Full wwPDB X-ray Structure Validation Report (i)

Jun 13, 2024 – 01:25 AM EDT

PDB ID	:	3DLP
Title	:	4-Chlorobenzoyl-CoA Ligase/Synthetase, Mutant D402P, bound to 4CB
Authors	:	Wu, R.; Cao, J.; Reger, A.S.; Lu, X.; Gulick, A.M.; Dunaway-Mariano, D.
Deposited on	:	2008-06-28
Resolution	:	2.60 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 (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

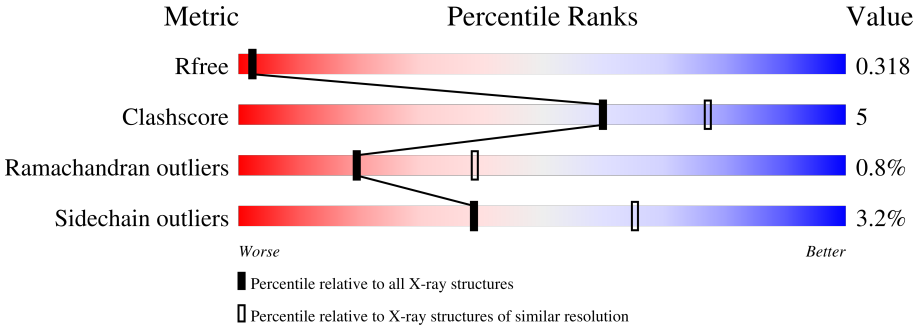
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.36.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 2.60 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	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)

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 of 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%

Mol	Chain	Length	Quality of chain
1	X	504	85% 14%

2 Entry composition (i)

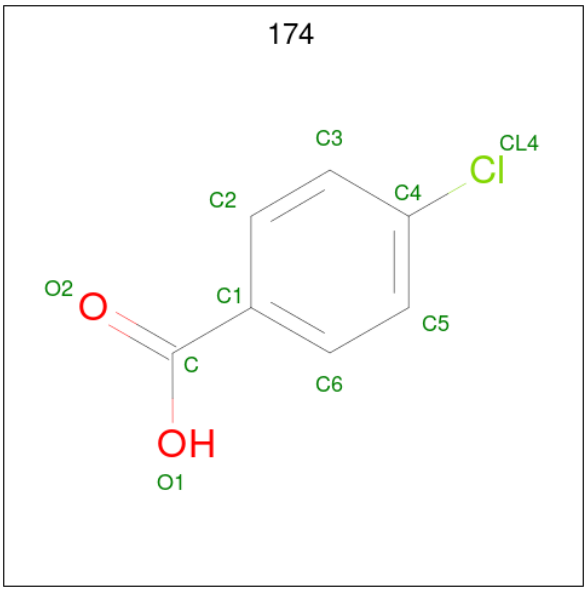
There are 3 unique types of molecules in this entry. The entry contains 3766 atoms, of which 0 are hydrogens and 0 are deuteriums.

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-Chlorobenzoate CoA Ligase/Synthetase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	X	504	3735	2363	667	692	13	0	0	0

- Molecule 2 is 4-CHLORO-BENZOIC ACID (three-letter code: 174) (formula: $C_7H_5ClO_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	Cl	O		
2	X	1	10	7	1	2	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	X	21	21	21	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. 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. 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-Chlorobenzoate CoA Ligase/Synthetase

Chain X:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α, β, γ	127.92Å 127.92Å 71.23Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	30.00 – 2.60 29.96 – 2.60	Depositor EDS
% Data completeness (in resolution range)	94.1 (30.00-2.60) 94.1 (29.96-2.60)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.26 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.206 , 0.252 0.282 , 0.318	Depositor DCC
R_{free} test set	992 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å^2)	62.4	Xtriage
Anisotropy	0.037	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 30.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.034 for -h,-k,l	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	3766	wwPDB-VP
Average B, all atoms (Å^2)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.26% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]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.

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: 174

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	0.43	2/3807 (0.1%)	0.52	0/5196

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	X	49	ASP	CG-OD1	11.89	1.52	1.25
1	X	49	ASP	C-N	5.80	1.43	1.33

There are no bond angle outliers.

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	3735	0	3709	34	0
2	X	10	0	4	1	0
3	X	21	0	0	0	0
All	All	3766	0	3713	34	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 5.

All (34) 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:109:VAL:HG12	1:X:110:GLY:H	1.34	0.92
1:X:109:VAL:HG12	1:X:110:GLY:N	2.09	0.66
1:X:444:VAL:HG23	1:X:476:PRO:HA	1.80	0.63
1:X:52:ARG:H	1:X:55:GLN:NE2	1.97	0.62
1:X:45:ARG:HD3	1:X:141:TYR:CZ	2.40	0.56
1:X:390:THR:HB	1:X:391:PRO:HD2	1.89	0.54
1:X:94:ALA:HA	1:X:117:ILE:HD13	1.90	0.52
1:X:83:LEU:HD12	1:X:159:PHE:CE1	2.44	0.52
1:X:304:TYR:HB3	1:X:313:LEU:HB2	1.92	0.51
1:X:45:ARG:HH21	1:X:132:LEU:HD23	1.75	0.51
1:X:431:VAL:HG21	1:X:493:VAL:HG21	1.93	0.50
1:X:160:TYR:CE2	1:X:170:ALA:HB2	2.47	0.49
1:X:181:ARG:HG2	1:X:310:MET:HB2	1.95	0.49
1:X:68:VAL:HG13	1:X:215:LEU:HD21	1.95	0.48
1:X:428:THR:HB	1:X:451:ARG:HG2	1.95	0.48
1:X:56:ARG:HH21	1:X:101:GLU:HB2	1.78	0.47
1:X:345:VAL:HB	1:X:349:GLU:HB2	1.95	0.47
1:X:383:THR:O	1:X:400:ARG:NH2	2.48	0.47
1:X:109:VAL:CG1	1:X:110:GLY:H	2.14	0.47
1:X:431:VAL:HG23	1:X:485:LEU:HD13	1.97	0.46
1:X:214:VAL:HG12	1:X:225:TYR:HE1	1.81	0.46
1:X:97:ILE:HG23	1:X:102:MET:HG3	1.99	0.45
1:X:401:VAL:N	1:X:402:PRO:HD2	2.32	0.45
1:X:14:ARG:NH2	1:X:222:ASP:OD2	2.43	0.44
1:X:32:HIS:O	1:X:36:ARG:HG2	2.18	0.44
1:X:413:HIS:HA	1:X:414:PRO:HD2	1.85	0.44
1:X:280:ALA:HA	1:X:303:ILE:O	2.18	0.43
1:X:113:VAL:O	1:X:117:ILE:HG22	2.19	0.42
1:X:345:VAL:C	1:X:347:ASN:H	2.22	0.42
1:X:305:GLY:HA3	2:X:909:174:C4	2.50	0.42
1:X:334:ILE:HD12	1:X:389:TRP:CD1	2.55	0.42
1:X:445:THR:HG23	1:X:478:ARG:HB3	2.01	0.41
1:X:180:SER:OG	1:X:360:SER:HB3	2.21	0.40
1:X:5:ASN:HB2	1:X:75:HIS:CD2	2.56	0.40

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	X	502/504 (100%)	471 (94%)	27 (5%)	4 (1%)	19 39

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	X	503	SER
1	X	346	ALA
1	X	165	THR
1	X	348	GLY

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	X	376/400 (94%)	364 (97%)	12 (3%)	39 65

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	X	45	ARG
1	X	99	ARG
1	X	162	SER
1	X	175	GLN
1	X	188	GLN
1	X	249	PHE
1	X	278	THR

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Mol	Chain	Res	Type
1	X	300	LYS
1	X	347	ASN
1	X	362	PHE
1	X	415	SER
1	X	502	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	X	18	HIS
1	X	55	GLN
1	X	154	GLN
1	X	175	GLN
1	X	188	GLN
1	X	242	GLN
1	X	311	ASN
1	X	491	ASN

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)

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	174	X	909	-	10,10,10	1.18	1 (10%)	13,13,13	1.18	0

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	174	X	909	-	-	0/4/4/4	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	X	909	174	C4-CL4	2.50	1.80	1.74

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	X	909	174	1	0

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)

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

6.5 Other polymers (i)

Unable to reproduce the depositors R factor - this section is therefore empty.