



# Full wwPDB X-ray Structure Validation Report ⓘ

Sep 22, 2021 – 12:09 AM EDT

PDB ID : 7K9Q  
Title : Co-crystal structure of alpha glucosidase with compound 4  
Authors : Karade, S.S.; Mariuzza, R.A.  
Deposited on : 2020-09-29  
Resolution : 2.30 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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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 : 2.23.1  
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) : 2.23.1

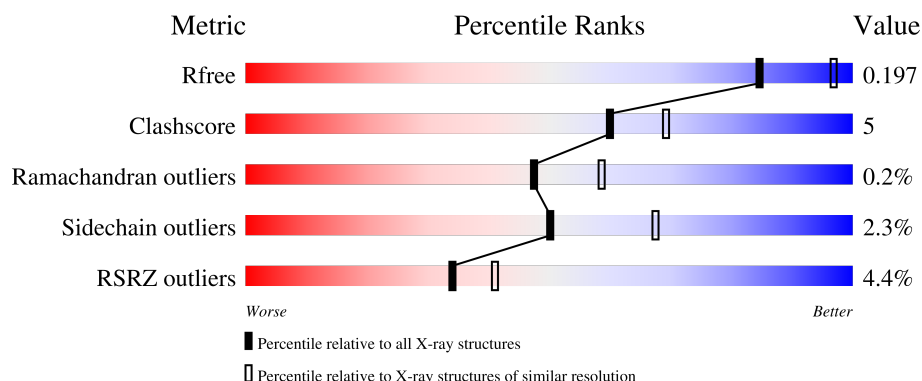
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.30 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	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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 style="width: 100%; height: 10px; background: linear-gradient(to right, red, orange, yellow, green, grey);"></div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> <span>%</span> <span>76%</span> <span>10%</span> <span>13%</span> </div> </div>
1	C	977	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red, orange, yellow, green, grey);"></div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> <span>4%</span> <span>79%</span> <span>8%</span> <span>12%</span> </div> </div>
2	B	547	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red, orange, yellow, green, grey);"></div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> <span>3%</span> <span>15%</span> <span>84%</span> </div> </div>
2	D	547	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red, orange, yellow, green, grey);"></div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> <span>4%</span> <span>14%</span> <span>84%</span> </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
7	SO4	A	1031	-	-	X	-

## 2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 16268 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 Alpha glucosidase 2 alpha neutral subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	853	Total	C	N	O	S	0	7	0
			6886	4412	1191	1255	28			
1	C	857	Total	C	N	O	S	0	9	0
			6941	4447	1199	1265	30			

There are 88 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	2	MET	-	initiating methionine	UNP A1A4T2
A	3	GLY	-	expression tag	UNP A1A4T2
A	4	ILE	-	expression tag	UNP A1A4T2
A	5	LEU	-	expression tag	UNP A1A4T2
A	6	PRO	-	expression tag	UNP A1A4T2
A	7	SER	-	expression tag	UNP A1A4T2
A	8	PRO	-	expression tag	UNP A1A4T2
A	9	GLY	-	expression tag	UNP A1A4T2
A	10	MET	-	expression tag	UNP A1A4T2
A	11	PRO	-	expression tag	UNP A1A4T2
A	12	ALA	-	expression tag	UNP A1A4T2
A	13	LEU	-	expression tag	UNP A1A4T2
A	14	LEU	-	expression tag	UNP A1A4T2
A	15	SER	-	expression tag	UNP A1A4T2
A	16	LEU	-	expression tag	UNP A1A4T2
A	17	VAL	-	expression tag	UNP A1A4T2
A	18	SER	-	expression tag	UNP A1A4T2
A	19	LEU	-	expression tag	UNP A1A4T2
A	20	LEU	-	expression tag	UNP A1A4T2
A	21	SER	-	expression tag	UNP A1A4T2
A	22	VAL	-	expression tag	UNP A1A4T2
A	23	LEU	-	expression tag	UNP A1A4T2
A	24	LEU	-	expression tag	UNP A1A4T2
A	25	MET	-	expression tag	UNP A1A4T2
A	26	GLY	-	expression tag	UNP A1A4T2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	27	CYS	-	expression tag	UNP A1A4T2
A	28	VAL	-	expression tag	UNP A1A4T2
A	29	ALA	-	expression tag	UNP A1A4T2
A	30	GLU	-	expression tag	UNP A1A4T2
A	31	THR	-	expression tag	UNP A1A4T2
A	32	GLY	-	expression tag	UNP A1A4T2
A	97	ASP	ASN	engineered mutation	UNP A1A4T2
A	967	SER	-	expression tag	UNP A1A4T2
A	968	ALA	-	expression tag	UNP A1A4T2
A	969	TRP	-	expression tag	UNP A1A4T2
A	970	SER	-	expression tag	UNP A1A4T2
A	971	HIS	-	expression tag	UNP A1A4T2
A	972	PRO	-	expression tag	UNP A1A4T2
A	973	GLN	-	expression tag	UNP A1A4T2
A	974	PHE	-	expression tag	UNP A1A4T2
A	975	GLU	-	expression tag	UNP A1A4T2
A	976	LYS	-	expression tag	UNP A1A4T2
A	977	LEU	-	expression tag	UNP A1A4T2
A	978	GLU	-	expression tag	UNP A1A4T2
C	2	MET	-	initiating methionine	UNP A1A4T2
C	3	GLY	-	expression tag	UNP A1A4T2
C	4	ILE	-	expression tag	UNP A1A4T2
C	5	LEU	-	expression tag	UNP A1A4T2
C	6	PRO	-	expression tag	UNP A1A4T2
C	7	SER	-	expression tag	UNP A1A4T2
C	8	PRO	-	expression tag	UNP A1A4T2
C	9	GLY	-	expression tag	UNP A1A4T2
C	10	MET	-	expression tag	UNP A1A4T2
C	11	PRO	-	expression tag	UNP A1A4T2
C	12	ALA	-	expression tag	UNP A1A4T2
C	13	LEU	-	expression tag	UNP A1A4T2
C	14	LEU	-	expression tag	UNP A1A4T2
C	15	SER	-	expression tag	UNP A1A4T2
C	16	LEU	-	expression tag	UNP A1A4T2
C	17	VAL	-	expression tag	UNP A1A4T2
C	18	SER	-	expression tag	UNP A1A4T2
C	19	LEU	-	expression tag	UNP A1A4T2
C	20	LEU	-	expression tag	UNP A1A4T2
C	21	SER	-	expression tag	UNP A1A4T2
C	22	VAL	-	expression tag	UNP A1A4T2
C	23	LEU	-	expression tag	UNP A1A4T2
C	24	LEU	-	expression tag	UNP A1A4T2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	25	MET	-	expression tag	UNP A1A4T2
C	26	GLY	-	expression tag	UNP A1A4T2
C	27	CYS	-	expression tag	UNP A1A4T2
C	28	VAL	-	expression tag	UNP A1A4T2
C	29	ALA	-	expression tag	UNP A1A4T2
C	30	GLU	-	expression tag	UNP A1A4T2
C	31	THR	-	expression tag	UNP A1A4T2
C	32	GLY	-	expression tag	UNP A1A4T2
C	97	ASP	ASN	engineered mutation	UNP A1A4T2
C	967	SER	-	expression tag	UNP A1A4T2
C	968	ALA	-	expression tag	UNP A1A4T2
C	969	TRP	-	expression tag	UNP A1A4T2
C	970	SER	-	expression tag	UNP A1A4T2
C	971	HIS	-	expression tag	UNP A1A4T2
C	972	PRO	-	expression tag	UNP A1A4T2
C	973	GLN	-	expression tag	UNP A1A4T2
C	974	PHE	-	expression tag	UNP A1A4T2
C	975	GLU	-	expression tag	UNP A1A4T2
C	976	LYS	-	expression tag	UNP A1A4T2
C	977	LEU	-	expression tag	UNP A1A4T2
C	978	GLU	-	expression tag	UNP A1A4T2

- 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
			614	362	102	140	10			
2	D	88	Total	C	N	O	S	0	0	0
			641	382	105	144	10			

There are 88 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	LEU	-	expression tag	UNP O08795
B	522	GLU	-	expression tag	UNP O08795
B	523	THR	-	expression tag	UNP O08795
B	524	LYS	-	expression tag	UNP O08795
B	525	HIS	-	expression tag	UNP O08795
B	526	HIS	-	expression tag	UNP O08795
B	527	HIS	-	expression tag	UNP O08795
B	528	HIS	-	expression tag	UNP O08795
B	529	HIS	-	expression tag	UNP O08795
B	530	HIS	-	expression tag	UNP O08795
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

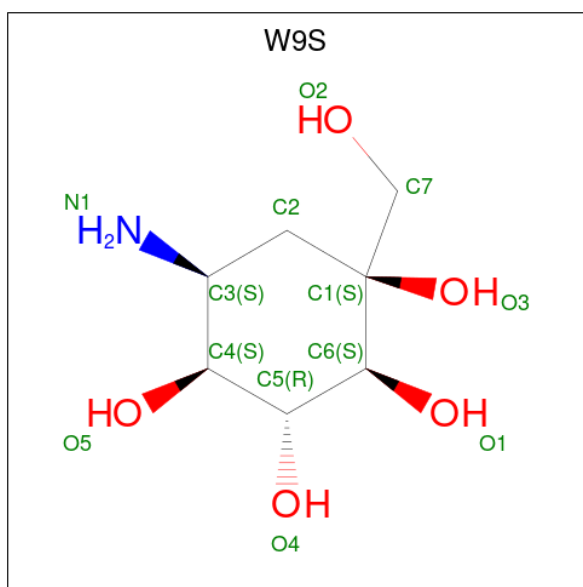
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Chain	Residue	Modelled	Actual	Comment	Reference
D	-9	GLY	-	expression tag	UNP O08795
D	-8	MET	-	expression tag	UNP O08795
D	-7	PRO	-	expression tag	UNP O08795
D	-6	ALA	-	expression tag	UNP O08795
D	-5	LEU	-	expression tag	UNP O08795
D	-4	LEU	-	expression 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	LEU	-	expression tag	UNP O08795
D	522	GLU	-	expression tag	UNP O08795
D	523	THR	-	expression tag	UNP O08795
D	524	LYS	-	expression tag	UNP O08795
D	525	HIS	-	expression tag	UNP O08795
D	526	HIS	-	expression tag	UNP O08795
D	527	HIS	-	expression tag	UNP O08795
D	528	HIS	-	expression tag	UNP O08795
D	529	HIS	-	expression tag	UNP O08795
D	530	HIS	-	expression tag	UNP O08795

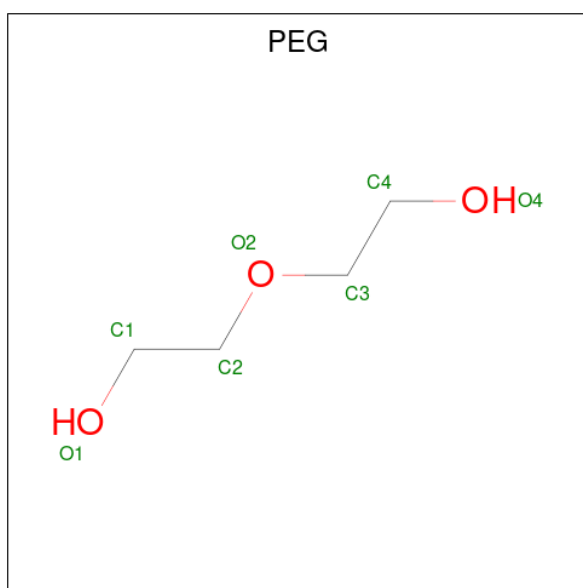
- Molecule 3 is (1S,2S,3R,4S,5S)-5-amino-1-(hydroxymethyl)cyclohexane-1,2,3,4-tetrol (three-letter code: W9S) (formula: C<sub>7</sub>H<sub>15</sub>NO<sub>5</sub>) (labeled as "Ligand of Interest" by depositor).





Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			13	7	1	5		
3	C	1	Total	C	N	O	0	0
			13	7	1	5		

- Molecule 4 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula:  $C_4H_{10}O_3$ ).



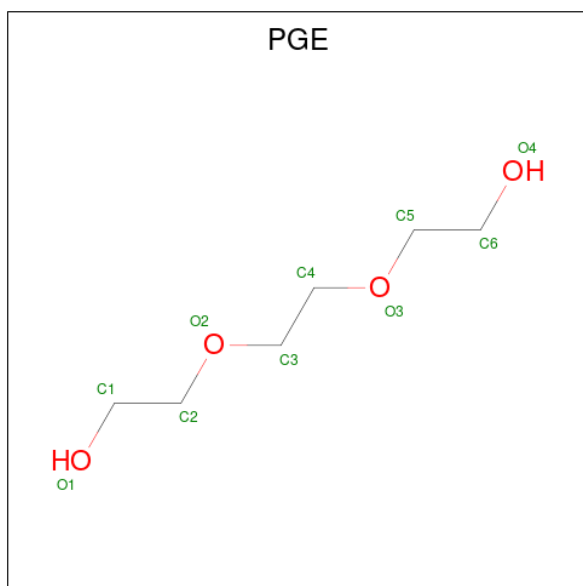
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			7	4	3		
4	A	1	Total	C	O	0	0
			7	4	3		

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

- Molecule 5 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula:  $C_6H_{14}O_4$ ).



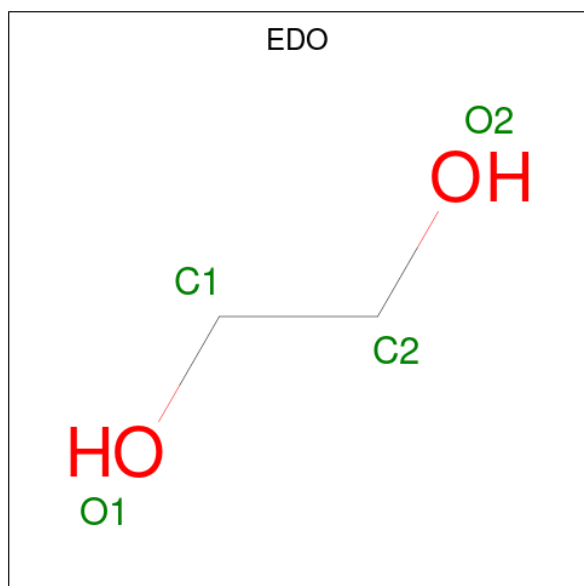
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			10	6	4		
5	A	1	Total	C	O	0	0
			10	6	4		
5	B	1	Total	C	O	0	0
			10	6	4		

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

- Molecule 6 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula:  $C_2H_6O_2$ ).



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

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

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

- Molecule 7 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



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

- Molecule 8 is CALCIUM ION (three-letter code: CA) (formula: Ca).

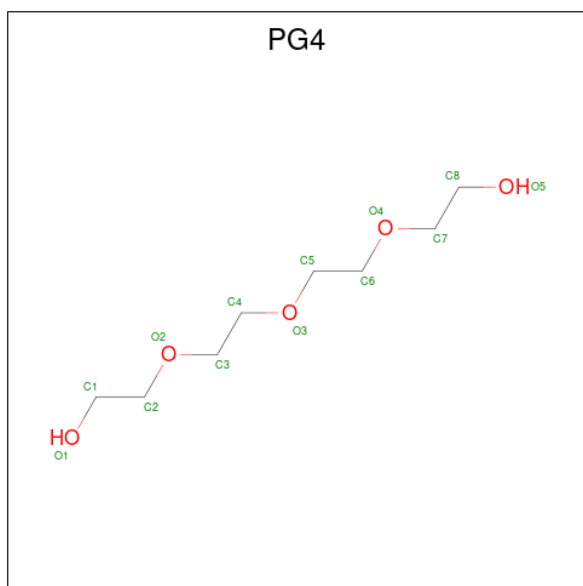
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	B	2	Total	Ca	0	0
			2	2		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	D	2	Total	Ca	0	0
			2	2		

- Molecule 9 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula:  $C_8H_{18}O_5$ ).

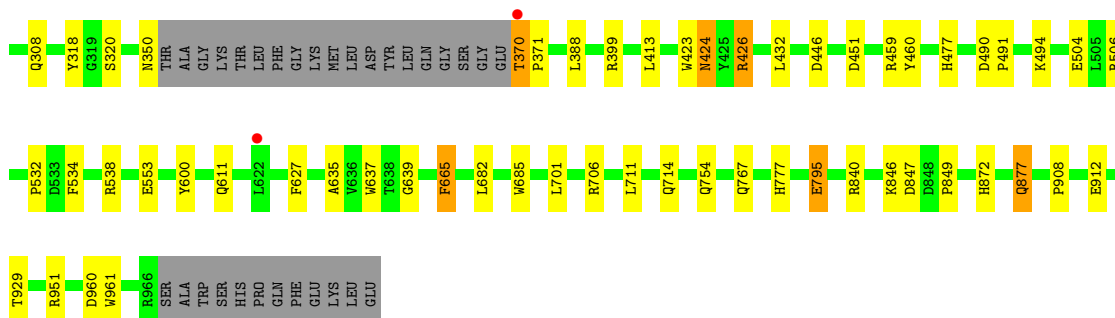


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	D	1	Total	C	O	0	0
			13	8	5		

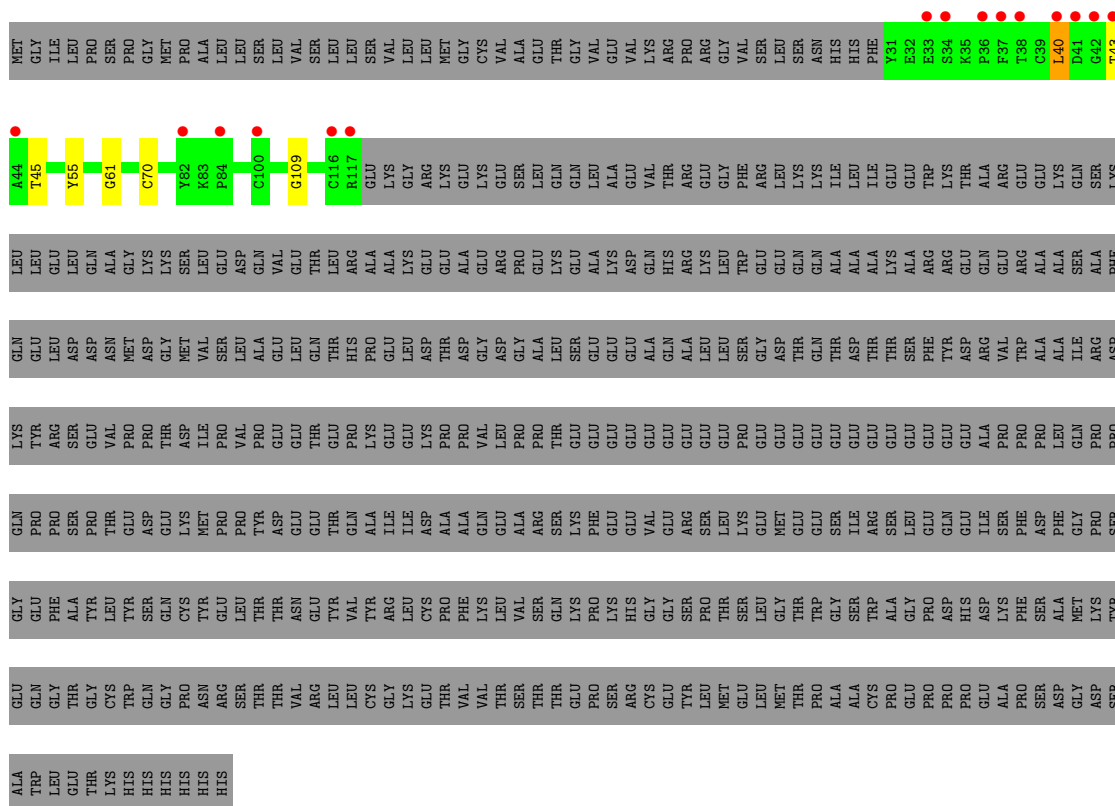
- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	428	Total	O	0	0
			428	428		
10	B	24	Total	O	0	0
			24	24		
10	C	384	Total	O	0	0
			384	384		
10	D	35	Total	O	0	0
			35	35		

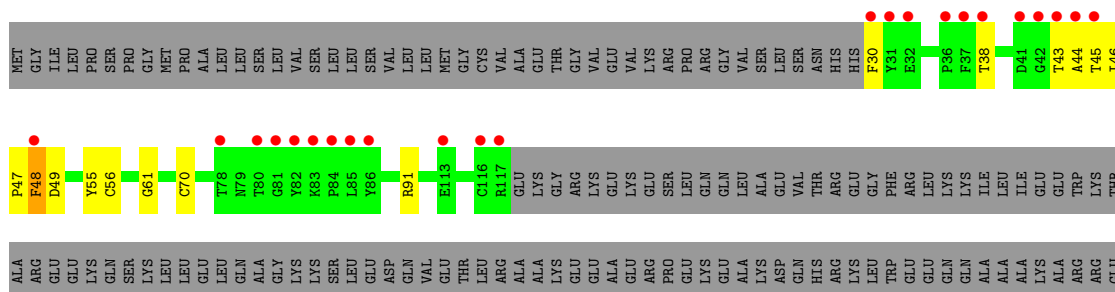




- Molecule 2: Glucosidase 2 subunit beta



- 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, $\alpha$ , $\beta$ , $\gamma$	102.88Å 102.88Å 241.70Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	42.49 – 2.30 50.01 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.9 (42.49-2.30) 94.6 (50.01-2.30)	Depositor EDS
$R_{merge}$	0.13	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	0.65 (at 2.29Å)	Xtriage
Refinement program	PHENIX 1.18.2_3874	Depositor
R, $R_{free}$	0.172 , 0.197 0.172 , 0.197	Depositor DCC
$R_{free}$ test set	1995 reflections (1.58%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	36.5	Xtriage
Anisotropy	0.171	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 38.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.018 for -h,-k,l 0.064 for h,-h-k,-l 0.033 for -k,-h,-l	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	16268	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.55% 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: PG4, SO4, PGE, PEG, CA, W9S, EDO

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	0.29	0/7118	0.50	0/9694
1	C	0.28	0/7180	0.51	2/9773 (0.0%)
2	B	0.31	0/625	0.59	1/856 (0.1%)
2	D	0.28	0/653	0.58	0/891
All	All	0.28	0/15576	0.51	3/21214 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	151	LEU	CA-CB-CG	5.75	128.51	115.30
1	C	134	ASP	CB-CG-OD2	-5.18	113.64	118.30
2	B	40	LEU	CA-CB-CG	5.17	127.19	115.30

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	6886	0	6613	66	0
1	C	6941	0	6685	53	0
2	B	614	0	492	3	0
2	D	641	0	539	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	13	0	0	0	0
3	C	13	0	0	0	0
4	A	42	0	60	5	0
4	C	21	0	30	1	0
4	D	7	0	10	0	0
5	A	20	0	28	2	0
5	B	10	0	14	0	0
5	C	10	0	14	3	0
6	A	72	0	108	7	0
6	B	16	0	24	1	0
6	C	40	0	60	5	0
6	D	4	0	6	0	0
7	A	20	0	0	4	0
7	C	10	0	0	0	0
8	B	2	0	0	0	0
8	D	2	0	0	0	0
9	D	13	0	18	2	0
10	A	428	0	0	17	0
10	B	24	0	0	0	0
10	C	384	0	0	21	0
10	D	35	0	0	4	0
All	All	16268	0	14701	137	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.

All (137) 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:72:ASP:O	10:C:1101:HOH:O	1.93	0.86
2:B:109:GLY:H	6:B:1906:EDO:H12	1.43	0.84
1:A:519:ASP:H	6:A:1022:EDO:H11	1.43	0.84
1:A:97:ASP:OD2	10:A:1101:HOH:O	1.97	0.83
1:C:167:LEU:O	10:C:1102:HOH:O	1.99	0.78
1:A:121:ALA:O	10:A:1102:HOH:O	2.01	0.77
7:A:1031:SO4:O3	10:A:1104:HOH:O	2.04	0.75
1:C:33:VAL:N	10:C:1107:HOH:O	2.19	0.75
1:C:308:GLN:OE1	10:C:1104:HOH:O	2.05	0.75
1:A:442:ASN:ND2	7:A:1031:SO4:O2	2.19	0.74
5:C:1003:PGE:O1	10:C:1103:HOH:O	2.04	0.73
1:C:413:LEU:HD22	6:C:1013:EDO:H12	1.71	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:48:PHE:O	10:D:1301:HOH:O	2.07	0.72
1:A:159:ASP:OD2	10:A:1106:HOH:O	2.08	0.71
1:C:960:ASP:HB3	4:C:1010:PEG:H41	1.73	0.71
1:C:350:ASN:OD1	10:C:1105:HOH:O	2.08	0.70
1:A:167:LEU:O	10:A:1107:HOH:O	2.11	0.69
2:D:44:ALA:O	10:D:1302:HOH:O	2.10	0.69
1:C:110:ARG:HH12	1:C:184:PRO:HG3	1.58	0.69
1:A:114:ARG:H	4:A:1011:PEG:H42	1.59	0.67
1:A:174:GLY:O	10:A:1108:HOH:O	2.12	0.66
5:C:1003:PGE:O4	10:C:1106:HOH:O	2.11	0.66
1:A:760:SER:HB2	4:A:1002:PEG:H41	1.76	0.66
1:C:110:ARG:NH1	10:C:1113:HOH:O	2.26	0.66
1:A:795:GLU:HB3	10:A:1130:HOH:O	1.97	0.64
1:C:553:GLU:HB3	6:C:1004:EDO:H22	1.78	0.64
1:A:692:GLN:OE1	10:A:1110:HOH:O	2.16	0.63
1:C:506:ARG:HD3	10:C:1138:HOH:O	1.99	0.63
1:C:293:THR:HG22	6:C:1015:EDO:H11	1.80	0.62
1:C:61:ARG:HD2	1:C:154:GLN:HB2	1.80	0.61
1:A:682:LEU:HD23	1:A:711:LEU:HD11	1.83	0.61
1:C:754:GLN:HB3	10:C:1182:HOH:O	2.00	0.61
1:C:112:ARG:NH2	1:C:179:GLU:O	2.34	0.61
5:A:1003:PGE:O4	10:A:1111:HOH:O	2.16	0.60
7:A:1031:SO4:O1	10:A:1109:HOH:O	2.15	0.59
1:C:795:GLU:HB3	10:C:1244:HOH:O	2.03	0.58
2:D:56:CYS:SG	9:D:1204:PG4:H42	2.44	0.57
1:A:112:ARG:NH2	1:A:179:GLU:O	2.37	0.57
1:A:310:GLU:HG2	4:A:1025:PEG:H32	1.88	0.56
2:D:47:PRO:HB2	2:D:49:ASP:OD1	2.06	0.56
1:C:168:LEU:HD21	1:C:388:LEU:HD13	1.88	0.54
1:A:426:ARG:NH2	10:A:1103:HOH:O	2.03	0.54
1:C:423:TRP:O	1:C:701:LEU:HA	2.08	0.53
1:C:506:ARG:HG3	10:C:1217:HOH:O	2.07	0.53
4:A:1025:PEG:O1	10:A:1113:HOH:O	2.18	0.53
1:A:293:THR:HG22	6:A:1023:EDO:H12	1.90	0.53
1:C:682:LEU:HD23	1:C:711:LEU:HD11	1.90	0.53
1:C:426:ARG:NH2	10:C:1125:HOH:O	2.40	0.53
2:D:38:THR:HG22	2:D:45:THR:HG23	1.89	0.53
1:A:459:ARG:NH1	1:A:494:LYS:HE2	2.24	0.52
1:A:423:TRP:O	1:A:701:LEU:HA	2.09	0.52
1:A:473:ASN:HB3	10:A:1368:HOH:O	2.09	0.52
1:C:370:THR:N	1:C:371:PRO:HD2	2.25	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:277:HIS:ND1	10:C:1119:HOH:O	2.34	0.51
2:D:30:PHE:N	10:D:1305:HOH:O	2.43	0.51
1:A:250:GLU:OE1	1:A:259:LYS:NZ	2.32	0.50
1:C:491:PRO:O	1:C:532:PRO:HD2	2.10	0.50
5:C:1003:PGE:H42	10:C:1103:HOH:O	2.12	0.50
1:A:311:LEU:HD22	1:A:650:ILE:HD13	1.93	0.50
1:A:370:THR:N	1:A:371:PRO:HD2	2.27	0.50
1:A:55:PRO:HB3	1:A:173:ARG:HB3	1.94	0.49
1:C:61:ARG:HG3	1:C:153:ALA:O	2.12	0.49
2:B:61:GLY:HA2	2:B:70:CYS:SG	2.53	0.49
2:D:61:GLY:HA2	2:D:70:CYS:SG	2.52	0.49
1:A:460:TYR:CE2	1:A:490:ASP:HB2	2.47	0.49
1:A:506:ARG:O	10:A:1114:HOH:O	2.19	0.49
1:C:951:ARG:HG3	2:D:55:TYR:CE2	2.48	0.49
9:D:1204:PG4:H41	10:D:1313:HOH:O	2.13	0.49
1:C:259:LYS:HD2	10:C:1421:HOH:O	2.13	0.48
1:A:523:TRP:CD2	4:A:1014:PEG:H12	2.48	0.48
2:D:43:THR:OG1	2:D:44:ALA:N	2.47	0.48
1:C:257:ASP:OD2	10:C:1108:HOH:O	2.20	0.48
1:A:951:ARG:HG3	2:B:55:TYR:CE2	2.49	0.47
1:C:929:THR:HB	1:C:961:TRP:HB3	1.96	0.47
1:A:491:PRO:O	1:A:532:PRO:HD2	2.14	0.47
1:C:320:SER:O	1:C:627:PHE:HA	2.15	0.47
1:C:42:ASP:N	10:C:1116:HOH:O	2.29	0.46
1:C:877:GLN:NE2	6:C:1009:EDO:H21	2.30	0.46
1:A:336:PHE:HB3	1:A:387:PHE:HB2	1.96	0.46
1:A:644:GLU:OE1	10:A:1115:HOH:O	2.21	0.46
1:A:286:ASP:OD1	1:A:291:LYS:NZ	2.44	0.46
1:C:292:VAL:HG12	1:C:294:GLU:H	1.81	0.46
1:A:519:ASP:N	6:A:1022:EDO:H11	2.23	0.45
1:A:849:PRO:HB2	1:A:912:GLU:HB3	1.98	0.45
1:A:424:ASN:OD1	1:A:451:ASP:HB3	2.17	0.45
1:C:399:ARG:NH1	10:C:1140:HOH:O	2.50	0.45
1:C:432:LEU:HD22	1:C:477[A]:HIS:ND1	2.32	0.44
1:C:460:TYR:CE2	1:C:490:ASP:HB2	2.52	0.44
1:A:396:ASP:OD1	6:A:1008:EDO:O2	2.36	0.44
1:A:794:GLN:C	1:A:795:GLU:HG2	2.37	0.44
1:C:158:LEU:HB2	1:C:170:VAL:HB	1.99	0.44
1:A:945:THR:OG1	10:A:1105:HOH:O	2.08	0.44
1:A:154:GLN:HA	1:A:155:PRO:HA	1.89	0.44
1:A:732:PHE:HE1	6:A:1021:EDO:H22	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:133:ARG:HG3	1:C:138:VAL:HG22	2.00	0.43
1:A:69:LEU:HD11	1:A:128:LEU:HB2	2.01	0.43
1:A:158:LEU:HB2	1:A:170:VAL:HB	2.00	0.43
1:C:163:ASP:HB3	1:C:164:ARG:H	1.69	0.43
1:A:426:ARG:HB3	7:A:1028:SO4:O3	2.19	0.43
1:C:424:ASN:OD1	1:C:451:ASP:HB3	2.19	0.43
1:A:447:VAL:HG11	1:A:486:VAL:HG23	2.00	0.43
1:A:767:GLN:HG3	1:A:777:HIS:ND1	2.34	0.42
1:C:767:GLN:HG3	1:C:777:HIS:ND1	2.35	0.42
1:C:846:LYS:HB2	6:C:1013:EDO:O1	2.18	0.42
1:A:929:THR:HB	1:A:961:TRP:HB3	2.01	0.42
1:C:635:ALA:HB2	1:C:665:PHE:CD2	2.54	0.42
1:A:343:THR:HA	1:A:378:MET:O	2.19	0.42
1:A:432:LEU:HD22	1:A:477[A]:HIS:ND1	2.34	0.42
1:A:534:PHE:HB3	1:A:600:TYR:HB3	2.01	0.42
1:A:720:ARG:CZ	6:A:1005:EDO:H12	2.50	0.42
1:A:746:PRO:HG2	1:A:749:ARG:HG2	2.00	0.42
1:C:847:ASP:HB3	1:C:908:PRO:HG2	2.02	0.42
1:A:426:ARG:O	1:A:467:ARG:HD2	2.20	0.42
1:A:656:LEU:HD23	1:A:656:LEU:HA	1.89	0.42
1:A:278:VAL:HG23	1:A:290:LEU:HB2	2.02	0.41
1:A:500:ARG:NH2	10:A:1136:HOH:O	2.39	0.41
1:A:531:TYR:CZ	1:A:570:VAL:HG22	2.55	0.41
1:A:567:GLU:N	1:A:568:PRO:HA	2.35	0.41
1:C:504:GLU:OE2	10:C:1109:HOH:O	2.21	0.41
1:C:849:PRO:HB2	1:C:912:GLU:HB3	2.02	0.41
1:A:113:TYR:CZ	1:A:593:ILE:HG22	2.56	0.41
1:A:163:ASP:HB3	1:A:164:ARG:H	1.63	0.41
1:A:318:TYR:CE2	1:A:639:GLY:HA3	2.56	0.41
1:A:884:LEU:HG	1:A:899:ALA:HB3	2.03	0.41
1:A:910:TRP:CG	5:A:1009:PGE:H2	2.56	0.41
1:C:426:ARG:NH2	10:C:1151:HOH:O	2.54	0.41
1:A:702:ASP:OD2	6:A:1017:EDO:O2	2.36	0.41
1:A:755:TYR:CE2	1:A:792:PRO:HG2	2.56	0.40
1:C:840:ARG:HH21	2:D:91:ARG:HG2	1.86	0.40
1:A:102:ARG:HA	1:A:384:ILE:O	2.21	0.40
1:C:318:TYR:CE2	1:C:639:GLY:HA3	2.56	0.40
1:C:152:THR:HB	1:C:157:ARG:HB3	2.04	0.40
1:C:534:PHE:HB3	1:C:600:TYR:HB3	2.03	0.40
1:C:459:ARG:NH1	1:C:494:LYS:HE2	2.36	0.40
1:A:648:LEU:HD13	1:A:685:TRP:CG	2.56	0.40

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	854/977 (87%)	828 (97%)	25 (3%)	1 (0%)	51	64
1	C	860/977 (88%)	833 (97%)	26 (3%)	1 (0%)	51	64
2	B	85/547 (16%)	79 (93%)	5 (6%)	1 (1%)	13	14
2	D	86/547 (16%)	80 (93%)	6 (7%)	0	100	100
All	All	1885/3048 (62%)	1820 (97%)	62 (3%)	3 (0%)	47	58

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	43	THR
1	A	872	HIS
1	C	872	HIS

### 5.3.2 Protein sidechains [i](#)

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	743/846 (88%)	730 (98%)	13 (2%)	60	76
1	C	751/846 (89%)	730 (97%)	21 (3%)	43	60
2	B	67/478 (14%)	65 (97%)	2 (3%)	41	57
2	D	73/478 (15%)	71 (97%)	2 (3%)	44	61

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1634/2648 (62%)	1596 (98%)	38 (2%)	50 67

All (38) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	67	LEU
1	A	69	LEU
1	A	84	LYS
1	A	129	SER
1	A	144	GLU
1	A	370	THR
1	A	424	ASN
1	A	426	ARG
1	A	446	ASP
1	A	637	TRP
1	A	665	PHE
1	A	685	TRP
1	A	706	ARG
2	B	40	LEU
2	B	45	THR
1	C	107	GLU
1	C	109	ARG
1	C	110	ARG
1	C	130	VAL
1	C	137	SER
1	C	151	LEU
1	C	161	LEU
1	C	168	LEU
1	C	253	LYS
1	C	370	THR
1	C	424	ASN
1	C	426	ARG
1	C	446	ASP
1	C	538	ARG
1	C	637	TRP
1	C	665	PHE
1	C	685	TRP
1	C	706	ARG
1	C	714	GLN
1	C	795	GLU
1	C	877	GLN
2	D	46	ILE

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Mol	Chain	Res	Type
2	D	48	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	C	877	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 60 ligands modelled in this entry, 4 are monoatomic - leaving 56 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	PEG	A	1011	-	6,6,6	0.51	0	5,5,5	0.28	0
7	SO4	A	1030	-	4,4,4	0.16	0	6,6,6	0.12	0
5	PGE	A	1003	-	9,9,9	0.31	0	8,8,8	0.28	0
4	PEG	A	1012	-	6,6,6	0.48	0	5,5,5	0.27	0
6	EDO	A	1017	-	3,3,3	0.49	0	2,2,2	0.42	0
6	EDO	A	1004	-	3,3,3	0.40	0	2,2,2	0.41	0
6	EDO	C	1015	-	3,3,3	0.44	0	2,2,2	0.27	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
6	EDO	B	1907	-	3,3,3	0.47	0	2,2,2	0.34	0
6	EDO	C	1007	-	3,3,3	0.49	0	2,2,2	0.28	0
5	PGE	C	1003	-	9,9,9	0.34	0	8,8,8	0.31	0
6	EDO	C	1012	-	3,3,3	0.42	0	2,2,2	0.44	0
6	EDO	A	1005	-	3,3,3	0.47	0	2,2,2	0.31	0
3	W9S	C	1001	-	13,13,13	0.80	0	17,20,20	0.96	1 (5%)
6	EDO	A	1008	-	3,3,3	0.41	0	2,2,2	0.57	0
4	PEG	D	1201	-	6,6,6	0.48	0	5,5,5	0.38	0
7	SO4	A	1028	-	4,4,4	0.15	0	6,6,6	0.11	0
5	PGE	A	1009	-	9,9,9	0.33	0	8,8,8	0.28	0
6	EDO	A	1021	-	3,3,3	0.51	0	2,2,2	0.28	0
7	SO4	A	1031	-	4,4,4	0.14	0	6,6,6	0.21	0
4	PEG	C	1010	-	6,6,6	0.48	0	5,5,5	0.26	0
4	PEG	A	1002	-	6,6,6	0.46	0	5,5,5	0.35	0
6	EDO	A	1006	-	3,3,3	0.42	0	2,2,2	0.48	0
4	PEG	A	1025	-	6,6,6	0.53	0	5,5,5	0.41	0
3	W9S	A	1001	-	13,13,13	0.84	1 (7%)	17,20,20	0.94	1 (5%)
4	PEG	C	1008	-	6,6,6	0.49	0	5,5,5	0.27	0
4	PEG	A	1014	-	6,6,6	0.48	0	5,5,5	0.44	0
6	EDO	B	1901	-	3,3,3	0.49	0	2,2,2	0.33	0
6	EDO	A	1013	-	3,3,3	0.48	0	2,2,2	0.27	0
6	EDO	B	1906	-	3,3,3	0.43	0	2,2,2	0.44	0
6	EDO	A	1018	-	3,3,3	0.47	0	2,2,2	0.41	0
6	EDO	A	1016	-	3,3,3	0.45	0	2,2,2	0.30	0
6	EDO	A	1024	-	3,3,3	0.45	0	2,2,2	0.45	0
7	SO4	C	1016	-	4,4,4	0.13	0	6,6,6	0.11	0
7	SO4	C	1017	-	4,4,4	0.16	0	6,6,6	0.08	0
5	PGE	B	1904	-	9,9,9	0.32	0	8,8,8	0.32	0
6	EDO	A	1027	-	3,3,3	0.50	0	2,2,2	0.27	0
6	EDO	D	1205	-	3,3,3	0.48	0	2,2,2	0.30	0
6	EDO	C	1002	-	3,3,3	0.43	0	2,2,2	0.45	0
6	EDO	A	1026	-	3,3,3	0.43	0	2,2,2	0.39	0
6	EDO	A	1020	-	3,3,3	0.50	0	2,2,2	0.27	0
4	PEG	C	1011	-	6,6,6	0.48	0	5,5,5	0.26	0
6	EDO	A	1015	-	3,3,3	0.46	0	2,2,2	0.40	0
6	EDO	C	1005	-	3,3,3	0.44	0	2,2,2	0.42	0
6	EDO	C	1013	-	3,3,3	0.41	0	2,2,2	0.62	0
6	EDO	C	1009	-	3,3,3	0.47	0	2,2,2	0.30	0
4	PEG	A	1007	-	6,6,6	0.47	0	5,5,5	0.35	0
6	EDO	C	1014	-	3,3,3	0.45	0	2,2,2	0.44	0
9	PG4	D	1204	-	12,12,12	0.53	0	11,11,11	0.35	0
6	EDO	A	1023	-	3,3,3	0.48	0	2,2,2	0.43	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
6	EDO	A	1010	-	3,3,3	0.46	0	2,2,2	0.32	0
6	EDO	A	1022	-	3,3,3	0.48	0	2,2,2	0.30	0
6	EDO	C	1004	-	3,3,3	0.48	0	2,2,2	0.27	0
6	EDO	A	1019	-	3,3,3	0.45	0	2,2,2	0.47	0
6	EDO	B	1905	-	3,3,3	0.45	0	2,2,2	0.38	0
7	SO4	A	1029	-	4,4,4	0.16	0	6,6,6	0.11	0
6	EDO	C	1006	-	3,3,3	0.55	0	2,2,2	0.16	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
4	PEG	A	1011	-	-	2/4/4/4	-
5	PGE	A	1003	-	-	1/7/7/7	-
4	PEG	A	1012	-	-	3/4/4/4	-
6	EDO	A	1017	-	-	0/1/1/1	-
6	EDO	A	1004	-	-	1/1/1/1	-
6	EDO	C	1015	-	-	0/1/1/1	-
6	EDO	B	1907	-	-	0/1/1/1	-
6	EDO	C	1007	-	-	0/1/1/1	-
5	PGE	C	1003	-	-	5/7/7/7	-
6	EDO	C	1012	-	-	1/1/1/1	-
6	EDO	A	1005	-	-	0/1/1/1	-
3	W9S	C	1001	-	-	0/3/26/26	0/1/1/1
6	EDO	A	1008	-	-	0/1/1/1	-
4	PEG	D	1201	-	-	3/4/4/4	-
5	PGE	A	1009	-	-	6/7/7/7	-
6	EDO	A	1021	-	-	0/1/1/1	-
4	PEG	C	1010	-	-	3/4/4/4	-
4	PEG	A	1002	-	-	4/4/4/4	-
6	EDO	A	1006	-	-	1/1/1/1	-
4	PEG	A	1025	-	-	2/4/4/4	-
3	W9S	A	1001	-	-	2/3/26/26	0/1/1/1
4	PEG	C	1008	-	-	2/4/4/4	-
4	PEG	A	1014	-	-	2/4/4/4	-
6	EDO	B	1901	-	-	1/1/1/1	-
6	EDO	A	1013	-	-	1/1/1/1	-
6	EDO	B	1906	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	EDO	A	1018	-	-	0/1/1/1	-
6	EDO	A	1016	-	-	1/1/1/1	-
6	EDO	A	1024	-	-	1/1/1/1	-
5	PGE	B	1904	-	-	5/7/7/7	-
6	EDO	A	1027	-	-	0/1/1/1	-
6	EDO	D	1205	-	-	0/1/1/1	-
6	EDO	C	1002	-	-	0/1/1/1	-
6	EDO	A	1026	-	-	1/1/1/1	-
6	EDO	A	1020	-	-	0/1/1/1	-
4	PEG	C	1011	-	-	3/4/4/4	-
6	EDO	A	1015	-	-	1/1/1/1	-
6	EDO	C	1005	-	-	0/1/1/1	-
6	EDO	C	1013	-	-	0/1/1/1	-
6	EDO	C	1009	-	-	0/1/1/1	-
4	PEG	A	1007	-	-	2/4/4/4	-
6	EDO	C	1014	-	-	1/1/1/1	-
9	PG4	D	1204	-	-	6/10/10/10	-
6	EDO	A	1023	-	-	0/1/1/1	-
6	EDO	A	1010	-	-	1/1/1/1	-
6	EDO	A	1022	-	-	0/1/1/1	-
6	EDO	C	1004	-	-	1/1/1/1	-
6	EDO	A	1019	-	-	1/1/1/1	-
6	EDO	B	1905	-	-	0/1/1/1	-
6	EDO	C	1006	-	-	1/1/1/1	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1001	W9S	O3-C1	-2.01	1.41	1.44

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	1001	W9S	C2-C3-C4	2.65	114.55	110.58
3	A	1001	W9S	C2-C3-C4	2.38	114.15	110.58

There are no chirality outliers.

All (65) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1001	W9S	O3-C1-C7-O2
5	C	1003	PGE	O1-C1-C2-O2
5	C	1003	PGE	O2-C3-C4-O3
9	D	1204	PG4	O3-C5-C6-O4
4	A	1002	PEG	O1-C1-C2-O2
4	A	1025	PEG	O1-C1-C2-O2
4	C	1010	PEG	O1-C1-C2-O2
4	C	1010	PEG	O2-C3-C4-O4
5	B	1904	PGE	O3-C5-C6-O4
4	D	1201	PEG	C4-C3-O2-C2
4	A	1002	PEG	C4-C3-O2-C2
5	C	1003	PGE	C4-C3-O2-C2
4	A	1011	PEG	O1-C1-C2-O2
4	C	1011	PEG	O1-C1-C2-O2
4	C	1011	PEG	O2-C3-C4-O4
4	A	1007	PEG	O2-C3-C4-O4
6	A	1010	EDO	O1-C1-C2-O2
9	D	1204	PG4	O2-C3-C4-O3
4	A	1014	PEG	O2-C3-C4-O4
4	D	1201	PEG	O2-C3-C4-O4
9	D	1204	PG4	O4-C7-C8-O5
4	A	1007	PEG	O1-C1-C2-O2
5	A	1009	PGE	O3-C5-C6-O4
5	A	1009	PGE	C4-C3-O2-C2
5	A	1009	PGE	O2-C3-C4-O3
6	A	1026	EDO	O1-C1-C2-O2
6	C	1006	EDO	O1-C1-C2-O2
4	A	1012	PEG	C1-C2-O2-C3
5	B	1904	PGE	O1-C1-C2-O2
4	D	1201	PEG	C1-C2-O2-C3
5	C	1003	PGE	C1-C2-O2-C3
5	A	1009	PGE	C6-C5-O3-C4
4	A	1002	PEG	C1-C2-O2-C3
4	C	1008	PEG	C1-C2-O2-C3
4	C	1010	PEG	C4-C3-O2-C2
3	A	1001	W9S	C6-C1-C7-O2
4	A	1002	PEG	O2-C3-C4-O4
5	A	1009	PGE	O1-C1-C2-O2
9	D	1204	PG4	O1-C1-C2-O2
5	C	1003	PGE	C6-C5-O3-C4
6	A	1013	EDO	O1-C1-C2-O2
6	C	1014	EDO	O1-C1-C2-O2
5	B	1904	PGE	C3-C4-O3-C5

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Mol	Chain	Res	Type	Atoms
9	D	1204	PG4	C1-C2-O2-C3
4	A	1012	PEG	O2-C3-C4-O4
5	A	1009	PGE	C3-C4-O3-C5
9	D	1204	PG4	C4-C3-O2-C2
4	A	1012	PEG	C4-C3-O2-C2
6	A	1004	EDO	O1-C1-C2-O2
6	A	1006	EDO	O1-C1-C2-O2
6	A	1016	EDO	O1-C1-C2-O2
6	A	1024	EDO	O1-C1-C2-O2
6	C	1004	EDO	O1-C1-C2-O2
6	C	1012	EDO	O1-C1-C2-O2
5	B	1904	PGE	C4-C3-O2-C2
4	A	1011	PEG	C4-C3-O2-C2
4	A	1014	PEG	C4-C3-O2-C2
4	A	1025	PEG	C4-C3-O2-C2
5	B	1904	PGE	O2-C3-C4-O3
4	C	1008	PEG	O2-C3-C4-O4
6	A	1015	EDO	O1-C1-C2-O2
6	B	1901	EDO	O1-C1-C2-O2
5	A	1003	PGE	O3-C5-C6-O4
6	A	1019	EDO	O1-C1-C2-O2
4	C	1011	PEG	C4-C3-O2-C2

There are no ring outliers.

22 monomers are involved in 30 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1011	PEG	1	0
5	A	1003	PGE	1	0
6	A	1017	EDO	1	0
6	C	1015	EDO	1	0
5	C	1003	PGE	3	0
6	A	1005	EDO	1	0
6	A	1008	EDO	1	0
7	A	1028	SO4	1	0
5	A	1009	PGE	1	0
6	A	1021	EDO	1	0
7	A	1031	SO4	3	0
4	C	1010	PEG	1	0
4	A	1002	PEG	1	0
4	A	1025	PEG	2	0
4	A	1014	PEG	1	0

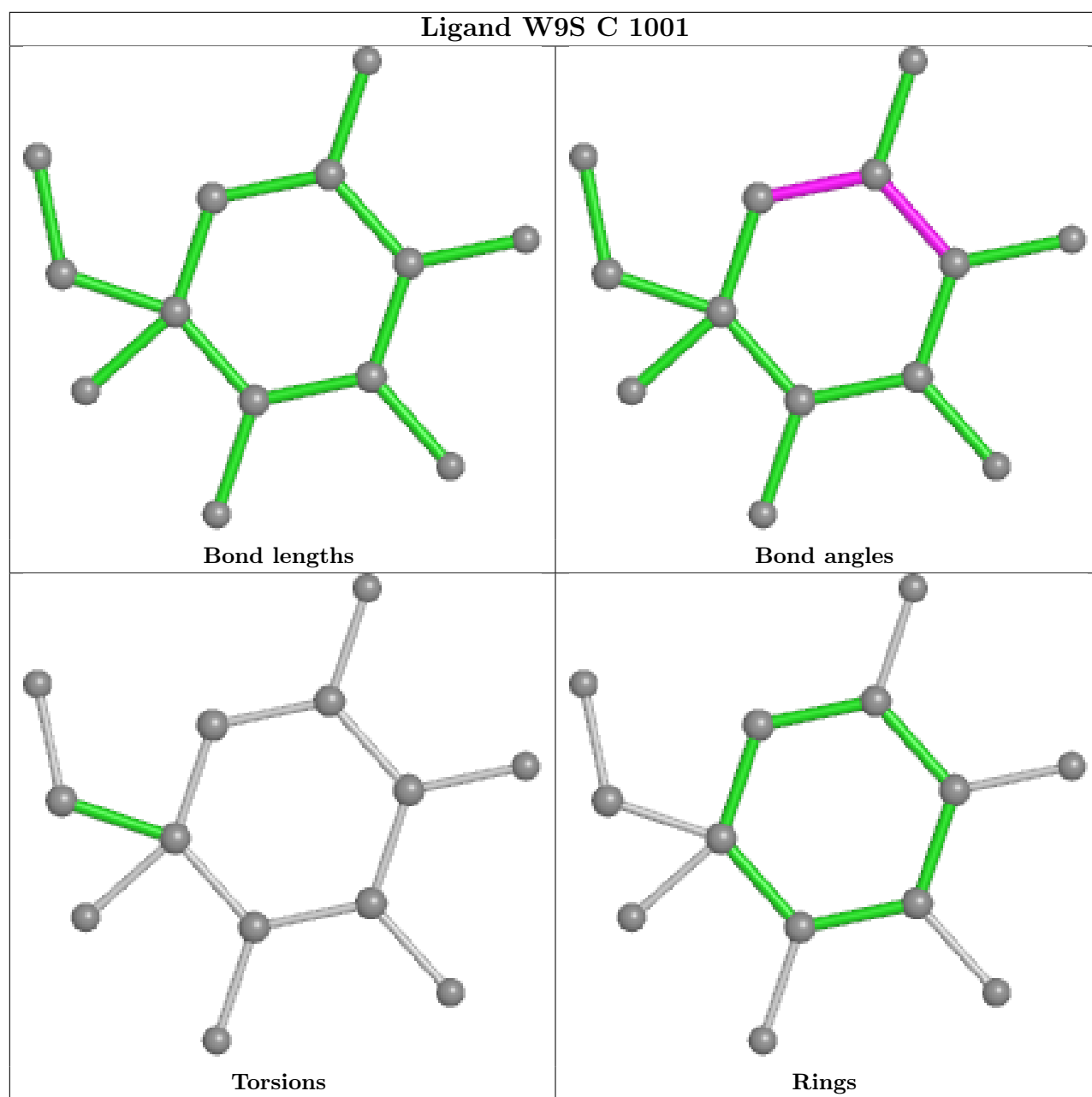
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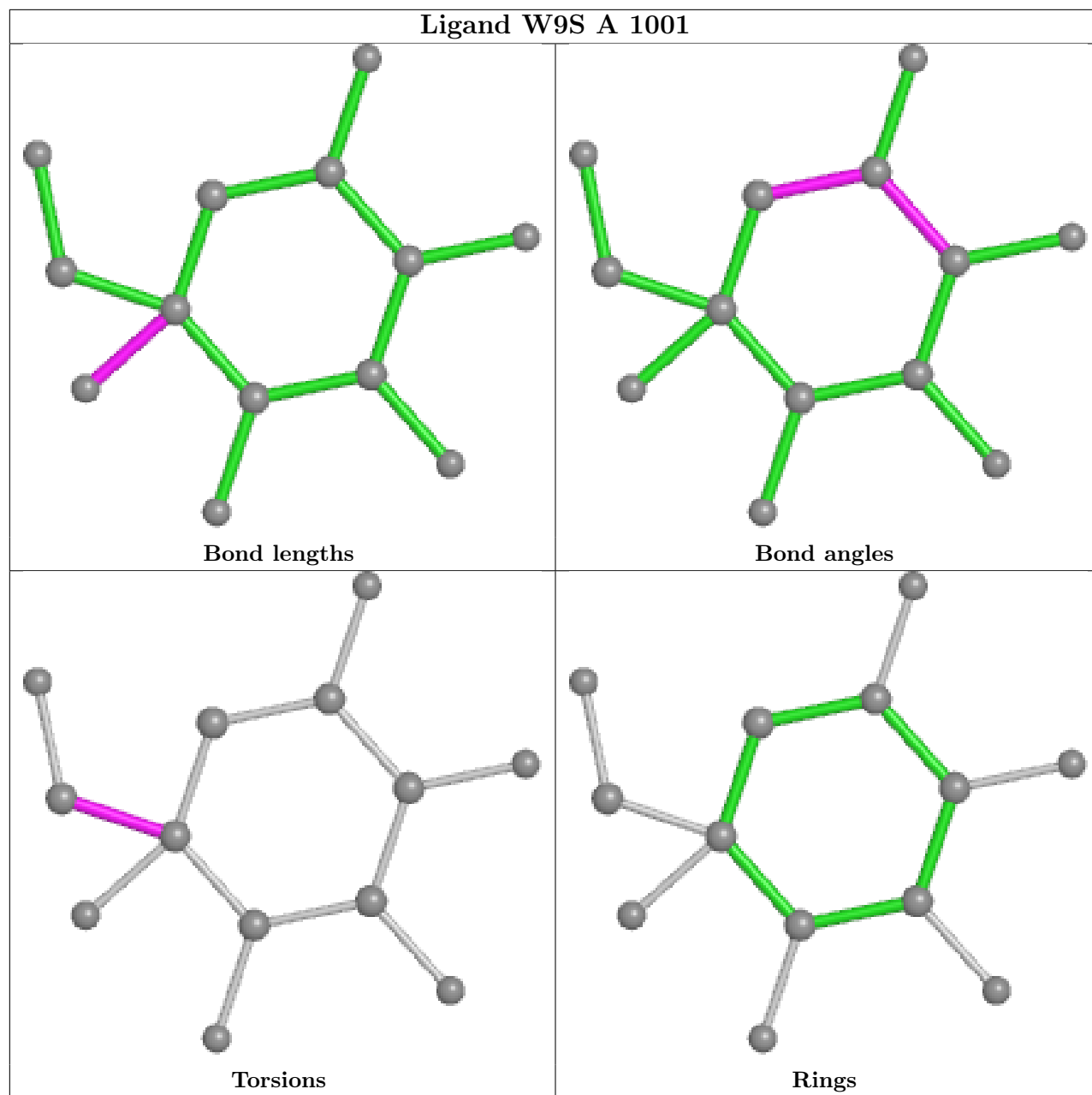
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	1906	EDO	1	0
6	C	1013	EDO	2	0
6	C	1009	EDO	1	0
9	D	1204	PG4	2	0
6	A	1023	EDO	1	0
6	A	1022	EDO	2	0
6	C	1004	EDO	1	0

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 ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	853/977 (87%)	-0.26	5 (0%) 89 92	26, 39, 61, 80	0
1	C	857/977 (87%)	0.02	40 (4%) 31 38	28, 43, 77, 100	0
2	B	87/547 (15%)	0.43	15 (17%) 1 1	33, 54, 87, 95	0
2	D	88/547 (16%)	0.85	23 (26%) 0 0	35, 55, 93, 100	0
All	All	1885/3048 (61%)	-0.05	83 (4%) 34 41	26, 42, 75, 100	0

All (83) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	43	THR	9.6
2	D	81	GLY	7.1
2	D	80	THR	5.2
2	D	30	PHE	5.1
1	C	135	ASP	5.1
2	B	117	ARG	4.6
2	D	117	ARG	4.6
2	D	82	TYR	4.5
1	C	136	ASN	4.4
1	A	247	ALA	4.1
1	C	61	ARG	4.0
2	D	45	THR	3.9
1	C	184	PRO	3.9
1	C	185	ARG	3.9
1	C	156	PHE	3.7
2	D	83	LYS	3.7
2	B	42	GLY	3.5
1	C	153	ALA	3.5
1	C	138	VAL	3.5
2	D	44	ALA	3.4
2	D	48	PHE	3.4

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Mol	Chain	Res	Type	RSRZ
2	B	41	ASP	3.4
1	C	164	ARG	3.4
2	D	78	THR	3.4
1	C	140	LEU	3.3
2	D	31	TYR	3.3
1	C	131	SER	3.2
1	C	128	LEU	3.2
2	D	41	ASP	3.2
1	A	109	ARG	3.1
2	B	40	LEU	3.1
1	C	69	LEU	3.1
1	C	137	SER	3.1
1	C	150	ILE	3.0
1	C	370	THR	3.0
2	B	84	PRO	2.9
2	B	82	TYR	2.9
2	B	34	SER	2.9
1	C	133	ARG	2.9
2	D	84	PRO	2.8
1	C	81	GLU	2.8
2	B	44	ALA	2.7
2	D	32	GLU	2.7
2	D	36	PRO	2.7
1	C	163	ASP	2.6
1	C	132	GLY	2.6
1	C	142	VAL	2.6
2	D	42	GLY	2.6
1	C	60	TYR	2.6
2	B	43	THR	2.6
1	C	152	THR	2.5
2	D	38	THR	2.5
1	C	74	LEU	2.5
1	A	636	VAL	2.5
1	C	244	GLU	2.5
1	C	55	PRO	2.5
2	B	36	PRO	2.5
2	B	33	GLU	2.4
1	C	63	LEU	2.4
2	B	116	CYS	2.4
1	C	66	THR	2.4
1	C	126	ALA	2.4
1	C	129	SER	2.3

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Mol	Chain	Res	Type	RSRZ
2	D	86	TYR	2.3
1	C	62	ALA	2.3
2	D	113	GLU	2.3
2	B	38	THR	2.3
1	C	79	ILE	2.3
2	D	37	PHE	2.3
1	C	154	GLN	2.2
1	A	164	ARG	2.2
1	C	622	LEU	2.2
2	D	85	LEU	2.2
2	B	37	PHE	2.2
1	C	155	PRO	2.2
1	C	165	SER	2.2
1	C	76	VAL	2.1
1	C	141	THR	2.1
1	A	637	TRP	2.1
1	C	149	ILE	2.1
2	B	100	CYS	2.1
2	D	116	CYS	2.1
1	C	89	LEU	2.1

## 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	EDO	A	1017	4/4	0.72	0.33	44,48,52,54	0
6	EDO	A	1024	4/4	0.72	0.33	64,67,68,70	0
4	PEG	D	1201	7/7	0.75	0.23	54,63,65,65	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
6	EDO	B	1907	4/4	0.75	0.24	53,58,60,61	0
9	PG4	D	1204	13/13	0.76	0.21	54,59,69,71	0
6	EDO	A	1015	4/4	0.79	0.23	63,65,66,66	0
6	EDO	C	1006	4/4	0.81	0.15	43,49,51,52	0
6	EDO	A	1020	4/4	0.81	0.17	54,59,61,62	0
5	PGE	C	1003	10/10	0.82	0.39	60,67,70,78	0
6	EDO	A	1022	4/4	0.83	0.28	48,54,55,60	0
4	PEG	A	1011	7/7	0.84	0.21	48,58,59,68	0
4	PEG	A	1012	7/7	0.85	0.16	47,59,64,69	0
4	PEG	C	1008	7/7	0.86	0.17	47,50,53,55	0
6	EDO	B	1901	4/4	0.86	0.18	49,52,56,56	0
4	PEG	A	1007	7/7	0.86	0.14	58,62,67,68	0
6	EDO	C	1005	4/4	0.86	0.17	47,51,52,55	0
4	PEG	A	1014	7/7	0.86	0.24	56,57,64,67	0
6	EDO	A	1010	4/4	0.86	0.20	61,62,64,65	0
6	EDO	A	1013	4/4	0.87	0.16	54,58,62,64	0
6	EDO	B	1905	4/4	0.87	0.29	60,65,66,70	0
7	SO4	A	1031	5/5	0.87	0.39	49,56,68,85	0
4	PEG	C	1010	7/7	0.87	0.30	49,58,65,67	0
5	PGE	A	1003	10/10	0.88	0.27	49,57,60,64	0
6	EDO	C	1014	4/4	0.88	0.14	55,59,63,72	0
5	PGE	B	1904	10/10	0.89	0.35	53,66,71,74	0
5	PGE	A	1009	10/10	0.89	0.19	50,59,64,68	0
6	EDO	C	1009	4/4	0.89	0.17	57,62,62,67	0
7	SO4	A	1028	5/5	0.90	0.23	61,75,87,91	0
4	PEG	A	1025	7/7	0.90	0.32	50,53,57,59	0
7	SO4	C	1016	5/5	0.90	0.17	65,66,70,91	0
6	EDO	C	1004	4/4	0.90	0.24	51,52,57,64	0
4	PEG	C	1011	7/7	0.91	0.19	58,61,65,66	0
4	PEG	A	1002	7/7	0.91	0.23	53,55,62,63	0
6	EDO	A	1018	4/4	0.91	0.18	48,51,55,57	0
6	EDO	A	1005	4/4	0.92	0.20	50,53,53,61	0
6	EDO	C	1015	4/4	0.92	0.17	57,57,57,61	0
6	EDO	C	1012	4/4	0.92	0.16	45,46,51,51	0
6	EDO	A	1026	4/4	0.93	0.16	49,52,54,64	0
6	EDO	A	1006	4/4	0.93	0.17	45,48,52,64	0
7	SO4	A	1030	5/5	0.93	0.29	63,69,79,98	0
6	EDO	C	1007	4/4	0.94	0.15	52,56,59,59	0
6	EDO	A	1021	4/4	0.94	0.13	44,45,46,49	0
6	EDO	B	1906	4/4	0.94	0.17	48,50,52,60	0
7	SO4	A	1029	5/5	0.94	0.35	73,79,86,92	0
6	EDO	A	1019	4/4	0.95	0.18	51,53,55,56	0

*Continued on next page...*

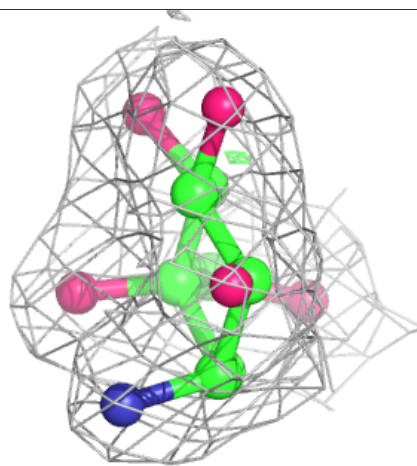
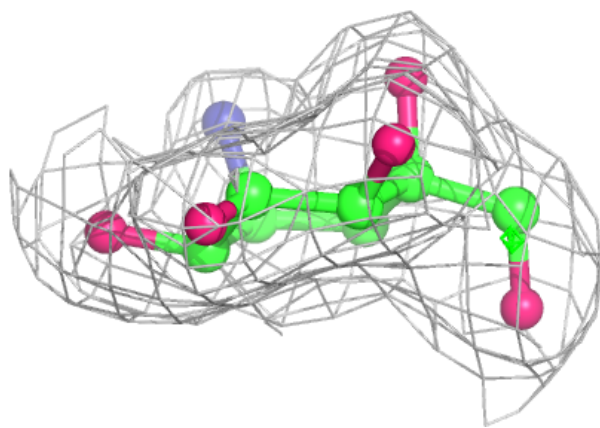
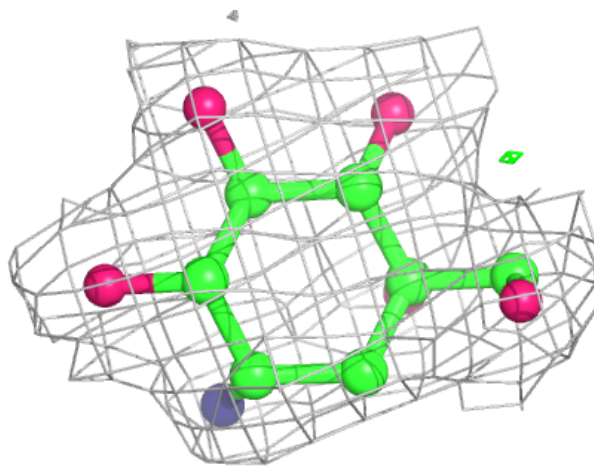
*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
6	EDO	A	1004	4/4	0.95	0.23	44,47,47,54	0
6	EDO	C	1002	4/4	0.95	0.17	40,44,50,55	0
6	EDO	C	1013	4/4	0.95	0.14	41,41,47,55	0
6	EDO	A	1016	4/4	0.96	0.10	40,41,46,48	0
6	EDO	A	1023	4/4	0.96	0.09	41,41,44,54	0
6	EDO	A	1008	4/4	0.96	0.21	42,42,47,49	0
3	W9S	A	1001	13/13	0.96	0.20	28,33,38,44	0
3	W9S	C	1001	13/13	0.97	0.15	29,34,38,38	0
7	SO4	C	1017	5/5	0.97	0.17	69,74,83,92	0
6	EDO	A	1027	4/4	0.97	0.32	39,45,52,53	0
8	CA	B	1903	1/1	0.98	0.07	38,38,38,38	0
8	CA	D	1203	1/1	0.98	0.10	40,40,40,40	0
6	EDO	D	1205	4/4	0.98	0.14	52,56,56,57	0
8	CA	B	1902	1/1	0.99	0.04	48,48,48,48	0
8	CA	D	1202	1/1	0.99	0.06	42,42,42,42	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 W9S A 1001:**

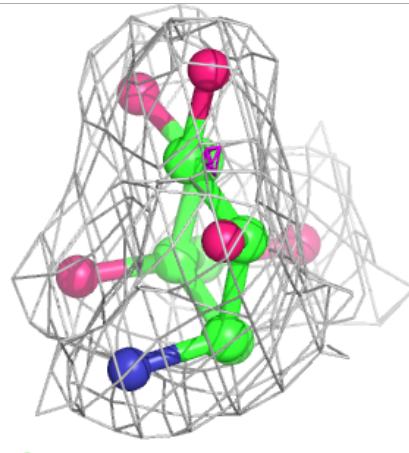
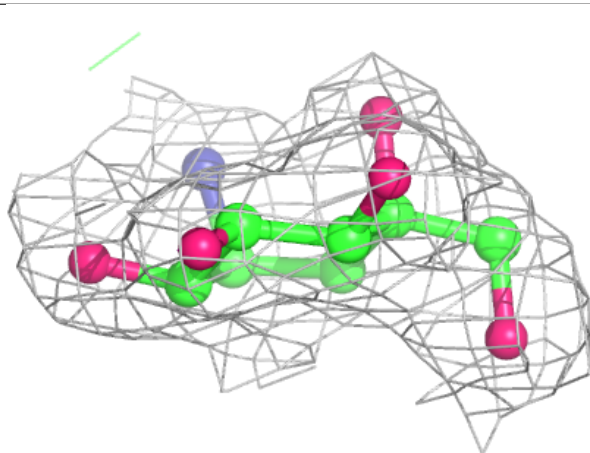
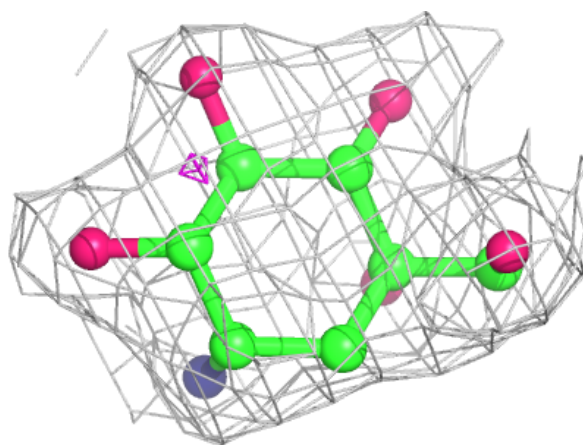
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





**Electron density around W9S C 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.