

# wwPDB X-ray Structure Validation Summary Report (i)

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PDB ID : 6SXL

> Title : Crystal structure of CrtE

Authors : Feng, Y.; Morgan, R.M.L.; Nixon, P.J.

2019-09-26 Deposited on

2.50 Å(reported) Resolution

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

MolProbity 4.02b-467

> 1.8.5 (274361), CSD as541be (2020) Mogul

Xtriage (Phenix) 1.13 EDS 2.13.1

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)

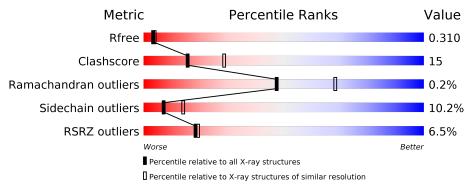
Validation Pipeline (wwPDB-VP) 2.13.1

## 1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.50 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	Similar resolution
Metric	$(\# \mathrm{Entries})$	$(\#  ext{Entries},  ext{resolution range}( ext{Å}))$
$R_{free}$	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 on 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					
1	A	277	75%	22%	•			
2	В	258	10%	28%	•			



## 2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 3963 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 Geranylgeranyl pyrophosphate synthase.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace	
1	Λ	977	Total	С	N	О	S	0	0	0
1	A	211	2036	1285	344	396	11	0	0	0

There are 15 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	ALA	deletion	UNP B1XJV9
A	?	-	GLU	deletion	UNP B1XJV9
A	?	-	$\operatorname{GLU}$	deletion	UNP B1XJV9
A	?	-	LEU	deletion	UNP B1XJV9
A	?	-	$\operatorname{GLY}$	deletion	UNP B1XJV9
A	?	-	LYS	deletion	UNP B1XJV9
A	?	-	THR	deletion	UNP B1XJV9
A	?	-	ALA	deletion	UNP B1XJV9
A	?	-	GLY	deletion	UNP B1XJV9
A	?	-	LYS	deletion	UNP B1XJV9
A	?	-	ASP	deletion	UNP B1XJV9
A	?	-	LEU	deletion	UNP B1XJV9
A	?	-	GLU	$\operatorname{deletion}$	UNP B1XJV9
A	?	-	ALA	deletion	UNP B1XJV9
A	?	-	GLN	deletion	UNP B1XJV9

• Molecule 2 is a protein called Geranylgeranyl pyrophosphate synthase.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace	
2	В	258	Total 1888	C 1191	N 322	O 364	S 11	0	0	0

There are 33 discrepancies between the modelled and reference sequences:

	toblade	Wiodelied	Actual	Comment	Reference
В	19	ALA	GLU	$\operatorname{conflict}$	UNP B1XJV9

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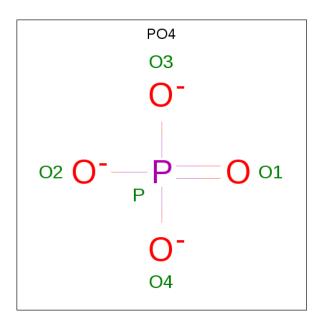


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Chain	Residue	Modelled	Actual	Comment	Reference
В	?	-	LYS	deletion	UNP B1XJV9
В	?	-	THR	deletion	UNP B1XJV9
В	?	-	ASP	deletion	UNP B1XJV9
В	?	-	VAL	deletion	UNP B1XJV9
В	?	-	ALA	deletion	UNP B1XJV9
В	?	-	VAL	deletion	UNP B1XJV9
В	?	-	ALA	deletion	UNP B1XJV9
В	?	-	GLU	deletion	UNP B1XJV9
В	?	-	GLU	deletion	UNP B1XJV9
В	?	-	LEU	deletion	UNP B1XJV9
В	?	-	GLY	deletion	UNP B1XJV9
В	?	-	LYS	deletion	UNP B1XJV9
В	?	-	THR	deletion	UNP B1XJV9
В	?	-	ALA	deletion	UNP B1XJV9
В	?	-	GLY	deletion	UNP B1XJV9
В	?	-	LYS	deletion	UNP B1XJV9
В	?	-	ASP	deletion	UNP B1XJV9
В	?	-	LEU	deletion	UNP B1XJV9
В	?	-	GLU	deletion	UNP B1XJV9
В	?	-	ALA	deletion	UNP B1XJV9
В	?	-	GLN	deletion	UNP B1XJV9
В	?	-	LYS	deletion	UNP B1XJV9
В	?	-	VAL	deletion	UNP B1XJV9
В	?	-	THR	deletion	UNP B1XJV9
В	?	-	TYR	deletion	UNP B1XJV9
В	?	-	PRO	deletion	UNP B1XJV9
В	?	-	SER	deletion	UNP B1XJV9
В	?	-	LEU	deletion	UNP B1XJV9
В	?	-	TRP	deletion	UNP B1XJV9
В	?	-	GLY	deletion	UNP B1XJV9
В	?	-	ILE	deletion	UNP B1XJV9
В	?	-	LEU	deletion	UNP B1XJV9

• Molecule 3 is PHOSPHATE ION (three-letter code: PO4) (formula: O<sub>4</sub>P).





Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total O P 5 4 1	0	0
3	В	1	Total O P 5 4 1	0	0

#### • Molecule 4 is water.

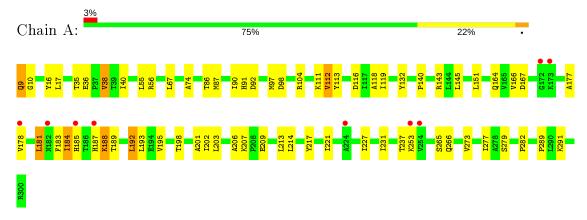
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	19	Total O 19 19	0	0
4	В	10	Total O 10 10	0	0



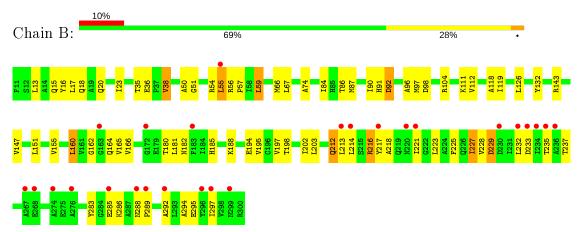
# 3 Residue-property plots (i)

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: Geranylgeranyl pyrophosphate synthase



• Molecule 2: Geranylgeranyl pyrophosphate synthase





## 4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants	70.20Å 89.47Å 107.32Å	Depositor
a, b, c, $\alpha$ , $\beta$ , $\gamma$	90.00° 90.00° 90.00°	Depositor
Resolution (Å)	68.82 - 2.50	Depositor
resolution (A)	68.72 - 2.50	EDS
% Data completeness	99.9 (68.82-2.50)	Depositor
(in resolution range)	100.0 (68.72-2.50)	EDS
$R_{merge}$	0.03	Depositor
$R_{sym}$	(Not available)	Depositor
$< I/\sigma(I) > 1$	2.27 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
P. P.	0.243 , 0.306	Depositor
$R, R_{free}$	0.245 , $0.310$	DCC
$R_{free}$ test set	1205  reflections  (5.02%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	55.3	Xtriage
Anisotropy	0.568	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$ , $B_{sol}(Å^2)$	0.32, 56.3	EDS
L-test for twinning <sup>2</sup>	$ < L > = 0.50, < L^2> = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	3963	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	77.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 5.36% of the height of the origin peak. No significant pseudotranslation is detected.

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



<sup>&</sup>lt;sup>1</sup>Intensities 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: PO4

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		
MIOI	Chain	RMSZ	# Z >5	RMSZ	# Z  > 5	
1	A	0.41	0/2060	0.77	0/2799	
2	В	0.38	0/1910	0.79	$1/2596 \ (0.0\%)$	
All	All	0.39	0/3970	0.78	1/5395~(0.0%)	

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	$\mathbf{Z}$	$\mathbf{Observed}(^o)$	$\mathbf{Ideal}(^o)$
2	В	229	ASP	CB-CA-C	5.18	120.76	110.40

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	2036	0	2015	61	0
2	В	1888	0	1871	56	0
3	A	5	0	0	0	0
3	В	5	0	0	0	0
4	A	19	0	0	4	0
4	В	10	0	0	1	0
All	All	3963	0	3886	115	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 15.

The worst 5 of 115 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	$egin{aligned}  ext{Interatomic} \  ext{distance} \ ( ext{Å}) \end{aligned}$	$egin{aligned}  ext{Clash} \  ext{overlap } ( ext{Å}) \end{aligned}$
2:B:13:LEU:HD13	2:B:292:ALA:HB3	1.44	0.98
1:A:167:ASP:HA	1:A:185:HIS:NE2	1.91	0.86
1:A:213:LEU:HD11	1:A:279:SER:HB2	1.60	0.83
1:A:56:ARG:HG2	1:A:192:LEU:HD11	1.61	0.83
2:B:198:THR:O	2:B:202:ILE:HG13	1.85	0.76

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	${f ntiles}$
1	A	$271/277 \ (98\%)$	257 (95%)	13 (5%)	1 (0%)	34	54
2	В	$250/258 \ (97\%)$	230 (92%)	20 (8%)	0	100	100
All	All	521/535~(97%)	487 (94%)	33 (6%)	1 (0%)	47	68

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	282	PRO

#### 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 sidechain conformation was



analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles		
1	A	203/220 (92%)	188 (93%)	15 (7%)	13 27		
2	В	188/203 (93%)	163 (87%)	25 (13%)	4 7		
All	All	391/423 (92%)	351 (90%)	40 (10%)	7 14		

5 of 40 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	В	23	ILE
2	В	92	ASP
2	В	233	ASP
2	В	55	LEU
2	В	98	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	15	GLN
2	В	185	HIS

#### 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)

2 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	T	Chain	Dog	T in le	B	ond leng	$_{ m gths}$	В	ond ang	gles
MIOI	Type	Chain	m Res	Link	Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z >2
3	PO4	В	401	_	4,4,4	0.61	0	6,6,6	0.62	0
3	PO4	A	401	-	4,4,4	0.74	0	6,6,6	0.47	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

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)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	В	3
1	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	В	237:THR	С	263:GLU	N	19.74
1	A	237:THR	С	253:LYS	N	15.62
1	В	172:GLY	С	179:GLU	N	12.91
1	В	279:SER	С	281:GLU	N	7.31



### 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	<RSRZ $>$	$\#\mathrm{RSRZ}{>}2$	$\mathbf{OWAB}(\mathrm{\AA}^2)$	Q < 0.9
1	A	$277/277 \ (100\%)$	0.19	9 (3%) 47 51	36, 58, 116, 160	0
2	В	$258/258 \; (100\%)$	0.70	26 (10%) 7 6	38, 82, 161, 211	1 (0%)
All	All	535/535~(100%)	0.44	35 (6%) 18 19	36, 69, 143, 211	1 (0%)

The worst 5 of 35 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	В	236	ALA	8.9
2	В	172	GLY	7.8
2	В	230	ASP	7.0
2	В	235	THR	5.2
2	В	288	ASN	5.0

### 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,  $95^{th}$  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	${f B\text{-factors}}({f \AA}^2)$	Q < 0.9
3	PO4	A	401	5/5	0.85	0.14	99,115,125,135	0
3	PO4	В	401	5/5	0.86	0.17	102,103,115,120	0

# 6.5 Other polymers (i)

There are no such residues in this entry.

