



# wwPDB X-ray Structure Validation Summary Report

Feb 28, 2014 – 12:17 AM GMT

PDB ID : 3DR7  
Title : GDP-perosamine synthase from Caulobacter crescentus with bound GDP-3-deoxyperosamine  
Authors : Holden, H.M.; Cook, P.D.; Carney, A.E.  
Deposited on : 2008-07-10  
Resolution : 1.70 Å(reported)

This is a wwPDB validation summary report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

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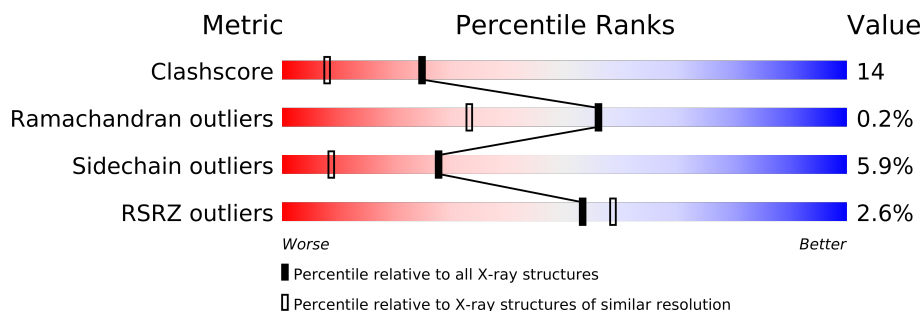
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.15 2013
Xtriage (Phenix)	:	dev-1323
EDS	:	stable22639
Percentile statistics	:	21963
Refmac	:	5.8.0049
CCP4	:	6.3.0 (Settle)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 1.70 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))
Clashscore	79885	2929 (1.70-1.70)
Ramachandran outliers	78287	2878 (1.70-1.70)
Sidechain outliers	78261	2878 (1.70-1.70)
RSRZ outliers	66119	2456 (1.70-1.70)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	391	
1	B	391	
1	C	391	
1	D	391	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
2	GPD	D	501	-	X
3	EDO	B	1040	-	X
3	EDO	D	1041	-	X

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 12605 atoms, of which 0 are hydrogen and 0 are deuterium.

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 Putative perosamine synthetase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	368	Total	C	N	O	P	S	0	2	0
			2855	1803	501	532	1	18			
1	B	367	Total	C	N	O	P	S	0	6	0
			2881	1820	507	535	1	18			
1	C	367	Total	C	N	O	P	S	0	0	0
			2837	1790	499	529	1	18			
1	D	367	Total	C	N	O	P	S	0	0	0
			2837	1790	499	529	1	18			

There are 180 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	EXPRESSION TAG	UNP O85354
A	-18	GLY	-	EXPRESSION TAG	UNP O85354
A	-17	SER	-	EXPRESSION TAG	UNP O85354
A	-16	SER	-	EXPRESSION TAG	UNP O85354
A	-15	HIS	-	EXPRESSION TAG	UNP O85354
A	-14	HIS	-	EXPRESSION TAG	UNP O85354
A	-13	HIS	-	EXPRESSION TAG	UNP O85354
A	-12	HIS	-	EXPRESSION TAG	UNP O85354
A	-11	HIS	-	EXPRESSION TAG	UNP O85354
A	-10	HIS	-	EXPRESSION TAG	UNP O85354
A	-9	SER	-	EXPRESSION TAG	UNP O85354
A	-8	SER	-	EXPRESSION TAG	UNP O85354
A	-7	GLU	-	EXPRESSION TAG	UNP O85354
A	-6	ASN	-	EXPRESSION TAG	UNP O85354
A	-5	LEU	-	EXPRESSION TAG	UNP O85354
A	-4	TYR	-	EXPRESSION TAG	UNP O85354
A	-3	PHE	-	EXPRESSION TAG	UNP O85354
A	-2	GLN	-	EXPRESSION TAG	UNP O85354
A	-1	GLY	-	EXPRESSION TAG	UNP O85354
A	0	HIS	-	EXPRESSION TAG	UNP O85354
A	1	MET	-	EXPRESSION TAG	UNP O85354

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Chain	Residue	Modelled	Actual	Comment	Reference
A	2	SER	-	EXPRESSION TAG	UNP O85354
A	3	ASP	-	EXPRESSION TAG	UNP O85354
A	4	LEU	-	EXPRESSION TAG	UNP O85354
A	5	PRO	-	EXPRESSION TAG	UNP O85354
A	6	ARG	-	EXPRESSION TAG	UNP O85354
A	7	ILE	-	EXPRESSION TAG	UNP O85354
A	8	SER	-	EXPRESSION TAG	UNP O85354
A	9	VAL	-	EXPRESSION TAG	UNP O85354
A	10	ALA	-	EXPRESSION TAG	UNP O85354
A	11	ALA	-	EXPRESSION TAG	UNP O85354
A	12	PRO	-	EXPRESSION TAG	UNP O85354
A	13	ARG	-	EXPRESSION TAG	UNP O85354
A	14	LEU	-	EXPRESSION TAG	UNP O85354
A	15	ASP	-	EXPRESSION TAG	UNP O85354
A	16	GLY	-	EXPRESSION TAG	UNP O85354
A	17	ASN	-	EXPRESSION TAG	UNP O85354
A	18	GLU	-	EXPRESSION TAG	UNP O85354
A	19	ARG	-	EXPRESSION TAG	UNP O85354
A	20	ASP	-	EXPRESSION TAG	UNP O85354
A	21	TYR	-	EXPRESSION TAG	UNP O85354
A	22	VAL	-	EXPRESSION TAG	UNP O85354
A	23	LEU	-	EXPRESSION TAG	UNP O85354
A	24	GLU	-	EXPRESSION TAG	UNP O85354
A	25	CYS	-	EXPRESSION TAG	UNP O85354
B	-19	MET	-	EXPRESSION TAG	UNP O85354
B	-18	GLY	-	EXPRESSION TAG	UNP O85354
B	-17	SER	-	EXPRESSION TAG	UNP O85354
B	-16	SER	-	EXPRESSION TAG	UNP O85354
B	-15	HIS	-	EXPRESSION TAG	UNP O85354
B	-14	HIS	-	EXPRESSION TAG	UNP O85354
B	-13	HIS	-	EXPRESSION TAG	UNP O85354
B	-12	HIS	-	EXPRESSION TAG	UNP O85354
B	-11	HIS	-	EXPRESSION TAG	UNP O85354
B	-10	HIS	-	EXPRESSION TAG	UNP O85354
B	-9	SER	-	EXPRESSION TAG	UNP O85354
B	-8	SER	-	EXPRESSION TAG	UNP O85354
B	-7	GLU	-	EXPRESSION TAG	UNP O85354
B	-6	ASN	-	EXPRESSION TAG	UNP O85354
B	-5	LEU	-	EXPRESSION TAG	UNP O85354
B	-4	TYR	-	EXPRESSION TAG	UNP O85354
B	-3	PHE	-	EXPRESSION TAG	UNP O85354
B	-2	GLN	-	EXPRESSION TAG	UNP O85354

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-1	GLY	-	EXPRESSION TAG	UNP O85354
B	0	HIS	-	EXPRESSION TAG	UNP O85354
B	1	MET	-	EXPRESSION TAG	UNP O85354
B	2	SER	-	EXPRESSION TAG	UNP O85354
B	3	ASP	-	EXPRESSION TAG	UNP O85354
B	4	LEU	-	EXPRESSION TAG	UNP O85354
B	5	PRO	-	EXPRESSION TAG	UNP O85354
B	6	ARG	-	EXPRESSION TAG	UNP O85354
B	7	ILE	-	EXPRESSION TAG	UNP O85354
B	8	SER	-	EXPRESSION TAG	UNP O85354
B	9	VAL	-	EXPRESSION TAG	UNP O85354
B	10	ALA	-	EXPRESSION TAG	UNP O85354
B	11	ALA	-	EXPRESSION TAG	UNP O85354
B	12	PRO	-	EXPRESSION TAG	UNP O85354
B	13	ARG	-	EXPRESSION TAG	UNP O85354
B	14	LEU	-	EXPRESSION TAG	UNP O85354
B	15	ASP	-	EXPRESSION TAG	UNP O85354
B	16	GLY	-	EXPRESSION TAG	UNP O85354
B	17	ASN	-	EXPRESSION TAG	UNP O85354
B	18	GLU	-	EXPRESSION TAG	UNP O85354
B	19	ARG	-	EXPRESSION TAG	UNP O85354
B	20	ASP	-	EXPRESSION TAG	UNP O85354
B	21	TYR	-	EXPRESSION TAG	UNP O85354
B	22	VAL	-	EXPRESSION TAG	UNP O85354
B	23	LEU	-	EXPRESSION TAG	UNP O85354
B	24	GLU	-	EXPRESSION TAG	UNP O85354
B	25	CYS	-	EXPRESSION TAG	UNP O85354
C	-19	MET	-	EXPRESSION TAG	UNP O85354
C	-18	GLY	-	EXPRESSION TAG	UNP O85354
C	-17	SER	-	EXPRESSION TAG	UNP O85354
C	-16	SER	-	EXPRESSION TAG	UNP O85354
C	-15	HIS	-	EXPRESSION TAG	UNP O85354
C	-14	HIS	-	EXPRESSION TAG	UNP O85354
C	-13	HIS	-	EXPRESSION TAG	UNP O85354
C	-12	HIS	-	EXPRESSION TAG	UNP O85354
C	-11	HIS	-	EXPRESSION TAG	UNP O85354
C	-10	HIS	-	EXPRESSION TAG	UNP O85354
C	-9	SER	-	EXPRESSION TAG	UNP O85354
C	-8	SER	-	EXPRESSION TAG	UNP O85354
C	-7	GLU	-	EXPRESSION TAG	UNP O85354
C	-6	ASN	-	EXPRESSION TAG	UNP O85354
C	-5	LEU	-	EXPRESSION TAG	UNP O85354

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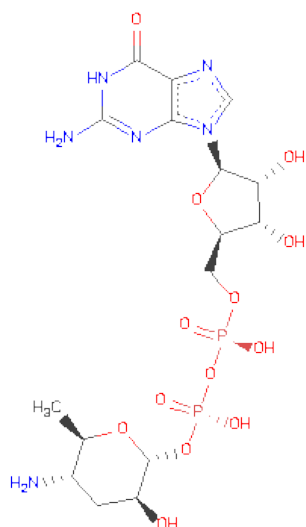
Chain	Residue	Modelled	Actual	Comment	Reference
C	-4	TYR	-	EXPRESSION TAG	UNP O85354
C	-3	PHE	-	EXPRESSION TAG	UNP O85354
C	-2	GLN	-	EXPRESSION TAG	UNP O85354
C	-1	GLY	-	EXPRESSION TAG	UNP O85354
C	0	HIS	-	EXPRESSION TAG	UNP O85354
C	1	MET	-	EXPRESSION TAG	UNP O85354
C	2	SER	-	EXPRESSION TAG	UNP O85354
C	3	ASP	-	EXPRESSION TAG	UNP O85354
C	4	LEU	-	EXPRESSION TAG	UNP O85354
C	5	PRO	-	EXPRESSION TAG	UNP O85354
C	6	ARG	-	EXPRESSION TAG	UNP O85354
C	7	ILE	-	EXPRESSION TAG	UNP O85354
C	8	SER	-	EXPRESSION TAG	UNP O85354
C	9	VAL	-	EXPRESSION TAG	UNP O85354
C	10	ALA	-	EXPRESSION TAG	UNP O85354
C	11	ALA	-	EXPRESSION TAG	UNP O85354
C	12	PRO	-	EXPRESSION TAG	UNP O85354
C	13	ARG	-	EXPRESSION TAG	UNP O85354
C	14	LEU	-	EXPRESSION TAG	UNP O85354
C	15	ASP	-	EXPRESSION TAG	UNP O85354
C	16	GLY	-	EXPRESSION TAG	UNP O85354
C	17	ASN	-	EXPRESSION TAG	UNP O85354
C	18	GLU	-	EXPRESSION TAG	UNP O85354
C	19	ARG	-	EXPRESSION TAG	UNP O85354
C	20	ASP	-	EXPRESSION TAG	UNP O85354
C	21	TYR	-	EXPRESSION TAG	UNP O85354
C	22	VAL	-	EXPRESSION TAG	UNP O85354
C	23	LEU	-	EXPRESSION TAG	UNP O85354
C	24	GLU	-	EXPRESSION TAG	UNP O85354
C	25	CYS	-	EXPRESSION TAG	UNP O85354
D	-19	MET	-	EXPRESSION TAG	UNP O85354
D	-18	GLY	-	EXPRESSION TAG	UNP O85354
D	-17	SER	-	EXPRESSION TAG	UNP O85354
D	-16	SER	-	EXPRESSION TAG	UNP O85354
D	-15	HIS	-	EXPRESSION TAG	UNP O85354
D	-14	HIS	-	EXPRESSION TAG	UNP O85354
D	-13	HIS	-	EXPRESSION TAG	UNP O85354
D	-12	HIS	-	EXPRESSION TAG	UNP O85354
D	-11	HIS	-	EXPRESSION TAG	UNP O85354
D	-10	HIS	-	EXPRESSION TAG	UNP O85354
D	-9	SER	-	EXPRESSION TAG	UNP O85354
D	-8	SER	-	EXPRESSION TAG	UNP O85354

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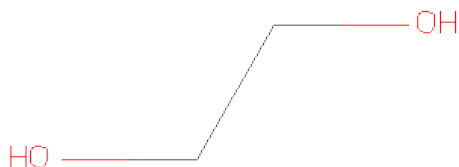
Chain	Residue	Modelled	Actual	Comment	Reference
D	-7	GLU	-	EXPRESSION TAG	UNP O85354
D	-6	ASN	-	EXPRESSION TAG	UNP O85354
D	-5	LEU	-	EXPRESSION TAG	UNP O85354
D	-4	TYR	-	EXPRESSION TAG	UNP O85354
D	-3	PHE	-	EXPRESSION TAG	UNP O85354
D	-2	GLN	-	EXPRESSION TAG	UNP O85354
D	-1	GLY	-	EXPRESSION TAG	UNP O85354
D	0	HIS	-	EXPRESSION TAG	UNP O85354
D	1	MET	-	EXPRESSION TAG	UNP O85354
D	2	SER	-	EXPRESSION TAG	UNP O85354
D	3	ASP	-	EXPRESSION TAG	UNP O85354
D	4	LEU	-	EXPRESSION TAG	UNP O85354
D	5	PRO	-	EXPRESSION TAG	UNP O85354
D	6	ARG	-	EXPRESSION TAG	UNP O85354
D	7	ILE	-	EXPRESSION TAG	UNP O85354
D	8	SER	-	EXPRESSION TAG	UNP O85354
D	9	VAL	-	EXPRESSION TAG	UNP O85354
D	10	ALA	-	EXPRESSION TAG	UNP O85354
D	11	ALA	-	EXPRESSION TAG	UNP O85354
D	12	PRO	-	EXPRESSION TAG	UNP O85354
D	13	ARG	-	EXPRESSION TAG	UNP O85354
D	14	LEU	-	EXPRESSION TAG	UNP O85354
D	15	ASP	-	EXPRESSION TAG	UNP O85354
D	16	GLY	-	EXPRESSION TAG	UNP O85354
D	17	ASN	-	EXPRESSION TAG	UNP O85354
D	18	GLU	-	EXPRESSION TAG	UNP O85354
D	19	ARG	-	EXPRESSION TAG	UNP O85354
D	20	ASP	-	EXPRESSION TAG	UNP O85354
D	21	TYR	-	EXPRESSION TAG	UNP O85354
D	22	VAL	-	EXPRESSION TAG	UNP O85354
D	23	LEU	-	EXPRESSION TAG	UNP O85354
D	24	GLU	-	EXPRESSION TAG	UNP O85354
D	25	CYS	-	EXPRESSION TAG	UNP O85354

- Molecule 2 is (2R,3S,5S,6R)-5-AMINO-3-HYDROXY-6-METHYL-OXAN-2-YL (three-letter code: GPD) (formula: C<sub>16</sub>H<sub>26</sub>N<sub>6</sub>O<sub>13</sub>P<sub>2</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			37	16	6	13	2		
2	A	1	Total	C	N	O	P	0	0
			37	16	6	13	2		
2	D	1	Total	C	N	O	P	0	0
			37	16	6	13	2		
2	D	1	Total	C	N	O	P	0	0
			37	16	6	13	2		

- Molecule 3 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula:  $C_2H_6O_2$ ).





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

- Molecule 4 is water.

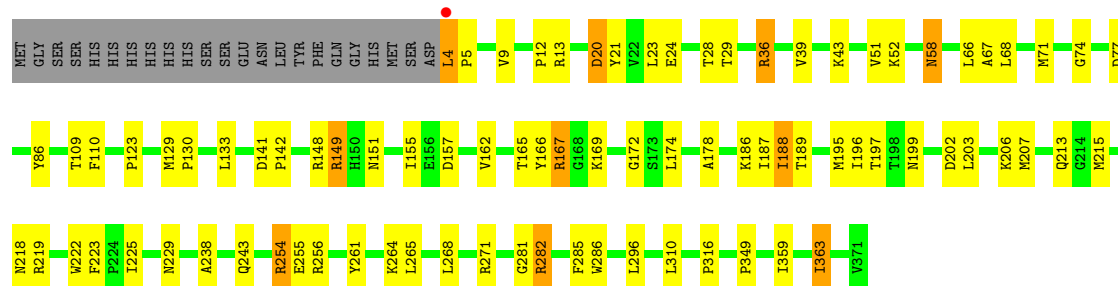
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	318	Total	O	0	0
			318	318		
4	B	287	Total	O	0	0
			287	287		
4	C	195	Total	O	0	0
			195	195		
4	D	239	Total	O	0	0
			239	239		

### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

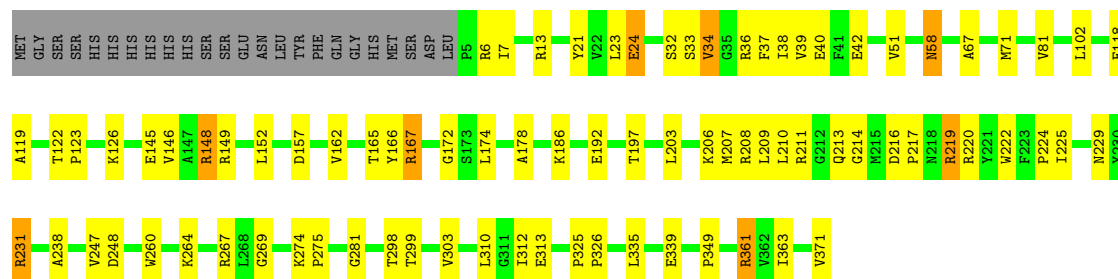
#### • Molecule 1: Putative perosamine synthetase

Chain A: 



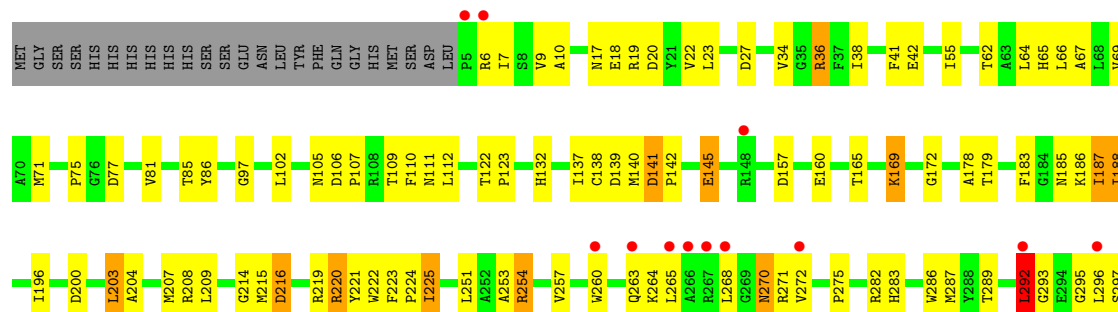
#### • Molecule 1: Putative perosamine synthetase

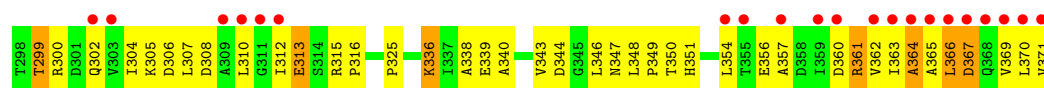
Chain B: 



#### • Molecule 1: Putative perosamine synthetase

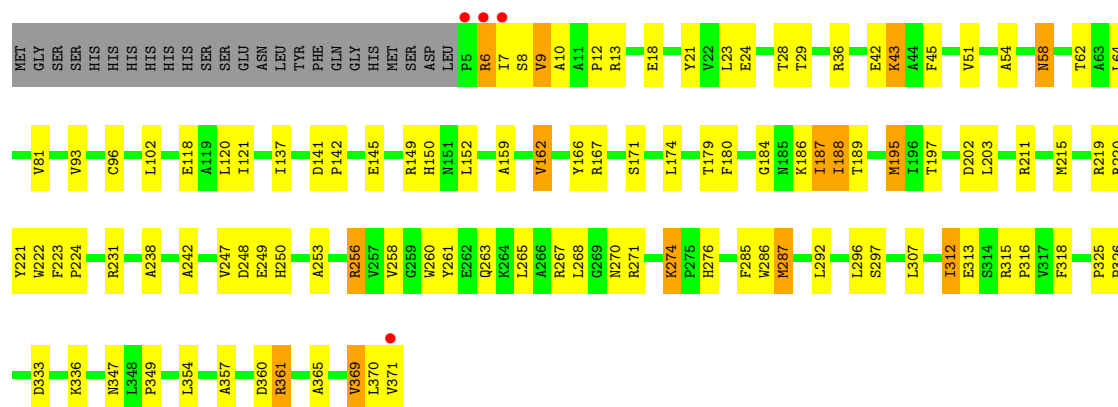
Chain C: 





• Molecule 1: Putative perosamine synthetase

Chain D: 



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	50.41Å 152.23Å 105.75Å 90.00° 101.83° 90.00°	Depositor
Resolution (Å)	30.00 – 1.70 42.80 – 1.70	Depositor EDS
% Data completeness (in resolution range)	94.6 (30.00-1.70) 94.6 (42.80-1.70)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.09	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	0.69 (at 1.70Å)	Xtriage
Refinement program	TNT	Depositor
R, $R_{free}$	0.197 , 0.263 0.196 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	9.0	Xtriage
Anisotropy	0.406	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 60.2	EDS
Estimated twinning fraction	0.033 for h,-k,-h-l	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 161554 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	12605	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.21% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: GPD, EDO, IT1

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	0.75	0/2890	1.23	13/3928 (0.3%)
1	B	0.73	0/2916	1.19	9/3962 (0.2%)
1	C	0.67	0/2869	1.15	8/3898 (0.2%)
1	D	0.71	2/2869 (0.1%)	1.14	7/3898 (0.2%)
All	All	0.72	2/11544 (0.0%)	1.18	37/15686 (0.2%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	371	VAL	CB-CG1	-6.52	1.39	1.52
1	D	371	VAL	C-OXT	-5.79	1.12	1.23

The worst 5 of 37 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	361	ARG	NE-CZ-NH1	8.81	124.71	120.30
1	A	271	ARG	NE-CZ-NH2	8.63	124.62	120.30
1	D	120	LEU	CB-CG-CD2	-8.18	97.09	111.00
1	B	361	ARG	NE-CZ-NH2	-8.08	116.26	120.30
1	A	149	ARG	NE-CZ-NH2	-7.94	116.33	120.30

There are no chirality outliers.

There are no planarity outliers.

### 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit,

and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2855	0	2844	59	0
1	B	2881	0	2874	62	0
1	C	2837	0	2822	130	0
1	D	2837	0	2821	71	0
2	A	74	0	46	10	0
2	D	74	0	48	12	0
3	B	4	0	6	0	0
3	D	4	0	6	3	0
4	A	318	0	0	3	0
4	B	287	0	0	6	0
4	C	195	0	0	5	0
4	D	239	0	0	3	0
All	All	12605	0	11467	321	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 14.

The worst 5 of 321 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:186:IT1:C4A	2:D:501:GPD:HN4B	1.44	1.31
1:D:276:HIS:HB2	3:D:1041:EDO:H12	1.36	1.05
1:D:186:IT1:C4A	2:D:501:GPD:N4A	2.23	1.01
1:A:186:IT1:C4A	2:A:500:GPD:HN4B	1.72	1.01
1:C:264:LYS:HB2	1:C:363:ILE:HD12	1.48	0.95

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	367/391 (94%)	358 (98%)	9 (2%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	370/391 (95%)	358 (97%)	12 (3%)	0	100	100
1	C	364/391 (93%)	341 (94%)	21 (6%)	2 (0%)	38	17
1	D	364/391 (93%)	350 (96%)	13 (4%)	1 (0%)	50	27
All	All	1465/1564 (94%)	1407 (96%)	55 (4%)	3 (0%)	56	33

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	292	LEU
1	C	364	ALA
1	D	184	GLY

### 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	299/318 (94%)	284 (95%)	15 (5%)	34	12
1	B	302/318 (95%)	292 (97%)	10 (3%)	50	25
1	C	296/318 (93%)	273 (92%)	23 (8%)	18	4
1	D	296/318 (93%)	274 (93%)	22 (7%)	20	4
All	All	1193/1272 (94%)	1123 (94%)	70 (6%)	28	9

5 of 70 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	169	LYS
1	C	270	ASN
1	D	267	ARG
1	C	187	ILE
1	C	220	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 11 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	105	ASN
1	C	250	HIS
1	D	58	ASN
1	C	91	ASN
1	C	347	ASN

### 5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

4 non-standard protein/DNA/RNA residues are modelled in this entry.

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	$\# Z  > 2$
1	IT1	A	186	1	24,24,25	3.90	7 (29%)	30,32,34	1.46	6 (20%)
1	IT1	B	186	1	24,24,25	3.29	5 (20%)	30,32,34	1.65	7 (23%)
1	IT1	C	186	1	24,24,25	3.89	5 (20%)	30,32,34	1.50	6 (20%)
1	IT1	D	186	1	24,24,25	3.88	6 (25%)	30,32,34	1.38	5 (16%)

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
1	IT1	A	186	1	-	0/15/17/19	0/1/1/1
1	IT1	B	186	1	-	0/15/17/19	0/1/1/1
1	IT1	C	186	1	-	0/15/17/19	0/1/1/1
1	IT1	D	186	1	-	0/15/17/19	0/1/1/1

The worst 5 of 23 bond length outliers are listed below:



Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	186	IT1	O-C	17.70	1.23	1.11
1	C	186	IT1	O-C	17.64	1.23	1.11
1	A	186	IT1	O-C	17.61	1.23	1.11
1	B	186	IT1	O-C	14.79	1.21	1.11
1	A	186	IT1	CA-C	3.41	1.54	1.48

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	186	IT1	OP4-C5A-C5	4.40	118.20	109.26
1	A	186	IT1	CD-CG-CB	3.54	126.53	113.64
1	C	186	IT1	C-CA-N	3.53	117.35	113.83
1	C	186	IT1	CG-CB-CA	-3.23	101.90	113.13
1	B	186	IT1	P-OP4-C5A	-3.20	109.70	121.22

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

6 ligands are modelled in this entry.

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	$\# Z  > 2$
2	GPD	A	500	-	40,40,40	1.04	3 (7%)	59,62,62	1.71	11 (18%)
2	GPD	A	501	-	40,40,40	2.53	17 (42%)	59,62,62	6.45	19 (32%)
3	EDO	B	1040	-	3,3,3	0.53	0	2,2,2	0.44	0
3	EDO	D	1041	-	3,3,3	0.58	0	2,2,2	0.10	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	GPD	D	500	-	40,40,40	1.09	2 (5%)	59,62,62	2.26	9 (15%)
2	GPD	D	501	-	40,40,40	0.94	3 (7%)	59,62,62	1.74	12 (20%)

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
2	GPD	A	500	-	-	0/21/53/53	0/2/4/4
2	GPD	A	501	-	-	0/21/53/53	1/2/4/4
3	EDO	B	1040	-	-	0/1/1/1	0/0/0/0
3	EDO	D	1041	-	-	0/1/1/1	0/0/0/0
2	GPD	D	500	-	-	0/21/53/53	0/2/4/4
2	GPD	D	501	-	-	0/21/53/53	0/2/4/4

The worst 5 of 25 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	GPD	P2-O1G	-6.81	1.41	1.60
2	A	501	GPD	C4-N9	-5.96	1.29	1.37
2	A	501	GPD	C2-N1	-5.04	1.28	1.36
2	A	501	GPD	P-O1P	-4.68	1.34	1.55
2	A	501	GPD	C2-N2	-3.45	1.27	1.32

The worst 5 of 51 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501	GPD	C6-C5-N7	-40.91	128.63	134.14
2	A	501	GPD	O4'-C1'-N9	18.97	126.08	108.44
2	D	500	GPD	C6-C5-N7	-10.96	132.66	134.14
2	D	500	GPD	O4'-C1'-N9	7.50	115.42	108.44
2	A	501	GPD	N3-C4-N9	7.38	137.74	126.91

There are no chirality outliers.

There are no torsion outliers.

All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	501	GPD	C1G-C2G-C3G-C4G-C5G-O5G

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	368/391 (94%)	-0.02	1 (0%) 91 95	5, 13, 37, 75	0
1	B	367/391 (93%)	-0.03	0 100 100	5, 14, 39, 80	0
1	C	367/391 (93%)	0.50	33 (8%) 10 12	5, 21, 64, 90	0
1	D	367/391 (93%)	0.11	4 (1%) 77 83	4, 18, 46, 74	0
All	All	1469/1564 (93%)	0.14	38 (2%) 53 58	4, 16, 51, 90	0

The worst 5 of 38 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	371	VAL	11.4
1	C	362	VAL	6.5
1	C	363	ILE	6.3
1	C	366	LEU	6.2
1	C	369	VAL	5.4

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

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> 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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
1	IT1	B	186	24/25	0.11	0.47	2,8,17,22	0
1	IT1	A	186	24/25	0.11	-0.10	2,9,16,24	0
1	IT1	D	186	24/25	0.10	-0.63	1,14,21,28	0
1	IT1	C	186	24/25	0.10	-0.63	1,13,18,26	0

### 6.3 Carbohydrates

There are no carbohydrates in this entry.

### 6.4 Ligands

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> 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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
3	EDO	D	1041	4/4	0.24	9.74	23,23,31,50	0
3	EDO	B	1040	4/4	0.15	5.48	17,32,32,36	0
2	GPD	D	501	37/37	0.16	2.40	25,61,99,99	0
2	GPD	A	500	37/37	0.12	0.54	16,31,99,99	0
2	GPD	D	500	37/37	0.11	0.01	20,30,82,99	0
2	GPD	A	501	37/37	0.08	-0.62	6,18,35,69	0

### 6.5 Other polymers

There are no such residues in this entry.