



Full wwPDB X-ray Structure Validation Report

Apr 29, 2014 – 12:11 AM EDT

PDB ID : 4O47
Title : Crystal structure of uncleaved guinea pig L-asparaginase type III
Authors : Schalk, A.M.; Lavie, A.
Deposited on : 2013-12-18
Resolution : 1.90 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>

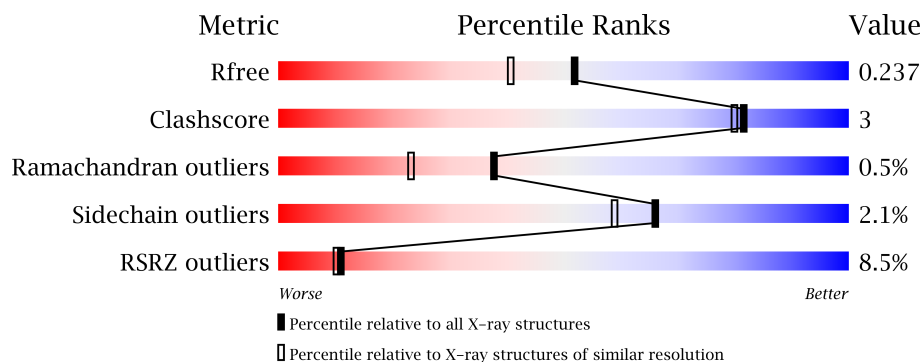
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.16 November 2013
Xtriage (Phenix) : dev-1439
EDS : stable22978
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) : stable22978

1 Overall quality at a glance

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))
R_{free}	66092	3684 (1.90-1.90)
Clashscore	79885	4465 (1.90-1.90)
Ramachandran outliers	78287	4413 (1.90-1.90)
Sidechain outliers	78261	4414 (1.90-1.90)
RSRZ outliers	66119	3686 (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. 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	332	
1	B	332	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4456 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 Uncharacterized protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	295	Total	C	N	O	S	0	4	0
			2157	1328	396	418	15			
1	B	290	Total	C	N	O	S	0	3	0
			2119	1307	390	408	14			

There are 46 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-22	MET	-	EXPRESSION TAG	UNP H0VQC8
A	-21	GLY	-	EXPRESSION TAG	UNP H0VQC8
A	-20	SER	-	EXPRESSION TAG	UNP H0VQC8
A	-19	SER	-	EXPRESSION TAG	UNP H0VQC8
A	-18	HIS	-	EXPRESSION TAG	UNP H0VQC8
A	-17	HIS	-	EXPRESSION TAG	UNP H0VQC8
A	-16	HIS	-	EXPRESSION TAG	UNP H0VQC8
A	-15	HIS	-	EXPRESSION TAG	UNP H0VQC8
A	-14	HIS	-	EXPRESSION TAG	UNP H0VQC8
A	-13	HIS	-	EXPRESSION TAG	UNP H0VQC8
A	-12	SER	-	EXPRESSION TAG	UNP H0VQC8
A	-11	SER	-	EXPRESSION TAG	UNP H0VQC8
A	-10	GLY	-	EXPRESSION TAG	UNP H0VQC8
A	-9	GLY	-	EXPRESSION TAG	UNP H0VQC8
A	-8	ASN	-	EXPRESSION TAG	UNP H0VQC8
A	-7	GLU	-	EXPRESSION TAG	UNP H0VQC8
A	-6	ASN	-	EXPRESSION TAG	UNP H0VQC8
A	-5	LEU	-	EXPRESSION TAG	UNP H0VQC8
A	-4	TYR	-	EXPRESSION TAG	UNP H0VQC8
A	-3	PHE	-	EXPRESSION TAG	UNP H0VQC8
A	-2	GLN	-	EXPRESSION TAG	UNP H0VQC8
A	-1	GLY	-	EXPRESSION TAG	UNP H0VQC8
A	0	HIS	-	EXPRESSION TAG	UNP H0VQC8
B	-22	MET	-	EXPRESSION TAG	UNP H0VQC8
B	-21	GLY	-	EXPRESSION TAG	UNP H0VQC8

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-20	SER	-	EXPRESSION TAG	UNP H0VQC8
B	-19	SER	-	EXPRESSION TAG	UNP H0VQC8
B	-18	HIS	-	EXPRESSION TAG	UNP H0VQC8
B	-17	HIS	-	EXPRESSION TAG	UNP H0VQC8
B	-16	HIS	-	EXPRESSION TAG	UNP H0VQC8
B	-15	HIS	-	EXPRESSION TAG	UNP H0VQC8
B	-14	HIS	-	EXPRESSION TAG	UNP H0VQC8
B	-13	HIS	-	EXPRESSION TAG	UNP H0VQC8
B	-12	SER	-	EXPRESSION TAG	UNP H0VQC8
B	-11	SER	-	EXPRESSION TAG	UNP H0VQC8
B	-10	GLY	-	EXPRESSION TAG	UNP H0VQC8
B	-9	GLY	-	EXPRESSION TAG	UNP H0VQC8
B	-8	ASN	-	EXPRESSION TAG	UNP H0VQC8
B	-7	GLU	-	EXPRESSION TAG	UNP H0VQC8
B	-6	ASN	-	EXPRESSION TAG	UNP H0VQC8
B	-5	LEU	-	EXPRESSION TAG	UNP H0VQC8
B	-4	TYR	-	EXPRESSION TAG	UNP H0VQC8
B	-3	PHE	-	EXPRESSION TAG	UNP H0VQC8
B	-2	GLN	-	EXPRESSION TAG	UNP H0VQC8
B	-1	GLY	-	EXPRESSION TAG	UNP H0VQC8
B	0	HIS	-	EXPRESSION TAG	UNP H0VQC8

- Molecule 2 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	1	Total Na 1 1	0	0
2	A	1	Total Na 1 1	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	104	Total O 104 104	0	0
3	B	74	Total O 74 74	0	0

4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	114.87Å 114.87Å 138.97Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	28.73 – 1.90 29.19 – 1.90	Depositor EDS
% Data completeness (in resolution range)	98.2 (28.73-1.90) 98.2 (29.19-1.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.05	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.46 (at 1.91Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.193 , 0.213 0.215 , 0.237	Depositor DCC
R_{free} test set	4120 reflections (5.27%)	DCC
Wilson B-factor (Å ²)	31.4	Xtriage
Anisotropy	0.653	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 47.6	EDS
Estimated twinning fraction	0.036 for -h,-k,l	Xtriage
L-test for twinning	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 83782 reflections	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	4456	wwPDB-VP
Average B, all atoms (Å ²)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.47% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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: NA

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	0.66	0/2188	0.83	1/2949 (0.0%)
1	B	0.63	0/2147	0.77	0/2893
All	All	0.64	0/4335	0.80	1/5842 (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	5	LEU	CA-CB-CG	-6.92	99.38	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 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 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	2157	0	2164	18	0
1	B	2119	0	2132	11	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	104	0	0	3	0
3	B	74	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	4456	0	4296	27	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 3.

All (27) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:203:ILE:HD13	3:B:559:HOH:O	1.90	0.71
1:A:16:SER:O	1:A:18:GLU:N	2.23	0.70
1:A:10:GLY:HA3	1:A:166:LEU:O	1.93	0.68
1:A:147:ARG:CZ	1:A:166:LEU:HD21	2.23	0.67
1:A:80:SER:HB3	1:A:201:PRO:HA	1.79	0.65
1:B:65:HIS:HD2	3:B:512:HOH:O	1.82	0.62
1:A:3:PRO:HG3	1:A:176[B]:CYS:SG	2.40	0.61
1:A:227:LYS:HE3	1:B:115:CYS:SG	2.43	0.58
1:A:65:HIS:HD2	3:A:505:HOH:O	1.87	0.57
1:B:71:GLU:O	1:B:152:ARG:NH2	2.42	0.51
1:B:147:ARG:NH1	1:B:166:LEU:HD21	2.25	0.51
1:B:289:VAL:HG22	1:B:294:VAL:HG22	1.92	0.51
1:A:200[B]:SER:N	1:A:201:PRO:CD	2.75	0.49
1:A:200[A]:SER:N	1:A:201:PRO:CD	2.76	0.48
1:A:257:LYS:O	1:A:261:LYS:HA	2.14	0.46
1:A:1:MET:CE	1:A:174:LEU:HD21	2.46	0.46
1:A:173:ALA:O	1:A:180:VAL:HA	2.16	0.45
1:A:243:LYS:HE2	3:A:596:HOH:O	2.16	0.45
1:A:240:GLN:NE2	3:A:596:HOH:O	2.48	0.45
1:A:24:ARG:NH2	1:A:304:THR:HG23	2.32	0.45
1:A:115:CYS:SG	1:B:227:LYS:HE3	2.57	0.44
1:B:147:ARG:CZ	1:B:166:LEU:HD21	2.47	0.44
1:B:266:LEU:HD12	1:B:266:LEU:C	2.38	0.43
1:A:182:TYR:CE2	1:A:207:GLY:HA3	2.53	0.43
1:B:240:GLN:O	1:B:241:GLY:O	2.38	0.42
1:A:1:MET:HE3	1:A:174:LEU:HD21	2.02	0.41
1:B:62:ASN:ND2	1:B:167:GLY:O	2.54	0.41

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	293/332 (88%)	283 (97%)	9 (3%)	1 (0%)	50	37
1	B	287/332 (86%)	276 (96%)	9 (3%)	2 (1%)	30	15
All	All	580/664 (87%)	559 (96%)	18 (3%)	3 (0%)	38	23

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	17	CYS
1	B	241	GLY
1	B	302	ASP

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	221/249 (89%)	217 (98%)	4 (2%)	71	66
1	B	216/249 (87%)	211 (98%)	5 (2%)	63	55
All	All	437/498 (88%)	428 (98%)	9 (2%)	66	59

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	LEU
1	A	17	CYS
1	A	19	ARG
1	A	116	PHE
1	B	5	LEU
1	B	22	ARG

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Mol	Chain	Res	Type
1	B	116	PHE
1	B	203	ILE
1	B	243	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	65	HIS
1	A	72	ASN
1	B	65	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, 2 are 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.

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, 95th 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 ²)	Q<0.9
1	A	295/332 (88%)	0.26	21 (7%) 16 15	26, 35, 65, 94	0
1	B	290/332 (87%)	0.43	29 (10%) 8 7	28, 41, 76, 100	0
All	All	585/664 (88%)	0.35	50 (8%) 11 10	26, 38, 73, 100	0

All (50) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	309	CYS	7.9
1	B	309	CYS	7.4
1	B	300	LEU	4.7
1	A	17	CYS	4.2
1	A	150	LYS	4.1
1	B	301	ASN	3.9
1	A	18	GLU	3.8
1	A	0	HIS	3.8
1	A	300	LEU	3.5
1	A	301	ASN	3.3
1	B	146	LYS	3.2
1	B	11	GLY	3.2
1	B	305	VAL	3.0
1	B	308	LEU	3.0
1	B	137	GLU	2.9
1	B	150	LYS	2.9
1	B	0	HIS	2.8
1	B	7	VAL	2.8
1	B	267	ILE	2.7
1	A	152	ARG	2.6
1	B	9	GLY	2.6
1	B	307	ASP	2.6
1	A	16	SER	2.6
1	A	19	ARG	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	169	VAL	2.5
1	B	302	ASP	2.5
1	A	184	THR	2.5
1	B	241	GLY	2.3
1	A	267	ILE	2.3
1	A	55	LEU	2.3
1	B	149	GLU	2.3
1	B	143	ARG	2.3
1	B	242	GLY	2.3
1	B	244	THR	2.3
1	A	166	LEU	2.3
1	B	152	ARG	2.3
1	A	169	VAL	2.3
1	A	9	GLY	2.2
1	A	182	TYR	2.2
1	B	142	GLU	2.1
1	A	7	VAL	2.1
1	A	172	VAL	2.1
1	A	170	GLY	2.1
1	B	147	ARG	2.1
1	B	184	THR	2.1
1	B	141	THR	2.0
1	B	166	LEU	2.0
1	B	170	GLY	2.0
1	B	8	HIS	2.0
1	A	151	GLU	2.0

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, 95th 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(\AA^2)	Q<0.9
2	NA	A	401	1/1	0.04	-1.50	35,35,35,35	0
2	NA	B	401	1/1	0.04	-1.53	35,35,35,35	0

6.5 Other polymers ⓘ

There are no such residues in this entry.