



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 10:18 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 Full wwPDB X-ray Structure Validation 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

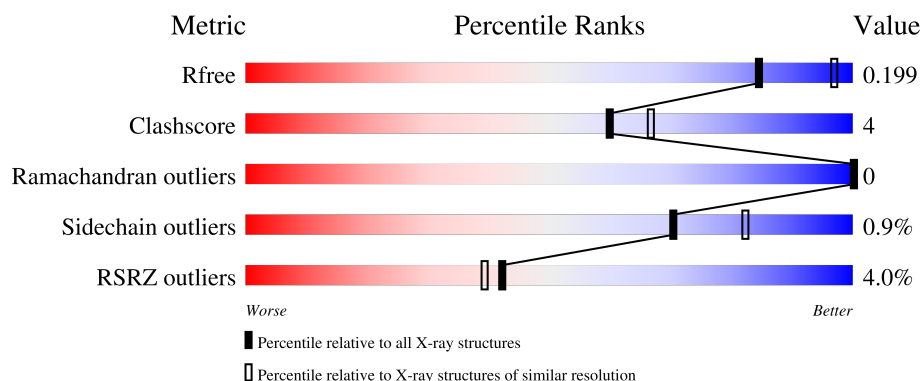
1 Overall quality at a glance

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% 39%
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:

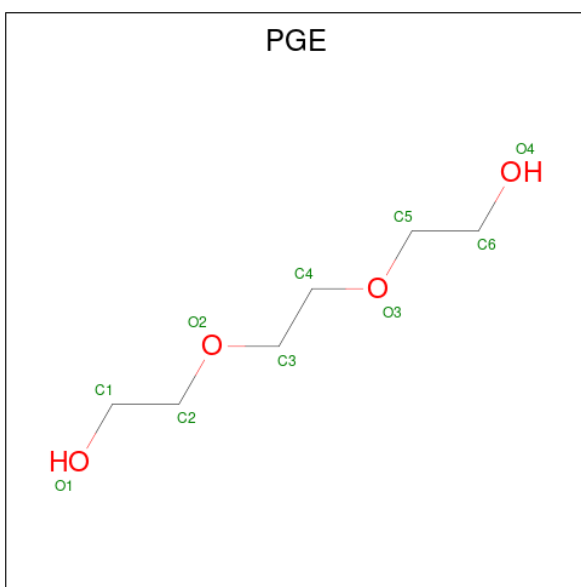
Chain	Residue	Modelled	Actual	Comment	Reference
B	-16	MET	-	initiating methionine	UNP O08795
B	-15	GLY	-	expression tag	UNP O08795
B	-14	ILE	-	expression tag	UNP O08795
B	-13	LEU	-	expression tag	UNP O08795
B	-12	PRO	-	expression tag	UNP O08795
B	-11	SER	-	expression tag	UNP O08795
B	-10	PRO	-	expression 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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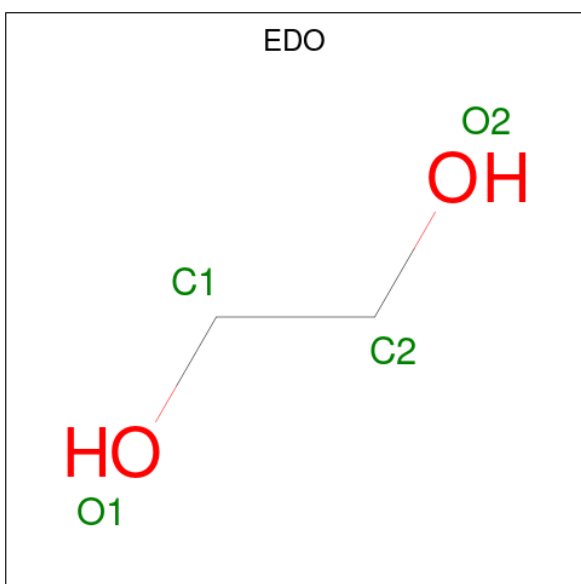
Chain	Residue	Modelled	Actual	Comment	Reference
D	-12	PRO	-	expression tag	UNP O08795
D	-11	SER	-	expression tag	UNP O08795
D	-10	PRO	-	expression tag	UNP O08795
D	-9	GLY	-	expression tag	UNP O08795
D	-8	MET	-	expression tag	UNP O08795
D	-7	PRO	-	expression tag	UNP O08795
D	-6	ALA	-	expression tag	UNP 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: C₂H₆O₂).



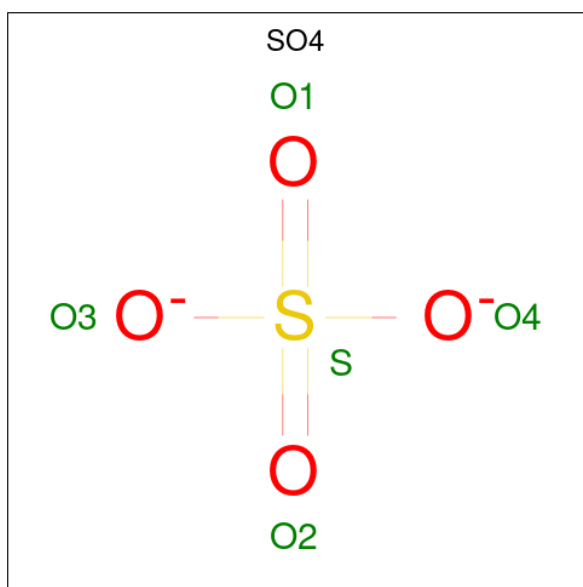
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	G	1	Total C O 4 2 2	0	0
6	H	1	Total C O 4 2 2	0	0
6	H	1	Total C O 4 2 2	0	0
6	A	1	Total C O 4 2 2	0	0
6	A	1	Total C O 4 2 2	0	0
6	A	1	Total C O 4 2 2	0	0
6	A	1	Total C O 4 2 2	0	0
6	A	1	Total C O 4 2 2	0	0
6	A	1	Total C O 4 2 2	0	0
6	A	1	Total C O 4 2 2	0	0
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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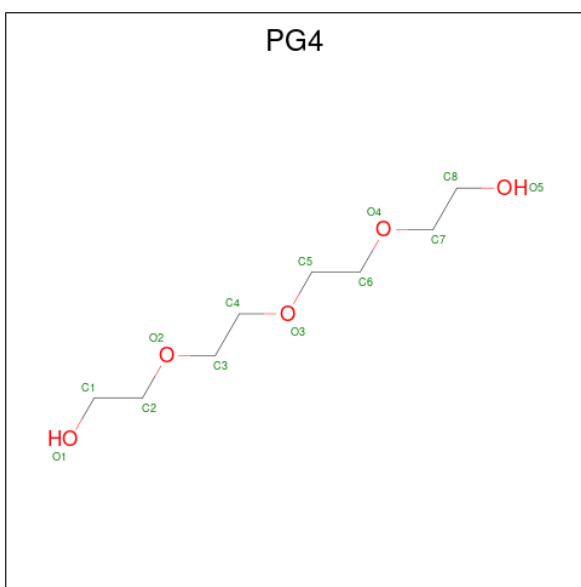
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	C	1	Total C O 4 2 2	0	0
6	C	1	Total C O 4 2 2	0	0
6	C	1	Total C O 4 2 2	0	0
6	C	1	Total C O 4 2 2	0	0
6	C	1	Total C O 4 2 2	0	0
6	C	1	Total C O 4 2 2	0	0
6	C	1	Total C O 4 2 2	0	0
6	C	1	Total C O 4 2 2	0	0
6	C	1	Total C O 4 2 2	0	0
6	C	1	Total C O 4 2 2	0	0
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 (CCD ID: SO4) (formula: O₄S).



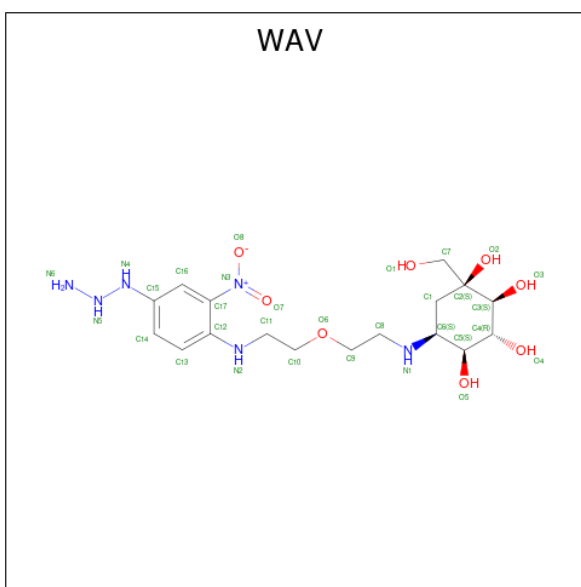
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	G	1	Total	O	S	0	0
			5	4	1		
7	A	1	Total	O	S	0	0
			5	4	1		
7	B	1	Total	O	S	0	0
			5	4	1		
7	J	1	Total	O	S	0	0
			5	4	1		
7	J	1	Total	O	S	0	0
			5	4	1		
7	C	1	Total	O	S	0	0
			5	4	1		
7	C	1	Total	O	S	0	0
			5	4	1		
7	C	1	Total	O	S	0	0
			5	4	1		

- 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).



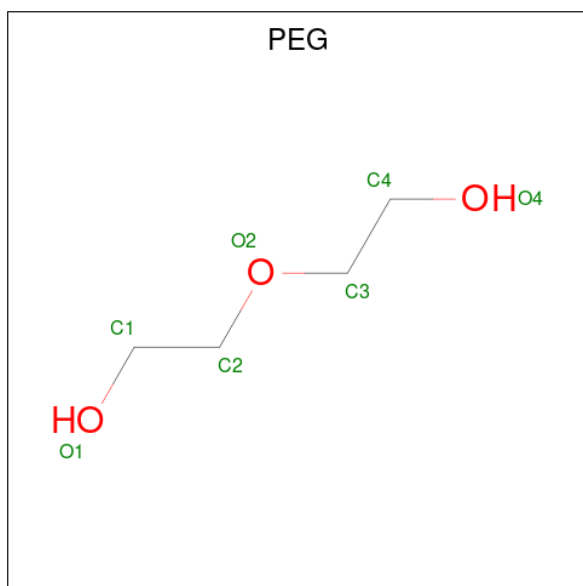
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	A	1	Total	C	N	O	0	0
			31	17	6	8		

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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		

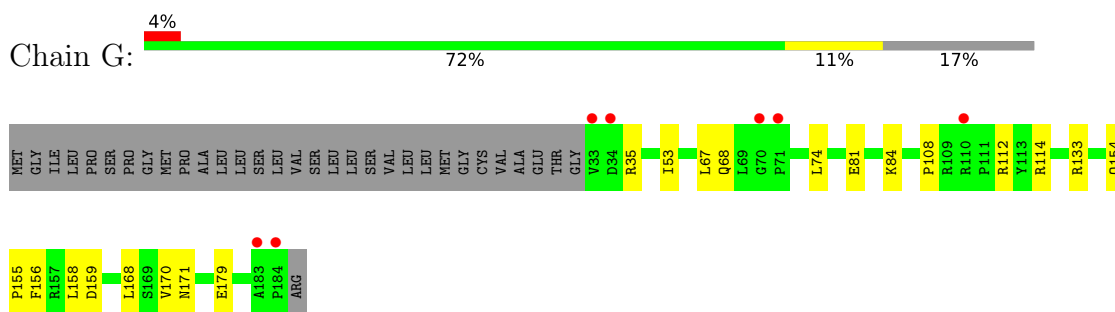
- Molecule 12 is water.

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		

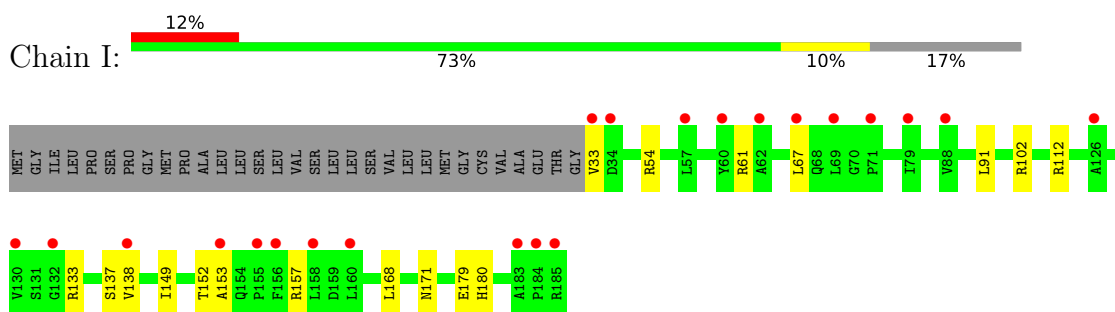
3 Residue-property plots [i](#)

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.

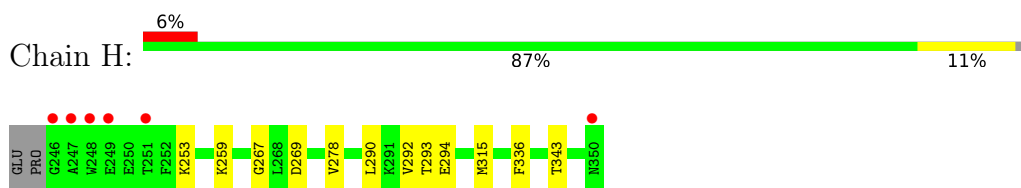
- Molecule 1: Neutral alpha-glucosidase AB Trypsin-cleaved Fragment #1



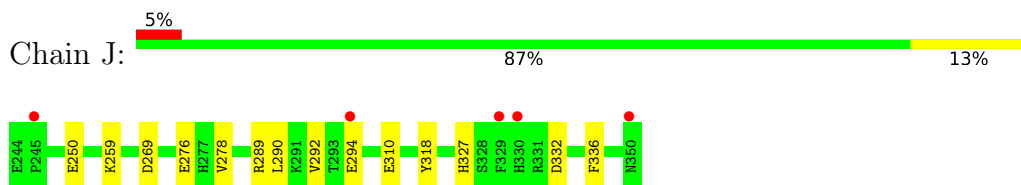
- Molecule 1: Neutral alpha-glucosidase AB Trypsin-cleaved Fragment #1



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



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



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

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.

All (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
1:G:156:PHE:O	12:G:1201:HOH:O	2.01	0.77
3:C:907:THR:H	6:C:1021:EDO:H11	1.50	0.77
3:C:385:ASP:OD2	12:C:1102:HOH:O	2.03	0.77
4:D:83:LYS:HD3	4:D:83:LYS:H	1.50	0.77
1:I:61:ARG:NH2	12:I:1703:HOH:O	2.12	0.74
1:G:159:ASP:OD2	12:G:1202:HOH:O	2.10	0.69
3:A:754[A]:GLN:HG3	3:A:769:MET:HE2	1.78	0.66
3:A:760:SER:HB2	10:A:1014:PEG:H31	1.76	0.66
3:A:385:ASP:OD2	12:A:1104:HOH:O	2.14	0.66
3:A:796:GLU:OE1	12:A:1103:HOH:O	2.13	0.66
3:C:607[B]:ASP:OD2	3:C:611:GLN:NE2	2.30	0.65
1:I:153:ALA:C	12:I:1701:HOH:O	2.40	0.65
3:A:518:SER:HA	5:A:1007:PGE:H32	1.77	0.64
3:A:607[B]:ASP:OD2	3:A:611:GLN:NE2	2.31	0.63
1:I:133:ARG:HD2	1:I:138:VAL:HG22	1.79	0.63
2:H:293:THR:HG22	6:H:1303:EDO:H21	1.82	0.61
2:H:294:GLU:OE2	12:H:1401:HOH:O	2.16	0.61
10:I:1601:PEG:O4	12:I:1704:HOH:O	2.17	0.60
3:A:480:SER:HA	10:B:1801:PEG:H11	1.83	0.60
3:C:423:TRP:O	3:C:701:LEU:HA	2.03	0.59
1:G:35:ARG:HD2	2:H:315:MET:HE1	1.85	0.58
2:J:336:PHE:HB3	3:C:387:PHE:HB2	1.85	0.58
6:C:1017:EDO:O1	12:C:1103:HOH:O	2.18	0.57
1:I:112:ARG:NH2	1:I:179:GLU:O	2.38	0.57
3:A:423:TRP:O	3:A:701:LEU:HA	2.04	0.57
1:G:81:GLU:O	1:G:84:LYS:NZ	2.38	0.56
1:G:112:ARG:NH2	1:G:179:GLU:O	2.39	0.56
4:B:59:LYS:HE3	10:B:1802:PEG:H41	1.88	0.56
3:A:865:GLU:OE2	12:A:1106:HOH:O	2.18	0.56
3:C:506:ARG:HH12	6:C:1002:EDO:H21	1.69	0.56
6:A:1006:EDO:O2	12:A:1105:HOH:O	2.18	0.55
2:H:292:VAL:HG12	2:H:294:GLU:H	1.71	0.55
9:A:1001:WAV:C11	9:A:1001:WAV:O7	2.55	0.54
9:C:1001:WAV:C11	9:C:1001:WAV:O7	2.55	0.54
3:A:766:ASP:OD2	12:A:1107:HOH:O	2.18	0.54
3:C:447:VAL:HG11	3:C:486:VAL:HG23	1.90	0.54
3:C:491:PRO:O	3:C:532:PRO:HD2	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:460:TYR:CE2	3:C:490:ASP:HB2	2.44	0.53
2:H:336:PHE:HB3	3:A:387:PHE:HB2	1.90	0.53
3:A:399:ARG:NH1	12:A:1111:HOH:O	2.27	0.52
3:C:960:ASP:HB3	10:C:1016:PEG:H41	1.90	0.52
1:G:158:LEU:HB2	1:G:170:VAL:HB	1.90	0.52
3:A:459:ARG:NH1	3:A:494:LYS:HE2	2.24	0.52
3:A:847:ASP:HB3	3:A:908:PRO:HG2	1.91	0.52
3:C:458:LYS:HG2	3:C:525:TRP:HB3	1.92	0.52
3:C:682:LEU:HD23	3:C:711:LEU:HD11	1.92	0.52
4:D:61:GLY:HA2	4:D:70:CYS:SG	2.50	0.51
1:I:180:HIS:ND1	12:I:1702:HOH:O	2.11	0.51
2:J:278:VAL:HG23	2:J:290:LEU:HB2	1.92	0.51
1:G:67:LEU:HD11	1:G:74:LEU:HD11	1.91	0.51
3:C:426:ARG:NH2	12:C:1107:HOH:O	2.29	0.51
2:J:327:HIS:ND1	2:J:332:ASP:OD1	2.37	0.51
1:G:108:PRO:HA	12:G:1218:HOH:O	2.10	0.50
3:A:491:PRO:O	3:A:532:PRO:HD2	2.11	0.50
3:C:758:ASP:OD2	3:C:790:TYR:OH	2.22	0.50
3:C:796:GLU:OE1	12:C:1104:HOH:O	2.20	0.50
3:C:847:ASP:HB3	3:C:908:PRO:HG2	1.93	0.49
3:A:447:VAL:HG11	3:A:486:VAL:HG23	1.94	0.49
1:G:171:ASN:HA	2:H:269:ASP:OD1	2.13	0.49
3:C:895:VAL:HG13	10:C:1016:PEG:H31	1.94	0.49
3:A:966:ARG:NH1	12:A:1109:HOH:O	2.25	0.49
2:J:250:GLU:OE1	2:J:259:LYS:NZ	2.39	0.49
3:C:424:ASN:OD1	3:C:451:ASP:HB3	2.12	0.48
2:J:276:GLU:O	2:J:289:ARG:NH2	2.40	0.48
3:A:767:GLN:HG3	3:A:777:HIS:ND1	2.29	0.48
2:J:292:VAL:HG12	2:J:294:GLU:H	1.79	0.47
3:C:534:PHE:HB3	3:C:600:TYR:HB3	1.95	0.47
3:A:424:ASN:OD1	3:A:451:ASP:HB3	2.14	0.47
3:A:450:LEU:HG	3:A:485:LEU:HD21	1.96	0.47
3:C:472:LEU:HD22	10:C:1006:PEG:H41	1.96	0.47
4:B:83:LYS:HD3	4:B:83:LYS:N	2.20	0.47
2:J:318:TYR:CE2	3:C:639:GLY:HA3	2.49	0.47
1:G:133:ARG:NH2	12:G:1211:HOH:O	2.47	0.46
3:A:370:THR:N	3:A:371:PRO:HD2	2.30	0.46
3:C:370:THR:N	3:C:371:PRO:HD2	2.31	0.45
1:G:114:ARG:H	5:G:1101:PGE:H5	1.82	0.45
3:A:478:LEU:CD1	3:A:485:LEU:HD12	2.47	0.45
1:I:91:LEU:HD21	1:I:149:ILE:HG21	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:G:1101:PGE:H52	3:A:588:TRP:CZ2	2.52	0.45
3:A:865:GLU:OE1	6:A:1017:EDO:O1	2.35	0.45
3:A:458:LYS:HG2	3:A:525:TRP:HB3	1.97	0.45
1:I:153:ALA:CA	12:I:1701:HOH:O	2.63	0.45
1:I:168:LEU:HD11	3:C:388:LEU:HD13	1.98	0.44
1:G:53:ILE:HB	3:A:376:ARG:HH22	1.82	0.44
3:A:648:LEU:HD13	3:A:685:TRP:CG	2.52	0.44
3:A:884:LEU:HG	3:A:899:ALA:HB3	1.99	0.43
3:A:635:ALA:HB2	3:A:665:PHE:CD2	2.54	0.43
4:B:61:GLY:HA2	4:B:70:CYS:SG	2.59	0.43
2:H:267:GLY:HA2	3:A:377:TRP:O	2.19	0.43
3:A:460:TYR:CE2	3:A:490:ASP:HB2	2.53	0.43
3:C:432:LEU:HD22	3:C:477[A]:HIS:ND1	2.34	0.43
3:C:450:LEU:HG	3:C:485:LEU:HD21	2.00	0.43
2:H:259:LYS:HD2	12:A:1302:HOH:O	2.19	0.43
3:A:534:PHE:HB3	3:A:600:TYR:HB3	2.01	0.43
4:D:42:GLY:N	12:D:1504:HOH:O	2.50	0.43
1:I:33:VAL:HG12	2:J:310:GLU:CD	2.43	0.43
1:G:154:GLN:HA	1:G:155:PRO:HA	1.93	0.43
2:H:259:LYS:HE3	2:H:259:LYS:HB2	1.89	0.43
3:C:806:LYS:HB3	3:C:806:LYS:HE3	1.62	0.43
3:C:892:SER:HB3	3:C:965:LEU:HB2	2.01	0.42
3:A:567:GLU:N	3:A:568:PRO:HA	2.35	0.42
4:B:40:LEU:HD13	4:B:62:SER:HB2	2.00	0.42
1:I:152:THR:HB	1:I:157:ARG:HB3	2.01	0.42
3:A:496:ASP:OD1	3:C:498:GLY:HA3	2.20	0.42
3:C:767:GLN:HG3	3:C:777:HIS:ND1	2.34	0.42
3:A:732:PHE:HD1	6:A:1019:EDO:H11	1.84	0.42
3:C:419:HIS:HB3	3:C:449:TRP:NE1	2.34	0.42
3:C:906:GLU:HA	6:C:1021:EDO:H12	2.01	0.42
1:I:102:ARG:HA	3:C:384:ILE:O	2.20	0.42
2:H:278:VAL:HG23	2:H:290:LEU:HB2	2.01	0.42
2:H:343:THR:HA	3:A:378:MET:O	2.20	0.42
3:C:671:GLY:H	3:C:685:TRP:CG	2.38	0.41
1:I:54:ARG:O	12:I:1705:HOH:O	2.21	0.41
1:I:171:ASN:HA	2:J:269:ASP:OD1	2.20	0.41
3:C:755:TYR:CE2	3:C:792:PRO:HG2	2.56	0.41
1:I:54:ARG:N	12:I:1705:HOH:O	2.40	0.41
3:C:423:TRP:CD2	3:C:701:LEU:HB2	2.56	0.41
3:C:846:LYS:HB2	6:C:1013:EDO:H22	2.00	0.41
3:C:578[A]:MET:HE2	3:C:578[A]:MET:HB2	1.99	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:59:LYS:HD2	6:D:1402:EDO:H22	2.03	0.41
3:A:758:ASP:OD2	3:A:790:TYR:OH	2.31	0.40
3:C:565:MET:HE3	3:C:569:SER:HB3	2.03	0.40
2:H:253:LYS:HA	2:H:253:LYS:HD2	1.86	0.40
4:D:64:GLU:HB3	4:D:67:THR:OG1	2.21	0.40
1:G:35:ARG:HA	1:G:35:ARG:HD3	1.69	0.40
10:C:1006:PEG:H12	10:C:1006:PEG:H31	1.91	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	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

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	68	GLN
1	G	168	LEU
3	A	424	ASN
3	A	446	ASP
3	A	500	ARG
1	I	67	LEU
1	I	137	SER
3	C	424	ASN
3	C	446	ASP
3	C	769	MET
3	C	797	VAL
3	C	936	ARG
3	C	966	ARG
4	D	34	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	G	77	HIS
1	G	154	GLN
2	H	255	HIS
3	A	436	GLN

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Mol	Chain	Res	Type
3	A	545	ASN
3	A	647	HIS
1	I	77	HIS
3	C	473	ASN
3	C	545	ASN
3	C	563	ASN
3	C	859	GLN
4	D	76	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	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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
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
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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
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	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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	-
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	-

All (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

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
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
9	C	1001	WAV	C17-N3	4.70	1.54	1.45
9	A	1001	WAV	O2-C2	-4.68	1.36	1.44
9	A	1001	WAV	C17-N3	4.52	1.54	1.45
9	A	1001	WAV	C12-N2	4.12	1.48	1.37
9	A	1001	WAV	C14-C15	4.09	1.46	1.39
9	C	1001	WAV	C12-N2	4.08	1.48	1.37
9	C	1001	WAV	C14-C15	3.95	1.45	1.39
9	C	1001	WAV	C2-C3	3.68	1.57	1.53
9	A	1001	WAV	C2-C3	3.15	1.56	1.53
9	A	1001	WAV	C16-C17	2.88	1.44	1.39
9	A	1001	WAV	C16-C15	-2.83	1.34	1.39
9	C	1001	WAV	C16-C15	-2.81	1.34	1.39
9	C	1001	WAV	C16-C17	2.65	1.44	1.39
9	A	1001	WAV	C11-C10	2.62	1.59	1.50
9	C	1001	WAV	C11-C10	2.49	1.59	1.50
9	C	1001	WAV	C11-N2	2.15	1.50	1.45
9	C	1001	WAV	C15-N4	2.07	1.46	1.39
9	A	1001	WAV	C11-N2	2.05	1.50	1.45
9	A	1001	WAV	C15-N4	2.01	1.45	1.39

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.

All (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
9	C	1001	WAV	C13-C12-N2-C11
5	A	1007	PGE	C3-C4-O3-C5

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Mol	Chain	Res	Type	Atoms
5	A	1008	PGE	O1-C1-C2-O2
8	A	1002	PG4	O4-C7-C8-O5
5	G	1101	PGE	C4-C3-O2-C2
5	A	1008	PGE	O2-C3-C4-O3
5	A	1003	PGE	O1-C1-C2-O2
5	A	1007	PGE	O1-C1-C2-O2
5	A	1008	PGE	O3-C5-C6-O4
10	B	1801	PEG	O2-C3-C4-O4
9	A	1001	WAV	C10-C11-N2-C12
9	C	1001	WAV	C10-C11-N2-C12
9	A	1001	WAV	N1-C8-C9-O6
9	C	1001	WAV	N1-C8-C9-O6
8	H	1301	PG4	O4-C7-C8-O5
10	C	1006	PEG	O2-C3-C4-O4
10	D	1403	PEG	O2-C3-C4-O4
5	A	1003	PGE	O3-C5-C6-O4
10	C	1022	PEG	O2-C3-C4-O4
10	B	1801	PEG	C1-C2-O2-C3
10	A	1014	PEG	O2-C3-C4-O4
10	C	1003	PEG	O1-C1-C2-O2
10	C	1006	PEG	C1-C2-O2-C3
10	C	1016	PEG	O1-C1-C2-O2
10	C	1016	PEG	O2-C3-C4-O4
5	G	1101	PGE	O1-C1-C2-O2
6	A	1017	EDO	O1-C1-C2-O2
6	A	1019	EDO	O1-C1-C2-O2
8	H	1301	PG4	O2-C3-C4-O3
9	A	1001	WAV	C9-C8-N1-C6
9	C	1001	WAV	C9-C8-N1-C6
8	A	1002	PG4	C5-C6-O4-C7
10	B	1801	PEG	C4-C3-O2-C2
5	A	1021	PGE	C1-C2-O2-C3
5	A	1008	PGE	C6-C5-O3-C4
10	C	1006	PEG	C4-C3-O2-C2
8	H	1301	PG4	C8-C7-O4-C6
10	D	1403	PEG	C1-C2-O2-C3
10	I	1601	PEG	O1-C1-C2-O2
10	J	1201	PEG	O2-C3-C4-O4
10	D	1403	PEG	O1-C1-C2-O2
10	B	1802	PEG	C1-C2-O2-C3
10	D	1403	PEG	C4-C3-O2-C2
8	H	1301	PG4	C1-C2-O2-C3

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Mol	Chain	Res	Type	Atoms
8	H	1301	PG4	O3-C5-C6-O4
10	B	1802	PEG	O1-C1-C2-O2
5	A	1003	PGE	C6-C5-O3-C4
5	A	1003	PGE	C4-C3-O2-C2
6	A	1006	EDO	O1-C1-C2-O2
6	C	1005	EDO	O1-C1-C2-O2
9	A	1001	WAV	C11-C10-O6-C9
9	C	1001	WAV	C11-C10-O6-C9
6	A	1018	EDO	O1-C1-C2-O2
6	C	1017	EDO	O1-C1-C2-O2
6	C	1021	EDO	O1-C1-C2-O2
5	A	1007	PGE	C1-C2-O2-C3
10	C	1022	PEG	C1-C2-O2-C3
9	A	1001	WAV	C3-C2-C7-O1
8	A	1002	PG4	C6-C5-O3-C4
5	G	1101	PGE	C6-C5-O3-C4
5	A	1003	PGE	C3-C4-O3-C5
6	A	1005	EDO	O1-C1-C2-O2
6	A	1009	EDO	O1-C1-C2-O2
6	C	1009	EDO	O1-C1-C2-O2
5	A	1007	PGE	C4-C3-O2-C2
5	A	1007	PGE	O3-C5-C6-O4
6	C	1010	EDO	O1-C1-C2-O2
6	C	1012	EDO	O1-C1-C2-O2
6	C	1018	EDO	O1-C1-C2-O2
8	A	1002	PG4	C1-C2-O2-C3
10	J	1201	PEG	O1-C1-C2-O2
8	A	1002	PG4	O2-C3-C4-O3
5	G	1101	PGE	C1-C2-O2-C3
8	A	1002	PG4	O3-C5-C6-O4
6	A	1011	EDO	O1-C1-C2-O2
6	C	1002	EDO	O1-C1-C2-O2
6	C	1020	EDO	O1-C1-C2-O2
10	A	1014	PEG	C1-C2-O2-C3

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

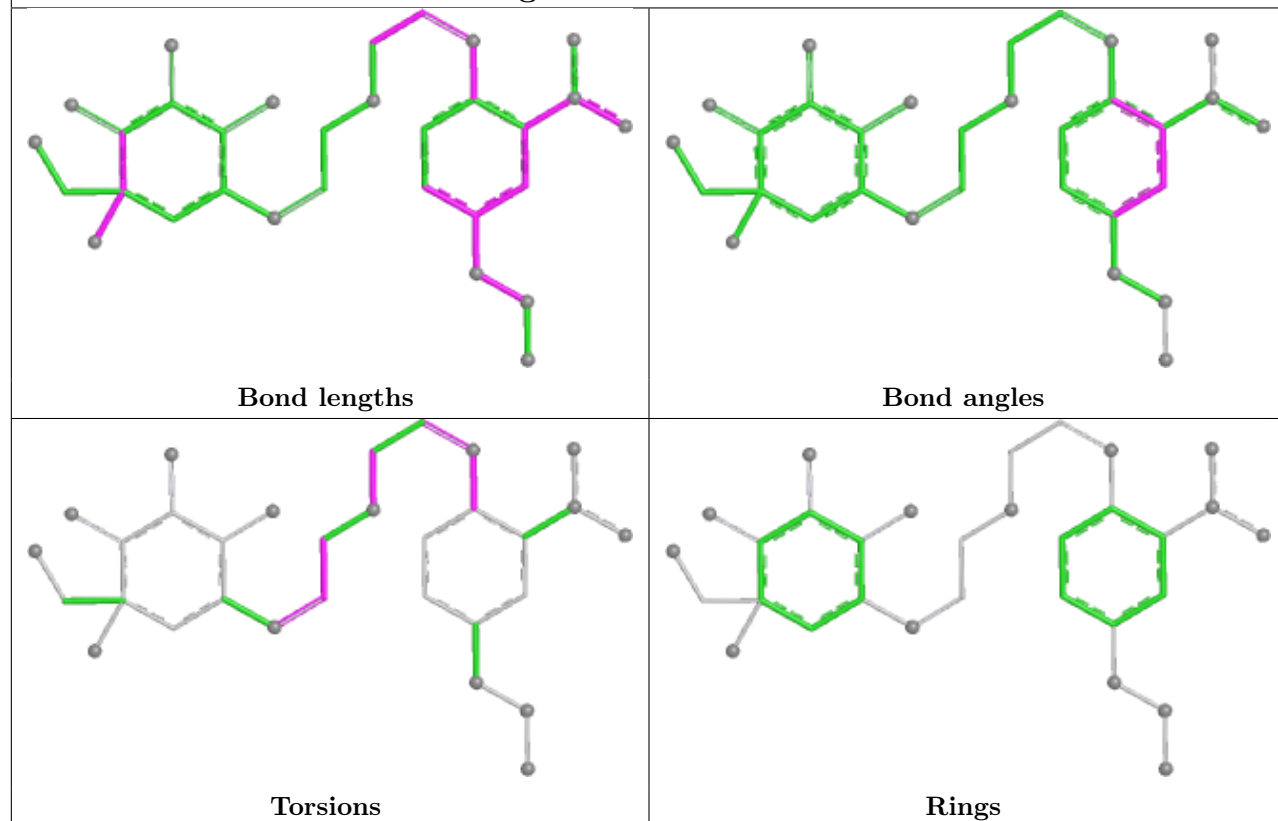
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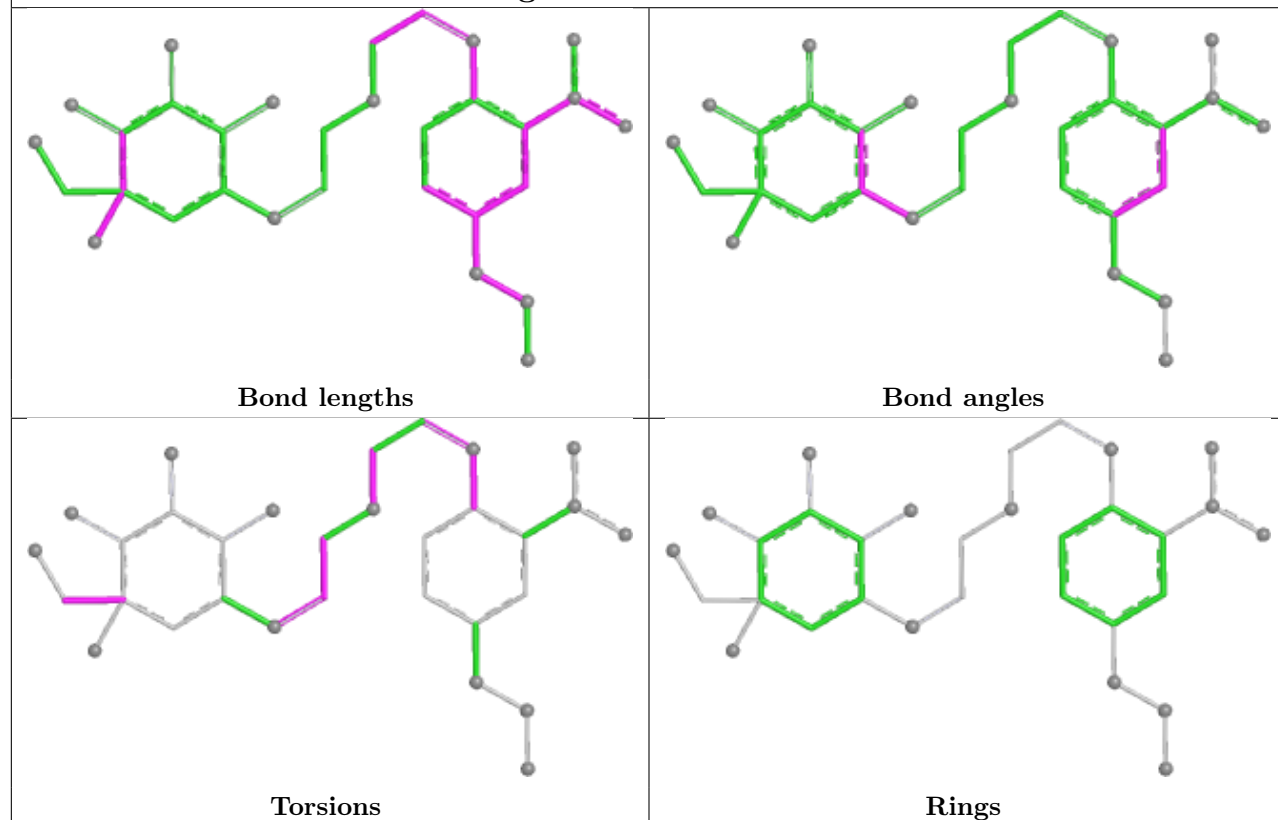
Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	C	1001	WAV	1	0
6	C	1002	EDO	1	0
9	A	1001	WAV	1	0
6	H	1303	EDO	1	0
10	C	1006	PEG	2	0
5	A	1007	PGE	1	0
10	C	1016	PEG	2	0
6	C	1013	EDO	1	0
6	A	1017	EDO	1	0
10	B	1802	PEG	1	0
6	A	1006	EDO	1	0
5	G	1101	PGE	2	0
6	A	1019	EDO	1	0
10	A	1014	PEG	1	0
6	C	1017	EDO	1	0
10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

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, 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%)

All (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
4	D	80	THR	4.4
1	I	185	ARG	4.2
3	A	370	THR	4.2
2	J	350	ASN	4.1
1	I	184	PRO	4.1
3	C	370	THR	4.0
2	H	350	ASN	4.0
4	B	43	THR	3.8
2	J	329	PHE	3.8
1	I	183	ALA	3.5
1	G	71	PRO	3.5

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Mol	Chain	Res	Type	RSRZ
4	B	80	THR	3.5
2	H	246	GLY	3.5
4	D	34	SER	3.4
2	H	247	ALA	3.4
4	B	81	GLY	3.4
4	B	38	THR	3.3
1	I	69	LEU	3.3
4	B	36	PRO	3.3
2	H	251	THR	3.2
4	B	82	TYR	3.2
4	B	83	LYS	3.1
4	D	44	ALA	3.1
4	D	82	TYR	3.1
4	B	44	ALA	3.1
1	I	153	ALA	3.0
2	H	248	TRP	3.0
1	I	57	LEU	2.9
4	D	117	ARG	2.9
1	I	33	VAL	2.9
3	A	785	HIS	2.9
1	I	138	VAL	2.8
1	I	34	ASP	2.8
2	J	245	PRO	2.7
4	D	36	PRO	2.7
3	C	795	GLU	2.7
1	I	130	VAL	2.7
4	D	78	THR	2.7
4	D	83	LYS	2.7
2	J	294	GLU	2.6
4	D	38	THR	2.6
3	C	442	ASN	2.5
1	G	33	VAL	2.5
1	G	70	GLY	2.5
4	D	45	THR	2.5
1	I	79	ILE	2.5
1	G	34	ASP	2.5
1	I	67	LEU	2.4
1	I	71	PRO	2.4
1	I	155	PRO	2.4
4	B	46	ILE	2.4
1	I	158	LEU	2.4
1	I	62	ALA	2.4

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Mol	Chain	Res	Type	RSRZ
4	D	46	ILE	2.3
1	G	110	ARG	2.3
1	I	156	PHE	2.3
4	D	81	GLY	2.3
1	I	160	LEU	2.2
4	B	42	GLY	2.2
4	B	45	THR	2.2
4	B	78	THR	2.2
3	C	808	HIS	2.2
1	I	126	ALA	2.2
1	I	88	VAL	2.2
1	I	60	TYR	2.2
4	B	117	ARG	2.1
2	J	330	HIS	2.1
4	B	40	LEU	2.1
2	H	249	GLU	2.1
3	C	785	HIS	2.1
1	I	132	GLY	2.1

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
7	SO4	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

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
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
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

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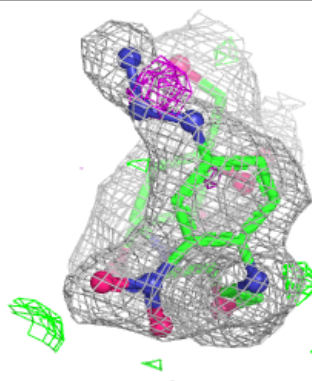
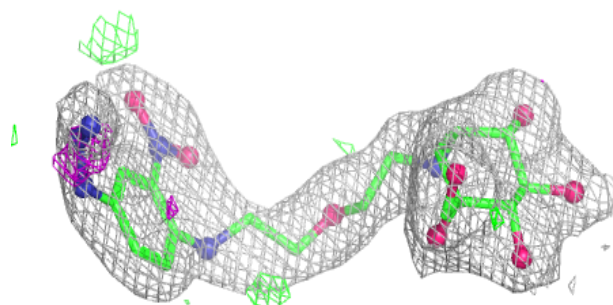
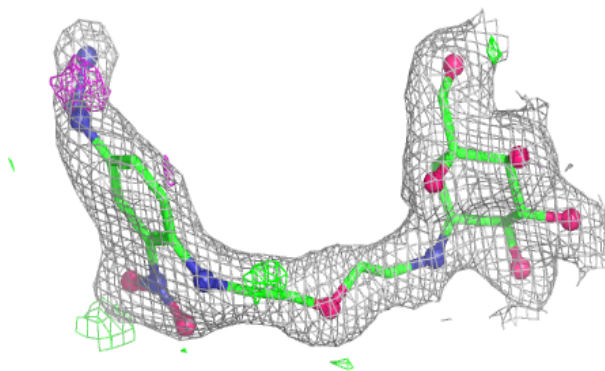
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	EDO	C	1004	4/4	0.92	0.12	46,54,55,59	0
6	EDO	A	1015	4/4	0.93	0.10	41,43,46,54	0
6	EDO	A	1006	4/4	0.93	0.10	50,50,51,65	0
6	EDO	A	1020	4/4	0.93	0.17	49,53,55,58	0
6	EDO	A	1012	4/4	0.94	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

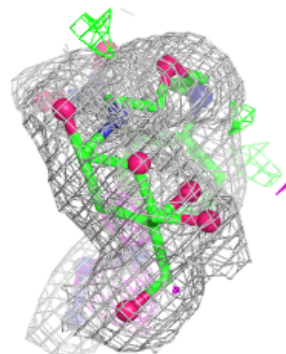
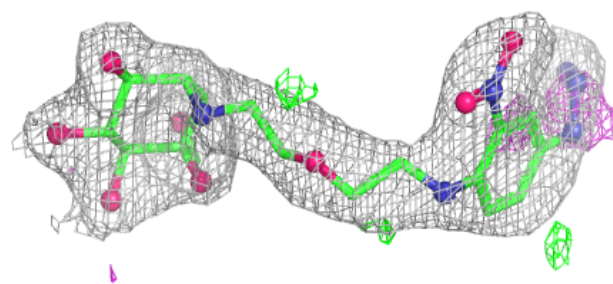
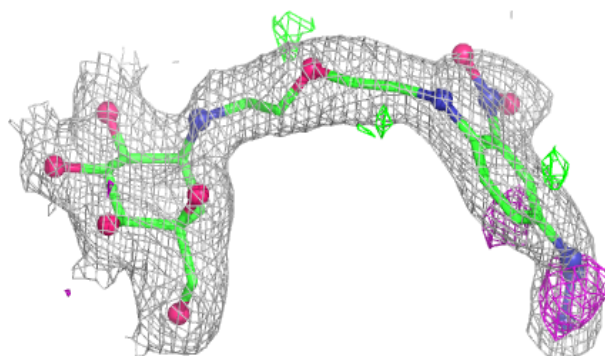
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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