Full wwPDB X-ray Structure Validation Report (i)

Aug 6, 2023 – 08:32 PM EDT

PDB ID	:	1JX9
Title	:	Penicillin Acylase, mutant
Authors	:	Hensgens, C.M.H.; Keizer, E.; Snijder, H.J.; Dijkstra, B.W.
Deposited on	:	2001-09-06
Resolution	:	2.28 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:

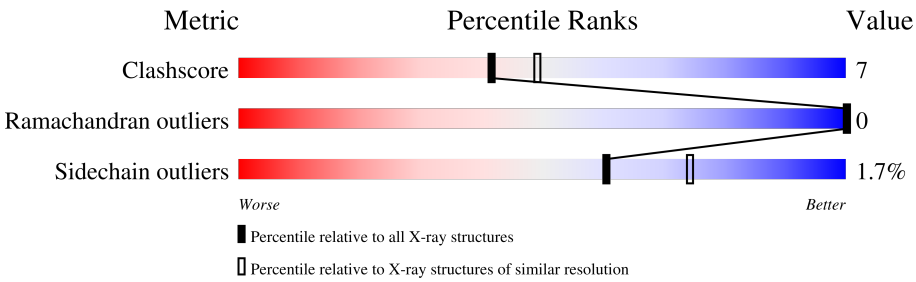
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

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 2.28 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	141614	7711 (2.30-2.26)
Ramachandran outliers	138981	7597 (2.30-2.26)
Sidechain outliers	138945	7598 (2.30-2.26)

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%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	209	84% 14% •
2	B	557	83% 16% •

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 6484 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 penicillin G acylase alpha subunit.

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

- Molecule 2 is a protein called penicillin G acylase beta subunit.

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

There are 2 discrepancies between the modelled and reference sequences:

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

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

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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	109	109	109	0	0
4	B	307	Total	O	0	0
			307	307		

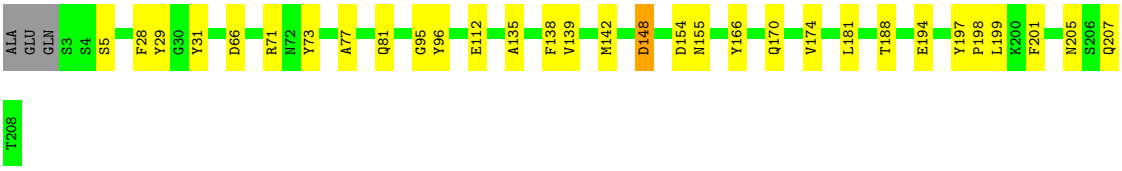
3 Residue-property plots (i)

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.

Note EDS was not executed.

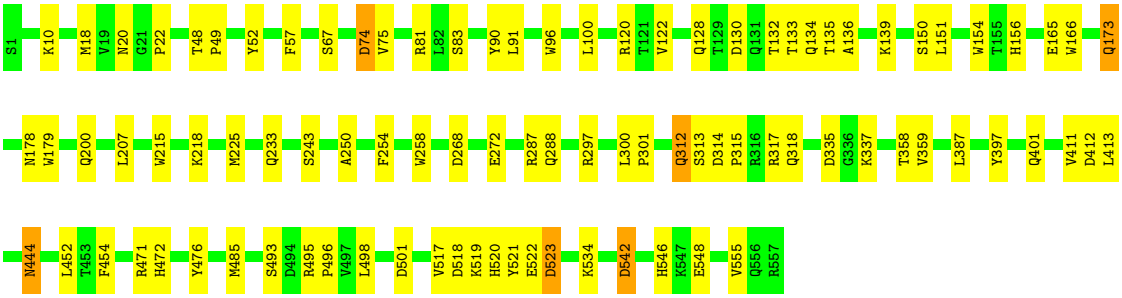
• Molecule 1: penicillin G acylase alpha subunit

Chain A:



• Molecule 2: penicillin G acylase beta subunit

Chain B:



4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	50.59Å 63.97Å 64.02Å 72.61° 74.09° 73.68°	Depositor
Resolution (Å)	29.88 – 2.28	Depositor
% Data completeness (in resolution range)	100.0 (29.88-2.28)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
Refinement program	REFMAC 5.0, CNS	Depositor
R, R_{free}	0.166 , 0.223	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6484	wwPDB-VP
Average B, all atoms (Å^2)	19.0	wwPDB-VP

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	A	0.55	0/1699	0.77	3/2305 (0.1%)
2	B	0.54	1/4535 (0.0%)	0.79	8/6184 (0.1%)
All	All	0.55	1/6234 (0.0%)	0.78	11/8489 (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	5.33	1.31	1.25

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	542	ASP	CB-CG-OD2	6.59	124.23	118.30
2	B	74	ASP	CB-CG-OD2	6.20	123.88	118.30
2	B	523	ASP	CB-CG-OD2	6.06	123.75	118.30
1	A	66	ASP	CB-CG-OD2	5.97	123.68	118.30
2	B	412	ASP	CB-CG-OD2	5.81	123.53	118.30
1	A	148	ASP	CB-CG-OD2	5.70	123.43	118.30
2	B	518	ASP	CB-CG-OD2	5.63	123.37	118.30
2	B	501	ASP	CB-CG-OD2	5.31	123.08	118.30
2	B	130	ASP	CB-CG-OD2	5.24	123.02	118.30
2	B	335	ASP	CB-CG-OD2	5.14	122.92	118.30
1	A	154	ASP	CB-CG-OD2	5.08	122.87	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	A	1657	0	1604	30	0
2	B	4410	0	4240	70	0
3	B	1	0	0	0	0
4	A	109	0	0	2	0
4	B	307	0	0	12	0
All	All	6484	0	5844	83	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 7.

All (83) 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:A:199:LEU:HG	2:B:225:MET:HE1	1.43	1.00
1:A:142:MET:SD	4:B:895:HOH:O	2.22	0.96
1:A:199:LEU:HG	2:B:225:MET:CE	1.96	0.94
2:B:337:LYS:HD3	4:B:626:HOH:O	1.76	0.85
1:A:181:LEU:HD21	1:A:201:PHE:HB2	1.63	0.81
2:B:287:ARG:NH1	2:B:288:GLN:OE1	2.15	0.79
1:A:199:LEU:CG	2:B:225:MET:CE	2.67	0.73
1:A:199:LEU:HD11	2:B:225:MET:HE2	1.73	0.70
1:A:199:LEU:CG	2:B:225:MET:HE1	2.21	0.69
1:A:194:GLU:OE2	2:B:233:GLN:HG3	1.94	0.67
2:B:471:ARG:HH22	2:B:522:GLU:CD	2.00	0.65
2:B:337:LYS:HE2	4:B:655:HOH:O	1.95	0.65
2:B:268:ASP:O	2:B:272:GLU:HG3	1.97	0.64
2:B:444:ASN:C	2:B:444:ASN:HD22	2.00	0.64
2:B:337:LYS:CD	4:B:626:HOH:O	2.42	0.63
1:A:5:SER:HB2	2:B:555:VAL:O	2.00	0.62
2:B:318:GLN:CD	4:B:872:HOH:O	2.41	0.58
1:A:199:LEU:CD1	2:B:225:MET:HE2	2.33	0.58
2:B:18:MET:O	2:B:485:MET:HA	2.04	0.57
1:A:181:LEU:CD2	1:A:201:PHE:HB2	2.34	0.57
2:B:314:ASP:O	2:B:317:ARG:HB3	2.05	0.57
2:B:315:PRO:HA	2:B:318:GLN:HG2	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:318:GLN:HB3	4:B:872:HOH:O	2.06	0.55
2:B:318:GLN:NE2	4:B:872:HOH:O	2.38	0.55
1:A:166:TYR:HB3	1:A:170:GLN:HB3	1.88	0.55
2:B:517:VAL:HG13	2:B:521:TYR:CB	2.38	0.54
1:A:71:ARG:NH1	2:B:128:GLN:HG2	2.23	0.53
2:B:359:VAL:HG22	2:B:413:LEU:HD13	1.90	0.53
2:B:493:SER:HB2	2:B:498:LEU:HD11	1.91	0.53
1:A:29:TYR:HA	1:A:95:GLY:O	2.09	0.53
2:B:132:THR:HG21	2:B:134:GLN:HE21	1.75	0.52
2:B:150:SER:HB3	2:B:173:GLN:OE1	2.10	0.51
1:A:199:LEU:CG	2:B:225:MET:HE2	2.41	0.51
1:A:188:THR:HA	2:B:243:SER:O	2.12	0.50
1:A:142:MET:CE	4:B:895:HOH:O	2.56	0.50
1:A:174:VAL:HG22	2:B:411:VAL:HG22	1.94	0.50
2:B:132:THR:HG22	2:B:133:THR:H	1.76	0.50
2:B:300:LEU:HB3	2:B:301:PRO:HD3	1.94	0.49
2:B:297:ARG:HD2	4:B:908:HOH:O	2.11	0.49
2:B:135:THR:HG22	2:B:136:ALA:N	2.27	0.49
2:B:495:ARG:NH1	2:B:542:ASP:OD1	2.47	0.48
2:B:542:ASP:O	2:B:546:HIS:HD2	1.96	0.48
2:B:471:ARG:NH2	2:B:522:GLU:CD	2.67	0.48
2:B:90:TYR:OH	2:B:122:VAL:HG23	2.15	0.47
2:B:100:LEU:HD12	2:B:120:ARG:HD3	1.96	0.47
2:B:517:VAL:HG13	2:B:521:TYR:HB3	1.96	0.46
1:A:148:ASP:OD2	2:B:139:LYS:NZ	2.45	0.46
2:B:444:ASN:C	2:B:444:ASN:ND2	2.68	0.45
2:B:81:ARG:HE	2:B:91:LEU:HD22	1.82	0.45
2:B:397:TYR:O	2:B:401:GLN:HG2	2.16	0.45
1:A:135:ALA:O	1:A:139:VAL:HG23	2.16	0.45
2:B:452:LEU:HB2	2:B:476:TYR:HA	1.98	0.45
2:B:523:ASP:OD1	2:B:523:ASP:N	2.50	0.45
2:B:519:LYS:HG3	2:B:520:HIS:CD2	2.52	0.45
1:A:170:GLN:HB2	4:A:298:HOH:O	2.16	0.44
2:B:132:THR:CG2	2:B:134:GLN:NE2	2.79	0.44
1:A:155:ASN:OD1	2:B:254:PHE:HB3	2.18	0.44
1:A:138:PHE:HA	2:B:52:TYR:CE1	2.53	0.43
2:B:151:LEU:HD23	2:B:151:LEU:C	2.39	0.43
2:B:156:HIS:HD2	4:B:653:HOH:O	2.01	0.43
1:A:71:ARG:NH2	4:A:247:HOH:O	2.49	0.43
1:A:207:GLN:HA	2:B:215:TRP:CZ2	2.53	0.43
1:A:28:PHE:O	1:A:96:TYR:HA	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:22:PRO:HG3	2:B:57:PHE:CZ	2.52	0.43
1:A:77:ALA:O	1:A:81:GLN:HG3	2.19	0.42
2:B:74:ASP:OD1	2:B:75:VAL:HG23	2.19	0.42
2:B:312:GLN:HG3	2:B:313:SER:N	2.34	0.42
2:B:454:PHE:HB2	2:B:471:ARG:HB2	2.02	0.42
2:B:200:GLN:NE2	2:B:218:LYS:HG2	2.33	0.42
2:B:67:SER:HA	2:B:178:ASN:O	2.20	0.42
2:B:250:ALA:HB2	2:B:258:TRP:CE3	2.55	0.42
2:B:358:THR:HB	2:B:413:LEU:HB3	2.02	0.42
2:B:472:HIS:HB3	4:B:721:HOH:O	2.19	0.42
1:A:197:TYR:HA	1:A:198:PRO:HD3	1.84	0.41
2:B:312:GLN:HE21	2:B:312:GLN:HB2	1.60	0.41
2:B:10:LYS:HE3	2:B:10:LYS:HB3	1.92	0.41
2:B:166:TRP:CH2	2:B:179:TRP:HB3	2.55	0.41
2:B:337:LYS:HB2	4:B:655:HOH:O	2.20	0.41
1:A:166:TYR:O	1:A:170:GLN:HB2	2.21	0.41
2:B:48:THR:HA	2:B:49:PRO:HD3	1.96	0.41
1:A:205:ASN:HB2	2:B:207:LEU:HD12	2.02	0.40
2:B:83:SER:HB2	2:B:96:TRP:CH2	2.57	0.40
2:B:495:ARG:HA	2:B:496:PRO:HD3	1.86	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	A	204/209 (98%)	199 (98%)	5 (2%)	0	100	100
2	B	555/557 (100%)	544 (98%)	11 (2%)	0	100	100
All	All	759/766 (99%)	743 (98%)	16 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	A	178/180 (99%)	175 (98%)	3 (2%)	60	74
2	B	459/459 (100%)	451 (98%)	8 (2%)	60	74
All	All	637/639 (100%)	626 (98%)	11 (2%)	60	74

All (11) 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	154	TRP
2	B	173	GLN
2	B	312	GLN
2	B	387	LEU
2	B	444	ASN
2	B	534	LYS
2	B	548	GLU

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

Mol	Chain	Res	Type
2	B	110	ASN
2	B	134	GLN
2	B	156	HIS
2	B	233	GLN
2	B	273	GLN
2	B	292	GLN
2	B	312	GLN
2	B	318	GLN
2	B	444	ASN
2	B	472	HIS
2	B	546	HIS

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)

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)

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates (i)

EDS was not executed - this section is therefore empty.

6.4 Ligands (i)

EDS was not executed - this section is therefore empty.

6.5 Other polymers (i)

EDS was not executed - this section is therefore empty.