



# wwPDB X-ray Structure Validation Summary Report ⓘ

May 13, 2020 – 01:38 am BST

PDB ID : 3OUR  
Title : Crystal structure of complex between EIIA and a novel pyruvate decarboxylase  
Authors : Jeong, C.S.; An, Y.J.; Cha, S.S.  
Deposited on : 2010-09-15  
Resolution : 2.20 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](mailto: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  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
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) : 2.11

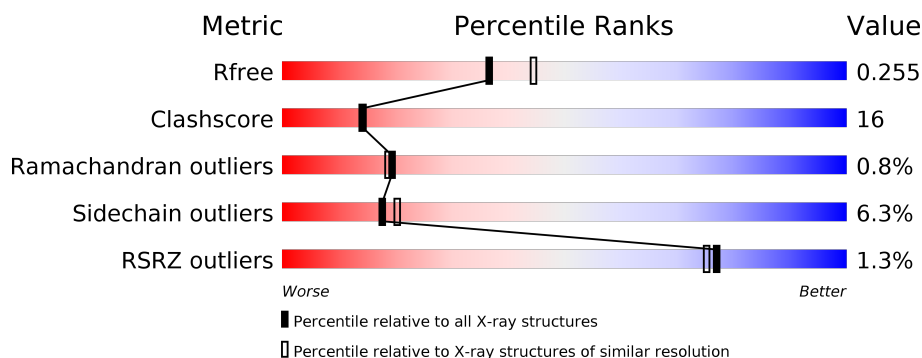
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.20 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	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	435	<div> <div>%</div> <div> <div></div> <div>65%</div> <div>24%</div> <div>•</div> <div>9%</div> </div> </div>
1	C	435	<div> <div>2%</div> <div> <div></div> <div>63%</div> <div>26%</div> <div>•</div> <div>9%</div> </div> </div>
1	E	435	<div> <div>2%</div> <div> <div></div> <div>64%</div> <div>24%</div> <div>•</div> <div>9%</div> </div> </div>
1	G	435	<div> <div>%</div> <div> <div></div> <div>63%</div> <div>25%</div> <div>•</div> <div>9%</div> </div> </div>
2	B	183	<div> <div>%</div> <div> <div></div> <div>51%</div> <div>28%</div> <div>•</div> <div>18%</div> </div> </div>
2	D	183	<div> <div>%</div> <div> <div></div> <div>54%</div> <div>20%</div> <div>8%</div> <div>•</div> <div>18%</div> </div> </div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	F	183	<div><div></div><div>57%</div><div>22%</div><div>• •</div><div>18%</div></div>
2	H	183	<div><div></div><div>55%</div><div>23%</div><div>•</div><div>18%</div></div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 17650 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 UPF0255 protein VV1\_0328.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	394	Total	C	N	O	S	0	0	0
			3018	1931	509	563	15			
1	C	394	Total	C	N	O	S	0	0	0
			3079	1966	522	576	15			
1	E	396	Total	C	N	O	S	0	0	0
			3048	1947	517	569	15			
1	G	396	Total	C	N	O	S	0	0	0
			3098	1979	525	579	15			

There are 80 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	EXPRESSION TAG	UNP Q8DF91
A	-18	ARG	-	EXPRESSION TAG	UNP Q8DF91
A	-17	GLY	-	EXPRESSION TAG	UNP Q8DF91
A	-16	SER	-	EXPRESSION TAG	UNP Q8DF91
A	-15	HIS	-	EXPRESSION TAG	UNP Q8DF91
A	-14	HIS	-	EXPRESSION TAG	UNP Q8DF91
A	-13	HIS	-	EXPRESSION TAG	UNP Q8DF91
A	-12	HIS	-	EXPRESSION TAG	UNP Q8DF91
A	-11	HIS	-	EXPRESSION TAG	UNP Q8DF91
A	-10	HIS	-	EXPRESSION TAG	UNP Q8DF91
A	-9	GLY	-	EXPRESSION TAG	UNP Q8DF91
A	-8	SER	-	EXPRESSION TAG	UNP Q8DF91
A	-7	ALA	-	EXPRESSION TAG	UNP Q8DF91
A	-6	CYS	-	EXPRESSION TAG	UNP Q8DF91
A	-5	GLU	-	EXPRESSION TAG	UNP Q8DF91
A	-4	LEU	-	EXPRESSION TAG	UNP Q8DF91
A	-3	GLY	-	EXPRESSION TAG	UNP Q8DF91
A	-2	THR	-	EXPRESSION TAG	UNP Q8DF91
A	-1	PRO	-	EXPRESSION TAG	UNP Q8DF91
A	0	ASN	-	EXPRESSION TAG	UNP Q8DF91
C	-19	MET	-	EXPRESSION TAG	UNP Q8DF91

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
C	-18	ARG	-	EXPRESSION TAG	UNP Q8DF91
C	-17	GLY	-	EXPRESSION TAG	UNP Q8DF91
C	-16	SER	-	EXPRESSION TAG	UNP Q8DF91
C	-15	HIS	-	EXPRESSION TAG	UNP Q8DF91
C	-14	HIS	-	EXPRESSION TAG	UNP Q8DF91
C	-13	HIS	-	EXPRESSION TAG	UNP Q8DF91
C	-12	HIS	-	EXPRESSION TAG	UNP Q8DF91
C	-11	HIS	-	EXPRESSION TAG	UNP Q8DF91
C	-10	HIS	-	EXPRESSION TAG	UNP Q8DF91
C	-9	GLY	-	EXPRESSION TAG	UNP Q8DF91
C	-8	SER	-	EXPRESSION TAG	UNP Q8DF91
C	-7	ALA	-	EXPRESSION TAG	UNP Q8DF91
C	-6	CYS	-	EXPRESSION TAG	UNP Q8DF91
C	-5	GLU	-	EXPRESSION TAG	UNP Q8DF91
C	-4	LEU	-	EXPRESSION TAG	UNP Q8DF91
C	-3	GLY	-	EXPRESSION TAG	UNP Q8DF91
C	-2	THR	-	EXPRESSION TAG	UNP Q8DF91
C	-1	PRO	-	EXPRESSION TAG	UNP Q8DF91
C	0	ASN	-	EXPRESSION TAG	UNP Q8DF91
E	-19	MET	-	EXPRESSION TAG	UNP Q8DF91
E	-18	ARG	-	EXPRESSION TAG	UNP Q8DF91
E	-17	GLY	-	EXPRESSION TAG	UNP Q8DF91
E	-16	SER	-	EXPRESSION TAG	UNP Q8DF91
E	-15	HIS	-	EXPRESSION TAG	UNP Q8DF91
E	-14	HIS	-	EXPRESSION TAG	UNP Q8DF91
E	-13	HIS	-	EXPRESSION TAG	UNP Q8DF91
E	-12	HIS	-	EXPRESSION TAG	UNP Q8DF91
E	-11	HIS	-	EXPRESSION TAG	UNP Q8DF91
E	-10	HIS	-	EXPRESSION TAG	UNP Q8DF91
E	-9	GLY	-	EXPRESSION TAG	UNP Q8DF91
E	-8	SER	-	EXPRESSION TAG	UNP Q8DF91
E	-7	ALA	-	EXPRESSION TAG	UNP Q8DF91
E	-6	CYS	-	EXPRESSION TAG	UNP Q8DF91
E	-5	GLU	-	EXPRESSION TAG	UNP Q8DF91
E	-4	LEU	-	EXPRESSION TAG	UNP Q8DF91
E	-3	GLY	-	EXPRESSION TAG	UNP Q8DF91
E	-2	THR	-	EXPRESSION TAG	UNP Q8DF91
E	-1	PRO	-	EXPRESSION TAG	UNP Q8DF91
E	0	ASN	-	EXPRESSION TAG	UNP Q8DF91
G	-19	MET	-	EXPRESSION TAG	UNP Q8DF91
G	-18	ARG	-	EXPRESSION TAG	UNP Q8DF91
G	-17	GLY	-	EXPRESSION TAG	UNP Q8DF91

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
G	-16	SER	-	EXPRESSION TAG	UNP Q8DF91
G	-15	HIS	-	EXPRESSION TAG	UNP Q8DF91
G	-14	HIS	-	EXPRESSION TAG	UNP Q8DF91
G	-13	HIS	-	EXPRESSION TAG	UNP Q8DF91
G	-12	HIS	-	EXPRESSION TAG	UNP Q8DF91
G	-11	HIS	-	EXPRESSION TAG	UNP Q8DF91
G	-10	HIS	-	EXPRESSION TAG	UNP Q8DF91
G	-9	GLY	-	EXPRESSION TAG	UNP Q8DF91
G	-8	SER	-	EXPRESSION TAG	UNP Q8DF91
G	-7	ALA	-	EXPRESSION TAG	UNP Q8DF91
G	-6	CYS	-	EXPRESSION TAG	UNP Q8DF91
G	-5	GLU	-	EXPRESSION TAG	UNP Q8DF91
G	-4	LEU	-	EXPRESSION TAG	UNP Q8DF91
G	-3	GLY	-	EXPRESSION TAG	UNP Q8DF91
G	-2	THR	-	EXPRESSION TAG	UNP Q8DF91
G	-1	PRO	-	EXPRESSION TAG	UNP Q8DF91
G	0	ASN	-	EXPRESSION TAG	UNP Q8DF91

- Molecule 2 is a protein called Phosphotransferase system IIA component.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	150	Total	C	N	O	S	0	0	0
			1121	714	177	228	2			
2	D	150	Total	C	N	O	S	0	0	0
			1117	713	178	224	2			
2	F	150	Total	C	N	O	S	0	0	0
			1121	715	178	226	2			
2	H	150	Total	C	N	O	S	0	0	0
			1121	714	177	228	2			

There are 56 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-13	MET	-	EXPRESSION TAG	UNP Q8DFJ9
B	-12	ARG	-	EXPRESSION TAG	UNP Q8DFJ9
B	-11	GLY	-	EXPRESSION TAG	UNP Q8DFJ9
B	-10	SER	-	EXPRESSION TAG	UNP Q8DFJ9
B	-9	HIS	-	EXPRESSION TAG	UNP Q8DFJ9
B	-8	HIS	-	EXPRESSION TAG	UNP Q8DFJ9
B	-7	HIS	-	EXPRESSION TAG	UNP Q8DFJ9
B	-6	HIS	-	EXPRESSION TAG	UNP Q8DFJ9
B	-5	HIS	-	EXPRESSION TAG	UNP Q8DFJ9

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
B	-4	HIS	-	EXPRESSION TAG	UNP Q8DFJ9
B	-3	GLY	-	EXPRESSION TAG	UNP Q8DFJ9
B	-2	SER	-	EXPRESSION TAG	UNP Q8DFJ9
B	-1	ASP	-	EXPRESSION TAG	UNP Q8DFJ9
B	0	THR	-	EXPRESSION TAG	UNP Q8DFJ9
D	-13	MET	-	EXPRESSION TAG	UNP Q8DFJ9
D	-12	ARG	-	EXPRESSION TAG	UNP Q8DFJ9
D	-11	GLY	-	EXPRESSION TAG	UNP Q8DFJ9
D	-10	SER	-	EXPRESSION TAG	UNP Q8DFJ9
D	-9	HIS	-	EXPRESSION TAG	UNP Q8DFJ9
D	-8	HIS	-	EXPRESSION TAG	UNP Q8DFJ9
D	-7	HIS	-	EXPRESSION TAG	UNP Q8DFJ9
D	-6	HIS	-	EXPRESSION TAG	UNP Q8DFJ9
D	-5	HIS	-	EXPRESSION TAG	UNP Q8DFJ9
D	-4	HIS	-	EXPRESSION TAG	UNP Q8DFJ9
D	-3	GLY	-	EXPRESSION TAG	UNP Q8DFJ9
D	-2	SER	-	EXPRESSION TAG	UNP Q8DFJ9
D	-1	ASP	-	EXPRESSION TAG	UNP Q8DFJ9
D	0	THR	-	EXPRESSION TAG	UNP Q8DFJ9
F	-13	MET	-	EXPRESSION TAG	UNP Q8DFJ9
F	-12	ARG	-	EXPRESSION TAG	UNP Q8DFJ9
F	-11	GLY	-	EXPRESSION TAG	UNP Q8DFJ9
F	-10	SER	-	EXPRESSION TAG	UNP Q8DFJ9
F	-9	HIS	-	EXPRESSION TAG	UNP Q8DFJ9
F	-8	HIS	-	EXPRESSION TAG	UNP Q8DFJ9
F	-7	HIS	-	EXPRESSION TAG	UNP Q8DFJ9
F	-6	HIS	-	EXPRESSION TAG	UNP Q8DFJ9
F	-5	HIS	-	EXPRESSION TAG	UNP Q8DFJ9
F	-4	HIS	-	EXPRESSION TAG	UNP Q8DFJ9
F	-3	GLY	-	EXPRESSION TAG	UNP Q8DFJ9
F	-2	SER	-	EXPRESSION TAG	UNP Q8DFJ9
F	-1	ASP	-	EXPRESSION TAG	UNP Q8DFJ9
F	0	THR	-	EXPRESSION TAG	UNP Q8DFJ9
H	-13	MET	-	EXPRESSION TAG	UNP Q8DFJ9
H	-12	ARG	-	EXPRESSION TAG	UNP Q8DFJ9
H	-11	GLY	-	EXPRESSION TAG	UNP Q8DFJ9
H	-10	SER	-	EXPRESSION TAG	UNP Q8DFJ9
H	-9	HIS	-	EXPRESSION TAG	UNP Q8DFJ9
H	-8	HIS	-	EXPRESSION TAG	UNP Q8DFJ9
H	-7	HIS	-	EXPRESSION TAG	UNP Q8DFJ9
H	-6	HIS	-	EXPRESSION TAG	UNP Q8DFJ9
H	-5	HIS	-	EXPRESSION TAG	UNP Q8DFJ9

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
H	-4	HIS	-	EXPRESSION TAG	UNP Q8DFJ9
H	-3	GLY	-	EXPRESSION TAG	UNP Q8DFJ9
H	-2	SER	-	EXPRESSION TAG	UNP Q8DFJ9
H	-1	ASP	-	EXPRESSION TAG	UNP Q8DFJ9
H	0	THR	-	EXPRESSION TAG	UNP Q8DFJ9

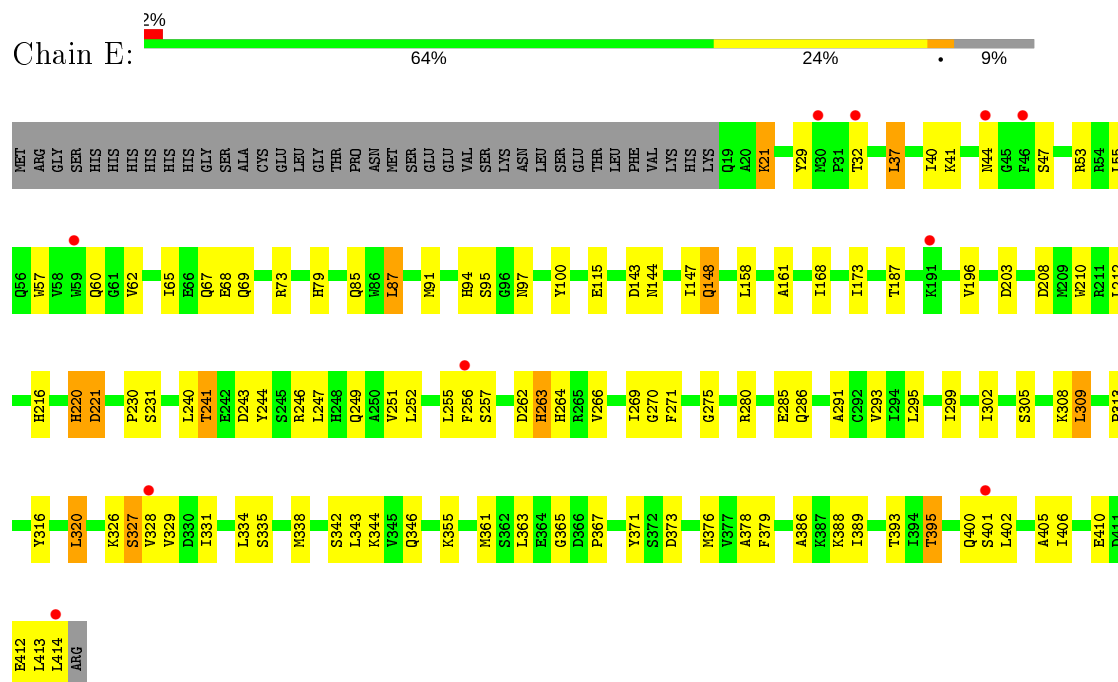
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	120	Total O 120 120	0	0
3	B	74	Total O 74 74	0	0
3	C	212	Total O 212 212	0	0
3	D	75	Total O 75 75	0	0
3	E	159	Total O 159 159	0	0
3	F	52	Total O 52 52	0	0
3	G	157	Total O 157 157	0	0
3	H	78	Total O 78 78	0	0

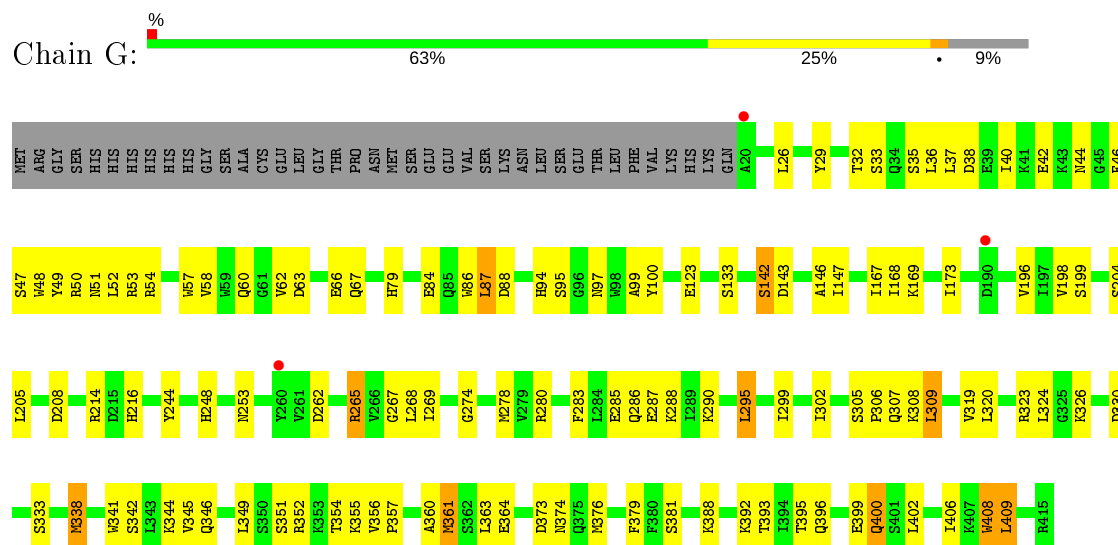




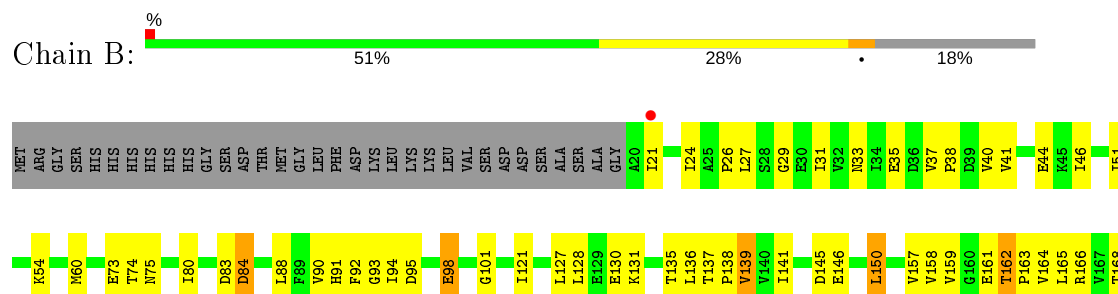
• Molecule 1: UPF0255 protein VV1\_0328



• Molecule 1: UPF0255 protein VV1\_0328



• Molecule 2: Phosphotransferase system IIA component



K169

- Molecule 2: Phosphotransferase system IIA component

Chain D: 

MET ARG GLY SER HIS HIS HIS HIS GLY SER ASP THR MET GLY LEU PHE ASP LYS LEU LYS LEU VAL SER ASP ASP SER ALA ALA GLY A20 A21 L27 L28 E35 D39 V40 V41 F42 A43 E44 K45 I46 V47 I51 A52 I53 K54 P55 N58 V61

K70 E73 T74 N75 F78 S79 D84 E87 L88 H91 F92 G93 I94 D95 T96 V97 E98 L99 E102 T105 E109 D118 T119 V120 I121 L125 E129 E130 K131 S134 T135 L136 T137 P138 E144 V140 I141 S142 N143 E146 I147 L150 T162 R166

V167 T168 K169

- Molecule 2: Phosphotransferase system IIA component

Chain F: 

MET ARG GLY SER HIS HIS HIS HIS GLY SER ASP THR MET GLY LEU PHE ASP LYS LEU LYS LEU VAL SER ASP ASP SER ALA ALA GLY A20 A21 L27 N33 I34 E35 D39 V40 V41 F42 A43 E44 K45 I46 V47 G50 V61 N65 I68 F72

E73 T74 N75 D84 L88 H91 F92 T96 V97 K100 G101 R106 E109 E110 K115 A116 L127 L128 E129 E130 K131 P138 V139 V140 I141 D145 K148 E149 L150 N151 V159 T162 P163 V164 L165 R166 K169

- Molecule 2: Phosphotransferase system IIA component

Chain H: 

MET ARG GLY SER HIS HIS HIS HIS GLY SER ASP THR MET GLY LEU PHE ASP LYS LEU LYS LEU VAL SER ASP ASP SER ALA ALA GLY A20 A21 I24 I34 V37 P38 D39 V40 V41 I46 V47 I51 A52 P55 K59 M60 V61 I68

E73 T74 N75 L88 F89 V90 F92 G93 D95 T96 V97 E98 L99 T105 R106 E109 E110 G111 Q112 G117 I121 L127 L128 E129 E130 K131 T135 L136 T137 P138 I147 K148 E149 L150 V159 G160 L165 R166 V167 T168 K169

## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	322.87Å 62.07Å 126.36Å 90.00° 110.80° 90.00°	Depositor
Resolution (Å)	49.37 – 2.20 49.37 – 2.19	Depositor EDS
% Data completeness (in resolution range)	90.5 (49.37-2.20) 98.4 (49.37-2.19)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.60 (at 2.18Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.201 , 0.248 0.208 , 0.255	Depositor DCC
$R_{free}$ test set	5953 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	29.2	Xtriage
Anisotropy	0.264	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 52.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.020 for -h-2*k,l	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	17650	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 14.29% of the height of the origin peak. No significant pseudotranslation is detected.*

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

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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	0.43	0/3092	0.67	1/4211 (0.0%)
1	C	0.43	0/3152	0.67	0/4279
1	E	0.41	0/3119	0.64	0/4241
1	G	0.44	0/3172	0.65	0/4306
2	B	0.49	0/1135	0.77	0/1539
2	D	0.46	0/1131	0.76	2/1533 (0.1%)
2	F	0.48	0/1135	0.80	2/1538 (0.1%)
2	H	0.50	0/1135	0.80	1/1539 (0.1%)
All	All	0.44	0/17071	0.69	6/23186 (0.0%)

There are no bond length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	88	LEU	CA-CB-CG	6.68	130.67	115.30
2	D	27	LEU	CA-CB-CG	6.08	129.29	115.30
2	F	88	LEU	CA-CB-CG	5.79	128.62	115.30
2	D	88	LEU	CA-CB-CG	5.54	128.04	115.30
1	A	330	ASP	N-CA-C	-5.14	97.12	111.00

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3018	0	2882	91	0
1	C	3079	0	2994	89	0
1	E	3048	0	2941	95	0
1	G	3098	0	3024	90	0
2	B	1121	0	1137	42	0
2	D	1117	0	1140	54	0
2	F	1121	0	1144	32	0
2	H	1121	0	1137	47	0
3	A	120	0	0	4	0
3	B	74	0	0	1	0
3	C	212	0	0	3	0
3	D	75	0	0	5	0
3	E	159	0	0	2	0
3	F	52	0	0	3	0
3	G	157	0	0	3	0
3	H	78	0	0	3	0
All	All	17650	0	16399	516	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 16.

The worst 5 of 516 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)
2:H:127:LEU:HD11	2:H:131:LYS:HE2	1.30	1.11
1:E:410:GLU:OE1	1:E:414:LEU:HD12	1.58	1.04
2:B:37:VAL:HB	2:B:94:ILE:HD11	1.50	0.94
1:C:118:ASN:H	1:C:118:ASN:HD22	1.15	0.94
1:E:97:ASN:HD22	1:E:100:TYR:H	1.21	0.88

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	392/435 (90%)	341 (87%)	42 (11%)	9 (2%)	6	3
1	C	390/435 (90%)	356 (91%)	29 (7%)	5 (1%)	12	9
1	E	394/435 (91%)	366 (93%)	24 (6%)	4 (1%)	15	14
1	G	394/435 (91%)	368 (93%)	26 (7%)	0	100	100
2	B	148/183 (81%)	139 (94%)	9 (6%)	0	100	100
2	D	148/183 (81%)	138 (93%)	10 (7%)	0	100	100
2	F	148/183 (81%)	138 (93%)	10 (7%)	0	100	100
2	H	148/183 (81%)	142 (96%)	6 (4%)	0	100	100
All	All	2162/2472 (88%)	1988 (92%)	156 (7%)	18 (1%)	19	19

5 of 18 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	46	PHE
1	A	350	SER
1	C	326	LYS
1	C	329	VAL
1	E	241	THR

### 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	310/377 (82%)	297 (96%)	13 (4%)	30	38
1	C	325/377 (86%)	314 (97%)	11 (3%)	37	47
1	E	316/377 (84%)	303 (96%)	13 (4%)	30	39
1	G	328/377 (87%)	309 (94%)	19 (6%)	20	23
2	B	125/153 (82%)	114 (91%)	11 (9%)	10	10
2	D	124/153 (81%)	102 (82%)	22 (18%)	2	1
2	F	125/153 (82%)	112 (90%)	13 (10%)	7	6
2	H	125/153 (82%)	115 (92%)	10 (8%)	12	12

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	1778/2120 (84%)	1666 (94%)	112 (6%)	18	20

5 of 112 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	D	135	THR
1	E	148	GLN
2	H	41	VAL
2	D	143	ASN
2	D	167	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 54 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	375	GLN
1	E	85	GLN
1	G	307	GLN
2	D	58	ASN
1	E	51	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

There are no ligands in this entry.



## 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, 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	394/435 (90%)	0.08	6 (1%) 73 72	17, 42, 66, 73	0
1	C	394/435 (90%)	-0.11	7 (1%) 68 66	13, 36, 63, 80	0
1	E	396/435 (91%)	-0.13	10 (2%) 57 55	15, 38, 61, 73	0
1	G	396/435 (91%)	-0.23	3 (0%) 86 85	15, 34, 54, 61	0
2	B	150/183 (81%)	-0.39	1 (0%) 87 86	16, 29, 46, 53	0
2	D	150/183 (81%)	-0.31	1 (0%) 87 86	19, 31, 48, 58	0
2	F	150/183 (81%)	-0.42	0 100 100	18, 27, 44, 50	0
2	H	150/183 (81%)	-0.48	0 100 100	16, 26, 45, 61	0
All	All	2180/2472 (88%)	-0.18	28 (1%) 77 75	13, 34, 61, 80	0

The worst 5 of 28 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	390	SER	4.2
1	C	260	TYR	3.2
1	A	259	PRO	2.9
1	G	20	ALA	2.8
1	E	32	THR	2.7

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

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

### 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.