wwPDB X-ray Structure Validation Summary Report (i)

Dec 15, 2024 – 10:53 PM EST

PDB ID	:	7KBJ
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 (i) 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 (i)) were used in the production of this report:

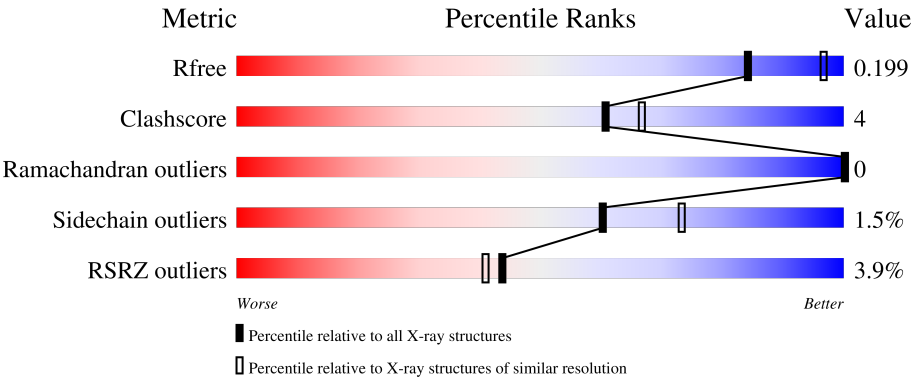
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.21
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.004 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.40

1 Overall quality at a glance (i)

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}	164625	7167 (2.24-2.20)
Clashscore	180529	8096 (2.24-2.20)
Ramachandran outliers	177936	8010 (2.24-2.20)
Sidechain outliers	177891	8011 (2.24-2.20)
RSRZ outliers	164620	7166 (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 <=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	11% 74% 9% 17%
2	H	107	6% 88% 9%
2	J	107	5% 90% 10%
3	A	609	88% 10%

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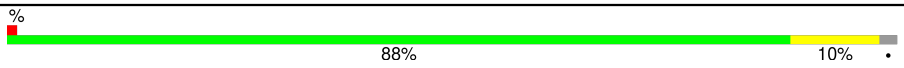
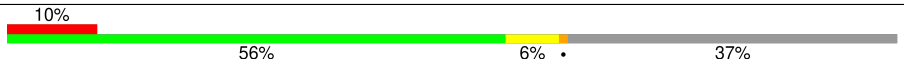
Mol	Chain	Length	Quality of chain
3	C	609	
4	B	134	
4	D	134	

2 Entry composition (i)

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	C	N	O	S	0	0	0
			607	362	99	136	10			
4	D	84	Total	C	N	O	S	0	0	0
			622	371	102	139	10			

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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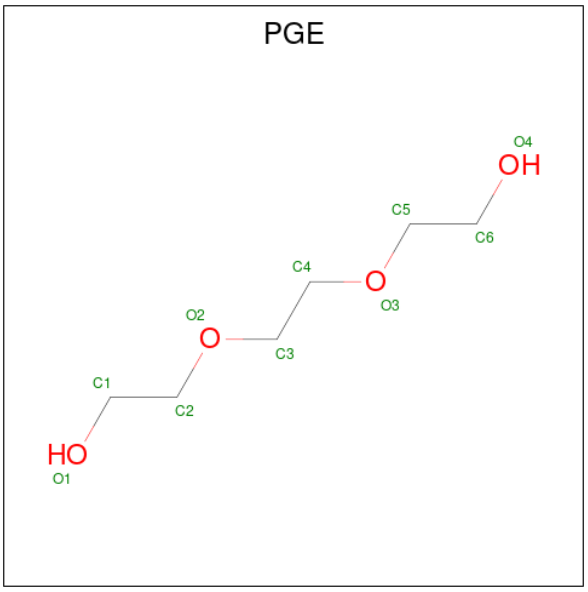
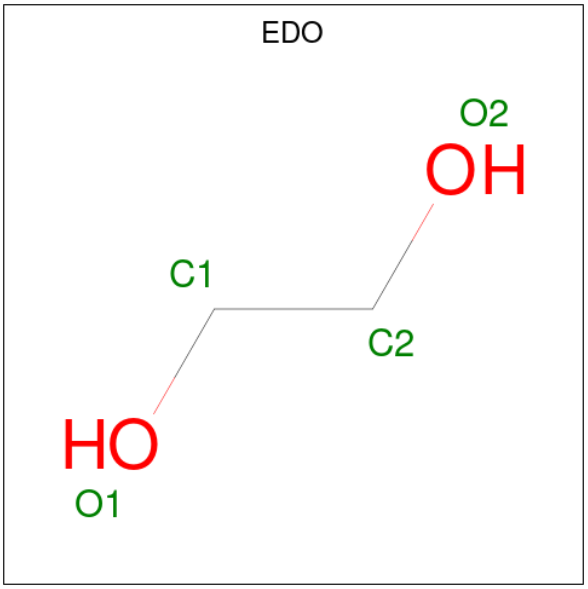
Chain	Residue	Modelled	Actual	Comment	Reference
D	-12	PRO	-	expression tag	UNP O08795
D	-11	SER	-	expression tag	UNP O08795
D	-10	PRO	-	expression tag	UNP O08795
D	-9	GLY	-	expression tag	UNP O08795
D	-8	MET	-	expression tag	UNP O08795
D	-7	PRO	-	expression tag	UNP O08795
D	-6	ALA	-	expression tag	UNP 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 (three-letter code: PGE) (formula: $C_6H_{14}O_4$).



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

- Molecule 6 is 1,2-ETHANEDIOL (three-letter code: 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
6	C	1	Total C O 4 2 2	0	0

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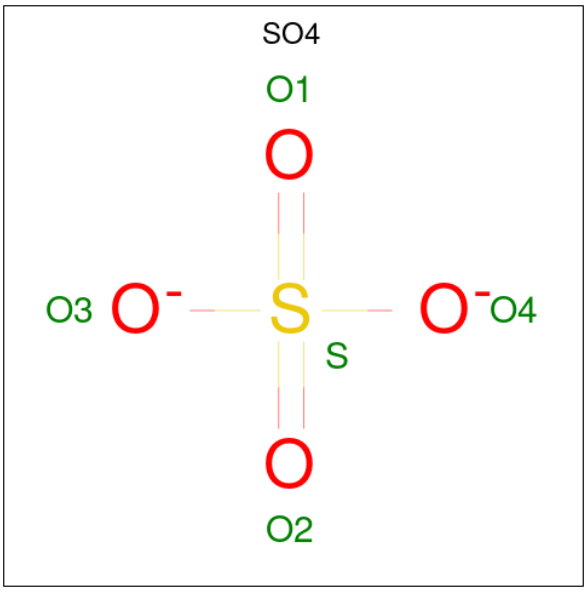
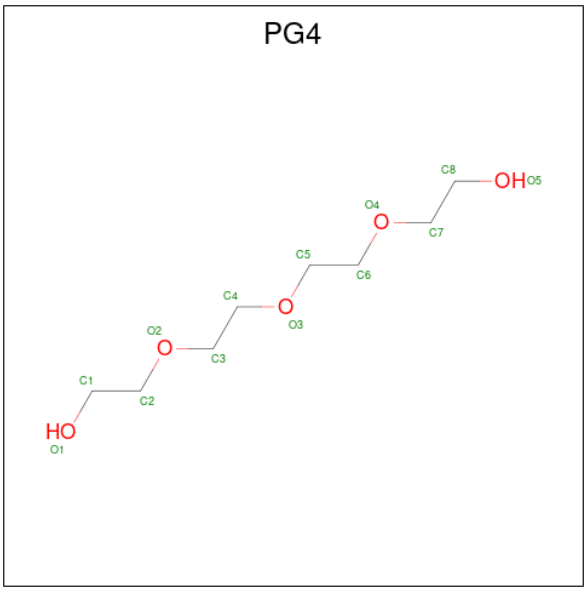
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	C	1	Total C O 4 2 2	0	0
6	C	1	Total C O 4 2 2	0	0
6	C	1	Total C O 4 2 2	0	0
6	C	1	Total C O 4 2 2	0	0
6	C	1	Total C O 4 2 2	0	0
6	C	1	Total C O 4 2 2	0	0
6	C	1	Total C O 4 2 2	0	0
6	C	1	Total C O 4 2 2	0	0
6	C	1	Total C O 4 2 2	0	0
6	C	1	Total C O 4 2 2	0	0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

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



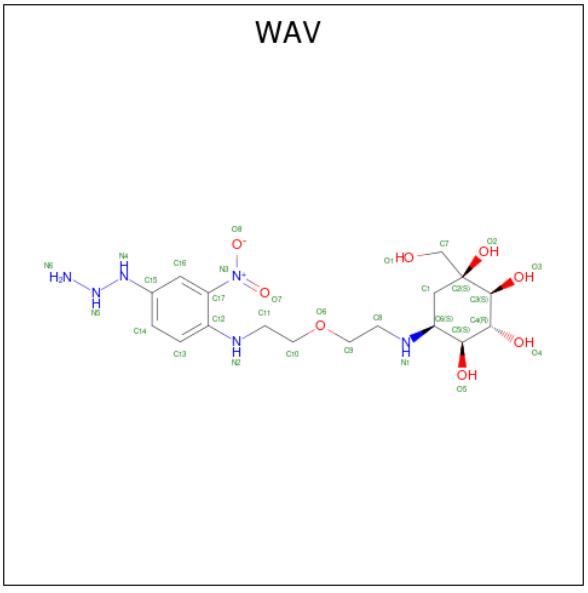
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	G	1	Total O S 5 4 1	0	0
7	A	1	Total O S 5 4 1	0	0
7	B	1	Total O S 5 4 1	0	0
7	J	1	Total O S 5 4 1	0	0
7	J	1	Total O S 5 4 1	0	0
7	C	1	Total O S 5 4 1	0	0
7	C	1	Total O S 5 4 1	0	0
7	C	1	Total O S 5 4 1	0	0

- Molecule 8 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: $C_8H_{18}O_5$).



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

- 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 (three-letter code: WAV) (formula: $C_{17}H_{30}N_6O_8$) (labeled as "Ligand of Interest" by depositor).



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

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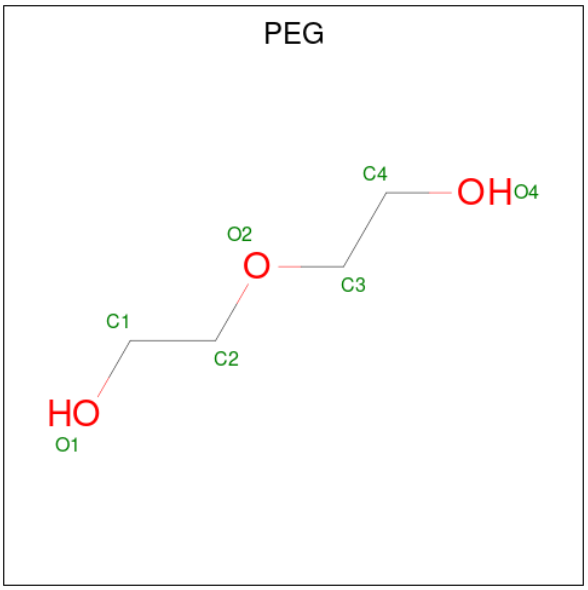
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	C	1	Total C N O 31 17 6 8	0	0

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



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

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

- Molecule 11 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

- Molecule 12 is water.

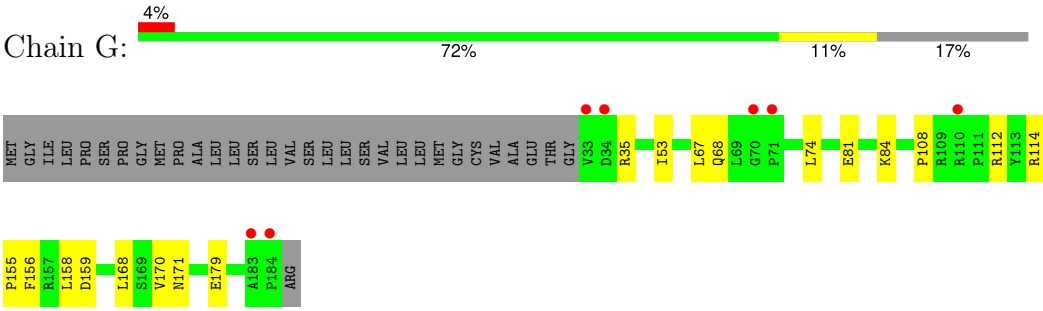
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
12	G	85	Total O 85 85	0	0
12	H	62	Total O 62 62	0	0
12	A	358	Total O 358 358	0	0
12	B	41	Total O 41 41	0	0
12	I	47	Total O 47 47	0	0
12	J	55	Total O 55 55	0	0
12	C	315	Total O 315 315	0	0
12	D	40	Total O 40 40	0	0

3 Residue-property plots

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

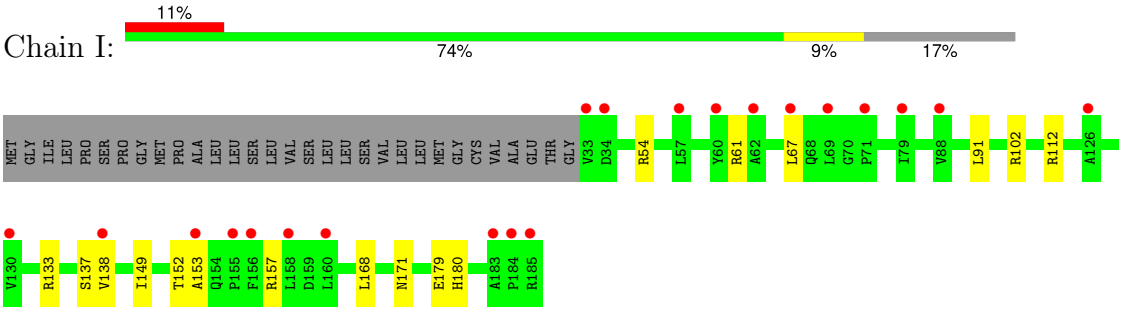
• Molecule 1: Neutral alpha-glucosidase AB Trypsin-cleaved Fragment #1

Chain G:



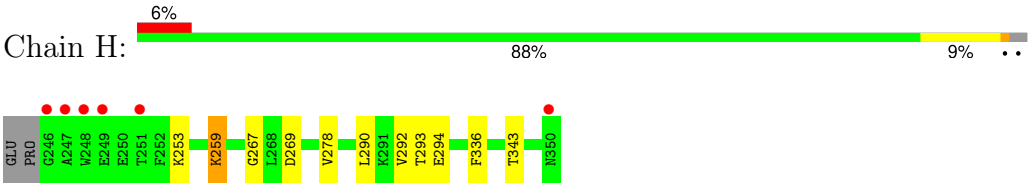
• Molecule 1: Neutral alpha-glucosidase AB Trypsin-cleaved Fragment #1

Chain I:



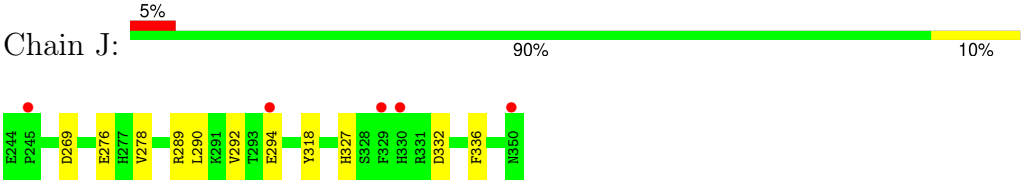
• Molecule 2: Neutral alpha-glucosidase AB Trypsin-cleaved Fragment #2

Chain H:



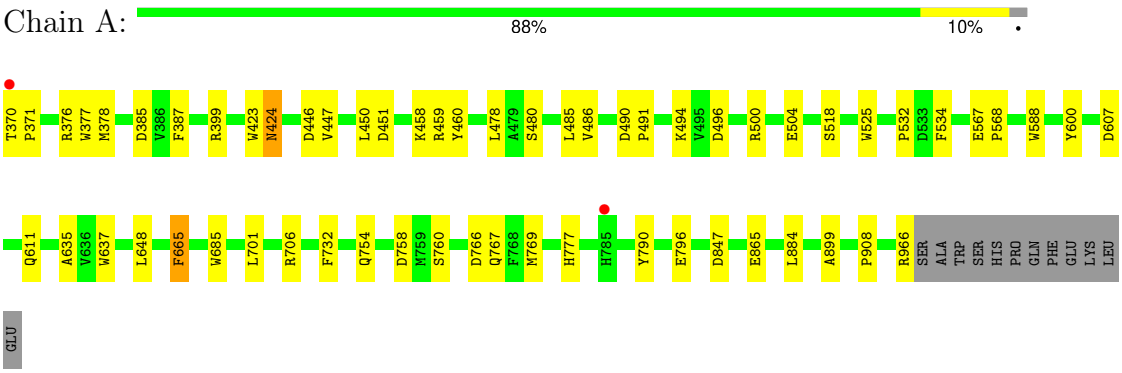
• Molecule 2: Neutral alpha-glucosidase AB Trypsin-cleaved Fragment #2

Chain J:



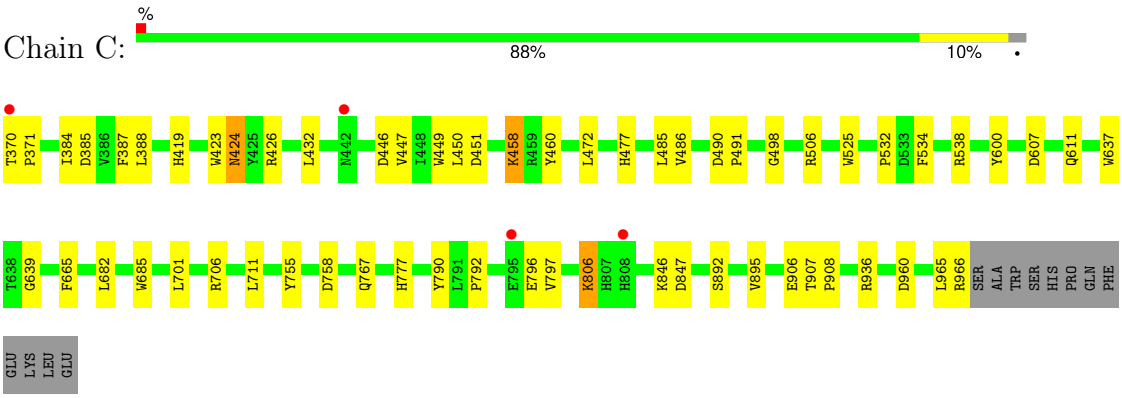
• Molecule 3: Neutral alpha-glucosidase AB Trypsin-cleaved Fragment #3

Chain A:



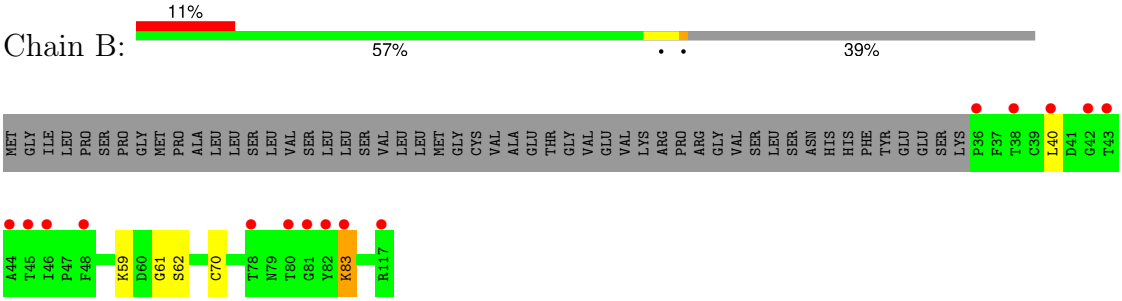
• Molecule 3: Neutral alpha-glucosidase AB Trypsin-cleaved Fragment #3

Chain C:



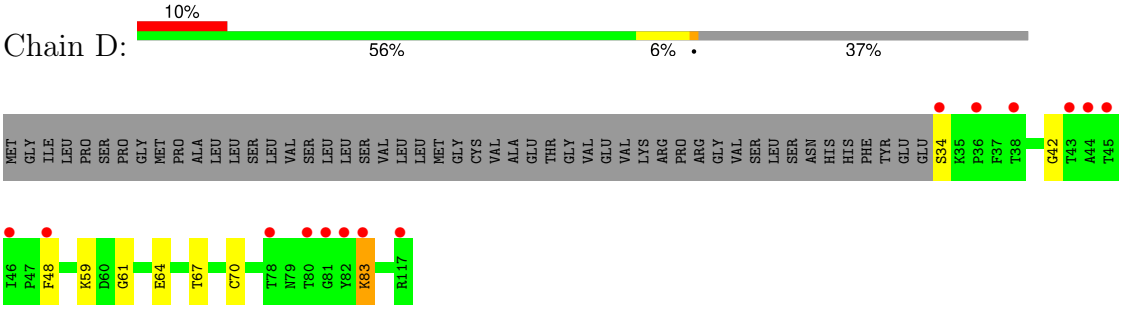
• Molecule 4: Glucosidase 2 subunit beta

Chain B:



• Molecule 4: Glucosidase 2 subunit beta

Chain D:



4 Data and refinement statistics (i)

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
$< I/\sigma(I) >$ [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	137977 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]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PGE, PG4, SO4, CA, WAV, 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	G	0.31	0/1229	0.56	1/1666 (0.1%)
1	I	0.29	0/1233	0.54	0/1672
2	H	0.36	0/865	0.54	0/1181
2	J	0.32	0/891	0.53	0/1216
3	A	0.35	0/5082	0.55	0/6919
3	C	0.34	0/5078	0.54	0/6914
4	B	0.33	0/619	0.57	0/842
4	D	0.31	0/634	0.57	0/862
All	All	0.34	0/15631	0.54	1/21272 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	G	168	LEU	CA-CB-CG	5.18	127.21	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	13	0
1	I	1213	0	1240	14	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	H	837	0	783	11	0
2	J	859	0	809	7	0
3	A	4889	0	4676	38	0
3	C	4885	0	4670	36	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	125	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 125 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%)	135 (99%)	1 (1%)	81 89
1	I	136/163 (83%)	134 (98%)	2 (2%)	60 73
2	H	90/92 (98%)	89 (99%)	1 (1%)	70 81
2	J	93/92 (101%)	93 (100%)	0	100 100
3	A	528/529 (100%)	522 (99%)	6 (1%)	70 81
3	C	527/529 (100%)	516 (98%)	11 (2%)	48 61
4	B	71/116 (61%)	70 (99%)	1 (1%)	62 75
4	D	73/116 (63%)	71 (97%)	2 (3%)	40 51
All	All	1654/1800 (92%)	1630 (98%)	24 (2%)	60 73

5 of 24 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	C	637	TRP
3	C	706	ARG
3	C	685	TRP
3	C	797	VAL
3	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
3	C	808	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 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	1007	-	9,9,9	0.37	0	8,8,8	0.35	0
8	PG4	A	1002	-	12,12,12	0.54	0	11,11,11	0.27	0
6	EDO	G	1102	-	3,3,3	0.40	0	2,2,2	0.47	0
6	EDO	C	1019	-	3,3,3	0.48	0	2,2,2	0.40	0
6	EDO	D	1402	-	3,3,3	0.45	0	2,2,2	0.24	0
6	EDO	A	1015	-	3,3,3	0.42	0	2,2,2	0.24	0
6	EDO	C	1011	-	3,3,3	0.48	0	2,2,2	0.32	0
7	SO4	J	1202	-	4,4,4	0.32	0	6,6,6	0.24	0
10	PEG	A	1010	-	6,6,6	0.52	0	5,5,5	0.35	0
6	EDO	A	1019	-	3,3,3	0.33	0	2,2,2	0.65	0
6	EDO	C	1010	-	3,3,3	0.48	0	2,2,2	0.24	0
7	SO4	B	1803	-	4,4,4	0.27	0	6,6,6	0.04	0
5	PGE	A	1003	-	9,9,9	0.36	0	8,8,8	0.35	0
10	PEG	C	1016	-	6,6,6	0.50	0	5,5,5	0.27	0
6	EDO	C	1020	-	3,3,3	0.44	0	2,2,2	0.45	0
6	EDO	A	1006	-	3,3,3	0.49	0	2,2,2	0.31	0
7	SO4	G	1103	-	4,4,4	0.26	0	6,6,6	0.11	0
6	EDO	C	1017	-	3,3,3	0.45	0	2,2,2	0.48	0
6	EDO	A	1011	-	3,3,3	0.41	0	2,2,2	0.48	0
6	EDO	C	1012	-	3,3,3	0.48	0	2,2,2	0.35	0
6	EDO	C	1021	-	3,3,3	0.46	0	2,2,2	0.29	0
10	PEG	C	1022	-	6,6,6	0.50	0	5,5,5	0.26	0
6	EDO	A	1009	-	3,3,3	0.36	0	2,2,2	0.72	0
6	EDO	D	1401	-	3,3,3	0.51	0	2,2,2	0.18	0
6	EDO	A	1017	-	3,3,3	0.38	0	2,2,2	0.47	0
5	PGE	A	1008	-	9,9,9	0.29	0	8,8,8	0.31	0
5	PGE	A	1021	-	9,9,9	0.41	0	8,8,8	0.32	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
6	EDO	A	1012	-	3,3,3	0.48	0	2,2,2	0.34	0
6	EDO	A	1013	-	3,3,3	0.43	0	2,2,2	0.34	0
6	EDO	H	1302	-	3,3,3	0.57	0	2,2,2	0.13	0
6	EDO	C	1002	-	3,3,3	0.49	0	2,2,2	0.25	0
6	EDO	C	1005	-	3,3,3	0.47	0	2,2,2	0.30	0
7	SO4	C	1023	-	4,4,4	0.23	0	6,6,6	0.30	0
6	EDO	C	1004	-	3,3,3	0.44	0	2,2,2	0.37	0
6	EDO	C	1018	-	3,3,3	0.44	0	2,2,2	0.44	0
6	EDO	H	1303	-	3,3,3	0.42	0	2,2,2	0.42	0
9	WAV	C	1001	-	32,32,32	3.09	12 (37%)	35,44,44	1.13	2 (5%)
10	PEG	C	1006	-	6,6,6	0.51	0	5,5,5	0.34	0
6	EDO	A	1016	-	3,3,3	0.43	0	2,2,2	0.41	0
10	PEG	A	1014	-	6,6,6	0.49	0	5,5,5	0.33	0
6	EDO	C	1008	-	3,3,3	0.37	0	2,2,2	0.47	0
6	EDO	C	1013	-	3,3,3	0.40	0	2,2,2	0.62	0
10	PEG	B	1801	-	6,6,6	0.55	0	5,5,5	0.45	0
10	PEG	B	1802	-	6,6,6	0.49	0	5,5,5	0.34	0
6	EDO	A	1018	-	3,3,3	0.47	0	2,2,2	0.36	0
8	PG4	H	1301	-	12,12,12	0.56	0	11,11,11	0.30	0
6	EDO	C	1014	-	3,3,3	0.52	0	2,2,2	0.33	0
10	PEG	I	1601	-	6,6,6	0.49	0	5,5,5	0.29	0
6	EDO	A	1004	-	3,3,3	0.39	0	2,2,2	0.42	0
10	PEG	D	1403	-	6,6,6	0.49	0	5,5,5	0.30	0
9	WAV	A	1001	-	32,32,32	3.09	12 (37%)	35,44,44	1.06	2 (5%)
5	PGE	G	1101	-	9,9,9	0.33	0	8,8,8	0.34	0
7	SO4	A	1022	-	4,4,4	0.23	0	6,6,6	0.25	0
6	EDO	A	1020	-	3,3,3	0.49	0	2,2,2	0.44	0
10	PEG	C	1003	-	6,6,6	0.48	0	5,5,5	0.44	0
7	SO4	C	1024	-	4,4,4	0.25	0	6,6,6	0.14	0
6	EDO	C	1007	-	3,3,3	0.43	0	2,2,2	0.44	0
10	PEG	J	1201	-	6,6,6	0.48	0	5,5,5	0.42	0
7	SO4	C	1025	-	4,4,4	0.23	0	6,6,6	0.17	0
7	SO4	J	1203	-	4,4,4	0.24	0	6,6,6	0.18	0
6	EDO	C	1015	-	3,3,3	0.45	0	2,2,2	0.73	0
6	EDO	A	1005	-	3,3,3	0.39	0	2,2,2	0.91	0
6	EDO	C	1009	-	3,3,3	0.40	0	2,2,2	0.45	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	1007	-	-	5/7/7/7	-
8	PG4	A	1002	-	-	6/10/10/10	-
6	EDO	G	1102	-	-	0/1/1/1	-
6	EDO	C	1019	-	-	0/1/1/1	-
6	EDO	D	1402	-	-	0/1/1/1	-
6	EDO	A	1015	-	-	0/1/1/1	-
6	EDO	C	1011	-	-	0/1/1/1	-
10	PEG	A	1010	-	-	0/4/4/4	-
6	EDO	A	1019	-	-	1/1/1/1	-
6	EDO	C	1010	-	-	1/1/1/1	-
10	PEG	C	1016	-	-	2/4/4/4	-
5	PGE	A	1003	-	-	5/7/7/7	-
6	EDO	C	1020	-	-	1/1/1/1	-
6	EDO	A	1006	-	-	1/1/1/1	-
6	EDO	C	1017	-	-	1/1/1/1	-
6	EDO	A	1011	-	-	1/1/1/1	-
6	EDO	C	1012	-	-	1/1/1/1	-
6	EDO	C	1021	-	-	1/1/1/1	-
10	PEG	C	1022	-	-	2/4/4/4	-
6	EDO	A	1009	-	-	1/1/1/1	-
6	EDO	D	1401	-	-	0/1/1/1	-
6	EDO	A	1017	-	-	1/1/1/1	-
5	PGE	A	1008	-	-	4/7/7/7	-
5	PGE	A	1021	-	-	1/7/7/7	-
6	EDO	A	1012	-	-	0/1/1/1	-
6	EDO	A	1013	-	-	0/1/1/1	-
6	EDO	H	1302	-	-	0/1/1/1	-
6	EDO	C	1002	-	-	1/1/1/1	-
6	EDO	C	1005	-	-	1/1/1/1	-
6	EDO	C	1004	-	-	0/1/1/1	-
6	EDO	C	1018	-	-	1/1/1/1	-
6	EDO	H	1303	-	-	0/1/1/1	-
9	WAV	C	1001	-	-	6/17/43/43	0/2/2/2
6	EDO	A	1016	-	-	0/1/1/1	-
10	PEG	A	1014	-	-	2/4/4/4	-
6	EDO	C	1008	-	-	0/1/1/1	-
6	EDO	C	1013	-	-	0/1/1/1	-
10	PEG	B	1801	-	-	3/4/4/4	-
10	PEG	B	1802	-	-	2/4/4/4	-
6	EDO	A	1018	-	-	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	C	1014	-	-	0/1/1/1	-
10	PEG	I	1601	-	-	1/4/4/4	-
6	EDO	A	1004	-	-	0/1/1/1	-
10	PEG	D	1403	-	-	4/4/4/4	-
9	WAV	A	1001	-	-	7/17/43/43	0/2/2/2
5	PGE	G	1101	-	-	4/7/7/7	-
6	EDO	A	1020	-	-	0/1/1/1	-
10	PEG	C	1003	-	-	1/4/4/4	-
10	PEG	J	1201	-	-	3/4/4/4	-
6	EDO	C	1007	-	-	0/1/1/1	-
10	PEG	C	1006	-	-	3/4/4/4	-
6	EDO	C	1015	-	-	0/1/1/1	-
6	EDO	A	1005	-	-	1/1/1/1	-
6	EDO	C	1009	-	-	1/1/1/1	-

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(^{o})	Ideal(^{o})
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

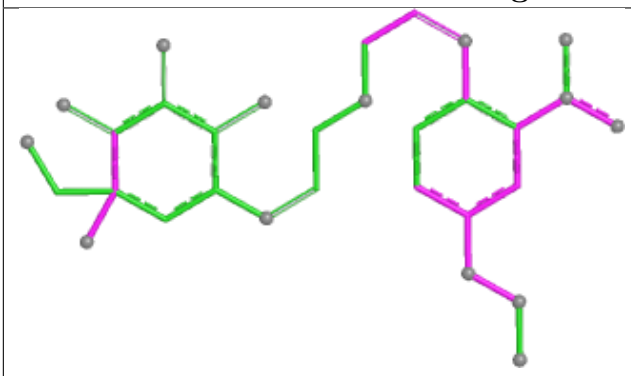
There are no ring outliers.

19 monomers are involved in 23 short contacts:

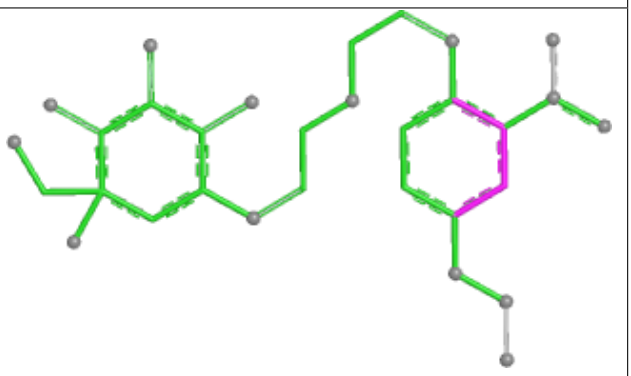
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1007	PGE	1	0
6	D	1402	EDO	1	0
6	A	1019	EDO	1	0
10	C	1016	PEG	2	0
6	A	1006	EDO	1	0
6	C	1017	EDO	1	0
6	C	1021	EDO	2	0
6	A	1017	EDO	1	0
6	C	1002	EDO	1	0
6	H	1303	EDO	1	0
9	C	1001	WAV	1	0
10	C	1006	PEG	2	0
10	A	1014	PEG	1	0
6	C	1013	EDO	1	0
10	B	1801	PEG	1	0
10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

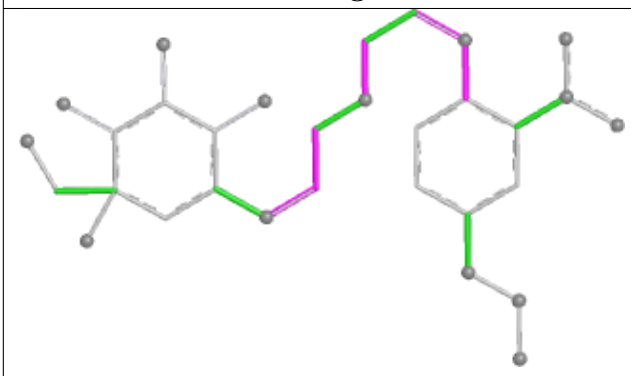
Ligand WAV C 1001



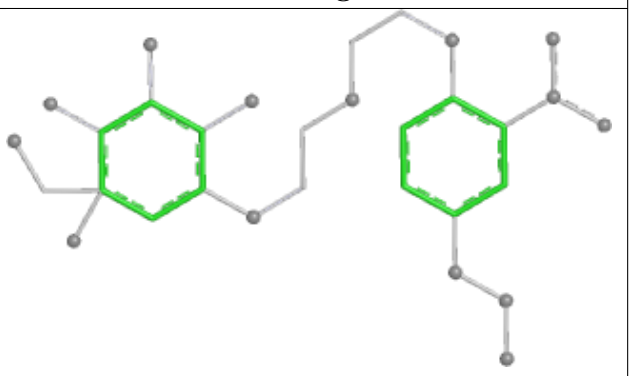
Bond lengths



Bond angles

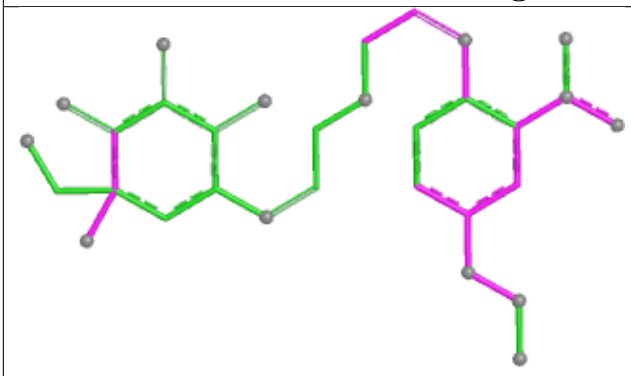


Torsions

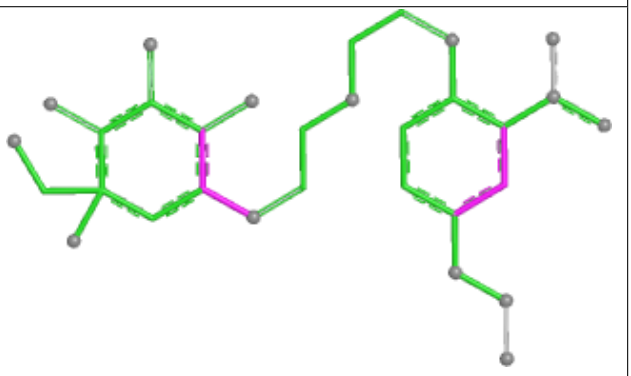


Rings

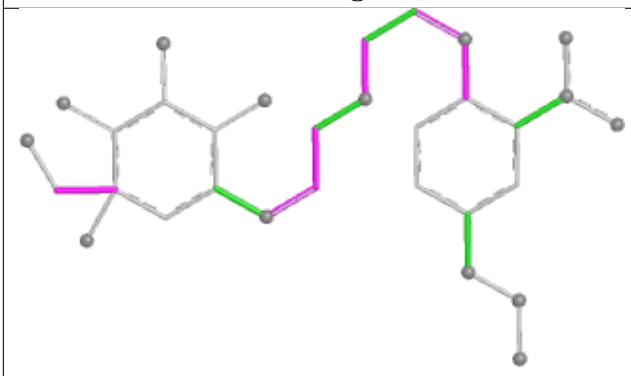
Ligand WAV A 1001



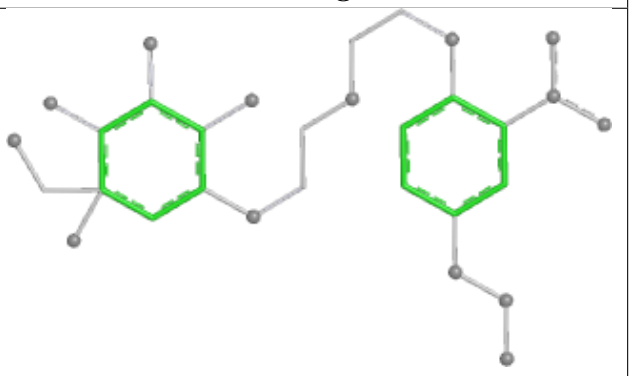
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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%)	0.09	7 (4%) 38 35	29, 43, 73, 106	0
1	I	153/184 (83%)	1.10	21 (13%) 8 6	36, 66, 88, 96	0
2	H	105/107 (98%)	-0.24	6 (5%) 30 28	24, 33, 71, 81	0
2	J	107/107 (100%)	0.23	5 (4%) 37 35	30, 47, 76, 101	1 (0%)
3	A	597/609 (98%)	-0.65	2 (0%) 90 89	15, 31, 52, 75	10 (1%)
3	C	597/609 (98%)	-0.42	4 (0%) 84 82	15, 35, 55, 92	10 (1%)
4	B	82/134 (61%)	0.53	15 (18%) 4 4	32, 48, 87, 102	0
4	D	84/134 (62%)	0.54	14 (16%) 5 4	29, 49, 95, 103	0
All	All	1877/2068 (90%)	-0.20	74 (3%) 44 41	15, 37, 75, 106	21 (1%)

The worst 5 of 74 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	B	48	PHE	5.6
1	G	184	PRO	5.3
4	D	43	THR	4.4
4	D	48	PHE	4.3
4	D	80	THR	4.3

6.2 Non-standard residues in protein, DNA, RNA chains

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

6.3 Carbohydrates

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} 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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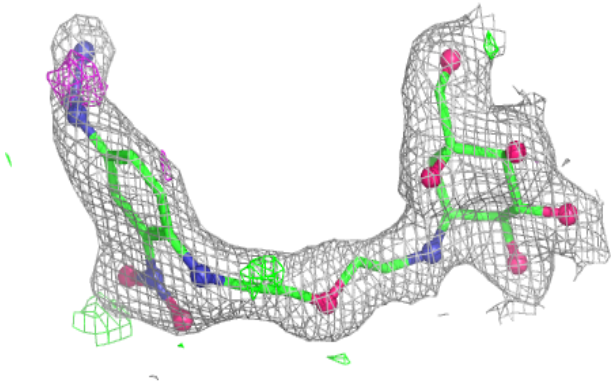
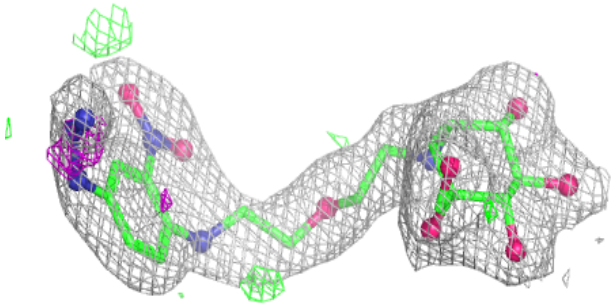
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	EDO	C	1021	4/4	0.91	0.13	50,54,60,71	0
6	EDO	D	1401	4/4	0.91	0.12	46,49,49,50	0
6	EDO	D	1402	4/4	0.91	0.13	53,53,58,70	0
5	PGE	G	1101	10/10	0.91	0.12	44,56,61,62	0
6	EDO	C	1015	4/4	0.91	0.16	40,45,55,63	0
6	EDO	C	1017	4/4	0.92	0.13	42,47,51,55	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

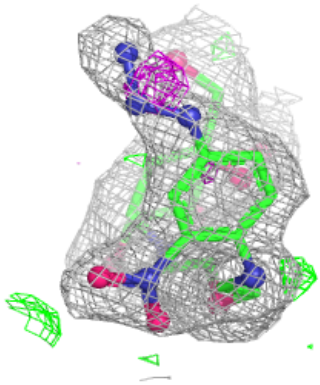
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

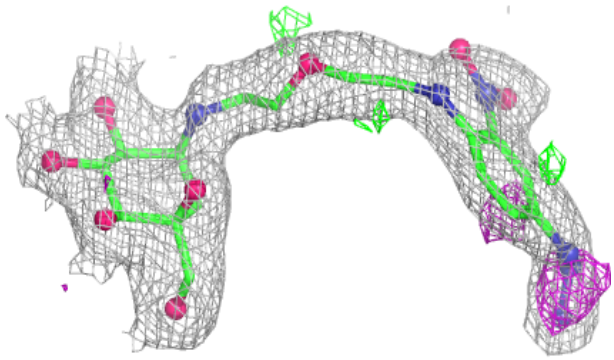


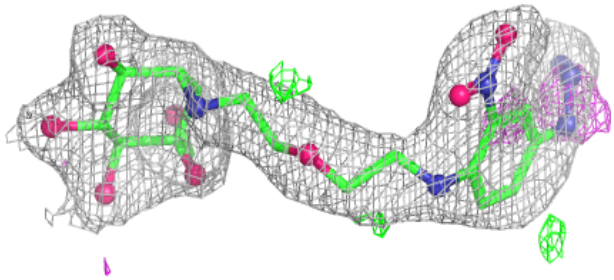


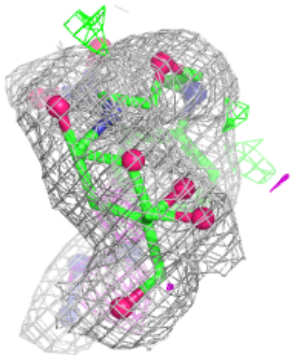


Electron density around WAV C 1001:

$2mF_o$-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.