



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 27, 2021 – 02:13 PM EDT

PDB ID : 7KAD
Title : Co-crystal structure of alpha glucosidase with compound 6
Authors : Karade, S.S.; Mariuzza, R.A.
Deposited on : 2020-09-30
Resolution : 2.51 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

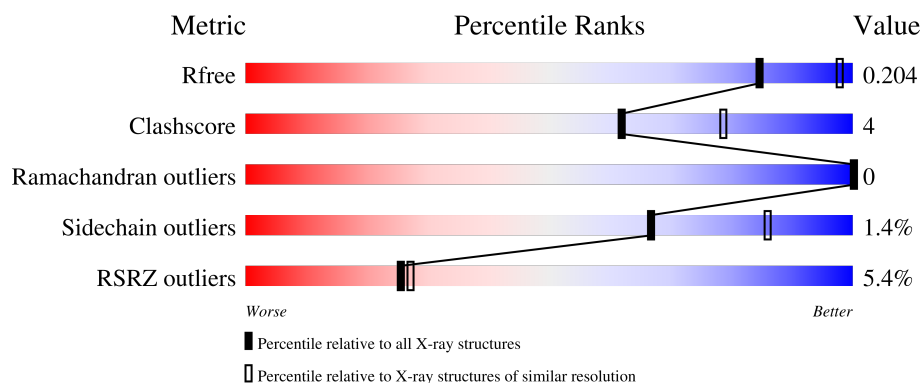
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.51 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	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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

Mol	Chain	Length	Quality of chain
1	A	977	<div> <div>2%</div> <div>78%</div> <div>9%</div> <div>13%</div> </div>
1	C	977	<div> <div>5%</div> <div>78%</div> <div>10%</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>15%</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
4	EDO	A	1020	-	-	-	X
5	PGE	A	1016	-	-	-	X
7	SO4	A	1034	-	-	X	-
7	SO4	A	1037	-	-	X	-
7	SO4	C	1028	-	-	-	X

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 15939 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	7	0
			6903	4426	1189	1258	30			
1	C	857	Total	C	N	O	S	0	8	0
			6903	4425	1198	1250	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
			623	371	102	140	10			
2	D	87	Total	C	N	O	S	0	0	0
			624	374	103	137	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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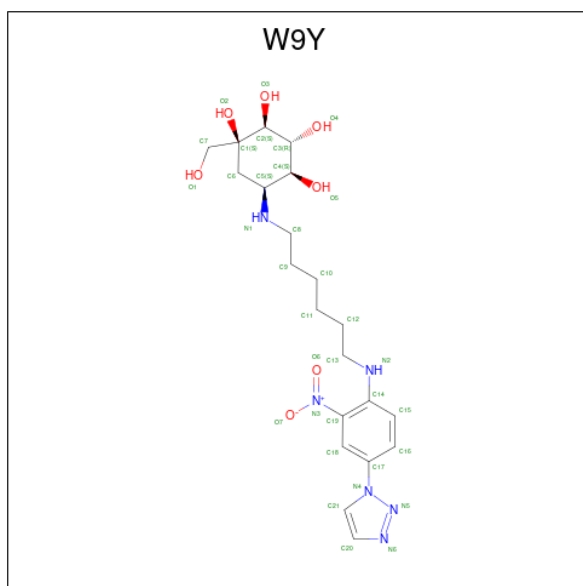
Chain	Residue	Modelled	Actual	Comment	Reference
D	-16	MET	-	initiating methionine	UNP O08795
D	-15	GLY	-	expression tag	UNP O08795
D	-14	ILE	-	expression tag	UNP O08795
D	-13	LEU	-	expression tag	UNP O08795
D	-12	PRO	-	expression tag	UNP O08795
D	-11	SER	-	expression tag	UNP O08795
D	-10	PRO	-	expression 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-[(6-{[2-nitro-4-(1H-1,2,3-triazol-1-yl)phenyl]amino}hexyl)amino]cyclohexane-1,2,3,4-tetrol (three-letter code: W9Y) (formula: C₂₁H₃₂N₆O₇) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			34	21	6	7		
3	C	1	Total	C	N	O	0	0
			34	21	6	7		

- Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



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

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

- Molecule 5 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: C₆H₁₄O₄).



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

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



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

- Molecule 7 is SULFATE ION (three-letter code: SO4) (formula: O₄S).

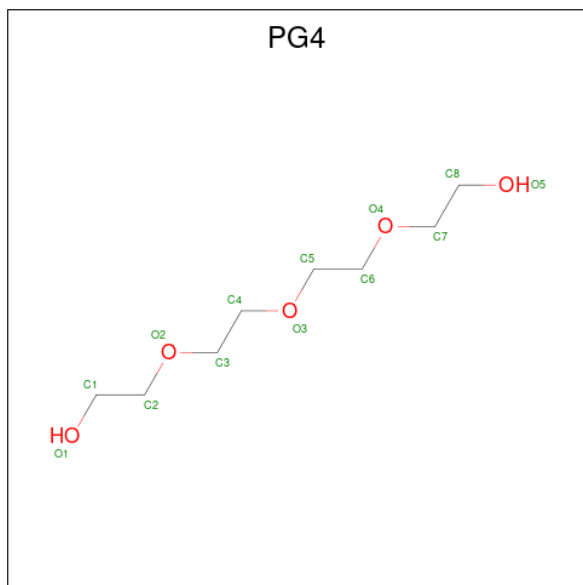


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	O	S	0	0
			5	4	1		
7	A	1	Total	O	S	0	0
			5	4	1		
7	A	1	Total	O	S	0	0
			5	4	1		
7	A	1	Total	O	S	0	0
			5	4	1		
7	C	1	Total	O	S	0	0
			5	4	1		
7	C	1	Total	O	S	0	0
			5	4	1		
7	C	1	Total	O	S	0	0
			5	4	1		
7	C	1	Total	O	S	0	0
			5	4	1		
7	C	1	Total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

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

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

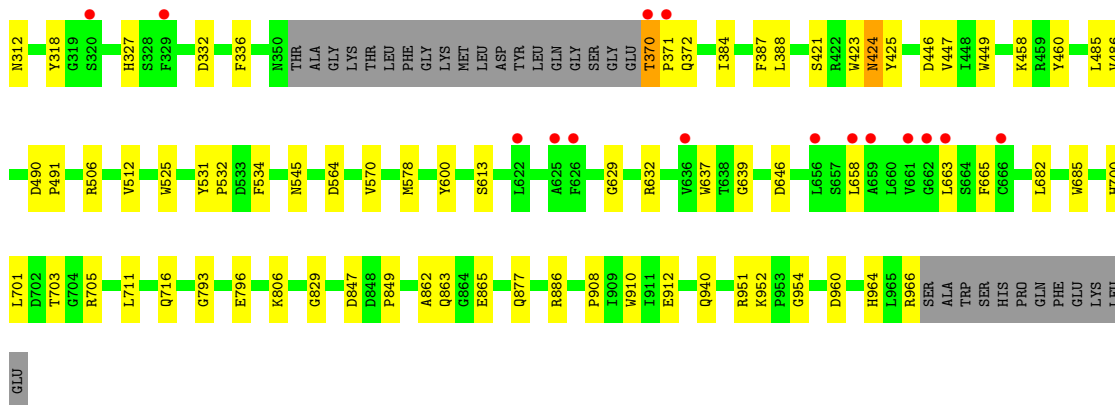
- Molecule 9 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: C₈H₁₈O₅).



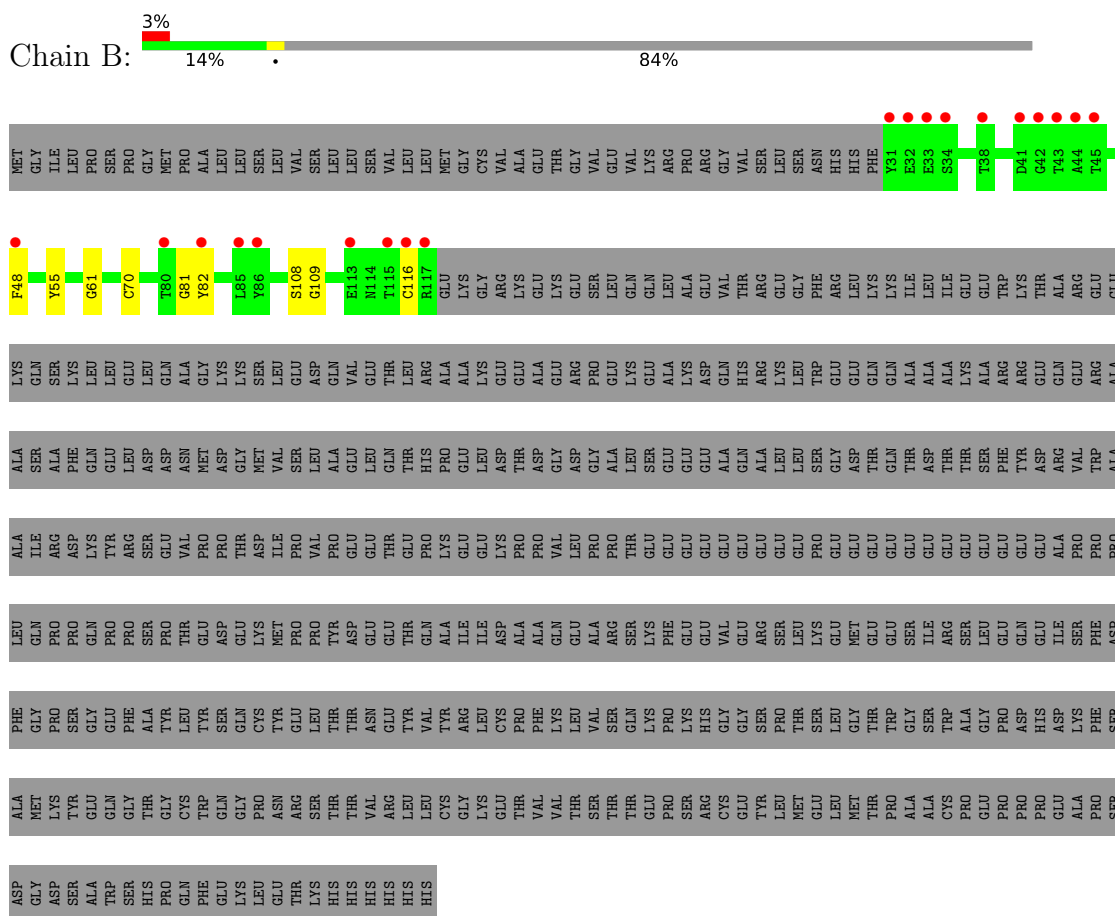
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	C	1	Total C O 13 8 5	0	0

- Molecule 10 is water.

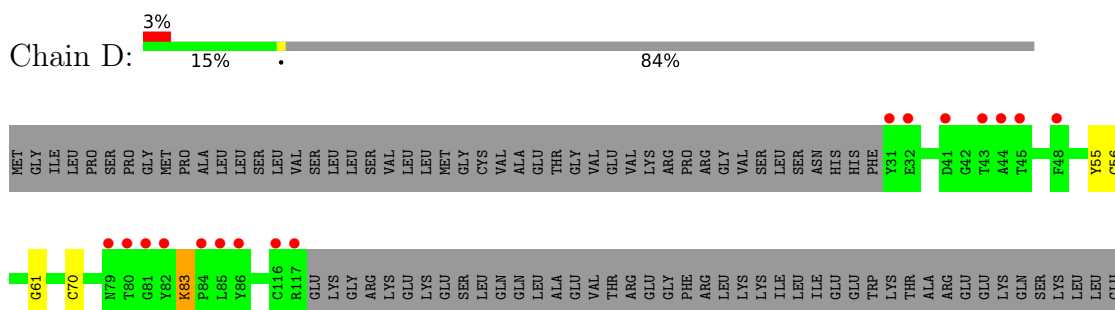
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	A	228	Total O 228 228	0	0
10	B	15	Total O 15 15	0	0
10	C	195	Total O 195 195	0	0
10	D	15	Total O 15 15	0	0



- Molecule 2: Glucosidase 2 subunit beta



- Molecule 2: Glucosidase 2 subunit beta



HIS	THR	ALA	SER	SER	LEU
PRO	GLY	TYR	PRO	GLU	GLN
GLN	CYS	LEU	THR	VAL	ALA
PHE	TRP	TYR	GLU	MET	GLY
GLU	GLN	SER	ASP	PRO	LYS
LYS	GLY	GLN	GLU	THR	GLY
LEU	PRO	CYS	LYS	ASP	MET
LEU	ASN	TYR	MET	ILE	SER
GLU	ASN	TYR	PRO	PRO	LEU
THR	ARG	GLU	ILE	VAL	GLU
LYS	SER	LEU	PRO	VAL	ASP
HIS	THR	THR	THR	ALA	GLN
HIS	THR	THR	THR	ALA	GLN
HIS	VAL	ASN	GLU	GLU	THR
HIS	ARG	GLU	GLU	THR	THR
HIS	LEU	TYR	THR	GLU	LEU
HIS	CYS	VAL	PRO	GLU	ALA
	GLY	ARG	ILE	GLY	ALA
	LYS	LEU	ILE	GLU	LYS
	GLU	CYS	ASP	LYS	GLU
	THR	PRO	ALA	THR	GLU
	VAL	PHE	ALA	PRO	THR
	VAL	LYS	GLN	ASP	ALA
	THR	LEU	GLU	ASP	GLY
	SER	VAL	ALA	GLY	ARG
	THR	SER	ARG	PRO	PRO
	THR	GLN	SER	PRO	GLU
	GLU	LYS	LYS	THR	LYS
	PRO	PRO	PHE	GLU	GLU
	SER	LYS	GLU	GLU	ALA
	ARG	HIS	GLU	GLU	LYS
	CYS	GLY	VAL	GLU	ASP
	GLU	TYR	GLU	GLU	GLN
	LEU	SER	LEU	GLU	ALA
	MET	GLU	LYS	PRO	THR
	LEU	LEU	GLU	GLU	TRP
	MET	GLY	MET	ASP	GLU
	THR	TRP	GLU	THR	GLN
	PRO	ALA	GLY	GLN	GLN
	ALA	SER	ILE	THR	ALA
	CYS	TRP	ARG	ASP	ALA
	PRO	ALA	SER	THR	LYS
	GLU	GLY	LEU	THR	ALA
	PRO	PRO	GLU	SER	ARG
	PRO	PRO	GLU	PHE	ARG
	PRO	ASP	GLN	TYR	ALA
	GLU	ASP	GLU	ASP	ALA
	ALA	ASP	ILE	ARG	ILE
	ALA	LYS	SER	VAL	ARG
	PRO	PHE	PHE	TRP	ALA
	SER	SER	ALA	ALA	ALA
	GLY	MET	GLY	ILE	SER
	ASP	LYS	PRO	GLN	ALA
	SER	TYR	SER	PRO	ALA
	ALA	GLU	GLY	GLN	PHE
	TRP	GLN	GLU	TYR	GLN
	SER	GLY	PHE	ARG	LEU

4 Data and refinement statistics

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, α , β , γ	102.69Å 102.69Å 240.28Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	42.28 – 2.51 42.28 – 2.51	Depositor EDS
% Data completeness (in resolution range)	99.9 (42.28-2.51) 94.9 (42.28-2.51)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.93 (at 2.51Å)	Xtriage
Refinement program	PHENIX 1.14_3228	Depositor
R, R_{free}	0.172 , 0.203 0.174 , 0.204	Depositor DCC
R_{free} test set	2037 reflections (2.09%)	wwPDB-VP
Wilson B-factor (Å ²)	41.8	Xtriage
Anisotropy	0.071	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 46.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.013 for -h,-k,l 0.042 for h,-h-k,-l 0.026 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	15939	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 2.49% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PEG, PG4, W9Y, CA, SO4, PGE, EDO

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.26	0/7132	0.47	0/9711
1	C	0.26	0/7136	0.46	0/9718
2	B	0.25	0/635	0.51	0/870
2	D	0.26	0/636	0.49	0/868
All	All	0.26	0/15539	0.47	0/21167

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

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	6903	0	6645	63	0
1	C	6903	0	6632	56	0
2	B	623	0	508	7	0
2	D	624	0	516	4	0
3	A	34	0	0	2	0
3	C	34	0	0	0	0
4	A	72	0	108	12	0
4	B	12	0	18	2	0
4	C	48	0	70	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	50	0	68	4	0
5	C	10	0	14	1	0
6	A	56	0	80	4	0
6	C	35	0	50	1	0
7	A	25	0	0	5	0
7	C	40	0	0	0	0
8	B	2	0	0	0	0
8	D	2	0	0	0	0
9	C	13	0	18	0	0
10	A	228	0	0	6	0
10	B	15	0	0	2	0
10	C	195	0	0	9	0
10	D	15	0	0	1	0
All	All	15939	0	14727	134	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 (134) 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:A:1001:W9Y:C20	4:A:1002:EDO:O1	2.00	1.09
1:A:150:ILE:O	10:A:1101:HOH:O	1.83	0.95
2:D:56:CYS:O	10:D:701:HOH:O	1.98	0.82
1:A:293:THR:HA	4:A:1011:EDO:H22	1.65	0.79
2:B:48:PHE:O	10:B:701:HOH:O	2.03	0.77
6:A:1017:PEG:H12	4:A:1018:EDO:H22	1.66	0.76
1:C:716:GLN:OE1	10:C:1101:HOH:O	2.05	0.73
2:D:83:LYS:HD3	2:D:83:LYS:H	1.55	0.71
1:C:506:ARG:HH12	4:C:1014:EDO:H11	1.55	0.70
1:A:143:ALA:O	10:A:1102:HOH:O	2.11	0.68
1:C:336:PHE:HB3	1:C:387:PHE:HB2	1.77	0.66
1:C:863:GLN:NE2	10:C:1103:HOH:O	2.17	0.65
1:A:380:GLU:OE1	10:A:1103:HOH:O	2.15	0.65
1:A:902:LYS:NZ	7:A:1034:SO4:O1	2.30	0.64
1:A:423:TRP:O	1:A:701:LEU:HA	2.00	0.62
4:C:1002:EDO:H22	10:C:1165:HOH:O	1.97	0.62
1:A:696:ARG:N	7:A:1037:SO4:O1	2.33	0.61
1:C:423:TRP:O	1:C:701:LEU:HA	2.00	0.60
1:C:964[A]:HIS:HD2	1:C:966:ARG:HG2	1.67	0.60
1:A:336:PHE:HB3	1:A:387:PHE:HB2	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:53:ILE:HD13	4:A:1031:EDO:H12	1.85	0.58
1:C:168:LEU:HD11	1:C:388:LEU:HD13	1.85	0.58
1:A:114:ARG:HB2	5:A:1004:PGE:H12	1.86	0.56
1:C:545:ASN:HB3	4:C:1011:EDO:H12	1.88	0.56
1:A:278:VAL:HG23	1:A:290:LEU:HB2	1.88	0.56
1:A:902:LYS:NZ	7:A:1034:SO4:S	2.78	0.56
1:A:112:ARG:NH2	1:A:179:GLU:O	2.39	0.55
1:A:428:GLU:HB2	4:A:1029:EDO:H12	1.88	0.55
1:C:865:GLU:OE2	1:C:886:ARG:NH2	2.39	0.55
1:C:458:LYS:HG2	1:C:525:TRP:HB3	1.89	0.55
1:A:645:TRP:HE1	6:A:1025:PEG:H31	1.72	0.54
1:C:564:ASP:OD2	10:C:1104:HOH:O	2.18	0.54
2:B:108:SER:H	4:B:602:EDO:H12	1.72	0.54
1:C:292:VAL:HG12	1:C:294:GLU:H	1.73	0.53
2:B:109:GLY:H	4:B:602:EDO:H12	1.73	0.52
1:A:645:TRP:NE1	6:A:1025:PEG:H31	2.24	0.52
1:A:447:VAL:HG11	1:A:486:VAL:HG23	1.91	0.52
1:C:629:GLY:O	1:C:632[A]:ARG:HG2	2.11	0.51
1:A:114:ARG:H	5:A:1004:PGE:H2	1.75	0.51
1:C:271:SER:HB3	1:C:372:GLN:NE2	2.25	0.51
2:B:82:TYR:HB2	2:B:116:CYS:HB3	1.92	0.50
1:A:884:LEU:HG	1:A:899:ALA:HB3	1.93	0.50
1:C:682:LEU:HD23	1:C:711:LEU:HD11	1.94	0.49
1:A:458:LYS:HG2	1:A:525:TRP:HB3	1.93	0.49
1:C:246:GLY:O	1:C:259:LYS:NZ	2.46	0.49
1:A:460:TYR:CE2	1:A:490:ASP:HB2	2.48	0.49
1:C:960:ASP:HB3	6:C:1007:PEG:H41	1.93	0.49
1:C:112:ARG:NH2	1:C:264:THR:O	2.45	0.48
1:C:146:PRO:HG2	1:C:162:GLU:HG3	1.94	0.48
1:A:427:ASP:HB2	4:A:1029:EDO:H11	1.95	0.48
1:A:148:LYS:NZ	1:A:163:ASP:O	2.30	0.48
1:C:81:GLU:O	1:C:84:LYS:NZ	2.34	0.48
2:D:61:GLY:HA2	2:D:70:CYS:SG	2.53	0.48
1:A:370:THR:N	1:A:371:PRO:HD2	2.29	0.48
1:C:491:PRO:O	1:C:532:PRO:HD2	2.14	0.48
1:C:700:HIS:HB3	1:C:703:THR:HG23	1.96	0.48
1:C:423:TRP:CD2	1:C:701:LEU:HB2	2.49	0.47
1:C:849:PRO:HB2	1:C:912:GLU:HB3	1.96	0.47
1:A:424:ASN:HD22	1:A:425:TYR:N	2.11	0.47
2:B:81:GLY:N	10:B:703:HOH:O	2.48	0.47
1:C:613:SER:HB3	10:C:1240:HOH:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:61:ARG:HB2	1:A:154:GLN:HG2	1.97	0.47
1:A:171:ASN:HA	1:A:269:ASP:OD1	2.14	0.47
1:A:459:ARG:NH1	1:A:494:LYS:HE2	2.30	0.47
1:C:60:TYR:OH	10:C:1105:HOH:O	2.20	0.47
1:A:534:PHE:HB3	1:A:600:TYR:HB3	1.96	0.47
1:C:327:HIS:ND1	1:C:332:ASP:OD1	2.32	0.47
1:C:793:GLY:HA3	1:C:796:GLU:HG3	1.97	0.47
1:A:156:PHE:O	10:A:1105:HOH:O	2.21	0.46
1:A:460:TYR:CZ	1:A:490:ASP:HB2	2.49	0.46
2:B:61:GLY:HA2	2:B:70:CYS:SG	2.56	0.46
1:C:447:VAL:HG11	1:C:486:VAL:HG23	1.97	0.46
1:C:705:ARG:NH1	10:C:1117:HOH:O	2.31	0.46
1:C:370:THR:N	1:C:371:PRO:HD2	2.30	0.46
1:A:421:SER:HB2	1:A:449:TRP:HB2	1.98	0.46
1:C:460:TYR:CE2	1:C:490:ASP:HB2	2.51	0.46
1:A:951:ARG:HG3	2:B:55:TYR:CE1	2.50	0.46
1:A:700:HIS:HB3	1:A:703:THR:HG23	1.98	0.46
1:A:802:GLN:HG3	10:A:1291:HOH:O	2.14	0.46
1:A:668:ALA:N	7:A:1037:SO4:O4	2.49	0.45
6:A:1017:PEG:H31	6:A:1017:PEG:H11	1.64	0.45
1:C:318:TYR:CE2	1:C:639:GLY:HA3	2.51	0.45
1:A:491:PRO:O	1:A:532:PRO:HD2	2.16	0.45
1:C:629:GLY:O	1:C:632[B]:ARG:HG2	2.17	0.44
1:C:910:TRP:CE3	1:C:954:GLY:HA2	2.53	0.44
1:A:292:VAL:HG12	1:A:294:GLU:H	1.82	0.44
1:A:80:HIS:HE2	4:A:1031:EDO:H22	1.83	0.44
1:A:73:ALA:HB2	1:A:92:GLN:HG2	2.00	0.44
1:A:183:ALA:HA	1:A:184:PRO:HD3	1.88	0.44
1:A:520:TYR:HE2	1:A:579:LEU:HD12	1.83	0.44
1:A:432:LEU:HD22	1:A:477[A]:HIS:ND1	2.32	0.43
1:C:424:ASN:HD22	1:C:425:TYR:N	2.15	0.43
1:C:951:ARG:HG3	2:D:55:TYR:CE1	2.53	0.43
1:A:635:ALA:HA	1:A:665:PHE:HB3	2.00	0.43
1:C:646:ASP:HB2	10:C:1170:HOH:O	2.18	0.43
1:A:538:ARG:HG2	4:A:1012:EDO:H12	2.01	0.43
1:A:635:ALA:HB2	1:A:665:PHE:CD2	2.54	0.43
1:C:512:VAL:HG11	1:C:578[B]:MET:SD	2.59	0.42
1:A:424:ASN:OD1	1:A:451:ASP:HB3	2.20	0.42
1:A:538:ARG:HG2	4:A:1012:EDO:H21	2.01	0.42
1:A:847:ASP:HB3	1:A:908:PRO:HG2	1.99	0.42
1:C:531:TYR:CZ	1:C:570:VAL:HG22	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:318:TYR:CE2	1:A:639:GLY:HA3	2.54	0.42
1:A:523:TRP:CG	4:A:1002:EDO:H11	2.55	0.42
1:A:259:LYS:HE3	1:A:259:LYS:HB2	1.86	0.42
1:A:113:TYR:CZ	1:A:593:ILE:HG22	2.55	0.42
1:A:567:GLU:N	1:A:568:PRO:HA	2.35	0.42
1:A:670:VAL:HG23	7:A:1037:SO4:O3	2.20	0.42
1:C:952:LYS:NZ	5:C:1006:PGE:H22	2.35	0.42
3:A:1001:W9Y:C20	4:A:1002:EDO:HO1	2.26	0.42
1:A:342:GLU:OE1	1:A:580:LYS:NZ	2.45	0.42
1:C:964[A]:HIS:CD2	1:C:966:ARG:HG2	2.50	0.42
1:C:847:ASP:HB3	1:C:908:PRO:HG2	2.02	0.42
1:C:158:LEU:HB2	1:C:170:VAL:HB	2.02	0.41
1:C:102:ARG:HA	1:C:384:ILE:O	2.20	0.41
1:C:278:VAL:HG23	1:C:290:LEU:HB2	2.01	0.41
1:C:865:GLU:H	4:C:1009:EDO:C1	2.32	0.41
1:C:506:ARG:NH1	10:C:1118:HOH:O	2.31	0.41
1:C:534:PHE:HB3	1:C:600:TYR:HB3	2.03	0.41
1:A:585:TYR:CE2	5:A:1004:PGE:H62	2.56	0.41
1:A:307:PHE:CE2	1:A:308:GLN:HG3	2.56	0.41
1:A:538:ARG:NH1	10:A:1142:HOH:O	2.53	0.41
5:A:1007:PGE:H4	5:A:1007:PGE:H22	1.77	0.41
1:C:169:SER:OG	1:C:271:SER:HB2	2.21	0.41
1:C:485:LEU:HD23	1:C:486:VAL:N	2.36	0.41
1:A:396:ASP:HA	4:A:1008:EDO:H12	2.03	0.41
1:C:829:GLY:HA2	1:C:862:ALA:HA	2.03	0.41
1:A:67:LEU:HD11	1:A:74:LEU:HD11	2.03	0.40
1:C:658:LEU:HD22	1:C:663:LEU:HD22	2.04	0.40
1:C:307:PHE:CE2	1:C:308:GLN:HG3	2.56	0.40
1:C:421:SER:HB2	1:C:449:TRP:HB2	2.03	0.40
1:A:331:ARG:HG2	1:A:332:ASP:H	1.86	0.40
1:A:910:TRP:CE3	1:A:954:GLY:HA2	2.57	0.40
1:C:285:ALA:O	1:C:312:ASN:N	2.53	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	855/977 (88%)	826 (97%)	29 (3%)	0	100	100
1	C	859/977 (88%)	829 (96%)	30 (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	1884/3062 (62%)	1819 (96%)	65 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	87
1	C	742/846 (88%)	731 (98%)	11 (2%)	65	85
2	B	69/485 (14%)	69 (100%)	0	100	100
2	D	68/485 (14%)	67 (98%)	1 (2%)	65	85
All	All	1626/2662 (61%)	1604 (99%)	22 (1%)	67	86

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	36	SER
1	A	65	ASP
1	A	259	LYS
1	A	370	THR
1	A	424	ASN
1	A	446	ASP
1	A	637	TRP
1	A	665	PHE

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Mol	Chain	Res	Type
1	A	706	ARG
1	A	863	GLN
1	C	160	LEU
1	C	164	ARG
1	C	370	THR
1	C	424	ASN
1	C	446	ASP
1	C	637	TRP
1	C	665	PHE
1	C	685	TRP
1	C	806	LYS
1	C	877	GLN
1	C	940	GLN
2	D	83	LYS

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	545	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 72 ligands modelled in this entry, 4 are monoatomic - leaving 68 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The

Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	PGE	A	1007	-	9,9,9	0.32	0	8,8,8	0.27	0
6	PEG	C	1010	-	6,6,6	0.49	0	5,5,5	0.33	0
6	PEG	A	1017	-	6,6,6	0.50	0	5,5,5	0.23	0
4	EDO	C	1009	-	3,3,3	0.43	0	2,2,2	0.40	0
6	PEG	A	1023	-	6,6,6	0.18	0	5,5,5	0.09	0
6	PEG	C	1017	-	6,6,6	0.11	0	5,5,5	0.11	0
3	W9Y	C	1001	-	34,36,36	2.46	11 (32%)	41,50,50	1.85	7 (17%)
4	EDO	A	1031	-	3,3,3	0.45	0	2,2,2	0.36	0
7	SO4	A	1036	-	4,4,4	0.14	0	6,6,6	0.06	0
7	SO4	C	1024	-	4,4,4	0.14	0	6,6,6	0.14	0
9	PG4	C	1020	-	12,12,12	0.52	0	11,11,11	0.17	0
4	EDO	A	1018	-	3,3,3	0.46	0	2,2,2	0.25	0
4	EDO	A	1002	-	3,3,3	0.25	0	2,2,2	0.17	0
4	EDO	A	1012	-	3,3,3	0.49	0	2,2,2	0.20	0
4	EDO	C	1011	-	3,3,3	0.45	0	2,2,2	0.33	0
7	SO4	C	1026	-	4,4,4	0.13	0	6,6,6	0.10	0
7	SO4	A	1034	-	4,4,4	0.15	0	6,6,6	0.13	0
6	PEG	A	1019	-	6,6,6	0.48	0	5,5,5	0.28	0
6	PEG	A	1025	-	6,6,6	0.47	0	5,5,5	0.30	0
7	SO4	C	1028	-	4,4,4	0.12	0	6,6,6	0.11	0
4	EDO	A	1003	-	3,3,3	0.46	0	2,2,2	0.32	0
4	EDO	A	1015	-	3,3,3	0.23	0	2,2,2	0.28	0
4	EDO	C	1004	-	3,3,3	0.49	0	2,2,2	0.24	0
6	PEG	A	1024	-	6,6,6	0.48	0	5,5,5	0.28	0
4	EDO	A	1020	-	3,3,3	0.45	0	2,2,2	0.41	0
6	PEG	A	1014	-	6,6,6	0.48	0	5,5,5	0.25	0
4	EDO	A	1022	-	3,3,3	0.46	0	2,2,2	0.39	0
6	PEG	A	1009	-	6,6,6	0.49	0	5,5,5	0.29	0
4	EDO	C	1012	-	3,3,3	0.46	0	2,2,2	0.36	0
7	SO4	A	1037	-	4,4,4	0.24	0	6,6,6	0.39	0
4	EDO	A	1008	-	3,3,3	0.43	0	2,2,2	0.46	0
4	EDO	A	1021	-	3,3,3	0.47	0	2,2,2	0.28	0
4	EDO	C	1003	-	3,3,3	0.44	0	2,2,2	0.46	0
4	EDO	A	1027	-	3,3,3	0.46	0	2,2,2	0.33	0
4	EDO	B	602	-	3,3,3	0.41	0	2,2,2	0.47	0
4	EDO	B	603	-	3,3,3	0.47	0	2,2,2	0.31	0
4	EDO	C	1005	-	3,3,3	0.49	0	2,2,2	0.25	0
7	SO4	A	1033	-	4,4,4	0.14	0	6,6,6	0.05	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	EDO	C	1018	-	3,3,3	0.49	0	2,2,2	0.51	0
7	SO4	C	1027	-	4,4,4	0.14	0	6,6,6	0.10	0
4	EDO	C	1014	-	3,3,3	0.34	0	2,2,2	0.27	0
5	PGE	C	1006	-	9,9,9	0.33	0	8,8,8	0.27	0
3	W9Y	A	1001	-	34,36,36	2.48	10 (29%)	41,50,50	1.82	10 (24%)
6	PEG	C	1019	-	6,6,6	0.49	0	5,5,5	0.31	0
4	EDO	C	1008	-	3,3,3	0.44	0	2,2,2	0.37	0
7	SO4	C	1025	-	4,4,4	0.12	0	6,6,6	0.19	0
6	PEG	C	1007	-	6,6,6	0.48	0	5,5,5	0.26	0
7	SO4	C	1022	-	4,4,4	0.13	0	6,6,6	0.10	0
4	EDO	A	1006	-	3,3,3	0.51	0	2,2,2	0.20	0
6	PEG	C	1015	-	6,6,6	0.47	0	5,5,5	0.25	0
7	SO4	C	1021	-	4,4,4	0.14	0	6,6,6	0.11	0
5	PGE	A	1026	-	9,9,9	0.31	0	8,8,8	0.36	0
5	PGE	A	1004	-	9,9,9	0.32	0	8,8,8	0.26	0
4	EDO	C	1016	-	3,3,3	0.15	0	2,2,2	0.18	0
6	PEG	A	1028	-	6,6,6	0.48	0	5,5,5	0.29	0
4	EDO	A	1013	-	3,3,3	0.43	0	2,2,2	0.40	0
7	SO4	C	1023	-	4,4,4	0.13	0	6,6,6	0.11	0
4	EDO	A	1029	-	3,3,3	0.47	0	2,2,2	0.27	0
4	EDO	A	1010	-	3,3,3	0.51	0	2,2,2	0.16	0
4	EDO	C	1002	-	3,3,3	0.46	0	2,2,2	0.23	0
5	PGE	A	1005	-	9,9,9	0.31	0	8,8,8	0.31	0
4	EDO	A	1011	-	3,3,3	0.42	0	2,2,2	0.49	0
5	PGE	A	1016	-	9,9,9	0.32	0	8,8,8	0.31	0
7	SO4	A	1035	-	4,4,4	0.13	0	6,6,6	0.08	0
4	EDO	C	1013	-	3,3,3	0.52	0	2,2,2	0.22	0
4	EDO	B	601	-	3,3,3	0.45	0	2,2,2	0.36	0
4	EDO	A	1030	-	3,3,3	0.45	0	2,2,2	0.38	0
4	EDO	A	1032	-	3,3,3	0.45	0	2,2,2	0.34	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	PGE	A	1007	-	-	4/7/7/7	-
6	PEG	C	1010	-	-	3/4/4/4	-
6	PEG	A	1017	-	-	1/4/4/4	-
4	EDO	C	1009	-	-	1/1/1/1	-
6	PEG	A	1023	-	-	3/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	PEG	C	1017	-	-	3/4/4/4	-
3	W9Y	C	1001	-	-	9/20/45/45	0/3/3/3
4	EDO	A	1031	-	-	0/1/1/1	-
9	PG4	C	1020	-	-	7/10/10/10	-
4	EDO	A	1018	-	-	0/1/1/1	-
4	EDO	A	1002	-	-	0/1/1/1	-
4	EDO	A	1012	-	-	1/1/1/1	-
4	EDO	C	1011	-	-	1/1/1/1	-
6	PEG	A	1019	-	-	0/4/4/4	-
6	PEG	A	1025	-	-	2/4/4/4	-
4	EDO	A	1003	-	-	0/1/1/1	-
4	EDO	A	1015	-	-	1/1/1/1	-
4	EDO	C	1004	-	-	0/1/1/1	-
6	PEG	A	1024	-	-	2/4/4/4	-
4	EDO	A	1020	-	-	1/1/1/1	-
6	PEG	A	1014	-	-	1/4/4/4	-
4	EDO	A	1022	-	-	0/1/1/1	-
6	PEG	A	1009	-	-	4/4/4/4	-
4	EDO	C	1012	-	-	0/1/1/1	-
4	EDO	A	1008	-	-	0/1/1/1	-
4	EDO	A	1021	-	-	1/1/1/1	-
4	EDO	C	1003	-	-	0/1/1/1	-
4	EDO	A	1027	-	-	1/1/1/1	-
4	EDO	B	602	-	-	1/1/1/1	-
4	EDO	B	603	-	-	1/1/1/1	-
4	EDO	C	1005	-	-	1/1/1/1	-
4	EDO	C	1018	-	-	1/1/1/1	-
4	EDO	C	1014	-	-	0/1/1/1	-
5	PGE	C	1006	-	-	3/7/7/7	-
3	W9Y	A	1001	-	-	15/20/45/45	0/3/3/3
6	PEG	C	1019	-	-	3/4/4/4	-
4	EDO	C	1008	-	-	1/1/1/1	-
6	PEG	C	1007	-	-	1/4/4/4	-
4	EDO	A	1006	-	-	0/1/1/1	-
6	PEG	C	1015	-	-	3/4/4/4	-
5	PGE	A	1026	-	-	4/7/7/7	-
5	PGE	A	1004	-	-	6/7/7/7	-
4	EDO	C	1016	-	-	1/1/1/1	-
6	PEG	A	1028	-	-	3/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	EDO	A	1013	-	-	0/1/1/1	-
4	EDO	A	1029	-	-	1/1/1/1	-
4	EDO	A	1010	-	-	0/1/1/1	-
4	EDO	C	1002	-	-	0/1/1/1	-
5	PGE	A	1005	-	-	2/7/7/7	-
4	EDO	A	1011	-	-	0/1/1/1	-
5	PGE	A	1016	-	-	5/7/7/7	-
4	EDO	C	1013	-	-	1/1/1/1	-
4	EDO	B	601	-	-	1/1/1/1	-
4	EDO	A	1030	-	-	0/1/1/1	-
4	EDO	A	1032	-	-	0/1/1/1	-

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1001	W9Y	O6-N3	9.99	1.39	1.22
3	C	1001	W9Y	O6-N3	9.11	1.38	1.22
3	C	1001	W9Y	O2-C1	-4.66	1.36	1.44
3	A	1001	W9Y	O2-C1	-4.64	1.36	1.44
3	A	1001	W9Y	N5-N4	-4.56	1.30	1.37
3	C	1001	W9Y	N5-N4	-3.90	1.31	1.37
3	A	1001	W9Y	O3-C2	-3.43	1.35	1.42
3	C	1001	W9Y	C18-C17	-3.04	1.34	1.38
3	C	1001	W9Y	O4-C3	-2.99	1.35	1.43
3	C	1001	W9Y	C14-N2	2.92	1.45	1.37
3	C	1001	W9Y	O3-C2	-2.89	1.37	1.42
3	C	1001	W9Y	N6-N5	-2.83	1.30	1.34
3	C	1001	W9Y	C6-C1	-2.76	1.50	1.53
3	C	1001	W9Y	O5-C4	-2.57	1.36	1.43
3	A	1001	W9Y	C5-N1	-2.55	1.42	1.47
3	A	1001	W9Y	O4-C3	-2.49	1.37	1.43
3	C	1001	W9Y	C18-C19	-2.29	1.35	1.39
3	A	1001	W9Y	C8-N1	-2.28	1.42	1.47
3	A	1001	W9Y	C14-N2	2.26	1.43	1.37
3	A	1001	W9Y	O5-C4	-2.25	1.37	1.43
3	A	1001	W9Y	N6-N5	-2.05	1.31	1.34

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	1001	W9Y	C16-C17-N4	7.39	125.61	119.15
3	A	1001	W9Y	C17-N4-N5	4.80	126.94	117.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1001	W9Y	C21-N4-N5	-4.72	107.91	112.72
3	C	1001	W9Y	C18-C17-N4	-4.22	113.69	119.07
3	A	1001	W9Y	C18-C19-C14	-3.96	117.94	121.53
3	C	1001	W9Y	C15-C14-N2	-3.03	116.64	121.80
3	C	1001	W9Y	C21-N4-N5	-2.79	109.88	112.72
3	A	1001	W9Y	C6-C5-N1	-2.67	106.19	112.11
3	C	1001	W9Y	O2-C1-C6	-2.66	102.78	108.36
3	C	1001	W9Y	C17-N4-N5	2.63	122.53	117.19
3	A	1001	W9Y	C19-C14-N2	-2.61	118.74	123.33
3	A	1001	W9Y	C18-C17-N4	2.43	122.17	119.07
3	A	1001	W9Y	C6-C1-C7	-2.40	106.69	110.17
3	A	1001	W9Y	C4-C5-N1	-2.35	105.37	109.66
3	A	1001	W9Y	C4-C3-C2	2.31	114.47	111.30
3	C	1001	W9Y	C8-N1-C5	-2.06	111.29	114.20
3	A	1001	W9Y	C15-C14-C19	2.04	121.60	118.58

There are no chirality outliers.

All (100) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1001	W9Y	C9-C8-N1-C5
6	C	1017	PEG	C1-C2-O2-C3
5	C	1006	PGE	O2-C3-C4-O3
9	C	1020	PG4	O3-C5-C6-O4
5	A	1016	PGE	O2-C3-C4-O3
3	A	1001	W9Y	N1-C8-C9-C10
3	C	1001	W9Y	N1-C8-C9-C10
3	A	1001	W9Y	C11-C12-C13-N2
5	A	1004	PGE	C3-C4-O3-C5
5	A	1026	PGE	O3-C5-C6-O4
5	A	1005	PGE	O2-C3-C4-O3
6	A	1017	PEG	C1-C2-O2-C3
5	A	1016	PGE	O1-C1-C2-O2
6	A	1023	PEG	O1-C1-C2-O2
6	A	1025	PEG	O2-C3-C4-O4
6	C	1010	PEG	O1-C1-C2-O2
3	A	1001	W9Y	C9-C10-C11-C12
5	A	1004	PGE	O2-C3-C4-O3
6	A	1009	PEG	O2-C3-C4-O4
3	C	1001	W9Y	C16-C17-N4-N5
3	C	1001	W9Y	C10-C11-C12-C13
6	A	1009	PEG	C1-C2-O2-C3

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Mol	Chain	Res	Type	Atoms
5	A	1016	PGE	O3-C5-C6-O4
6	C	1010	PEG	O2-C3-C4-O4
6	C	1017	PEG	O2-C3-C4-O4
4	A	1015	EDO	O1-C1-C2-O2
4	A	1021	EDO	O1-C1-C2-O2
4	A	1027	EDO	O1-C1-C2-O2
4	A	1029	EDO	O1-C1-C2-O2
4	B	601	EDO	O1-C1-C2-O2
4	B	602	EDO	O1-C1-C2-O2
4	B	603	EDO	O1-C1-C2-O2
4	C	1005	EDO	O1-C1-C2-O2
4	C	1009	EDO	O1-C1-C2-O2
6	A	1028	PEG	O2-C3-C4-O4
3	A	1001	W9Y	C6-C5-N1-C8
5	A	1004	PGE	O1-C1-C2-O2
5	A	1004	PGE	O3-C5-C6-O4
6	A	1014	PEG	O2-C3-C4-O4
6	C	1015	PEG	O2-C3-C4-O4
9	C	1020	PG4	O1-C1-C2-O2
9	C	1020	PG4	C4-C3-O2-C2
5	A	1007	PGE	O1-C1-C2-O2
3	A	1001	W9Y	C12-C13-N2-C14
6	A	1024	PEG	O2-C3-C4-O4
6	A	1028	PEG	C4-C3-O2-C2
3	A	1001	W9Y	C16-C17-N4-N5
3	A	1001	W9Y	C18-C17-N4-N5
3	C	1001	W9Y	C18-C17-N4-N5
4	A	1012	EDO	O1-C1-C2-O2
3	A	1001	W9Y	C18-C19-N3-O6
3	A	1001	W9Y	O2-C1-C7-O1
6	A	1009	PEG	C4-C3-O2-C2
5	A	1016	PGE	C1-C2-O2-C3
5	A	1005	PGE	C4-C3-O2-C2
6	C	1019	PEG	C1-C2-O2-C3
6	C	1007	PEG	O1-C1-C2-O2
4	A	1020	EDO	O1-C1-C2-O2
6	A	1023	PEG	C1-C2-O2-C3
5	A	1004	PGE	C4-C3-O2-C2
6	C	1019	PEG	O2-C3-C4-O4
9	C	1020	PG4	O4-C7-C8-O5
5	A	1007	PGE	C4-C3-O2-C2
3	C	1001	W9Y	C11-C10-C9-C8

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Mol	Chain	Res	Type	Atoms
5	A	1004	PGE	C1-C2-O2-C3
4	C	1016	EDO	O1-C1-C2-O2
4	C	1018	EDO	O1-C1-C2-O2
3	A	1001	W9Y	C19-C14-N2-C13
6	A	1009	PEG	O1-C1-C2-O2
6	A	1028	PEG	C1-C2-O2-C3
6	C	1019	PEG	C4-C3-O2-C2
5	C	1006	PGE	C1-C2-O2-C3
6	C	1017	PEG	O1-C1-C2-O2
5	A	1026	PGE	C1-C2-O2-C3
5	A	1007	PGE	C1-C2-O2-C3
5	A	1026	PGE	C6-C5-O3-C4
6	C	1015	PEG	C4-C3-O2-C2
5	C	1006	PGE	C3-C4-O3-C5
9	C	1020	PG4	O2-C3-C4-O3
6	A	1024	PEG	C1-C2-O2-C3
3	A	1001	W9Y	C4-C5-N1-C8
6	A	1025	PEG	C1-C2-O2-C3
9	C	1020	PG4	C6-C5-O3-C4
6	C	1015	PEG	C1-C2-O2-C3
5	A	1016	PGE	C3-C4-O3-C5
4	C	1008	EDO	O1-C1-C2-O2
4	C	1011	EDO	O1-C1-C2-O2
3	C	1001	W9Y	C11-C12-C13-N2
6	A	1023	PEG	C4-C3-O2-C2
3	C	1001	W9Y	C18-C19-N3-O6
3	A	1001	W9Y	C16-C17-N4-C21
3	A	1001	W9Y	C18-C17-N4-C21
3	C	1001	W9Y	C16-C17-N4-C21
3	C	1001	W9Y	C18-C17-N4-C21
9	C	1020	PG4	C5-C6-O4-C7
4	C	1013	EDO	O1-C1-C2-O2
5	A	1007	PGE	O2-C3-C4-O3
3	A	1001	W9Y	C10-C11-C12-C13
6	C	1010	PEG	C1-C2-O2-C3
5	A	1026	PGE	O2-C3-C4-O3

There are no ring outliers.

21 monomers are involved in 32 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1007	PGE	1	0

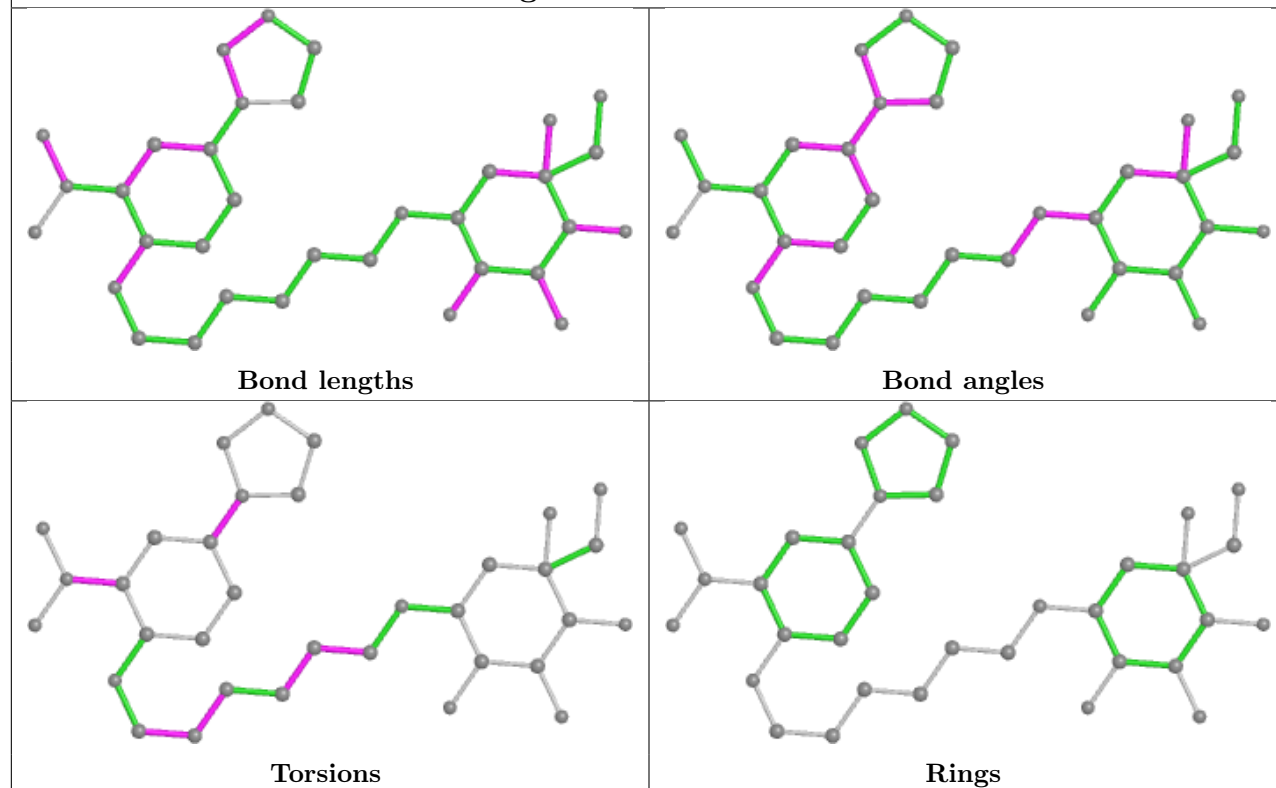
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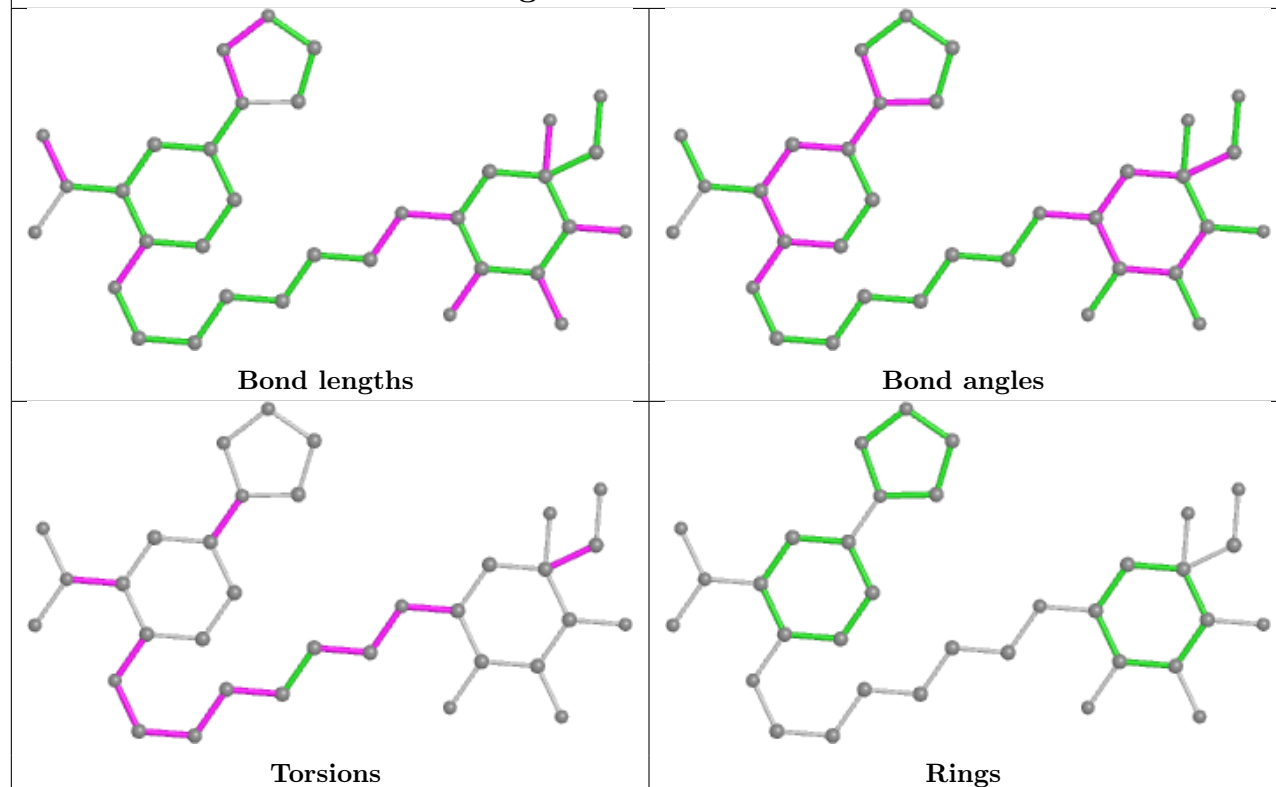
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	1017	PEG	2	0
4	C	1009	EDO	1	0
4	A	1031	EDO	2	0
4	A	1018	EDO	1	0
4	A	1002	EDO	3	0
4	A	1012	EDO	2	0
4	C	1011	EDO	1	0
7	A	1034	SO4	2	0
6	A	1025	PEG	2	0
7	A	1037	SO4	3	0
4	A	1008	EDO	1	0
4	B	602	EDO	2	0
4	C	1014	EDO	1	0
5	C	1006	PGE	1	0
3	A	1001	W9Y	2	0
6	C	1007	PEG	1	0
5	A	1004	PGE	3	0
4	A	1029	EDO	2	0
4	C	1002	EDO	1	0
4	A	1011	EDO	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 W9Y C 1001



Ligand W9Y 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	A	854/977 (87%)	-0.22	20 (2%) 60 63	31, 42, 67, 125	0
1	C	857/977 (87%)	-0.01	47 (5%) 25 26	32, 48, 86, 107	0
2	B	87/554 (15%)	0.55	19 (21%) 0 0	40, 59, 99, 121	0
2	D	87/554 (15%)	0.58	16 (18%) 1 1	37, 59, 105, 116	0
All	All	1885/3062 (61%)	-0.05	102 (5%) 25 27	31, 46, 84, 125	0

All (102) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	184	PRO	9.3
2	D	81	GLY	6.7
2	D	43	THR	6.7
2	B	82	TYR	4.7
2	B	48	PHE	4.6
2	B	43	THR	4.5
1	A	183	ALA	4.5
1	C	370	THR	4.3
1	A	33	VAL	4.1
1	A	247	ALA	4.1
2	D	31	TYR	4.0
2	D	82	TYR	4.0
1	A	251	THR	3.9
1	C	185	ARG	3.9
1	A	248	TRP	3.7
2	D	44	ALA	3.6
1	A	246	GLY	3.5
1	C	69	LEU	3.5
2	B	85	LEU	3.5
2	D	84	PRO	3.4
2	D	32	GLU	3.4

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Mol	Chain	Res	Type	RSRZ
2	D	80	THR	3.2
1	C	141	THR	3.1
1	C	184	PRO	3.1
1	A	254	THR	3.1
1	C	164	ARG	3.0
2	D	117	ARG	3.0
2	B	44	ALA	3.0
2	B	34	SER	3.0
1	A	249	GLU	3.0
1	C	136	ASN	3.0
1	A	666	CYS	2.9
2	B	45	THR	2.9
2	B	42	GLY	2.9
1	C	138	VAL	2.9
2	D	85	LEU	2.9
2	B	41	ASP	2.9
1	C	137	SER	2.9
2	B	86	TYR	2.9
1	C	35	ARG	2.9
2	B	32	GLU	2.9
2	B	38	THR	2.9
1	C	148	LYS	2.8
1	C	144	GLU	2.8
1	C	33	VAL	2.7
2	B	31	TYR	2.7
1	C	129	SER	2.7
2	B	117	ARG	2.7
2	D	45	THR	2.6
1	C	165	SER	2.6
2	B	33	GLU	2.6
1	C	74	LEU	2.6
1	C	127	ARG	2.6
1	A	637	TRP	2.6
1	C	626	PHE	2.6
1	C	625	ALA	2.5
2	D	41	ASP	2.5
1	C	131	SER	2.5
1	C	245	PRO	2.5
1	A	34	ASP	2.4
1	C	251	THR	2.4
1	C	64	LEU	2.4
2	B	116	CYS	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	163	ASP	2.4
1	C	663	LEU	2.3
1	C	130	VAL	2.3
1	A	253	LYS	2.3
1	A	252	PHE	2.3
1	C	329	PHE	2.3
2	D	48	PHE	2.3
1	C	63	LEU	2.3
1	C	661	VAL	2.3
2	B	115	THR	2.3
1	C	34	ASP	2.3
1	C	126	ALA	2.3
1	C	666	CYS	2.2
1	A	164	ARG	2.2
1	C	55	PRO	2.2
2	D	86	TYR	2.2
1	C	659	ALA	2.2
1	C	282	PRO	2.2
2	B	113	GLU	2.2
1	C	658	LEU	2.2
1	C	662	GLY	2.2
2	D	116	CYS	2.2
1	C	143	ALA	2.1
1	C	636	VAL	2.1
1	A	623	SER	2.1
2	B	80	THR	2.1
1	C	132	GLY	2.1
1	C	66	THR	2.0
1	C	320	SER	2.0
1	A	658	LEU	2.0
1	C	139	GLU	2.0
1	C	622	LEU	2.0
2	D	79	ASN	2.0
1	A	655	CYS	2.0
1	C	128	LEU	2.0
1	C	371	PRO	2.0
1	A	622	LEU	2.0
1	C	79	ILE	2.0
1	C	656	LEU	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(\AA^2)	Q<0.9
4	EDO	C	1013	4/4	0.52	0.27	70,73,83,95	0
6	PEG	A	1023	7/7	0.60	0.30	68,81,98,102	0
4	EDO	A	1015	4/4	0.71	0.28	79,84,95,102	0
4	EDO	A	1020	4/4	0.74	0.53	78,80,84,95	0
5	PGE	A	1016	10/10	0.77	0.41	58,73,80,84	0
4	EDO	C	1016	4/4	0.77	0.28	79,82,85,86	0
7	SO4	C	1028	5/5	0.77	0.44	92,93,103,129	0
6	PEG	A	1025	7/7	0.78	0.32	56,63,78,85	0
4	EDO	A	1010	4/4	0.80	0.21	48,57,58,62	0
6	PEG	A	1019	7/7	0.82	0.21	62,66,73,90	0
4	EDO	C	1012	4/4	0.82	0.33	72,74,77,78	0
5	PGE	A	1007	10/10	0.82	0.25	66,71,80,80	0
4	EDO	A	1003	4/4	0.82	0.27	66,67,68,71	0
4	EDO	A	1012	4/4	0.83	0.28	58,59,68,73	0
4	EDO	C	1018	4/4	0.83	0.22	62,83,84,92	0
5	PGE	A	1005	10/10	0.83	0.21	57,65,77,79	0
4	EDO	C	1005	4/4	0.84	0.27	57,59,64,64	0
9	PG4	C	1020	13/13	0.84	0.20	58,65,83,84	0
4	EDO	C	1004	4/4	0.85	0.17	56,61,63,73	0
6	PEG	A	1009	7/7	0.85	0.16	57,63,67,72	0
6	PEG	C	1017	7/7	0.85	0.27	72,73,80,83	0
6	PEG	A	1017	7/7	0.85	0.27	61,73,79,84	0
4	EDO	A	1006	4/4	0.85	0.23	50,54,55,56	0
4	EDO	B	603	4/4	0.86	0.22	61,64,66,67	0
6	PEG	A	1014	7/7	0.86	0.25	55,61,79,87	0
6	PEG	A	1028	7/7	0.86	0.22	63,68,72,78	0
7	SO4	A	1034	5/5	0.87	0.34	83,97,114,135	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
7	SO4	C	1027	5/5	0.87	0.52	77,82,87,111	0
4	EDO	C	1014	4/4	0.87	0.13	62,65,73,85	0
5	PGE	C	1006	10/10	0.87	0.21	57,69,77,88	0
7	SO4	A	1037	5/5	0.88	0.47	62,70,79,103	0
3	W9Y	A	1001	34/34	0.88	0.19	30,59,97,106	0
6	PEG	C	1019	7/7	0.88	0.22	56,65,71,73	0
5	PGE	A	1026	10/10	0.88	0.36	57,70,78,82	0
7	SO4	C	1024	5/5	0.89	0.40	79,89,110,130	0
3	W9Y	C	1001	34/34	0.89	0.20	36,64,99,107	0
7	SO4	A	1036	5/5	0.89	0.40	83,84,113,129	0
6	PEG	C	1010	7/7	0.89	0.28	54,67,73,73	0
5	PGE	A	1004	10/10	0.90	0.24	58,67,71,73	0
7	SO4	C	1026	5/5	0.90	0.44	76,84,103,113	0
4	EDO	A	1030	4/4	0.90	0.46	62,64,76,83	0
7	SO4	A	1033	5/5	0.90	0.35	94,109,115,128	0
7	SO4	C	1022	5/5	0.90	0.22	61,69,77,109	0
4	EDO	C	1003	4/4	0.91	0.13	47,54,55,65	0
4	EDO	A	1027	4/4	0.91	0.31	41,59,60,61	0
4	EDO	A	1002	4/4	0.91	0.26	67,68,68,84	0
7	SO4	C	1025	5/5	0.91	0.43	72,77,98,113	0
4	EDO	C	1008	4/4	0.91	0.26	44,66,71,74	0
4	EDO	A	1031	4/4	0.91	0.18	52,64,64,65	0
4	EDO	A	1008	4/4	0.91	0.23	40,56,65,72	0
4	EDO	C	1002	4/4	0.91	0.28	50,56,65,68	0
7	SO4	C	1021	5/5	0.92	0.27	81,88,95,107	0
7	SO4	A	1035	5/5	0.92	0.43	76,77,104,111	0
6	PEG	A	1024	7/7	0.92	0.38	58,69,73,77	0
4	EDO	A	1013	4/4	0.92	0.36	46,49,64,67	0
4	EDO	A	1011	4/4	0.93	0.20	48,51,53,53	0
4	EDO	A	1029	4/4	0.93	0.17	53,55,56,57	0
4	EDO	B	601	4/4	0.93	0.10	50,55,65,66	0
6	PEG	C	1007	7/7	0.93	0.31	48,66,71,87	0
4	EDO	C	1009	4/4	0.93	0.23	58,59,60,68	0
6	PEG	C	1015	7/7	0.94	0.28	52,59,73,76	0
4	EDO	A	1018	4/4	0.94	0.22	58,59,62,66	0
4	EDO	A	1032	4/4	0.94	0.48	55,58,59,67	0
4	EDO	C	1011	4/4	0.94	0.24	55,56,58,58	0
4	EDO	A	1021	4/4	0.95	0.14	49,50,51,59	0
8	CA	D	601	1/1	0.95	0.08	56,56,56,56	0
7	SO4	C	1023	5/5	0.95	0.24	56,76,79,94	0
4	EDO	B	602	4/4	0.97	0.16	41,52,65,65	0
4	EDO	A	1022	4/4	0.97	0.09	46,49,52,53	0

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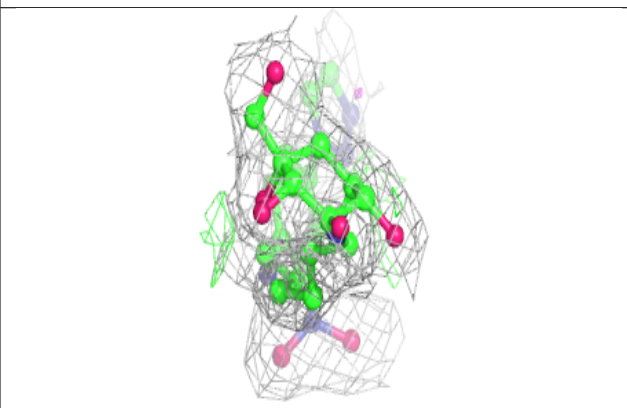
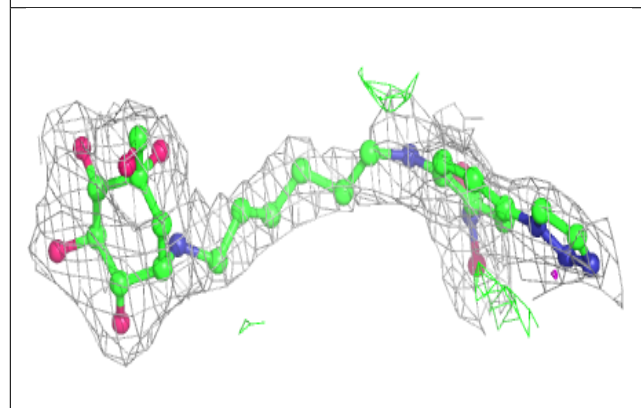
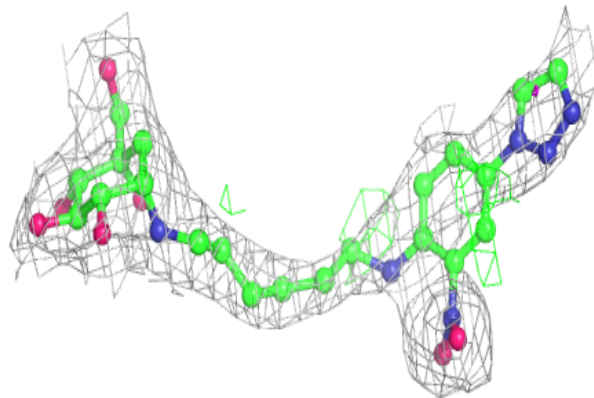
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
8	CA	B	604	1/1	0.98	0.08	46,46,46,46	0
8	CA	D	602	1/1	0.99	0.09	44,44,44,44	0
8	CA	B	605	1/1	0.99	0.05	53,53,53,53	0

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.

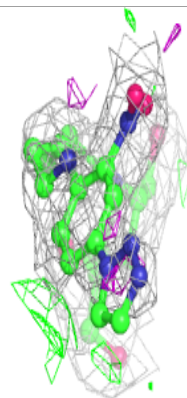
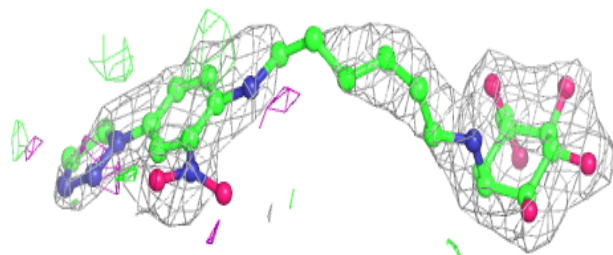
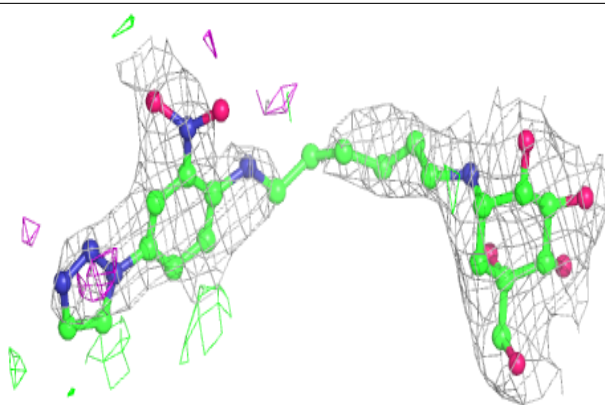
Electron density around W9Y A 1001:

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 W9Y 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.