



# wwPDB X-ray Structure Validation Summary Report ⓘ

Sep 27, 2021 – 02:10 PM EDT

PDB ID : 7KB8  
Title : Co-crystal structure of alpha glucosidase with compound 8  
Authors : Karade, S.S.; Mariuzza, R.A.  
Deposited on : 2020-10-01  
Resolution : 2.38 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.

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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 : 2.23.2  
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) : 2.23.2

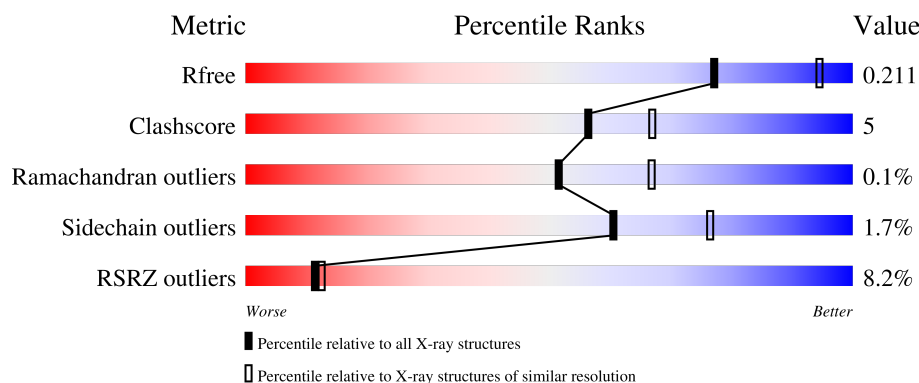
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.38 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	5509 (2.40-2.36)
Clashscore	141614	6082 (2.40-2.36)
Ramachandran outliers	138981	5973 (2.40-2.36)
Sidechain outliers	138945	5975 (2.40-2.36)
RSRZ outliers	127900	5397 (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	977	<div> <div>5%</div> <div>78%</div> <div>9%</div> <div>13%</div> </div>
1	C	977	<div> <div>7%</div> <div>78%</div> <div>9%</div> <div>12%</div> </div>
2	B	554	<div> <div>3%</div> <div>14%</div> <div>84%</div> </div>
2	D	554	<div> <div>3%</div> <div>12%</div> <div>84%</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
6	PEG	C	1512	-	-	X	-

## 2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 15963 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 Isoform 2 of Neutral alpha-glucosidase AB.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	854	Total	C	N	O	S	0	4	0
			6898	4419	1192	1259	28			
1	C	857	Total	C	N	O	S	0	8	0
			6894	4420	1184	1260	30			

There are 88 discrepancies between the modelled and reference sequences:

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

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

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Chain	Residue	Modelled	Actual	Comment	Reference
C	25	MET	-	expression tag	UNP Q8BHN3-2
C	26	GLY	-	expression tag	UNP Q8BHN3-2
C	27	CYS	-	expression tag	UNP Q8BHN3-2
C	28	VAL	-	expression tag	UNP Q8BHN3-2
C	29	ALA	-	expression tag	UNP Q8BHN3-2
C	30	GLU	-	expression tag	UNP Q8BHN3-2
C	31	THR	-	expression tag	UNP Q8BHN3-2
C	32	GLY	-	expression tag	UNP Q8BHN3-2
C	97	ASP	ASN	engineered mutation	UNP Q8BHN3-2
C	967	SER	-	expression tag	UNP Q8BHN3-2
C	968	ALA	-	expression tag	UNP Q8BHN3-2
C	969	TRP	-	expression tag	UNP Q8BHN3-2
C	970	SER	-	expression tag	UNP Q8BHN3-2
C	971	HIS	-	expression tag	UNP Q8BHN3-2
C	972	PRO	-	expression tag	UNP Q8BHN3-2
C	973	GLN	-	expression tag	UNP Q8BHN3-2
C	974	PHE	-	expression tag	UNP Q8BHN3-2
C	975	GLU	-	expression tag	UNP Q8BHN3-2
C	976	LYS	-	expression tag	UNP Q8BHN3-2
C	977	LEU	-	expression tag	UNP Q8BHN3-2
C	978	GLU	-	expression tag	UNP Q8BHN3-2

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	87	Total	C	N	O	S	0	0	0
			624	371	102	141	10			
2	D	87	Total	C	N	O	S	0	0	0
			632	377	104	141	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

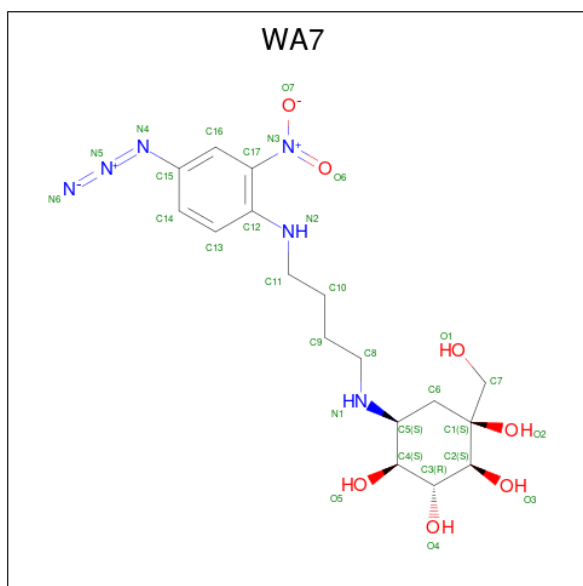
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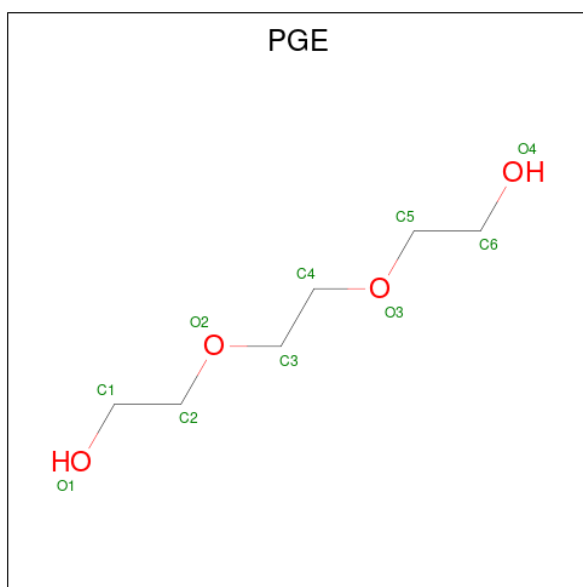
Chain	Residue	Modelled	Actual	Comment	Reference
D	529	GLU	-	expression tag	UNP O08795
D	530	THR	-	expression tag	UNP O08795
D	531	LYS	-	expression tag	UNP O08795
D	532	HIS	-	expression tag	UNP O08795
D	533	HIS	-	expression tag	UNP O08795
D	534	HIS	-	expression tag	UNP O08795
D	535	HIS	-	expression tag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

- Molecule 3 is (1S,2S,3R,4S,5S)-1-(hydroxymethyl)-5-[(4-{[2-nitro-4-(triazan-1-yl)phenyl]amino}butyl)amino]cyclohexane-1,2,3,4-tetrol (three-letter code: WA7) (formula: C<sub>17</sub>H<sub>26</sub>N<sub>6</sub>O<sub>7</sub>) (labeled as "Ligand of Interest" by depositor).



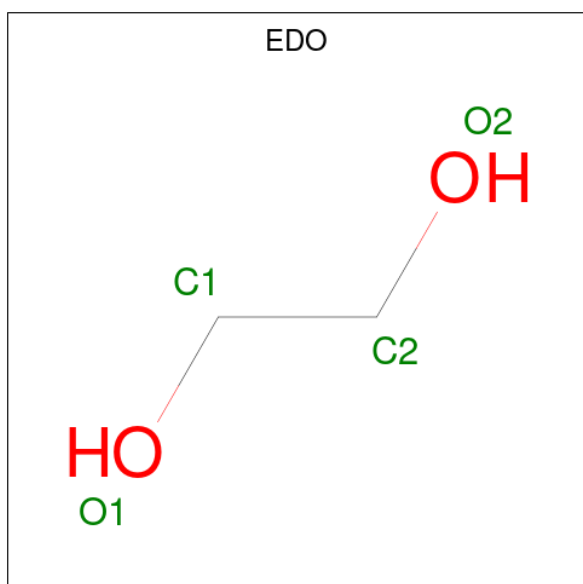
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			30	17	6	7		
3	C	1	Total	C	N	O	0	0
			30	17	6	7		

- Molecule 4 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: C<sub>6</sub>H<sub>14</sub>O<sub>4</sub>).



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	A	1	Total	C	O	0	0
			10	6	4		
4	C	1	Total	C	O	0	0
			10	6	4		

- Molecule 5 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



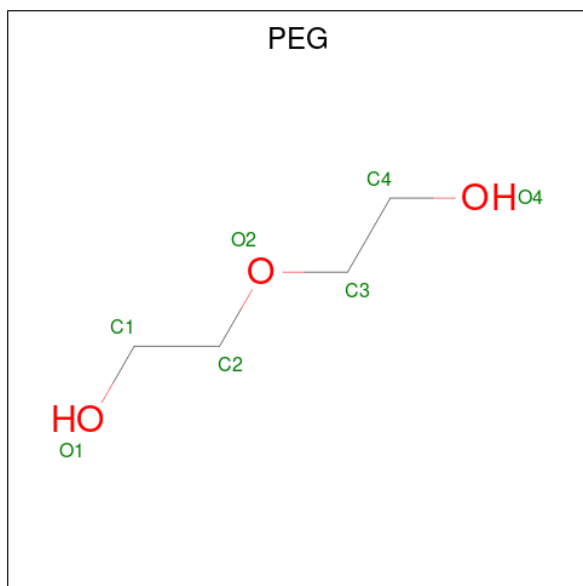
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 4 2 2	0	0
5	A	1	Total C O 4 2 2	0	0
5	A	1	Total C O 4 2 2	0	0
5	A	1	Total C O 4 2 2	0	0
5	A	1	Total C O 4 2 2	0	0
5	A	1	Total C O 4 2 2	0	0
5	A	1	Total C O 4 2 2	0	0
5	A	1	Total C O 4 2 2	0	0
5	B	1	Total C O 4 2 2	0	0
5	B	1	Total C O 4 2 2	0	0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

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

- Molecule 6 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
6	A	1	Total C O 7 4 3	0	0
6	A	1	Total C O 7 4 3	0	0

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

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

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

- Molecule 8 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	C	1	Total	O	S	0	0
			5	4	1		
8	C	1	Total	O	S	0	0
			5	4	1		

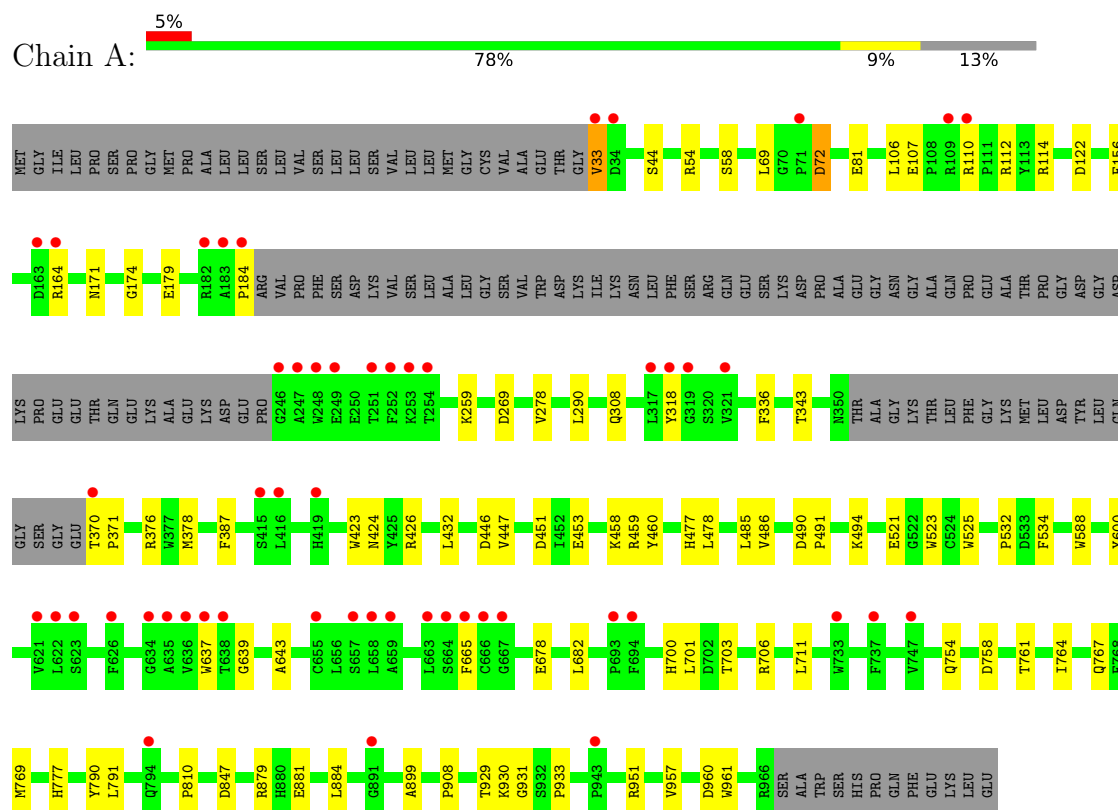
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	315	Total	O	0	0
			315	315		
9	B	13	Total	O	0	0
			13	13		
9	C	247	Total	O	0	0
			247	247		
9	D	15	Total	O	0	0
			15	15		

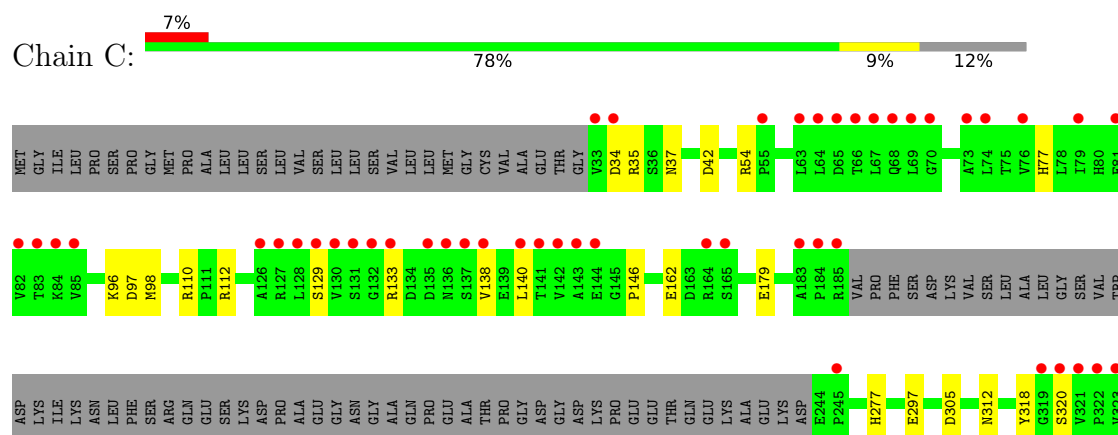
### 3 Residue-property plots

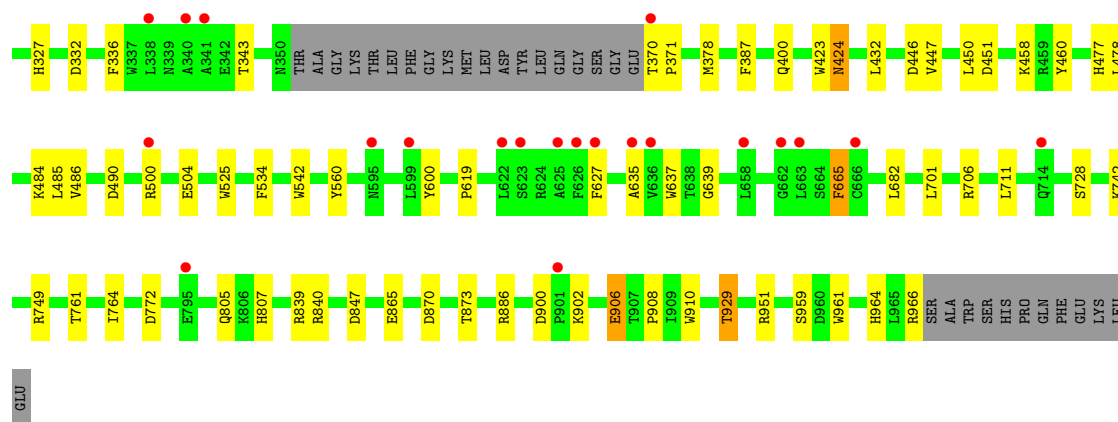
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Isoform 2 of Neutral alpha-glucosidase AB

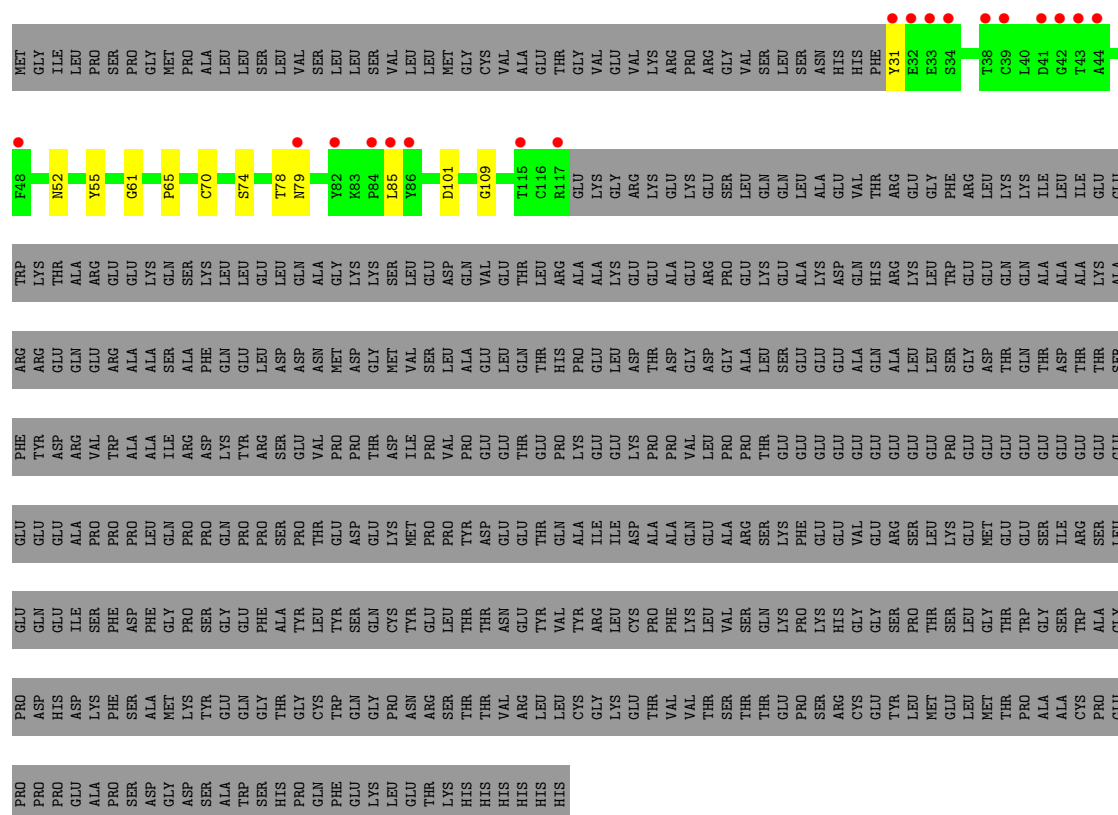


#### • Molecule 1: Isoform 2 of Neutral alpha-glucosidase AB

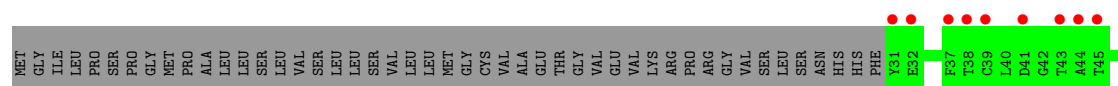




● Molecule 2: Glucosidase 2 subunit beta



● Molecule 2: Glucosidase 2 subunit beta





CYS	PRO	ALA	TRP	ARG	GLU	THR	ALA	ILE	Y55
PRO	GLU	GLY	GLY	SER	GLU	THR	LYS	GLU	C58
PRO	PRO	PRO	GLU	GLU	GLU	PHE	ARG	TRP	
PRO	PRO	ASP	GLN	GLN	GLU	TYR	ARG	LYS	G61
GLU	ALA	ASP	GLU	GLU	GLU	ASP	GLJ	THR	S62
GLU	GLU	ASP	ILE	ILE	ALA	ARG	GLN	ALA	D63
PRO	PRO	PHE	PHE	SER	PRO	TRP	ARG	ARG	C70
SER	SER	SER	ASP	ASP	PRO	PRO	ALA	GLU	P71
ASP	ASP	MET	PHE	PHE	LEU	ALA	ALA	LYS	N72
GLY	GLY	MET	GLY	GLY	GLN	ILE	SER	GLN	
ASP	LYS	LYS	LYS	PRO	PRO	ARG	ALA	SER	T78
SER	SER	TYR	SER	SER	PRO	ASP	PHE	LYS	N79
ALA	ALA	GLU	GLY	GLY	GLN	LYS	GLN	LEU	T80
TRP	TRP	GLN	GLN	GLY	PRO	TYR	GLU	LEU	G81
SER	SER	GLY	PHE	PHE	PRO	ARG	LEU	GLU	Y82
HIS	HIS	THR	ALA	ALA	SER	SER	ASP	LEU	K83
PRO	PRO	GLY	TYR	TYR	PRO	GLU	ASP	LEU	
GLN	GLN	CYS	CYS	LEU	THR	VAL	ASN	ALA	P84
PHE	PHE	TRP	TRP	TRP	GLU	PRO	MET	GLY	L85
GLU	GLU	GLN	GLN	SER	ASP	PRO	ASP	LYS	Y86
LYS	LYS	GLY	GLY	GLN	GLU	THR	GLY	LYS	I87
LEU	LEU	PRO	PRO	CYS	LYS	ASP	MET	SER	L88
GLU	GLU	ASN	TYR	TYR	MET	ILE	VAL	LEU	S89
THR	THR	SER	GLU	GLU	PRO	PRO	LEU	GLU	S90
LYS	LYS	ARG	LEU	LEU	PRO	VAL	LEU	ASP	R91
HIS	HIS	THR	THR	THR	TYR	PRO	ALA	GLN	C99
HIS	HIS	VAL	VAL	ASN	GLU	GLU	GLU	VAL	C100
HIS	HIS	ARG	GLU	GLU	GLU	THR	GLN	GLU	D101
HIS	HIS	LEU	LEU	VAL	THR	GLU	THR	LEU	
HIS	HIS	LEU	LEU	VAL	GLN	PRO	HIS	ARG	C116
		CYS	CYS	TYR	ALA	LYS	PRO	ALA	R117
		LYS	LYS	ARG	ILE	GLU	GLU	ALA	GLU
		GLU	GLU	CYS	ILE	GLU	LEU	LYS	LYS
		THR	THR	TYR	THR	LYS	ASP	GLY	GLY
		VAL	VAL	PHE	ALA	PRO	THR	GLU	ARG
		VAL	VAL	LYS	GLN	VAL	ASP	ALA	LYS
		THR	THR	LEU	GLU	LEU	ASP	ARG	GLU
		SER	SER	VAL	ALA	PRO	GLY	PRO	SER
		THR	THR	SER	ARG	PRO	ALA	GLU	LEU
		THR	THR	GLN	SER	THR	LEU	LYS	GLN
		GLU	GLU	LYS	GLY	GLU	SER	GLU	GLN
		PRO	PRO	PRO	PHE	GLU	GLU	ALA	LEU
		SER	SER	LYS	GLU	GLU	GLU	LYS	ALA
		ARG	ARG	HIS	GLU	GLU	GLU	ASP	GLU
		CYS	CYS	GLY	VAL	GLU	ALA	GLN	VAL
		GLU	GLU	GLY	GLU	GLU	GLN	HIS	THR
		TYR	TYR	SER	ARG	GLU	ALA	ARG	ARG
		LEU	LEU	PRO	SER	GLU	LEU	LYS	GLY
		MET	MET	THR	THR	PRO	SER	TRP	PHE
		GLU	GLU	SER	LYS	GLU	GLY	GLU	ARG
		LEU	LEU	LEU	GLU	GLU	GLY	GLU	LYS
		THR	THR	THR	THR	GLU	THR	GLN	ILE
		MET	MET	GLY	THR	GLU	ASP	ALA	THR
		PRO	PRO	TRP	TRP	GLU	THR	GLN	GLU
		ALA	ALA	SER	THR	GLU	THR	ALA	ILE

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	102.78Å 102.78Å 240.12Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	40.02 – 2.38 43.24 – 2.38	Depositor EDS
% Data completeness (in resolution range)	99.7 (40.02-2.38) 93.5 (43.24-2.38)	Depositor EDS
$R_{merge}$	0.12	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	0.75 (at 2.39Å)	Xtriage
Refinement program	PHENIX 1.14_3228	Depositor
R, $R_{free}$	0.174 , 0.210 0.174 , 0.211	Depositor DCC
$R_{free}$ test set	1979 reflections (1.76%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	41.5	Xtriage
Anisotropy	0.241	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 40.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.008 for -h,-k,l 0.038 for h,-h-k,-l 0.020 for -k,-h,-l	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	15963	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.54% 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: WA7, PGE, SO4, CA, EDO, PEG

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	0.38	0/7120	0.58	0/9694
1	C	0.38	0/7130	0.57	1/9714 (0.0%)
2	B	0.34	0/636	0.60	0/870
2	D	0.35	0/644	0.61	0/880
All	All	0.37	0/15530	0.58	1/21158 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	886	ARG	NE-CZ-NH2	-6.29	117.16	120.30

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	6898	0	6646	63	0
1	C	6894	0	6599	61	0
2	B	624	0	504	9	0
2	D	632	0	530	17	0
3	A	30	0	0	0	0
3	C	30	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	40	0	56	7	0
4	C	10	0	14	1	0
5	A	32	0	46	4	0
5	B	16	0	23	4	0
5	C	68	0	100	9	0
5	D	8	0	12	0	0
6	A	42	0	60	3	0
6	B	7	0	10	0	0
6	C	21	0	30	13	0
6	D	7	0	10	2	0
7	B	2	0	0	0	0
7	D	2	0	0	0	0
8	C	10	0	0	1	0
9	A	315	0	0	10	0
9	B	13	0	0	2	0
9	C	247	0	0	13	0
9	D	15	0	0	1	0
All	All	15963	0	14640	149	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 5.

The worst 5 of 149 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:37:ASN:OD1	9:C:1601:HOH:O	1.82	0.97
1:C:840:ARG:HB3	6:C:1512:PEG:H32	1.61	0.81
1:C:619:PRO:O	9:C:1602:HOH:O	1.99	0.80
1:A:521:GLU:H	5:A:1019:EDO:H11	1.47	0.80
1:C:54:ARG:O	9:C:1603:HOH:O	2.00	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	852/977 (87%)	820 (96%)	31 (4%)	1 (0%)	51	67
1	C	859/977 (88%)	825 (96%)	34 (4%)	0	100	100
2	B	85/554 (15%)	82 (96%)	3 (4%)	0	100	100
2	D	85/554 (15%)	82 (96%)	3 (4%)	0	100	100
All	All	1881/3062 (61%)	1809 (96%)	71 (4%)	1 (0%)	51	67

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	643	ALA

### 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	747/846 (88%)	737 (99%)	10 (1%)	69	82
1	C	742/846 (88%)	732 (99%)	10 (1%)	69	82
2	B	69/485 (14%)	67 (97%)	2 (3%)	42	60
2	D	71/485 (15%)	66 (93%)	5 (7%)	15	21
All	All	1629/2662 (61%)	1602 (98%)	27 (2%)	60	76

5 of 27 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	312	ASN
1	C	637	TRP
2	D	83	LYS
1	C	446	ASP
1	C	665	PHE

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

sidechains are listed below:

Mol	Chain	Res	Type
1	A	424	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 monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 55 ligands modelled in this entry, 4 are monoatomic - leaving 51 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	$\# Z  > 2$
5	EDO	B	602	-	3,3,3	0.58	0	2,2,2	0.15	0
4	PGE	C	1505	-	9,9,9	0.39	0	8,8,8	0.32	0
5	EDO	A	1012	-	3,3,3	0.63	0	2,2,2	0.31	0
5	EDO	C	1511	-	3,3,3	0.47	0	2,2,2	0.45	0
6	PEG	A	1017	-	6,6,6	0.47	0	5,5,5	0.31	0
5	EDO	C	1519	-	3,3,3	0.49	0	2,2,2	0.22	0
6	PEG	C	1508	-	6,6,6	0.49	0	5,5,5	0.31	0
8	SO4	C	1523	-	4,4,4	0.18	0	6,6,6	0.41	0
4	PGE	A	1002	-	9,9,9	0.39	0	8,8,8	0.56	0
8	SO4	C	1524	-	4,4,4	0.17	0	6,6,6	0.23	0
5	EDO	C	1509	-	3,3,3	0.46	0	2,2,2	0.53	0
5	EDO	C	1503	-	3,3,3	0.64	0	2,2,2	0.16	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
6	PEG	A	1011	-	6,6,6	0.49	0	5,5,5	0.26	0
5	EDO	C	1517	-	3,3,3	0.50	0	2,2,2	0.30	0
5	EDO	A	1015	-	3,3,3	0.50	0	2,2,2	0.62	0
5	EDO	A	1019	-	3,3,3	0.56	0	2,2,2	0.23	0
4	PGE	A	1006	-	9,9,9	0.34	0	8,8,8	0.49	0
5	EDO	C	1515	-	3,3,3	0.75	0	2,2,2	0.46	0
5	EDO	C	1521	-	3,3,3	0.23	0	2,2,2	0.13	0
5	EDO	A	1016	-	3,3,3	0.53	0	2,2,2	0.40	0
4	PGE	A	1008	-	9,9,9	0.22	0	8,8,8	0.15	0
5	EDO	B	605	-	3,3,3	0.60	0	2,2,2	0.33	0
5	EDO	C	1507	-	3,3,3	0.62	0	2,2,2	0.16	0
3	WA7	C	1502	-	29,31,31	2.93	10 (34%)	35,43,43	1.27	3 (8%)
6	PEG	C	1504	-	6,6,6	0.50	0	5,5,5	0.40	0
5	EDO	A	1018	-	3,3,3	0.46	0	2,2,2	0.45	0
6	PEG	C	1512	-	6,6,6	0.46	0	5,5,5	0.93	0
5	EDO	C	1506	-	3,3,3	0.52	0	2,2,2	0.39	0
6	PEG	A	1005	-	6,6,6	0.53	0	5,5,5	0.62	0
5	EDO	C	1510	-	3,3,3	0.47	0	2,2,2	0.14	0
4	PGE	A	1007	-	9,9,9	0.42	0	8,8,8	0.38	0
5	EDO	C	1516	-	3,3,3	0.40	0	2,2,2	0.80	0
3	WA7	A	1001	-	29,31,31	3.27	12 (41%)	35,43,43	1.59	6 (17%)
5	EDO	A	1013	-	3,3,3	0.47	0	2,2,2	0.42	0
5	EDO	D	603	-	3,3,3	0.45	0	2,2,2	0.40	0
5	EDO	A	1003	-	3,3,3	0.57	0	2,2,2	0.26	0
5	EDO	D	601	-	3,3,3	0.57	0	2,2,2	0.16	0
5	EDO	B	604	-	3,3,3	0.44	0	2,2,2	0.40	0
6	PEG	D	602	-	6,6,6	0.13	0	5,5,5	0.18	0
5	EDO	C	1501	-	3,3,3	0.50	0	2,2,2	0.40	0
5	EDO	C	1518	-	3,3,3	0.45	0	2,2,2	0.64	0
5	EDO	C	1520	-	3,3,3	0.37	0	2,2,2	0.72	0
5	EDO	C	1513	-	3,3,3	0.56	0	2,2,2	0.26	0
5	EDO	A	1014	-	3,3,3	0.69	0	2,2,2	0.11	0
6	PEG	A	1010	-	6,6,6	0.50	0	5,5,5	0.30	0
5	EDO	C	1522	-	3,3,3	0.59	0	2,2,2	0.29	0
6	PEG	A	1009	-	6,6,6	0.35	0	5,5,5	0.15	0
5	EDO	C	1514	-	3,3,3	0.55	0	2,2,2	0.16	0
6	PEG	A	1004	-	6,6,6	0.52	0	5,5,5	0.39	0
6	PEG	B	601	-	6,6,6	0.51	0	5,5,5	0.43	0
5	EDO	B	603	-	3,3,3	0.49	0	2,2,2	0.30	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
5	EDO	B	602	-	-	1/1/1/1	-
4	PGE	C	1505	-	-	4/7/7/7	-
5	EDO	A	1012	-	-	0/1/1/1	-
5	EDO	C	1511	-	-	0/1/1/1	-
6	PEG	A	1017	-	-	1/4/4/4	-
5	EDO	C	1519	-	-	1/1/1/1	-
6	PEG	C	1508	-	-	2/4/4/4	-
4	PGE	A	1002	-	-	3/7/7/7	-
5	EDO	C	1509	-	-	0/1/1/1	-
5	EDO	C	1503	-	-	1/1/1/1	-
6	PEG	A	1011	-	-	0/4/4/4	-
5	EDO	C	1517	-	-	0/1/1/1	-
5	EDO	A	1015	-	-	1/1/1/1	-
5	EDO	A	1019	-	-	0/1/1/1	-
4	PGE	A	1006	-	-	3/7/7/7	-
5	EDO	C	1515	-	-	1/1/1/1	-
5	EDO	C	1521	-	-	0/1/1/1	-
5	EDO	A	1016	-	-	0/1/1/1	-
4	PGE	A	1008	-	-	5/7/7/7	-
5	EDO	B	605	-	-	1/1/1/1	-
5	EDO	C	1507	-	-	0/1/1/1	-
3	WA7	C	1502	-	-	8/17/42/42	0/2/2/2
6	PEG	C	1504	-	-	3/4/4/4	-
5	EDO	A	1018	-	-	1/1/1/1	-
6	PEG	C	1512	-	-	0/4/4/4	-
5	EDO	C	1506	-	-	0/1/1/1	-
6	PEG	A	1005	-	-	0/4/4/4	-
5	EDO	C	1510	-	-	1/1/1/1	-
4	PGE	A	1007	-	-	3/7/7/7	-
5	EDO	C	1516	-	-	1/1/1/1	-
3	WA7	A	1001	-	-	8/17/42/42	0/2/2/2
5	EDO	A	1013	-	-	1/1/1/1	-
5	EDO	D	603	-	-	1/1/1/1	-
5	EDO	A	1003	-	-	0/1/1/1	-
5	EDO	D	601	-	-	1/1/1/1	-
5	EDO	B	604	-	-	1/1/1/1	-
6	PEG	D	602	-	-	3/4/4/4	-
5	EDO	C	1501	-	-	0/1/1/1	-
5	EDO	C	1518	-	-	1/1/1/1	-
5	EDO	C	1520	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	EDO	C	1513	-	-	0/1/1/1	-
5	EDO	A	1014	-	-	1/1/1/1	-
6	PEG	A	1010	-	-	1/4/4/4	-
5	EDO	C	1522	-	-	1/1/1/1	-
6	PEG	A	1009	-	-	1/4/4/4	-
5	EDO	C	1514	-	-	1/1/1/1	-
6	PEG	A	1004	-	-	2/4/4/4	-
6	PEG	B	601	-	-	2/4/4/4	-
5	EDO	B	603	-	-	1/1/1/1	-

The worst 5 of 22 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1001	WA7	O6-N3	13.61	1.45	1.22
3	C	1502	WA7	O6-N3	10.82	1.41	1.22
3	A	1001	WA7	N5-N4	5.27	1.39	1.24
3	C	1502	WA7	N5-N4	5.09	1.39	1.24
3	C	1502	WA7	O2-C1	-4.24	1.37	1.44

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1001	WA7	C11-N2-C12	-4.01	113.75	123.39
3	C	1502	WA7	C17-C12-N2	-3.82	116.62	123.33
3	A	1001	WA7	C15-N4-N5	3.77	123.51	116.02
3	C	1502	WA7	O6-N3-C17	-3.63	112.83	119.03
3	A	1001	WA7	O6-N3-C17	3.62	125.22	119.03

There are no chirality outliers.

5 of 68 torsion outliers are listed below:

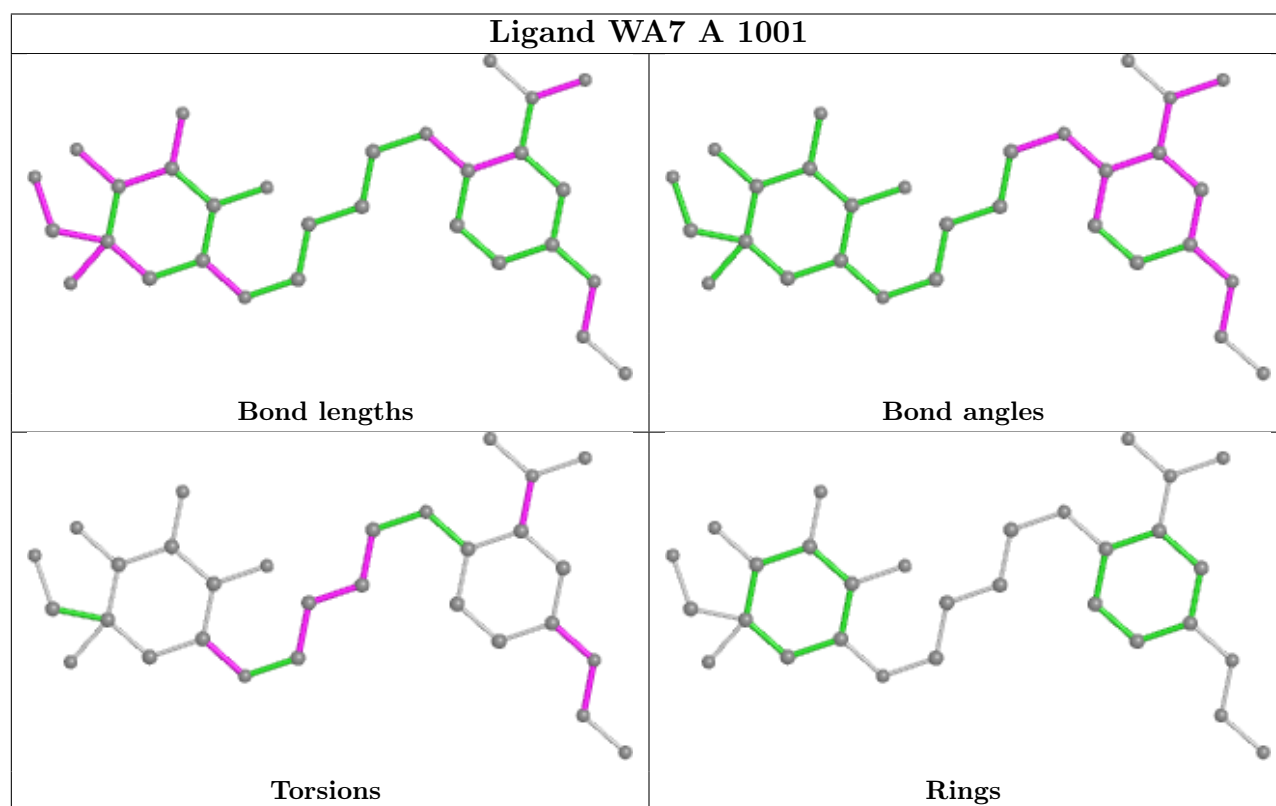
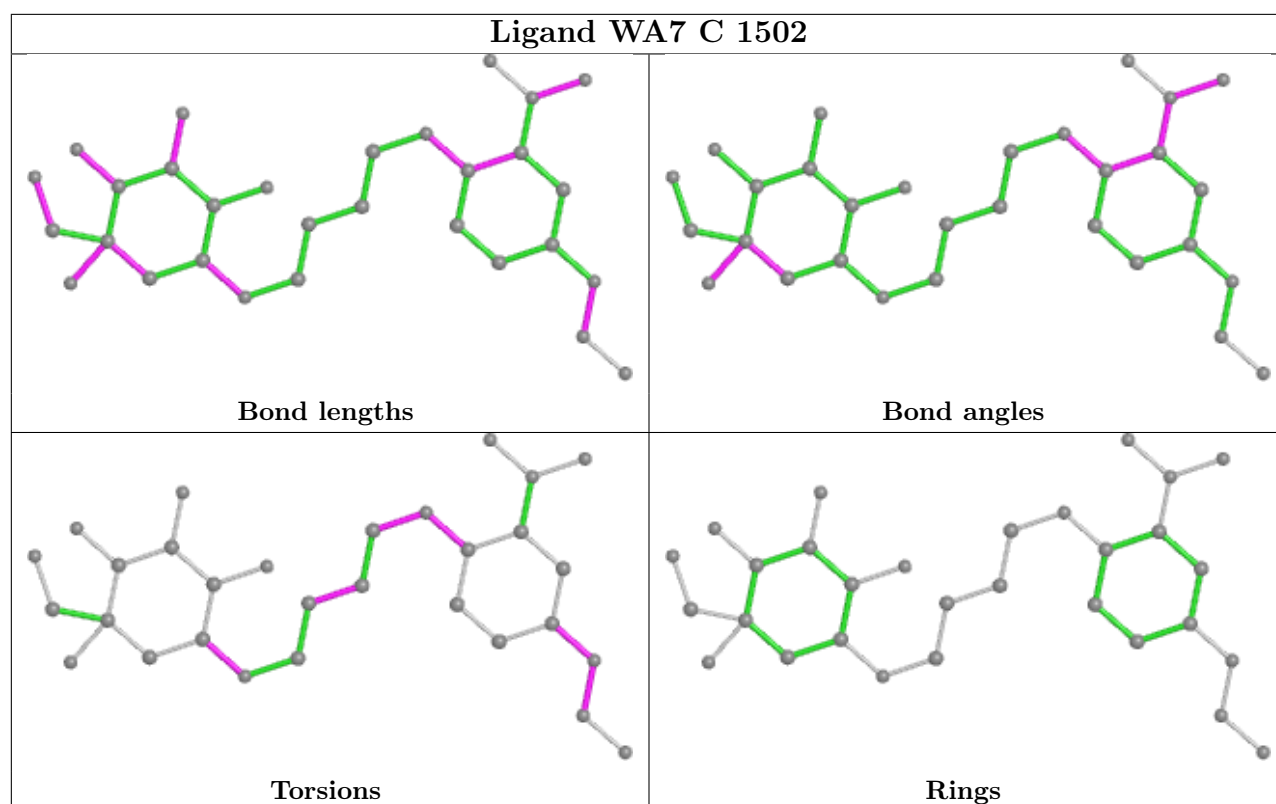
Mol	Chain	Res	Type	Atoms
3	A	1001	WA7	C6-C5-N1-C8
3	A	1001	WA7	C14-C15-N4-N5
3	A	1001	WA7	C16-C15-N4-N5
3	A	1001	WA7	C15-N4-N5-N6
3	C	1502	WA7	C14-C15-N4-N5

There are no ring outliers.

22 monomers are involved in 44 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	602	EDO	1	0
4	C	1505	PGE	1	0
5	C	1519	EDO	1	0
8	C	1524	SO4	1	0
5	C	1503	EDO	1	0
5	A	1015	EDO	2	0
5	A	1019	EDO	1	0
4	A	1006	PGE	3	0
4	A	1008	PGE	3	0
5	B	605	EDO	1	0
6	C	1504	PEG	1	0
6	C	1512	PEG	12	0
6	A	1005	PEG	2	0
4	A	1007	PGE	1	0
5	C	1516	EDO	3	0
5	A	1013	EDO	1	0
5	B	604	EDO	2	0
6	D	602	PEG	2	0
5	C	1518	EDO	2	0
5	C	1520	EDO	1	0
5	C	1513	EDO	1	0
6	A	1009	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 ⓘ

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	854/977 (87%)	0.02	52 (6%) 21 23	30, 43, 69, 106	0
1	C	857/977 (87%)	0.20	69 (8%) 12 13	32, 48, 82, 102	0
2	B	87/554 (15%)	0.63	18 (20%) 1 1	38, 59, 92, 101	0
2	D	87/554 (15%)	0.68	15 (17%) 1 1	41, 60, 94, 104	0
All	All	1885/3062 (61%)	0.16	154 (8%) 11 12	30, 46, 82, 106	0

The worst 5 of 154 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	184	PRO	9.6
2	D	43	THR	8.3
2	D	81	GLY	7.8
2	B	43	THR	6.5
2	D	31	TYR	5.9

### 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.

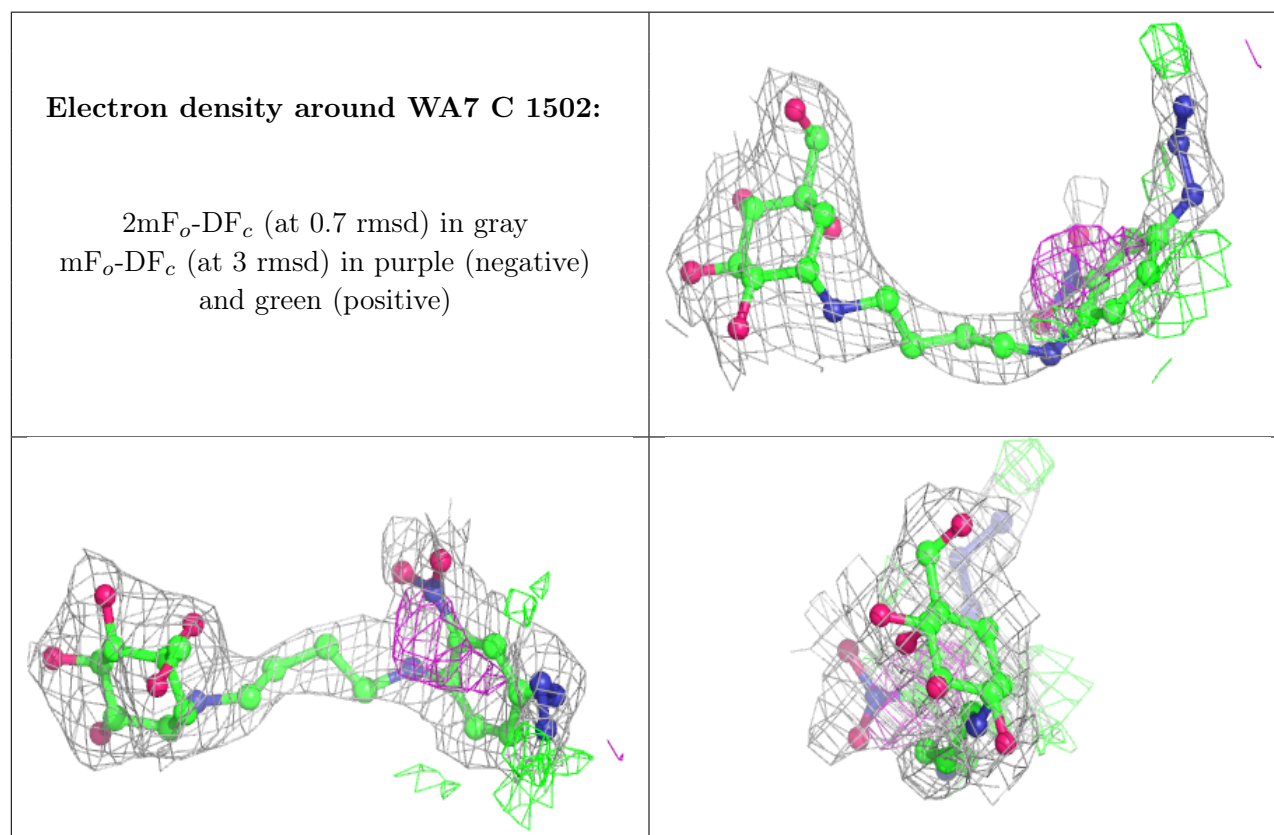
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
5	EDO	B	605	4/4	0.68	0.35	53,61,62,75	0
5	EDO	A	1015	4/4	0.69	0.25	54,57,61,85	0
6	PEG	B	601	7/7	0.70	0.37	58,67,74,76	0
5	EDO	C	1510	4/4	0.75	0.26	70,78,78,79	0
5	EDO	C	1522	4/4	0.76	0.36	62,63,64,83	0
5	EDO	A	1014	4/4	0.78	0.18	42,52,59,70	0
5	EDO	C	1515	4/4	0.78	0.26	36,49,58,64	0
6	PEG	D	602	7/7	0.81	0.28	62,69,74,75	0
5	EDO	C	1507	4/4	0.82	0.20	63,66,66,73	0
5	EDO	B	602	4/4	0.82	0.26	54,61,68,70	0
4	PGE	A	1002	10/10	0.82	0.20	50,66,73,79	0
6	PEG	C	1512	7/7	0.84	0.31	50,52,61,63	0
4	PGE	A	1008	10/10	0.84	0.23	79,84,92,102	0
6	PEG	C	1508	7/7	0.85	0.25	58,67,75,80	0
3	WA7	C	1502	30/30	0.85	0.18	35,59,81,85	0
4	PGE	A	1007	10/10	0.85	0.30	50,65,74,79	0
5	EDO	D	601	4/4	0.86	0.15	58,63,66,71	0
5	EDO	A	1013	4/4	0.86	0.17	64,66,67,67	0
5	EDO	C	1503	4/4	0.86	0.24	59,59,61,62	0
5	EDO	C	1517	4/4	0.86	0.16	61,67,68,73	0
4	PGE	C	1505	10/10	0.86	0.24	54,65,71,77	0
6	PEG	A	1004	7/7	0.87	0.16	51,62,68,73	0
6	PEG	A	1010	7/7	0.88	0.17	53,59,66,68	0
3	WA7	A	1001	30/30	0.88	0.15	36,60,82,94	0
5	EDO	B	603	4/4	0.88	0.15	58,62,64,81	0
5	EDO	C	1521	4/4	0.88	0.20	86,92,100,104	0
6	PEG	A	1009	7/7	0.88	0.31	60,62,71,72	0
6	PEG	C	1504	7/7	0.89	0.30	53,66,70,73	0
5	EDO	A	1018	4/4	0.89	0.43	54,55,58,61	0
5	EDO	C	1514	4/4	0.90	0.16	53,63,65,65	0
6	PEG	A	1005	7/7	0.90	0.22	43,54,64,65	0
5	EDO	C	1516	4/4	0.90	0.14	49,51,54,56	0
5	EDO	C	1513	4/4	0.91	0.16	51,54,54,62	0
4	PGE	A	1006	10/10	0.91	0.28	49,62,74,75	0
5	EDO	D	603	4/4	0.91	0.26	54,63,64,65	0
5	EDO	A	1019	4/4	0.92	0.29	55,60,63,66	0
5	EDO	C	1519	4/4	0.92	0.34	63,67,73,74	0
5	EDO	C	1506	4/4	0.92	0.09	46,57,60,63	0
5	EDO	A	1012	4/4	0.92	0.25	53,55,60,76	0
5	EDO	C	1501	4/4	0.92	0.12	54,58,63,70	0
6	PEG	A	1017	7/7	0.93	0.15	54,64,69,72	0
5	EDO	C	1509	4/4	0.93	0.17	56,56,64,70	0
6	PEG	A	1011	7/7	0.93	0.28	60,62,66,69	0

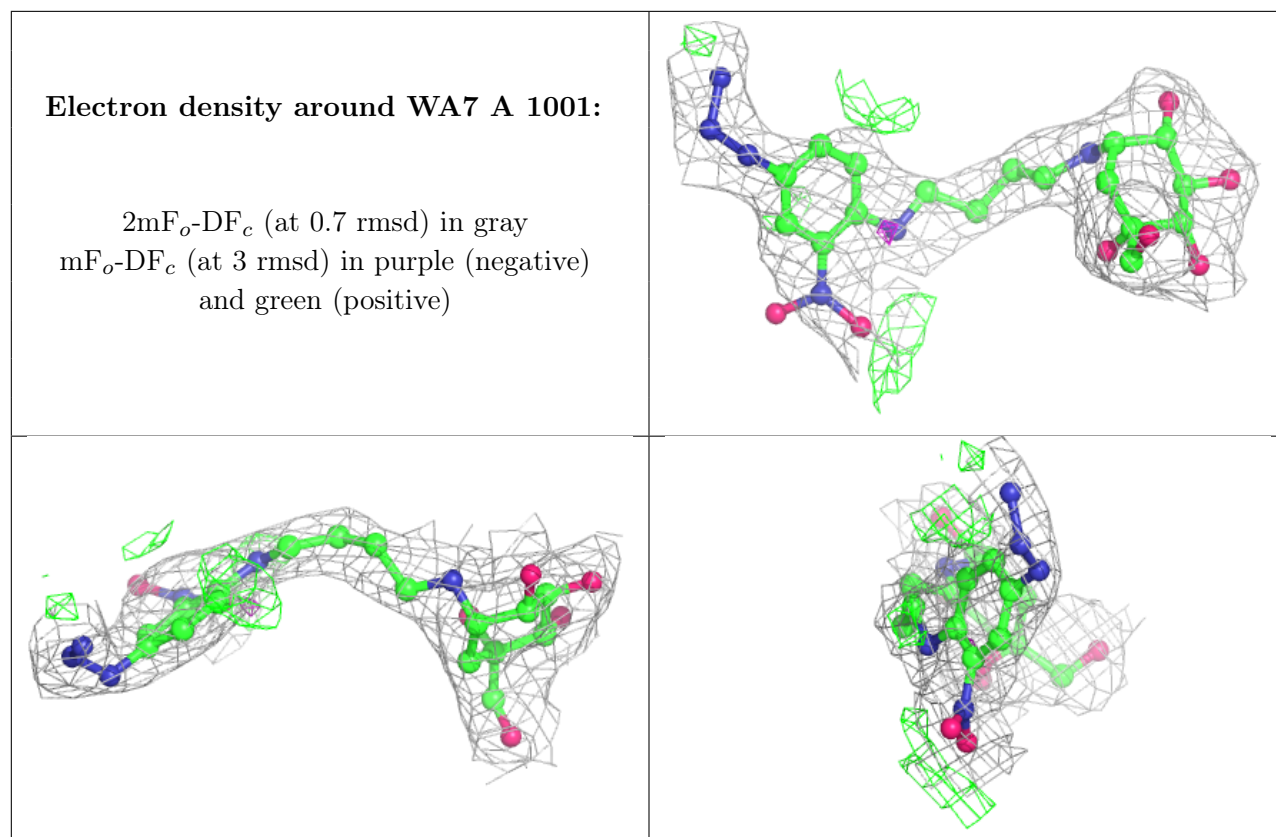
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
5	EDO	C	1520	4/4	0.94	0.21	58,60,65,70	0
5	EDO	A	1016	4/4	0.94	0.10	47,53,54,56	0
5	EDO	A	1003	4/4	0.94	0.21	46,52,52,53	0
5	EDO	C	1511	4/4	0.94	0.12	44,47,49,71	0
8	SO4	C	1523	5/5	0.94	0.16	61,67,82,104	0
8	SO4	C	1524	5/5	0.94	0.26	73,79,90,97	0
5	EDO	B	604	4/4	0.95	0.20	54,54,62,64	0
5	EDO	C	1518	4/4	0.96	0.23	49,55,61,66	0
7	CA	D	605	1/1	0.97	0.10	45,45,45,45	0
7	CA	D	604	1/1	0.98	0.06	51,51,51,51	0
7	CA	B	607	1/1	0.98	0.05	51,51,51,51	0
7	CA	B	606	1/1	0.99	0.09	45,45,45,45	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.





## 6.5 Other polymers [i](#)

There are no such residues in this entry.