



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 10, 2026 – 08:53 AM UTC

PDB ID : 7K9Q / pdb_00007k9q
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 wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at 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>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

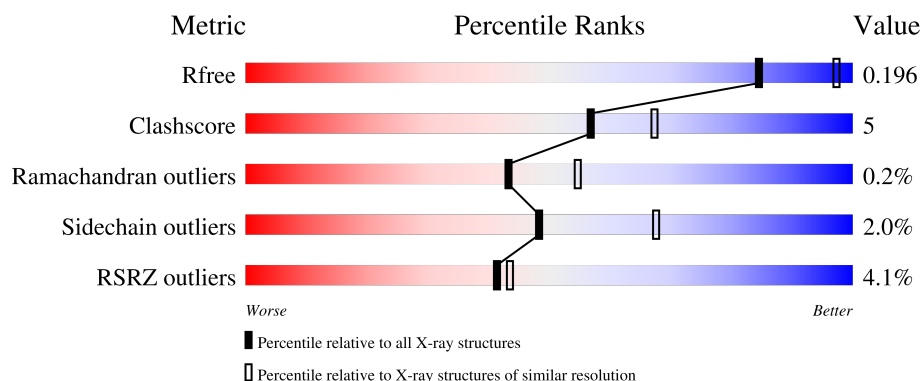
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

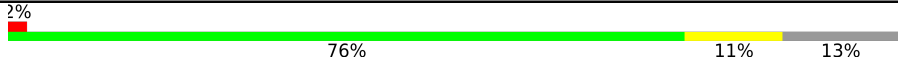
The reported resolution of this entry is 2.30 Å.

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}	180053	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (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 ≥ 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	
1	C	977	
2	B	547	
2	D	547	

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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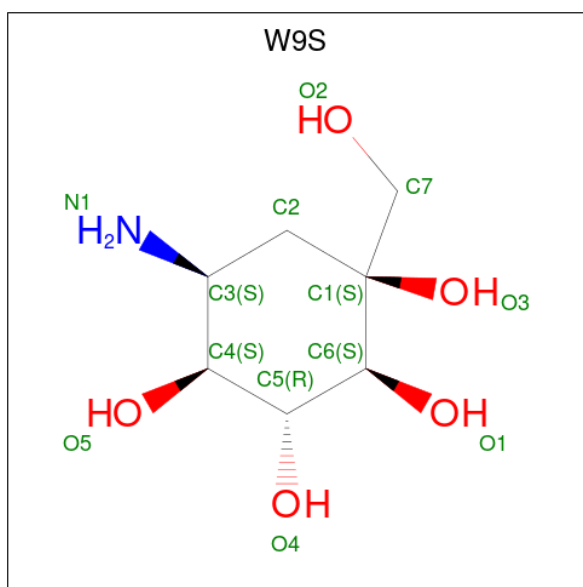
Chain	Residue	Modelled	Actual	Comment	Reference
B	-7	PRO	-	expression tag	UNP O08795
B	-6	ALA	-	expression tag	UNP O08795
B	-5	LEU	-	expression tag	UNP O08795
B	-4	LEU	-	expression tag	UNP O08795
B	-3	SER	-	expression tag	UNP O08795
B	-2	LEU	-	expression tag	UNP O08795
B	-1	VAL	-	expression tag	UNP O08795
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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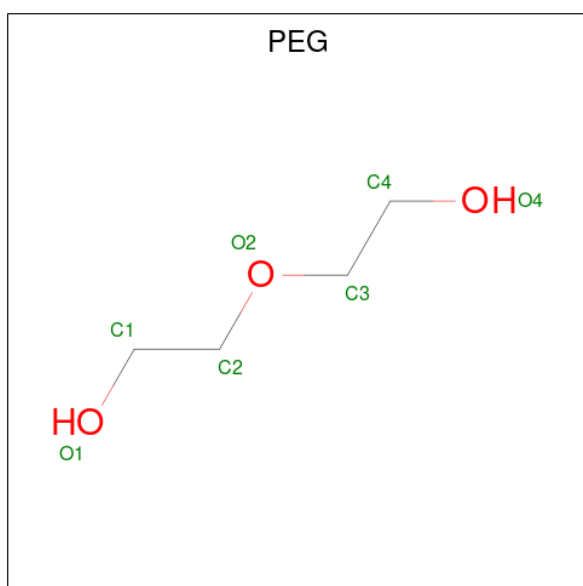
Chain	Residue	Modelled	Actual	Comment	Reference
D	-9	GLY	-	expression tag	UNP O08795
D	-8	MET	-	expression tag	UNP O08795
D	-7	PRO	-	expression tag	UNP O08795
D	-6	ALA	-	expression tag	UNP O08795
D	-5	LEU	-	expression tag	UNP O08795
D	-4	LEU	-	expression tag	UNP O08795
D	-3	SER	-	expression tag	UNP O08795
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 (CCD ID: W9S) (formula: C₇H₁₅NO₅) (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 (CCD ID: PEG) (formula: $C_4H_{10}O_3$).



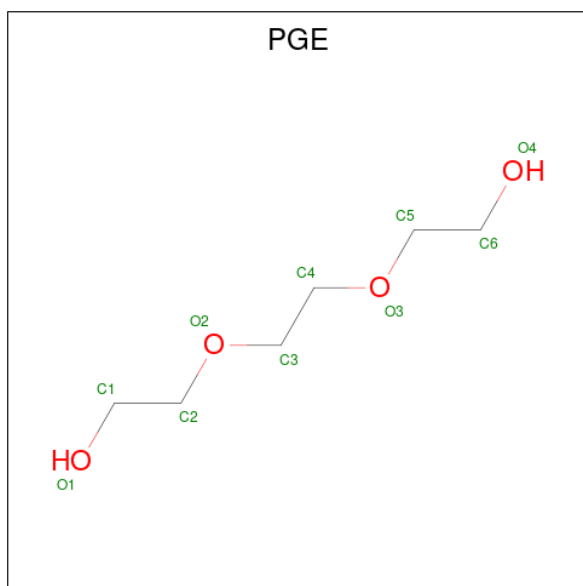
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			7	4	3		
4	A	1	Total	C	O	0	0
			7	4	3		

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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 (CCD ID: PGE) (formula: $C_6H_{14}O_4$).



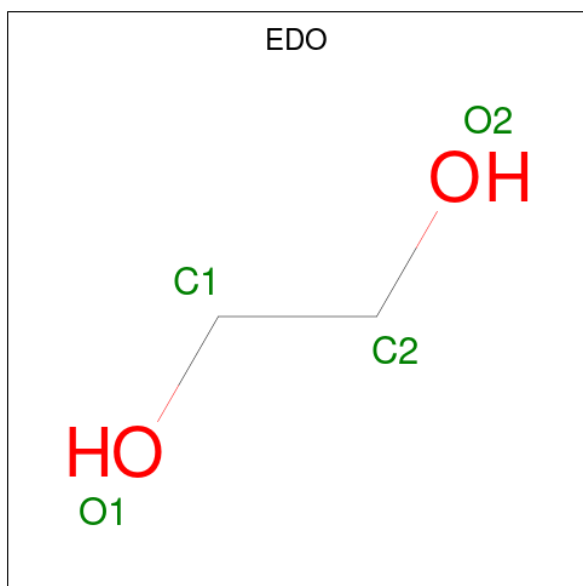
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			10	6	4		
5	A	1	Total	C	O	0	0
			10	6	4		
5	B	1	Total	C	O	0	0
			10	6	4		

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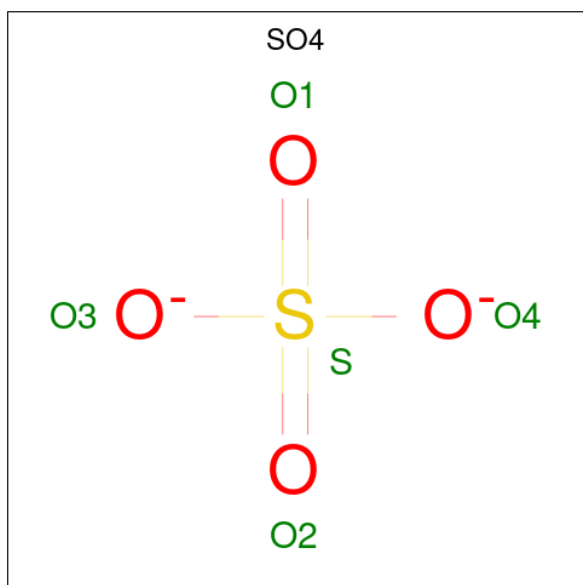
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			4	2	2		
6	A	1	Total	C	O	0	0
			4	2	2		
6	A	1	Total	C	O	0	0
			4	2	2		
6	A	1	Total	C	O	0	0
			4	2	2		
6	A	1	Total	C	O	0	0
			4	2	2		
6	A	1	Total	C	O	0	0
			4	2	2		
6	B	1	Total	C	O	0	0
			4	2	2		
6	B	1	Total	C	O	0	0
			4	2	2		
6	B	1	Total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

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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 (CCD ID: SO4) (formula: O₄S).



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 (CCD ID: CA) (formula: Ca).

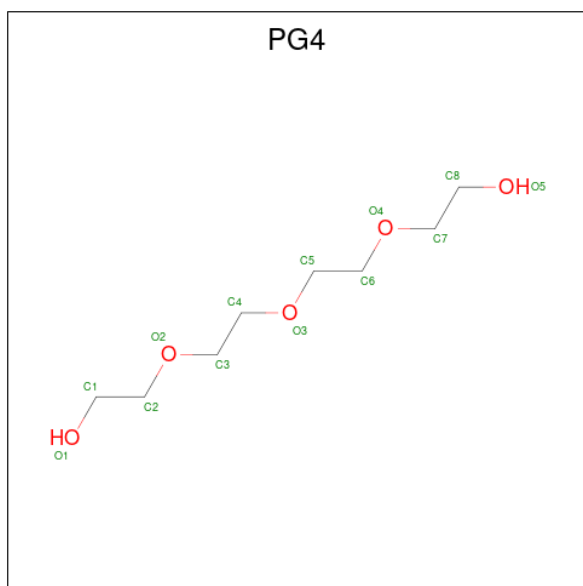
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	B	2	Total	Ca	0	0
			2	2		

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

- Molecule 9 is TETRAETHYLENE GLYCOL (CCD ID: PG4) (formula: $C_8H_{18}O_5$).



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

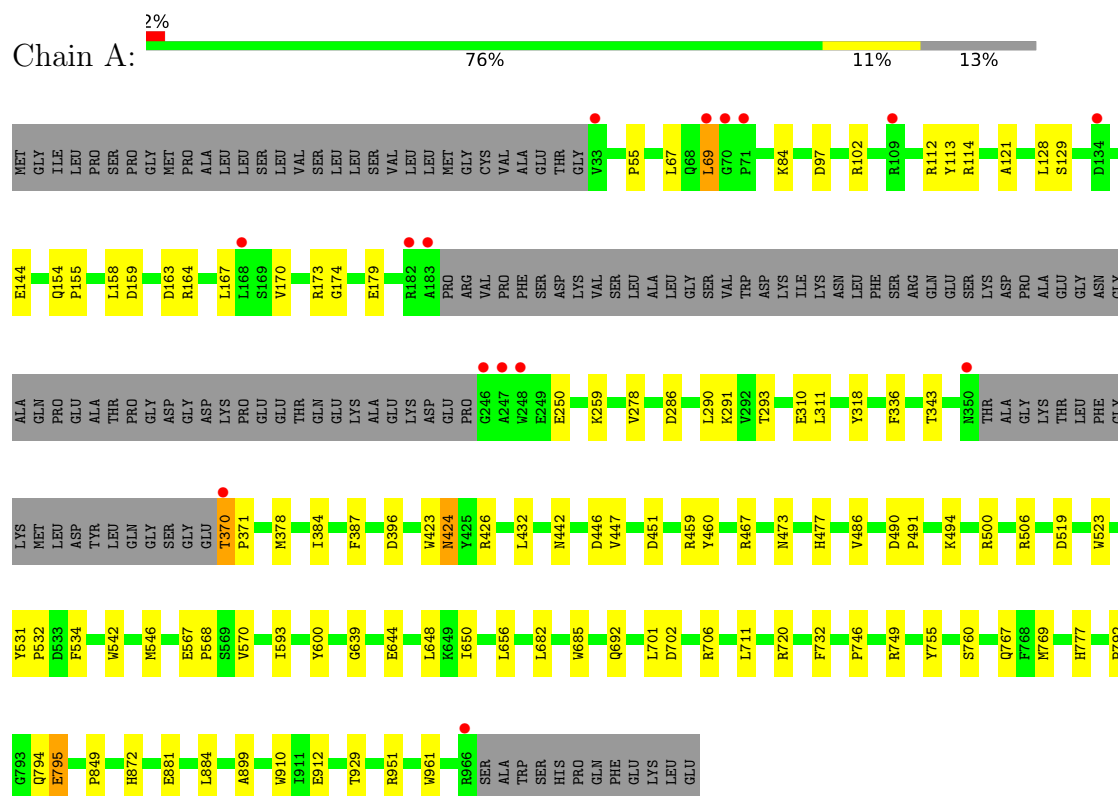
- Molecule 10 is water.

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		

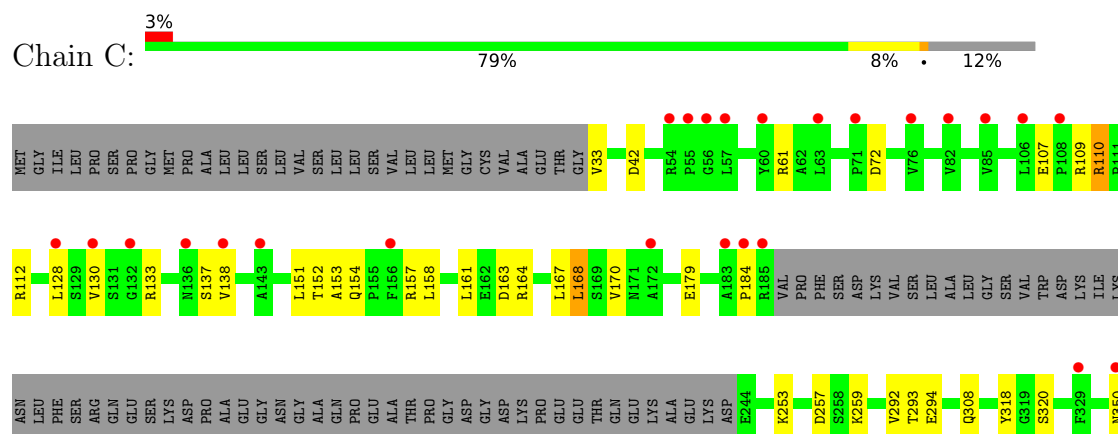
3 Residue-property plots [i](#)

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

- Molecule 1: Alpha glucosidase 2 alpha neutral subunit



- Molecule 1: Alpha glucosidase 2 alpha neutral subunit





ASP	ALA	PHE	LEU	ALA	ALA
GLY	MET	GLY	GLN	ILE	SER
ASP	LYS	PRO	PRO	ARG	SER
SER	TYR	SER	PRO	ASP	PHE
ALA	GLU	GLY	GLN	LYS	GLU
TRP	GLN	GLU	PRO	TYR	LEU
LEU	GLY	PHE	PRO	ARG	LEU
GLU	THR	ALA	SER	SER	ASP
THR	GLY	TYR	PRO	GLU	ASN
LYS	CYS	LEU	THR	VAL	ASP
HIS	TRP	TYR	GLU	PRO	MET
HIS	GLN	SER	ASP	PRO	ASP
HIS	GLY	GLN	GLU	THR	GLY
HIS	PRO	CYS	LYS	ASP	MET
HIS	ASN	TYR	MET	ILE	VAL
HIS	ARG	GLU	PRO	PRO	SER
	SER	LEU	PRO	VAL	LEU
	THR	THR	TYR	PRO	ALA
	THR	THR	ASP	GLU	GLU
	VAL	ASN	GLU	GLU	LEU
	ARG	GLU	THR	THR	GLN
	LEU	TYR	THR	GLU	THR
	LEU	VAL	GLN	PRO	HIS
	CYS	TYR	ALA	LYS	PRO
	GLY	ARG	ILE	GLU	GLU
	LYS	LEU	ILE	GLU	LEU
	GLU	CYS	ASP	LYS	ASP
	THR	PRO	ALA	PRO	THR
	VAL	PHE	ALA	PRO	ASP
	VAL	LYS	GLN	VAL	GLY
	THR	LEU	GLU	LEU	ASP
	SER	LEU	GLU	GLU	GLU
	PRO	PRO	PHE	GLU	GLU
	SER	LYS	THR	GLU	GLU
	ARG	HIS	GLU	GLU	GLU
	GLY	GLY	VAL	GLU	ALA
	GLN	GLY	GLU	GLU	GLN
	TYR	SER	ARG	GLU	ALA
	LEU	PRO	SER	GLU	LEU
	THR	THR	LEU	GLU	THR
	PRO	PRO	GLU	GLU	THR
	ALA	ALA	ILE	GLU	THR
	CYS	TRP	ARG	GLU	THR
	PRO	ALA	SER	GLU	SER
	GLU	GLY	LEU	GLU	PHE
	PRO	PRO	GLU	GLU	THR
	PRO	ASP	GLN	GLU	TYR
	GLU	HIS	ILE	ALA	ASP
	GLU	ASP	ILE	ALA	ARG
	ALA	LYS	GLU	PRO	VAL
	PRO	PHE	PHE	PRO	THR
	SER	SER	ASP	PRO	ALA

4 Data and refinement statistics

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, α , β , γ	102.88Å 102.88Å 241.70Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	42.49 – 2.30 42.49 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.9 (42.49-2.30) 94.6 (42.49-2.30)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.65 (at 2.29Å)	Xtriage
Refinement program	PHENIX 1.18.2_3874	Depositor
R, R_{free}	0.172 , 0.197 0.173 , 0.196	Depositor DCC
R_{free} test set	1995 reflections (1.58%)	wwPDB-VP
Wilson B-factor (Å ²)	36.5	Xtriage
Anisotropy	0.171	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 34.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	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 ²)	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.*

¹Intensities estimated from amplitudes.

²Theoretical 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: PGE, SO4, CA, W9S, PG4, PEG, 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	0.18	0/7118	0.42	0/9694
1	C	0.17	0/7180	0.42	0/9773
2	B	0.23	0/625	0.46	0/856
2	D	0.21	0/653	0.48	0/891
All	All	0.18	0/15576	0.43	0/21214

There are no bond length outliers.

There are no bond angle outliers.

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	68	0
1	C	6941	0	6685	52	0
2	B	614	0	492	3	0
2	D	641	0	539	10	0
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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	16	0
10	B	24	0	0	0	0
10	C	384	0	0	20	0
10	D	35	0	0	4	0
All	All	16268	0	14701	138	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 138 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

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%)	48	60
1	C	860/977 (88%)	833 (97%)	26 (3%)	1 (0%)	48	60
2	B	85/547 (16%)	79 (93%)	5 (6%)	1 (1%)	10	12
2	D	86/547 (16%)	80 (93%)	6 (7%)	0	100	100
All	All	1885/3048 (62%)	1820 (97%)	62 (3%)	3 (0%)	43	55

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 ⓘ

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%)	733 (99%)	10 (1%)	61	77
1	C	751/846 (89%)	733 (98%)	18 (2%)	43	62
2	B	67/478 (14%)	65 (97%)	2 (3%)	36	53
2	D	73/478 (15%)	71 (97%)	2 (3%)	39	58
All	All	1634/2648 (62%)	1602 (98%)	32 (2%)	48	67

5 of 32 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	795	GLU
1	C	877	GLN
1	C	107	GLU
2	B	45	THR
2	D	46	ILE

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

Mol	Chain	Res	Type
1	A	330	HIS
1	A	692	GLN
1	C	77	HIS
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 oligosaccharides 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	$\# Z > 2$
6	EDO	C	1012	-	3,3,3	0.39	0	2,2,2	0.48	0
6	EDO	A	1005	-	3,3,3	0.44	0	2,2,2	0.36	0
6	EDO	A	1022	-	3,3,3	0.45	0	2,2,2	0.35	0
4	PEG	A	1014	-	6,6,6	0.49	0	5,5,5	0.44	0
7	SO4	C	1016	-	4,4,4	0.24	0	6,6,6	0.08	0
6	EDO	C	1004	-	3,3,3	0.45	0	2,2,2	0.32	0
7	SO4	A	1031	-	4,4,4	0.25	0	6,6,6	0.21	0
6	EDO	C	1009	-	3,3,3	0.44	0	2,2,2	0.35	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	EDO	A	1006	-	3,3,3	0.39	0	2,2,2	0.52	0
6	EDO	A	1019	-	3,3,3	0.42	0	2,2,2	0.50	0
6	EDO	A	1013	-	3,3,3	0.45	0	2,2,2	0.32	0
5	PGE	C	1003	-	9,9,9	0.35	0	8,8,8	0.30	0
6	EDO	C	1013	-	3,3,3	0.38	0	2,2,2	0.64	0
5	PGE	B	1904	-	9,9,9	0.33	0	8,8,8	0.32	0
4	PEG	C	1011	-	6,6,6	0.49	0	5,5,5	0.26	0
6	EDO	A	1008	-	3,3,3	0.38	0	2,2,2	0.60	0
6	EDO	A	1020	-	3,3,3	0.47	0	2,2,2	0.32	0
6	EDO	C	1005	-	3,3,3	0.42	0	2,2,2	0.45	0
6	EDO	C	1014	-	3,3,3	0.42	0	2,2,2	0.48	0
6	EDO	A	1004	-	3,3,3	0.38	0	2,2,2	0.45	0
4	PEG	A	1011	-	6,6,6	0.53	0	5,5,5	0.28	0
6	EDO	A	1016	-	3,3,3	0.42	0	2,2,2	0.35	0
7	SO4	C	1017	-	4,4,4	0.26	0	6,6,6	0.04	0
4	PEG	A	1007	-	6,6,6	0.49	0	5,5,5	0.35	0
6	EDO	A	1021	-	3,3,3	0.48	0	2,2,2	0.32	0
4	PEG	D	1201	-	6,6,6	0.49	0	5,5,5	0.38	0
6	EDO	A	1018	-	3,3,3	0.44	0	2,2,2	0.45	0
6	EDO	C	1007	-	3,3,3	0.46	0	2,2,2	0.33	0
7	SO4	A	1030	-	4,4,4	0.27	0	6,6,6	0.15	0
3	W9S	A	1001	-	13,13,13	0.80	1 (7%)	17,20,20	0.92	1 (5%)
6	EDO	B	1905	-	3,3,3	0.42	0	2,2,2	0.43	0
6	EDO	C	1006	-	3,3,3	0.51	0	2,2,2	0.21	0
6	EDO	A	1026	-	3,3,3	0.40	0	2,2,2	0.43	0
4	PEG	A	1002	-	6,6,6	0.48	0	5,5,5	0.35	0
6	EDO	D	1205	-	3,3,3	0.45	0	2,2,2	0.34	0
7	SO4	A	1028	-	4,4,4	0.25	0	6,6,6	0.10	0
6	EDO	B	1907	-	3,3,3	0.44	0	2,2,2	0.39	0
7	SO4	A	1029	-	4,4,4	0.27	0	6,6,6	0.14	0
6	EDO	A	1027	-	3,3,3	0.47	0	2,2,2	0.32	0
4	PEG	C	1010	-	6,6,6	0.49	0	5,5,5	0.25	0
6	EDO	C	1015	-	3,3,3	0.41	0	2,2,2	0.31	0
6	EDO	B	1906	-	3,3,3	0.40	0	2,2,2	0.48	0
6	EDO	B	1901	-	3,3,3	0.46	0	2,2,2	0.38	0
6	EDO	C	1002	-	3,3,3	0.40	0	2,2,2	0.49	0
3	W9S	C	1001	-	13,13,13	0.78	0	17,20,20	0.93	1 (5%)
5	PGE	A	1009	-	9,9,9	0.34	0	8,8,8	0.28	0
6	EDO	A	1015	-	3,3,3	0.43	0	2,2,2	0.44	0
6	EDO	A	1017	-	3,3,3	0.46	0	2,2,2	0.46	0
6	EDO	A	1023	-	3,3,3	0.45	0	2,2,2	0.47	0
6	EDO	A	1024	-	3,3,3	0.42	0	2,2,2	0.48	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
9	PG4	D	1204	-	12,12,12	0.54	0	11,11,11	0.35	0
5	PGE	A	1003	-	9,9,9	0.32	0	8,8,8	0.28	0
4	PEG	C	1008	-	6,6,6	0.51	0	5,5,5	0.27	0
6	EDO	A	1010	-	3,3,3	0.44	0	2,2,2	0.36	0
4	PEG	A	1012	-	6,6,6	0.49	0	5,5,5	0.27	0
4	PEG	A	1025	-	6,6,6	0.54	0	5,5,5	0.40	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
6	EDO	C	1012	-	-	1/1/1/1	-
6	EDO	A	1005	-	-	0/1/1/1	-
6	EDO	A	1022	-	-	0/1/1/1	-
4	PEG	A	1014	-	-	2/4/4/4	-
6	EDO	C	1004	-	-	1/1/1/1	-
6	EDO	C	1009	-	-	0/1/1/1	-
6	EDO	A	1006	-	-	1/1/1/1	-
6	EDO	A	1019	-	-	1/1/1/1	-
6	EDO	A	1013	-	-	1/1/1/1	-
5	PGE	C	1003	-	-	5/7/7/7	-
6	EDO	C	1013	-	-	0/1/1/1	-
5	PGE	B	1904	-	-	5/7/7/7	-
4	PEG	C	1011	-	-	3/4/4/4	-
6	EDO	A	1008	-	-	0/1/1/1	-
6	EDO	A	1020	-	-	0/1/1/1	-
6	EDO	C	1005	-	-	0/1/1/1	-
6	EDO	C	1014	-	-	1/1/1/1	-
6	EDO	A	1004	-	-	1/1/1/1	-
4	PEG	A	1011	-	-	2/4/4/4	-
6	EDO	A	1016	-	-	1/1/1/1	-
4	PEG	A	1007	-	-	2/4/4/4	-
6	EDO	A	1021	-	-	0/1/1/1	-
4	PEG	D	1201	-	-	3/4/4/4	-
6	EDO	A	1018	-	-	0/1/1/1	-
6	EDO	C	1007	-	-	0/1/1/1	-
3	W9S	A	1001	-	-	2/3/26/26	0/1/1/1
6	EDO	B	1905	-	-	0/1/1/1	-
6	EDO	C	1006	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	EDO	A	1026	-	-	1/1/1/1	-
4	PEG	A	1002	-	-	4/4/4/4	-
6	EDO	D	1205	-	-	0/1/1/1	-
6	EDO	B	1907	-	-	0/1/1/1	-
6	EDO	A	1027	-	-	0/1/1/1	-
4	PEG	C	1010	-	-	3/4/4/4	-
6	EDO	C	1015	-	-	0/1/1/1	-
6	EDO	B	1906	-	-	0/1/1/1	-
6	EDO	B	1901	-	-	1/1/1/1	-
6	EDO	C	1002	-	-	0/1/1/1	-
3	W9S	C	1001	-	-	0/3/26/26	0/1/1/1
5	PGE	A	1009	-	-	6/7/7/7	-
6	EDO	A	1015	-	-	1/1/1/1	-
6	EDO	A	1017	-	-	0/1/1/1	-
6	EDO	A	1023	-	-	0/1/1/1	-
6	EDO	A	1024	-	-	1/1/1/1	-
9	PG4	D	1204	-	-	6/10/10/10	-
5	PGE	A	1003	-	-	1/7/7/7	-
4	PEG	C	1008	-	-	2/4/4/4	-
6	EDO	A	1010	-	-	1/1/1/1	-
4	PEG	A	1012	-	-	4/4/4/4	-
4	PEG	A	1025	-	-	2/4/4/4	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1001	W9S	O3-C1	-2.05	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	2.72	114.55	110.58
3	A	1001	W9S	C2-C3-C4	2.44	114.15	110.58

There are no chirality outliers.

5 of 66 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	C	1003	PGE	O1-C1-C2-O2
5	C	1003	PGE	O2-C3-C4-O3

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Mol	Chain	Res	Type	Atoms
4	A	1025	PEG	O1-C1-C2-O2
4	C	1010	PEG	O1-C1-C2-O2
4	C	1010	PEG	O2-C3-C4-O4

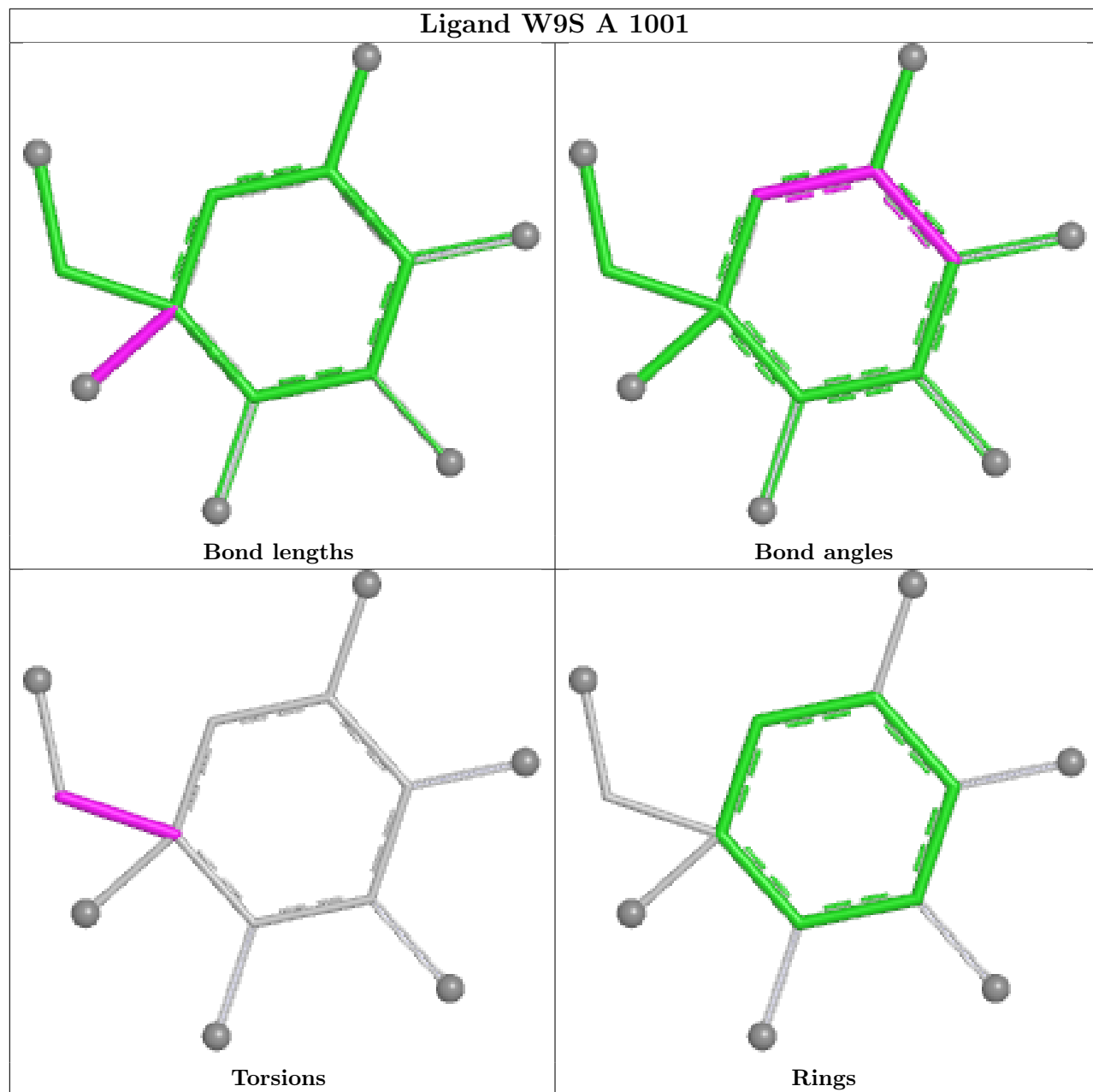
There are no ring outliers.

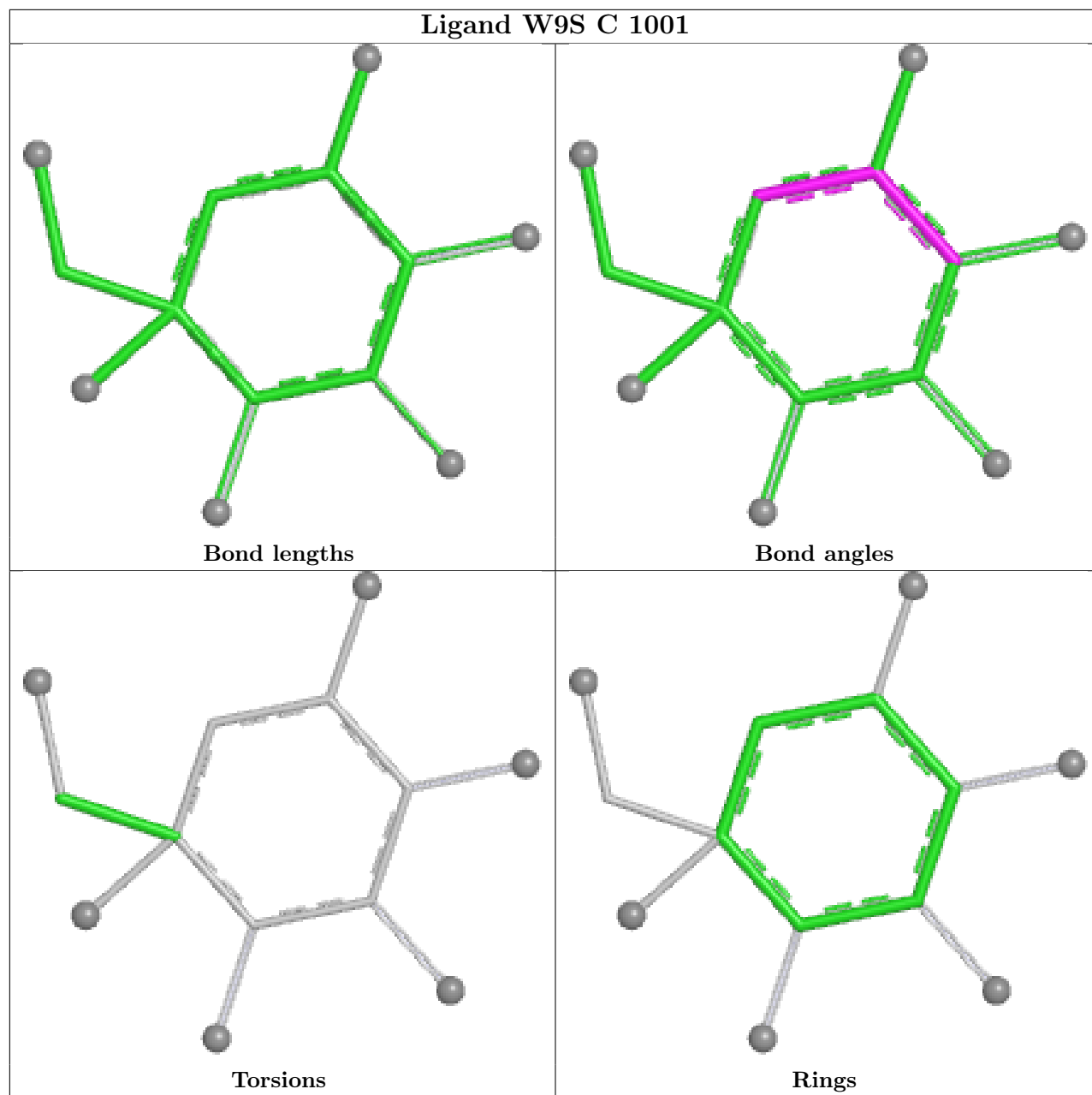
22 monomers are involved in 30 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	1005	EDO	1	0
6	A	1022	EDO	2	0
4	A	1014	PEG	1	0
6	C	1004	EDO	1	0
7	A	1031	SO4	3	0
6	C	1009	EDO	1	0
5	C	1003	PGE	3	0
6	C	1013	EDO	2	0
6	A	1008	EDO	1	0
4	A	1011	PEG	1	0
6	A	1021	EDO	1	0
4	A	1002	PEG	1	0
7	A	1028	SO4	1	0
4	C	1010	PEG	1	0
6	C	1015	EDO	1	0
6	B	1906	EDO	1	0
5	A	1009	PGE	1	0
6	A	1017	EDO	1	0
6	A	1023	EDO	1	0
9	D	1204	PG4	2	0
5	A	1003	PGE	1	0
4	A	1025	PEG	2	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, 95th 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 ²)	Q<0.9
1	A	853/977 (87%)	-0.20	15 (1%) 67 69	20, 38, 61, 80	7 (0%)
1	C	857/977 (87%)	0.07	30 (3%) 47 49	20, 43, 77, 100	9 (1%)
2	B	87/547 (15%)	0.62	13 (14%) 5 6	33, 54, 87, 95	0
2	D	88/547 (16%)	0.82	20 (22%) 2 2	35, 55, 93, 100	0
All	All	1885/3048 (61%)	0.01	78 (4%) 41 43	20, 42, 75, 100	16 (0%)

The worst 5 of 78 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	43	THR	5.2
1	A	247	ALA	4.3
2	D	48	PHE	4.1
2	B	32	GLU	4.1
2	D	44	ALA	4.0

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 oligosaccharides 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, 95th 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
7	SO4	A	1029	5/5	0.69	0.19	73,79,86,92	0
4	PEG	D	1201	7/7	0.70	0.21	54,63,65,65	0
6	EDO	C	1009	4/4	0.75	0.19	57,62,62,67	0
6	EDO	A	1024	4/4	0.75	0.20	64,67,68,70	0
7	SO4	A	1028	5/5	0.76	0.17	61,75,87,91	0
6	EDO	A	1015	4/4	0.76	0.18	63,65,66,66	0
5	PGE	C	1003	10/10	0.77	0.19	60,67,70,78	0
4	PEG	A	1025	7/7	0.80	0.16	50,53,57,59	0
5	PGE	A	1009	10/10	0.81	0.19	50,59,64,68	0
6	EDO	C	1014	4/4	0.81	0.17	55,59,63,72	0
4	PEG	A	1007	7/7	0.81	0.15	58,62,67,68	0
6	EDO	B	1907	4/4	0.81	0.15	53,58,60,61	0
6	EDO	B	1901	4/4	0.82	0.16	49,52,56,56	0
6	EDO	A	1017	4/4	0.83	0.21	44,48,52,54	0
5	PGE	B	1904	10/10	0.83	0.18	53,66,71,74	0
7	SO4	A	1030	5/5	0.83	0.12	63,69,79,98	0
6	EDO	C	1005	4/4	0.84	0.17	47,51,52,55	0
6	EDO	A	1020	4/4	0.84	0.15	54,59,61,62	0
4	PEG	A	1011	7/7	0.84	0.14	48,58,59,68	0
9	PG4	D	1204	13/13	0.84	0.17	54,59,69,71	0
7	SO4	A	1031	5/5	0.85	0.38	49,56,68,85	0
6	EDO	B	1905	4/4	0.85	0.15	60,65,66,70	0
6	EDO	A	1013	4/4	0.86	0.16	54,58,62,64	0
4	PEG	C	1010	7/7	0.86	0.14	49,58,65,67	0
4	PEG	A	1014	7/7	0.87	0.15	56,57,64,67	0
6	EDO	C	1004	4/4	0.88	0.16	51,52,57,64	0
4	PEG	C	1008	7/7	0.88	0.16	47,50,53,55	0
6	EDO	C	1006	4/4	0.88	0.18	43,49,51,52	0
6	EDO	B	1906	4/4	0.88	0.13	48,50,52,60	0
7	SO4	C	1016	5/5	0.88	0.21	65,66,70,91	0
7	SO4	C	1017	5/5	0.88	0.08	69,74,83,92	0
4	PEG	A	1012	7/7	0.88	0.16	47,59,64,69	0
6	EDO	A	1010	4/4	0.89	0.12	61,62,64,65	0
4	PEG	A	1002	7/7	0.89	0.12	53,55,62,63	0
6	EDO	A	1022	4/4	0.89	0.12	48,54,55,60	0
4	PEG	C	1011	7/7	0.89	0.12	58,61,65,66	0
5	PGE	A	1003	10/10	0.90	0.12	49,57,60,64	0
6	EDO	A	1005	4/4	0.90	0.12	50,53,53,61	0
6	EDO	C	1007	4/4	0.90	0.16	52,56,59,59	0
6	EDO	C	1012	4/4	0.91	0.14	45,46,51,51	0
6	EDO	A	1006	4/4	0.91	0.12	45,48,52,64	0
6	EDO	A	1018	4/4	0.91	0.17	48,51,55,57	0
6	EDO	A	1004	4/4	0.92	0.15	44,47,47,54	0

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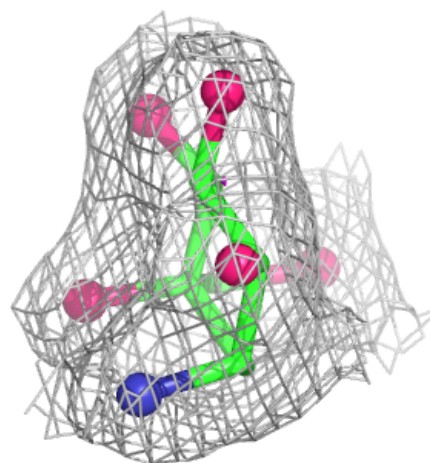
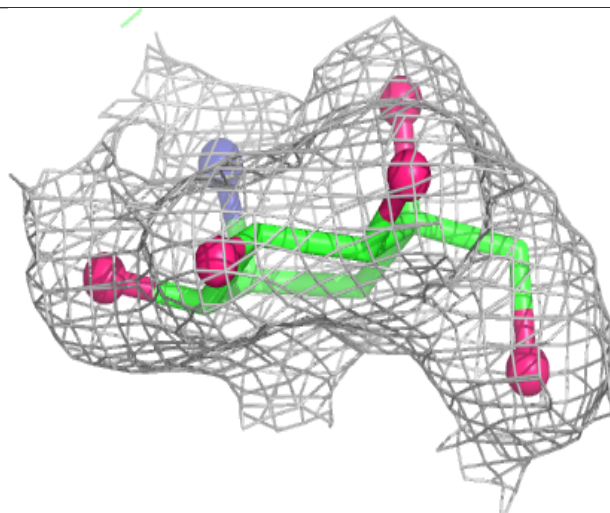
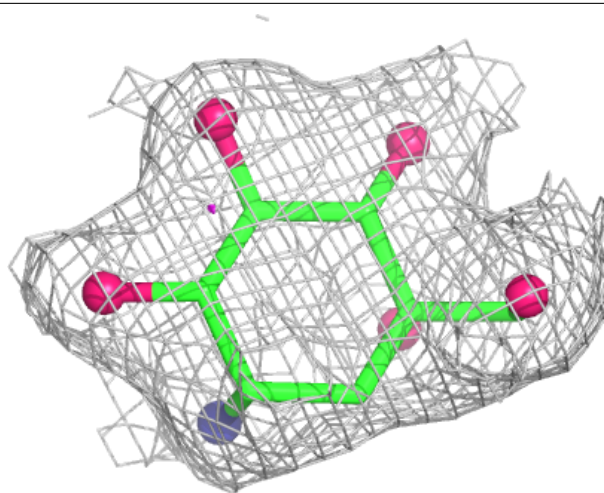
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	EDO	A	1019	4/4	0.93	0.10	51,53,55,56	0
6	EDO	C	1002	4/4	0.93	0.11	40,44,50,55	0
6	EDO	A	1021	4/4	0.93	0.14	44,45,46,49	0
6	EDO	A	1026	4/4	0.93	0.11	49,52,54,64	0
6	EDO	A	1008	4/4	0.94	0.14	42,42,47,49	0
6	EDO	C	1013	4/4	0.94	0.11	41,41,47,55	0
6	EDO	D	1205	4/4	0.95	0.09	52,56,56,57	0
6	EDO	A	1027	4/4	0.95	0.16	39,45,52,53	0
6	EDO	A	1016	4/4	0.95	0.09	40,41,46,48	0
6	EDO	C	1015	4/4	0.95	0.10	57,57,57,61	0
3	W9S	C	1001	13/13	0.96	0.06	29,34,38,38	0
3	W9S	A	1001	13/13	0.96	0.06	28,33,38,44	0
6	EDO	A	1023	4/4	0.97	0.06	41,41,44,54	0
8	CA	B	1903	1/1	0.99	0.02	38,38,38,38	0
8	CA	D	1202	1/1	0.99	0.03	42,42,42,42	0
8	CA	D	1203	1/1	0.99	0.03	40,40,40,40	0
8	CA	B	1902	1/1	0.99	0.03	48,48,48,48	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.

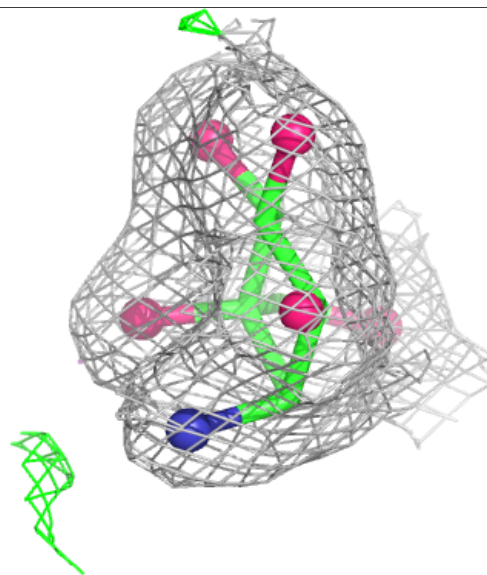
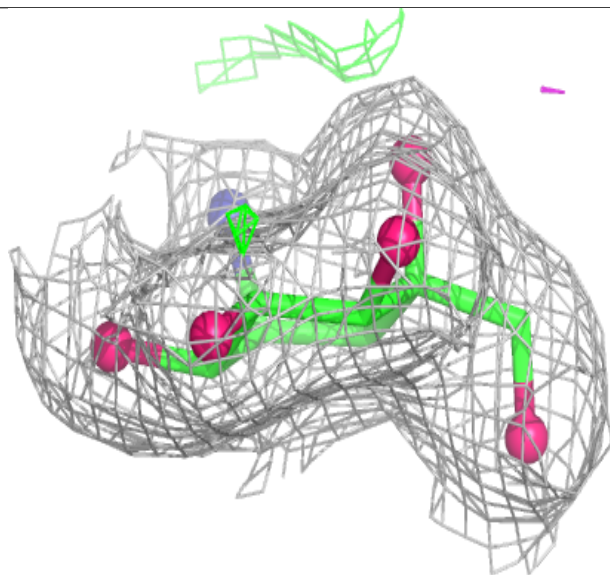
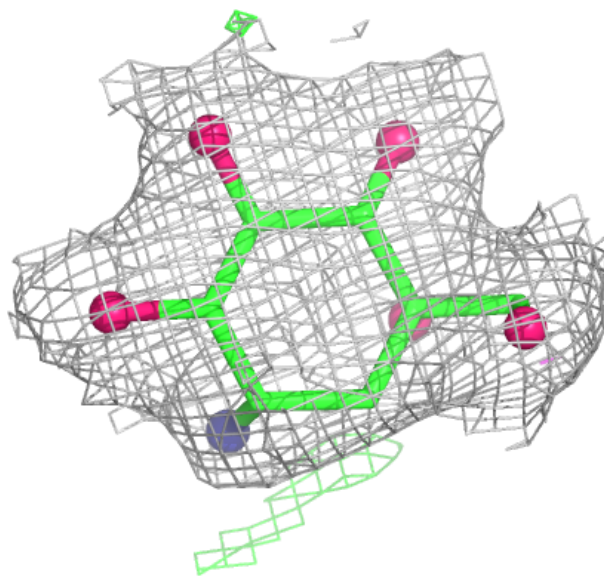
Electron density around W9S C 1001:

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



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)



6.5 Other polymers [i](#)

There are no such residues in this entry.