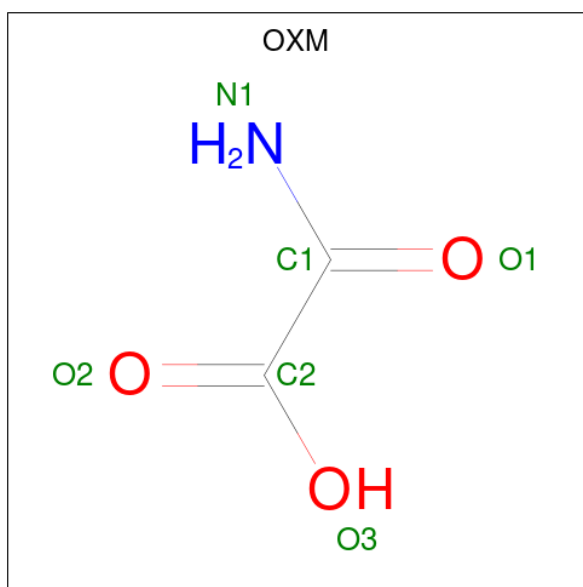
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	D	1	Total	C	H	O	0	0
			17	6	8	3		

- Molecule 7 is HEXAETHYLENE GLYCOL (three-letter code: P6G) (formula:  $C_{12}H_{26}O_7$ ).



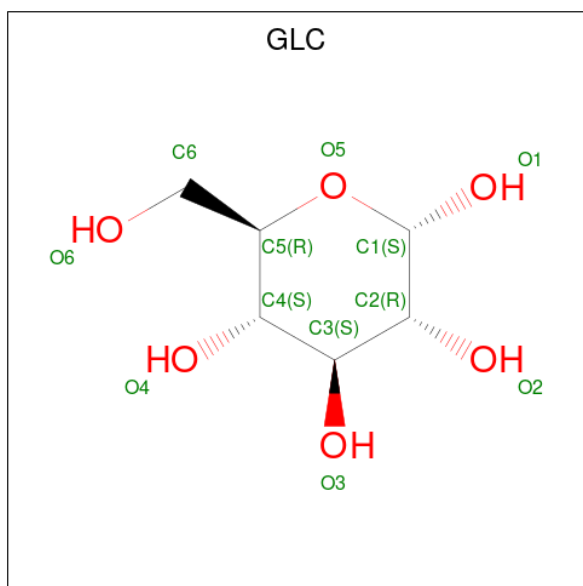
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	A	1	Total	C	H	O	0	0
			45	12	26	7		
7	A	1	Total	C	H	O	0	0
			30	9	16	5		
7	A	1	Total	C	H	O	0	0
			45	12	26	7		
7	C	1	Total	C	H	O	0	0
			45	12	26	7		
7	C	1	Total	C	H	O	0	0
			45	12	26	7		

- Molecule 8 is OXAMIC ACID (three-letter code: OXM) (formula:  $C_2H_3NO_3$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
8	A	1	Total	C	H	N	O	0	0
			8	2	2	1	3		

- Molecule 9 is alpha-D-glucopyranose (three-letter code: GLC) (formula: C<sub>6</sub>H<sub>12</sub>O<sub>6</sub>).

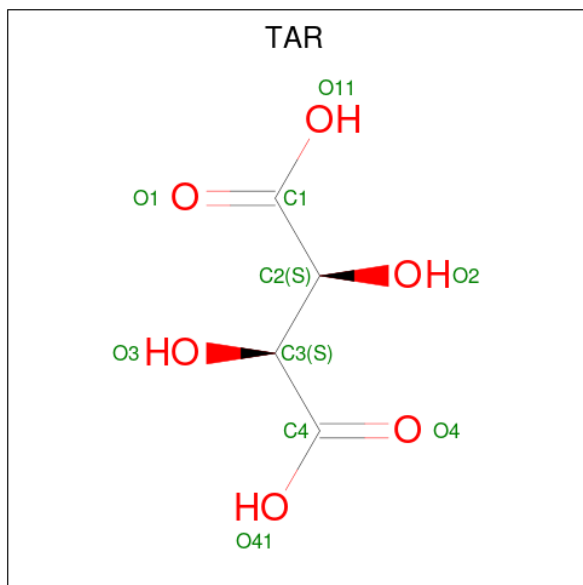


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	A	1	Total	C	H	O	0	0
			24	6	12	6		
9	C	1	Total	C	H	O	0	0
			24	6	12	6		

- Molecule 10 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	B	2	Total Ca 2 2	0	0
10	D	2	Total Ca 2 2	0	0

- Molecule 11 is D(-)-TARTARIC ACID (three-letter code: TAR) (formula: C<sub>4</sub>H<sub>6</sub>O<sub>6</sub>).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	C	1	Total C H O 14 4 4 6	0	0

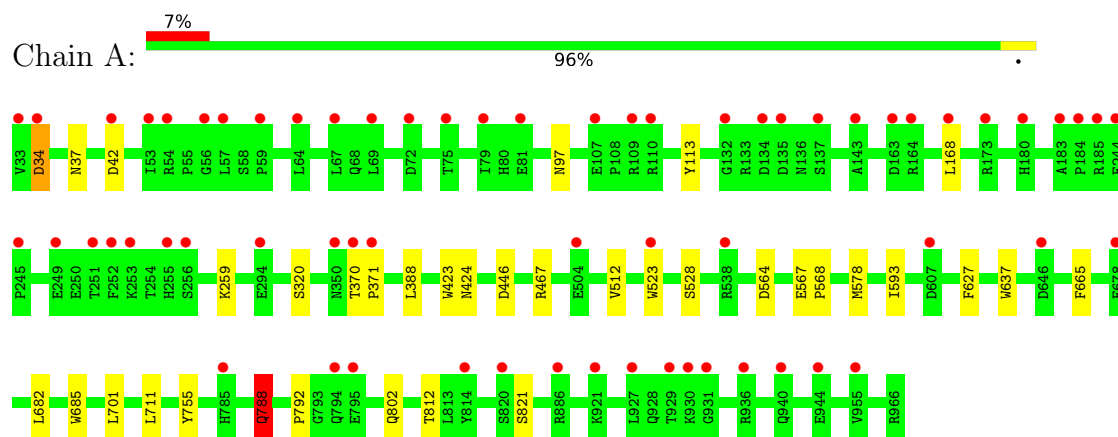
- Molecule 12 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
12	A	210	Total O 210 210	0	0
12	B	17	Total O 17 17	0	0
12	C	191	Total O 191 191	0	0
12	D	13	Total O 13 13	0	0

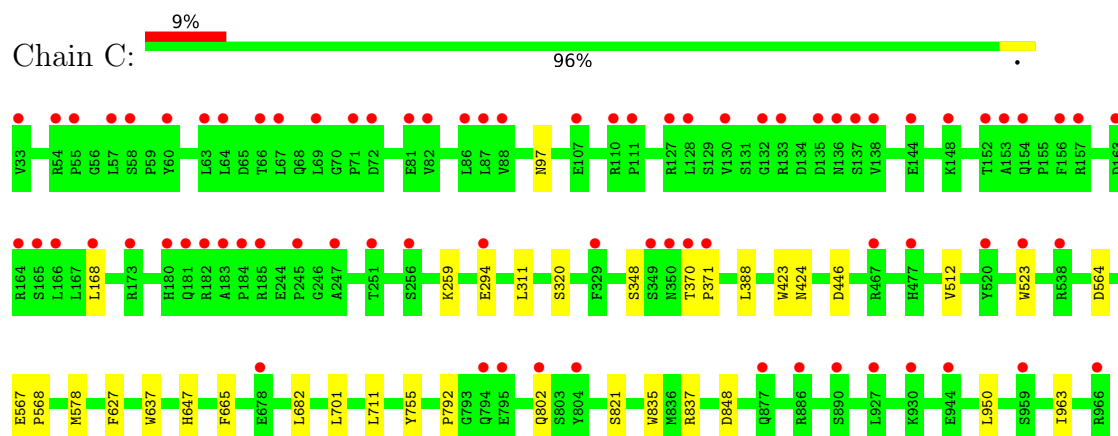
### 3 Residue-property plots [i](#)

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

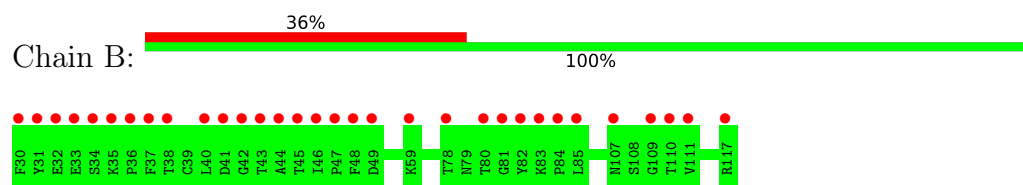
- Molecule 1: Neutral alpha-glucosidase AB



- Molecule 1: Neutral alpha-glucosidase AB



- Molecule 2: Glucosidase 2 subunit beta



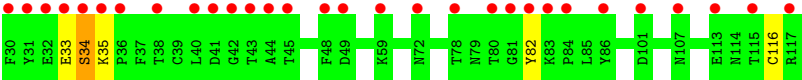
- Molecule 2: Glucosidase 2 subunit beta

Chain D: 

34%

94%

5% •





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	102.14Å 170.74Å 125.99Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	87.66 – 2.37 87.66 – 2.37	Depositor EDS
% Data completeness (in resolution range)	99.3 (87.66-2.37) 99.3 (87.66-2.37)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.24	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.81 (at 2.37Å)	Xtriage
Refinement program	BUSTER 2.10.2	Depositor
R, $R_{free}$	0.221 , 0.253 0.234 , 0.266	Depositor DCC
$R_{free}$ test set	4422 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	25.2	Xtriage
Anisotropy	0.270	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.43 , 51.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	30841	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 24.10 % 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 4.0910e-03. 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: CA, EDO, P6G, GLC, PG4, OXM, NAG, TAR, FMT

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	0.48	0/7225	0.69	4/9830 (0.0%)
1	C	0.53	0/7215	0.69	0/9818
2	B	0.49	0/677	0.69	0/920
2	D	0.61	0/677	0.77	1/920 (0.1%)
All	All	0.51	0/15794	0.69	5/21488 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	467	ARG	CB-CG-CD	7.16	130.22	111.60
1	A	467	ARG	CA-CB-CG	-6.11	99.97	113.40
2	D	34	SER	C-N-CA	5.75	136.07	121.70
1	A	788	GLN	CB-CG-CD	5.08	124.80	111.60
1	A	34	ASP	N-CA-CB	5.06	119.71	110.60

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	6977	6743	6755	18	0
1	C	6970	6735	6747	29	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	663	538	568	0	0
2	D	663	555	568	1	0
3	A	28	0	26	7	0
3	C	28	0	26	7	0
4	A	12	0	18	3	0
4	C	20	6	29	14	0
5	A	30	2	17	0	0
5	C	24	0	12	1	0
6	A	17	20	20	0	0
6	B	20	21	21	0	0
6	C	17	20	20	0	0
6	D	9	8	8	0	0
7	A	52	68	68	0	0
7	C	38	52	52	1	0
8	A	6	2	2	0	0
9	A	12	12	12	1	0
9	C	12	12	12	1	0
10	B	2	0	0	0	0
10	D	2	0	0	0	0
11	C	10	4	4	0	0
12	A	210	0	0	0	0
12	B	17	0	0	0	0
12	C	191	0	0	1	0
12	D	13	0	0	0	0
All	All	16043	14798	14985	58	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 2.

The worst 5 of 58 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:97:ASN:HD21	3:A:1001:NAG:C1	1.25	1.46
1:C:97:ASN:HD21	3:C:1001:NAG:C1	1.27	1.44
1:A:97:ASN:ND2	3:A:1001:NAG:C1	2.10	1.14
1:C:97:ASN:ND2	3:C:1001:NAG:C1	2.11	1.14
1:C:848:ASP:HB3	4:C:1006:EDO:H22	1.26	1.11

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	863/857 (101%)	837 (97%)	26 (3%)	0	100	100
1	C	862/857 (101%)	836 (97%)	26 (3%)	0	100	100
2	B	86/88 (98%)	84 (98%)	2 (2%)	0	100	100
2	D	86/88 (98%)	81 (94%)	5 (6%)	0	100	100
All	All	1897/1890 (100%)	1838 (97%)	59 (3%)	0	100	100

There are no Ramachandran outliers to report.

### 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	760/748 (102%)	749 (99%)	11 (1%)	62	78
1	C	759/748 (102%)	751 (99%)	8 (1%)	70	83
2	B	77/77 (100%)	77 (100%)	0	100	100
2	D	77/77 (100%)	74 (96%)	3 (4%)	27	43
All	All	1673/1650 (101%)	1651 (99%)	22 (1%)	65	80

5 of 22 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	424	ASN
1	C	637	TRP
1	C	523	TRP

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Mol	Chain	Res	Type
1	C	665	PHE
1	A	528[B]	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	37	ASN
1	A	97	ASN
1	A	725	GLN
1	C	97	ASN

### 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 oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 51 ligands modelled in this entry, 1 is modelled with single atom and 4 are monoatomic - leaving 46 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	EDO	A	1005	-	3,3,3	0.76	0	2,2,2	0.11	0
5	FMT	A	1009	-	2,2,2	1.08	0	1,1,1	1.10	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
8	OXM	A	1020	-	5,5,5	0.45	0	4,6,6	1.64	1 (25%)
5	FMT	C	1013	-	2,2,2	1.30	0	1,1,1	1.20	0
3	NAG	C	1002	-	14,14,15	0.41	0	17,19,21	2.09	1 (5%)
6	PG4	B	204	-	8,8,12	0.38	0	7,7,11	0.39	0
9	GLC	C	1022	-	12,12,12	0.57	0	17,17,17	0.66	0
5	FMT	A	1007	-	2,2,2	1.68	1 (50%)	1,1,1	0.84	0
4	EDO	C	1005	-	3,3,3	0.93	0	2,2,2	0.05	0
3	NAG	A	1002	-	14,14,15	0.41	0	17,19,21	2.16	1 (5%)
6	PG4	A	1015	-	7,7,12	0.26	0	6,6,11	0.17	0
6	PG4	B	201	-	10,10,12	0.30	0	9,9,11	0.44	0
4	EDO	A	1003	-	3,3,3	0.97	0	2,2,2	0.40	0
5	FMT	C	1007	-	2,2,2	1.16	0	1,1,1	1.12	0
5	FMT	A	1008	-	2,2,2	1.14	0	1,1,1	1.10	0
7	P6G	C	1019	-	18,18,18	0.28	0	17,17,17	0.24	0
6	PG4	C	1017	-	8,8,12	0.38	0	7,7,11	0.35	0
7	P6G	A	1017	-	18,18,18	0.16	0	17,17,17	0.20	0
5	FMT	A	1006	-	2,2,2	1.15	0	1,1,1	1.08	0
7	P6G	C	1018	-	18,18,18	0.27	0	17,17,17	0.40	0
6	PG4	D	203	-	8,8,12	0.42	0	7,7,11	0.38	0
5	FMT	C	1011	-	2,2,2	1.69	1 (50%)	1,1,1	1.08	0
6	PG4	C	1016	-	7,7,12	0.24	0	6,6,11	0.18	0
6	PG4	A	1016	-	8,8,12	0.35	0	7,7,11	0.34	0
5	FMT	A	1014	-	2,2,2	1.33	0	1,1,1	0.89	0
4	EDO	A	1004	-	3,3,3	0.77	0	2,2,2	0.20	0
5	FMT	A	1012	-	2,2,2	1.90	1 (50%)	1,1,1	0.65	0
11	TAR	C	1021	-	9,9,9	0.22	0	12,12,12	0.54	0
5	FMT	C	1015	-	2,2,2	1.50	1 (50%)	1,1,1	0.83	0
3	NAG	A	1001	-	14,14,15	0.36	0	17,19,21	1.57	3 (17%)
4	EDO	C	1004	-	3,3,3	0.67	0	2,2,2	0.22	0
5	FMT	A	1019	-	2,2,2	1.52	1 (50%)	1,1,1	0.81	0
9	GLC	A	1021	-	12,12,12	0.26	0	17,17,17	0.87	1 (5%)
5	FMT	C	1014	-	2,2,2	1.27	0	1,1,1	1.11	0
4	EDO	C	1006	-	3,3,3	0.86	0	2,2,2	0.26	0
4	EDO	C	1003	-	3,3,3	0.51	0	2,2,2	0.41	0
5	FMT	A	1011	-	2,2,2	1.20	0	1,1,1	0.98	0
5	FMT	C	1012	-	2,2,2	1.05	0	1,1,1	1.18	0
4	EDO	C	1020	-	3,3,3	0.60	0	2,2,2	0.12	0
5	FMT	A	1010	-	2,2,2	1.33	0	1,1,1	1.10	0
7	P6G	A	1022	-	18,18,18	0.32	0	17,17,17	0.40	0
5	FMT	C	1008	-	2,2,2	1.47	1 (50%)	1,1,1	0.80	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
7	P6G	A	1018	-	13,13,18	0.23	0	12,12,17	0.30	0
5	FMT	A	1013	-	2,2,2	1.36	0	1,1,1	1.02	0
3	NAG	C	1001	-	14,14,15	0.31	0	17,19,21	1.62	3 (17%)

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	EDO	A	1005	-	-	1/1/1/1	-
8	OXM	A	1020	-	-	0/3/4/4	-
3	NAG	C	1002	-	-	2/6/23/26	0/1/1/1
6	PG4	B	204	-	-	4/6/6/10	-
9	GLC	C	1022	-	-	0/2/22/22	0/1/1/1
4	EDO	C	1005	-	-	1/1/1/1	-
3	NAG	A	1002	-	-	2/6/23/26	0/1/1/1
6	PG4	A	1015	-	-	0/5/5/10	-
4	EDO	A	1003	-	-	0/1/1/1	-
7	P6G	C	1019	-	-	5/16/16/16	-
6	PG4	C	1017	-	-	2/6/6/10	-
7	P6G	A	1017	-	-	0/16/16/16	-
7	P6G	C	1018	-	-	8/16/16/16	-
6	PG4	D	203	-	-	4/6/6/10	-
6	PG4	C	1016	-	-	0/5/5/10	-
6	PG4	A	1016	-	-	2/6/6/10	-
4	EDO	A	1004	-	-	1/1/1/1	-
11	TAR	C	1021	-	-	6/12/12/12	-
3	NAG	A	1001	-	-	0/6/23/26	0/1/1/1
4	EDO	C	1004	-	-	1/1/1/1	-
9	GLC	A	1021	-	-	0/2/22/22	0/1/1/1
4	EDO	C	1006	-	-	0/1/1/1	-
4	EDO	C	1003	-	-	1/1/1/1	-
4	EDO	C	1020	-	-	1/1/1/1	-
7	P6G	A	1022	-	-	8/16/16/16	-
7	P6G	A	1018	-	-	4/11/11/16	-
3	NAG	C	1001	-	-	0/6/23/26	0/1/1/1
6	PG4	B	201	-	-	5/8/8/10	-

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1012	FMT	O2-C	2.51	1.41	1.28
5	C	1011	FMT	O2-C	2.39	1.40	1.28
5	A	1007	FMT	O2-C	2.36	1.40	1.28
5	C	1015	FMT	O2-C	2.08	1.39	1.28
5	C	1008	FMT	O2-C	2.06	1.39	1.28

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1002	NAG	O5-C1-C2	-8.29	98.20	111.29
3	C	1002	NAG	O5-C1-C2	-7.99	98.67	111.29
3	C	1001	NAG	C1-C2-N2	-4.44	102.91	110.49
3	A	1001	NAG	C1-C2-N2	-4.27	103.19	110.49
3	C	1001	NAG	C1-O5-C5	-3.49	107.47	112.19

There are no chirality outliers.

5 of 58 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
11	C	1021	TAR	O2-C2-C3-O3
11	C	1021	TAR	C1-C2-C3-O3
11	C	1021	TAR	O2-C2-C3-C4
7	A	1018	P6G	O4-C5-C6-O7
6	B	201	PG4	O1-C1-C2-O2

There are no ring outliers.

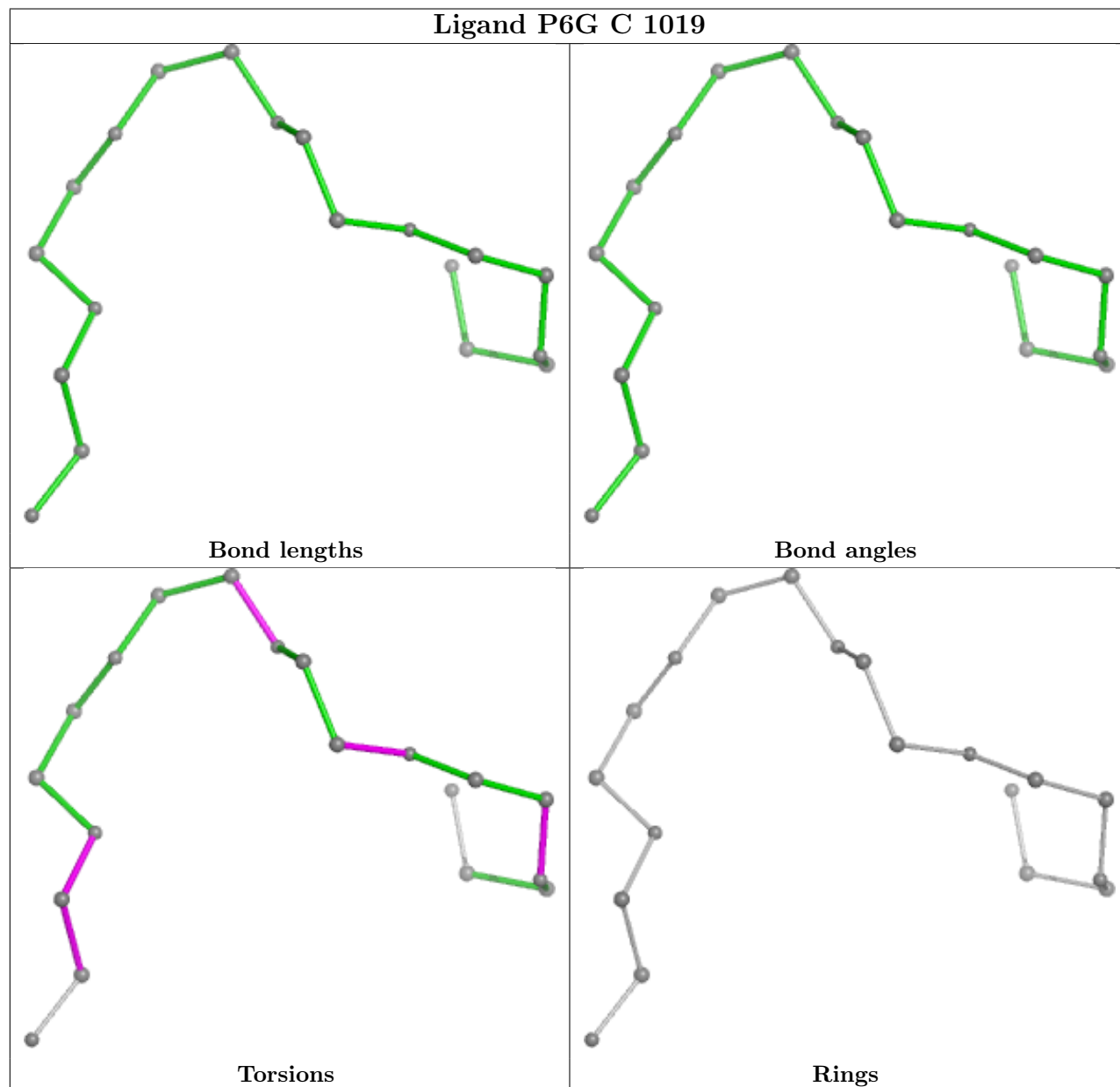
10 monomers are involved in 34 short contacts:

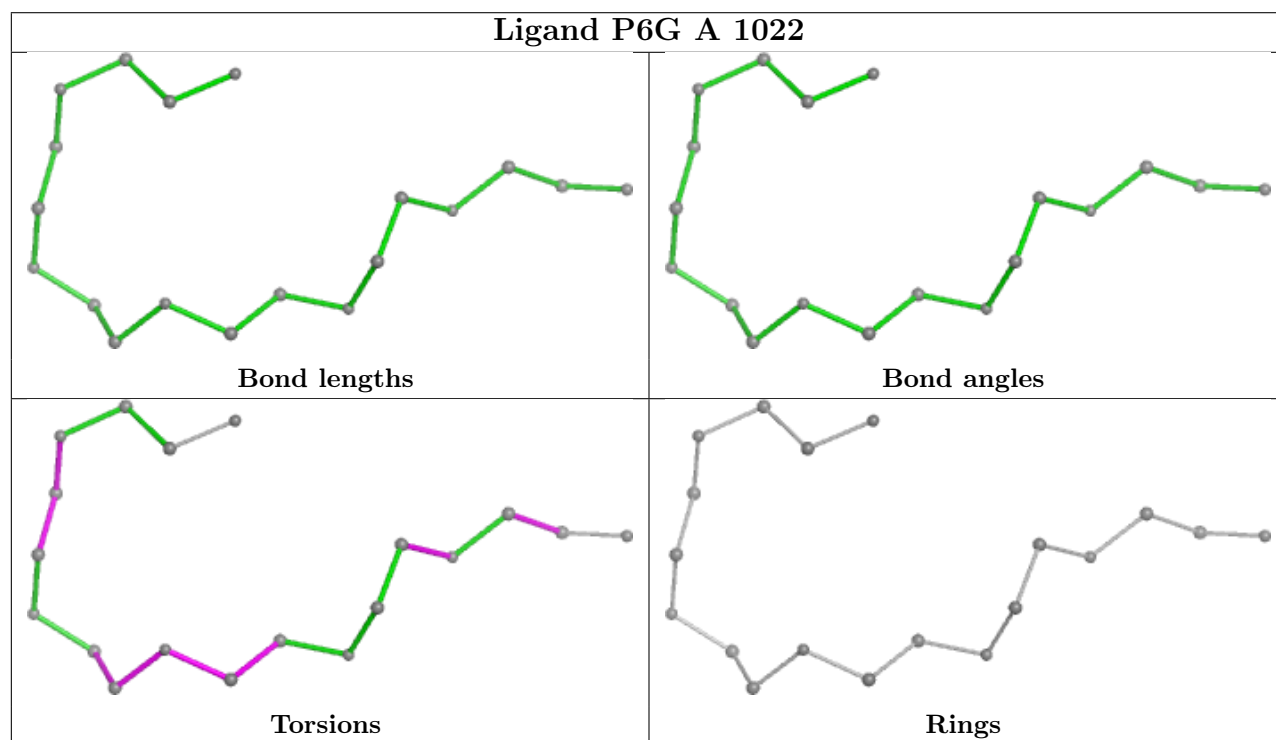
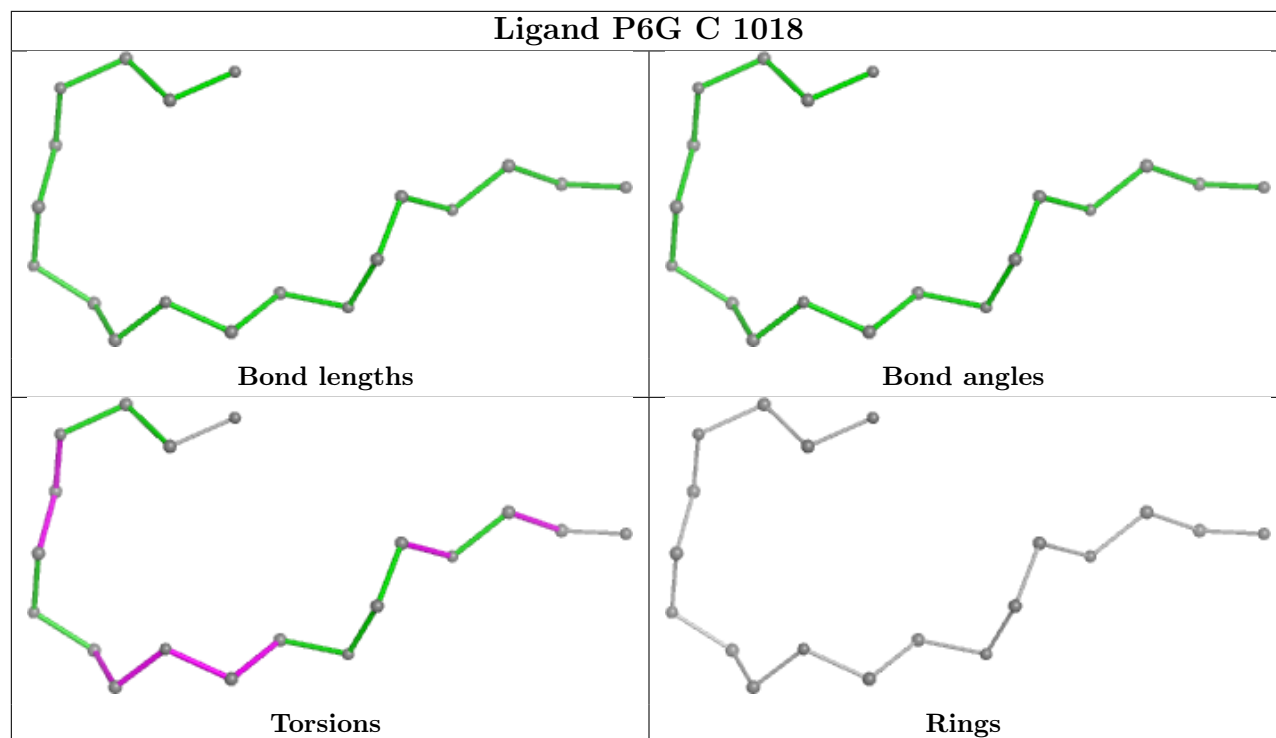
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1005	EDO	3	0
3	C	1002	NAG	4	0
9	C	1022	GLC	1	0
4	C	1005	EDO	3	0
3	A	1002	NAG	4	0
7	C	1018	P6G	1	0
3	A	1001	NAG	7	0
9	A	1021	GLC	1	0
4	C	1006	EDO	11	0
3	C	1001	NAG	7	0

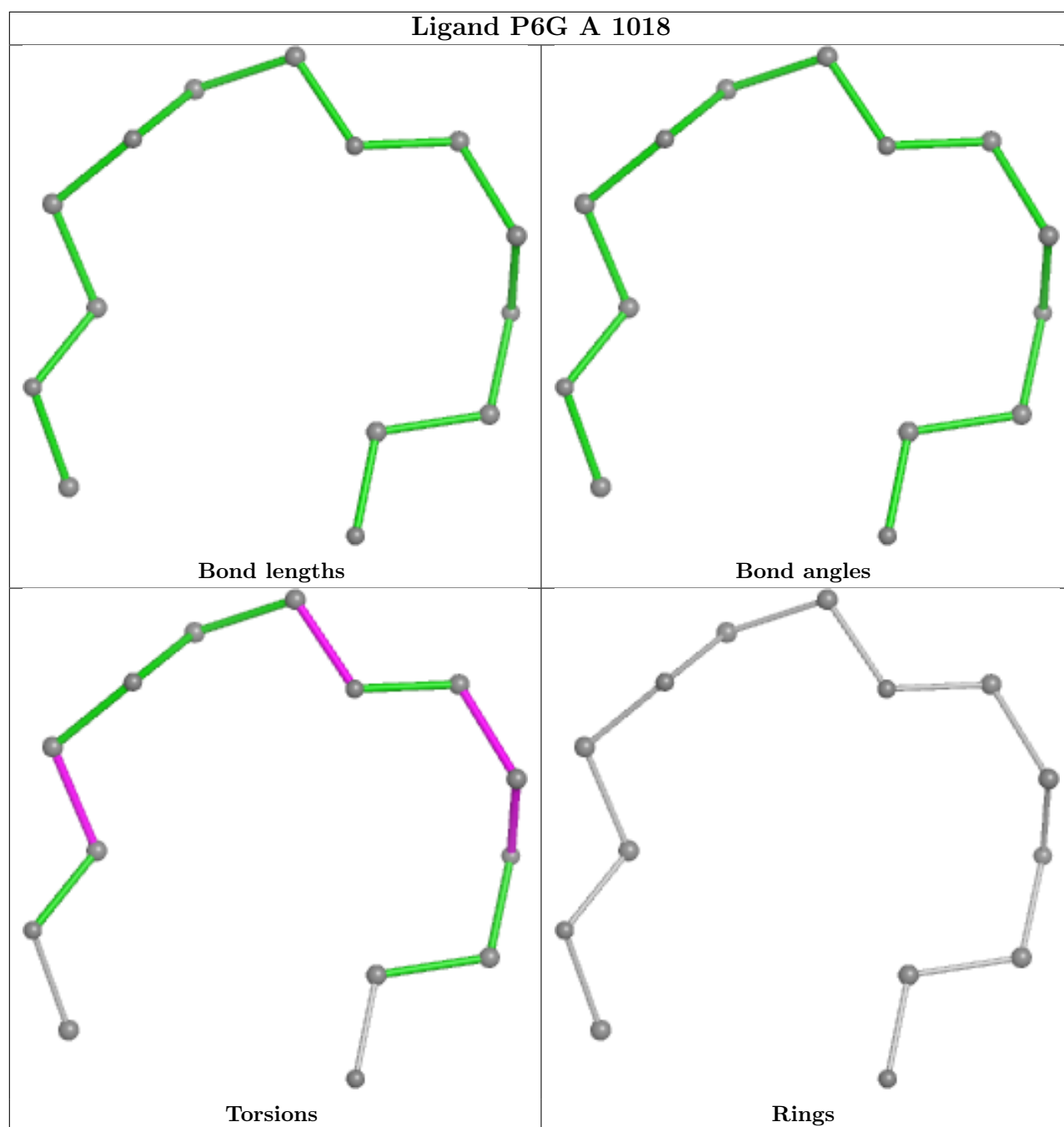
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In



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







## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	2
1	C	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	185:ARG	C	244:GLU	N	15.76
1	C	185:ARG	C	244:GLU	N	15.19
1	A	350:ASN	C	370:THR	N	7.78
1	C	350:ASN	C	370:THR	N	7.77

## 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	857/857 (100%)	0.44	64 (7%)	22 22	8, 27, 53, 84	12 (1%)
1	C	857/857 (100%)	0.53	77 (8%)	17 17	11, 29, 60, 88	11 (1%)
2	B	88/88 (100%)	1.68	32 (36%)	1 1	18, 42, 81, 99	0
2	D	88/88 (100%)	1.54	30 (34%)	1 1	24, 44, 79, 99	0
All	All	1890/1890 (100%)	0.59	203 (10%)	12 12	8, 29, 61, 99	23 (1%)

The worst 5 of 203 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	44	ALA	8.1
1	C	370	THR	6.6
2	D	34	SER	6.5
2	B	43	THR	6.3
2	B	31	TYR	6.3

### 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 monosaccharides in this entry.

### 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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( $\text{\AA}^2$ )	Q<0.9
6	PG4	B	201	11/13	0.47	0.42	55,75,88,89	0
6	PG4	A	1015	8/13	0.61	0.28	62,63,66,66	0
11	TAR	C	1021	10/10	0.61	0.30	89,91,98,99	0
7	P6G	C	1018	19/19	0.62	0.27	55,82,93,93	0
5	FMT	C	1009	1/3	0.62	0.56	30,30,30,30	0
5	FMT	A	1011	3/3	0.63	0.39	70,70,74,77	0
5	FMT	A	1014	3/3	0.65	0.27	73,73,74,74	0
5	FMT	C	1013	3/3	0.65	0.22	55,55,56,58	0
6	PG4	C	1016	8/13	0.66	0.31	78,79,81,81	0
6	PG4	A	1016	9/13	0.67	0.28	49,67,77,77	0
7	P6G	C	1019	19/19	0.67	0.34	68,90,107,107	0
7	P6G	A	1017	19/19	0.67	0.30	68,76,92,93	0
4	EDO	A	1004	4/4	0.68	0.25	49,53,54,58	0
6	PG4	C	1017	9/13	0.68	0.22	34,54,66,66	0
4	EDO	C	1004	4/4	0.70	0.30	63,65,66,66	0
5	FMT	A	1007	3/3	0.70	0.39	58,58,63,65	0
4	EDO	A	1003	4/4	0.70	0.23	35,39,40,40	0
3	NAG	C	1002	14/15	0.71	0.23	44,54,58,60	0
3	NAG	A	1002	14/15	0.72	0.18	38,50,55,59	0
5	FMT	A	1008	3/3	0.72	0.29	52,52,55,55	0
5	FMT	C	1015	3/3	0.72	0.23	56,56,58,59	0
7	P6G	A	1022	19/19	0.74	0.21	41,67,75,76	0
5	FMT	C	1014	3/3	0.74	0.32	76,76,76,77	0
6	PG4	B	204	9/13	0.75	0.27	57,59,68,68	0
5	FMT	A	1010	3/3	0.75	0.19	51,51,53,54	0
4	EDO	C	1005	4/4	0.75	0.26	35,42,45,48	0
5	FMT	C	1011	3/3	0.75	0.18	35,35,41,46	0
5	FMT	A	1006	3/3	0.76	0.23	34,34,40,43	0
6	PG4	D	203	9/13	0.78	0.25	59,61,62,62	0
5	FMT	C	1007	3/3	0.79	0.21	41,41,41,42	0
5	FMT	C	1010	2/3	0.79	0.16	27,27,27,29	0
8	OXM	A	1020	6/6	0.79	0.25	42,55,58,58	0
5	FMT	C	1008	3/3	0.79	0.29	63,63,65,65	0
7	P6G	A	1018	14/19	0.80	0.18	32,39,63,64	0
4	EDO	A	1005	4/4	0.80	0.18	35,37,37,39	0
4	EDO	C	1003	4/4	0.82	0.15	32,33,36,40	0
5	FMT	A	1019	3/3	0.83	0.30	32,33,34,34	0
4	EDO	C	1020	4/4	0.85	0.17	38,41,46,46	0
5	FMT	C	1012	3/3	0.86	0.12	48,48,48,49	0
5	FMT	A	1012	3/3	0.86	0.13	35,35,35,39	0
5	FMT	A	1013	3/3	0.87	0.14	42,42,43,43	0
3	NAG	C	1001	14/15	0.88	0.12	26,32,34,35	0
5	FMT	A	1009	3/3	0.89	0.15	49,49,51,51	0

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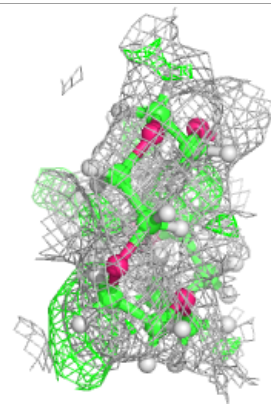
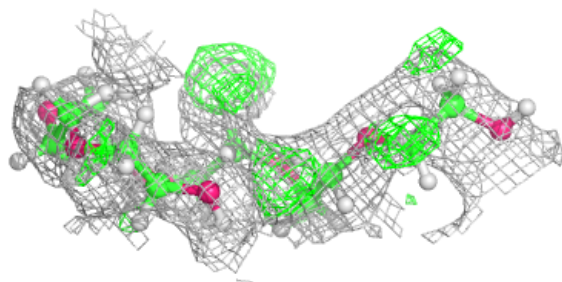
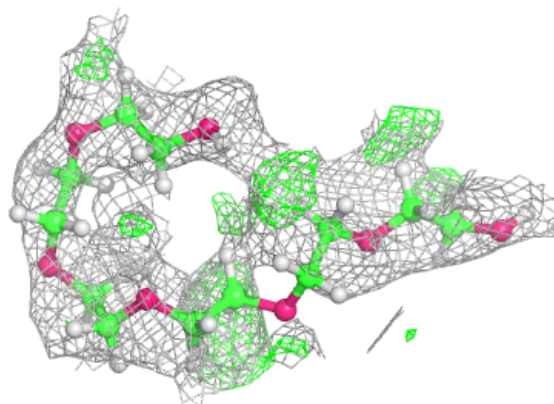
*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	NAG	A	1001	14/15	0.90	0.12	19,40,43,44	0
9	GLC	C	1022	12/12	0.94	0.08	17,22,24,24	0
4	EDO	C	1006	4/4	0.94	0.15	15,19,22,26	0
9	GLC	A	1021	12/12	0.95	0.07	13,21,32,36	0
10	CA	B	203	1/1	0.96	0.04	24,24,24,24	0
10	CA	B	202	1/1	0.98	0.03	27,27,27,27	0
10	CA	D	202	1/1	0.99	0.02	23,23,23,23	0
10	CA	D	201	1/1	0.99	0.02	25,25,25,25	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.

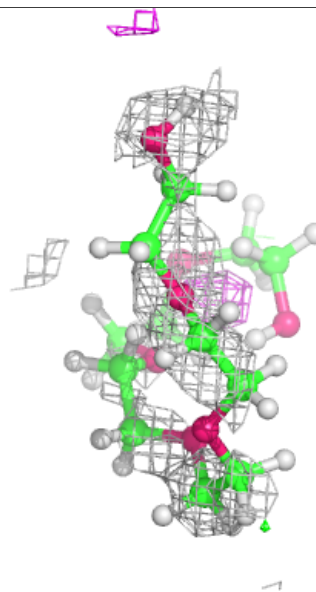
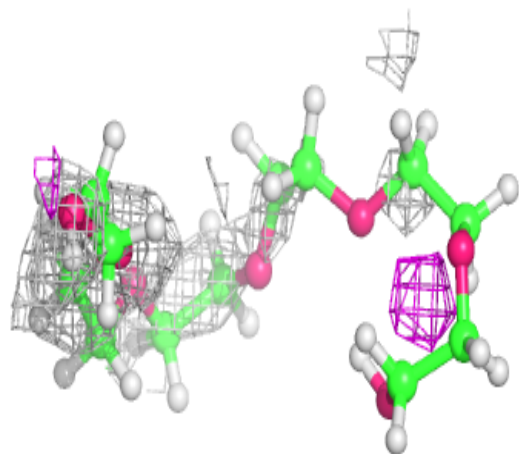
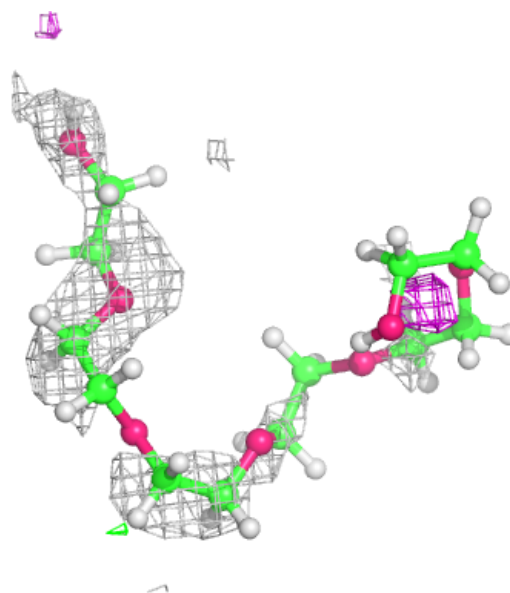
**Electron density around P6G C 1018:**

2mF<sub>o</sub>-DF<sub>c</sub> (at 0.7 rmsd) in gray  
mF<sub>o</sub>-DF<sub>c</sub> (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around P6G C 1019:**

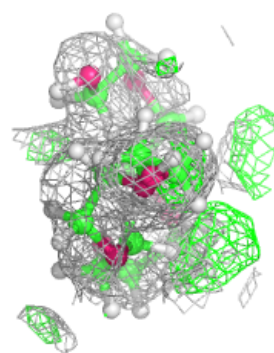
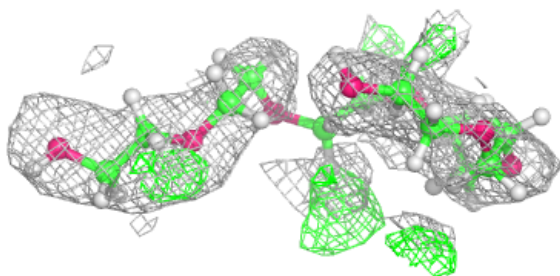
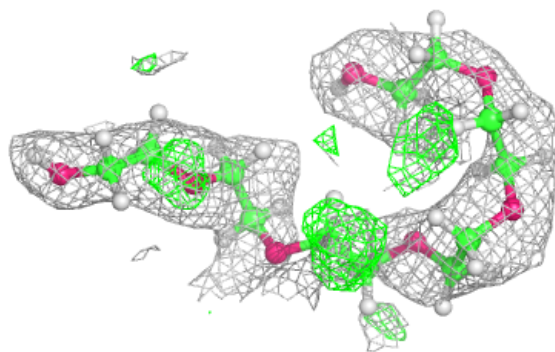
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

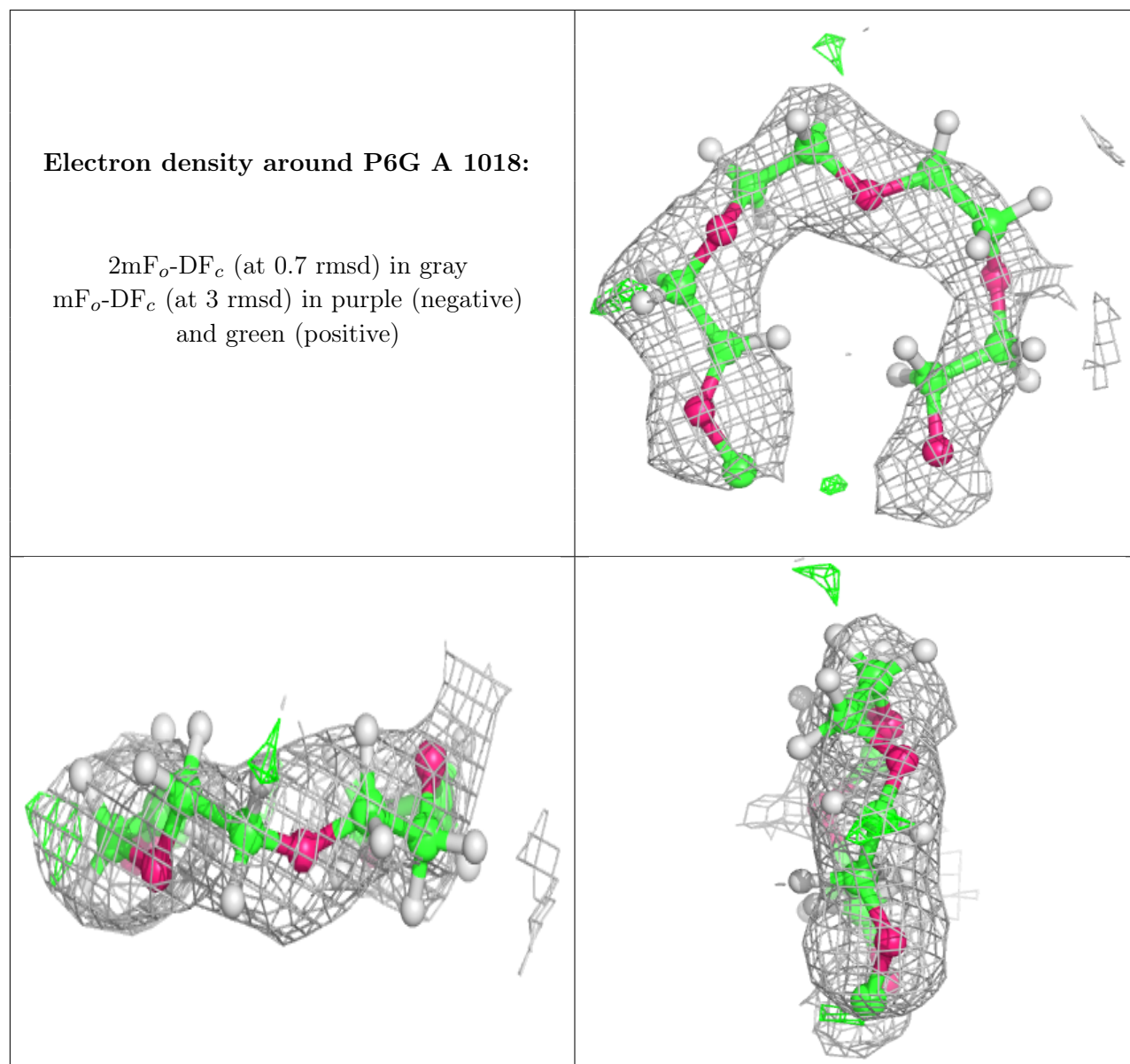




**Electron density around P6G A 1022:**

$2mF_o-DF_c$  (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.