

wwPDB X-ray Structure Validation Summary Report (i)

Aug 14, 2023 – 02:26 pm BST

PDB ID	:	8A29
Title	:	Apo 1-deoxy-D-xylulose 5-phosphate synthase from Pseudomonas aeruginosa
Authors	:	Hamid, R.; Adam, S.; Lacour, A.; Monjas, L.; Hirsch, A.
Deposited on	:	2022-06-02
Resolution	:	2.10 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org A user guide is available at https://www.wwpdb.org/validation/2017/XrayValidationReportHelp with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
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)	:	2.35

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: $X\text{-}RAY\;DIFFRACTION$

The reported resolution of this entry is 2.10 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.



Motric	Whole archive	Similar resolution		
IVIEUTIC	$(\# { m Entries})$	$(\# { m Entries}, { m resolution} { m range}({ m \AA}))$		
R _{free}	130704	5197 (2.10-2.10)		
Clashscore	141614	5710 (2.10-2.10)		
Ramachandran outliers	138981	5647 (2.10-2.10)		
Sidechain outliers	138945	5648 (2.10-2.10)		
RSRZ outliers	127900	5083 (2.10-2.10)		

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

Mol	Chain	Length	Quality of chain		
			5%		
1	А	622	83%	6%	10%
			4%		
1	В	622	84%	6%	9%
			4%		
1	С	622	86%	·	10%
			8%		
1	D	622	81% 8	%	11%
			4%		
1	E	622	84%	6%	10%



Mol	Chain	Length	Quality of chain		
			3%		
1	\mathbf{F}	622	85%	5%	11%



2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 53080 atoms, of which 25331 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.

Mol	Chain	Residues			Atom	IS			ZeroOcc	AltConf	Trace		
1	Δ	557	Total	С	Η	Ν	0	S	0	0 0	0		
1	Л	001	8442	2684	4197	735	805	21	0	0	0		
1	В	563	Total	С	Η	Ν	0	S	0	2	0		
1	D	505	8569	2719	4267	748	814	21	0	2	0		
1	С	С	C	C 559	Total	С	Η	Ν	0	S	0	2	0
1	U	009	8524	2707	4240	748	809	20	0	2	0		
1	л	554	Total	С	Η	Ν	Ο	\mathbf{S}	0	0	0		
	D		8393	2669	4171	734	799	20	0	0	0		
1	F	560	Total	С	Η	Ν	Ο	\mathbf{S}	0	0	0		
	500	8451	2698	4187	739	806	21	0	0	0			
1 F	F	556	Total	С	Η	Ν	0	S	0	0	0		
	550	8452	2685	4205	738	804	20	U	0	U			

• Molecule 1 is a protein called 1-deoxy-D-xylulose-5-phosphate synthase.

There are 204 discrepancies between the modelled and reference sequences:

Chain Residue		Modelled	Actual	Comment	Reference
А	1	MET	-	initiating methionine	UNP B7V7R4
А	2	GLY	-	expression tag	UNP B7V7R4
А	3	SER	-	expression tag	UNP B7V7R4
А	4	SER	-	expression tag	UNP B7V7R4
А	5	HIS	-	expression tag	UNP B7V7R4
А	6	HIS	-	expression tag	UNP B7V7R4
А	7	HIS	-	expression tag	UNP B7V7R4
А	8	HIS	-	expression tag	UNP B7V7R4
А	9	HIS	-	expression tag	UNP B7V7R4
А	10	HIS	-	expression tag	UNP B7V7R4
А	11	SER	-	expression tag	UNP B7V7R4
А	12	SER	-	expression tag	UNP B7V7R4
А	13	GLY	-	expression tag	UNP B7V7R4
А	14	LEU	-	expression tag	UNP B7V7R4
A	15	VAL	-	expression tag	UNP B7V7R4
A	16	PRO	-	expression tag	UNP B7V7R4
A	17	ARG	-	expression tag	UNP B7V7R4



Chain	Residue	Modelled	Actual	Comment	Reference
А	18	GLY	-	expression tag	UNP B7V7R4
А	19	SER	-	expression tag	UNP B7V7R4
А	20	MET	-	expression tag	UNP B7V7R4
А	21	GLU	-	expression tag	UNP B7V7R4
А	22	ASN	-	expression tag	UNP B7V7R4
А	23	LEU	-	expression tag	UNP B7V7R4
А	24	TYR	-	expression tag	UNP B7V7R4
А	25	PHE	-	expression tag	UNP B7V7R4
А	26	GLN	-	expression tag	UNP B7V7R4
А	27	SER	-	expression tag	UNP B7V7R4
А	28	HIS	-	expression tag	UNP B7V7R4
А	235	GLY	-	linker	UNP B7V7R4
А	236	GLY	-	linker	UNP B7V7R4
А	237	GLY	-	linker	UNP B7V7R4
А	238	GLY	-	linker	UNP B7V7R4
А	239	GLY	-	linker	UNP B7V7R4
А	240	GLY	-	linker	UNP B7V7R4
В	1	MET	-	initiating methionine	UNP B7V7R4
В	2	GLY	-	expression tag	UNP B7V7R4
В	3	SER	-	expression tag	UNP B7V7R4
В	4	SER	-	expression tag	UNP B7V7R4
В	5	HIS	-	expression tag	UNP B7V7R4
В	6	HIS	-	expression tag	UNP B7V7R4
В	7	HIS	-	expression tag	UNP B7V7R4
В	8	HIS	-	expression tag	UNP B7V7R4
В	9	HIS	-	expression tag	UNP B7V7R4
В	10	HIS	-	expression tag	UNP B7V7R4
В	11	SER	-	expression tag	UNP B7V7R4
В	12	SER	-	expression tag	UNP B7V7R4
В	13	GLY	-	expression tag	UNP B7V7R4
В	14	LEU	-	expression tag	UNP B7V7R4
В	15	VAL	_	expression tag	UNP B7V7R4
В	16	PRO	-	expression tag	UNP B7V7R4
В	17	ARG	_	expression tag	UNP B7V7R4
В	18	GLY	-	expression tag	UNP B7V7R4
В	19	SER	_	expression tag	UNP B7V7R4
В	20	MET	-	expression tag	UNP B7V7R4
В	21	GLU	-	expression tag	UNP B7V7R4
В	22	ASN	-	expression tag	UNP B7V7R4
В	23	LEU	-	expression tag	UNP B7V7R4
В	24	TYR	-	expression tag	UNP B7V7R4
В	25	PHE	_	expression tag	UNP B7V7R4



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1 Continued	trom	nromanic	naae
Continucu	110116	$p_{1}c_{0}a_{0}a_{0}$	payc
	5	1	1 5

Chain Residue		Modelled	Actual	Comment	Reference
В	26	GLN	-	expression tag	UNP B7V7R4
В	27	SER	-	expression tag	UNP B7V7R4
В	28	HIS	-	expression tag	UNP B7V7R4
В	235	GLY	-	linker	UNP B7V7R4
В	236	GLY	-	linker	UNP B7V7R4
В	237	GLY	-	linker	UNP B7V7R4
В	238	GLY	-	linker	UNP B7V7R4
В	239	GLY	-	linker	UNP B7V7R4
В	240	GLY	-	linker	UNP B7V7R4
С	1	MET	-	initiating methionine	UNP B7V7R4
С	2	GLY	-	expression tag	UNP B7V7R4
С	3	SER	-	expression tag	UNP B7V7R4
С	4	SER	-	expression tag	UNP B7V7R4
С	5	HIS	-	expression tag	UNP B7V7R4
С	6	HIS	-	expression tag	UNP B7V7R4
С	7	HIS	-	expression tag	UNP B7V7R4
С	8	HIS	-	expression tag	UNP B7V7R4
С	9	HIS	-	expression tag	UNP B7V7R4
С	10	HIS	-	expression tag	UNP B7V7R4
С	11	SER	-	expression tag	UNP B7V7R4
С	12	SER	-	expression tag	UNP B7V7R4
С	13	GLY	-	expression tag	UNP B7V7R4
С	14	LEU	-	expression tag	UNP B7V7R4
C	15	VAL	-	expression tag	UNP B7V7R4
C	16	PRO	-	expression tag	UNP B7V7R4
C	17	ARG	-	expression tag	UNP B7V7R4
C	18	GLY	-	expression tag	UNP B7V7R4
C	19	SER	-	expression tag	UNP B7V7R4
C	20	MET	-	expression tag	UNP B7V7R4
C	21	GLU	-	expression tag	UNP B7V7R4
C	22	ASN	-	expression tag	UNP B7V7R4
C	23	LEU	-	expression tag	UNP B7V7R4
C	24	TYR	-	expression tag	UNP B7V7R4
C	25	PHE	-	expression tag	UNP B7V7R4
C	26	GLN	-	expression tag	UNP B7V7R4
C	27	SER	-	expression tag	UNP B7V7R4
C	28	HIS	-	expression tag	UNP B7V7R4
C	235	GLY	-	linker	UNP B7V7R4
C	236	GLY	-	linker	UNP B7V7R4
C	237	GLY	-	linker	UNP B7V7R4
C	238	GLY	-	linker	UNP B7V7R4
C	239	GLY	-	linker	UNP B7V7R4



Chain Residue		Modelled	Actual	Comment	Reference
С	240	GLY	-	linker	UNP B7V7R4
D	1	MET	-	initiating methionine	UNP B7V7R4
D	2	GLY	-	expression tag	UNP B7V7R4
D	3	SER	-	expression tag	UNP B7V7R4
D	4	SER	-	expression tag	UNP B7V7R4
D	5	HIS	-	expression tag	UNP B7V7R4
D	6	HIS	-	expression tag	UNP B7V7R4
D	7	HIS	-	expression tag	UNP B7V7R4
D	8	HIS	-	expression tag	UNP B7V7R4
D	9	HIS	-	expression tag	UNP B7V7R4
D	10	HIS	-	expression tag	UNP B7V7R4
D	11	SER	-	expression tag	UNP B7V7R4
D	12	SER	-	expression tag	UNP B7V7R4
D	13	GLY	-	expression tag	UNP B7V7R4
D	14	LEU	-	expression tag	UNP B7V7R4
D	15	VAL	-	expression tag	UNP B7V7R4
D	16	PRO	-	expression tag	UNP B7V7R4
D	17	ARG	-	expression tag	UNP B7V7R4
D	18	GLY	-	expression tag	UNP B7V7R4
D	19	SER	-	expression tag	UNP B7V7R4
D	20	MET	-	expression tag	UNP B7V7R4
D	21	GLU	-	expression tag	UNP B7V7R4
D	22	ASN	-	expression tag	UNP B7V7R4
D	23	LEU	-	expression tag	UNP B7V7R4
D	24	TYR	-	expression tag	UNP B7V7R4
D	25	PHE	-	expression tag	UNP B7V7R4
D	26	GLN	-	expression tag	UNP B7V7R4
D	27	SER	-	expression tag	UNP B7V7R4
D	28	HIS	-	expression tag	UNP B7V7R4
D	235	GLY	-	linker	UNP B7V7R4
D	236	GLY	-	linker	UNP B7V7R4
D	237	GLY	-	linker	UNP B7V7R4
D	238	GLY	-	linker	UNP B7V7R4
D	239	GLY	-	linker	UNP B7V7R4
D	240	GLY	-	linker	UNP B7V7R4
E	1	MET	-	initiating methionine	UNP $B7V7R\overline{4}$
E	2	GLY	-	expression tag	UNP B7V7R4
E	3	SER	-	expression tag	UNP B7V7R4
E	4	SER	-	expression tag	UNP $B7V7R\overline{4}$
E	5	HIS	-	expression tag	UNP B7V7R4
E	6	HIS	-	expression tag	UNP B7V7R4
E	7	HIS	-	expression tag	UNP B7V7R4



Chain	Residue	Modelled	Actual	Comment	Reference
Е	8	HIS	-	expression tag	UNP B7V7R4
Е	9	HIS	-	expression tag	UNP B7V7R4
Е	10	HIS	-	expression tag	UNP B7V7R4
Е	11	SER	-	expression tag	UNP B7V7R4
Е	12	SER	-	expression tag	UNP B7V7R4
Е	13	GLY	-	expression tag	UNP B7V7R4
Е	14	LEU	-	expression tag	UNP B7V7R4
Е	15	VAL	-	expression tag	UNP B7V7R4
Е	16	PRO	-	expression tag	UNP B7V7R4
Е	17	ARG	-	expression tag	UNP B7V7R4
Е	18	GLY	-	expression tag	UNP B7V7R4
Е	19	SER	-	expression tag	UNP B7V7R4
Е	20	MET	-	expression tag	UNP B7V7R4
E	21	GLU	-	expression tag	UNP B7V7R4
Е	22	ASN	-	expression tag	UNP B7V7R4
Е	23	LEU	-	expression tag	UNP B7V7R4
E	24	TYR	-	expression tag	UNP B7V7R4
Е	25	PHE	-	expression tag	UNP B7V7R4
Е	26	GLN	-	expression tag	UNP B7V7R4
E	27	SER	-	expression tag	UNP B7V7R4
Ε	28	HIS	-	expression tag	UNP B7V7R4
E	235	GLY	-	linker	UNP B7V7R4
Е	236	GLY	-	linker	UNP B7V7R4
Ε	237	GLY	-	linker	UNP B7V7R4
Е	238	GLY	-	linker	UNP B7V7R4
Е	239	GLY	-	linker	UNP B7V7R4
Ε	240	GLY	-	linker	UNP B7V7R4
F	1	MET	-	initiating methionine	UNP B7V7R4
F	2	GLY	-	expression tag	UNP B7V7R4
F	3	SER	-	expression tag	UNP B7V7R4
F	4	SER	-	expression tag	UNP B7V7R4
F	5	HIS	-	expression tag	UNP B7V7R4
F	6	HIS	-	expression tag	UNP B7V7R4
F	7	HIS	-	expression tag	UNP B7V7R4
F	8	HIS	-	expression tag	UNP B7V7R4
F	9	HIS	-	expression tag	UNP B7V7R4
F	10	HIS		expression tag	UNP B7V7R4
F	11	SER	-	expression tag	UNP B7V7R4
F	12	SER	-	expression tag	UNP B7V7R4
F	13	GLY	-	expression tag	UNP B7V7R4
F	14	LEU	-	expression tag	UNP B7V7R4
F	15	VAL	-	expression tag	UNP B7V7R4



Chain	Residue	Modelled	Actual	$\operatorname{Comment}$	Reference
F	16	PRO	-	expression tag	UNP B7V7R4
F	17	ARG	-	expression tag	UNP B7V7R4
F	18	GLY	-	expression tag	UNP B7V7R4
F	19	SER	-	expression tag	UNP B7V7R4
F	20	MET	-	expression tag	UNP B7V7R4
F	21	GLU	-	expression tag	UNP B7V7R4
F	22	ASN	-	expression tag	UNP B7V7R4
F	23	LEU	-	expression tag	UNP B7V7R4
F	24	TYR	-	expression tag	UNP B7V7R4
F	25	PHE	-	expression tag	UNP B7V7R4
F	26	GLN	-	expression tag	UNP B7V7R4
F	27	SER	-	expression tag	UNP B7V7R4
F	28	HIS	-	expression tag	UNP B7V7R4
F	235	GLY	-	linker	UNP B7V7R4
F	236	GLY	-	linker	UNP B7V7R4
F	237	GLY	-	linker	UNP B7V7R4
F	238	GLY	-	linker	UNP B7V7R4
F	239	GLY	-	linker	UNP B7V7R4
F	240	GLY	-	linker	UNP B7V7R4

• Molecule 2 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	А	1	Total C H O 14 3 8 3	0	0
2	D	1	Total C H O 14 3 8 3	0	0



Continued from previous page...

Mol	Chain	Residues	A	ton	ns		ZeroOcc	AltConf
0	F	1	Total	С	Η	0	0	0
	Ľ	1	14	3	8	3	0	0
9	F	1	Total	С	Η	Ο	0	0
	Ľ	1	14	3	8	3	0	0
2	F	1	Total	С	Η	Ο	0	0
2	Ľ	1	14	3	8	3	0	0
2	F	1	Total	С	Η	0	0	0
2	Ľ	1	14	3	8	3	0	
2	F	1	Total	С	Η	Ο	0	0
2	Ľ	1	14	3	8	3	0	0
2	F	1	Total	C	Η	0		0
	T,	1	14	3	8	3		0

• Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	А	2	Total Mg 2 2	0	0
3	В	4	Total Mg 4 4	0	0
3	С	2	Total Mg 2 2	0	0
3	D	1	Total Mg 1 1	0	0
3	Ε	2	Total Mg 2 2	0	0
3	F	2	Total Mg 2 2	0	0

• Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	А	1	Total Cl 1 1	0	0
4	В	1	Total Cl 1 1	0	0

• Molecule 5 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	А	1	Total Na 1 1	0	0



Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	С	1	Total Na 1 1	0	0
5	D	1	Total Na 1 1	0	0
5	Е	1	Total Na 1 1	0	0
5	F	1	Total Na 1 1	0	0

• Molecule 6 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	А	2	Total Ca 2 2	0	0
6	В	1	Total Ca 1 1	0	0
6	С	1	Total Ca 1 1	0	0
6	D	4	Total Ca 4 4	0	0
6	Е	2	Total Ca 2 2	0	0
6	F	2	Total Ca 2 2	0	0

• Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	А	326	Total O 326 326	0	0
7	В	384	Total O 384 384	0	0
7	С	311	Total O 311 311	0	0
7	D	337	Total O 337 337	0	0
7	Е	356	Total O 356 356	0	0
7	F	391	Total O 391 391	0	0



3 Residue-property plots (i)

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



• Molecule 1: 1-deoxy-D-xylulose-5-phosphate synthase



• Molecule 1: 1-deoxy-D-xylulose-5-phosphate synthase

Chain D:	81%	8%	11%
MET CLY SER SER SER SER HIS HIS HIS HIS SER HIS SER RIS SER CLY CLU PRO AND AND AND AND AND AND AND AND AND AND	LEU TYR PHE GLN GLN HIS MET FRO FRO CLN CLN CLN CLN CLN CLN CLN CLN CLN CLN	600 641 641 743 743 743 744 744 647 647 848 848 849	15 15 15 16 16 16 16 16 16 16 16 16
D68 B69 B69 B69 B71 B71 <td>Y118 Y118 L123 L123 L123 H123 M164 M168 B178</td> <td>M194 V211 V211 L213 L213 MET SER ILLE SER SER SER SER SER SER</td> <td>VASN VASN GLY GLY GLY SER SER ASN TYR ALA</td>	Y118 Y118 L123 L123 L123 H123 M164 M168 B178	M194 V211 V211 L213 L213 MET SER ILLE SER SER SER SER SER SER	VASN VASN GLY GLY GLY SER SER ASN TYR ALA
LYS ILE GLY GLY CLY CLY CLY CLY CLY CLY CL24 CL24 CL24 CL24 CL24 CL24 CL24 CL24	T267 1268 R260 N270 N270 N271 N271 N271 V282 V282 C289 F290 F290	E295 E295 1296 P296 P297 P297 P297 P297 P295 F296 E206 E10 E10	CLY CLY SER ALA PRO LYS LYS LYS LYS K347
L352 Y363 Y366 A367 A367 A367 A368 A367 A368 A367 A373 Y391 F391 F391 F395 F391 F391 F395 F391 F391 F395 F391 F395 F391 F395 F395 F395 F395 F395 F395 F305 F305 F305 F305 F305 F305 F305 F30	F435 D436 1439 L440 L440 L460 L460 L464 R502 R502 R502	V330 F534 L546 E571 L578 L578 R821 R821	
• Molecule 1: 1-deoxy-D-xylu	lose-5-phosphate synt	hase	
Chain E:	84%	6%	10%
MET CLY CLY SER SER HIS HIS HIS HIS HIS SER HIS SER RIS SER CLY CLU PRO CLU SER RIS SER ASU	LEU: TYR TYR GLN GLN GLN HIS M29 E35 E35 E35 E35 E35 E35 E35 E35 E35	D62 L63 L70 Y100 F102 F102 F118	1133 1150 1192 1193 1194 1208
D217 MET SER MET SER SER HIS ASN VAL ASL VAL LEU CLY CLY GLY GLY CIY CIY	GLY GLY 7252 1253 1253 1253 1253 1253 1254 1275 1251 1251 1251 1251 1251 1251 1251	A291 P292 L295 L295 CLU ALA ALA ALA ALA CLY	ALA ALA PRO LYS LYS LYS THR G317 B361 R362
V366 A367 1566 A369 A369 A373 A373 A369 M380 1291 1291 1291 1291 1291 1291 1291 129	1404 1418 1418 8451 8452 0453 0453 1453 8524 8524	V530 D531 D531 E446 G563 G563 G563 G563 G563 A10 A10 A10 A10 A10 A10 A10 A10 A10 A10	
• Molecule 1: 1-deoxy-D-xylu	lose-5-phosphate synt	hase	
Chain F:	85%	5%	11%
MET SER SER SER SER HIS HIS HIS HIS SER HIS SER HIS SER ASC CU MET ASC ASC ASC ASC ASC ASC ASC ASC ASC ASC	LES	E60 E64 D68 V110 V113 V113 V113	L133 T152 S158 A192 N216
D217 MET SER SER SER TLE TLE ASN ASN ASN ASN ASN ASN ASN ASN ASN ASN	GLY GLY FRO GLY FRO GLY GLY F1243 F245 F245 F245 F245 F260 F260 F261 F261 F262 F263 M270 W270	R272 B273 D273 D273 E307 E307 ALA PR0 G17 SER ALA ALA ALA IVS	THN THN C317 L339 L339 V366 V366 A367 A367 A369







4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants	116.44Å 137.63Å 232.08Å	Depositor
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor
$Percelution(\hat{\lambda})$	48.59 - 2.10	Depositor
Resolution (A)	48.59 - 2.10	EDS
% Data completeness	99.9 (48.59-2.10)	Depositor
(in resolution range)	99.9 (48.59-2.10)	EDS
R_{merge}	0.06	Depositor
R _{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	1.93 (at 2.10Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487, PHENIX 1.20.1_4487	Depositor
D D.	0.171 , 0.224	Depositor
$\mathbf{n}, \mathbf{n}_{free}$	0.171 , 0.224	DCC
R_{free} test set	10811 reflections (4.99%)	wwPDB-VP
Wilson B-factor $(Å^2)$	27.3	Xtriage
Anisotropy	0.533	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	0.44, 51.2	EDS
L-test for twinning ²	$< L >=0.50, < L^2>=0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	53080	wwPDB-VP
Average B, all atoms $(Å^2)$	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 18.87% of the height of the origin peak. No significant pseudotranslation is detected.

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.



¹Intensities estimated from amplitudes.

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: CL, MG, NA, GOL, CA

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).

Mal	Chain	Bond lengths		Bond angles		
MOI	Unam	RMSZ	# Z > 5	RMSZ	# Z > 5	
1	А	0.51	0/4329	0.70	0/5869	
1	В	0.54	0/4390	0.70	0/5951	
1	С	0.53	0/4372	0.70	0/5926	
1	D	0.54	0/4305	0.68	0/5837	
1	Е	0.52	0/4350	0.70	2/5899~(0.0%)	
1	F	0.55	0/4331	0.70	0/5872	
All	All	0.53	0/26077	0.70	2/35354~(0.0%)	

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	F	0	1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	Е	453	ASP	CB-CG-OD1	6.29	123.96	118.30
1	Е	531	ASP	CB-CG-OD2	-5.39	113.45	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	F	618	ARG	Sidechain



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	А	4245	4197	4210	24	0
1	В	4302	4267	4274	20	0
1	С	4284	4240	4257	13	0
1	D	4222	4171	4194	32	0
1	Е	4264	4187	4236	23	0
1	F	4247	4205	4214	17	0
2	А	6	8	8	0	0
2	D	6	8	8	0	0
2	Е	12	16	16	0	0
2	F	24	32	31	0	0
3	А	2	0	0	0	0
3	В	4	0	0	0	0
3	С	2	0	0	0	0
3	D	1	0	0	0	0
3	Е	2	0	0	0	0
3	F	2	0	0	0	0
4	А	1	0	0	0	0
4	В	1	0	0	0	0
5	А	1	0	0	0	0
5	С	1	0	0	0	0
5	D	1	0	0	0	0
5	Е	1	0	0	0	0
5	F	1	0	0	0	0
6	А	2	0	0	0	0
6	В	1	0	0	0	0
6	С	1	0	0	0	0
6	D	4	0	0	0	0
6	Ε	2	0	0	0	0
6	F	2	0	0	0	0
7	А	326	0	0	3	0
7	В	384	0	0	1	0
7	С	311	0	0	2	0
7	D	337	0	0	2	0
7	Е	356	0	0	0	0
7	F	391	0	0	1	0
All	All	27749	25331	25448	127	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 2.

The worst 5 of 127 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:D:256:ILE:HD11	1:D:282:VAL:HG22	1.48	0.93
1:A:33:LEU:O	1:A:33:LEU:HD23	1.71	0.91
1:B:39:GLU:OE1	7:B:801:HOH:O	2.00	0.79
1:A:38:ARG:HH12	1:A:307:GLU:HB2	1.48	0.78
1:A:509:LEU:HD21	1:A:546:LEU:HD13	1.80	0.64

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Perce	ntiles
1	А	551/622~(89%)	534 (97%)	16 (3%)	1 (0%)	47	49
1	В	559/622~(90%)	540 (97%)	19 (3%)	0	100	100
1	С	555/622~(89%)	540 (97%)	14 (2%)	1 (0%)	47	49
1	D	548/622~(88%)	531 (97%)	17 (3%)	0	100	100
1	Ε	554/622~(89%)	537~(97%)	17 (3%)	0	100	100
1	F	550/622~(88%)	532 (97%)	18 (3%)	0	100	100
All	All	3317/3732~(89%)	3214 (97%)	101 (3%)	2(0%)	51	54

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	С	526	ASP
1	А	218	MET



5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Perce	ntiles
1	А	440/490~(90%)	435~(99%)	5 (1%)	73	79
1	В	446/490~(91%)	443 (99%)	3 (1%)	84	88
1	С	444/490 (91%)	441 (99%)	3 (1%)	84	88
1	D	437/490~(89%)	432 (99%)	5 (1%)	73	79
1	Ε	442/490~(90%)	440 (100%)	2 (0%)	88	92
1	F	440/490 (90%)	436 (99%)	4 (1%)	78	84
All	All	2649/2940~(90%)	2627 (99%)	22 (1%)	81	86

 $5~{\rm of}~22$ residues with a non-rotameric side chain are listed below:

Mol	Chain	Res	Type
1	D	244	LEU
1	Е	524	SER
1	Е	474	ARG
1	F	68	ASP
1	В	255	PRO

Sometimes side chains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such side chains are listed below:

Mol	Chain	Res	Type
1	А	490	GLN
1	Е	135	GLN
1	Е	617	GLN

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 40 ligands modelled in this entry, 32 are monoatomic - leaving 8 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	Dec	Tink	B	ond leng	gths	E	Bond ang	gles
	туре	Unain	nes		Counts	RMSZ	# Z >2	Counts	RMSZ	# Z >2
2	GOL	E	702	-	5,5,5	1.46	0	5,5,5	0.42	0
2	GOL	А	701	-	5,5,5	1.00	0	5,5,5	0.90	0
2	GOL	E	701	-	5,5,5	0.95	0	$5,\!5,\!5$	0.97	0
2	GOL	F	702	-	5,5,5	1.17	1 (20%)	$5,\!5,\!5$	0.86	0
2	GOL	D	701	-	5,5,5	0.95	0	5,5,5	1.00	0
2	GOL	F	701	-	5,5,5	1.33	1 (20%)	5,5,5	0.80	0
2	GOL	F	703	-	5,5,5	2.43	1 (20%)	5,5,5	0.80	0
2	GOL	F	704	-	5,5,5	2.56	3 (60%)	5,5,5	0.90	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
2	GOL	Е	702	-	-	4/4/4/4	-
2	GOL	А	701	-	-	0/4/4/4	-
2	GOL	Е	701	-	-	2/4/4/4	-
2	GOL	F	702	-	-	1/4/4/4	-
2	GOL	D	701	-	-	2/4/4/4	-
2	GOL	F	701	-	-	4/4/4/4	-
2	GOL	F	703	-	-	2/4/4/4	-
2	GOL	F	704	_	_	2/4/4/4	_



Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	703	GOL	O2-C2	-4.99	1.28	1.43
2	F	704	GOL	O2-C2	3.97	1.55	1.43
2	F	704	GOL	C3-C2	2.75	1.63	1.51
2	F	701	GOL	C1-C2	2.11	1.60	1.51
2	F	702	GOL	O2-C2	-2.10	1.37	1.43

The worst 5 of 6 bond length outliers are listed below:

There are no bond angle outliers.

There are no chirality outliers.

5 of 17 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	Е	702	GOL	C1-C2-C3-O3
2	D	701	GOL	C1-C2-C3-O3
2	Е	701	GOL	C1-C2-C3-O3
2	F	701	GOL	O1-C1-C2-C3
2	F	701	GOL	C1-C2-C3-O3

There are no ring outliers.

No monomer is involved in short contacts.

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 (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	$\langle RSRZ \rangle$	#RSRZ>2	$OWAB(Å^2)$	Q<0.9
1	А	557/622~(89%)	0.28	28 (5%) 28 34	19, 29, 49, 88	0
1	В	563/622~(90%)	0.23	24 (4%) 35 41	17, 26, 43, 90	0
1	С	559/622~(89%)	0.25	22 (3%) 39 45	17, 28, 47, 79	0
1	D	554/622~(89%)	0.52	52 (9%) 8 11	17, 29, 57, 90	0
1	Ε	560/622~(90%)	0.28	23 (4%) 37 43	18, 27, 46, 83	0
1	F	556/622~(89%)	0.26	16 (2%) 51 57	16, 25, 44, 71	0
All	All	3349/3732~(89%)	0.30	165 (4%) 29 35	16, 27, 49, 90	0

The worst 5 of 165 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	В	621	ARG	5.7
1	D	75	LEU	5.2
1	F	307	GLU	4.9
1	D	306	LEU	4.8
1	А	219	SER	4.8

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, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	$B-factors(A^2)$	Q < 0.9
2	GOL	А	701	6/6	0.69	0.31	52,62,67,72	0
2	GOL	D	701	6/6	0.74	0.26	48,57,64,66	0
2	GOL	Е	701	6/6	0.75	0.22	59,73,83,87	0
2	GOL	Е	702	6/6	0.75	0.22	29,46,55,66	0
2	GOL	F	701	6/6	0.77	0.26	35,50,66,66	0
2	GOL	F	703	6/6	0.81	0.18	32,40,60,60	0
3	MG	С	701	1/1	0.82	0.13	40,40,40,40	0
3	MG	В	703	1/1	0.83	0.35	37,37,37,37	0
2	GOL	F	704	6/6	0.83	0.17	19,40,48,48	0
6	CA	А	707	1/1	0.83	0.11	66,66,66,66	0
5	NA	D	703	1/1	0.85	0.05	54,54,54,54	0
6	CA	А	706	1/1	0.86	0.14	$61,\!61,\!61,\!61$	0
4	CL	В	705	1/1	0.89	0.14	$65,\!65,\!65,\!65$	0
6	CA	С	704	1/1	0.91	0.18	$67,\!67,\!67,\!67$	0
3	MG	F	706	1/1	0.93	0.30	39,39,39,39	0
3	MG	А	702	1/1	0.93	0.23	34,34,34,34	0
3	MG	В	701	1/1	0.93	0.12	28,28,28,28	0
3	MG	D	702	1/1	0.94	0.22	43,43,43,43	0
3	MG	Е	703	1/1	0.94	0.27	37,37,37,37	0
5	NA	F	707	1/1	0.95	0.08	37,37,37,37	0
3	MG	F	705	1/1	0.95	0.11	35,35,35,35	0
5	NA	А	705	1/1	0.95	0.17	29,29,29,29	0
4	CL	А	704	1/1	0.95	0.15	50, 50, 50, 50	0
6	CA	F	709	1/1	0.95	0.20	$50,\!50,\!50,\!50$	0
6	CA	D	704	1/1	0.96	0.07	54,54,54,54	0
6	CA	D	705	1/1	0.96	0.25	49,49,49,49	0
6	CA	F	708	1/1	0.96	0.06	39,39,39,39	0
3	MG	В	702	1/1	0.96	0.13	26, 26, 26, 26	0
6	CA	В	706	1/1	0.97	0.05	63,63,63,63	0
6	CA	D	706	1/1	0.97	0.14	$69,\!69,\!69,\!69$	0
6	CA	D	707	1/1	0.97	0.06	38,38,38,38	0
6	CA	E	706	1/1	0.97	0.20	49,49,49,49	0
6	CA	Е	707	1/1	0.97	0.20	47,47,47,47	0
5	NA	E	705	1/1	0.97	0.07	24,24,24,24	0
3	MG	А	703	1/1	0.97	0.22	26,26,26,26	0
5	NA	С	703	1/1	0.98	0.10	26,26,26,26	0
3	MG	E	704	1/1	0.98	0.14	33,33,33,33	0



Mol	Type	Chain	Res	Atoms	RSCC	RSR	$\mathbf{B} ext{-factors}(\mathrm{\AA}^2)$	Q<0.9
2	GOL	F	702	6/6	0.98	0.10	$23,\!36,\!44,\!53$	0
3	MG	С	702	1/1	0.98	0.14	22,22,22,22	0
3	MG	В	704	1/1	0.99	0.50	$51,\!51,\!51,\!51$	0

Continued from previous page...

6.5 Other polymers (i)

There are no such residues in this entry.

