



# wwPDB X-ray Structure Validation Summary Report

Feb 27, 2014 – 04:07 PM GMT

PDB ID : 1JSL  
Title : Crystal structure of Erwinia chrysanthemi L-asparaginase complexed with 6-HYDROXY-D-NORLEUCINE  
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Deposited on : 2001-08-17  
Resolution : 1.70 Å(reported)

This is a wwPDB validation summary report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

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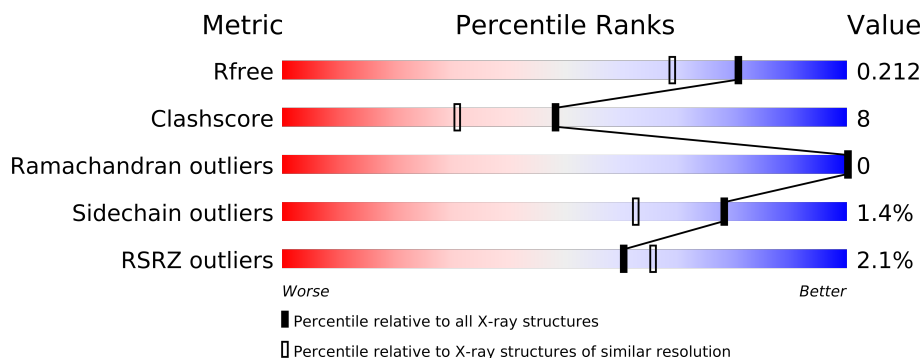
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.15 2013
Xtriage (Phenix)	:	dev-1323
EDS	:	stable22639
Percentile statistics	:	21963
Refmac	:	5.8.0049
CCP4	:	6.3.0 (Settle)
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 1.70 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))
$R_{free}$	66092	2456 (1.70-1.70)
Clashscore	79885	2929 (1.70-1.70)
Ramachandran outliers	78287	2878 (1.70-1.70)
Sidechain outliers	78261	2878 (1.70-1.70)
RSRZ outliers	66119	2456 (1.70-1.70)

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  $\geq 3$ , 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.

Mol	Chain	Length	Quality of chain
1	A	327	
1	B	327	
1	C	327	
1	D	327	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
3	1PE	A	2501	-	X
4	GOL	C	2603	-	X
4	GOL	D	2602	-	X

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 11215 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.

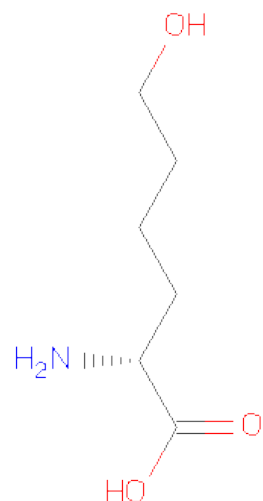
- Molecule 1 is a protein called L-asparaginase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	324	Total	C	N	O	S	0	9	0
			2510	1578	440	482	10			
1	B	324	Total	C	N	O	S	0	8	0
			2503	1570	438	486	9			
1	C	324	Total	C	N	O	S	0	6	0
			2492	1564	440	479	9			
1	D	324	Total	C	N	O	S	0	4	0
			2472	1551	435	477	9			

There are 16 discrepancies between the modelled and reference sequences:

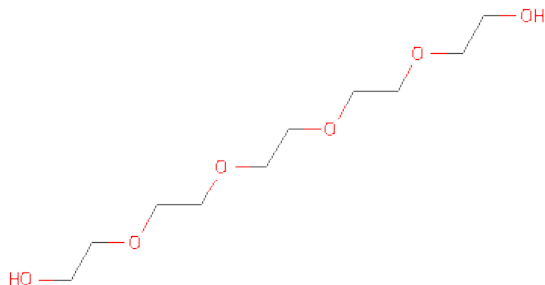
Chain	Residue	Modelled	Actual	Comment	Reference
A	156	ILE	LEU	VARIANT	UNP P06608
A	178	ARG	LYS	VARIANT	UNP P06608
A	267	LEU	MET	VARIANT	UNP P06608
A	274	MET	ILE	VARIANT	UNP P06608
B	156	ILE	LEU	VARIANT	UNP P06608
B	178	ARG	LYS	VARIANT	UNP P06608
B	267	LEU	MET	VARIANT	UNP P06608
B	274	MET	ILE	VARIANT	UNP P06608
C	156	ILE	LEU	VARIANT	UNP P06608
C	178	ARG	LYS	VARIANT	UNP P06608
C	267	LEU	MET	VARIANT	UNP P06608
C	274	MET	ILE	VARIANT	UNP P06608
D	156	ILE	LEU	VARIANT	UNP P06608
D	178	ARG	LYS	VARIANT	UNP P06608
D	267	LEU	MET	VARIANT	UNP P06608
D	274	MET	ILE	VARIANT	UNP P06608

- Molecule 2 is 6-HYDROXY-D-NORLEUCINE (three-letter code: DDO) (formula: C<sub>6</sub>H<sub>13</sub>NO<sub>3</sub>).



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		
2	C	1	Total	C	N	O	0	0
			10	6	1	3		
2	D	1	Total	C	N	O	0	0
			10	6	1	3		

- Molecule 3 is PENTAETHYLENE GLYCOL (three-letter code: 1PE) (formula: C<sub>10</sub>H<sub>22</sub>O<sub>6</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			16	10	6		

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	C	1	Total	C	O	0	0
			6	3	3		
4	D	1	Total	C	O	0	0
			6	3	3		
4	C	1	Total	C	O	0	0
			6	3	3		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	297	Total	O	0	1
			299	299		
5	B	273	Total	O	0	0
			273	273		
5	C	296	Total	O	0	0
			296	296		
5	D	293	Total	O	0	2
			296	296		



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	106.15Å 90.39Å 127.37Å 90.00° 91.38° 90.00°	Depositor
Resolution (Å)	20.00 – 1.70 19.95 – 1.70	Depositor EDS
% Data completeness (in resolution range)	(Not available) (20.00-1.70) 86.6 (19.95-1.70)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	0.08	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.14 (at 1.69Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.186 , 0.212 0.186 , 0.212	Depositor DCC
$R_{free}$ test set	1368 reflections (1.19%)	DCC
Wilson B-factor (Å <sup>2</sup> )	15.1	Xtriage
Anisotropy	0.660	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.43 , 46.6	EDS
Estimated twinning fraction	0.019 for -h,-k,l	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 122183 reflections	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	11215	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	19.0	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.*

<sup>1</sup>Intensities estimated from amplitudes.

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, DDO, 1PE

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	0.31	0/2546	0.63	1/3454 (0.0%)
1	B	0.31	0/2539	0.64	1/3443 (0.0%)
1	C	0.31	0/2528	0.64	0/3429
1	D	0.31	0/2508	0.64	1/3400 (0.0%)
All	All	0.31	0/10121	0.64	3/13726 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	284	VAL	N-CA-C	-5.45	96.28	111.00
1	B	284	VAL	N-CA-C	-5.22	96.90	111.00
1	A	284	VAL	N-CA-C	-5.01	97.48	111.00

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	2510	0	2558	62	0
1	B	2503	0	2535	44	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	2492	0	2534	28	0
1	D	2472	0	2513	27	0
2	A	10	0	10	3	0
2	B	10	0	10	1	0
2	C	10	0	10	0	0
2	D	10	0	10	1	0
3	A	16	0	22	7	0
4	C	12	0	14	1	0
4	D	6	0	7	1	0
5	A	299	0	0	8	0
5	B	273	0	0	6	0
5	C	296	0	0	3	0
5	D	296	0	0	4	0
All	All	11215	0	10223	159	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 8.

The worst 5 of 159 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:A:2401:DDO:HE1	5:A:2508[C]:HOH:O	1.30	1.27
1:A:153:MET:HB3	1:A:160[B]:ILE:HD11	1.17	1.15
1:A:43[B]:VAL:HB	1:A:136[B]:LEU:HD11	1.49	0.94
1:A:243:LYS:HZ3	3:A:2501:1PE:H131	1.33	0.93
1:A:153:MET:CB	1:A:160[B]:ILE:HD11	2.02	0.90

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	331/327 (101%)	324 (98%)	7 (2%)	0	100	100
1	B	330/327 (101%)	323 (98%)	7 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	327/327 (100%)	320 (98%)	7 (2%)	0	100	100
1	D	326/327 (100%)	320 (98%)	6 (2%)	0	100	100
All	All	1314/1308 (100%)	1287 (98%)	27 (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	271/264 (103%)	268 (99%)	3 (1%)	84	72
1	B	270/264 (102%)	262 (97%)	8 (3%)	53	29
1	C	268/264 (102%)	264 (98%)	4 (2%)	76	60
1	D	266/264 (101%)	265 (100%)	1 (0%)	95	92
All	All	1075/1056 (102%)	1059 (98%)	16 (2%)	78	60

5 of 16 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	136	LEU
1	B	145	LYS
1	C	4[B]	LEU
1	B	80	LEU
1	C	233	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 10 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	227	GLN
1	C	239	GLN
1	D	51	ASN
1	C	41	ASN
1	D	6	ASN

### 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 ⓘ

8 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	DDO	A	2401	1	9,9,9	0.56	0	10,10,10	0.90	0
3	1PE	A	2501	-	15,15,15	0.34	0	14,14,14	0.48	0
2	DDO	B	2402	1	9,9,9	0.58	0	10,10,10	0.81	0
2	DDO	C	2403	1	9,9,9	0.54	0	10,10,10	1.05	1 (10%)
4	GOL	C	2601	-	5,5,5	0.18	0	5,5,5	1.95	2 (40%)
4	GOL	C	2603	-	5,5,5	0.17	0	5,5,5	1.95	1 (20%)
2	DDO	D	2404	1	9,9,9	0.55	0	10,10,10	0.91	0
4	GOL	D	2602	-	5,5,5	0.16	0	5,5,5	2.01	1 (20%)

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	DDO	A	2401	1	-	0/9/9/9	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	1PE	A	2501	-	-	0/13/13/13	0/0/0/0
2	DDO	B	2402	1	-	0/9/9/9	0/0/0/0
2	DDO	C	2403	1	-	0/9/9/9	0/0/0/0
4	GOL	C	2601	-	-	0/4/4/4	0/0/0/0
4	GOL	C	2603	-	-	0/4/4/4	0/0/0/0
2	DDO	D	2404	1	-	0/9/9/9	0/0/0/0
4	GOL	D	2602	-	-	0/4/4/4	0/0/0/0

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	2602	GOL	C3-C2-C1	3.77	127.92	111.26
4	C	2603	GOL	C3-C2-C1	3.42	126.37	111.26
4	C	2601	GOL	C3-C2-C1	3.37	126.14	111.26
2	C	2403	DDO	C-CA-N	2.29	113.15	109.36
4	C	2601	GOL	O2-C2-C3	2.14	117.96	108.22

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

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	324/327 (99%)	-0.13	5 (1%) 70 76	9, 17, 29, 34	12 (3%)
1	B	324/327 (99%)	-0.05	12 (3%) 39 44	8, 17, 30, 34	12 (3%)
1	C	324/327 (99%)	-0.17	5 (1%) 70 76	11, 17, 27, 33	10 (3%)
1	D	324/327 (99%)	-0.18	6 (1%) 64 69	9, 16, 28, 37	8 (2%)
All	All	1296/1308 (99%)	-0.13	28 (2%) 60 64	8, 17, 29, 37	42 (3%)

The worst 5 of 28 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	160[A]	ILE	4.4
1	B	10[A]	LEU	3.9
1	B	213	GLY	3.7
1	D	21	ALA	3.5
1	D	212	ARG	3.4

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

There are no non-standard protein/DNA/RNA residues in this entry.

### 6.3 Carbohydrates

There are no carbohydrates in this entry.

### 6.4 Ligands

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> 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	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
4	GOL	D	2602	6/6	0.17	6.19	25,28,28,29	0
3	1PE	A	2501	16/16	0.17	3.74	29,32,37,38	0
4	GOL	C	2603	6/6	0.29	3.08	39,39,40,40	0
2	DDO	A	2401	10/10	0.12	1.43	18,19,21,21	0
2	DDO	C	2403	10/10	0.13	1.38	20,21,22,22	0
2	DDO	B	2402	10/10	0.12	1.13	21,22,24,24	0
4	GOL	C	2601	6/6	0.08	0.86	17,17,18,19	0
2	DDO	D	2404	10/10	0.11	0.62	17,19,20,21	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.