



Full wwPDB X-ray Structure Validation Report

Feb 27, 2014 – 04:36 PM GMT

PDB ID : 1K5Q
Title : PENICILLIN ACYLASE, MUTANT COMPLEXED WITH PAA
Authors : Hensgens, C.M.H.; Keizer, E.; Snijder, H.J.; Dijkstra, B.W.
Deposited on : 2001-10-12
Resolution : 2.34 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

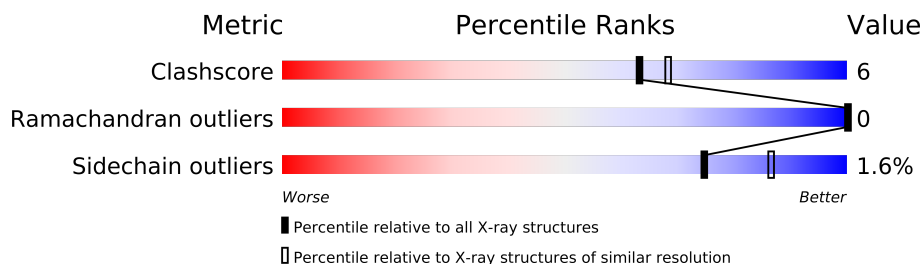
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 21963
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 2.34 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))
Clashscore	79885	1094 (2.36-2.32)
Ramachandran outliers	78287	1080 (2.36-2.32)
Sidechain outliers	78261	1081 (2.36-2.32)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	209	
2	B	557	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 6436 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 PENICILLIN G ACYLASE ALPHA SUBUNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	206	Total	C	N	O	S	0	0	0
			1657	1058	278	313	8			

- Molecule 2 is a protein called PENICILLIN G ACYLASE BETA SUBUNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	557	Total	C	N	O	S	0	0	0
			4410	2800	766	834	10			

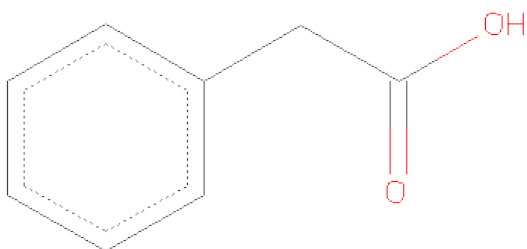
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	24	ALA	PHE	ENGINEERED	UNP P06875
B	148	LEU	VAL	ENGINEERED	UNP P06875

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Ca	0	0
			1	1		

- Molecule 4 is 2-PHENYLACETIC ACID (three-letter code: PAC) (formula: C₈H₈O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	C	O	0	0
			10	8	2		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	101	Total	O	0	0
			101	101		
5	B	257	Total	O	0	0
			257	257		

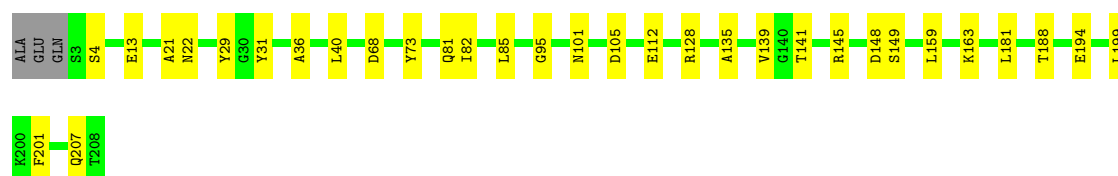
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

Note EDS was not executed.

• Molecule 1: PENICILLIN G ACYLASE ALPHA SUBUNIT

Chain A: 



• Molecule 2: PENICILLIN G ACYLASE BETA SUBUNIT

Chain B: 



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	50.76Å 63.96Å 64.24Å 72.86° 73.91° 73.50°	Depositor
Resolution (Å)	19.03 – 2.34	Depositor
% Data completeness (in resolution range)	92.9 (19.03-2.34)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.04	Depositor
Refinement program	REFMAC 5	Depositor
R, R_{free}	0.163 , 0.218	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6436	wwPDB-VP
Average B, all atoms (Å ²)	17.0	wwPDB-VP

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: CA, PAC

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	0.48	0/1699	0.71	3/2305 (0.1%)
2	B	0.50	1/4535 (0.0%)	0.74	5/6184 (0.1%)
All	All	0.49	1/6234 (0.0%)	0.73	8/8489 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	165	GLU	CD-OE2	6.88	1.33	1.25

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	68	ASP	CB-CG-OD2	6.32	123.98	118.30
1	A	148	ASP	CB-CG-OD2	6.18	123.86	118.30
2	B	13	ASP	CB-CG-OD2	6.16	123.84	118.30
2	B	542	ASP	CB-CG-OD2	6.00	123.70	118.30
2	B	403	ASP	CB-CG-OD2	5.80	123.52	118.30
2	B	523	ASP	CB-CG-OD2	5.54	123.28	118.30
2	B	381	ASP	CB-CG-OD2	5.24	123.01	118.30
1	A	105	ASP	CB-CG-OD2	5.11	122.90	118.30

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	1657	0	1604	21	0
2	B	4410	0	4240	56	0
3	B	1	0	0	0	0
4	B	10	0	7	0	0
5	A	101	0	0	1	0
5	B	257	0	0	3	0
All	All	6436	0	5851	66	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 6.

All (66) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:287:ARG:NH1	2:B:288:GLN:OE1	2.25	0.69
1:A:181:LEU:HD21	1:A:201:PHE:HB2	1.72	0.69
1:A:81:GLN:HB3	2:B:148:LEU:HD22	1.76	0.68
1:A:82:ILE:HG13	2:B:148:LEU:HD21	1.77	0.65
1:A:181:LEU:CD2	1:A:201:PHE:HB2	2.31	0.60
1:A:82:ILE:CG1	2:B:148:LEU:HD21	2.32	0.59
1:A:4:SER:HA	1:A:22:ASN:HD22	1.66	0.59
1:A:194:GLU:OE2	2:B:233:GLN:HG3	2.04	0.57
2:B:1:SER:HB3	2:B:23:GLN:H	1.69	0.57
2:B:1:SER:HB3	2:B:22:PRO:HA	1.89	0.55
2:B:67:SER:HA	2:B:178:ASN:O	2.06	0.55
2:B:250:ALA:HB2	2:B:258:TRP:CE3	2.41	0.55
2:B:318:GLN:HG3	5:B:737:HOH:O	2.07	0.55
2:B:82:LEU:HD11	2:B:136:ALA:HB2	1.89	0.53
2:B:526:LYS:HA	2:B:526:LYS:HE2	1.91	0.53
2:B:42:TYR:CZ	2:B:159:LYS:HE3	2.44	0.52
2:B:401:GLN:HA	2:B:401:GLN:NE2	2.23	0.52
2:B:1:SER:CB	2:B:22:PRO:HA	2.40	0.51
2:B:315:PRO:HA	2:B:318:GLN:CG	2.40	0.51
1:A:159:LEU:HD11	1:A:163:LYS:HE3	1.92	0.50
2:B:74:ASP:OD1	2:B:75:VAL:HG23	2.11	0.50
2:B:314:ASP:O	2:B:317:ARG:HB3	2.12	0.49
2:B:517:VAL:HG13	2:B:521:TYR:CB	2.43	0.48
1:A:101:ASN:ND2	1:A:128:ARG:HG3	2.28	0.48
2:B:22:PRO:HG3	2:B:57:PHE:CZ	2.48	0.48
2:B:44:VAL:HG11	2:B:158:MET:HB3	1.96	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:359:VAL:HG22	2:B:413:LEU:HD13	1.95	0.47
2:B:83:SER:HB2	2:B:96:TRP:CH2	2.49	0.47
2:B:132:THR:HG22	2:B:133:THR:H	1.80	0.47
1:A:85:LEU:HD22	2:B:152:LEU:HD11	1.97	0.46
2:B:486:ILE:N	2:B:486:ILE:HD12	2.31	0.45
2:B:16:ALA:HB2	2:B:186:GLY:HA2	1.99	0.45
2:B:472:HIS:HB3	5:B:626:HOH:O	2.16	0.45
1:A:29:TYR:HA	1:A:95:GLY:O	2.17	0.44
2:B:300:LEU:HB3	2:B:301:PRO:HD3	1.99	0.44
1:A:207:GLN:HA	2:B:215:TRP:CZ2	2.53	0.44
1:A:135:ALA:O	1:A:139:VAL:HG23	2.18	0.44
2:B:18:MET:O	2:B:485:MET:HA	2.17	0.44
2:B:520:HIS:NE2	2:B:548:GLU:OE2	2.51	0.44
2:B:274:LYS:HE2	2:B:277:LEU:HG	1.99	0.44
1:A:13:GLU:HB2	5:A:249:HOH:O	2.17	0.43
2:B:414:PHE:HD1	2:B:422:VAL:HG21	1.84	0.43
2:B:156:HIS:HD2	5:B:601:HOH:O	2.01	0.43
2:B:26:TRP:CE2	2:B:452:LEU:HD11	2.53	0.43
2:B:517:VAL:HG13	2:B:521:TYR:HB3	2.00	0.43
2:B:214:LYS:HG2	2:B:214:LYS:O	2.19	0.43
2:B:452:LEU:HB2	2:B:476:TYR:HA	2.01	0.43
2:B:287:ARG:HA	2:B:531:PHE:CE1	2.54	0.42
2:B:270:LEU:HD12	2:B:285:VAL:HG13	2.01	0.42
2:B:358:THR:HB	2:B:413:LEU:HB3	2.02	0.42
2:B:326:TRP:CD2	2:B:328:GLY:HA2	2.54	0.42
2:B:388:ASN:OD1	2:B:389:ILE:N	2.52	0.42
1:A:199:LEU:HG	2:B:225:MET:HE2	2.02	0.42
2:B:333:ASN:ND2	2:B:340:GLN:HG2	2.34	0.42
1:A:199:LEU:HG	2:B:225:MET:CE	2.49	0.42
2:B:319:LEU:O	2:B:322:THR:HB	2.20	0.41
2:B:100:LEU:HB2	2:B:120:ARG:HB3	2.02	0.41
1:A:141:THR:O	1:A:145:ARG:HB2	2.19	0.41
1:A:149:SER:HB3	2:B:253:LEU:HD11	2.02	0.41
1:A:188:THR:HA	2:B:243:SER:O	2.21	0.41
1:A:21:ALA:O	2:B:39:GLY:HA3	2.21	0.41
2:B:333:ASN:HD21	2:B:340:GLN:HA	1.86	0.40
1:A:36:ALA:O	1:A:40:LEU:HB2	2.20	0.40
2:B:303:LEU:HD21	2:B:350:TRP:CE2	2.57	0.40
2:B:348:ASN:ND2	2:B:374:SER:OG	2.54	0.40
2:B:387:LEU:HA	2:B:387:LEU:HD12	1.82	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	204/209 (98%)	197 (97%)	7 (3%)	0	100	100
2	B	555/557 (100%)	543 (98%)	12 (2%)	0	100	100
All	All	759/766 (99%)	740 (98%)	19 (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	A	178/180 (99%)	175 (98%)	3 (2%)	73	85
2	B	459/459 (100%)	452 (98%)	7 (2%)	76	88
All	All	637/639 (100%)	627 (98%)	10 (2%)	75	86

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

Mol	Chain	Res	Type
1	A	31	TYR
1	A	73	TYR
1	A	112	GLU
2	B	20	ASN
2	B	134	GLN
2	B	154	TRP
2	B	173	GLN
2	B	387	LEU
2	B	534	LYS
2	B	541	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	22	ASN
1	A	120	ASN
2	B	110	ASN
2	B	134	GLN
2	B	156	HIS
2	B	168	GLN
2	B	273	GLN
2	B	292	GLN
2	B	304	GLN
2	B	330	ASN
2	B	333	ASN
2	B	348	ASN
2	B	401	GLN
2	B	472	HIS
2	B	541	GLN
2	B	546	HIS

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

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	$\# Z > 2$
4	PAC	B	559	-	10,10,10	1.27	2 (20%)	12,12,12	1.04	1 (8%)

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
4	PAC	B	559	-	-	0/4/4/4	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	559	PAC	O1-C1	3.23	1.33	1.22
4	B	559	PAC	O2-C1	-2.25	1.22	1.30

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	559	PAC	O2-C1-C2	2.13	119.14	113.80

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

EDS was not executed - this section will therefore be empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates

EDS was not executed - this section will therefore be empty.

6.4 Ligands

EDS was not executed - this section will therefore be empty.

6.5 Other polymers

EDS was not executed - this section will therefore be empty.