



# wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 9, 2023 – 03:20 PM EDT

PDB ID : 7KRY  
Title : Co-crystal structure of alpha glucosidase with compound 11  
Authors : Karade, S.S.; Mariuzza, R.A.  
Deposited on : 2020-11-20  
Resolution : 2.55 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 : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.35.1  
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) : 2.35.1

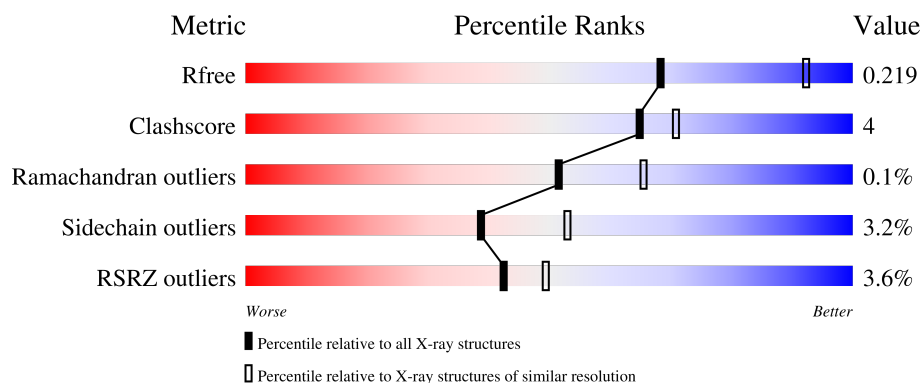
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.55 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	1284 (2.56-2.52)
Clashscore	141614	1332 (2.56-2.52)
Ramachandran outliers	138981	1315 (2.56-2.52)
Sidechain outliers	138945	1315 (2.56-2.52)
RSRZ outliers	127900	1272 (2.56-2.52)

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	955	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 12%, green 77%, grey 11%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>%</span> <span>77%</span> <span>12%</span> <span>11%</span> </div> </div>
1	C	955	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 3%, orange 1%, yellow 9%, green 80%, grey 10%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>3%</span> <span>80%</span> <span>9%</span> <span>10%</span> </div> </div>
2	B	554	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 2%, orange 1%, yellow 14%, green 85%, grey 0%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>2%</span> <span>14%</span> <span>85%</span> </div> </div>
2	D	554	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 3%, orange 1%, yellow 14%, green 85%, grey 0%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>3%</span> <span>14%</span> <span>85%</span> </div> </div>

## 2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 15587 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 Neutral alpha-glucosidase AB.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	854	Total	C	N	O	S	0	5	0
			6865	4402	1181	1252	30			
1	C	857	Total	C	N	O	S	0	4	0
			6892	4413	1186	1265	28			

There are 88 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	2	MET	-	initiating methionine	UNP Q8BHN3
A	3	GLY	-	expression tag	UNP Q8BHN3
A	4	ILE	-	expression tag	UNP Q8BHN3
A	5	LEU	-	expression tag	UNP Q8BHN3
A	6	PRO	-	expression tag	UNP Q8BHN3
A	7	SER	-	expression tag	UNP Q8BHN3
A	8	PRO	-	expression tag	UNP Q8BHN3
A	9	GLY	-	expression tag	UNP Q8BHN3
A	10	MET	-	expression tag	UNP Q8BHN3
A	11	PRO	-	expression tag	UNP Q8BHN3
A	12	ALA	-	expression tag	UNP Q8BHN3
A	13	LEU	-	expression tag	UNP Q8BHN3
A	14	LEU	-	expression tag	UNP Q8BHN3
A	15	SER	-	expression tag	UNP Q8BHN3
A	16	LEU	-	expression tag	UNP Q8BHN3
A	17	VAL	-	expression tag	UNP Q8BHN3
A	18	SER	-	expression tag	UNP Q8BHN3
A	19	LEU	-	expression tag	UNP Q8BHN3
A	20	LEU	-	expression tag	UNP Q8BHN3
A	21	SER	-	expression tag	UNP Q8BHN3
A	22	VAL	-	expression tag	UNP Q8BHN3
A	23	LEU	-	expression tag	UNP Q8BHN3
A	24	LEU	-	expression tag	UNP Q8BHN3
A	25	MET	-	expression tag	UNP Q8BHN3
A	26	GLY	-	expression tag	UNP Q8BHN3

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Chain	Residue	Modelled	Actual	Comment	Reference
A	27	CYS	-	expression tag	UNP Q8BHN3
A	28	VAL	-	expression tag	UNP Q8BHN3
A	29	ALA	-	expression tag	UNP Q8BHN3
A	30	GLU	-	expression tag	UNP Q8BHN3
A	31	THR	-	expression tag	UNP Q8BHN3
A	32	GLY	-	expression tag	UNP Q8BHN3
A	97	ASP	ASN	engineered mutation	UNP Q8BHN3
A	967	SER	-	expression tag	UNP Q8BHN3
A	968	ALA	-	expression tag	UNP Q8BHN3
A	969	TRP	-	expression tag	UNP Q8BHN3
A	970	SER	-	expression tag	UNP Q8BHN3
A	971	HIS	-	expression tag	UNP Q8BHN3
A	972	PRO	-	expression tag	UNP Q8BHN3
A	973	GLN	-	expression tag	UNP Q8BHN3
A	974	PHE	-	expression tag	UNP Q8BHN3
A	975	GLU	-	expression tag	UNP Q8BHN3
A	976	LYS	-	expression tag	UNP Q8BHN3
A	977	LEU	-	expression tag	UNP Q8BHN3
A	978	GLU	-	expression tag	UNP Q8BHN3
C	2	MET	-	initiating methionine	UNP Q8BHN3
C	3	GLY	-	expression tag	UNP Q8BHN3
C	4	ILE	-	expression tag	UNP Q8BHN3
C	5	LEU	-	expression tag	UNP Q8BHN3
C	6	PRO	-	expression tag	UNP Q8BHN3
C	7	SER	-	expression tag	UNP Q8BHN3
C	8	PRO	-	expression tag	UNP Q8BHN3
C	9	GLY	-	expression tag	UNP Q8BHN3
C	10	MET	-	expression tag	UNP Q8BHN3
C	11	PRO	-	expression tag	UNP Q8BHN3
C	12	ALA	-	expression tag	UNP Q8BHN3
C	13	LEU	-	expression tag	UNP Q8BHN3
C	14	LEU	-	expression tag	UNP Q8BHN3
C	15	SER	-	expression tag	UNP Q8BHN3
C	16	LEU	-	expression tag	UNP Q8BHN3
C	17	VAL	-	expression tag	UNP Q8BHN3
C	18	SER	-	expression tag	UNP Q8BHN3
C	19	LEU	-	expression tag	UNP Q8BHN3
C	20	LEU	-	expression tag	UNP Q8BHN3
C	21	SER	-	expression tag	UNP Q8BHN3
C	22	VAL	-	expression tag	UNP Q8BHN3
C	23	LEU	-	expression tag	UNP Q8BHN3
C	24	LEU	-	expression tag	UNP Q8BHN3

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Chain	Residue	Modelled	Actual	Comment	Reference
C	25	MET	-	expression tag	UNP Q8BHN3
C	26	GLY	-	expression tag	UNP Q8BHN3
C	27	CYS	-	expression tag	UNP Q8BHN3
C	28	VAL	-	expression tag	UNP Q8BHN3
C	29	ALA	-	expression tag	UNP Q8BHN3
C	30	GLU	-	expression tag	UNP Q8BHN3
C	31	THR	-	expression tag	UNP Q8BHN3
C	32	GLY	-	expression tag	UNP Q8BHN3
C	97	ASP	ASN	engineered mutation	UNP Q8BHN3
C	967	SER	-	expression tag	UNP Q8BHN3
C	968	ALA	-	expression tag	UNP Q8BHN3
C	969	TRP	-	expression tag	UNP Q8BHN3
C	970	SER	-	expression tag	UNP Q8BHN3
C	971	HIS	-	expression tag	UNP Q8BHN3
C	972	PRO	-	expression tag	UNP Q8BHN3
C	973	GLN	-	expression tag	UNP Q8BHN3
C	974	PHE	-	expression tag	UNP Q8BHN3
C	975	GLU	-	expression tag	UNP Q8BHN3
C	976	LYS	-	expression tag	UNP Q8BHN3
C	977	LEU	-	expression tag	UNP Q8BHN3
C	978	GLU	-	expression tag	UNP Q8BHN3

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	84	Total	C	N	O	S	0	0	0
			585	343	99	133	10			
2	D	84	Total	C	N	O	S	0	0	0
			601	359	97	135	10			

There are 102 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-16	MET	-	initiating methionine	UNP O08795
B	-15	GLY	-	expression tag	UNP O08795
B	-14	ILE	-	expression tag	UNP O08795
B	-13	LEU	-	expression tag	UNP O08795
B	-12	PRO	-	expression tag	UNP O08795
B	-11	SER	-	expression tag	UNP O08795
B	-10	PRO	-	expression tag	UNP O08795
B	-9	GLY	-	expression tag	UNP O08795
B	-8	MET	-	expression tag	UNP O08795

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-7	PRO	-	expression tag	UNP O08795
B	-6	ALA	-	expression tag	UNP O08795
B	-5	LEU	-	expression tag	UNP O08795
B	-4	LEU	-	expression tag	UNP O08795
B	-3	SER	-	expression tag	UNP O08795
B	-2	LEU	-	expression tag	UNP O08795
B	-1	VAL	-	expression tag	UNP O08795
B	0	SER	-	expression tag	UNP O08795
B	1	LEU	-	expression tag	UNP O08795
B	2	LEU	-	expression tag	UNP O08795
B	3	SER	-	expression tag	UNP O08795
B	4	VAL	-	expression tag	UNP O08795
B	5	LEU	-	expression tag	UNP O08795
B	6	LEU	-	expression tag	UNP O08795
B	7	MET	-	expression tag	UNP O08795
B	8	GLY	-	expression tag	UNP O08795
B	9	CYS	-	expression tag	UNP O08795
B	10	VAL	-	expression tag	UNP O08795
B	11	ALA	-	expression tag	UNP O08795
B	12	GLU	-	expression tag	UNP O08795
B	13	THR	-	expression tag	UNP O08795
B	14	GLY	-	expression tag	UNP O08795
B	518	SER	-	expression tag	UNP O08795
B	519	ALA	-	expression tag	UNP O08795
B	520	TRP	-	expression tag	UNP O08795
B	521	SER	-	expression tag	UNP O08795
B	522	HIS	-	expression tag	UNP O08795
B	523	PRO	-	expression tag	UNP O08795
B	524	GLN	-	expression tag	UNP O08795
B	525	PHE	-	expression tag	UNP O08795
B	526	GLU	-	expression tag	UNP O08795
B	527	LYS	-	expression tag	UNP O08795
B	528	LEU	-	expression tag	UNP O08795
B	529	GLU	-	expression tag	UNP O08795
B	530	THR	-	expression tag	UNP O08795
B	531	LYS	-	expression tag	UNP O08795
B	532	HIS	-	expression tag	UNP O08795
B	533	HIS	-	expression tag	UNP O08795
B	534	HIS	-	expression tag	UNP O08795
B	535	HIS	-	expression tag	UNP O08795
B	536	HIS	-	expression tag	UNP O08795
B	537	HIS	-	expression tag	UNP O08795

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-16	MET	-	initiating methionine	UNP O08795
D	-15	GLY	-	expression tag	UNP O08795
D	-14	ILE	-	expression tag	UNP O08795
D	-13	LEU	-	expression tag	UNP O08795
D	-12	PRO	-	expression tag	UNP O08795
D	-11	SER	-	expression tag	UNP O08795
D	-10	PRO	-	expression tag	UNP O08795
D	-9	GLY	-	expression tag	UNP O08795
D	-8	MET	-	expression tag	UNP O08795
D	-7	PRO	-	expression tag	UNP O08795
D	-6	ALA	-	expression tag	UNP O08795
D	-5	LEU	-	expression tag	UNP O08795
D	-4	LEU	-	expression tag	UNP O08795
D	-3	SER	-	expression tag	UNP O08795
D	-2	LEU	-	expression tag	UNP O08795
D	-1	VAL	-	expression tag	UNP O08795
D	0	SER	-	expression tag	UNP O08795
D	1	LEU	-	expression tag	UNP O08795
D	2	LEU	-	expression tag	UNP O08795
D	3	SER	-	expression tag	UNP O08795
D	4	VAL	-	expression tag	UNP O08795
D	5	LEU	-	expression tag	UNP O08795
D	6	LEU	-	expression tag	UNP O08795
D	7	MET	-	expression tag	UNP O08795
D	8	GLY	-	expression tag	UNP O08795
D	9	CYS	-	expression tag	UNP O08795
D	10	VAL	-	expression tag	UNP O08795
D	11	ALA	-	expression tag	UNP O08795
D	12	GLU	-	expression tag	UNP O08795
D	13	THR	-	expression tag	UNP O08795
D	14	GLY	-	expression tag	UNP O08795
D	518	SER	-	expression tag	UNP O08795
D	519	ALA	-	expression tag	UNP O08795
D	520	TRP	-	expression tag	UNP O08795
D	521	SER	-	expression tag	UNP O08795
D	522	HIS	-	expression tag	UNP O08795
D	523	PRO	-	expression tag	UNP O08795
D	524	GLN	-	expression tag	UNP O08795
D	525	PHE	-	expression tag	UNP O08795
D	526	GLU	-	expression tag	UNP O08795
D	527	LYS	-	expression tag	UNP O08795
D	528	LEU	-	expression tag	UNP O08795

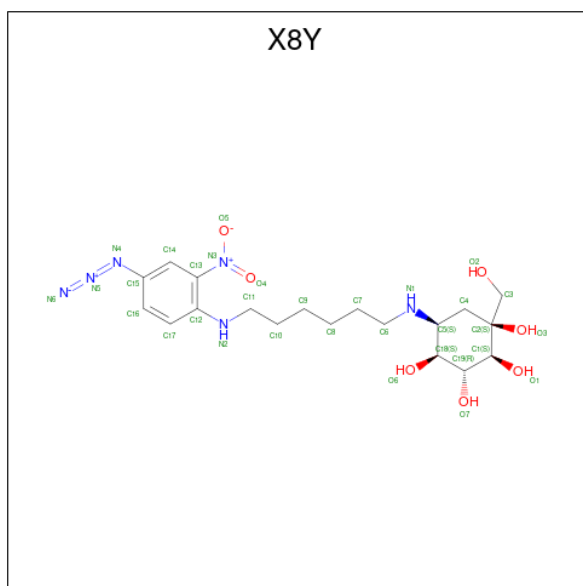
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Chain	Residue	Modelled	Actual	Comment	Reference
D	529	GLU	-	expression tag	UNP O08795
D	530	THR	-	expression tag	UNP O08795
D	531	LYS	-	expression tag	UNP O08795
D	532	HIS	-	expression tag	UNP O08795
D	533	HIS	-	expression tag	UNP O08795
D	534	HIS	-	expression tag	UNP O08795
D	535	HIS	-	expression tag	UNP O08795
D	536	HIS	-	expression tag	UNP O08795
D	537	HIS	-	expression tag	UNP O08795

- Molecule 3 is (1S,2S,3R,4S,5S)-5-({6-[(4-azido-2-nitrophenyl)amino]hexyl}amino)-1-(hydroxymethyl)cyclohexane-1,2,3,4-tetrol (three-letter code: X8Y) (formula: C<sub>19</sub>H<sub>30</sub>N<sub>6</sub>O<sub>7</sub>) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			32	19	6	7		
3	C	1	Total	C	N	O	0	0
			32	19	6	7		

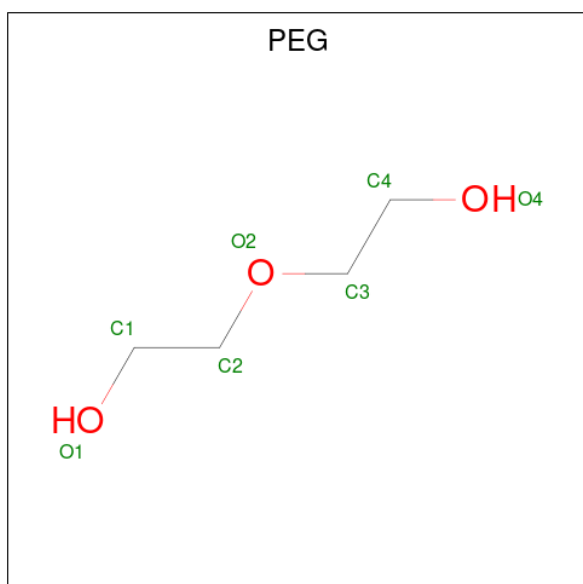
- Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).





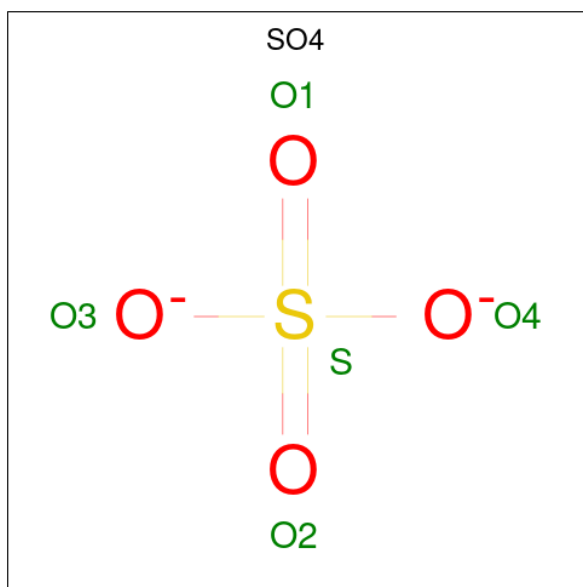
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		
4	C	1	Total	C	O	0	0
			4	2	2		

- Molecule 5 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula:  $C_4H_{10}O_3$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			7	4	3		
5	C	1	Total	C	O	0	0
			7	4	3		

- Molecule 6 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).

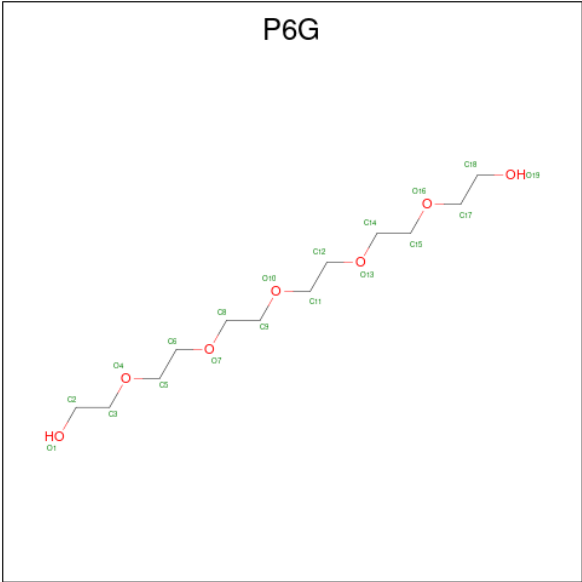


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	O	S	0	0
			5	4	1		
6	A	1	Total	O	S	0	0
			5	4	1		

- Molecule 7 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

- Molecule 8 is HEXAETHYLENE GLYCOL (three-letter code: P6G) (formula: C<sub>12</sub>H<sub>26</sub>O<sub>7</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	C	1	Total	C	O	0	0
			19	12	7		

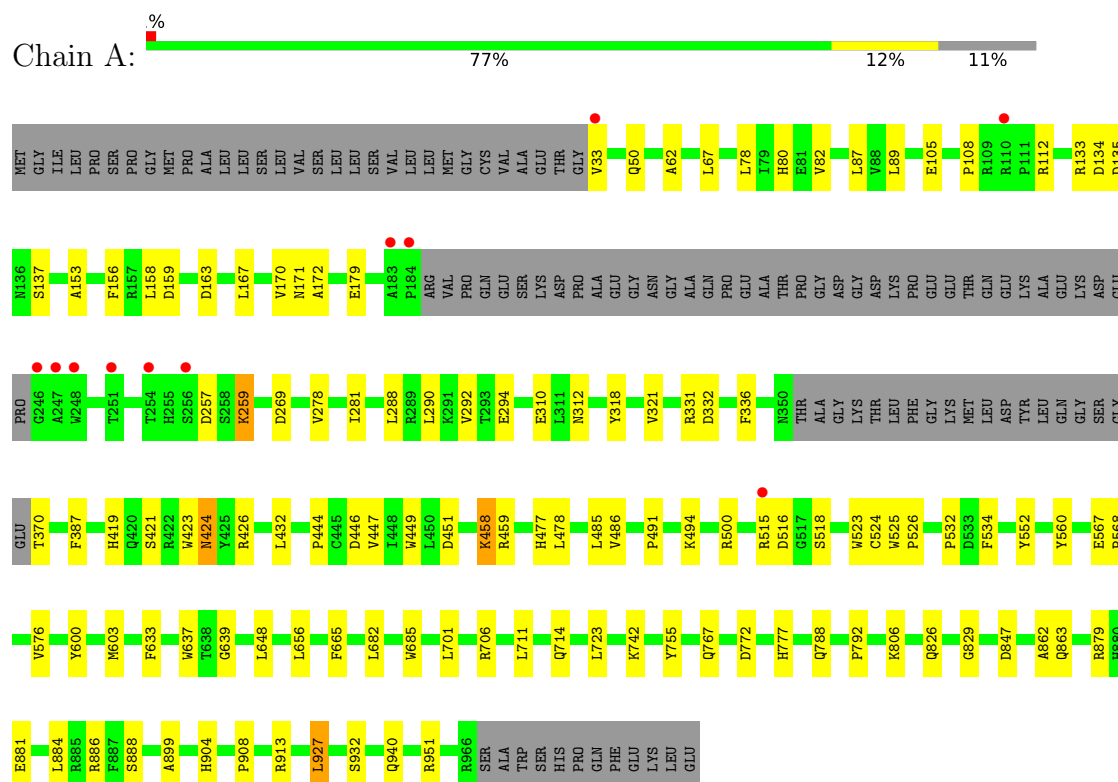
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	271	Total	O	0	0
			271	271		
9	B	11	Total	O	0	0
			11	11		
9	C	217	Total	O	0	0
			217	217		
9	D	14	Total	O	0	0
			14	14		

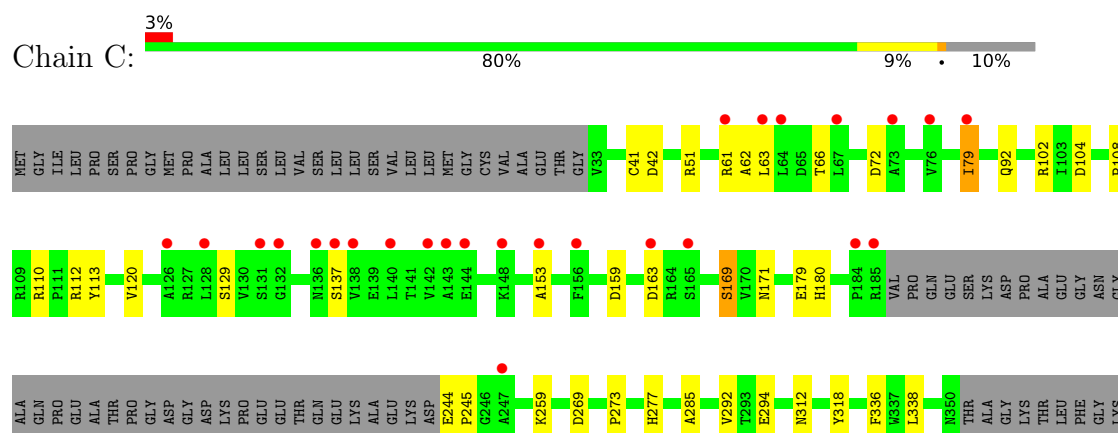
### 3 Residue-property plots

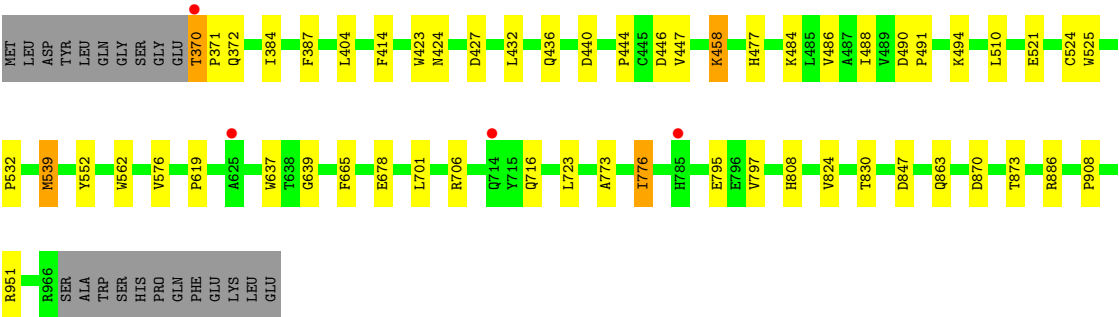
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Neutral alpha-glucosidase AB

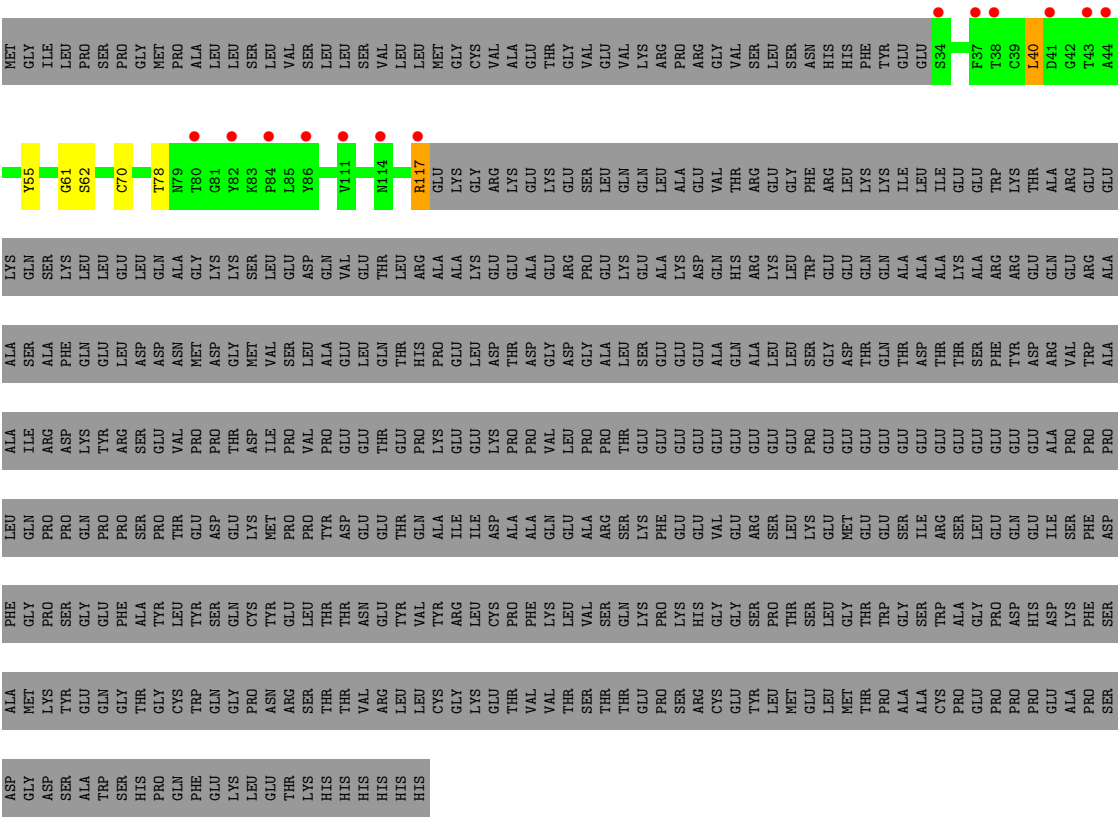


#### • Molecule 1: Neutral alpha-glucosidase AB

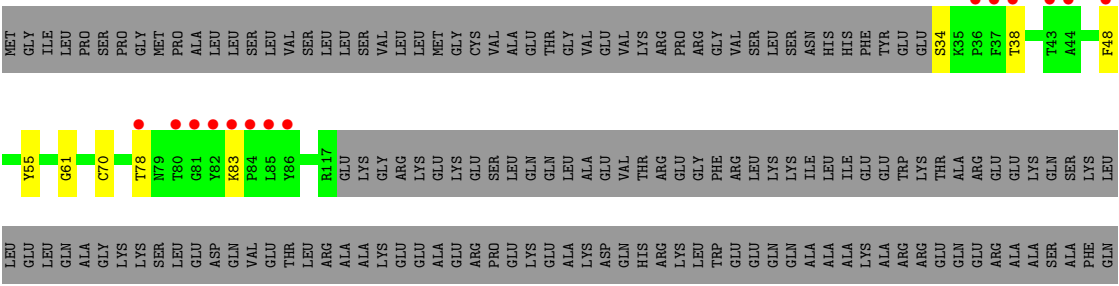




● Molecule 2: Glucosidase 2 subunit beta



● Molecule 2: Glucosidase 2 subunit beta



[illegible]

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	102.92Å 102.92Å 240.22Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	49.80 – 2.55 49.80 – 2.55	Depositor EDS
% Data completeness (in resolution range)	100.0 (49.80-2.55) 93.4 (49.80-2.55)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	0.90 (at 2.54Å)	Xtriage
Refinement program	PHENIX 1.18.2_3874	Depositor
R, $R_{free}$	0.181 , 0.219 0.181 , 0.219	Depositor DCC
$R_{free}$ test set	1989 reflections (2.15%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	43.1	Xtriage
Anisotropy	0.008	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 38.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.014 for -h,-k,l 0.043 for h,-h-k,-l 0.025 for -k,-h,-l	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	15587	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.63% 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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: PEG, P6G, EDO, SO4, CA, X8Y

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	0.42	0/7090	0.61	2/9658 (0.0%)
1	C	0.40	0/7112	0.60	0/9690
2	B	0.36	0/595	0.66	0/815
2	D	0.41	0/613	0.61	0/838
All	All	0.41	0/15410	0.61	2/21001 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	927	LEU	CA-CB-CG	5.80	128.64	115.30
1	A	772	ASP	CB-CG-OD1	5.55	123.30	118.30

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	6865	0	6591	64	0
1	C	6892	0	6600	49	0
2	B	585	0	468	4	0
2	D	601	0	490	3	0
3	A	32	0	0	0	0

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*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	32	0	0	1	0
4	A	16	0	23	5	0
4	C	4	0	6	0	0
5	A	7	0	10	1	0
5	C	7	0	10	1	0
6	A	10	0	0	1	0
7	B	2	0	0	0	0
7	D	2	0	0	0	0
8	C	19	0	26	0	0
9	A	271	0	0	14	0
9	B	11	0	0	0	0
9	C	217	0	0	12	0
9	D	14	0	0	1	0
All	All	15587	0	14224	121	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 4.

The worst 5 of 121 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:619:PRO:O	9:C:1201:HOH:O	1.91	0.89
1:A:159:ASP:OD2	9:A:1101:HOH:O	1.93	0.85
1:A:167:LEU:O	9:A:1102:HOH:O	2.00	0.80
1:A:134:ASP:O	9:A:1103:HOH:O	2.01	0.79
1:C:277:HIS:ND1	9:C:1207:HOH:O	2.15	0.78

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	853/955 (89%)	826 (97%)	26 (3%)	1 (0%)	51	65
1	C	855/955 (90%)	824 (96%)	30 (4%)	1 (0%)	51	65
2	B	82/554 (15%)	78 (95%)	4 (5%)	0	100	100
2	D	82/554 (15%)	77 (94%)	5 (6%)	0	100	100
All	All	1872/3018 (62%)	1805 (96%)	65 (4%)	2 (0%)	51	65

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	576	VAL
1	C	576	VAL

### 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	740/826 (90%)	717 (97%)	23 (3%)	40	54
1	C	743/826 (90%)	721 (97%)	22 (3%)	41	55
2	B	64/485 (13%)	61 (95%)	3 (5%)	26	35
2	D	67/485 (14%)	63 (94%)	4 (6%)	19	25
All	All	1614/2622 (62%)	1562 (97%)	52 (3%)	39	53

5 of 52 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	110	ARG
1	C	424	ASN
2	D	48	PHE
1	C	129	SER
1	C	169	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

Of 16 ligands modelled in this entry, 4 are monoatomic - leaving 12 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	X8Y	A	1001	-	31,33,33	2.91	6 (19%)	37,45,45	1.58	4 (10%)
8	P6G	C	1101	-	18,18,18	0.54	0	17,17,17	0.26	0
3	X8Y	C	1102	-	31,33,33	2.73	6 (19%)	37,45,45	1.35	5 (13%)
4	EDO	A	1006	-	3,3,3	0.83	0	2,2,2	0.55	0
6	SO4	A	1007	-	4,4,4	0.25	0	6,6,6	0.32	0
6	SO4	A	1008	-	4,4,4	0.19	0	6,6,6	0.31	0
5	PEG	A	1005	-	6,6,6	0.48	0	5,5,5	0.51	0
4	EDO	A	1002	-	3,3,3	0.67	0	2,2,2	0.42	0
4	EDO	A	1004	-	3,3,3	0.57	0	2,2,2	0.55	0
4	EDO	A	1003	-	3,3,3	0.68	0	2,2,2	0.35	0
5	PEG	C	1103	-	6,6,6	0.49	0	5,5,5	0.32	0
4	EDO	C	1104	-	3,3,3	0.49	0	2,2,2	0.21	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	X8Y	A	1001	-	-	14/19/44/44	0/2/2/2
8	P6G	C	1101	-	-	7/16/16/16	-
3	X8Y	C	1102	-	-	10/19/44/44	0/2/2/2
4	EDO	A	1006	-	-	0/1/1/1	-
5	PEG	A	1005	-	-	2/4/4/4	-
4	EDO	A	1002	-	-	1/1/1/1	-
4	EDO	A	1004	-	-	0/1/1/1	-
4	EDO	A	1003	-	-	1/1/1/1	-
5	PEG	C	1103	-	-	2/4/4/4	-
4	EDO	C	1104	-	-	1/1/1/1	-

The worst 5 of 12 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1001	X8Y	O4-N3	11.68	1.42	1.22
3	C	1102	X8Y	O4-N3	11.18	1.41	1.22
3	A	1001	X8Y	N5-N4	7.87	1.46	1.24
3	C	1102	X8Y	N5-N4	7.12	1.44	1.24
3	A	1001	X8Y	C12-N2	4.27	1.49	1.37

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1001	X8Y	C6-N1-C5	-6.53	104.97	114.20
3	A	1001	X8Y	C11-N2-C12	-3.09	115.96	123.39
3	C	1102	X8Y	C18-C5-N1	-3.05	104.10	109.66
3	C	1102	X8Y	C17-C12-N2	-3.02	116.66	121.80
3	C	1102	X8Y	C11-N2-C12	-2.93	116.33	123.39

There are no chirality outliers.

5 of 38 torsion outliers are listed below:

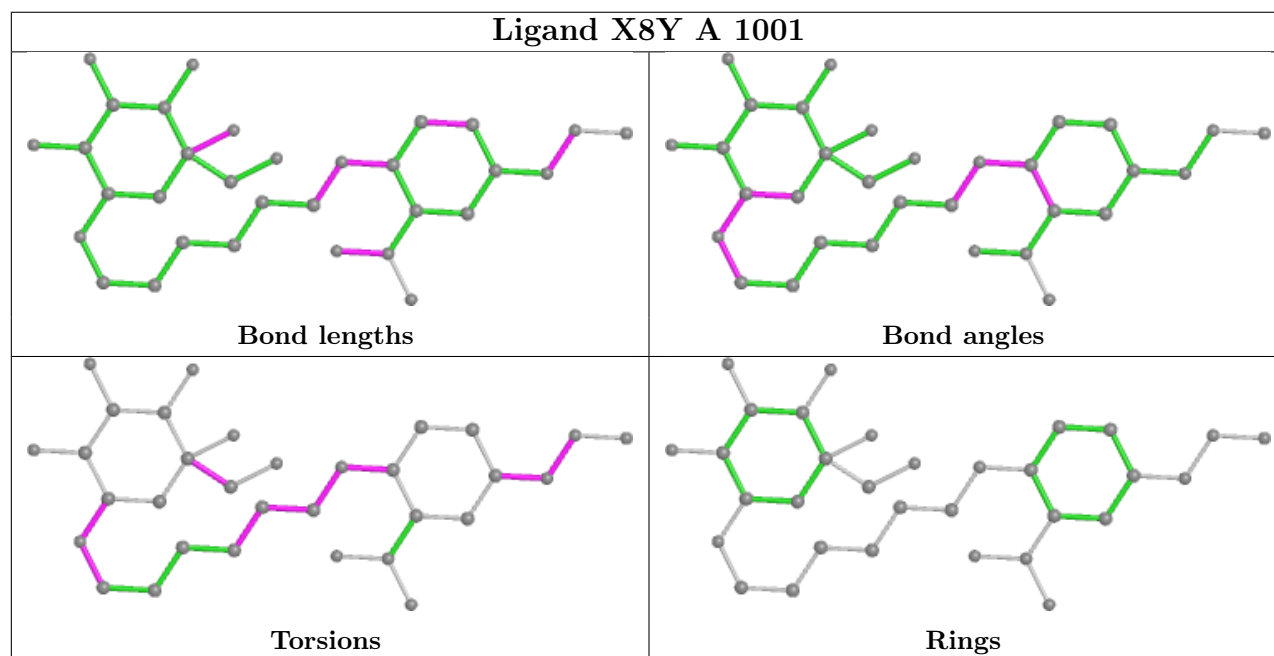
Mol	Chain	Res	Type	Atoms
3	A	1001	X8Y	C18-C5-N1-C6
3	A	1001	X8Y	C14-C15-N4-N5
3	A	1001	X8Y	C16-C15-N4-N5
3	A	1001	X8Y	C13-C12-N2-C11
3	A	1001	X8Y	C1-C2-C3-O2

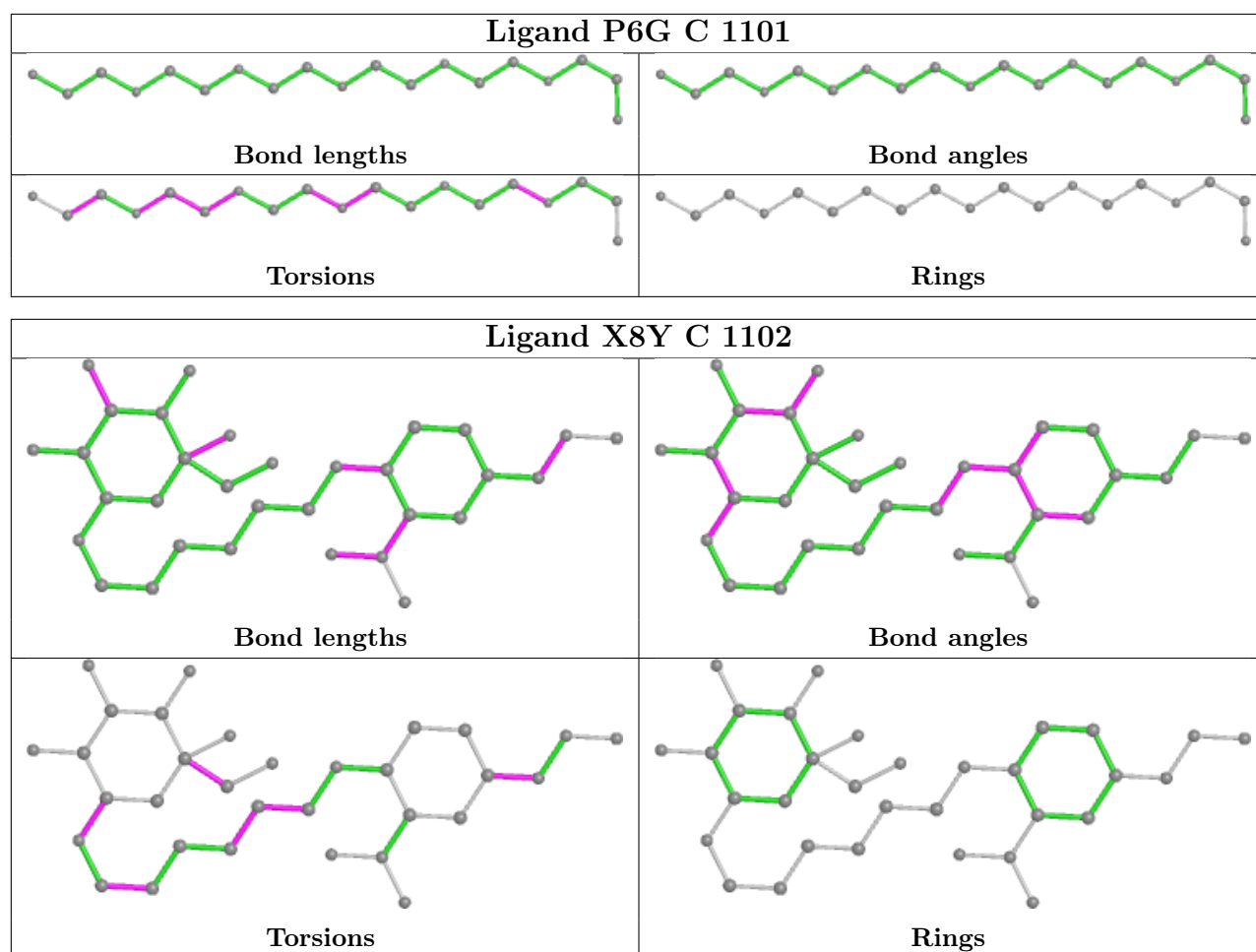
There are no ring outliers.

8 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	1102	X8Y	1	0
4	A	1006	EDO	1	0
6	A	1008	SO4	1	0
5	A	1005	PEG	1	0
4	A	1002	EDO	1	0
4	A	1004	EDO	2	0
4	A	1003	EDO	1	0
5	C	1103	PEG	1	0

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





## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.



## 6 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2		OWAB(Å <sup>2</sup> )	Q < 0.9
1	A	854/955 (89%)	-0.24	11 (1%)	77 82	33, 45, 67, 104	0
1	C	857/955 (89%)	-0.02	30 (3%)	44 51	34, 50, 88, 103	0
2	B	84/554 (15%)	0.47	13 (15%)	2 2	42, 60, 91, 96	0
2	D	84/554 (15%)	0.64	14 (16%)	1 1	43, 59, 91, 96	0
All	All	1879/3018 (62%)	-0.07	68 (3%)	42 49	33, 48, 84, 104	0

The worst 5 of 68 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	184	PRO	7.1
2	D	43	THR	7.0
2	D	81	GLY	5.3
2	D	82	TYR	5.0
2	B	43	THR	4.8

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

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

### 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

### 6.4 Ligands [i](#)

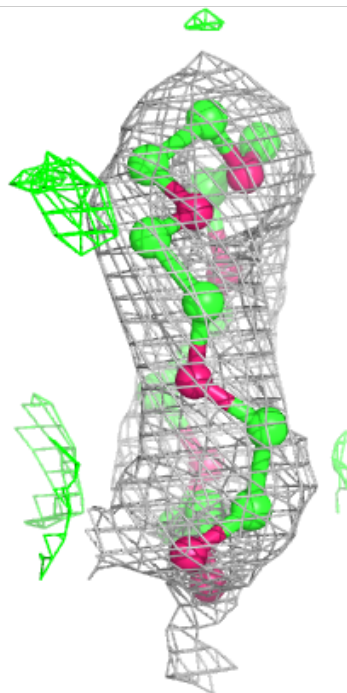
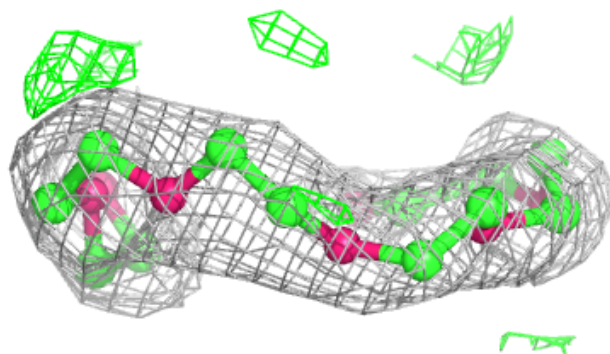
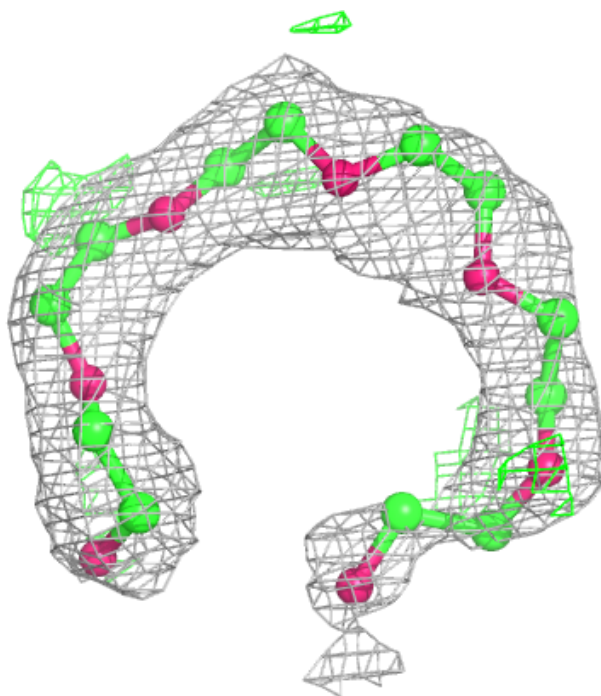
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q < 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
4	EDO	A	1003	4/4	0.81	0.24	63,64,68,72	0
4	EDO	A	1006	4/4	0.84	0.45	57,62,69,70	0
5	PEG	C	1103	7/7	0.84	0.17	61,70,73,74	0
4	EDO	C	1104	4/4	0.87	0.29	62,63,64,65	0
8	P6G	C	1101	19/19	0.87	0.18	63,72,76,76	0
3	X8Y	C	1102	32/32	0.90	0.20	37,49,71,74	0
5	PEG	A	1005	7/7	0.90	0.25	62,65,74,74	0
6	SO4	A	1007	5/5	0.92	0.17	64,64,67,91	0
3	X8Y	A	1001	32/32	0.93	0.20	36,44,65,68	0
4	EDO	A	1004	4/4	0.93	0.40	62,65,66,70	0
6	SO4	A	1008	5/5	0.96	0.19	66,68,73,83	0
4	EDO	A	1002	4/4	0.97	0.11	44,45,48,53	0
7	CA	D	601	1/1	0.98	0.07	55,55,55,55	0
7	CA	B	601	1/1	0.99	0.07	58,58,58,58	0
7	CA	D	602	1/1	0.99	0.08	46,46,46,46	0
7	CA	B	602	1/1	0.99	0.05	43,43,43,43	0

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

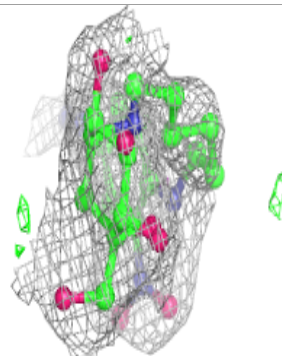
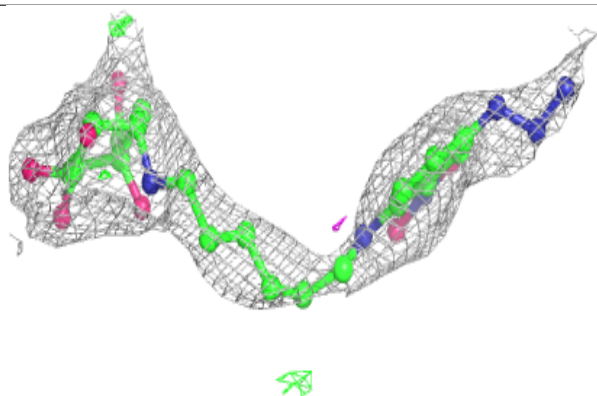
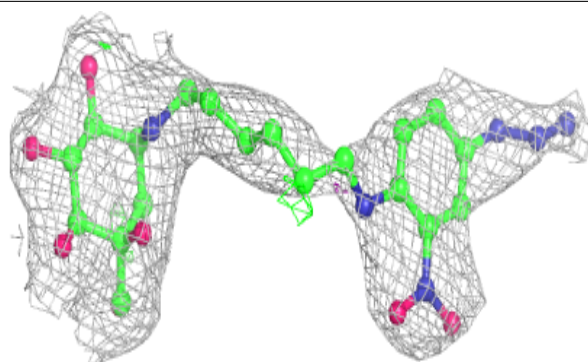
**Electron density around P6G C 1101:**

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

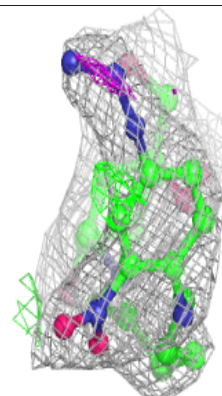
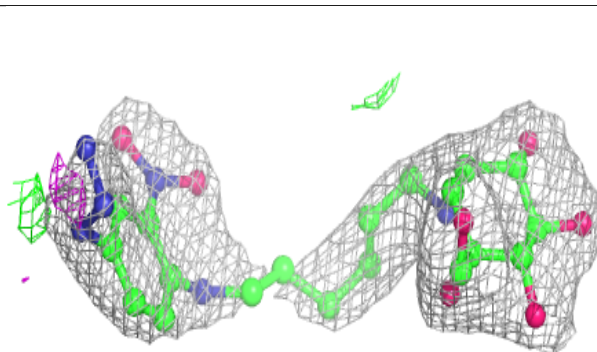
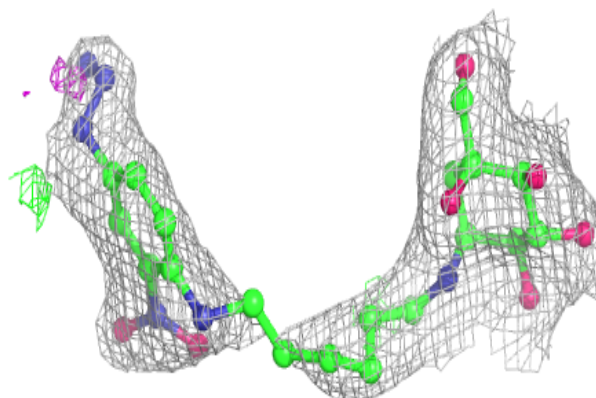


**Electron density around X8Y C 1102:**

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

**Electron density around X8Y A 1001:**

$2mF_o-DF_c$  (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.