



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 6, 2026 – 10:12 PM UTC

PDB ID : 7KBJ / pdb_00007kbj
Title : Co-crystal structure of alpha glucosidase with compound 9
Authors : Karade, S.S.; Mariuzza, R.A.
Deposited on : 2020-10-02
Resolution : 2.21 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

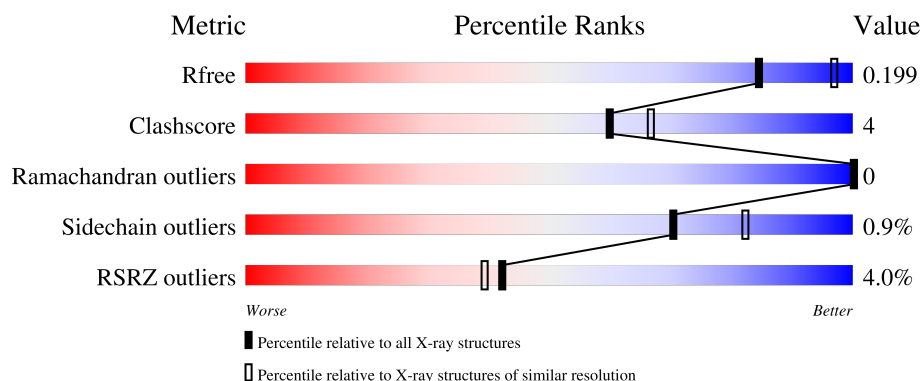
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.21 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	7682 (2.24-2.20)
Clashscore	190562	8402 (2.24-2.20)
Ramachandran outliers	187476	8303 (2.24-2.20)
Sidechain outliers	187428	8304 (2.24-2.20)
RSRZ outliers	180081	7683 (2.24-2.20)

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	G	184	4% 72% 11% 17%
1	I	184	12% 73% 10% 17%
2	H	107	6% 87% 11% .
2	J	107	5% 87% 13%
3	A	609	89% 9% .

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Mol	Chain	Length	Quality of chain
3	C	609	% 88% 10%
4	B	134	11% 57%
4	D	134	10% 56% 7% 37%

2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 16523 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Neutral alpha-glucosidase AB Trypsin-cleaved Fragment #1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	G	152	Total	C	N	O	S	0	0	0
			1209	758	223	224	4			
1	I	153	Total	C	N	O	S	0	0	0
			1213	760	224	225	4			

There are 64 discrepancies between the modelled and reference sequences:

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

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Chain	Residue	Modelled	Actual	Comment	Reference
G	27	CYS	-	expression tag	UNP Q8BHN3
G	28	VAL	-	expression tag	UNP Q8BHN3
G	29	ALA	-	expression tag	UNP Q8BHN3
G	30	GLU	-	expression tag	UNP Q8BHN3
G	31	THR	-	expression tag	UNP Q8BHN3
G	32	GLY	-	expression tag	UNP Q8BHN3
G	97	ASP	ASN	engineered mutation	UNP Q8BHN3
I	2	MET	-	initiating methionine	UNP Q8BHN3
I	3	GLY	-	expression tag	UNP Q8BHN3
I	4	ILE	-	expression tag	UNP Q8BHN3
I	5	LEU	-	expression tag	UNP Q8BHN3
I	6	PRO	-	expression tag	UNP Q8BHN3
I	7	SER	-	expression tag	UNP Q8BHN3
I	8	PRO	-	expression tag	UNP Q8BHN3
I	9	GLY	-	expression tag	UNP Q8BHN3
I	10	MET	-	expression tag	UNP Q8BHN3
I	11	PRO	-	expression tag	UNP Q8BHN3
I	12	ALA	-	expression tag	UNP Q8BHN3
I	13	LEU	-	expression tag	UNP Q8BHN3
I	14	LEU	-	expression tag	UNP Q8BHN3
I	15	SER	-	expression tag	UNP Q8BHN3
I	16	LEU	-	expression tag	UNP Q8BHN3
I	17	VAL	-	expression tag	UNP Q8BHN3
I	18	SER	-	expression tag	UNP Q8BHN3
I	19	LEU	-	expression tag	UNP Q8BHN3
I	20	LEU	-	expression tag	UNP Q8BHN3
I	21	SER	-	expression tag	UNP Q8BHN3
I	22	VAL	-	expression tag	UNP Q8BHN3
I	23	LEU	-	expression tag	UNP Q8BHN3
I	24	LEU	-	expression tag	UNP Q8BHN3
I	25	MET	-	expression tag	UNP Q8BHN3
I	26	GLY	-	expression tag	UNP Q8BHN3
I	27	CYS	-	expression tag	UNP Q8BHN3
I	28	VAL	-	expression tag	UNP Q8BHN3
I	29	ALA	-	expression tag	UNP Q8BHN3
I	30	GLU	-	expression tag	UNP Q8BHN3
I	31	THR	-	expression tag	UNP Q8BHN3
I	32	GLY	-	expression tag	UNP Q8BHN3
I	97	ASP	ASN	engineered mutation	UNP Q8BHN3

- Molecule 2 is a protein called Neutral alpha-glucosidase AB Trypsin-cleaved Fragment #2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	105	Total	C	N	O	S	0	0	0
			837	540	136	159	2			
2	J	107	Total	C	N	O	S	0	1	0
			859	555	139	163	2			

- Molecule 3 is a protein called Neutral alpha-glucosidase AB Trypsin-cleaved Fragment #3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	597	Total	C	N	O	S	0	10	0
			4889	3146	838	881	24			
3	C	597	Total	C	N	O	S	0	10	0
			4885	3144	838	879	24			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	967	SER	-	expression tag	UNP Q8BHN3
A	968	ALA	-	expression tag	UNP Q8BHN3
A	969	TRP	-	expression tag	UNP Q8BHN3
A	970	SER	-	expression tag	UNP Q8BHN3
A	971	HIS	-	expression tag	UNP Q8BHN3
A	972	PRO	-	expression tag	UNP Q8BHN3
A	973	GLN	-	expression tag	UNP Q8BHN3
A	974	PHE	-	expression tag	UNP Q8BHN3
A	975	GLU	-	expression tag	UNP Q8BHN3
A	976	LYS	-	expression tag	UNP Q8BHN3
A	977	LEU	-	expression tag	UNP Q8BHN3
A	978	GLU	-	expression tag	UNP Q8BHN3
C	967	SER	-	expression tag	UNP Q8BHN3
C	968	ALA	-	expression tag	UNP Q8BHN3
C	969	TRP	-	expression tag	UNP Q8BHN3
C	970	SER	-	expression tag	UNP Q8BHN3
C	971	HIS	-	expression tag	UNP Q8BHN3
C	972	PRO	-	expression tag	UNP Q8BHN3
C	973	GLN	-	expression tag	UNP Q8BHN3
C	974	PHE	-	expression tag	UNP Q8BHN3
C	975	GLU	-	expression tag	UNP Q8BHN3
C	976	LYS	-	expression tag	UNP Q8BHN3
C	977	LEU	-	expression tag	UNP Q8BHN3
C	978	GLU	-	expression tag	UNP Q8BHN3

- Molecule 4 is a protein called Glucosidase 2 subunit beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	B	82	Total 607	C 362	N 99	O 136	S 10	0	0	0
4	D	84	Total 622	C 371	N 102	O 139	S 10	0	0	0

There are 62 discrepancies between the modelled and reference sequences:

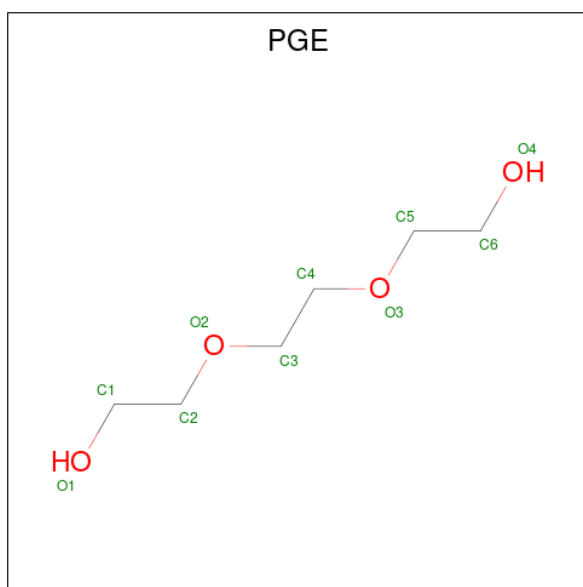
Chain	Residue	Modelled	Actual	Comment	Reference
B	-16	MET	-	initiating methionine	UNP O08795
B	-15	GLY	-	expression tag	UNP O08795
B	-14	ILE	-	expression tag	UNP O08795
B	-13	LEU	-	expression tag	UNP O08795
B	-12	PRO	-	expression tag	UNP O08795
B	-11	SER	-	expression tag	UNP O08795
B	-10	PRO	-	expression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

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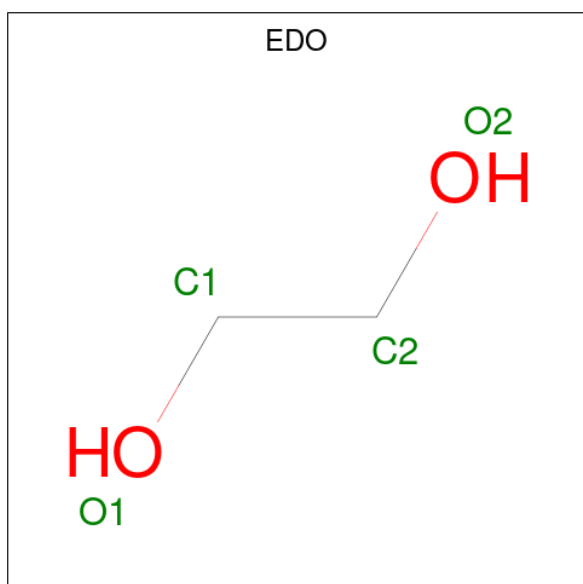
Chain	Residue	Modelled	Actual	Comment	Reference
D	-12	PRO	-	expression tag	UNP O08795
D	-11	SER	-	expression tag	UNP O08795
D	-10	PRO	-	expression tag	UNP O08795
D	-9	GLY	-	expression tag	UNP O08795
D	-8	MET	-	expression tag	UNP O08795
D	-7	PRO	-	expression tag	UNP O08795
D	-6	ALA	-	expression tag	UNP 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

- Molecule 5 is TRIETHYLENE GLYCOL (CCD ID: PGE) (formula: C₆H₁₄O₄).



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

- Molecule 6 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



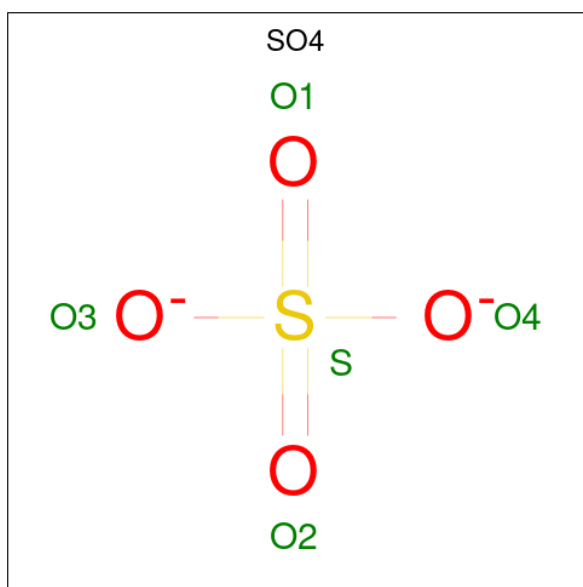
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	G	1	Total C O 4 2 2	0	0
6	H	1	Total C O 4 2 2	0	0
6	H	1	Total C O 4 2 2	0	0
6	A	1	Total C O 4 2 2	0	0
6	A	1	Total C O 4 2 2	0	0
6	A	1	Total C O 4 2 2	0	0
6	A	1	Total C O 4 2 2	0	0
6	A	1	Total C O 4 2 2	0	0
6	A	1	Total C O 4 2 2	0	0
6	A	1	Total C O 4 2 2	0	0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

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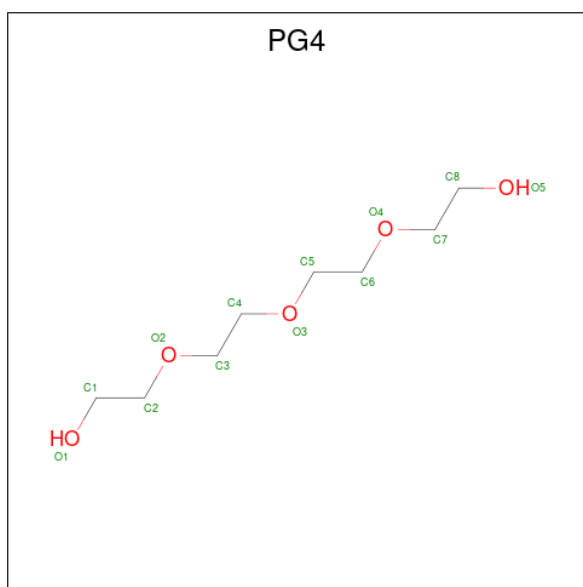
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	C	1	Total	C	O	0	0
			4	2	2		
6	C	1	Total	C	O	0	0
			4	2	2		
6	C	1	Total	C	O	0	0
			4	2	2		
6	C	1	Total	C	O	0	0
			4	2	2		
6	C	1	Total	C	O	0	0
			4	2	2		
6	C	1	Total	C	O	0	0
			4	2	2		
6	C	1	Total	C	O	0	0
			4	2	2		
6	C	1	Total	C	O	0	0
			4	2	2		
6	D	1	Total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



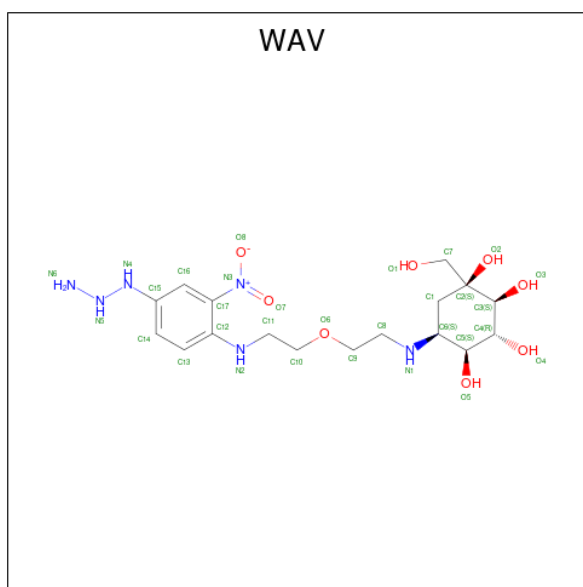
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	G	1	Total	O	S	0	0
			5	4	1		
7	A	1	Total	O	S	0	0
			5	4	1		
7	B	1	Total	O	S	0	0
			5	4	1		
7	J	1	Total	O	S	0	0
			5	4	1		
7	J	1	Total	O	S	0	0
			5	4	1		
7	C	1	Total	O	S	0	0
			5	4	1		
7	C	1	Total	O	S	0	0
			5	4	1		
7	C	1	Total	O	S	0	0
			5	4	1		

- Molecule 8 is TETRAETHYLENE GLYCOL (CCD ID: PG4) (formula: C₈H₁₈O₅).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	H	1	Total	C	O	0	0
			13	8	5		
8	A	1	Total	C	O	0	0
			13	8	5		

- Molecule 9 is (1S,2S,3R,4S,5S)-1-(hydroxymethyl)-5-{{2-(2-{{2-nitro-4-(triazan-1-yl)phenyl}amino}ethoxy)ethyl}amino}cyclohexane-1,2,3,4-tetrol (CCD ID: WAV) (formula: C₁₇H₃₀N₆O₈) (labeled as "Ligand of Interest" by depositor).



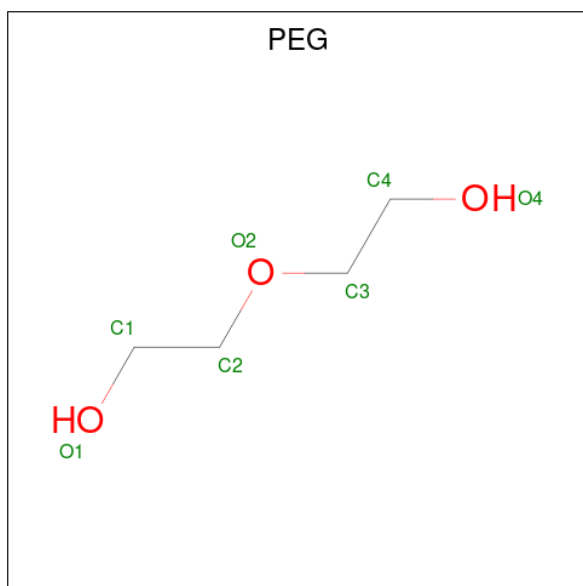
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	A	1	Total	C	N	O	0	0
			31	17	6	8		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	C	1	Total	C	N	O	0	0
			31	17	6	8		

- Molecule 10 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: $C_4H_{10}O_3$).



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

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

- Molecule 11 is CALCIUM ION (CCD ID: CA) (formula: Ca).

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

- Molecule 12 is water.

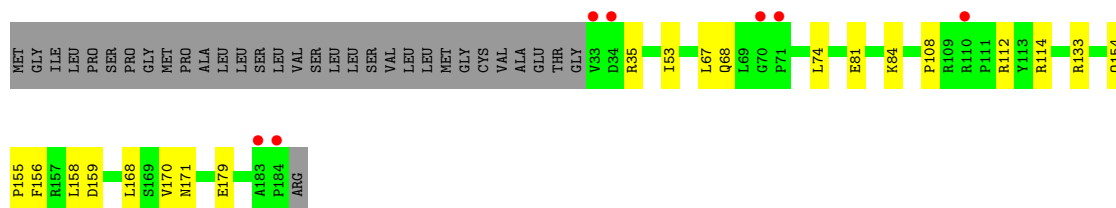
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	G	85	Total	O	0	0
			85	85		
12	H	62	Total	O	0	0
			62	62		
12	A	358	Total	O	0	0
			358	358		
12	B	41	Total	O	0	0
			41	41		
12	I	47	Total	O	0	0
			47	47		
12	J	55	Total	O	0	0
			55	55		
12	C	315	Total	O	0	0
			315	315		
12	D	40	Total	O	0	0
			40	40		

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.

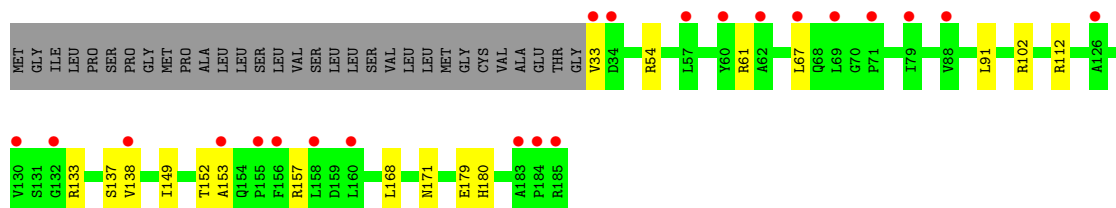
- Molecule 1: Neutral alpha-glucosidase AB Trypsin-cleaved Fragment #1

Chain G: 



- Molecule 1: Neutral alpha-glucosidase AB Trypsin-cleaved Fragment #1

Chain I: 



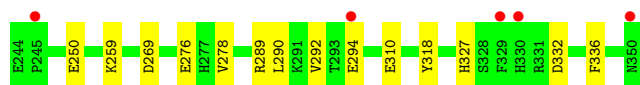
- Molecule 2: Neutral alpha-glucosidase AB Trypsin-cleaved Fragment #2

Chain H: 



- Molecule 2: Neutral alpha-glucosidase AB Trypsin-cleaved Fragment #2

Chain J: 



- Molecule 3: Neutral alpha-glucosidase AB Trypsin-cleaved Fragment #3

Category	Item	Value
A	A611	100
	A635	100
	A648	100
	A665	100
	A685	100
	A701	100
	A732	100
	A754	100
	A758	100
	A769	100
B	B611	100
	B635	100
	B648	100
	B665	100
	B685	100
	B701	100
	B732	100
	B754	100
	B758	100
	B769	100
C	C611	100
	C635	100
	C648	100
	C665	100
	C685	100
	C701	100
	C732	100
	C754	100
	C758	100
	C769	100
D	D611	100
	D635	100
	D648	100
	D665	100
	D685	100
	D701	100
	D732	100
	D754	100
	D758	100
	D769	100
E	E611	100
	E635	100
	E648	100
	E665	100
	E685	100
	E701	100
	E732	100
	E754	100
	E758	100
	E769	100
F	F611	100
	F635	100
	F648	100
	F665	100
	F685	100
	F701	100
	F732	100
	F754	100
	F758	100
	F769	100
G	G611	100
	G635	100
	G648	100
	G665	100
	G685	100
	G701	100
	G732	100
	G754	100
	G758	100
	G769	100
H	H611	100
	H635	100
	H648	100
	H665	100
	H685	100
	H701	100
	H732	100
	H754	100
	H758	100
	H769	100
I	I611	100
	I635	100
	I648	100
	I665	100
	I685	100
	I701	100
	I732	100
	I754	100
	I758	100
	I769	100
J	J611	100
	J635	100
	J648	100
	J665	100
	J685	100
	J701	100
	J732	100
	J754	100
	J758	100
	J769	100
K	K611	100
	K635	100
	K648	100
	K665	100
	K685	100
	K701	100
	K732	100
	K754	100
	K758	100
	K769	100
L	L611	100
	L635	100
	L648	100
	L665	100
	L685	100
	L701	100
	L732	100
	L754	100
	L758	100
	L769	100
M	M611	100
	M635	100
	M648	100
	M665	100
	M685	100
	M701	100
	M732	100
	M754	100
	M758	100
	M769	100
N	N611	100
	N635	100
	N648	100
	N665	100
	N685	100
	N701	100
	N732	100
	N754	100
	N758	100
	N769	100
O	O611	100
	O635	100
	O648	100
	O665	100
	O685	100
	O701	100
	O732	100
	O754	100
	O758	100
	O769	100
P	P611	100
	P635	100
	P648	100
	P665	100
	P685	100

Chain C: 88% 10% 2%

TRP	D607	T370
SER	P371	
HIS	Q611	
PRO	D385	
GLN	G639	
PHE	G671	
GLU	L682	
LYS	W835	
LEU	L701	
GLU	L711	
	Y755	
	D758	
	Q767	
	F768	
	H769	
	H777	
	H785	
	Y790	
	L791	
	P792	
	E795	
	E796	
	V797	
	K806	
	H807	
	H808	
	K846	
	D847	
	S892	
	V895	
	E906	
	T907	
	P908	
	R936	
	D960	
	L965	
	R966	
SER	A791	
ALA	Y600	

Chain B:

A44	T45	I46	P47	F48	K59	D60	G61	S62	C70	T78	N79	T80	G81	Y82	K83	R117	MET	GLY	ILE	LEU	PRO	SER	PRO	GLY	MET	PRO	ALA	LEU	LEU	SER	LEU	VAL	SER	LEU	LEU	SER	VAL	LEU	LEU	MET	GLY	CYS	VAL	ALA	GLU	THR	GLY	VAL	GLU	GLU	LYS	ARG	PRO	ARG	GLY	VAL	SER	LEU	SER	ASN	HIS	PHE	TYR	GLU	GLU	SER	LYS	P36	F37	T38	C39	L40	D41	G42	T43
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	------	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

Chain D:

4 Data and refinement statistics

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, α , β , γ	102.65Å 102.65Å 238.91Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	42.09 – 2.21 42.09 – 2.21	Depositor EDS
% Data completeness (in resolution range)	99.3 (42.09-2.21) 94.6 (42.09-2.21)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.56 (at 2.20Å)	Xtriage
Refinement program	PHENIX 1.18.2_3874	Depositor
R, R_{free}	0.167 , 0.200 0.167 , 0.199	Depositor DCC
R_{free} test set	2033 reflections (1.45%)	wwPDB-VP
Wilson B-factor (Å ²)	32.2	Xtriage
Anisotropy	0.178	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 43.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.012 for -h,-k,l 0.038 for h,-h-k,-l 0.024 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	16523	wwPDB-VP
Average B, all atoms (Å ²)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.52% 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: WAV, CA, PGE, PG4, SO4, EDO, PEG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	G	0.24	0/1229	0.48	0/1666
1	I	0.22	0/1233	0.49	0/1672
2	H	0.27	0/865	0.48	0/1181
2	J	0.22	0/891	0.45	0/1216
3	A	0.28	0/5082	0.50	0/6919
3	C	0.26	0/5078	0.48	0/6914
4	B	0.22	0/619	0.47	0/842
4	D	0.23	0/634	0.46	0/862
All	All	0.26	0/15631	0.48	0/21272

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	G	1209	0	1240	14	0
1	I	1213	0	1240	15	0
2	H	837	0	783	12	0
2	J	859	0	809	9	0
3	A	4889	0	4676	38	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	4885	0	4670	39	0
4	B	607	0	521	5	0
4	D	622	0	538	6	0
5	A	40	0	55	1	0
5	G	10	0	14	2	0
6	A	52	0	76	3	0
6	C	68	0	99	5	0
6	D	8	0	12	1	0
6	G	4	0	6	0	0
6	H	8	0	12	1	0
7	A	5	0	0	0	0
7	B	5	0	0	0	0
7	C	15	0	0	0	0
7	G	5	0	0	0	0
7	J	10	0	0	0	0
8	A	13	0	18	0	0
8	H	13	0	18	0	0
9	A	31	0	0	1	0
9	C	31	0	0	1	0
10	A	14	0	20	1	0
10	B	14	0	20	2	0
10	C	28	0	40	4	0
10	D	7	0	10	0	0
10	I	7	0	10	1	0
10	J	7	0	10	0	0
11	B	2	0	0	0	0
11	D	2	0	0	0	0
12	A	358	0	0	9	0
12	B	41	0	0	0	0
12	C	315	0	0	5	0
12	D	40	0	0	2	0
12	G	85	0	0	4	0
12	H	62	0	0	1	0
12	I	47	0	0	8	0
12	J	55	0	0	0	0
All	All	16523	0	14897	131	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 131 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)
3:C:538:ARG:NH1	12:C:1101:HOH:O	2.03	0.91
3:A:504:GLU:OE2	12:A:1101:HOH:O	1.92	0.87
4:B:83:LYS:H	4:B:83:LYS:HD3	1.40	0.86
1:I:153:ALA:O	12:I:1701:HOH:O	1.98	0.79
4:D:48:PHE:O	12:D:1501:HOH:O	2.00	0.78

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	G	150/184 (82%)	146 (97%)	4 (3%)	0	100	100
1	I	151/184 (82%)	146 (97%)	5 (3%)	0	100	100
2	H	103/107 (96%)	96 (93%)	7 (7%)	0	100	100
2	J	106/107 (99%)	98 (92%)	8 (8%)	0	100	100
3	A	605/609 (99%)	588 (97%)	17 (3%)	0	100	100
3	C	605/609 (99%)	587 (97%)	18 (3%)	0	100	100
4	B	80/134 (60%)	78 (98%)	2 (2%)	0	100	100
4	D	82/134 (61%)	80 (98%)	2 (2%)	0	100	100
All	All	1882/2068 (91%)	1819 (97%)	63 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	G	136/163 (83%)	134 (98%)	2 (2%)	57	71
1	I	136/163 (83%)	134 (98%)	2 (2%)	57	71
2	H	90/92 (98%)	90 (100%)	0	100	100
2	J	93/92 (101%)	93 (100%)	0	100	100
3	A	528/529 (100%)	525 (99%)	3 (1%)	78	88
3	C	527/529 (100%)	521 (99%)	6 (1%)	65	78
4	B	71/116 (61%)	71 (100%)	0	100	100
4	D	73/116 (63%)	72 (99%)	1 (1%)	59	73
All	All	1654/1800 (92%)	1640 (99%)	14 (1%)	70	84

5 of 14 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	C	424	ASN
3	C	446	ASP
4	D	34	SER
3	C	936	ARG
3	C	966	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 12 such sidechains are listed below:

Mol	Chain	Res	Type
3	C	473	ASN
3	C	545	ASN
4	D	76	HIS
3	C	563	ASN
3	A	436	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 67 ligands modelled in this entry, 4 are monoatomic - leaving 63 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	PGE	A	1021	-	9,9,9	0.41	0	8,8,8	0.32	0
6	EDO	C	1021	-	3,3,3	0.46	0	2,2,2	0.29	0
6	EDO	A	1004	-	3,3,3	0.39	0	2,2,2	0.42	0
6	EDO	D	1402	-	3,3,3	0.45	0	2,2,2	0.24	0
10	PEG	I	1601	-	6,6,6	0.49	0	5,5,5	0.29	0
7	SO4	A	1022	-	4,4,4	0.23	0	6,6,6	0.25	0
7	SO4	J	1202	-	4,4,4	0.32	0	6,6,6	0.24	0
9	WAV	C	1001	-	32,32,32	3.09	12 (37%)	35,44,44	1.13	2 (5%)
10	PEG	J	1201	-	6,6,6	0.48	0	5,5,5	0.42	0
6	EDO	C	1008	-	3,3,3	0.37	0	2,2,2	0.47	0
6	EDO	A	1016	-	3,3,3	0.43	0	2,2,2	0.41	0
7	SO4	G	1103	-	4,4,4	0.26	0	6,6,6	0.11	0
6	EDO	C	1002	-	3,3,3	0.49	0	2,2,2	0.25	0
8	PG4	A	1002	-	12,12,12	0.54	0	11,11,11	0.27	0
10	PEG	C	1003	-	6,6,6	0.48	0	5,5,5	0.44	0
6	EDO	C	1005	-	3,3,3	0.47	0	2,2,2	0.30	0
10	PEG	A	1010	-	6,6,6	0.52	0	5,5,5	0.35	0
6	EDO	G	1102	-	3,3,3	0.40	0	2,2,2	0.47	0
7	SO4	C	1025	-	4,4,4	0.23	0	6,6,6	0.17	0
6	EDO	C	1004	-	3,3,3	0.44	0	2,2,2	0.37	0
9	WAV	A	1001	-	32,32,32	3.09	12 (37%)	35,44,44	1.06	2 (5%)
6	EDO	H	1303	-	3,3,3	0.42	0	2,2,2	0.42	0
6	EDO	H	1302	-	3,3,3	0.57	0	2,2,2	0.13	0
6	EDO	A	1011	-	3,3,3	0.41	0	2,2,2	0.48	0
6	EDO	C	1010	-	3,3,3	0.48	0	2,2,2	0.24	0
7	SO4	C	1024	-	4,4,4	0.25	0	6,6,6	0.14	0
6	EDO	C	1012	-	3,3,3	0.48	0	2,2,2	0.35	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
10	PEG	C	1006	-	6,6,6	0.51	0	5,5,5	0.34	0
6	EDO	A	1009	-	3,3,3	0.36	0	2,2,2	0.72	0
10	PEG	C	1022	-	6,6,6	0.50	0	5,5,5	0.26	0
5	PGE	A	1003	-	9,9,9	0.36	0	8,8,8	0.35	0
10	PEG	D	1403	-	6,6,6	0.49	0	5,5,5	0.30	0
6	EDO	A	1005	-	3,3,3	0.39	0	2,2,2	0.91	0
5	PGE	A	1007	-	9,9,9	0.37	0	8,8,8	0.35	0
6	EDO	C	1018	-	3,3,3	0.44	0	2,2,2	0.44	0
6	EDO	C	1019	-	3,3,3	0.48	0	2,2,2	0.40	0
10	PEG	C	1016	-	6,6,6	0.50	0	5,5,5	0.27	0
7	SO4	J	1203	-	4,4,4	0.24	0	6,6,6	0.18	0
6	EDO	A	1012	-	3,3,3	0.48	0	2,2,2	0.34	0
6	EDO	C	1014	-	3,3,3	0.52	0	2,2,2	0.33	0
6	EDO	D	1401	-	3,3,3	0.51	0	2,2,2	0.18	0
6	EDO	C	1013	-	3,3,3	0.40	0	2,2,2	0.62	0
6	EDO	A	1017	-	3,3,3	0.38	0	2,2,2	0.47	0
10	PEG	B	1802	-	6,6,6	0.49	0	5,5,5	0.34	0
6	EDO	C	1009	-	3,3,3	0.40	0	2,2,2	0.45	0
8	PG4	H	1301	-	12,12,12	0.56	0	11,11,11	0.30	0
6	EDO	A	1018	-	3,3,3	0.47	0	2,2,2	0.36	0
6	EDO	A	1020	-	3,3,3	0.49	0	2,2,2	0.44	0
7	SO4	C	1023	-	4,4,4	0.23	0	6,6,6	0.30	0
6	EDO	A	1013	-	3,3,3	0.43	0	2,2,2	0.34	0
5	PGE	A	1008	-	9,9,9	0.29	0	8,8,8	0.31	0
6	EDO	A	1015	-	3,3,3	0.42	0	2,2,2	0.24	0
7	SO4	B	1803	-	4,4,4	0.27	0	6,6,6	0.04	0
6	EDO	C	1011	-	3,3,3	0.48	0	2,2,2	0.32	0
6	EDO	A	1006	-	3,3,3	0.49	0	2,2,2	0.31	0
5	PGE	G	1101	-	9,9,9	0.33	0	8,8,8	0.34	0
6	EDO	A	1019	-	3,3,3	0.33	0	2,2,2	0.65	0
6	EDO	C	1007	-	3,3,3	0.43	0	2,2,2	0.44	0
10	PEG	A	1014	-	6,6,6	0.49	0	5,5,5	0.33	0
6	EDO	C	1020	-	3,3,3	0.44	0	2,2,2	0.45	0
6	EDO	C	1017	-	3,3,3	0.45	0	2,2,2	0.48	0
10	PEG	B	1801	-	6,6,6	0.55	0	5,5,5	0.45	0
6	EDO	C	1015	-	3,3,3	0.45	0	2,2,2	0.73	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	PGE	A	1021	-	-	1/7/7/7	-
6	EDO	C	1021	-	-	1/1/1/1	-
6	EDO	A	1004	-	-	0/1/1/1	-
6	EDO	D	1402	-	-	0/1/1/1	-
10	PEG	I	1601	-	-	1/4/4/4	-
9	WAV	C	1001	-	-	6/17/43/43	0/2/2/2
10	PEG	J	1201	-	-	3/4/4/4	-
6	EDO	C	1008	-	-	0/1/1/1	-
6	EDO	A	1016	-	-	0/1/1/1	-
6	EDO	C	1002	-	-	1/1/1/1	-
8	PG4	A	1002	-	-	6/10/10/10	-
10	PEG	C	1003	-	-	1/4/4/4	-
6	EDO	C	1005	-	-	1/1/1/1	-
10	PEG	A	1010	-	-	0/4/4/4	-
6	EDO	G	1102	-	-	0/1/1/1	-
6	EDO	C	1004	-	-	0/1/1/1	-
9	WAV	A	1001	-	-	7/17/43/43	0/2/2/2
6	EDO	H	1303	-	-	0/1/1/1	-
6	EDO	H	1302	-	-	0/1/1/1	-
6	EDO	A	1011	-	-	1/1/1/1	-
6	EDO	C	1010	-	-	1/1/1/1	-
6	EDO	C	1012	-	-	1/1/1/1	-
10	PEG	C	1006	-	-	3/4/4/4	-
6	EDO	A	1009	-	-	1/1/1/1	-
10	PEG	C	1022	-	-	2/4/4/4	-
5	PGE	A	1003	-	-	5/7/7/7	-
10	PEG	D	1403	-	-	4/4/4/4	-
6	EDO	A	1005	-	-	1/1/1/1	-
5	PGE	A	1007	-	-	5/7/7/7	-
6	EDO	C	1018	-	-	1/1/1/1	-
6	EDO	C	1019	-	-	0/1/1/1	-
10	PEG	C	1016	-	-	2/4/4/4	-
6	EDO	A	1012	-	-	0/1/1/1	-
6	EDO	C	1014	-	-	0/1/1/1	-
6	EDO	D	1401	-	-	0/1/1/1	-
6	EDO	C	1013	-	-	0/1/1/1	-
6	EDO	A	1017	-	-	1/1/1/1	-
10	PEG	B	1802	-	-	2/4/4/4	-
6	EDO	C	1009	-	-	1/1/1/1	-
8	PG4	H	1301	-	-	5/10/10/10	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	EDO	A	1018	-	-	1/1/1/1	-
6	EDO	A	1020	-	-	0/1/1/1	-
6	EDO	A	1013	-	-	0/1/1/1	-
5	PGE	A	1008	-	-	4/7/7/7	-
6	EDO	A	1015	-	-	0/1/1/1	-
6	EDO	C	1011	-	-	0/1/1/1	-
6	EDO	A	1006	-	-	1/1/1/1	-
5	PGE	G	1101	-	-	4/7/7/7	-
6	EDO	A	1019	-	-	1/1/1/1	-
6	EDO	C	1007	-	-	0/1/1/1	-
10	PEG	A	1014	-	-	2/4/4/4	-
6	EDO	C	1020	-	-	1/1/1/1	-
6	EDO	C	1017	-	-	1/1/1/1	-
10	PEG	B	1801	-	-	3/4/4/4	-
6	EDO	C	1015	-	-	0/1/1/1	-

The worst 5 of 24 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	A	1001	WAV	O7-N3	11.58	1.42	1.22
9	C	1001	WAV	O7-N3	11.34	1.42	1.22
9	C	1001	WAV	N4-N5	-5.84	1.35	1.41
9	A	1001	WAV	N4-N5	-5.81	1.35	1.41
9	C	1001	WAV	O2-C2	-4.75	1.36	1.44

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	C	1001	WAV	C15-C16-C17	3.34	121.80	119.57
9	C	1001	WAV	C16-C17-C12	-2.23	119.51	121.55
9	A	1001	WAV	C5-C6-N1	-2.16	105.71	109.66
9	A	1001	WAV	C15-C16-C17	2.14	121.00	119.57

There are no chirality outliers.

5 of 82 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	A	1001	WAV	C13-C12-N2-C11
9	A	1001	WAV	C17-C12-N2-C11
9	C	1001	WAV	C17-C12-N2-C11
10	J	1201	PEG	C1-C2-O2-C3

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Mol	Chain	Res	Type	Atoms
9	C	1001	WAV	C13-C12-N2-C11

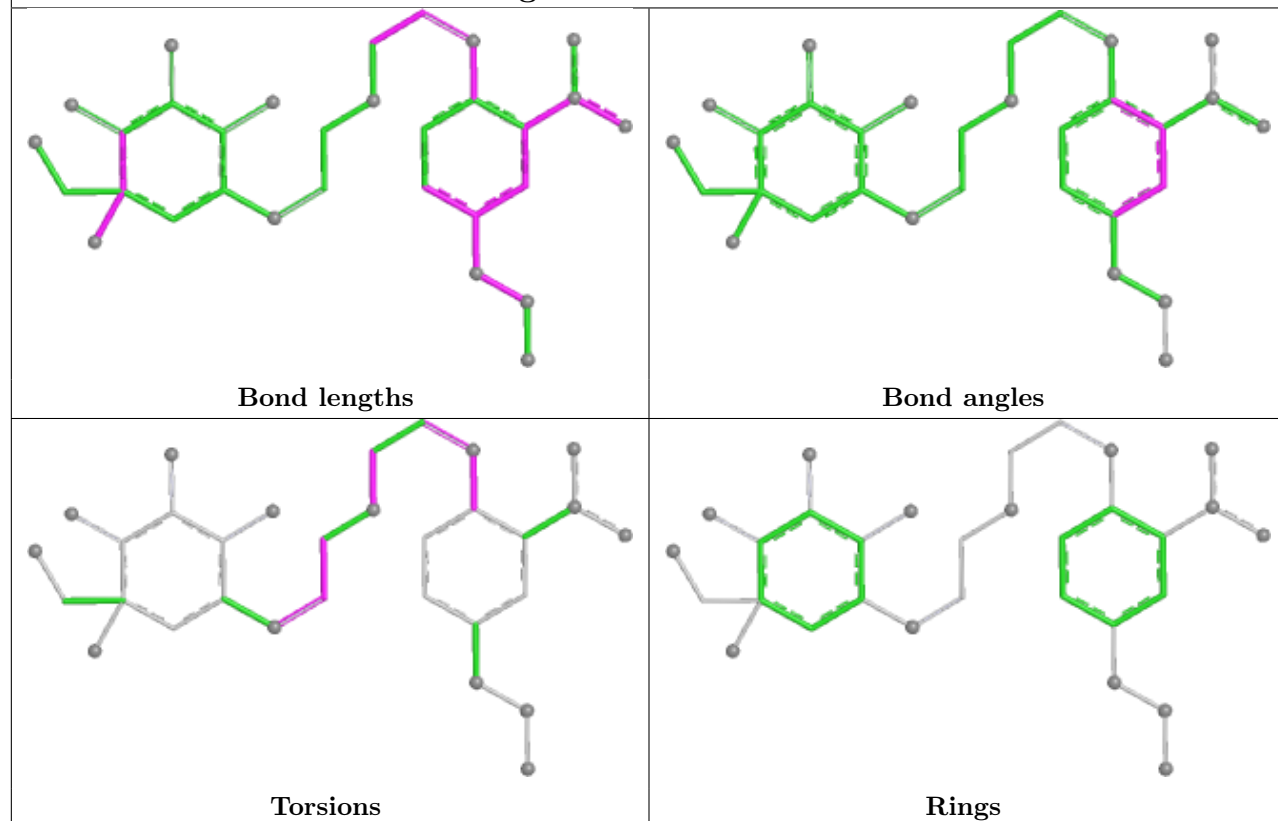
There are no ring outliers.

19 monomers are involved in 23 short contacts:

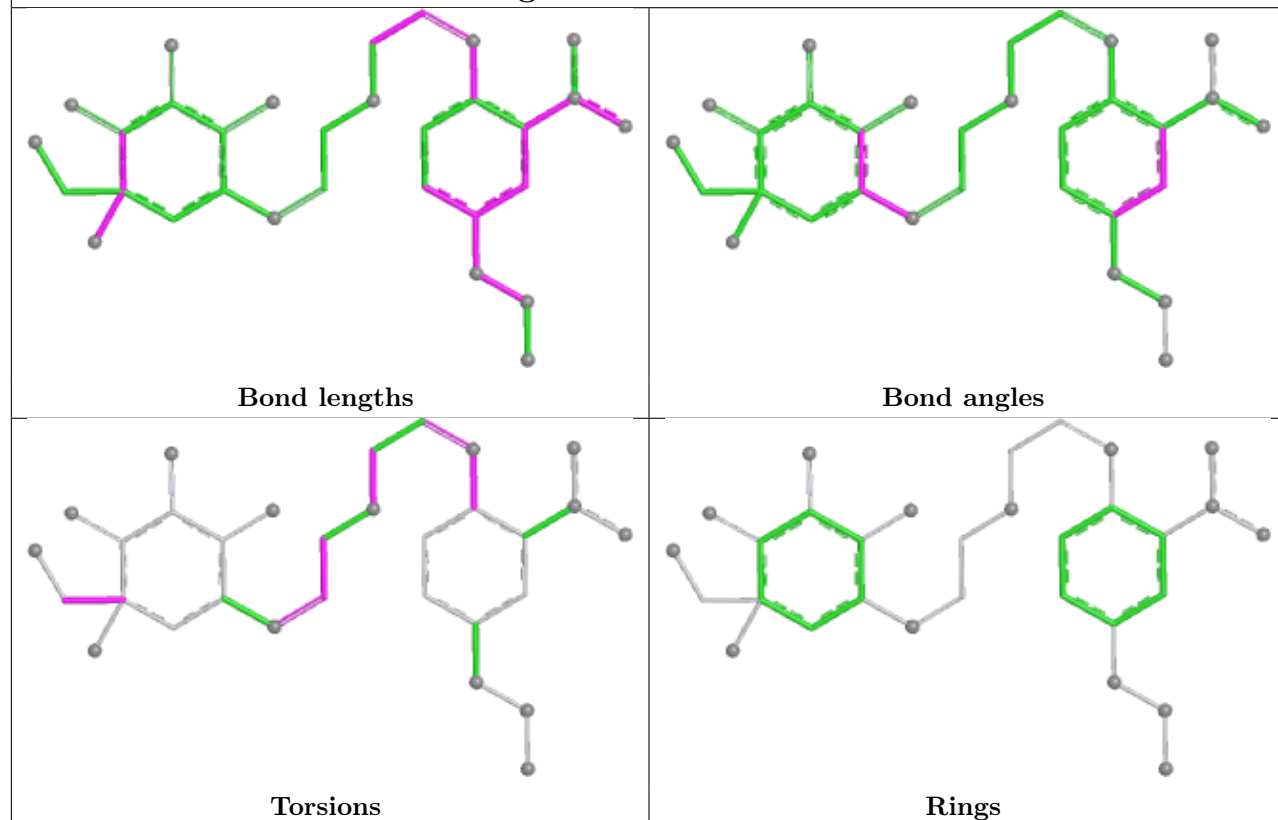
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	C	1021	EDO	2	0
6	D	1402	EDO	1	0
10	I	1601	PEG	1	0
9	C	1001	WAV	1	0
6	C	1002	EDO	1	0
9	A	1001	WAV	1	0
6	H	1303	EDO	1	0
10	C	1006	PEG	2	0
5	A	1007	PGE	1	0
10	C	1016	PEG	2	0
6	C	1013	EDO	1	0
6	A	1017	EDO	1	0
10	B	1802	PEG	1	0
6	A	1006	EDO	1	0
5	G	1101	PGE	2	0
6	A	1019	EDO	1	0
10	A	1014	PEG	1	0
6	C	1017	EDO	1	0
10	B	1801	PEG	1	0

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

Ligand WAV C 1001



Ligand WAV A 1001



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	G	152/184 (82%)	0.19	7 (4%) 37 34	29, 43, 73, 106	0
1	I	153/184 (83%)	1.19	22 (14%) 6 4	36, 66, 88, 96	0
2	H	105/107 (98%)	-0.14	6 (5%) 29 26	24, 33, 71, 81	0
2	J	107/107 (100%)	0.33	5 (4%) 36 33	30, 47, 76, 101	1 (0%)
3	A	597/609 (98%)	-0.55	2 (0%) 90 89	15, 31, 52, 75	10 (1%)
3	C	597/609 (98%)	-0.32	5 (0%) 82 81	15, 35, 55, 92	10 (1%)
4	B	82/134 (61%)	0.63	15 (18%) 3 2	32, 48, 87, 102	0
4	D	84/134 (62%)	0.64	14 (16%) 4 3	29, 49, 95, 103	0
All	All	1877/2068 (90%)	-0.10	76 (4%) 42 39	15, 37, 75, 106	21 (1%)

The worst 5 of 76 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	B	48	PHE	5.8
1	G	184	PRO	5.4
4	D	43	THR	4.5
4	D	48	PHE	4.5
1	G	183	ALA	4.4

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

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(Å ²)	Q<0.9
7	SO4	C	1025	5/5	0.58	0.15	84,86,98,120	0
7	SO4	G	1103	5/5	0.64	0.13	101,105,110,123	0
10	PEG	I	1601	7/7	0.75	0.20	71,78,82,94	0
6	EDO	C	1011	4/4	0.77	0.19	60,61,62,67	0
6	EDO	C	1005	4/4	0.78	0.21	55,67,70,82	0
10	PEG	A	1010	7/7	0.80	0.18	52,57,66,70	0
7	SO4	J	1202	5/5	0.81	0.18	65,80,84,122	0
6	EDO	C	1002	4/4	0.81	0.17	56,58,59,60	0
5	PGE	A	1021	10/10	0.81	0.18	53,62,75,77	0
7	SO4	B	1803	5/5	0.81	0.10	85,91,115,123	0
7	SO4	C	1024	5/5	0.82	0.12	72,78,91,104	0
7	SO4	J	1203	5/5	0.82	0.14	68,75,101,114	0
5	PGE	A	1007	10/10	0.83	0.17	49,57,73,76	0
10	PEG	C	1022	7/7	0.83	0.16	61,70,76,84	0
10	PEG	D	1403	7/7	0.83	0.17	56,62,75,78	0
8	PG4	A	1002	13/13	0.84	0.18	53,60,74,91	0
10	PEG	C	1003	7/7	0.85	0.16	41,55,64,72	0
10	PEG	J	1201	7/7	0.86	0.16	57,59,69,75	0
8	PG4	H	1301	13/13	0.86	0.15	54,62,75,85	0
10	PEG	B	1801	7/7	0.86	0.16	53,59,64,65	0
6	EDO	H	1302	4/4	0.86	0.20	45,51,52,52	0
10	PEG	B	1802	7/7	0.87	0.15	58,60,67,77	0
6	EDO	C	1007	4/4	0.87	0.14	36,49,57,59	0
5	PGE	A	1003	10/10	0.87	0.15	48,55,67,73	0
6	EDO	A	1005	4/4	0.88	0.19	42,42,54,56	0
10	PEG	C	1016	7/7	0.88	0.14	55,61,65,66	0
6	EDO	C	1012	4/4	0.88	0.17	45,54,61,65	0
6	EDO	C	1009	4/4	0.88	0.15	39,40,54,58	0
5	PGE	A	1008	10/10	0.89	0.14	55,67,78,78	0
7	SO4	C	1023	5/5	0.89	0.14	68,70,72,92	0
10	PEG	C	1006	7/7	0.89	0.13	53,53,67,67	0
7	SO4	A	1022	5/5	0.89	0.11	65,70,79,109	0
6	EDO	A	1013	4/4	0.89	0.17	50,57,61,70	0
6	EDO	C	1018	4/4	0.89	0.13	45,56,60,68	0
6	EDO	A	1019	4/4	0.90	0.17	42,42,49,53	0
6	EDO	A	1016	4/4	0.90	0.12	44,53,57,60	0
6	EDO	A	1018	4/4	0.91	0.12	50,52,53,55	0

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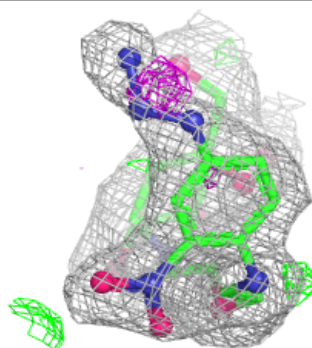
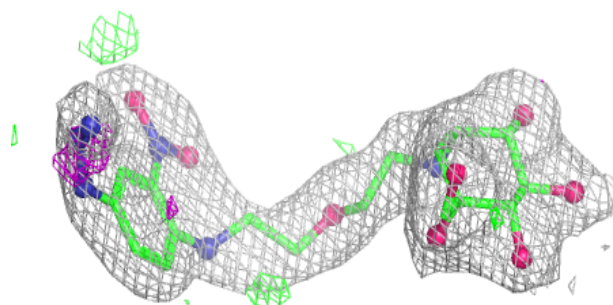
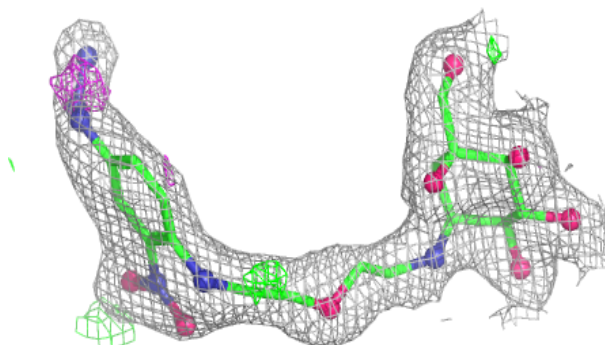
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	EDO	C	1021	4/4	0.91	0.13	50,54,60,71	0
6	EDO	D	1401	4/4	0.91	0.12	46,49,49,50	0
6	EDO	D	1402	4/4	0.91	0.13	53,53,58,70	0
5	PGE	G	1101	10/10	0.91	0.12	44,56,61,62	0
6	EDO	C	1015	4/4	0.91	0.16	40,45,55,63	0
6	EDO	C	1017	4/4	0.92	0.13	42,47,51,55	0
6	EDO	A	1011	4/4	0.92	0.16	40,48,55,57	0
10	PEG	A	1014	7/7	0.92	0.10	54,57,66,69	0
6	EDO	C	1019	4/4	0.92	0.12	42,42,52,60	0
6	EDO	C	1014	4/4	0.92	0.12	37,47,47,60	0
6	EDO	C	1004	4/4	0.92	0.12	46,54,55,59	0
6	EDO	A	1015	4/4	0.93	0.10	41,43,46,54	0
6	EDO	A	1006	4/4	0.93	0.10	50,50,51,65	0
6	EDO	A	1020	4/4	0.93	0.17	49,53,55,58	0
6	EDO	A	1012	4/4	0.94	0.14	35,47,47,53	0
9	WAV	A	1001	31/31	0.94	0.10	27,38,60,76	0
9	WAV	C	1001	31/31	0.94	0.11	25,47,62,82	0
6	EDO	C	1008	4/4	0.94	0.10	40,41,54,60	0
6	EDO	C	1020	4/4	0.94	0.09	44,44,49,61	0
6	EDO	A	1009	4/4	0.94	0.10	38,45,49,52	0
6	EDO	A	1017	4/4	0.94	0.12	40,52,53,60	0
6	EDO	C	1013	4/4	0.95	0.10	40,41,55,56	0
6	EDO	A	1004	4/4	0.95	0.10	42,45,46,72	0
6	EDO	C	1010	4/4	0.95	0.10	39,40,54,57	0
6	EDO	H	1303	4/4	0.97	0.07	36,41,45,46	0
6	EDO	G	1102	4/4	0.98	0.06	36,37,42,46	0
11	CA	B	1804	1/1	0.99	0.02	41,41,41,41	0
11	CA	B	1805	1/1	0.99	0.02	33,33,33,33	0
11	CA	D	1404	1/1	0.99	0.04	40,40,40,40	0
11	CA	D	1405	1/1	1.00	0.01	31,31,31,31	0

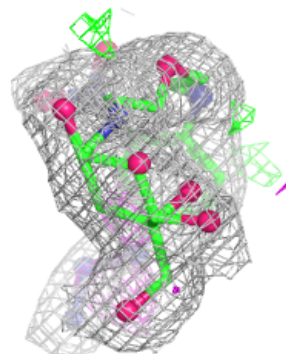
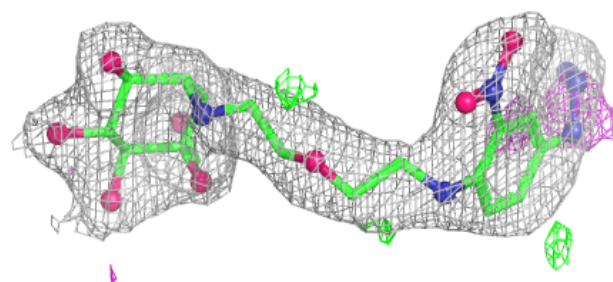
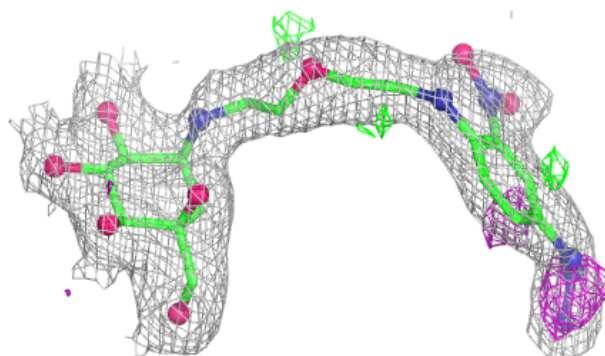
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around WAV 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 WAV 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.