



wwPDB X-ray Structure Validation Summary Report ⓘ

Sep 27, 2021 – 02:14 PM EDT

PDB ID : 7KB6
Title : Co-crystal structure of alpha glucosidase with compound 7
Authors : Karade, S.S.; Mariuzza, R.A.
Deposited on : 2020-10-01
Resolution : 2.20 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 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

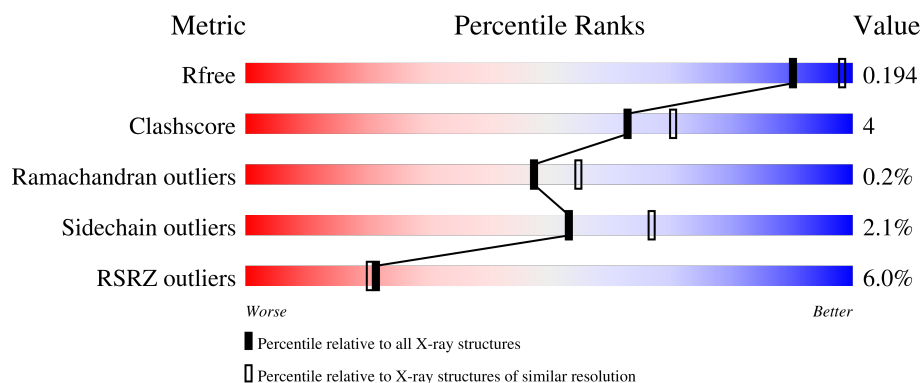
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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	<div> <div>2%</div> <div>78%</div> <div>9%</div> <div>13%</div> </div>
1	C	977	<div> <div>6%</div> <div>78%</div> <div>9%</div> <div>12%</div> </div>
2	B	554	<div> <div>3%</div> <div>14%</div> <div>85%</div> </div>
2	D	554	<div> <div>3%</div> <div>14%</div> <div>85%</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
4	EDO	A	1222	-	-	X	-
7	SO4	A	1240	-	-	-	X
7	SO4	C	1234	-	-	-	X
7	SO4	C	1235	-	-	X	-

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 16287 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	850	Total	C	N	O	S	0	8	0
			6878	4405	1188	1256	29			
1	C	856	Total	C	N	O	S	0	6	0
			6848	4391	1179	1249	29			

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	83	Total	C	N	O	S	0	0	0
			575	338	95	132	10			
2	D	83	Total	C	N	O	S	0	0	0
			591	353	95	133	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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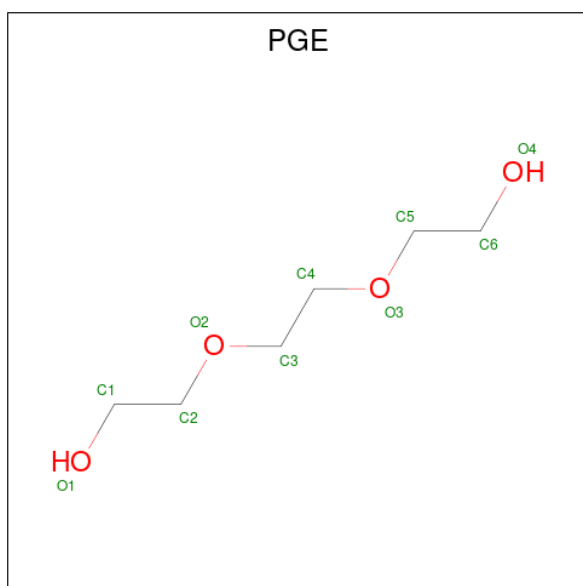
Chain	Residue	Modelled	Actual	Comment	Reference
D	-16	MET	-	initiating methionine	UNP O08795
D	-15	GLY	-	expression tag	UNP O08795
D	-14	ILE	-	expression tag	UNP O08795
D	-13	LEU	-	expression tag	UNP O08795
D	-12	PRO	-	expression tag	UNP O08795
D	-11	SER	-	expression tag	UNP O08795
D	-10	PRO	-	expression 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 TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: $C_6H_{14}O_4$).



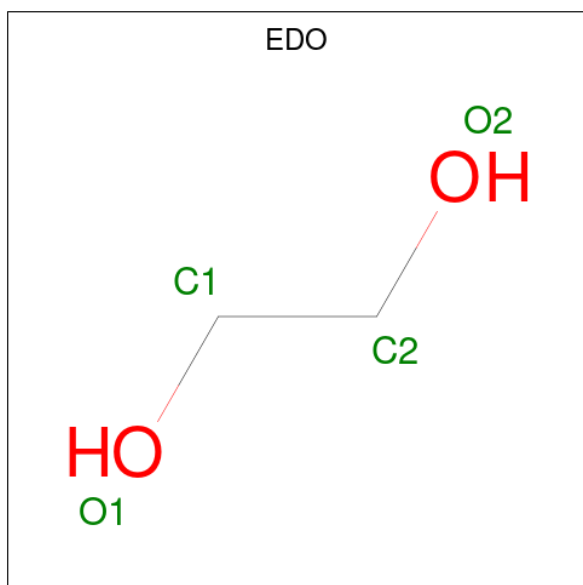
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 10 6 4	0	0
3	A	1	Total C O 10 6 4	0	0
3	A	1	Total C O 10 6 4	0	0
3	A	1	Total C O 10 6 4	0	0
3	A	1	Total C O 10 6 4	0	0
3	C	1	Total C O 10 6 4	0	0
3	C	1	Total C O 10 6 4	0	0

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

- Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



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

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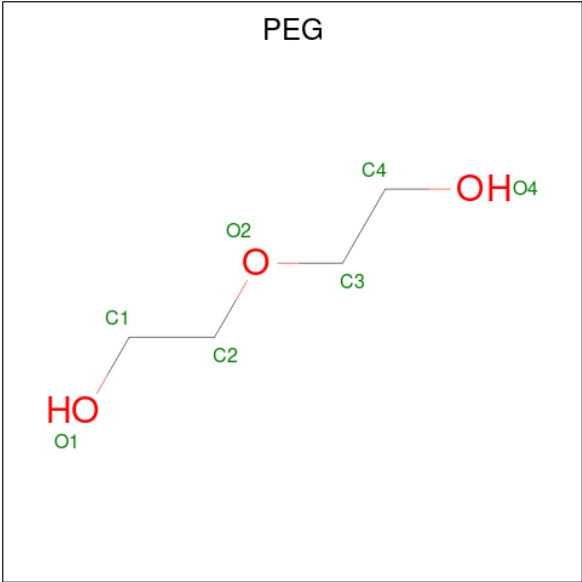
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 4 2 2	0	0
4	A	1	Total C O 4 2 2	0	0
4	A	1	Total C O 4 2 2	0	0
4	A	1	Total C O 4 2 2	0	0
4	A	1	Total C O 4 2 2	0	0
4	A	1	Total C O 4 2 2	0	0
4	A	1	Total C O 4 2 2	0	0
4	A	1	Total C O 4 2 2	0	0
4	A	1	Total C O 4 2 2	0	0
4	A	1	Total C O 4 2 2	0	0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

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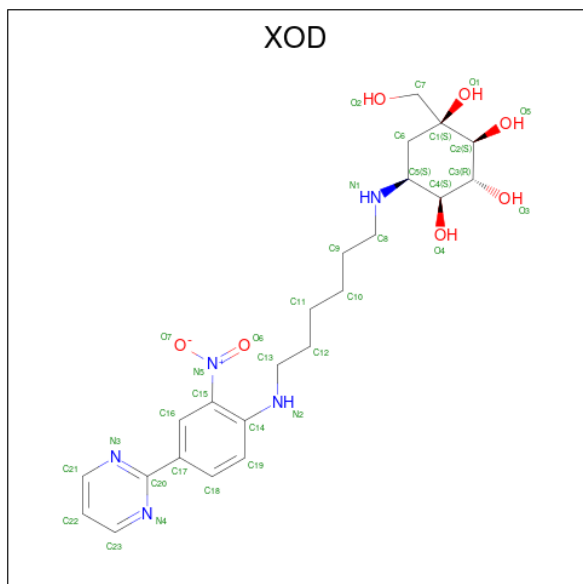
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	C	1	Total C O 4 2 2	0	0
4	C	1	Total C O 4 2 2	0	0
4	C	1	Total C O 4 2 2	0	0
4	C	1	Total C O 4 2 2	0	0
4	C	1	Total C O 4 2 2	0	0
4	C	1	Total C O 4 2 2	0	0
4	C	1	Total C O 4 2 2	0	0
4	C	1	Total C O 4 2 2	0	0
4	C	1	Total C O 4 2 2	0	0
4	C	1	Total C O 4 2 2	0	0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

- Molecule 5 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: C₄H₁₀O₃).



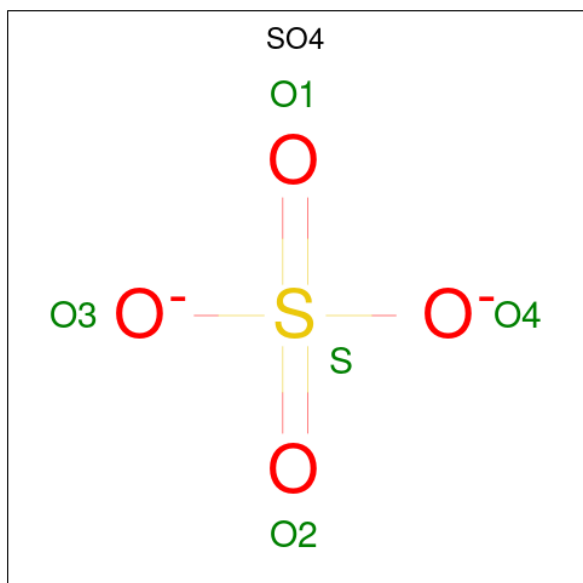
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			7	4	3		
5	A	1	Total	C	O	0	0
			7	4	3		
5	A	1	Total	C	O	0	0
			7	4	3		
5	A	1	Total	C	O	0	0
			7	4	3		
5	A	1	Total	C	O	0	0
			7	4	3		
5	A	1	Total	C	O	0	0
			7	4	3		
5	B	1	Total	C	O	0	0
			7	4	3		
5	C	1	Total	C	O	0	0
			7	4	3		
5	C	1	Total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

- Molecule 6 is (1S,2S,3R,4S,5S)-1-(hydroxymethyl)-5-[(6-{[2-nitro-4-(pyrimidin-2-yl)phenyl]amino}hexyl)amino]cyclohexane-1,2,3,4-tetrol (three-letter code: XOD) (formula: $C_{23}H_{33}N_5O_7$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	N	O	0	0
			35	23	5	7		
6	C	1	Total	C	N	O	0	0
			35	23	5	7		

- Molecule 7 is SULFATE ION (three-letter code: SO4) (formula: O_4S).

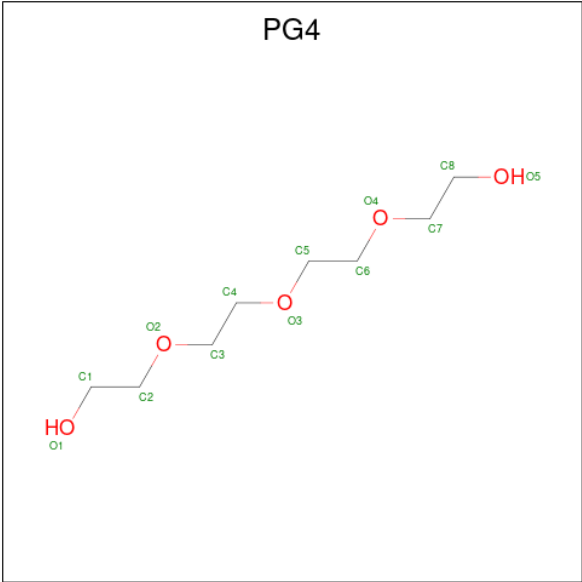


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total O S 5 4 1	0	0
7	A	1	Total O S 5 4 1	0	0
7	A	1	Total O S 5 4 1	0	0
7	A	1	Total O S 5 4 1	0	0
7	B	1	Total O S 5 4 1	0	0
7	C	1	Total O S 5 4 1	0	0
7	C	1	Total O S 5 4 1	0	0
7	C	1	Total O S 5 4 1	0	0
7	C	1	Total O S 5 4 1	0	0
7	C	1	Total O S 5 4 1	0	0

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

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

- Molecule 9 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: C₈H₁₈O₅).



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

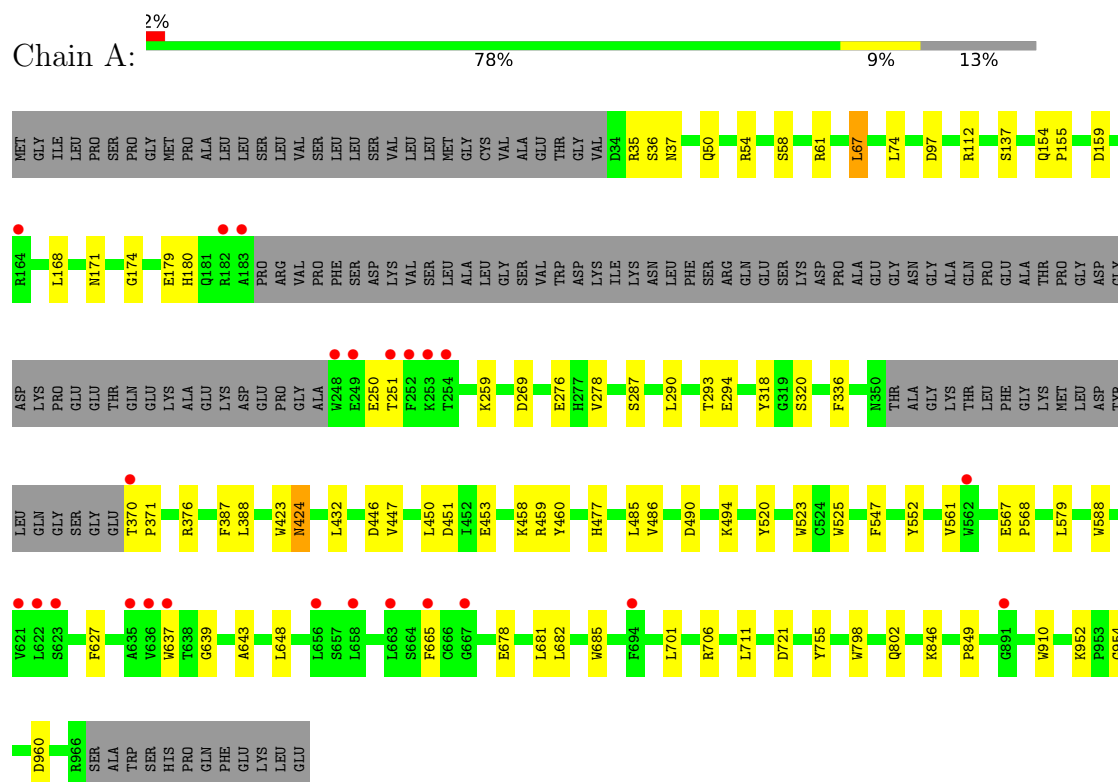
- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	438	Total	O	0	0
			438	438		
10	B	28	Total	O	0	0
			28	28		
10	C	379	Total	O	0	0
			379	379		
10	D	32	Total	O	0	0
			32	32		

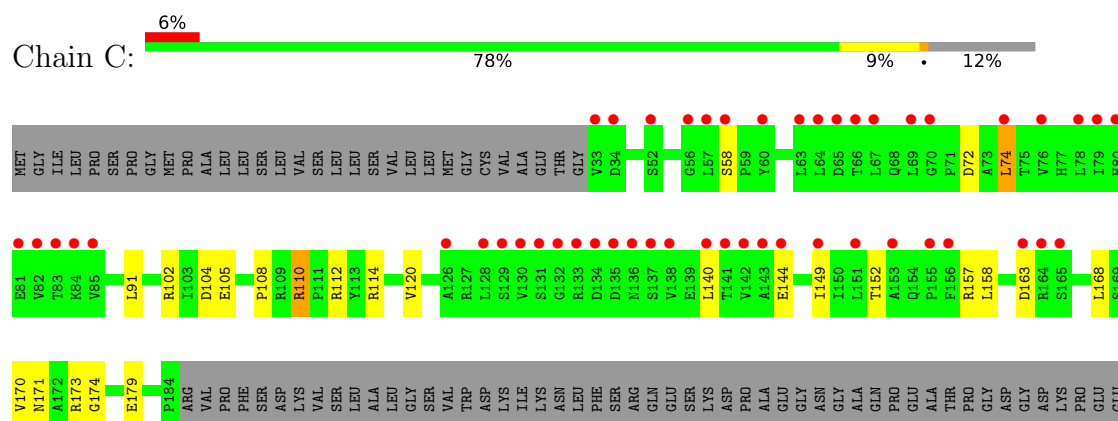
3 Residue-property plots [i](#)

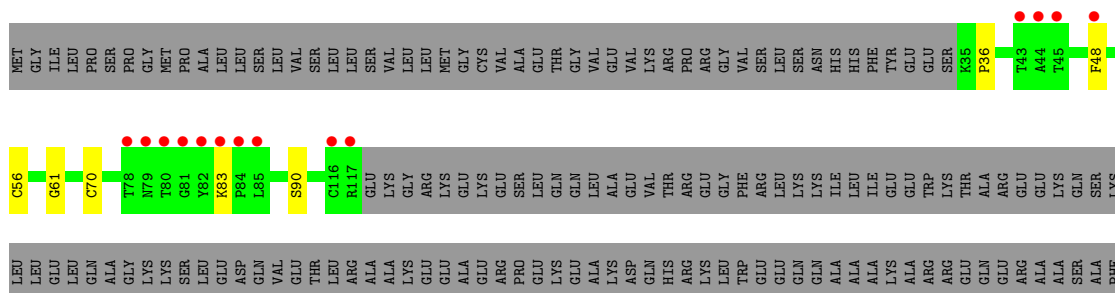
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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



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





[illegible]

4 Data and refinement statistics

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, α , β , γ	102.91Å 102.91Å 239.83Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	44.56 – 2.20 44.56 – 2.20	Depositor EDS
% Data completeness (in resolution range)	97.5 (44.56-2.20) 92.0 (44.56-2.20)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.01 (at 2.20Å)	Xtriage
Refinement program	PHENIX 1.18.2_3874	Depositor
R, R_{free}	0.167 , 0.194 0.167 , 0.194	Depositor DCC
R_{free} test set	1958 reflections (1.39%)	wwPDB-VP
Wilson B-factor (Å ²)	33.1	Xtriage
Anisotropy	0.300	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 45.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.009 for -h,-k,l 0.037 for h,-h-k,-l 0.022 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	16287	wwPDB-VP
Average B, all atoms (Å ²)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.51% 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: PG4, PGE, CA, XOD, PEG, SO4, 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	0.27	0/7095	0.48	0/9663
1	C	0.27	0/7069	0.47	0/9636
2	B	0.25	0/585	0.53	0/803
2	D	0.28	0/603	0.51	0/826
All	All	0.27	0/15352	0.48	0/20928

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	6878	0	6592	52	0
1	C	6848	0	6532	62	0
2	B	575	0	457	4	0
2	D	591	0	474	3	0
3	A	50	0	70	3	0
3	C	30	0	42	1	0
3	D	10	0	14	0	0
4	A	96	0	140	12	0
4	B	4	0	6	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	C	76	0	113	13	0
4	D	4	0	6	0	0
5	A	49	0	70	6	0
5	B	7	0	10	0	0
5	C	42	0	60	6	0
6	A	35	0	0	1	0
6	C	35	0	0	0	0
7	A	20	0	0	0	0
7	B	5	0	0	0	0
7	C	25	0	0	2	0
8	B	2	0	0	0	0
8	D	2	0	0	0	0
9	B	13	0	18	0	0
9	C	13	0	18	2	0
10	A	438	0	0	4	0
10	B	28	0	0	2	0
10	C	379	0	0	18	0
10	D	32	0	0	0	0
All	All	16287	0	14622	129	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

The worst 5 of 129 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:910:TRP:HE1	4:A:1222:EDO:H12	1.25	0.99
1:C:104:ASP:OD2	10:C:1302:HOH:O	1.92	0.88
1:A:180:HIS:O	10:A:1301:HOH:O	1.92	0.84
1:C:407:THR:H	4:C:1209:EDO:H21	1.40	0.84
1:A:97:ASP:OD2	10:A:1302:HOH:O	2.04	0.75

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%)	821 (96%)	30 (4%)	1 (0%)	51	60
1	C	856/977 (88%)	820 (96%)	36 (4%)	0	100	100
2	B	81/554 (15%)	77 (95%)	4 (5%)	0	100	100
2	D	81/554 (15%)	76 (94%)	3 (4%)	2 (2%)	5	3
All	All	1870/3062 (61%)	1794 (96%)	73 (4%)	3 (0%)	47	55

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	36	PRO
2	D	83	LYS
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	741/846 (88%)	728 (98%)	13 (2%)	59	72
1	C	730/846 (86%)	712 (98%)	18 (2%)	47	60
2	B	63/485 (13%)	62 (98%)	1 (2%)	62	76
2	D	65/485 (13%)	64 (98%)	1 (2%)	65	78
All	All	1599/2662 (60%)	1566 (98%)	33 (2%)	53	67

5 of 33 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	706	ARG
1	C	714	GLN
2	D	48	PHE
1	A	706	ARG
1	A	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	964	HIS

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 86 ligands modelled in this entry, 4 are monoatomic - leaving 82 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	EDO	C	1215	-	3,3,3	0.47	0	2,2,2	0.30	0
5	PEG	A	1228	-	6,6,6	0.49	0	5,5,5	0.20	0
4	EDO	A	1233	-	3,3,3	0.49	0	2,2,2	0.33	0
4	EDO	B	605	-	3,3,3	0.47	0	2,2,2	0.32	0
4	EDO	C	1222	-	3,3,3	0.49	0	2,2,2	0.28	0
3	PGE	A	1210	-	9,9,9	0.31	0	8,8,8	0.29	0
4	EDO	A	1226	-	3,3,3	0.51	0	2,2,2	0.21	0
3	PGE	A	1207	-	9,9,9	0.33	0	8,8,8	0.23	0
4	EDO	A	1213	-	3,3,3	0.48	0	2,2,2	0.28	0
4	EDO	A	1231	-	3,3,3	0.43	0	2,2,2	0.47	0
4	EDO	A	1225	-	3,3,3	0.43	0	2,2,2	0.44	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
5	PEG	C	1202	-	6,6,6	0.49	0	5,5,5	0.27	0
9	PG4	C	1230	-	12,12,12	0.52	0	11,11,11	0.23	0
5	PEG	A	1214	-	6,6,6	0.49	0	5,5,5	0.35	0
4	EDO	C	1204	-	3,3,3	0.46	0	2,2,2	0.34	0
4	EDO	C	1213	-	3,3,3	0.48	0	2,2,2	0.34	0
4	EDO	A	1211	-	3,3,3	0.43	0	2,2,2	0.42	0
4	EDO	C	1224	-	3,3,3	0.45	0	2,2,2	0.39	0
7	SO4	C	1234	-	4,4,4	0.14	0	6,6,6	0.05	0
4	EDO	A	1205	-	3,3,3	0.42	0	2,2,2	0.42	0
7	SO4	B	606	-	4,4,4	0.12	0	6,6,6	0.15	0
4	EDO	A	1227	-	3,3,3	0.52	0	2,2,2	0.65	0
4	EDO	A	1229	-	3,3,3	0.46	0	2,2,2	0.34	0
5	PEG	C	1211	-	6,6,6	0.50	0	5,5,5	0.26	0
5	PEG	C	1206	-	6,6,6	0.49	0	5,5,5	0.27	0
7	SO4	C	1233	-	4,4,4	0.15	0	6,6,6	0.08	0
4	EDO	A	1204	-	3,3,3	0.48	0	2,2,2	0.31	0
4	EDO	C	1221	-	3,3,3	0.44	0	2,2,2	0.41	0
5	PEG	C	1217	-	6,6,6	0.50	0	5,5,5	0.25	0
5	PEG	A	1220	-	6,6,6	0.49	0	5,5,5	0.23	0
3	PGE	C	1220	-	9,9,9	0.32	0	8,8,8	0.29	0
4	EDO	A	1219	-	3,3,3	0.44	0	2,2,2	0.42	0
4	EDO	C	1223	-	3,3,3	0.48	0	2,2,2	0.31	0
4	EDO	A	1203	-	3,3,3	0.42	0	2,2,2	0.43	0
4	EDO	A	1224	-	3,3,3	0.46	0	2,2,2	0.36	0
4	EDO	C	1228	-	3,3,3	0.47	0	2,2,2	0.36	0
3	PGE	A	1221	-	9,9,9	0.29	0	8,8,8	0.38	0
5	PEG	A	1208	-	6,6,6	0.49	0	5,5,5	0.30	0
4	EDO	C	1210	-	3,3,3	0.42	0	2,2,2	0.39	0
3	PGE	D	603	-	9,9,9	0.31	0	8,8,8	0.30	0
4	EDO	A	1236	-	3,3,3	0.44	0	2,2,2	0.49	0
6	XOD	A	1237	-	36,37,37	2.04	4 (11%)	44,51,51	1.64	7 (15%)
9	PG4	B	603	-	12,12,12	0.52	0	11,11,11	0.22	0
3	PGE	A	1223	-	9,9,9	0.31	0	8,8,8	0.27	0
7	SO4	C	1235	-	4,4,4	0.14	0	6,6,6	0.07	0
5	PEG	A	1212	-	6,6,6	0.50	0	5,5,5	0.28	0
5	PEG	B	604	-	6,6,6	0.48	0	5,5,5	0.24	0
5	PEG	C	1219	-	6,6,6	0.48	0	5,5,5	0.27	0
4	EDO	C	1207	-	3,3,3	0.46	0	2,2,2	0.27	0
7	SO4	C	1232	-	4,4,4	0.16	0	6,6,6	0.13	0
4	EDO	A	1235	-	3,3,3	0.46	0	2,2,2	0.36	0
4	EDO	D	604	-	3,3,3	0.46	0	2,2,2	0.41	0
7	SO4	A	1239	-	4,4,4	0.15	0	6,6,6	0.06	0
7	SO4	A	1238	-	4,4,4	0.14	0	6,6,6	0.05	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	SO4	C	1231	-	4,4,4	0.13	0	6,6,6	0.11	0
4	EDO	A	1216	-	3,3,3	0.43	0	2,2,2	0.42	0
4	EDO	C	1209	-	3,3,3	0.47	0	2,2,2	0.31	0
7	SO4	A	1241	-	4,4,4	0.14	0	6,6,6	0.06	0
5	PEG	A	1215	-	6,6,6	0.48	0	5,5,5	0.29	0
7	SO4	A	1240	-	4,4,4	0.14	0	6,6,6	0.06	0
3	PGE	C	1205	-	9,9,9	0.31	0	8,8,8	0.35	0
4	EDO	A	1206	-	3,3,3	0.47	0	2,2,2	0.32	0
6	XOD	C	1229	-	36,37,37	2.01	3 (8%)	44,51,51	1.70	10 (22%)
3	PGE	C	1208	-	9,9,9	0.35	0	8,8,8	0.25	0
4	EDO	C	1203	-	3,3,3	0.41	0	2,2,2	0.55	0
4	EDO	A	1234	-	3,3,3	0.44	0	2,2,2	0.41	0
4	EDO	C	1227	-	3,3,3	0.57	0	2,2,2	0.19	0
4	EDO	A	1222	-	3,3,3	0.43	0	2,2,2	0.41	0
4	EDO	C	1225	-	3,3,3	0.43	0	2,2,2	0.51	0
4	EDO	C	1214	-	3,3,3	0.46	0	2,2,2	0.38	0
4	EDO	C	1226	-	3,3,3	0.45	0	2,2,2	0.38	0
4	EDO	C	1218	-	3,3,3	0.48	0	2,2,2	0.30	0
5	PEG	A	1217	-	6,6,6	0.49	0	5,5,5	0.26	0
4	EDO	A	1230	-	3,3,3	0.46	0	2,2,2	0.31	0
4	EDO	A	1218	-	3,3,3	0.47	0	2,2,2	0.33	0
5	PEG	C	1212	-	6,6,6	0.47	0	5,5,5	0.24	0
3	PGE	A	1201	-	9,9,9	0.30	0	8,8,8	0.32	0
4	EDO	A	1209	-	3,3,3	0.47	0	2,2,2	0.23	0
4	EDO	A	1202	-	3,3,3	0.46	0	2,2,2	0.39	0
4	EDO	C	1201	-	3,3,3	0.39	0	2,2,2	0.59	0
4	EDO	C	1216	-	3,3,3	0.48	0	2,2,2	0.33	0
4	EDO	A	1232	-	3,3,3	0.48	0	2,2,2	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
4	EDO	C	1218	-	-	0/1/1/1	-
4	EDO	C	1215	-	-	0/1/1/1	-
5	PEG	A	1228	-	-	1/4/4/4	-
5	PEG	A	1217	-	-	2/4/4/4	-
5	PEG	C	1211	-	-	2/4/4/4	-
5	PEG	C	1206	-	-	2/4/4/4	-
4	EDO	A	1230	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	EDO	A	1233	-	-	1/1/1/1	-
4	EDO	B	605	-	-	0/1/1/1	-
4	EDO	C	1222	-	-	0/1/1/1	-
3	PGE	A	1210	-	-	0/7/7/7	-
4	EDO	A	1226	-	-	0/1/1/1	-
4	EDO	A	1218	-	-	0/1/1/1	-
4	EDO	A	1204	-	-	0/1/1/1	-
3	PGE	A	1207	-	-	1/7/7/7	-
5	PEG	A	1212	-	-	3/4/4/4	-
4	EDO	A	1213	-	-	0/1/1/1	-
4	EDO	C	1221	-	-	0/1/1/1	-
5	PEG	B	604	-	-	1/4/4/4	-
5	PEG	C	1219	-	-	1/4/4/4	-
4	EDO	C	1207	-	-	1/1/1/1	-
4	EDO	A	1235	-	-	0/1/1/1	-
4	EDO	D	604	-	-	0/1/1/1	-
4	EDO	A	1231	-	-	1/1/1/1	-
5	PEG	C	1217	-	-	2/4/4/4	-
4	EDO	A	1225	-	-	1/1/1/1	-
5	PEG	A	1220	-	-	2/4/4/4	-
5	PEG	C	1202	-	-	1/4/4/4	-
3	PGE	C	1220	-	-	3/7/7/7	-
4	EDO	A	1219	-	-	0/1/1/1	-
4	EDO	C	1223	-	-	1/1/1/1	-
4	EDO	A	1203	-	-	0/1/1/1	-
4	EDO	A	1216	-	-	0/1/1/1	-
4	EDO	A	1224	-	-	0/1/1/1	-
4	EDO	C	1209	-	-	0/1/1/1	-
4	EDO	C	1228	-	-	0/1/1/1	-
3	PGE	A	1221	-	-	4/7/7/7	-
5	PEG	A	1214	-	-	2/4/4/4	-
9	PG4	C	1230	-	-	4/10/10/10	-
5	PEG	C	1212	-	-	0/4/4/4	-
4	EDO	C	1204	-	-	0/1/1/1	-
5	PEG	A	1215	-	-	0/4/4/4	-
3	PGE	A	1201	-	-	3/7/7/7	-
4	EDO	C	1213	-	-	0/1/1/1	-
4	EDO	A	1211	-	-	0/1/1/1	-
3	PGE	C	1205	-	-	5/7/7/7	-
4	EDO	A	1209	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	PEG	A	1208	-	-	0/4/4/4	-
4	EDO	A	1202	-	-	0/1/1/1	-
4	EDO	A	1206	-	-	0/1/1/1	-
4	EDO	C	1201	-	-	0/1/1/1	-
4	EDO	C	1224	-	-	0/1/1/1	-
4	EDO	C	1216	-	-	0/1/1/1	-
4	EDO	A	1232	-	-	1/1/1/1	-
3	PGE	C	1208	-	-	1/7/7/7	-
6	XOD	C	1229	-	-	12/20/45/45	0/3/3/3
4	EDO	C	1210	-	-	0/1/1/1	-
4	EDO	A	1205	-	-	1/1/1/1	-
3	PGE	D	603	-	-	1/7/7/7	-
4	EDO	C	1203	-	-	0/1/1/1	-
4	EDO	A	1227	-	-	1/1/1/1	-
4	EDO	A	1236	-	-	0/1/1/1	-
4	EDO	A	1234	-	-	0/1/1/1	-
4	EDO	A	1229	-	-	0/1/1/1	-
4	EDO	C	1214	-	-	0/1/1/1	-
6	XOD	A	1237	-	-	9/20/45/45	0/3/3/3
4	EDO	C	1227	-	-	1/1/1/1	-
4	EDO	A	1222	-	-	0/1/1/1	-
9	PG4	B	603	-	-	7/10/10/10	-
4	EDO	C	1225	-	-	0/1/1/1	-
3	PGE	A	1223	-	-	5/7/7/7	-
4	EDO	C	1226	-	-	0/1/1/1	-

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	1237	XOD	O6-N5	10.65	1.40	1.22
6	C	1229	XOD	O6-N5	10.42	1.40	1.22
6	A	1237	XOD	C14-N2	3.29	1.46	1.37
6	C	1229	XOD	C14-N2	3.08	1.46	1.37
6	A	1237	XOD	O1-C1	-2.19	1.40	1.44

The worst 5 of 17 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	1237	XOD	C21-N3-C20	4.86	121.16	116.08
6	C	1229	XOD	C21-N3-C20	4.82	121.12	116.08
6	A	1237	XOD	C8-N1-C5	-3.96	108.60	114.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	1237	XOD	C23-N4-C20	3.63	119.87	116.08
6	C	1229	XOD	C4-C3-C2	-3.34	106.70	111.30

There are no chirality outliers.

5 of 84 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	1237	XOD	C14-C15-N5-O6
6	A	1237	XOD	C16-C15-N5-O6
6	C	1229	XOD	C15-C14-N2-C13
5	C	1211	PEG	O1-C1-C2-O2
5	A	1212	PEG	C4-C3-O2-C2

There are no ring outliers.

28 monomers are involved in 44 short contacts:

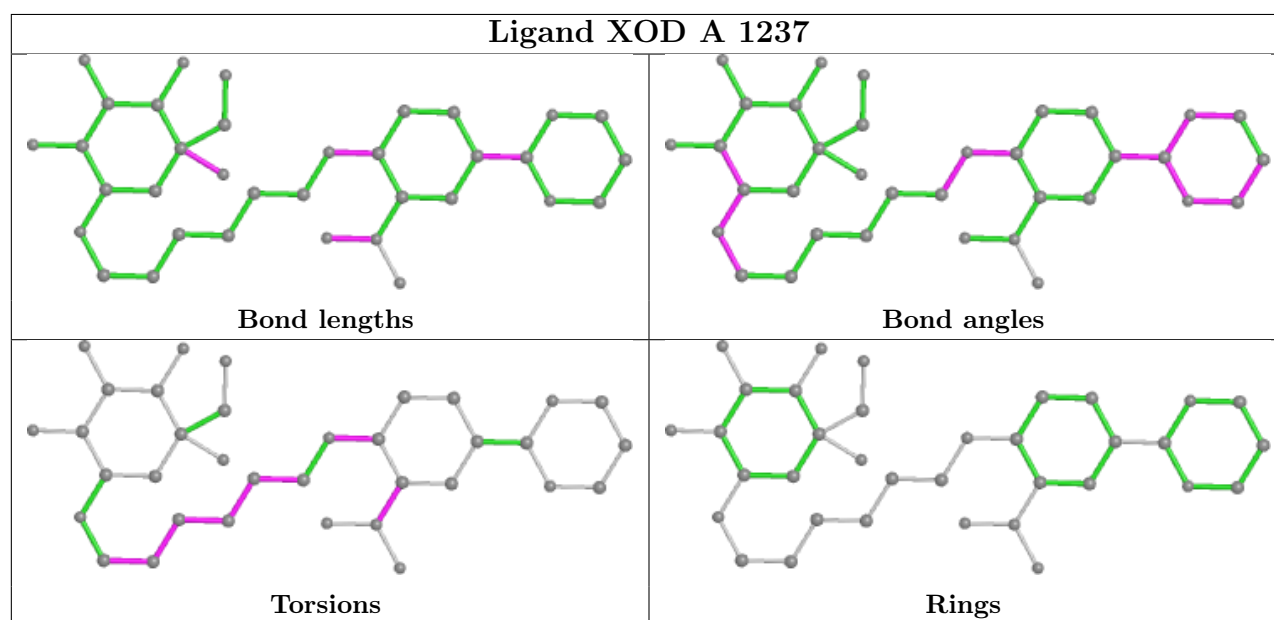
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	1215	EDO	1	0
4	A	1213	EDO	1	0
4	A	1225	EDO	1	0
5	C	1202	PEG	1	0
9	C	1230	PG4	2	0
5	A	1214	PEG	3	0
4	C	1204	EDO	3	0
4	A	1229	EDO	1	0
5	C	1211	PEG	2	0
5	C	1206	PEG	1	0
5	C	1217	PEG	2	0
4	A	1219	EDO	1	0
6	A	1237	XOD	1	0
3	A	1223	PGE	1	0
7	C	1235	SO4	2	0
5	A	1212	PEG	2	0
4	C	1209	EDO	2	0
5	A	1215	PEG	1	0
3	C	1208	PGE	1	0
4	C	1203	EDO	1	0
4	C	1227	EDO	1	0
4	A	1222	EDO	4	0
4	C	1225	EDO	1	0
4	C	1214	EDO	2	0

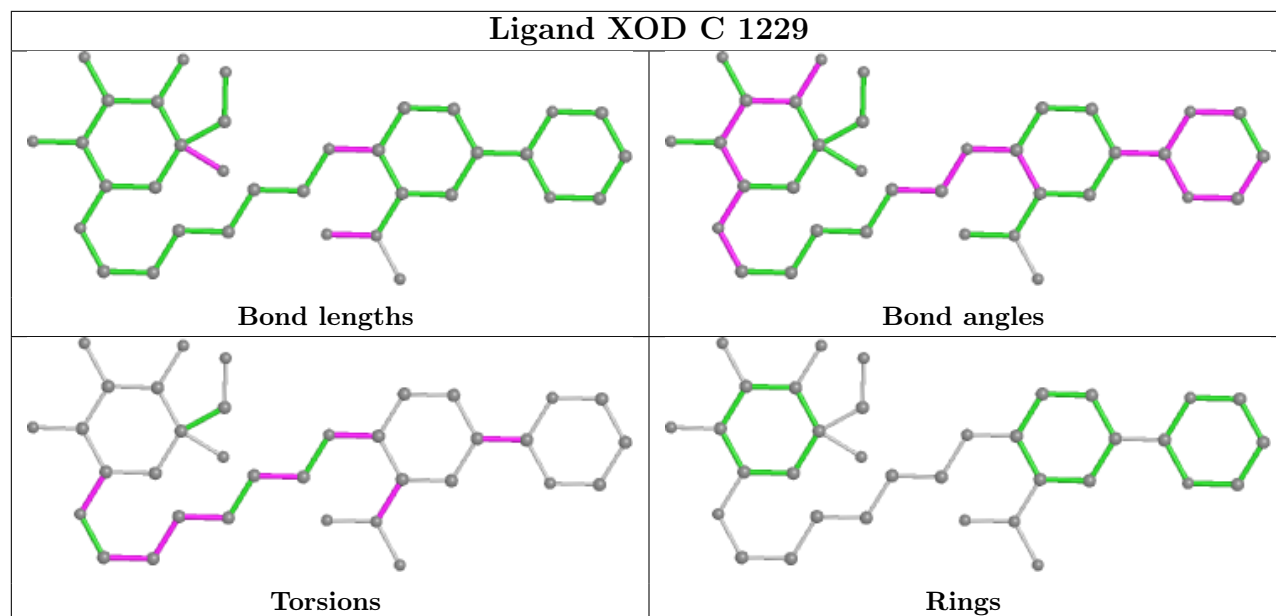
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1218	EDO	2	0
3	A	1201	PGE	2	0
4	C	1201	EDO	2	0
4	A	1232	EDO	2	0

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(Å²)	Q<0.9
1	A	850/977 (87%)	-0.26	24 (2%)	53	51	23, 35, 62, 106	0
1	C	856/977 (87%)	-0.09	57 (6%)	17	16	24, 40, 81, 110	0
2	B	83/554 (14%)	0.50	18 (21%)	0	0	30, 51, 85, 100	0
2	D	83/554 (14%)	0.43	14 (16%)	1	1	32, 50, 89, 108	0
All	All	1872/3062 (61%)	-0.12	113 (6%)	21	20	23, 38, 79, 110	0

The worst 5 of 113 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	81	GLY	8.1
2	D	82	TYR	6.3
1	C	370	THR	6.0
1	A	183	ALA	5.7
1	A	248	TRP	5.2

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, 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(\AA^2)	Q<0.9
4	EDO	C	1215	4/4	0.65	0.30	72,74,75,84	0
4	EDO	C	1209	4/4	0.66	0.27	50,55,69,76	0
3	PGE	C	1220	10/10	0.71	0.30	58,79,85,95	0
7	SO4	A	1240	5/5	0.72	0.55	109,135,152,170	0
4	EDO	A	1233	4/4	0.74	0.27	61,71,73,85	0
7	SO4	C	1234	5/5	0.76	0.60	135,143,159,180	0
5	PEG	A	1217	7/7	0.77	0.20	53,59,64,70	0
5	PEG	A	1212	7/7	0.78	0.19	59,64,77,80	0
5	PEG	A	1220	7/7	0.79	0.15	49,60,67,73	0
4	EDO	A	1235	4/4	0.80	0.21	67,71,74,76	0
4	EDO	A	1226	4/4	0.81	0.27	41,64,66,76	0
4	EDO	C	1218	4/4	0.82	0.12	59,65,69,70	0
7	SO4	A	1241	5/5	0.82	0.29	82,92,110,127	0
4	EDO	A	1206	4/4	0.82	0.17	55,68,71,76	0
4	EDO	C	1216	4/4	0.83	0.15	52,62,62,64	0
3	PGE	C	1208	10/10	0.83	0.27	46,77,85,86	0
9	PG4	B	603	13/13	0.83	0.22	58,67,76,77	0
4	EDO	C	1227	4/4	0.84	0.47	52,56,72,84	0
4	EDO	C	1210	4/4	0.84	0.20	49,56,68,77	0
3	PGE	C	1205	10/10	0.85	0.17	35,61,71,77	0
9	PG4	C	1230	13/13	0.85	0.17	53,72,78,93	0
4	EDO	A	1213	4/4	0.86	0.21	43,49,56,66	0
3	PGE	A	1207	10/10	0.86	0.28	50,65,73,74	0
5	PEG	A	1228	7/7	0.86	0.24	45,50,67,67	0
4	EDO	A	1227	4/4	0.86	0.22	49,52,61,68	0
5	PEG	C	1206	7/7	0.87	0.13	62,69,80,99	0
7	SO4	A	1238	5/5	0.87	0.21	80,97,131,154	0
4	EDO	C	1213	4/4	0.87	0.12	48,56,56,56	0
3	PGE	A	1221	10/10	0.87	0.26	56,72,78,78	0
7	SO4	C	1233	5/5	0.87	0.23	66,89,92,129	0
4	EDO	A	1204	4/4	0.87	0.11	57,57,60,66	0
4	EDO	A	1224	4/4	0.87	0.14	48,49,59,64	0
4	EDO	C	1223	4/4	0.87	0.30	62,63,66,77	0
4	EDO	A	1218	4/4	0.88	0.17	55,60,71,75	0
5	PEG	A	1208	7/7	0.88	0.16	51,62,65,78	0
4	EDO	C	1214	4/4	0.88	0.18	55,65,67,68	0
5	PEG	B	604	7/7	0.88	0.31	50,69,75,78	0
7	SO4	A	1239	5/5	0.89	0.39	79,81,121,131	0
4	EDO	A	1209	4/4	0.89	0.19	41,50,58,61	0
3	PGE	A	1223	10/10	0.89	0.16	56,64,79,88	0
7	SO4	B	606	5/5	0.89	0.33	65,68,101,107	0
4	EDO	C	1207	4/4	0.89	0.21	54,55,64,75	0
4	EDO	A	1229	4/4	0.89	0.18	48,61,68,80	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
5	PEG	C	1217	7/7	0.89	0.18	45,56,69,78	0
4	EDO	A	1230	4/4	0.89	0.26	56,58,61,63	0
5	PEG	C	1219	7/7	0.90	0.21	50,56,68,71	0
7	SO4	C	1232	5/5	0.90	0.16	76,86,97,131	0
3	PGE	D	603	10/10	0.90	0.22	54,74,78,79	0
5	PEG	C	1202	7/7	0.90	0.17	51,59,72,75	0
5	PEG	A	1214	7/7	0.90	0.15	47,54,68,74	0
5	PEG	A	1215	7/7	0.90	0.14	47,59,78,82	0
4	EDO	B	605	4/4	0.91	0.22	51,57,60,63	0
7	SO4	C	1235	5/5	0.91	0.30	75,83,117,119	0
6	XOD	C	1229	35/35	0.91	0.16	27,58,114,119	0
4	EDO	A	1234	4/4	0.91	0.35	49,59,60,74	0
5	PEG	C	1211	7/7	0.92	0.30	38,51,71,74	0
3	PGE	A	1210	10/10	0.92	0.28	48,60,73,81	0
4	EDO	A	1216	4/4	0.92	0.22	45,62,62,63	0
6	XOD	A	1237	35/35	0.92	0.19	23,53,104,113	0
4	EDO	C	1226	4/4	0.93	0.26	46,52,61,62	0
3	PGE	A	1201	10/10	0.93	0.24	51,63,70,70	0
7	SO4	C	1231	5/5	0.94	0.11	62,67,70,105	0
4	EDO	D	604	4/4	0.94	0.16	48,53,58,62	0
4	EDO	C	1204	4/4	0.94	0.10	39,49,51,55	0
5	PEG	C	1212	7/7	0.94	0.29	45,68,73,77	0
4	EDO	A	1222	4/4	0.94	0.15	42,49,58,60	0
4	EDO	A	1232	4/4	0.94	0.16	36,38,56,57	0
4	EDO	C	1203	4/4	0.94	0.14	35,42,52,57	0
4	EDO	A	1231	4/4	0.95	0.11	40,45,50,53	0
4	EDO	C	1221	4/4	0.95	0.18	40,48,59,65	0
4	EDO	A	1202	4/4	0.95	0.14	42,44,45,52	0
4	EDO	C	1224	4/4	0.95	0.28	56,57,59,81	0
4	EDO	A	1225	4/4	0.95	0.17	39,42,61,66	0
4	EDO	C	1228	4/4	0.96	0.16	46,50,50,53	0
4	EDO	A	1203	4/4	0.96	0.18	53,58,60,61	0
4	EDO	C	1225	4/4	0.96	0.14	54,60,70,74	0
4	EDO	C	1222	4/4	0.96	0.13	40,44,52,57	0
4	EDO	A	1205	4/4	0.96	0.09	43,49,55,57	0
4	EDO	C	1201	4/4	0.97	0.10	45,46,54,66	0
4	EDO	A	1236	4/4	0.97	0.25	56,59,64,70	0
4	EDO	A	1211	4/4	0.97	0.10	35,48,66,69	0
4	EDO	A	1219	4/4	0.98	0.09	35,39,48,52	0
8	CA	D	601	1/1	0.98	0.05	42,42,42,42	0
8	CA	B	602	1/1	0.99	0.05	33,33,33,33	0
8	CA	B	601	1/1	0.99	0.06	39,39,39,39	0

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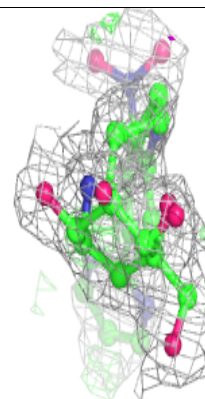
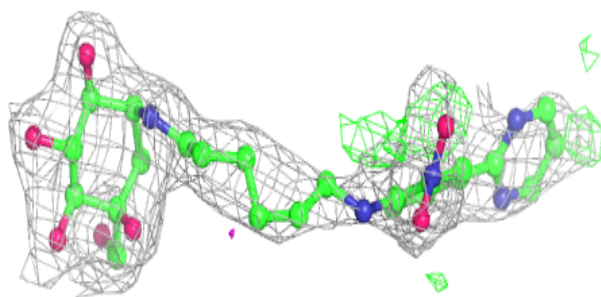
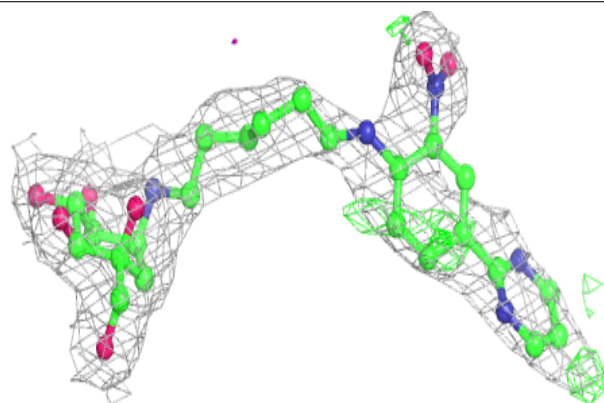
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
8	CA	D	602	1/1	1.00	0.04	32,32,32,32	0

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.

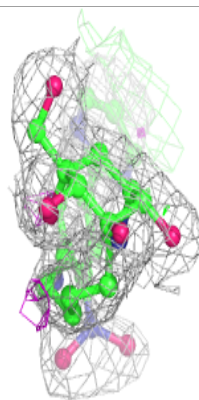
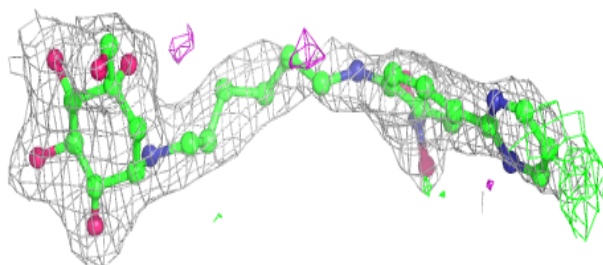
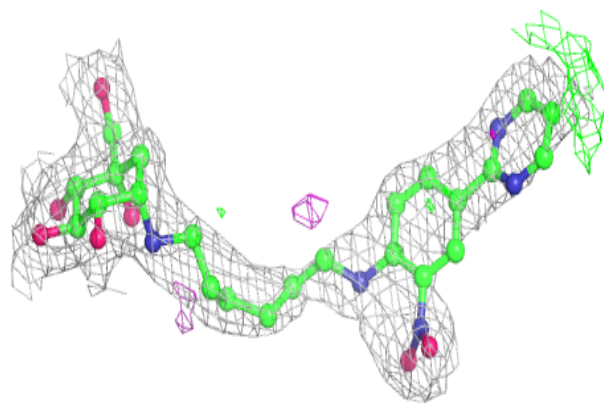
Electron density around XOD C 1229:

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 XOD A 1237:

$2mF_o - DF_c$ (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.