



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 13, 2018 – 01:51 pm GMT

PDB ID : 1T5H
Title : 4-Chlorobenzoyl-CoA Ligase/Synthetase unliganded, selenomethionine
Authors : Gulick, A.M.; Lu, X.; Dunaway-Mariano, D.
Deposited on : 2004-05-04
Resolution : 2.00 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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 ⓘ 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	:	trunk31020
Percentile statistics	:	20171227.v01 (using entries in the PDB archive December 27th 2017)
Refmac	:	5.8.0158
CCP4	:	7.0 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk31020

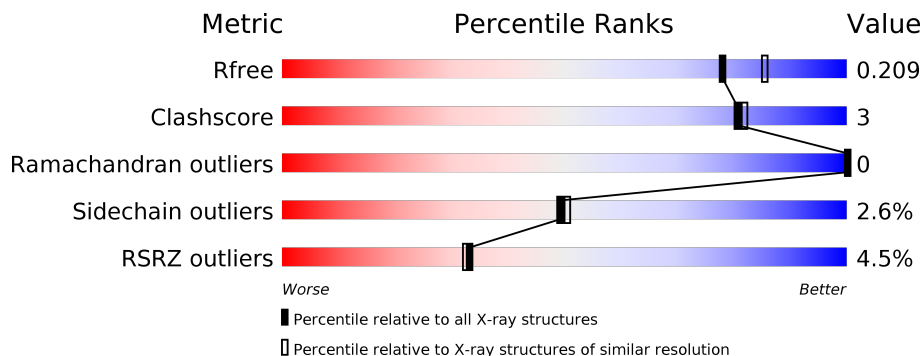
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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}	111664	7193 (2.00-2.00)
Clashscore	122126	8267 (2.00-2.00)
Ramachandran outliers	120053	8166 (2.00-2.00)
Sidechain outliers	120020	8165 (2.00-2.00)
RSRZ outliers	108989	7011 (2.00-2.00)

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. 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	X	504	<div> <div>4%</div> <div>91%</div> <div>7% ..</div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4077 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 4-chlorobenzoyl CoA ligase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	S	Se			
1	X	498	3736	2364	669	690	3	10	0	0	0

There are 21 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
X	1	MSE	MET	MODIFIED RESIDUE	UNP Q8GN86
X	7	MSE	MET	MODIFIED RESIDUE	UNP Q8GN86
X	43	ALA	-	SEE REMARK 999	UNP Q8GN86
X	45	ARG	GLY	SEE REMARK 999	UNP Q8GN86
X	78	GLY	-	SEE REMARK 999	UNP Q8GN86
X	102	MSE	MET	MODIFIED RESIDUE	UNP Q8GN86
X	151	GLU	ASP	SEE REMARK 999	UNP Q8GN86
X	152	PRO	ALA	SEE REMARK 999	UNP Q8GN86
X	185	MSE	MET	MODIFIED RESIDUE	UNP Q8GN86
X	203	MSE	MET	MODIFIED RESIDUE	UNP Q8GN86
X	259	ALA	-	SEE REMARK 999	UNP Q8GN86
X	284	MSE	MET	MODIFIED RESIDUE	UNP Q8GN86
X	310	MSE	MET	MODIFIED RESIDUE	UNP Q8GN86
X	315	MSE	MET	MODIFIED RESIDUE	UNP Q8GN86
X	317	GLN	HIS	SEE REMARK 999	UNP Q8GN86
X	318	PRO	ALA	SEE REMARK 999	UNP Q8GN86
X	324	MSE	MET	MODIFIED RESIDUE	UNP Q8GN86
X	404	MSE	MET	MODIFIED RESIDUE	UNP Q8GN86
X	428	THR	ALA	SEE REMARK 999	UNP Q8GN86
X	497	GLN	HIS	SEE REMARK 999	UNP Q8GN86
X	498	LEU	VAL	SEE REMARK 999	UNP Q8GN86

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

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

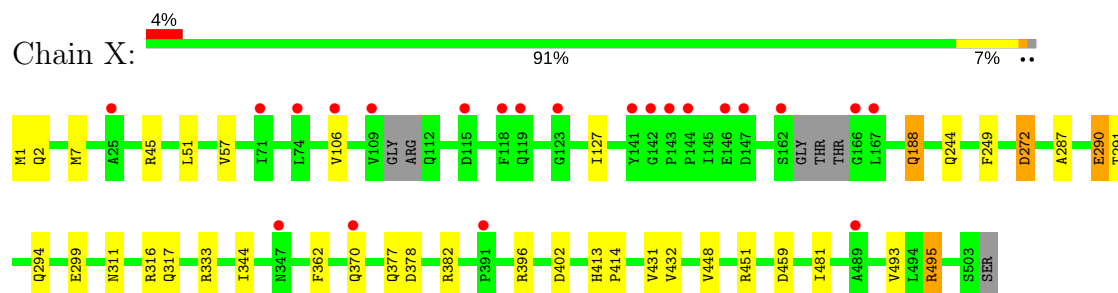
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	X	340	Total 340	O 340	0	0

3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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: 4-chlorobenzoyl CoA ligase



4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	124.98Å 124.98Å 69.00Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	25.00 – 2.00 24.93 – 2.00	Depositor EDS
% Data completeness (in resolution range)	98.7 (25.00-2.00) 98.7 (24.93-2.00)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.68 (at 2.01Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.183 , 0.206 0.184 , 0.209	Depositor DCC
R_{free} test set	2102 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	25.6	Xtriage
Anisotropy	0.432	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 42.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.033 for -h,-k,l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	4077	wwPDB-VP
Average B, all atoms (Å ²)	16.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.23% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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.

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: 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	X	0.42	0/3796	0.68	3/5156 (0.1%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	272	ASP	CB-CG-OD2	6.35	124.02	118.30
1	X	378	ASP	CB-CG-OD2	6.04	123.74	118.30
1	X	402	ASP	CB-CG-OD2	5.84	123.56	118.30

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	X	3736	0	3749	22	0
2	X	1	0	0	0	0
3	X	340	0	0	6	0
All	All	4077	0	3749	22	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 3.

All (22) 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:X:299:GLU:OE2	1:X:316:ARG:HD2	1.89	0.72
1:X:244:GLN:HG3	3:X:1208:HOH:O	1.91	0.69
1:X:287:ALA:O	1:X:290:GLU:HG3	1.97	0.64
1:X:333:ARG:HD3	1:X:344:ILE:HD11	1.82	0.62
1:X:448:VAL:CG2	1:X:481:ILE:HD13	2.31	0.61
1:X:188:GLN:HE21	1:X:311:ASN:HD22	1.49	0.60
1:X:495:ARG:NH1	3:X:1226:HOH:O	2.24	0.56
1:X:377:GLN:NE2	1:X:382:ARG:HH11	2.05	0.55
1:X:459:ASP:HB2	3:X:1209:HOH:O	2.06	0.54
1:X:188:GLN:HE21	1:X:311:ASN:ND2	2.07	0.52
1:X:333:ARG:HD3	1:X:344:ILE:CD1	2.38	0.52
1:X:432:VAL:O	1:X:495:ARG:NH2	2.42	0.52
1:X:51:LEU:HD21	1:X:57:VAL:HG21	1.93	0.51
1:X:396:ARG:HD3	3:X:1186:HOH:O	2.11	0.51
1:X:451:ARG:NH2	3:X:1263:HOH:O	2.39	0.49
1:X:299:GLU:HG3	1:X:317:GLN:HE21	1.79	0.47
1:X:431:VAL:HG21	1:X:493:VAL:HG11	1.96	0.47
1:X:287:ALA:O	1:X:291:THR:HG23	2.15	0.46
1:X:413:HIS:HA	1:X:414:PRO:HD2	1.87	0.45
1:X:2:GLN:HB3	1:X:7:MSE:HG3	2.00	0.44
1:X:106:VAL:HA	1:X:127:ILE:O	2.18	0.44
1:X:495:ARG:NH2	3:X:1195:HOH:O	2.40	0.43

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	X	492/504 (98%)	483 (98%)	9 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	X	382/390 (98%)	372 (97%)	10 (3%)	49 50

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	X	1	MSE
1	X	45	ARG
1	X	188	GLN
1	X	249	PHE
1	X	272	ASP
1	X	290	GLU
1	X	294	GLN
1	X	362	PHE
1	X	370	GLN
1	X	495	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	X	54	GLN
1	X	119	GLN
1	X	154	GLN
1	X	175	GLN
1	X	244	GLN
1	X	294	GLN
1	X	311	ASN
1	X	317	GLN
1	X	367	ASN
1	X	368	GLN
1	X	377	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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

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.

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, 95th 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 ²)	Q<0.9
1	X	488/504 (96%)	-0.10	22 (4%) 33 32	8, 14, 22, 26	0

All (22) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	X	109	VAL	5.8
1	X	141	TYR	4.6
1	X	489	ALA	4.4
1	X	162	SER	4.4
1	X	144	PRO	3.8
1	X	166	GLY	3.7
1	X	147	ASP	3.5
1	X	119	GLN	3.4
1	X	25	ALA	3.3
1	X	123	GLY	3.0
1	X	74	LEU	2.8
1	X	347	ASN	2.7
1	X	118	PHE	2.7
1	X	370	GLN	2.7
1	X	167	LEU	2.7
1	X	106	VAL	2.6
1	X	143	PRO	2.5
1	X	142	GLY	2.5
1	X	115	ASP	2.4
1	X	71	ILE	2.2
1	X	391	PRO	2.2
1	X	146	GLU	2.0

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 carbohydrates 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, 95th 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(\AA^2)	Q<0.9
2	CA	X	999	1/1	0.98	0.07	31,31,31,31	0

6.5 Other polymers [i](#)

There are no such residues in this entry.