



# wwPDB X-ray Structure Validation Summary Report i

Feb 27, 2014 – 12:58 PM GMT

PDB ID : 2W04  
Title : CO-COMPLEX STRUCTURE OF ACHROMOBACTIN SYNTHETASE  
PROTEIN D (ACSD) WITH CITRATE IN ATP BINDING SITE FROM  
PECTOBACTERIUM CHRYSANTHEMI  
Authors : Schmelz, S.; McMahon, S.A.; Kadi, N.; Song, L.; Oves-Costales, D.; Oke, M.;  
Liu, H.; Johnson, K.A.; Carter, L.; White, M.F.; Challis, G.L.; Naismith, J.H.  
Deposited on : 2008-08-08  
Resolution : 2.80 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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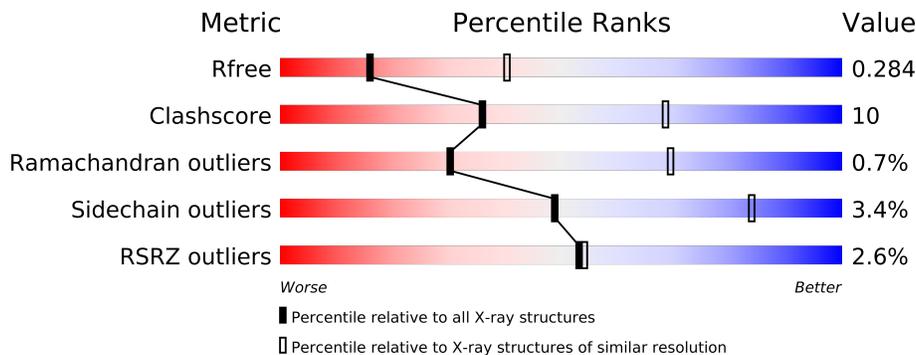
The following versions of software and data (see [references](#)) were used in the production of this report:

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 2.80 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	1799 (2.80-2.80)
Clashscore	79885	2295 (2.80-2.80)
Ramachandran outliers	78287	2252 (2.80-2.80)
Sidechain outliers	78261	2254 (2.80-2.80)
RSRZ outliers	66119	1802 (2.80-2.80)

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	620	
1	B	620	

## 2 Entry composition (i)

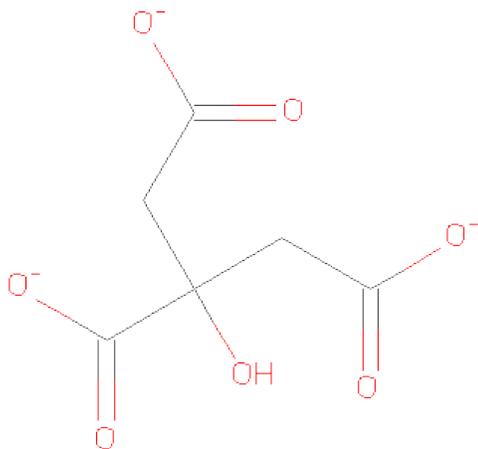
There are 3 unique types of molecules in this entry. The entry contains 9358 atoms, of which 0 are hydrogen and 0 are deuterium.

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 ACSD.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	575	4605	2929	834	822	20	0	0	0
1	B	575	4610	2931	836	823	20	0	0	0

- Molecule 2 is CITRATE ANION (three-letter code: FLC) (formula: C<sub>6</sub>H<sub>5</sub>O<sub>7</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
2	B	1	13	6	7	0	0

- Molecule 3 is water.

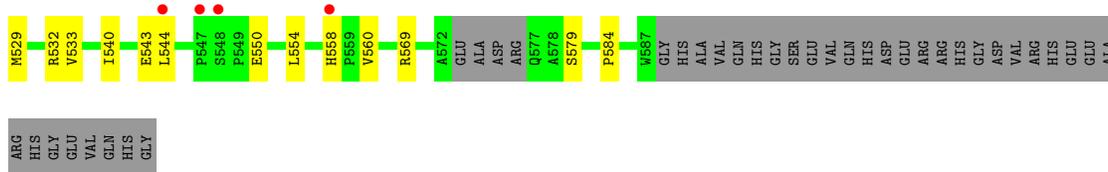
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	62	Total 62 O 62	0	0

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<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>		<b>ZeroOcc</b>	<b>AltConf</b>
3	B	68	Total	O	0	0
			68	68		





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	80.37Å 94.96Å 160.26Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	81.65 – 2.80 37.01 – 2.80	Depositor EDS
% Data completeness (in resolution range)	98.9 (81.65-2.80) 99.0 (37.01-2.80)	Depositor EDS
$R_{merge}$	0.16	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.60 (at 2.81Å)	Xtrriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.202 , 0.280 0.211 , 0.284	Depositor DCC
$R_{free}$ test set	1513 reflections (5.20%)	DCC
Wilson B-factor (Å <sup>2</sup> )	31.8	Xtrriage
Anisotropy	0.200	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , -10.0	EDS
Estimated twinning fraction	No twinning to report.	Xtrriage
L-test for twinning	$\langle  L  \rangle = 0.44$ , $\langle L^2 \rangle = 0.27$	Xtrriage
Outliers	1 of 30598 reflections (0.003%)	Xtrriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	9358	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	11.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.95% of the height of the origin peak. No significant pseudotranslation is detected.*

<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: FLC

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	0.61	0/4726	0.72	0/6423
1	B	0.63	1/4730 (0.0%)	0.73	1/6427 (0.0%)
All	All	0.62	1/9456 (0.0%)	0.72	1/12850 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	446	GLN	CG-CD	5.73	1.64	1.51

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	179	ARG	NE-CZ-NH1	5.50	123.05	120.30

There are no chirality outliers.

There are no planarity outliers.

### 5.2 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 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	4605	0	4515	98	0
1	B	4610	0	4527	95	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	13	0	5	0	0
3	A	62	0	0	5	0
3	B	68	0	0	8	0
All	All	9358	0	9047	190	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 10.

The worst 5 of 190 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:481:ASP:HA	3:B:2059:HOH:O	1.41	1.17
1:A:430:VAL:HG11	1:A:506:LEU:HD11	1.44	0.99
1:A:182:PRO:HB2	1:A:184:HIS:CE1	2.04	0.93
1:A:230:GLN:HG2	3:A:2026:HOH:O	1.73	0.88
1:B:446:GLN:HB3	3:B:2057:HOH:O	1.73	0.88

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	569/620 (92%)	542 (95%)	25 (4%)	2 (0%)	43 80
1	B	569/620 (92%)	542 (95%)	21 (4%)	6 (1%)	21 57
All	All	1138/1240 (92%)	1084 (95%)	46 (4%)	8 (1%)	30 69

5 of 8 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	302	ASN
1	A	184	HIS
1	B	43	ASP
1	B	101	ASP
1	A	101	ASP

### 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	485/522 (93%)	469 (97%)	16 (3%)	50	85
1	B	486/522 (93%)	469 (96%)	17 (4%)	48	83
All	All	971/1044 (93%)	938 (97%)	33 (3%)	49	84

5 of 33 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	493	TYR
1	B	162	SER
1	B	493	TYR
1	A	512	SER
1	B	7	ASP

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	135	GLN
1	A	247	GLN
1	A	257	GLN
1	B	230	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 (i)

1 ligand is 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	FLC	B	1588	-	5,12,12	4.43	2 (40%)	7,17,17	2.63	2 (28%)

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	FLC	B	1588	-	-	0/6/16/16	0/0/0/0

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1588	FLC	CA-CAC	8.63	1.54	1.49
2	B	1588	FLC	CG-CGC	4.65	1.52	1.49

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1588	FLC	CB-CA-CAC	5.75	123.60	115.01
2	B	1588	FLC	OHB-CB-CA	2.89	115.25	108.51

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 5.7 Other polymers (i)

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	575/620 (92%)	-0.15	17 (2%) 48 49	3, 11, 23, 34	0
1	B	575/620 (92%)	-0.09	13 (2%) 57 58	2, 11, 22, 34	3 (0%)
All	All	1150/1240 (92%)	-0.12	30 (2%) 53 54	2, 11, 23, 34	3 (0%)

The worst 5 of 30 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	482	ASP	5.1
1	A	481	ASP	3.8
1	A	480	ASP	3.7
1	A	476	ILE	3.6
1	A	483	ILE	3.6

### 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( $\text{\AA}^2$ )	Q<0.9
2	FLC	B	1588	13/13	0.22	0.58	4,10,15,17	0

## 6.5 Other polymers

There are no such residues in this entry.