



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 06:59 PM GMT

PDB ID : 1DJP
Title : CRYSTAL STRUCTURE OF PSEUDOMONAS 7A GLUTAMINASE-ASP
ARAGINASE WITH THE INHIBITOR DON COVALENTLY BOUND IN
THE ACTIVE SITE
Authors : Ortlund, E.; Lacount, M.W.; Lewinski, K.; Lebioda, L.
Deposited on : 1999-12-03
Resolution : 1.90 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
<http://wwpdb.org/validation/2016/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
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

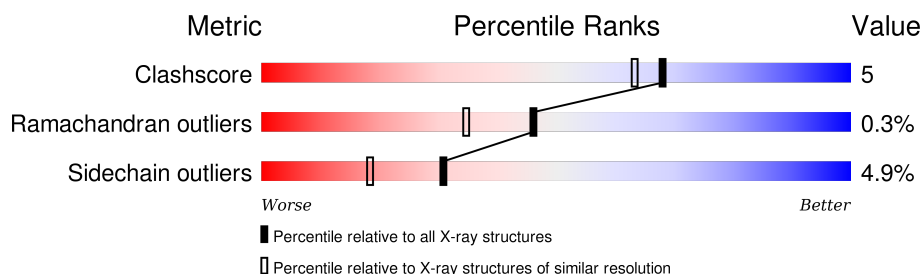
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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	102246	5398 (1.90-1.90)
Ramachandran outliers	100387	5338 (1.90-1.90)
Sidechain outliers	100360	5339 (1.90-1.90)

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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	330	 84% 15% •
1	B	330	 88% 12% •

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 5201 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.

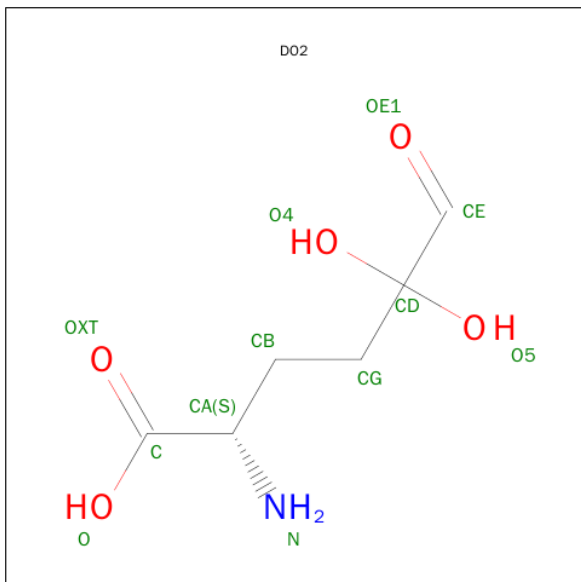
- Molecule 1 is a protein called GLUTAMINASE-ASPARAGINASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	330	Total	C	N	O	S	0	0	0
			2485	1550	440	487	8			
1	B	330	Total	C	N	O	S	0	0	0
			2485	1550	440	487	8			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1111	ASN	ASP	SEE REMARK 999	UNP P10182
A	1113	VAL	THR	SEE REMARK 999	UNP P10182
A	1114	GLN	LEU	SEE REMARK 999	UNP P10182
A	1115	LYS	ASN	SEE REMARK 999	UNP P10182
A	1263	VAL	LEU	SEE REMARK 999	UNP P10182
A	1264	VAL	THR	SEE REMARK 999	UNP P10182
A	1269	GLN	THR	SEE REMARK 999	UNP P10182
A	1273	ASN	THR	SEE REMARK 999	UNP P10182
A	1317	ALA	VAL	SEE REMARK 999	UNP P10182
A	1318	MET	GLU	SEE REMARK 999	UNP P10182
A	1319	VAL	LEU	SEE REMARK 999	UNP P10182
A	1322	THR	VAL	SEE REMARK 999	UNP P10182
B	3111	ASN	ASP	SEE REMARK 999	UNP P10182
B	3113	VAL	THR	SEE REMARK 999	UNP P10182
B	3114	GLN	LEU	SEE REMARK 999	UNP P10182
B	3115	LYS	ASN	SEE REMARK 999	UNP P10182
B	3263	VAL	LEU	SEE REMARK 999	UNP P10182
B	3264	VAL	THR	SEE REMARK 999	UNP P10182
B	3269	GLN	THR	SEE REMARK 999	UNP P10182
B	3273	ASN	THR	SEE REMARK 999	UNP P10182
B	3317	ALA	VAL	SEE REMARK 999	UNP P10182
B	3318	MET	GLU	SEE REMARK 999	UNP P10182
B	3319	VAL	LEU	SEE REMARK 999	UNP P10182
B	3322	THR	VAL	SEE REMARK 999	UNP P10182

- Molecule 2 is 5,5-DIHYDROXY-6-OXO-L-NORLEUCINE (three-letter code: DO2) (formula: $C_6H_{11}NO_5$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			10	6	1	3		
2	B	1	Total	C	N	O	0	0
			10	6	1	3		

- Molecule 3 is water.

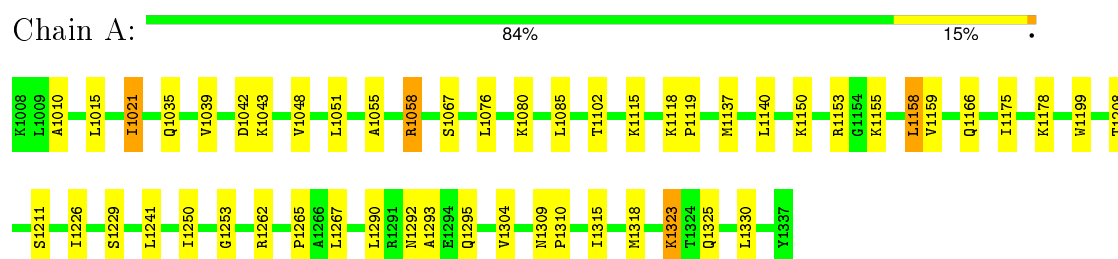
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	102	Total	O	0	0
			102	102		
3	B	109	Total	O	0	0
			109	109		

3 Residue-property plots

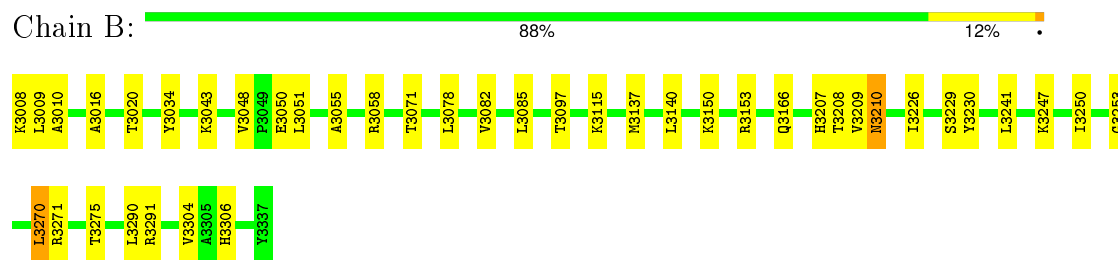
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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: GLUTAMINASE-ASPARAGINASE



• Molecule 1: GLUTAMINASE-ASPARAGINASE



4 Data and refinement statistics

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

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	78.51Å 135.91Å 137.58Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.35 – 1.90	Depositor
% Data completeness (in resolution range)	80.7 (48.35-1.90)	Depositor
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS 0.9	Depositor
R, R_{free}	0.189 , 0.228	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	5201	wwPDB-VP
Average B, all atoms (Å ²)	23.0	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: DO2

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	0.34	0/2520	0.62	1/3413 (0.0%)
1	B	0.35	0/2520	0.63	0/3413
All	All	0.34	0/5040	0.63	1/6826 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1158	LEU	CA-CB-CG	5.39	127.69	115.30

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	2485	0	2503	24	0
1	B	2485	0	2503	25	0
2	A	10	0	8	0	0
2	B	10	0	7	5	0
3	A	102	0	0	1	0
3	B	109	0	0	0	0
All	All	5201	0	5021	47	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 (47) 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:1159:VAL:HG22	1:A:1166:GLN:HB2	1.64	0.78
1:A:1039:VAL:HG13	1:A:1043:LYS:HD3	1.67	0.76
1:A:1021:ILE:H	1:A:1021:ILE:HD12	1.62	0.64
1:B:3150:LYS:HE2	1:B:3153:ARG:NH2	2.12	0.63
1:B:3207:HIS:H	1:B:3210:ASN:ND2	1.95	0.63
1:A:1150:LYS:HD2	1:A:1153:ARG:HD2	1.82	0.60
1:A:1323:LYS:NZ	1:A:1323:LYS:HB3	2.17	0.59
1:A:1058:ARG:HB2	1:A:1058:ARG:HH21	1.69	0.56
1:B:3304:VAL:HG12	1:B:3306:HIS:H	1.69	0.56
1:A:1229:SER:HB3	1:A:1253:GLY:HA2	1.86	0.56
1:B:3043:LYS:HD3	1:B:3043:LYS:O	2.06	0.55
1:B:3010:ALA:O	1:B:3055:ALA:HB1	2.07	0.55
1:B:3034:TYR:CE2	2:B:4001:DO2:HG	2.40	0.55
1:A:1048:VAL:O	1:A:1051:LEU:HB2	2.06	0.55
1:B:3034:TYR:CE2	2:B:4001:DO2:CG	2.88	0.55
1:B:3229:SER:HB3	1:B:3253:GLY:HA2	1.90	0.53
1:B:3048:VAL:O	1:B:3051:LEU:HB2	2.08	0.52
1:A:1010:ALA:O	1:A:1055:ALA:HB1	2.09	0.52
1:A:1226:ILE:HG12	1:A:1250:ILE:HB	1.92	0.51
1:B:3078:LEU:O	1:B:3082:VAL:HG23	2.12	0.50
1:B:3016:ALA:HA	1:B:3097:THR:OG1	2.13	0.49
1:B:3020:THR:CB	2:B:4001:DO2:OE1	2.57	0.48
1:B:3226:ILE:HG12	1:B:3250:ILE:HB	1.97	0.47
1:B:3291:ARG:HA	1:B:3304:VAL:HG21	1.97	0.46
1:B:3008:LYS:HG2	1:B:3009:LEU:H	1.82	0.45
1:A:1115:LYS:HE2	1:A:1211:SER:O	2.17	0.45
1:A:1155:LYS:HD3	1:A:1199:TRP:CZ3	2.52	0.45
1:A:1315:ILE:HD13	1:A:1318:MET:CE	2.46	0.45
1:B:3048:VAL:HB	1:B:3051:LEU:HD22	2.00	0.44
1:A:1175:ILE:HG21	1:A:1178:LYS:HE2	1.98	0.44
1:A:1021:ILE:H	1:A:1021:ILE:CD1	2.24	0.43
1:A:1290:LEU:HD23	1:A:1293:ALA:HB2	2.00	0.43
1:B:3207:HIS:H	1:B:3210:ASN:HD21	1.63	0.42
1:A:1262:ARG:NH1	1:B:3071:THR:HG23	2.34	0.42
1:B:3020:THR:HB	2:B:4001:DO2:OE1	2.20	0.42
1:A:1292:ASN:HA	1:A:1295:GLN:O	2.19	0.42
1:B:3034:TYR:HE2	2:B:4001:DO2:CG	2.32	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1265:PRO:HG2	3:A:307:HOH:O	2.20	0.41
1:A:1067:SER:HB2	1:A:1102:THR:OG1	2.21	0.41
1:A:1076:LEU:O	1:A:1080:LYS:HG3	2.21	0.41
1:B:3271:ARG:HA	1:B:3275:THR:O	2.21	0.41
1:A:1309:ASN:HB2	1:A:1310:PRO:CD	2.51	0.41
1:B:3270:LEU:HA	1:B:3270:LEU:HD12	1.91	0.41
1:B:3050:GLU:H	1:B:3050:GLU:CD	2.24	0.41
1:B:3137:MET:N	1:B:3137:MET:SD	2.91	0.40
1:A:1226:ILE:HD12	1:B:3230:TYR:CD1	2.57	0.40
1:A:1118:LYS:HA	1:A:1119:PRO:HD3	1.96	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	328/330 (99%)	317 (97%)	10 (3%)	1 (0%)	46	35
1	B	328/330 (99%)	319 (97%)	8 (2%)	1 (0%)	46	35
All	All	656/660 (99%)	636 (97%)	18 (3%)	2 (0%)	46	35

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1208	THR
1	B	3208	THR

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	265/265 (100%)	250 (94%)	15 (6%)	25	13
1	B	265/265 (100%)	254 (96%)	11 (4%)	36	24
All	All	530/530 (100%)	504 (95%)	26 (5%)	31	18

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1015	LEU
1	A	1021	ILE
1	A	1035	GLN
1	A	1042	ASP
1	A	1058	ARG
1	A	1085	LEU
1	A	1137	MET
1	A	1140	LEU
1	A	1158	LEU
1	A	1241	LEU
1	A	1267	LEU
1	A	1304	VAL
1	A	1323	LYS
1	A	1325	GLN
1	A	1330	LEU
1	B	3058	ARG
1	B	3085	LEU
1	B	3115	LYS
1	B	3140	LEU
1	B	3166	GLN
1	B	3209	VAL
1	B	3210	ASN
1	B	3241	LEU
1	B	3247	LYS
1	B	3270	LEU
1	B	3290	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1035	GLN

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Mol	Chain	Res	Type
1	A	1149	ASN
1	A	1166	GLN
1	A	1244	ASN
1	A	1269	GLN
1	A	1273	ASN
1	A	1285	GLN
1	A	1306	HIS
1	B	3166	GLN
1	B	3210	ASN
1	B	3217	GLN
1	B	3223	GLN
1	B	3269	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](#)

2 ligands are 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	DO2	A	4000	1	6,9,11	0.47	0	3,10,15	1.71	1 (33%)
2	DO2	B	4001	1	6,9,11	0.48	0	3,10,15	1.84	1 (33%)

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	DO2	A	4000	1	-	0/4/9/13	0/0/0/0
2	DO2	B	4001	1	-	0/4/9/13	0/0/0/0

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	4001	DO2	CB-CG-CD	-2.97	109.58	114.53
2	A	4000	DO2	CB-CG-CD	-2.73	109.99	114.53

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	4001	DO2	5	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 ⓘ

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.