



# Full wwPDB X-ray Structure Validation Report

Feb 27, 2014 – 11:05 PM GMT

PDB ID : 1PQW  
Title : Putative enoyl reductase domain of polyketide synthase  
Authors : Gogos, A.; Mu, H.; Shapiro, L.; Burley, S.K.; New York SGX Research Center  
for Structural Genomics (NYSGXRC)  
Deposited on : 2003-06-19  
Resolution : 2.66 Å(reported)

This is a full wwPDB validation 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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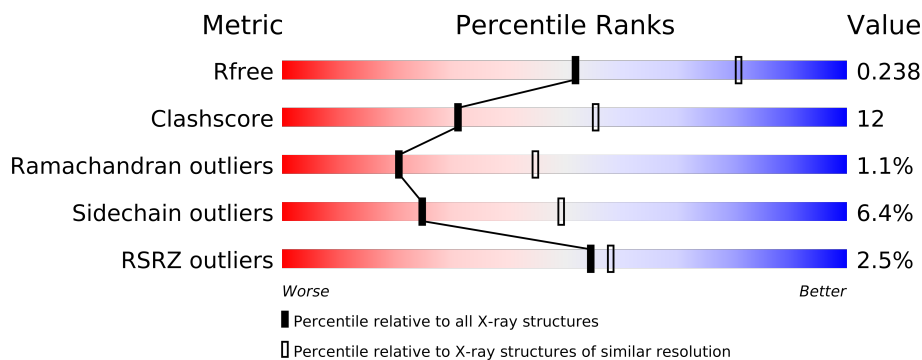
The following versions of software and data (see [references](#)) were used in the production of this report:

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 2.66 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))
$R_{free}$	66092	2232 (2.70-2.62)
Clashscore	79885	2700 (2.70-2.62)
Ramachandran outliers	78287	2657 (2.70-2.62)
Sidechain outliers	78261	2657 (2.70-2.62)
RSRZ outliers	66119	2234 (2.70-2.62)

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	198	
1	B	198	

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 2775 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 polyketide synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	183	Total	C	N	O	S	0	0	0
			1342	853	233	252	4			
1	B	175	Total	C	N	O	S	0	0	0
			1291	818	227	242	4			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	SER	-	CLONING ARTIFACT	UNP P96202
B	1	SER	-	CLONING ARTIFACT	UNP P96202

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Ca	0	0
			1	1		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	65	Total	O	0	0
			65	65		
3	B	76	Total	O	0	0
			76	76		



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	69.83Å 78.39Å 81.60Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	17.97 – 2.66 17.97 – 2.66	Depositor EDS
% Data completeness (in resolution range)	97.9 (17.97-2.66) 98.9 (17.97-2.66)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	0.08	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	5.03 (at 2.66Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.197 , 0.228 0.213 , 0.238	Depositor DCC
$R_{free}$ test set	657 reflections (4.98%)	DCC
Wilson B-factor (Å <sup>2</sup> )	28.8	Xtriage
Anisotropy	0.235	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 18.8	EDS
Estimated twinning fraction	0.016 for -h,l,k	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 24404 reflections	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	2775	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.13% 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: 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).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.40	0/1361	0.66	0/1845
1	B	0.39	0/1308	0.64	0/1771
All	All	0.40	0/2669	0.65	0/3616

There are no bond length outliers.

There are no bond angle outliers.

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	1342	0	1357	38	0
1	B	1291	0	1317	24	0
2	A	1	0	0	0	0
3	A	65	0	0	2	0
3	B	76	0	0	3	0
All	All	2775	0	2674	62	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 12.

All (62) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:69:THR:HG23	1:B:90:SER:HB3	1.32	1.09
1:A:195:VAL:HG12	1:A:196:THR:H	1.19	1.05
1:A:170:GLN:HA	1:A:170:GLN:HE21	1.24	1.01
1:B:46:SER:H	1:B:69:THR:HG22	1.35	0.90
1:A:195:VAL:HG12	1:A:196:THR:N	1.82	0.89
1:A:69:THR:HG23	1:A:90:SER:HB3	1.56	0.87
1:A:93:VAL:HG13	1:A:122:ARG:HG2	1.59	0.84
1:B:69:THR:CG2	1:B:90:SER:HB3	2.12	0.80
1:A:195:VAL:CG1	1:A:196:THR:H	1.95	0.77
1:A:46:SER:H	1:A:69:THR:HG22	1.56	0.70
1:A:60:LYS:HD2	1:A:193:LEU:HD11	1.75	0.68
1:B:42:VAL:HG23	1:B:110:VAL:HG23	1.76	0.67
1:A:25:THR:OG1	1:A:163:LEU:HD22	1.94	0.66
1:A:170:GLN:CA	1:A:170:GLN:HE21	2.07	0.65
1:A:170:GLN:NE2	1:A:170:GLN:HA	2.07	0.63
1:B:72:SER:O	1:B:76:ARG:HG3	1.97	0.63
1:A:175:ARG:O	1:A:179:GLN:HG3	1.99	0.62
1:B:20:GLY:O	1:B:24:LEU:HB2	2.01	0.60
1:B:112:LEU:HD13	3:B:203:HOH:O	2.02	0.60
1:B:42:VAL:HG23	1:B:110:VAL:CG2	2.32	0.59
1:A:167:LEU:O	1:A:171:PRO:HG3	2.03	0.58
1:A:195:VAL:CG1	1:A:196:THR:N	2.56	0.57
1:B:25:THR:OG1	1:B:163:LEU:HD22	2.04	0.57
1:A:173:ARG:HB3	1:A:173:ARG:NH2	2.22	0.55
1:A:120:ILE:O	1:A:124:VAL:HG23	2.07	0.55
1:A:120:ILE:HD11	1:A:141:VAL:HG12	1.87	0.55
1:B:196:THR:HG22	1:B:196:THR:O	2.07	0.54
1:A:69:THR:CG2	1:A:90:SER:HB3	2.31	0.53
1:A:69:THR:HG23	1:A:90:SER:CB	2.33	0.53
1:B:134:ILE:N	1:B:134:ILE:HD12	2.25	0.52
1:B:112:LEU:CD1	3:B:203:HOH:O	2.58	0.51
1:B:166:ASN:HB3	1:B:174:TYR:CE2	2.45	0.51
1:A:170:GLN:N	1:A:171:PRO:HD3	2.26	0.51
1:B:152:LEU:HA	1:B:156:ALA:HB3	1.92	0.51
1:A:48:THR:HG21	1:A:75:LYS:HD3	1.94	0.50
1:B:69:THR:HG23	1:B:90:SER:CB	2.24	0.50
1:A:173:ARG:HH21	1:A:173:ARG:CB	2.25	0.49
1:A:25:THR:HG1	1:A:163:LEU:HD22	1.75	0.49
1:A:15:GLU:HA	1:A:18:THR:HG22	1.94	0.48
1:A:27:TRP:CE3	1:A:181:ILE:HG12	2.49	0.48
1:A:67:TYR:HE2	1:A:102:LEU:HD23	1.78	0.48
1:B:178:LEU:O	1:B:182:LEU:HG	2.14	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:45:HIS:CD2	1:A:69:THR:HG21	2.50	0.47
1:A:173:ARG:NH2	1:A:173:ARG:CB	2.78	0.46
1:A:171:PRO:O	1:A:175:ARG:HG3	2.16	0.45
1:B:147:LEU:HD12	3:B:223:HOH:O	2.17	0.45
1:B:46:SER:N	1:B:69:THR:HG22	2.17	0.43
1:B:34:GLY:O	1:B:132:ARG:HD2	2.18	0.43
1:A:152:LEU:HA	1:A:156:ALA:HB3	2.00	0.43
1:A:93:VAL:CG1	1:A:93:VAL:O	2.66	0.43
1:B:127:LEU:HD11	1:B:133:PHE:HB2	2.00	0.42
1:A:20:GLY:O	1:A:24:LEU:HB2	2.20	0.42
1:A:24:LEU:HD12	1:A:24:LEU:HA	1.92	0.42
1:A:154:LYS:HB2	3:A:540:HOH:O	2.20	0.41
1:B:78:MET:HG3	1:B:196:THR:HB	2.02	0.41
1:A:48:THR:HB	3:A:505:HOH:O	2.21	0.41
1:A:110:VAL:HA	1:A:132:ARG:O	2.21	0.41
1:A:147:LEU:HD23	1:A:148:GLY:N	2.36	0.41
1:A:37:SER:HB2	1:A:38:PRO:HD2	2.03	0.41
1:B:24:LEU:HD12	1:B:24:LEU:HA	1.87	0.40
1:B:23:TYR:OH	1:B:192:VAL:HG13	2.21	0.40
1:B:128:ALA:O	1:B:129:PRO:C	2.60	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	181/198 (91%)	173 (96%)	5 (3%)	3 (2%)	14	30
1	B	171/198 (86%)	167 (98%)	3 (2%)	1 (1%)	33	63
All	All	352/396 (89%)	340 (97%)	8 (2%)	4 (1%)	21	45

All (4) Ramachandran outliers are listed below:



Mol	Chain	Res	Type
1	A	139	LYS
1	A	143	ALA
1	B	196	THR
1	A	195	VAL

### 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	134/154 (87%)	124 (92%)	10 (8%)	19	40
1	B	132/154 (86%)	125 (95%)	7 (5%)	32	60
All	All	266/308 (86%)	249 (94%)	17 (6%)	25	49

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	GLU
1	A	24	LEU
1	A	36	LEU
1	A	43	LEU
1	A	69	THR
1	A	110	VAL
1	A	112	LEU
1	A	147	LEU
1	A	170	GLN
1	A	176	GLN
1	B	24	LEU
1	B	36	LEU
1	B	43	LEU
1	B	69	THR
1	B	102	LEU
1	B	108	VAL
1	B	122	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	45	HIS
1	A	125	GLN
1	A	166	ASN
1	A	170	GLN

### 5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

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.

## 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	183/198 (92%)	-0.27	6 (3%) 44 47	13, 27, 53, 61	0
1	B	175/198 (88%)	-0.47	3 (1%) 67 71	11, 24, 40, 58	0
All	All	358/396 (90%)	-0.37	9 (2%) 54 58	11, 25, 48, 61	0

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	14	ASN	3.7
1	A	173	ARG	3.3
1	A	17	ALA	2.9
1	A	140	ASP	2.7
1	B	137	GLY	2.6
1	B	196	THR	2.2
1	B	138	LYS	2.1
1	A	15	GLU	2.1
1	A	141	VAL	2.0

### 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 ⓘ

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
2	CA	A	501	1/1	0.04	-3.15	35,35,35,35	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.