



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 27, 2021 – 02:10 PM EDT

PDB ID : 7KB8
Title : Co-crystal structure of alpha glucosidase with compound 8
Authors : Karade, S.S.; Mariuzza, R.A.
Deposited on : 2020-10-01
Resolution : 2.38 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.23.2
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.23.2

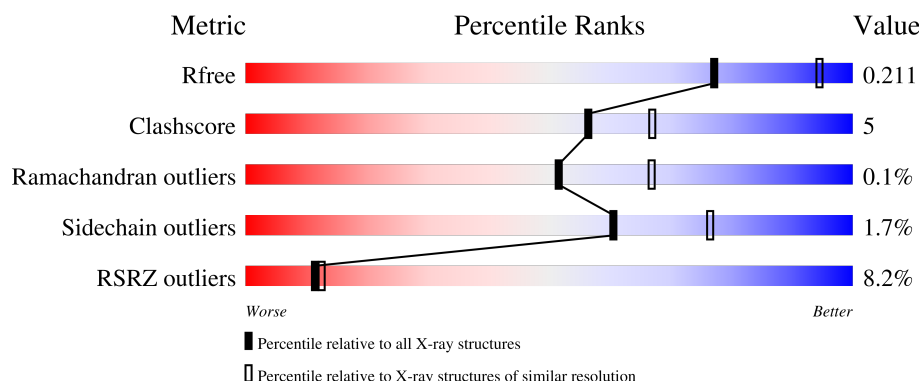
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.38 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	5509 (2.40-2.36)
Clashscore	141614	6082 (2.40-2.36)
Ramachandran outliers	138981	5973 (2.40-2.36)
Sidechain outliers	138945	5975 (2.40-2.36)
RSRZ outliers	127900	5397 (2.40-2.36)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	977	<div> <div>5%</div> <div>78%</div> <div>9%</div> <div>13%</div> </div>
1	C	977	<div> <div>7%</div> <div>78%</div> <div>9%</div> <div>12%</div> </div>
2	B	554	<div> <div>3%</div> <div>14%</div> <div>84%</div> </div>
2	D	554	<div> <div>3%</div> <div>12%</div> <div>84%</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	PEG	C	1512	-	-	X	-

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 15963 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Isoform 2 of Neutral alpha-glucosidase AB.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	854	Total	C	N	O	S	0	4	0
			6898	4419	1192	1259	28			
1	C	857	Total	C	N	O	S	0	8	0
			6894	4420	1184	1260	30			

There are 88 discrepancies between the modelled and reference sequences:

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

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Chain	Residue	Modelled	Actual	Comment	Reference
A	27	CYS	-	expression tag	UNP Q8BHN3-2
A	28	VAL	-	expression tag	UNP Q8BHN3-2
A	29	ALA	-	expression tag	UNP Q8BHN3-2
A	30	GLU	-	expression tag	UNP Q8BHN3-2
A	31	THR	-	expression tag	UNP Q8BHN3-2
A	32	GLY	-	expression tag	UNP Q8BHN3-2
A	97	ASP	ASN	engineered mutation	UNP Q8BHN3-2
A	967	SER	-	expression tag	UNP Q8BHN3-2
A	968	ALA	-	expression tag	UNP Q8BHN3-2
A	969	TRP	-	expression tag	UNP Q8BHN3-2
A	970	SER	-	expression tag	UNP Q8BHN3-2
A	971	HIS	-	expression tag	UNP Q8BHN3-2
A	972	PRO	-	expression tag	UNP Q8BHN3-2
A	973	GLN	-	expression tag	UNP Q8BHN3-2
A	974	PHE	-	expression tag	UNP Q8BHN3-2
A	975	GLU	-	expression tag	UNP Q8BHN3-2
A	976	LYS	-	expression tag	UNP Q8BHN3-2
A	977	LEU	-	expression tag	UNP Q8BHN3-2
A	978	GLU	-	expression tag	UNP Q8BHN3-2
C	2	MET	-	initiating methionine	UNP Q8BHN3-2
C	3	GLY	-	expression tag	UNP Q8BHN3-2
C	4	ILE	-	expression tag	UNP Q8BHN3-2
C	5	LEU	-	expression tag	UNP Q8BHN3-2
C	6	PRO	-	expression tag	UNP Q8BHN3-2
C	7	SER	-	expression tag	UNP Q8BHN3-2
C	8	PRO	-	expression tag	UNP Q8BHN3-2
C	9	GLY	-	expression tag	UNP Q8BHN3-2
C	10	MET	-	expression tag	UNP Q8BHN3-2
C	11	PRO	-	expression tag	UNP Q8BHN3-2
C	12	ALA	-	expression tag	UNP Q8BHN3-2
C	13	LEU	-	expression tag	UNP Q8BHN3-2
C	14	LEU	-	expression tag	UNP Q8BHN3-2
C	15	SER	-	expression tag	UNP Q8BHN3-2
C	16	LEU	-	expression tag	UNP Q8BHN3-2
C	17	VAL	-	expression tag	UNP Q8BHN3-2
C	18	SER	-	expression tag	UNP Q8BHN3-2
C	19	LEU	-	expression tag	UNP Q8BHN3-2
C	20	LEU	-	expression tag	UNP Q8BHN3-2
C	21	SER	-	expression tag	UNP Q8BHN3-2
C	22	VAL	-	expression tag	UNP Q8BHN3-2
C	23	LEU	-	expression tag	UNP Q8BHN3-2
C	24	LEU	-	expression tag	UNP Q8BHN3-2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	25	MET	-	expression tag	UNP Q8BHN3-2
C	26	GLY	-	expression tag	UNP Q8BHN3-2
C	27	CYS	-	expression tag	UNP Q8BHN3-2
C	28	VAL	-	expression tag	UNP Q8BHN3-2
C	29	ALA	-	expression tag	UNP Q8BHN3-2
C	30	GLU	-	expression tag	UNP Q8BHN3-2
C	31	THR	-	expression tag	UNP Q8BHN3-2
C	32	GLY	-	expression tag	UNP Q8BHN3-2
C	97	ASP	ASN	engineered mutation	UNP Q8BHN3-2
C	967	SER	-	expression tag	UNP Q8BHN3-2
C	968	ALA	-	expression tag	UNP Q8BHN3-2
C	969	TRP	-	expression tag	UNP Q8BHN3-2
C	970	SER	-	expression tag	UNP Q8BHN3-2
C	971	HIS	-	expression tag	UNP Q8BHN3-2
C	972	PRO	-	expression tag	UNP Q8BHN3-2
C	973	GLN	-	expression tag	UNP Q8BHN3-2
C	974	PHE	-	expression tag	UNP Q8BHN3-2
C	975	GLU	-	expression tag	UNP Q8BHN3-2
C	976	LYS	-	expression tag	UNP Q8BHN3-2
C	977	LEU	-	expression tag	UNP Q8BHN3-2
C	978	GLU	-	expression tag	UNP Q8BHN3-2

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	87	Total	C	N	O	S	0	0	0
			624	371	102	141	10			
2	D	87	Total	C	N	O	S	0	0	0
			632	377	104	141	10			

There are 102 discrepancies between the modelled and reference sequences:

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

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-7	PRO	-	expression tag	UNP O08795
B	-6	ALA	-	expression tag	UNP O08795
B	-5	LEU	-	expression tag	UNP O08795
B	-4	LEU	-	expression tag	UNP O08795
B	-3	SER	-	expression tag	UNP O08795
B	-2	LEU	-	expression tag	UNP O08795
B	-1	VAL	-	expression tag	UNP O08795
B	0	SER	-	expression tag	UNP O08795
B	1	LEU	-	expression tag	UNP O08795
B	2	LEU	-	expression tag	UNP O08795
B	3	SER	-	expression tag	UNP O08795
B	4	VAL	-	expression tag	UNP O08795
B	5	LEU	-	expression tag	UNP O08795
B	6	LEU	-	expression tag	UNP O08795
B	7	MET	-	expression tag	UNP O08795
B	8	GLY	-	expression tag	UNP O08795
B	9	CYS	-	expression tag	UNP O08795
B	10	VAL	-	expression tag	UNP O08795
B	11	ALA	-	expression tag	UNP O08795
B	12	GLU	-	expression tag	UNP O08795
B	13	THR	-	expression tag	UNP O08795
B	14	GLY	-	expression tag	UNP O08795
B	518	SER	-	expression tag	UNP O08795
B	519	ALA	-	expression tag	UNP O08795
B	520	TRP	-	expression tag	UNP O08795
B	521	SER	-	expression tag	UNP O08795
B	522	HIS	-	expression tag	UNP O08795
B	523	PRO	-	expression tag	UNP O08795
B	524	GLN	-	expression tag	UNP O08795
B	525	PHE	-	expression tag	UNP O08795
B	526	GLU	-	expression tag	UNP O08795
B	527	LYS	-	expression tag	UNP O08795
B	528	LEU	-	expression tag	UNP O08795
B	529	GLU	-	expression tag	UNP O08795
B	530	THR	-	expression tag	UNP O08795
B	531	LYS	-	expression tag	UNP O08795
B	532	HIS	-	expression tag	UNP O08795
B	533	HIS	-	expression tag	UNP O08795
B	534	HIS	-	expression tag	UNP O08795
B	535	HIS	-	expression tag	UNP O08795
B	536	HIS	-	expression tag	UNP O08795
B	537	HIS	-	expression tag	UNP O08795

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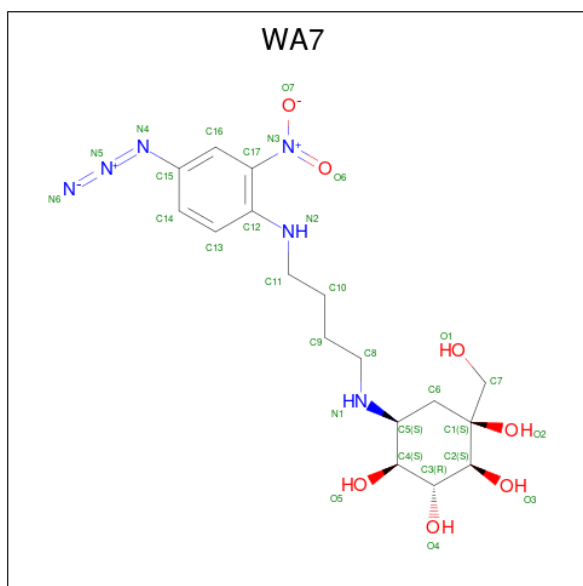
Chain	Residue	Modelled	Actual	Comment	Reference
D	-16	MET	-	initiating methionine	UNP O08795
D	-15	GLY	-	expression tag	UNP O08795
D	-14	ILE	-	expression tag	UNP O08795
D	-13	LEU	-	expression tag	UNP O08795
D	-12	PRO	-	expression tag	UNP O08795
D	-11	SER	-	expression tag	UNP O08795
D	-10	PRO	-	expression tag	UNP O08795
D	-9	GLY	-	expression tag	UNP O08795
D	-8	MET	-	expression tag	UNP O08795
D	-7	PRO	-	expression tag	UNP O08795
D	-6	ALA	-	expression tag	UNP O08795
D	-5	LEU	-	expression tag	UNP O08795
D	-4	LEU	-	expression tag	UNP O08795
D	-3	SER	-	expression tag	UNP O08795
D	-2	LEU	-	expression tag	UNP O08795
D	-1	VAL	-	expression tag	UNP O08795
D	0	SER	-	expression tag	UNP O08795
D	1	LEU	-	expression tag	UNP O08795
D	2	LEU	-	expression tag	UNP O08795
D	3	SER	-	expression tag	UNP O08795
D	4	VAL	-	expression tag	UNP O08795
D	5	LEU	-	expression tag	UNP O08795
D	6	LEU	-	expression tag	UNP O08795
D	7	MET	-	expression tag	UNP O08795
D	8	GLY	-	expression tag	UNP O08795
D	9	CYS	-	expression tag	UNP O08795
D	10	VAL	-	expression tag	UNP O08795
D	11	ALA	-	expression tag	UNP O08795
D	12	GLU	-	expression tag	UNP O08795
D	13	THR	-	expression tag	UNP O08795
D	14	GLY	-	expression tag	UNP O08795
D	518	SER	-	expression tag	UNP O08795
D	519	ALA	-	expression tag	UNP O08795
D	520	TRP	-	expression tag	UNP O08795
D	521	SER	-	expression tag	UNP O08795
D	522	HIS	-	expression tag	UNP O08795
D	523	PRO	-	expression tag	UNP O08795
D	524	GLN	-	expression tag	UNP O08795
D	525	PHE	-	expression tag	UNP O08795
D	526	GLU	-	expression tag	UNP O08795
D	527	LYS	-	expression tag	UNP O08795
D	528	LEU	-	expression tag	UNP O08795

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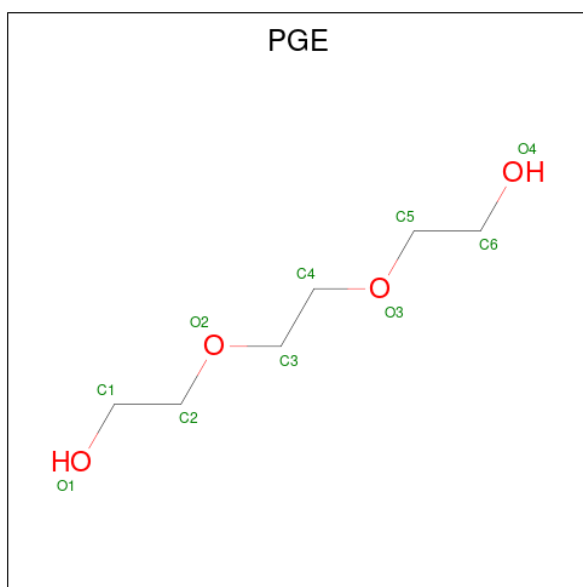
Chain	Residue	Modelled	Actual	Comment	Reference
D	529	GLU	-	expression tag	UNP O08795
D	530	THR	-	expression tag	UNP O08795
D	531	LYS	-	expression tag	UNP O08795
D	532	HIS	-	expression tag	UNP O08795
D	533	HIS	-	expression tag	UNP O08795
D	534	HIS	-	expression tag	UNP O08795
D	535	HIS	-	expression tag	UNP O08795
D	536	HIS	-	expression tag	UNP O08795
D	537	HIS	-	expression tag	UNP O08795

- Molecule 3 is (1S,2S,3R,4S,5S)-1-(hydroxymethyl)-5-[(4-{[2-nitro-4-(triazan-1-yl)phenyl]amino}butyl)amino]cyclohexane-1,2,3,4-tetrol (three-letter code: WA7) (formula: C₁₇H₂₆N₆O₇) (labeled as "Ligand of Interest" by depositor).



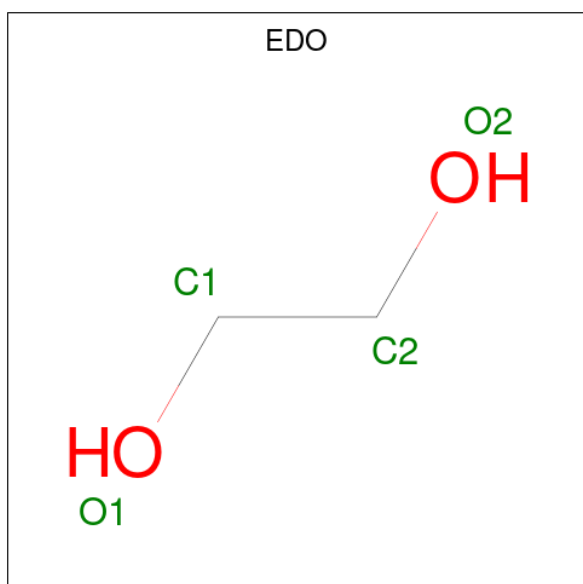
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			30	17	6	7		
3	C	1	Total	C	N	O	0	0
			30	17	6	7		

- Molecule 4 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: C₆H₁₄O₄).



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

- Molecule 5 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



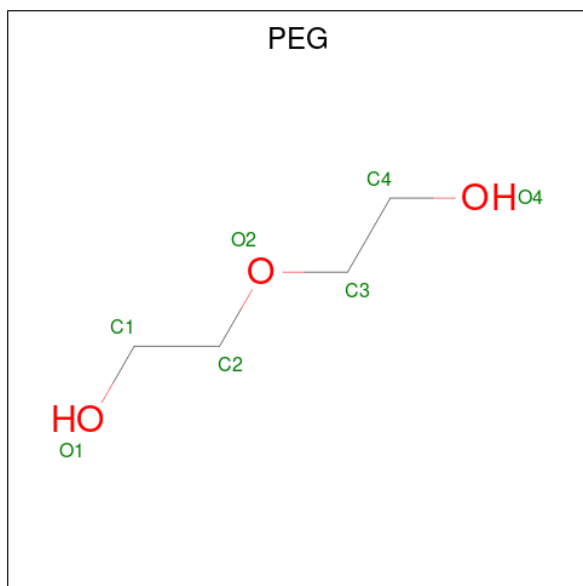
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 4 2 2	0	0
5	A	1	Total C O 4 2 2	0	0
5	A	1	Total C O 4 2 2	0	0
5	A	1	Total C O 4 2 2	0	0
5	A	1	Total C O 4 2 2	0	0
5	A	1	Total C O 4 2 2	0	0
5	A	1	Total C O 4 2 2	0	0
5	A	1	Total C O 4 2 2	0	0
5	B	1	Total C O 4 2 2	0	0
5	B	1	Total C O 4 2 2	0	0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

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

- Molecule 6 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: C₄H₁₀O₃).



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

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

- Molecule 7 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

- Molecule 8 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	C	1	Total	O	S	0	0
			5	4	1		
8	C	1	Total	O	S	0	0
			5	4	1		

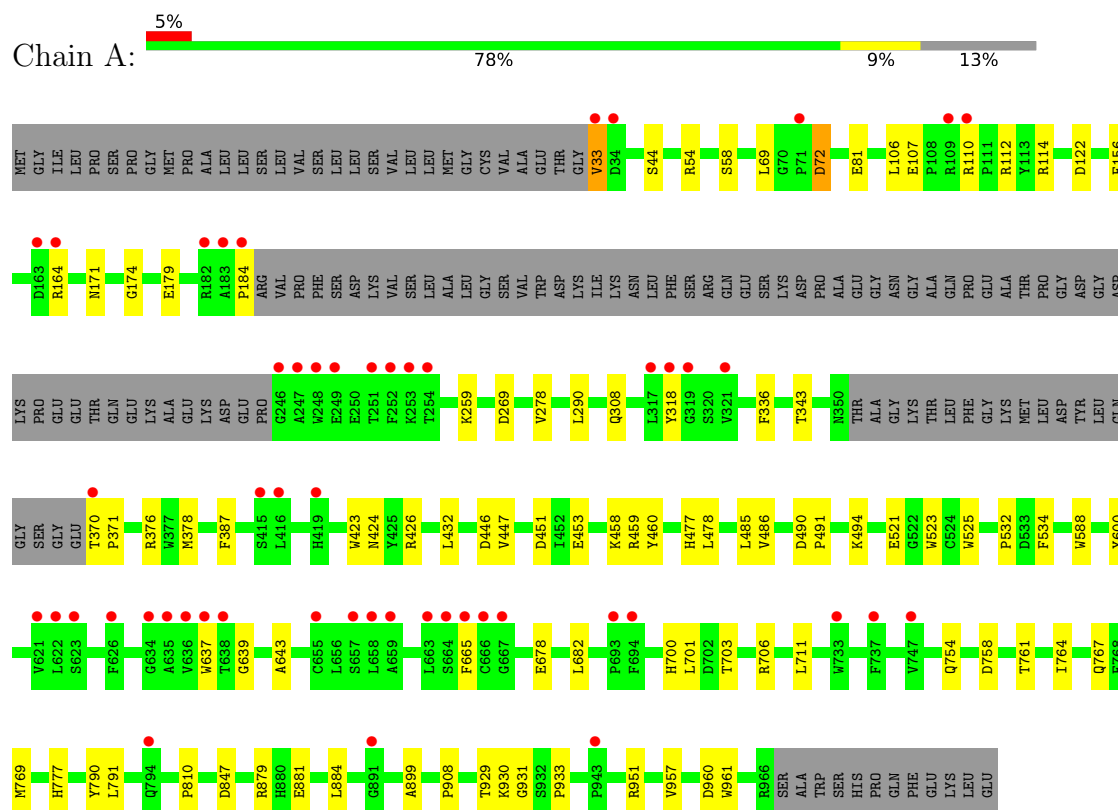
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	315	Total	O	0	0
			315	315		
9	B	13	Total	O	0	0
			13	13		
9	C	247	Total	O	0	0
			247	247		
9	D	15	Total	O	0	0
			15	15		

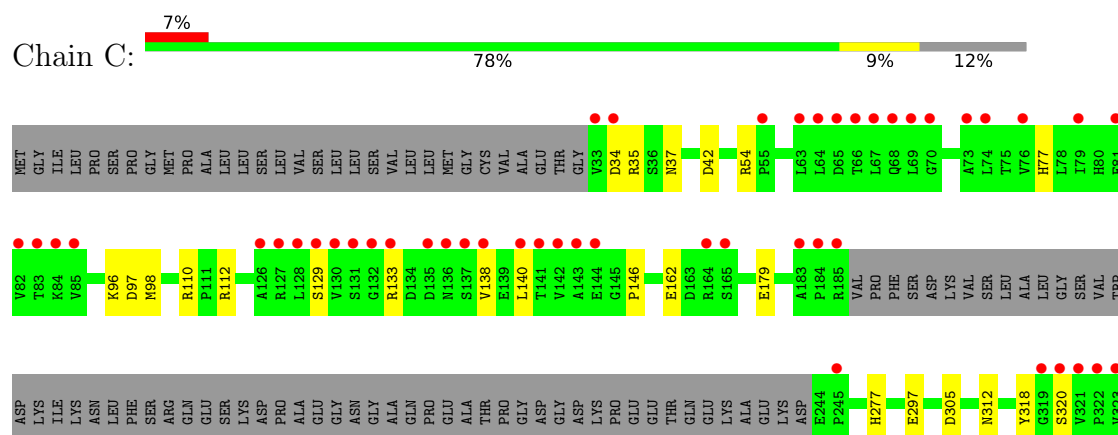
3 Residue-property plots

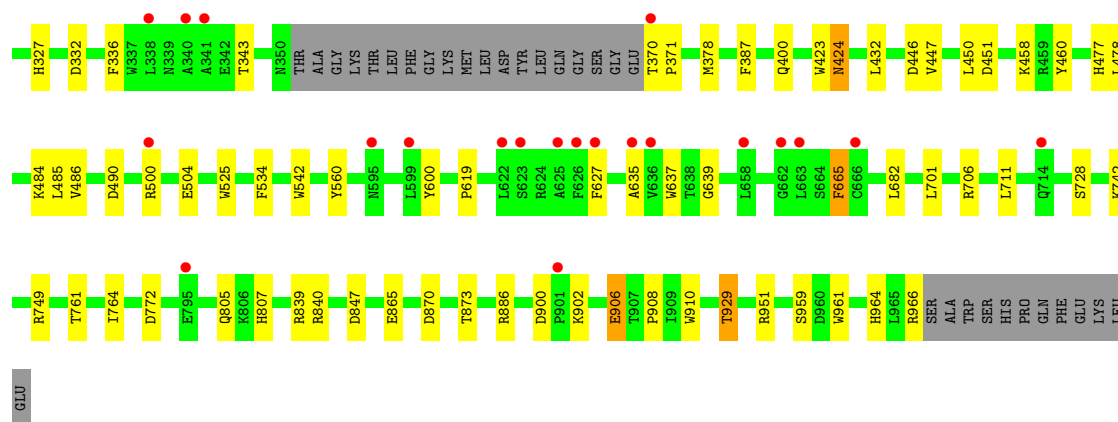
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

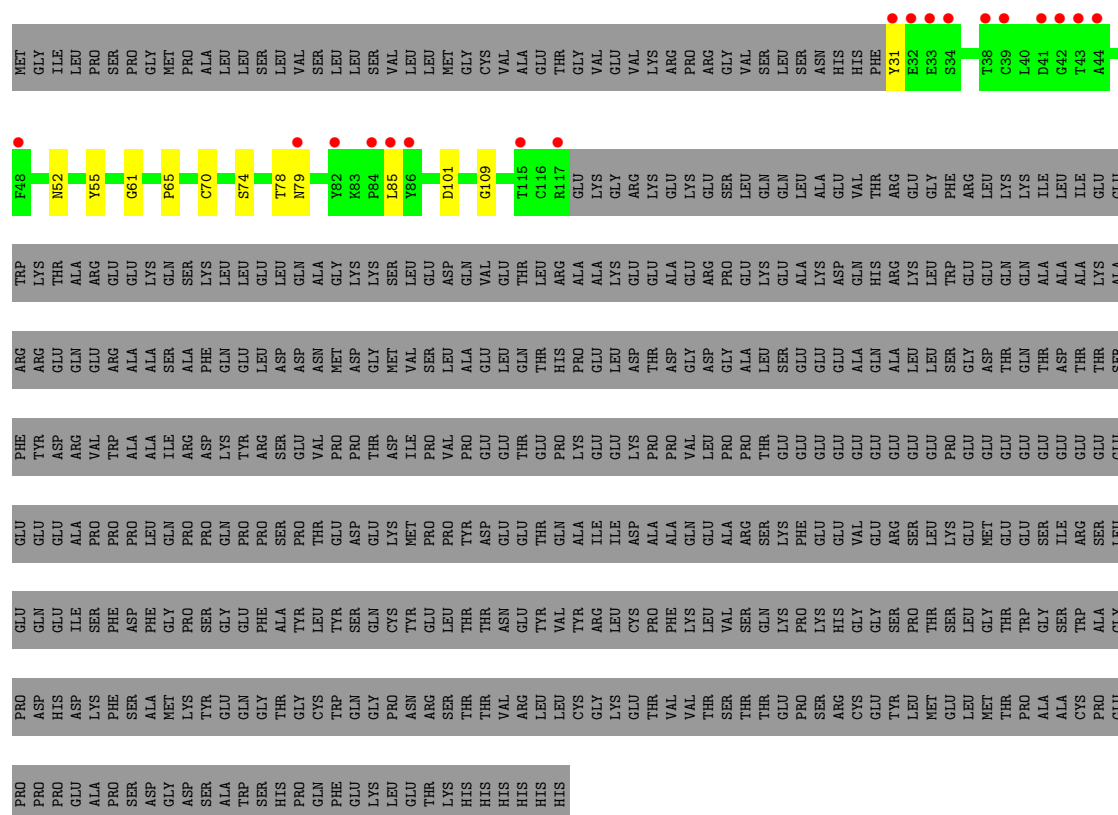


• Molecule 1: Isoform 2 of Neutral alpha-glucosidase AB

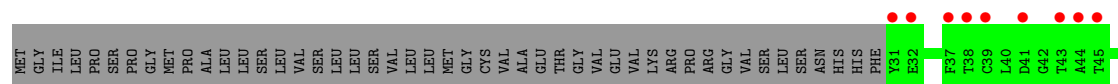




● Molecule 2: Glucosidase 2 subunit beta



● Molecule 2: Glucosidase 2 subunit beta



CYS	TRP	ARG	GLU	THR	ALA	ILE	Y55
PRO	ALA	SER	GLU	THR	LYS	GLU	
GLU	GLY	LEU	GLU	SER	ALA	GLU	C58
PRO	PRO	GLU	GLU	PHE	ARG	TRP	
PRO	ASP	GLN	GLU	TYR	ARG	LYS	G61
PRO	HIS	ILE	GLU	ASP	GLU	THR	S62
GLU	ASP	ILE	ALA	ARG	ALA	ALA	D63
ALA	LYS	SER	PRO	VAL	GLU	ARG	
PRO	PHE	PHE	PRO	TRP	GLU	GLU	C70
SER	ASP	ALA	PRO	ALA	ALA	LYS	F71
GLY	MET	PRO	GLN	ILE	SER	GLN	N72
ASP	LYS	PRO	PRO	ARG	ALA	SER	T78
SER	TYR	SER	PRO	ASP	ALA	GLN	N79
ALA	GLU	GLY	GLN	LYS	PHE	LYS	T80
TRP	GLN	GLU	PRO	TYR	GLN	LEU	G81
SER	GLY	PHE	PRO	ARG	LEU	LEU	Y82
HIS	THR	ALA	SER	SER	ASP	LEU	K83
PRO	GLY	TYR	PRO	GLU	ASP	GLN	P84
GLN	CYS	LEU	THR	VAL	ASN	ALA	L85
PHE	TRP	TYR	GLU	PRO	MET	GLY	Y86
GLU	GLN	SER	ASP	PRO	LYS	LYS	I87
LYS	GLY	GLN	GLU	THR	GLY	LYS	L88
LEU	PRO	CYS	LYS	ASP	MET	SER	S89
GLU	ASN	TYR	MET	ILE	VAL	LEU	S90
THR	ARG	GLU	PRO	PRO	SER	GLU	R91
LYS	SER	LEU	PRO	VAL	LEU	ASP	
HIS	THR	THR	TYR	PRO	ALA	GLN	C99
HIS	VAL	ASN	GLU	GLU	GLU	VAL	C100
HIS	ARG	GLU	GLU	THR	LEU	GLU	D101
HIS	LEU	TYR	THR	GLU	GLN	THR	
HIS	LEU	GLN	GLN	PRO	THR	LEU	G116
HIS	LEU	VAL	THR	GLU	HIS	ARG	R117
	CYS	GLY	ALA	LYS	PRO	ALA	GLU
	LYS	LEU	ILE	GLU	GLU	ALA	LYS
	THR	GLU	ILE	LEU	LYS	LEU	GLY
	GLU	CYS	ASP	LYS	ASP	GLU	ARG
	THR	PRO	ALA	PRO	THR	GLU	LYS
	VAL	PHE	ALA	PRO	ASP	ALA	GLU
	THR	LYS	GLN	VAL	GLY	GLU	LYS
	SER	LEU	GLU	LEU	ASP	ARG	GLU
	THR	VAL	ALA	PRO	GLY	SER	SER
	THR	SER	ARG	PRO	ALA	GLU	LEU
	GLU	GLN	SER	THR	LEU	LYS	GLN
	PRO	LYS	LYS	GLU	SER	GLU	GLN
	SER	PRO	PHE	GLU	ALA	ALA	LEU
	ARG	LYS	GLU	GLU	LYS	LYS	ALA
	CYS	HIS	GLU	GLU	ASP	ASP	GLU
	GLY	GLY	VAL	VAL	ALA	VAL	VAL
	TYR	SER	GLY	GLU	GLN	THR	THR
	LEU	PRO	ARG	GLU	ALA	ARG	ARG
	MET	THR	LEU	GLY	ASP	GLU	LEU
	THR	GLY	THR	GLU	THR	GLN	LYS
	PRO	TRP	GLY	GLU	THR	ALA	LYS
	ALA	SER	ILE	GLU	ASP	THR	ILE
							LEU

4 Data and refinement statistics

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, α , β , γ	102.78Å 102.78Å 240.12Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	40.02 – 2.38 43.24 – 2.38	Depositor EDS
% Data completeness (in resolution range)	99.7 (40.02-2.38) 93.5 (43.24-2.38)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.75 (at 2.39Å)	Xtriage
Refinement program	PHENIX 1.14_3228	Depositor
R, R_{free}	0.174 , 0.210 0.174 , 0.211	Depositor DCC
R_{free} test set	1979 reflections (1.76%)	wwPDB-VP
Wilson B-factor (Å ²)	41.5	Xtriage
Anisotropy	0.241	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 40.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.008 for -h,-k,l 0.038 for h,-h-k,-l 0.020 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	15963	wwPDB-VP
Average B, all atoms (Å ²)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.54% 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: WA7, PGE, SO4, CA, 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	A	0.38	0/7120	0.58	0/9694
1	C	0.38	0/7130	0.57	1/9714 (0.0%)
2	B	0.34	0/636	0.60	0/870
2	D	0.35	0/644	0.61	0/880
All	All	0.37	0/15530	0.58	1/21158 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	886	ARG	NE-CZ-NH2	-6.29	117.16	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	6898	0	6646	63	0
1	C	6894	0	6599	61	0
2	B	624	0	504	9	0
2	D	632	0	530	17	0
3	A	30	0	0	0	0
3	C	30	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	40	0	56	7	0
4	C	10	0	14	1	0
5	A	32	0	46	4	0
5	B	16	0	23	4	0
5	C	68	0	100	9	0
5	D	8	0	12	0	0
6	A	42	0	60	3	0
6	B	7	0	10	0	0
6	C	21	0	30	13	0
6	D	7	0	10	2	0
7	B	2	0	0	0	0
7	D	2	0	0	0	0
8	C	10	0	0	1	0
9	A	315	0	0	10	0
9	B	13	0	0	2	0
9	C	247	0	0	13	0
9	D	15	0	0	1	0
All	All	15963	0	14640	149	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (149) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:37:ASN:OD1	9:C:1601:HOH:O	1.82	0.97
1:C:840:ARG:HB3	6:C:1512:PEG:H32	1.61	0.81
1:C:619:PRO:O	9:C:1602:HOH:O	1.99	0.80
1:A:521:GLU:H	5:A:1019:EDO:H11	1.47	0.80
1:C:54:ARG:O	9:C:1603:HOH:O	2.00	0.78
1:A:114:ARG:H	4:A:1006:PGE:H22	1.48	0.78
2:D:88:LEU:HD23	6:D:602:PEG:H41	1.66	0.78
1:A:682:LEU:HD23	1:A:711:LEU:HD11	1.72	0.71
1:A:847:ASP:OD1	9:A:1102:HOH:O	2.08	0.71
1:C:305:ASP:OD1	9:C:1605:HOH:O	2.07	0.71
1:A:424:ASN:ND2	1:A:453:GLU:H	1.89	0.71
1:A:930:LYS:HA	4:A:1008:PGE:H5	1.73	0.71
1:C:772:ASP:OD1	9:C:1604:HOH:O	2.07	0.70
2:B:52:ASN:O	9:B:701:HOH:O	2.09	0.69
1:A:44:SER:OG	9:A:1103:HOH:O	2.09	0.68
1:C:277:HIS:ND1	9:C:1614:HOH:O	2.27	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:81:GLU:OE2	9:A:1104:HOH:O	2.11	0.68
2:D:117:ARG:NH1	9:D:701:HOH:O	2.27	0.67
1:A:424:ASN:ND2	1:A:451:ASP:HB3	2.10	0.66
1:A:156:PHE:O	9:A:1105:HOH:O	2.14	0.65
1:C:297:GLU:O	5:C:1520:EDO:O1	2.11	0.65
1:A:81:GLU:HG2	9:A:1267:HOH:O	1.95	0.65
1:A:588:TRP:HE1	4:A:1006:PGE:H52	1.62	0.65
1:A:426:ARG:HD3	8:C:1524:SO4:O4	1.98	0.64
1:A:957:VAL:O	9:A:1106:HOH:O	2.15	0.64
1:A:933:PRO:HA	4:A:1008:PGE:H22	1.79	0.63
2:B:31:TYR:N	9:B:702:HOH:O	2.31	0.63
1:C:865:GLU:H	5:C:1513:EDO:H21	1.63	0.63
6:C:1512:PEG:H31	2:D:91:ARG:HE	1.63	0.63
6:C:1512:PEG:H22	2:D:91:ARG:HH21	1.64	0.63
2:B:109:GLY:H	5:B:604:EDO:H21	1.63	0.62
1:A:447:VAL:HG11	1:A:486:VAL:HG23	1.82	0.61
1:A:879:ARG:NH1	1:A:881:GLU:OE1	2.34	0.61
1:A:423:TRP:O	1:A:701:LEU:HA	2.01	0.61
1:A:110:ARG:HH22	1:A:184:PRO:HG3	1.65	0.60
1:A:678:GLU:H	5:A:1015:EDO:H12	1.67	0.59
1:C:133:ARG:HG3	1:C:138:VAL:HG22	1.83	0.59
1:C:35:ARG:N	9:C:1623:HOH:O	2.36	0.59
1:A:703:THR:HG22	6:A:1005:PEG:H32	1.84	0.58
1:C:42:ASP:N	9:C:1613:HOH:O	2.26	0.58
1:A:459:ARG:NH1	1:A:494:LYS:HE2	2.19	0.58
6:C:1512:PEG:H31	2:D:91:ARG:CG	2.34	0.57
1:C:112:ARG:NH2	1:C:179:GLU:O	2.38	0.57
1:A:678:GLU:H	5:A:1015:EDO:C1	2.18	0.57
1:C:840:ARG:HA	6:C:1512:PEG:H12	1.86	0.57
1:C:847:ASP:HB3	1:C:908:PRO:HG2	1.86	0.56
1:A:112:ARG:NH2	1:A:179:GLU:O	2.38	0.56
1:C:929:THR:HG23	1:C:961:TRP:HB3	1.88	0.56
6:C:1512:PEG:H31	2:D:91:ARG:HG2	1.88	0.56
1:C:900:ASP:OD1	1:C:902:LYS:HG2	2.06	0.55
1:C:34:ASP:OD1	9:C:1608:HOH:O	2.18	0.55
1:C:542:TRP:O	5:C:1518:EDO:O1	2.25	0.55
1:C:484:LYS:NZ	5:C:1516:EDO:H12	2.22	0.55
1:C:96:LYS:HB3	5:C:1519:EDO:H11	1.89	0.55
1:C:336:PHE:HB3	1:C:387:PHE:HB2	1.88	0.55
2:B:65:PRO:O	5:B:605:EDO:H22	2.07	0.54
1:C:728:SER:OG	5:C:1503:EDO:H21	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:749:ARG:NH2	9:C:1630:HOH:O	2.42	0.52
1:A:931:GLY:H	4:A:1008:PGE:C5	2.22	0.52
1:C:423:TRP:O	1:C:701:LEU:HA	2.10	0.52
1:A:72:ASP:N	1:A:72:ASP:OD1	2.41	0.52
1:C:906:GLU:H	1:C:906:GLU:CD	2.10	0.52
1:C:542:TRP:CD1	5:C:1518:EDO:H11	2.45	0.52
1:A:336:PHE:HB3	1:A:387:PHE:HB2	1.92	0.51
1:A:110:ARG:NH2	9:A:1125:HOH:O	2.44	0.51
6:C:1512:PEG:H31	2:D:91:ARG:NE	2.25	0.51
1:C:484:LYS:HZ1	5:C:1516:EDO:H12	1.75	0.50
1:A:491:PRO:O	1:A:532:PRO:HD2	2.11	0.50
1:C:370:THR:N	1:C:371:PRO:HD2	2.27	0.50
1:C:320:SER:O	1:C:627:PHE:HA	2.12	0.50
1:A:370:THR:N	1:A:371:PRO:HD2	2.27	0.49
1:A:478:LEU:CD1	1:A:485:LEU:HD12	2.43	0.49
1:C:447:VAL:HG11	1:C:486:VAL:HG23	1.94	0.49
1:A:761:THR:HA	1:A:764:ILE:HG13	1.94	0.49
2:D:72:ASN:HA	6:D:602:PEG:H12	1.93	0.49
1:C:635:ALA:HB2	1:C:665:PHE:CD2	2.47	0.49
1:A:588:TRP:NE1	4:A:1006:PGE:H52	2.28	0.49
1:C:951:ARG:HG3	2:D:55:TYR:CE2	2.48	0.49
2:B:79:ASN:HA	2:B:101:ASP:HB3	1.95	0.49
1:C:560:TYR:OH	5:C:1516:EDO:H11	2.12	0.49
1:A:767:GLN:HG3	1:A:777:HIS:ND1	2.28	0.49
1:C:761:THR:HA	1:C:764:ILE:HG13	1.95	0.48
1:A:700:HIS:HB3	1:A:703:THR:HG23	1.95	0.48
1:A:110:ARG:NH2	1:A:184:PRO:HG3	2.29	0.48
1:C:910:TRP:CD2	4:C:1505:PGE:H3	2.49	0.48
1:C:458:LYS:HG2	1:C:525:TRP:HB3	1.95	0.48
1:C:343:THR:HA	1:C:378:MET:O	2.13	0.48
1:A:343:THR:HA	1:A:378:MET:O	2.14	0.47
1:C:839:ARG:HB3	6:C:1512:PEG:H41	1.96	0.47
1:A:523:TRP:CG	5:A:1013:EDO:H11	2.50	0.47
1:C:424:ASN:OD1	1:C:451:ASP:HB3	2.14	0.47
1:A:478:LEU:HD11	1:A:485:LEU:HD12	1.97	0.46
1:A:171:ASN:HA	1:A:269:ASP:OD1	2.15	0.46
2:B:109:GLY:N	5:B:604:EDO:H21	2.30	0.46
1:C:450:LEU:HG	1:C:485:LEU:HD21	1.97	0.46
1:C:805:GLN:HG2	1:C:807:HIS:CE1	2.50	0.46
1:C:327:HIS:ND1	1:C:332:ASP:OD1	2.38	0.46
1:A:58:SER:HB2	1:A:174:GLY:HA2	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:682:LEU:HD23	1:C:711:LEU:HD11	1.98	0.46
1:A:106:LEU:HG	1:A:107:GLU:HG3	1.98	0.46
2:B:61:GLY:HA2	2:B:70:CYS:SG	2.55	0.45
2:B:74:SER:HB3	5:B:602:EDO:H12	1.99	0.45
2:D:61:GLY:HA2	2:D:70:CYS:SG	2.56	0.45
1:C:959:SER:OG	6:C:1504:PEG:H22	2.16	0.45
1:C:460:TYR:CE2	1:C:490:ASP:HB2	2.52	0.45
6:C:1512:PEG:C2	2:D:91:ARG:HH21	2.29	0.44
2:D:79:ASN:HB3	2:D:116:CYS:SG	2.57	0.44
2:D:58:CYS:SG	2:D:63:ASP:HB3	2.58	0.44
1:C:110:ARG:NH2	9:C:1647:HOH:O	2.50	0.44
1:A:847:ASP:HB3	1:A:908:PRO:HG2	2.00	0.43
1:C:146:PRO:HG2	1:C:162:GLU:HG3	1.99	0.43
1:C:964[A]:HIS:HD2	1:C:966:ARG:HG2	1.83	0.43
1:C:478:LEU:CD1	1:C:485:LEU:HD12	2.49	0.43
1:A:259:LYS:HE3	1:A:259:LYS:HB2	1.85	0.43
1:A:758:ASP:OD2	1:A:790:TYR:OH	2.25	0.43
1:A:951:ARG:HG3	2:B:55:TYR:CE1	2.54	0.43
6:C:1512:PEG:H42	2:D:90:SER:O	2.19	0.43
1:A:791:LEU:O	1:A:810:PRO:HA	2.20	0.42
1:A:884:LEU:HG	1:A:899:ALA:HB3	2.01	0.42
4:A:1007:PGE:H4	9:A:1265:HOH:O	2.20	0.42
1:C:839:ARG:CA	6:C:1512:PEG:H41	2.50	0.42
1:A:929:THR:HB	1:A:961:TRP:HB3	2.01	0.42
1:C:42:ASP:HB2	9:C:1613:HOH:O	2.19	0.42
1:A:458:LYS:HG2	1:A:525:TRP:HB3	2.01	0.42
1:A:424:ASN:HD21	1:A:451:ASP:C	2.23	0.42
1:A:703:THR:CG2	6:A:1005:PEG:H32	2.49	0.42
1:C:500:ARG:HE	1:C:504:GLU:HG2	1.85	0.42
1:C:870:ASP:OD2	1:C:873:THR:OG1	2.24	0.41
1:A:432:LEU:HD22	1:A:477[A]:HIS:ND1	2.35	0.41
1:A:485:LEU:HD23	1:A:486:VAL:N	2.35	0.41
1:A:534:PHE:HB3	1:A:600:TYR:HB3	2.01	0.41
1:A:960:ASP:HB3	6:A:1009:PEG:H42	2.02	0.41
1:A:278:VAL:HG23	1:A:290:LEU:HB2	2.02	0.41
1:C:318:TYR:CE2	1:C:639:GLY:HA3	2.55	0.41
1:C:839:ARG:HA	6:C:1512:PEG:H41	2.02	0.41
1:C:129:SER:O	1:C:140:LEU:HA	2.21	0.41
1:A:33:VAL:HG12	1:A:308:GLN:O	2.21	0.41
1:A:754:GLN:HG3	1:A:769:MET:CE	2.51	0.41
1:A:259:LYS:HD2	9:A:1329:HOH:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:432:LEU:HD22	1:C:477[A]:HIS:ND1	2.36	0.41
1:C:742:LYS:NZ	9:C:1622:HOH:O	2.36	0.41
2:D:79:ASN:ND2	2:D:101:ASP:H	2.19	0.41
1:A:318:TYR:CE2	1:A:639:GLY:HA3	2.56	0.40
1:C:98:MET:SD	1:C:400:GLN:HB3	2.61	0.40
1:A:376:ARG:NH1	9:A:1101:HOH:O	1.99	0.40
2:D:79:ASN:HD21	2:D:99:CYS:HB3	1.86	0.40
2:D:79:ASN:OD1	2:D:79:ASN:N	2.54	0.40
1:A:460:TYR:CE2	1:A:490:ASP:HB2	2.57	0.40
1:C:534:PHE:HB3	1:C:600:TYR:HB3	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	852/977 (87%)	820 (96%)	31 (4%)	1 (0%)	51	67
1	C	859/977 (88%)	825 (96%)	34 (4%)	0	100	100
2	B	85/554 (15%)	82 (96%)	3 (4%)	0	100	100
2	D	85/554 (15%)	82 (96%)	3 (4%)	0	100	100
All	All	1881/3062 (61%)	1809 (96%)	71 (4%)	1 (0%)	51	67

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	643	ALA

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	747/846 (88%)	737 (99%)	10 (1%)	69	82
1	C	742/846 (88%)	732 (99%)	10 (1%)	69	82
2	B	69/485 (14%)	67 (97%)	2 (3%)	42	60
2	D	71/485 (15%)	66 (93%)	5 (7%)	15	21
All	All	1629/2662 (61%)	1602 (98%)	27 (2%)	60	76

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	33	VAL
1	A	54	ARG
1	A	69	LEU
1	A	72	ASP
1	A	122	ASP
1	A	164	ARG
1	A	446	ASP
1	A	637	TRP
1	A	665	PHE
1	A	706	ARG
2	B	78	THR
2	B	85	LEU
1	C	77	HIS
1	C	97	ASP
1	C	312	ASN
1	C	424	ASN
1	C	446	ASP
1	C	637	TRP
1	C	665	PHE
1	C	706	ARG
1	C	906	GLU
1	C	929	THR
2	D	78	THR
2	D	80	THR

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Mol	Chain	Res	Type
2	D	83	LYS
2	D	85	LEU
2	D	90	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	424	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 55 ligands modelled in this entry, 4 are monoatomic - leaving 51 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	EDO	B	602	-	3,3,3	0.58	0	2,2,2	0.15	0
4	PGE	C	1505	-	9,9,9	0.39	0	8,8,8	0.32	0
5	EDO	A	1012	-	3,3,3	0.63	0	2,2,2	0.31	0
5	EDO	C	1511	-	3,3,3	0.47	0	2,2,2	0.45	0
6	PEG	A	1017	-	6,6,6	0.47	0	5,5,5	0.31	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	EDO	C	1519	-	3,3,3	0.49	0	2,2,2	0.22	0
6	PEG	C	1508	-	6,6,6	0.49	0	5,5,5	0.31	0
8	SO4	C	1523	-	4,4,4	0.18	0	6,6,6	0.41	0
4	PGE	A	1002	-	9,9,9	0.39	0	8,8,8	0.56	0
8	SO4	C	1524	-	4,4,4	0.17	0	6,6,6	0.23	0
5	EDO	C	1509	-	3,3,3	0.46	0	2,2,2	0.53	0
5	EDO	C	1503	-	3,3,3	0.64	0	2,2,2	0.16	0
6	PEG	A	1011	-	6,6,6	0.49	0	5,5,5	0.26	0
5	EDO	C	1517	-	3,3,3	0.50	0	2,2,2	0.30	0
5	EDO	A	1015	-	3,3,3	0.50	0	2,2,2	0.62	0
5	EDO	A	1019	-	3,3,3	0.56	0	2,2,2	0.23	0
4	PGE	A	1006	-	9,9,9	0.34	0	8,8,8	0.49	0
5	EDO	C	1515	-	3,3,3	0.75	0	2,2,2	0.46	0
5	EDO	C	1521	-	3,3,3	0.23	0	2,2,2	0.13	0
5	EDO	A	1016	-	3,3,3	0.53	0	2,2,2	0.40	0
4	PGE	A	1008	-	9,9,9	0.22	0	8,8,8	0.15	0
5	EDO	B	605	-	3,3,3	0.60	0	2,2,2	0.33	0
5	EDO	C	1507	-	3,3,3	0.62	0	2,2,2	0.16	0
3	WA7	C	1502	-	29,31,31	2.93	10 (34%)	35,43,43	1.27	3 (8%)
6	PEG	C	1504	-	6,6,6	0.50	0	5,5,5	0.40	0
5	EDO	A	1018	-	3,3,3	0.46	0	2,2,2	0.45	0
6	PEG	C	1512	-	6,6,6	0.46	0	5,5,5	0.93	0
5	EDO	C	1506	-	3,3,3	0.52	0	2,2,2	0.39	0
6	PEG	A	1005	-	6,6,6	0.53	0	5,5,5	0.62	0
5	EDO	C	1510	-	3,3,3	0.47	0	2,2,2	0.14	0
4	PGE	A	1007	-	9,9,9	0.42	0	8,8,8	0.38	0
5	EDO	C	1516	-	3,3,3	0.40	0	2,2,2	0.80	0
3	WA7	A	1001	-	29,31,31	3.27	12 (41%)	35,43,43	1.59	6 (17%)
5	EDO	A	1013	-	3,3,3	0.47	0	2,2,2	0.42	0
5	EDO	D	603	-	3,3,3	0.45	0	2,2,2	0.40	0
5	EDO	A	1003	-	3,3,3	0.57	0	2,2,2	0.26	0
5	EDO	D	601	-	3,3,3	0.57	0	2,2,2	0.16	0
5	EDO	B	604	-	3,3,3	0.44	0	2,2,2	0.40	0
6	PEG	D	602	-	6,6,6	0.13	0	5,5,5	0.18	0
5	EDO	C	1501	-	3,3,3	0.50	0	2,2,2	0.40	0
5	EDO	C	1518	-	3,3,3	0.45	0	2,2,2	0.64	0
5	EDO	C	1520	-	3,3,3	0.37	0	2,2,2	0.72	0
5	EDO	C	1513	-	3,3,3	0.56	0	2,2,2	0.26	0
5	EDO	A	1014	-	3,3,3	0.69	0	2,2,2	0.11	0
6	PEG	A	1010	-	6,6,6	0.50	0	5,5,5	0.30	0
5	EDO	C	1522	-	3,3,3	0.59	0	2,2,2	0.29	0
6	PEG	A	1009	-	6,6,6	0.35	0	5,5,5	0.15	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	EDO	C	1514	-	3,3,3	0.55	0	2,2,2	0.16	0
6	PEG	A	1004	-	6,6,6	0.52	0	5,5,5	0.39	0
6	PEG	B	601	-	6,6,6	0.51	0	5,5,5	0.43	0
5	EDO	B	603	-	3,3,3	0.49	0	2,2,2	0.30	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	EDO	B	602	-	-	1/1/1/1	-
4	PGE	C	1505	-	-	4/7/7/7	-
5	EDO	A	1012	-	-	0/1/1/1	-
5	EDO	C	1511	-	-	0/1/1/1	-
6	PEG	A	1017	-	-	1/4/4/4	-
5	EDO	C	1519	-	-	1/1/1/1	-
6	PEG	C	1508	-	-	2/4/4/4	-
4	PGE	A	1002	-	-	3/7/7/7	-
5	EDO	C	1509	-	-	0/1/1/1	-
5	EDO	C	1503	-	-	1/1/1/1	-
6	PEG	A	1011	-	-	0/4/4/4	-
5	EDO	C	1517	-	-	0/1/1/1	-
5	EDO	A	1015	-	-	1/1/1/1	-
5	EDO	A	1019	-	-	0/1/1/1	-
4	PGE	A	1006	-	-	3/7/7/7	-
5	EDO	C	1515	-	-	1/1/1/1	-
5	EDO	C	1521	-	-	0/1/1/1	-
5	EDO	A	1016	-	-	0/1/1/1	-
4	PGE	A	1008	-	-	5/7/7/7	-
5	EDO	B	605	-	-	1/1/1/1	-
5	EDO	C	1507	-	-	0/1/1/1	-
3	WA7	C	1502	-	-	8/17/42/42	0/2/2/2
6	PEG	C	1504	-	-	3/4/4/4	-
5	EDO	A	1018	-	-	1/1/1/1	-
6	PEG	C	1512	-	-	0/4/4/4	-
5	EDO	C	1506	-	-	0/1/1/1	-
6	PEG	A	1005	-	-	0/4/4/4	-
5	EDO	C	1510	-	-	1/1/1/1	-
4	PGE	A	1007	-	-	3/7/7/7	-
5	EDO	C	1516	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	WA7	A	1001	-	-	8/17/42/42	0/2/2/2
5	EDO	A	1013	-	-	1/1/1/1	-
5	EDO	D	603	-	-	1/1/1/1	-
5	EDO	A	1003	-	-	0/1/1/1	-
5	EDO	D	601	-	-	1/1/1/1	-
5	EDO	B	604	-	-	1/1/1/1	-
6	PEG	D	602	-	-	3/4/4/4	-
5	EDO	C	1501	-	-	0/1/1/1	-
5	EDO	C	1518	-	-	1/1/1/1	-
5	EDO	C	1520	-	-	1/1/1/1	-
5	EDO	C	1513	-	-	0/1/1/1	-
5	EDO	A	1014	-	-	1/1/1/1	-
6	PEG	A	1010	-	-	1/4/4/4	-
5	EDO	C	1522	-	-	1/1/1/1	-
6	PEG	A	1009	-	-	1/4/4/4	-
5	EDO	C	1514	-	-	1/1/1/1	-
6	PEG	A	1004	-	-	2/4/4/4	-
6	PEG	B	601	-	-	2/4/4/4	-
5	EDO	B	603	-	-	1/1/1/1	-

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1001	WA7	O6-N3	13.61	1.45	1.22
3	C	1502	WA7	O6-N3	10.82	1.41	1.22
3	A	1001	WA7	N5-N4	5.27	1.39	1.24
3	C	1502	WA7	N5-N4	5.09	1.39	1.24
3	C	1502	WA7	O2-C1	-4.24	1.37	1.44
3	C	1502	WA7	C12-C17	-3.92	1.35	1.40
3	A	1001	WA7	O2-C1	-3.77	1.38	1.44
3	C	1502	WA7	C6-C1	-3.36	1.49	1.53
3	A	1001	WA7	C12-C17	-3.32	1.36	1.40
3	C	1502	WA7	O4-C3	-3.19	1.35	1.43
3	A	1001	WA7	O4-C3	-3.18	1.35	1.43
3	A	1001	WA7	C5-N1	-3.08	1.41	1.47
3	C	1502	WA7	C12-N2	3.07	1.45	1.37
3	A	1001	WA7	C6-C1	-2.92	1.50	1.53
3	A	1001	WA7	C7-C1	2.91	1.57	1.52
3	C	1502	WA7	C5-N1	-2.82	1.41	1.47
3	A	1001	WA7	C12-N2	2.71	1.45	1.37
3	A	1001	WA7	O3-C2	-2.71	1.37	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	1502	WA7	O1-C7	-2.71	1.33	1.42
3	C	1502	WA7	O3-C2	-2.34	1.38	1.42
3	A	1001	WA7	O1-C7	-2.20	1.34	1.42
3	A	1001	WA7	C3-C2	-2.08	1.49	1.53

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1001	WA7	C11-N2-C12	-4.01	113.75	123.39
3	C	1502	WA7	C17-C12-N2	-3.82	116.62	123.33
3	A	1001	WA7	C15-N4-N5	3.77	123.51	116.02
3	C	1502	WA7	O6-N3-C17	-3.63	112.83	119.03
3	A	1001	WA7	O6-N3-C17	3.62	125.22	119.03
3	A	1001	WA7	C13-C12-N2	-3.19	116.37	121.80
3	A	1001	WA7	C16-C17-C12	-3.03	118.78	121.53
3	A	1001	WA7	C17-C16-C15	2.39	121.61	119.32
3	C	1502	WA7	O2-C1-C6	-2.32	103.50	108.36

There are no chirality outliers.

All (68) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1001	WA7	C6-C5-N1-C8
3	A	1001	WA7	C14-C15-N4-N5
3	A	1001	WA7	C16-C15-N4-N5
3	A	1001	WA7	C15-N4-N5-N6
3	C	1502	WA7	C14-C15-N4-N5
3	C	1502	WA7	C16-C15-N4-N5
3	C	1502	WA7	C17-C12-N2-C11
4	C	1505	PGE	C4-C3-O2-C2
4	A	1008	PGE	O2-C3-C4-O3
4	A	1006	PGE	O2-C3-C4-O3
4	A	1007	PGE	O2-C3-C4-O3
3	C	1502	WA7	C13-C12-N2-C11
4	C	1505	PGE	O2-C3-C4-O3
6	C	1504	PEG	O1-C1-C2-O2
4	A	1006	PGE	O1-C1-C2-O2
6	B	601	PEG	O1-C1-C2-O2
3	A	1001	WA7	C11-C10-C9-C8
4	A	1002	PGE	O2-C3-C4-O3
5	B	604	EDO	O1-C1-C2-O2
5	C	1510	EDO	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
5	C	1514	EDO	O1-C1-C2-O2
5	C	1520	EDO	O1-C1-C2-O2
5	D	601	EDO	O1-C1-C2-O2
6	B	601	PEG	C4-C3-O2-C2
3	C	1502	WA7	C15-N4-N5-N6
3	C	1502	WA7	C6-C5-N1-C8
4	A	1007	PGE	O1-C1-C2-O2
6	D	602	PEG	O1-C1-C2-O2
4	A	1002	PGE	O3-C5-C6-O4
5	C	1516	EDO	O1-C1-C2-O2
5	C	1518	EDO	O1-C1-C2-O2
5	C	1522	EDO	O1-C1-C2-O2
3	C	1502	WA7	C10-C11-N2-C12
4	A	1008	PGE	O3-C5-C6-O4
5	A	1013	EDO	O1-C1-C2-O2
5	A	1015	EDO	O1-C1-C2-O2
5	B	603	EDO	O1-C1-C2-O2
5	C	1515	EDO	O1-C1-C2-O2
3	A	1001	WA7	N1-C8-C9-C10
3	A	1001	WA7	C9-C10-C11-N2
6	A	1017	PEG	O1-C1-C2-O2
6	C	1504	PEG	C1-C2-O2-C3
6	D	602	PEG	C1-C2-O2-C3
6	D	602	PEG	C4-C3-O2-C2
6	C	1508	PEG	C4-C3-O2-C2
4	A	1008	PGE	C6-C5-O3-C4
4	A	1008	PGE	C1-C2-O2-C3
6	A	1010	PEG	C1-C2-O2-C3
4	A	1002	PGE	C3-C4-O3-C5
4	C	1505	PGE	C3-C4-O3-C5
4	A	1008	PGE	O1-C1-C2-O2
6	A	1004	PEG	C1-C2-O2-C3
6	C	1504	PEG	O2-C3-C4-O4
6	C	1508	PEG	O2-C3-C4-O4
5	A	1018	EDO	O1-C1-C2-O2
5	B	602	EDO	O1-C1-C2-O2
5	D	603	EDO	O1-C1-C2-O2
4	A	1006	PGE	C1-C2-O2-C3
4	C	1505	PGE	O3-C5-C6-O4
6	A	1009	PEG	C4-C3-O2-C2
4	A	1007	PGE	C6-C5-O3-C4
3	A	1001	WA7	C16-C17-N3-O6

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Mol	Chain	Res	Type	Atoms
5	C	1519	EDO	O1-C1-C2-O2
3	C	1502	WA7	C11-C10-C9-C8
5	A	1014	EDO	O1-C1-C2-O2
5	B	605	EDO	O1-C1-C2-O2
5	C	1503	EDO	O1-C1-C2-O2
6	A	1004	PEG	C4-C3-O2-C2

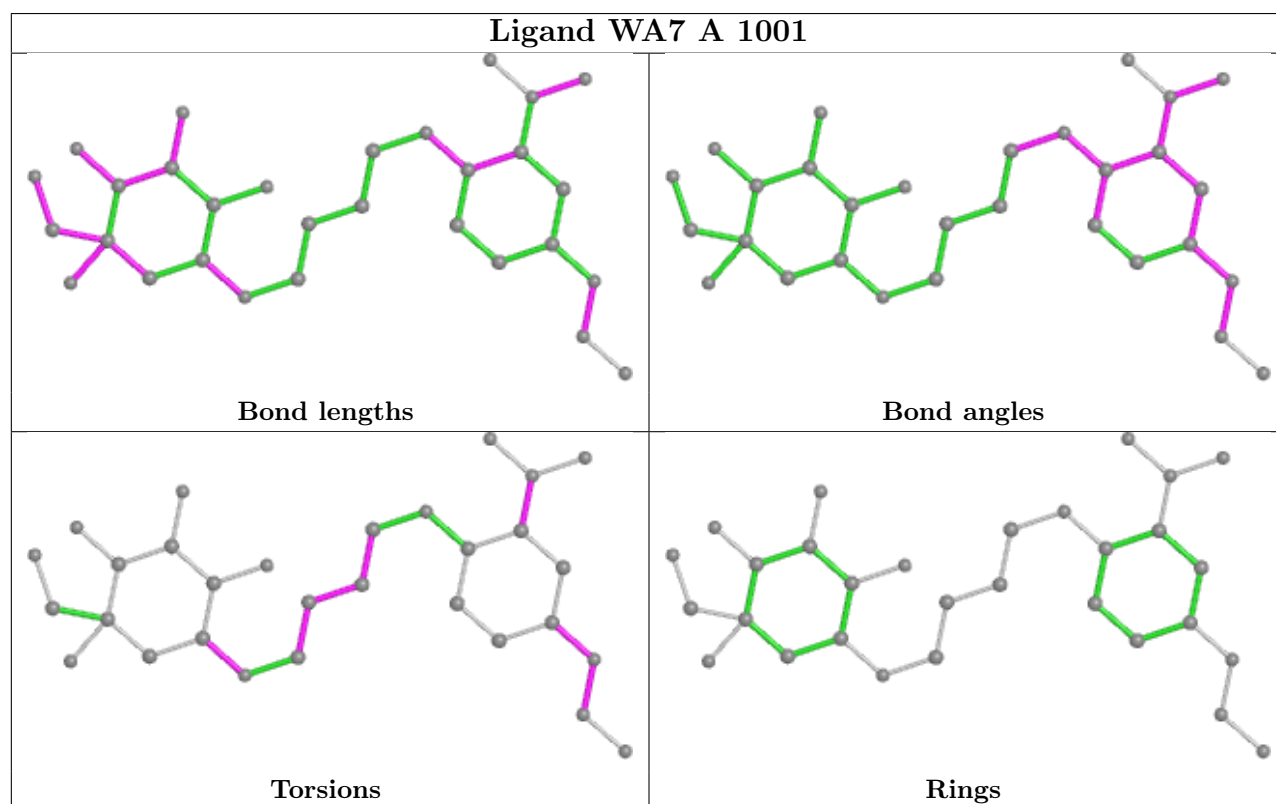
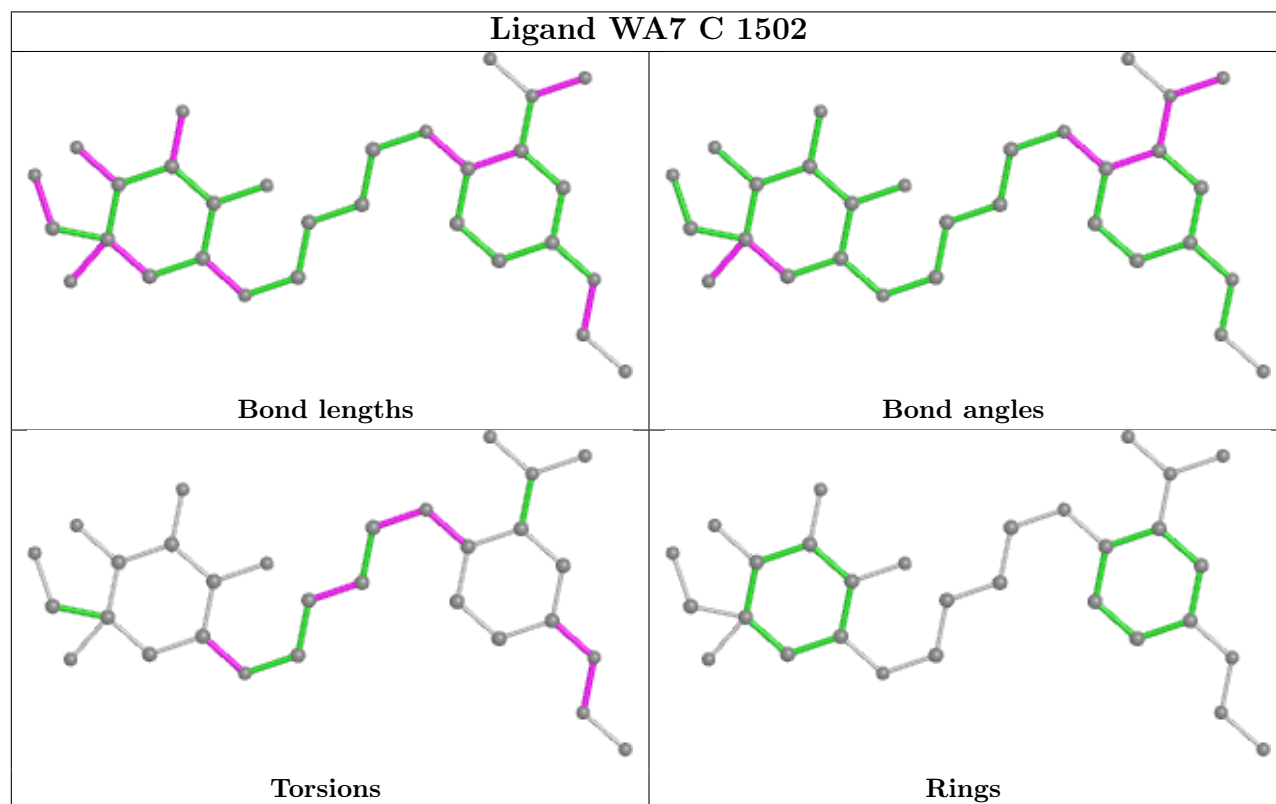
There are no ring outliers.

22 monomers are involved in 44 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	602	EDO	1	0
4	C	1505	PGE	1	0
5	C	1519	EDO	1	0
8	C	1524	SO4	1	0
5	C	1503	EDO	1	0
5	A	1015	EDO	2	0
5	A	1019	EDO	1	0
4	A	1006	PGE	3	0
4	A	1008	PGE	3	0
5	B	605	EDO	1	0
6	C	1504	PEG	1	0
6	C	1512	PEG	12	0
6	A	1005	PEG	2	0
4	A	1007	PGE	1	0
5	C	1516	EDO	3	0
5	A	1013	EDO	1	0
5	B	604	EDO	2	0
6	D	602	PEG	2	0
5	C	1518	EDO	2	0
5	C	1520	EDO	1	0
5	C	1513	EDO	1	0
6	A	1009	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.



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	A	854/977 (87%)	0.02	52 (6%) 21 23	30, 43, 69, 106	0
1	C	857/977 (87%)	0.20	69 (8%) 12 13	32, 48, 82, 102	0
2	B	87/554 (15%)	0.63	18 (20%) 1 1	38, 59, 92, 101	0
2	D	87/554 (15%)	0.68	15 (17%) 1 1	41, 60, 94, 104	0
All	All	1885/3062 (61%)	0.16	154 (8%) 11 12	30, 46, 82, 106	0

All (154) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	184	PRO	9.6
2	D	43	THR	8.3
2	D	81	GLY	7.8
2	B	43	THR	6.5
2	D	31	TYR	5.9
2	D	80	THR	5.8
1	C	34	ASP	5.3
1	C	184	PRO	5.2
1	C	185	ARG	5.0
2	B	48	PHE	4.9
1	C	143	ALA	4.8
2	D	82	TYR	4.7
1	C	128	LEU	4.6
1	C	370	THR	4.5
1	A	109	ARG	4.5
1	C	69	LEU	4.5
1	A	248	TRP	4.4
1	C	627	PHE	4.2
1	C	82	VAL	4.0
1	C	136	ASN	3.9
1	C	63	LEU	3.9

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Mol	Chain	Res	Type	RSRZ
2	D	117	ARG	3.9
1	C	129	SER	3.8
2	B	33	GLU	3.8
2	D	44	ALA	3.8
1	C	79	ILE	3.8
1	C	141	THR	3.7
1	A	636	VAL	3.7
1	C	73	ALA	3.5
2	D	32	GLU	3.5
2	B	41	ASP	3.5
1	A	183	ALA	3.5
1	A	635	ALA	3.5
1	A	33	VAL	3.4
1	C	137	SER	3.4
1	A	416	LEU	3.4
1	C	81	GLU	3.3
1	C	132	GLY	3.3
1	C	130	VAL	3.3
1	A	110	ARG	3.3
1	C	65	ASP	3.3
1	C	135	ASP	3.3
1	C	142	VAL	3.3
1	C	321	VAL	3.3
1	A	164	ARG	3.2
1	C	33	VAL	3.2
1	A	622	LEU	3.2
1	C	144	GLU	3.1
1	C	599	LEU	3.1
2	B	86	TYR	3.1
1	C	127	ARG	3.1
1	C	625	ALA	3.1
1	A	658	LEU	3.1
1	A	694	PHE	3.1
1	A	247	ALA	3.1
2	B	31	TYR	3.1
1	C	626	PHE	3.1
1	A	665	PHE	3.0
2	B	34	SER	3.0
1	A	246	GLY	3.0
2	B	42	GLY	3.0
1	A	252	PHE	3.0
1	A	370	THR	3.0

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Mol	Chain	Res	Type	RSRZ
2	D	41	ASP	3.0
1	A	254	THR	3.0
1	C	74	LEU	2.9
1	C	133	ARG	2.9
1	C	85	VAL	2.9
1	A	693	PRO	2.9
1	C	636	VAL	2.8
1	C	658	LEU	2.8
1	A	249	GLU	2.8
1	C	83	THR	2.8
1	C	663	LEU	2.8
2	B	117	ARG	2.8
2	B	32	GLU	2.8
2	D	45	THR	2.8
1	A	253	LYS	2.7
2	D	79	ASN	2.7
1	C	320	SER	2.7
1	A	667	GLY	2.7
1	A	666	CYS	2.7
1	A	251	THR	2.7
1	A	891	GLY	2.7
1	C	322	PRO	2.7
1	A	659	ALA	2.7
1	C	635	ALA	2.6
2	B	44	ALA	2.6
1	C	66	THR	2.6
1	C	67	LEU	2.6
1	C	622	LEU	2.6
1	A	637	TRP	2.6
1	A	319	GLY	2.6
1	A	626	PHE	2.5
1	C	131	SER	2.5
1	A	663	LEU	2.5
1	C	165	SER	2.5
1	A	71	PRO	2.5
1	A	415	SER	2.5
1	A	34	ASP	2.5
1	C	623	SER	2.5
2	B	82	TYR	2.5
2	D	39	CYS	2.5
1	A	621	VAL	2.4
1	A	163	ASP	2.4

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Mol	Chain	Res	Type	RSRZ
2	B	115	THR	2.4
2	D	38	THR	2.4
1	A	318	TYR	2.4
1	A	321	VAL	2.4
1	C	84	LYS	2.3
1	C	68	GLN	2.3
1	C	340	ALA	2.3
1	C	341	ALA	2.3
1	C	64	LEU	2.3
2	B	79	ASN	2.3
1	C	595	ASN	2.3
1	C	140	LEU	2.3
1	C	323	VAL	2.3
1	C	55	PRO	2.3
1	C	245	PRO	2.3
2	D	86	TYR	2.2
1	A	623	SER	2.2
1	A	182	ARG	2.2
1	A	664	SER	2.2
1	C	70	GLY	2.2
1	C	714	GLN	2.2
1	A	943	PRO	2.2
1	A	794	GLN	2.2
1	C	138	VAL	2.2
2	D	37	PHE	2.1
2	B	85	LEU	2.1
1	C	662	GLY	2.1
1	C	183	ALA	2.1
1	A	634	GLY	2.1
1	C	338	LEU	2.1
1	C	666	CYS	2.1
2	B	39	CYS	2.1
1	A	638	THR	2.1
1	C	126	ALA	2.1
1	C	319	GLY	2.1
2	B	84	PRO	2.1
2	B	38	THR	2.1
1	A	655	CYS	2.1
1	A	733	TRP	2.1
1	A	747	VAL	2.1
1	C	76	VAL	2.1
1	C	901	PRO	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	657	SER	2.0
1	A	737	PHE	2.0
1	A	317	LEU	2.0
1	C	500	ARG	2.0
1	A	419	HIS	2.0
1	C	795	GLU	2.0
1	C	164	ARG	2.0

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

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	EDO	B	605	4/4	0.68	0.35	53,61,62,75	0
5	EDO	A	1015	4/4	0.69	0.25	54,57,61,85	0
6	PEG	B	601	7/7	0.70	0.37	58,67,74,76	0
5	EDO	C	1510	4/4	0.75	0.26	70,78,78,79	0
5	EDO	C	1522	4/4	0.76	0.36	62,63,64,83	0
5	EDO	A	1014	4/4	0.78	0.18	42,52,59,70	0
5	EDO	C	1515	4/4	0.78	0.26	36,49,58,64	0
6	PEG	D	602	7/7	0.81	0.28	62,69,74,75	0
5	EDO	C	1507	4/4	0.82	0.20	63,66,66,73	0
5	EDO	B	602	4/4	0.82	0.26	54,61,68,70	0
4	PGE	A	1002	10/10	0.82	0.20	50,66,73,79	0
6	PEG	C	1512	7/7	0.84	0.31	50,52,61,63	0
4	PGE	A	1008	10/10	0.84	0.23	79,84,92,102	0
6	PEG	C	1508	7/7	0.85	0.25	58,67,75,80	0
3	WA7	C	1502	30/30	0.85	0.18	35,59,81,85	0
4	PGE	A	1007	10/10	0.85	0.30	50,65,74,79	0

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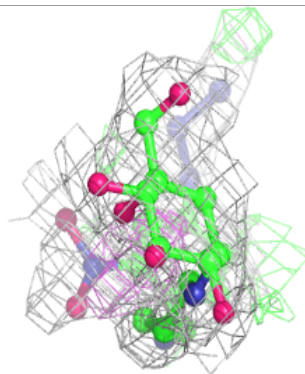
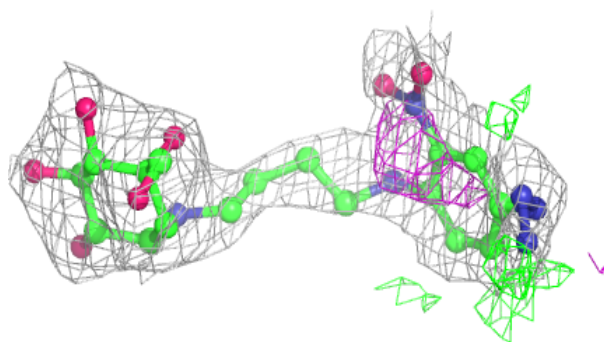
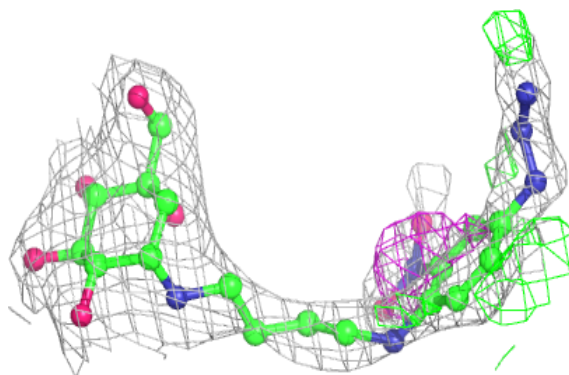
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
5	EDO	D	601	4/4	0.86	0.15	58,63,66,71	0
5	EDO	A	1013	4/4	0.86	0.17	64,66,67,67	0
5	EDO	C	1503	4/4	0.86	0.24	59,59,61,62	0
5	EDO	C	1517	4/4	0.86	0.16	61,67,68,73	0
4	PGE	C	1505	10/10	0.86	0.24	54,65,71,77	0
6	PEG	A	1004	7/7	0.87	0.16	51,62,68,73	0
6	PEG	A	1010	7/7	0.88	0.17	53,59,66,68	0
3	WA7	A	1001	30/30	0.88	0.15	36,60,82,94	0
5	EDO	B	603	4/4	0.88	0.15	58,62,64,81	0
5	EDO	C	1521	4/4	0.88	0.20	86,92,100,104	0
6	PEG	A	1009	7/7	0.88	0.31	60,62,71,72	0
6	PEG	C	1504	7/7	0.89	0.30	53,66,70,73	0
5	EDO	A	1018	4/4	0.89	0.43	54,55,58,61	0
5	EDO	C	1514	4/4	0.90	0.16	53,63,65,65	0
6	PEG	A	1005	7/7	0.90	0.22	43,54,64,65	0
5	EDO	C	1516	4/4	0.90	0.14	49,51,54,56	0
5	EDO	C	1513	4/4	0.91	0.16	51,54,54,62	0
4	PGE	A	1006	10/10	0.91	0.28	49,62,74,75	0
5	EDO	D	603	4/4	0.91	0.26	54,63,64,65	0
5	EDO	A	1019	4/4	0.92	0.29	55,60,63,66	0
5	EDO	C	1519	4/4	0.92	0.34	63,67,73,74	0
5	EDO	C	1506	4/4	0.92	0.09	46,57,60,63	0
5	EDO	A	1012	4/4	0.92	0.25	53,55,60,76	0
5	EDO	C	1501	4/4	0.92	0.12	54,58,63,70	0
6	PEG	A	1017	7/7	0.93	0.15	54,64,69,72	0
5	EDO	C	1509	4/4	0.93	0.17	56,56,64,70	0
6	PEG	A	1011	7/7	0.93	0.28	60,62,66,69	0
5	EDO	C	1520	4/4	0.94	0.21	58,60,65,70	0
5	EDO	A	1016	4/4	0.94	0.10	47,53,54,56	0
5	EDO	A	1003	4/4	0.94	0.21	46,52,52,53	0
5	EDO	C	1511	4/4	0.94	0.12	44,47,49,71	0
8	SO4	C	1523	5/5	0.94	0.16	61,67,82,104	0
8	SO4	C	1524	5/5	0.94	0.26	73,79,90,97	0
5	EDO	B	604	4/4	0.95	0.20	54,54,62,64	0
5	EDO	C	1518	4/4	0.96	0.23	49,55,61,66	0
7	CA	D	605	1/1	0.97	0.10	45,45,45,45	0
7	CA	D	604	1/1	0.98	0.06	51,51,51,51	0
7	CA	B	607	1/1	0.98	0.05	51,51,51,51	0
7	CA	B	606	1/1	0.99	0.09	45,45,45,45	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.

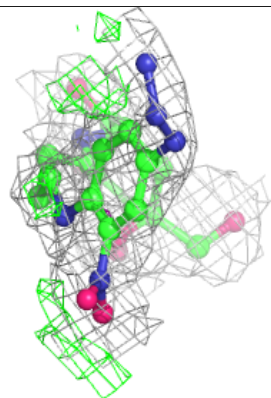
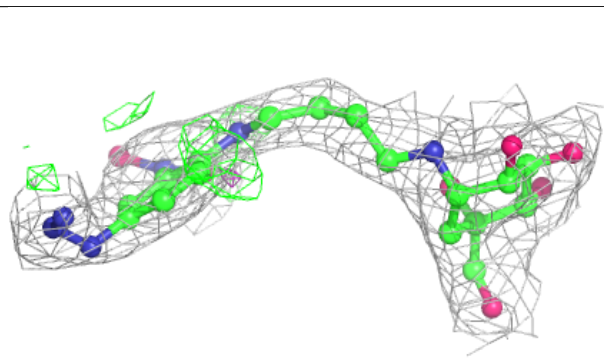
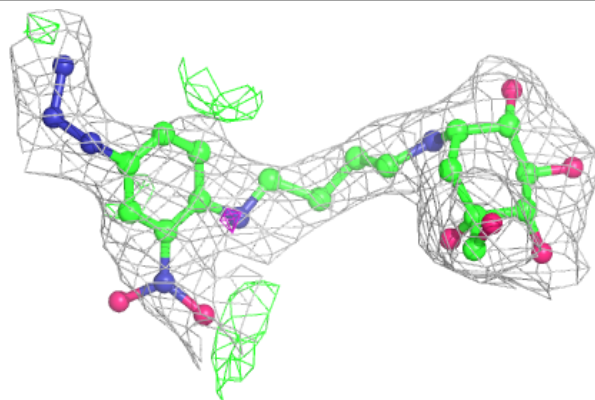
Electron density around WA7 C 1502:

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



Electron density around WA7 A 1001:

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



6.5 Other polymers [i](#)

There are no such residues in this entry.