wwPDB X-ray Structure Validation Summary Report (i)

Aug 22, 2023 – 08:34 AM EDT

PDB ID	:	2QJS
Title	:	Stenotrophomonas maltophilia L1 metallo-beta-lactamase Asp-120 Asn mutant
Authors	:	Crisp, J.; Conners, R.; Spencer, J.
Deposited on	:	2007-07-09
Resolution	:	2.25 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 (1)) were used in the production of this report:

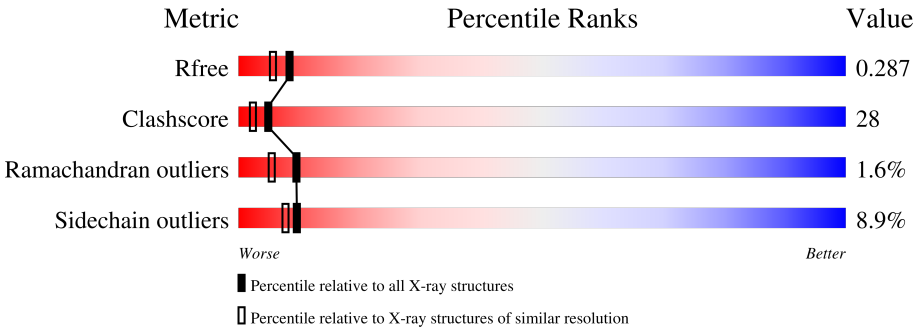
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation 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 2.25 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}	130704	1377 (2.26-2.26)
Clashscore	141614	1487 (2.26-2.26)
Ramachandran outliers	138981	1449 (2.26-2.26)
Sidechain outliers	138945	1450 (2.26-2.26)

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%

Mol	Chain	Length	Quality of chain
1	A	269	48% 39% 6% 8%
1	B	269	55% 32% 5% 8%
1	C	269	48% 39% 5% 8%
1	D	269	54% 33% • • 8%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 7820 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 Metallo-beta-lactamase L1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	248	Total	C	N	O	S	0	0	0
			1854	1162	337	347	8			
1	B	248	Total	C	N	O	S	0	0	0
			1854	1162	337	347	8			
1	C	248	Total	C	N	O	S	0	0	0
			1854	1162	337	347	8			
1	D	248	Total	C	N	O	S	0	0	0
			1854	1162	337	347	8			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	120	ASN	ASP	engineered mutation	UNP P52700
B	120	ASN	ASP	engineered mutation	UNP P52700
C	120	ASN	ASP	engineered mutation	UNP P52700
D	120	ASN	ASP	engineered mutation	UNP P52700

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Zn	0	0
			2	2		
2	B	2	Total	Zn	0	0
			2	2		
2	C	2	Total	Zn	0	0
			2	2		
2	D	2	Total	Zn	0	0
			2	2		

- Molecule 3 is water.

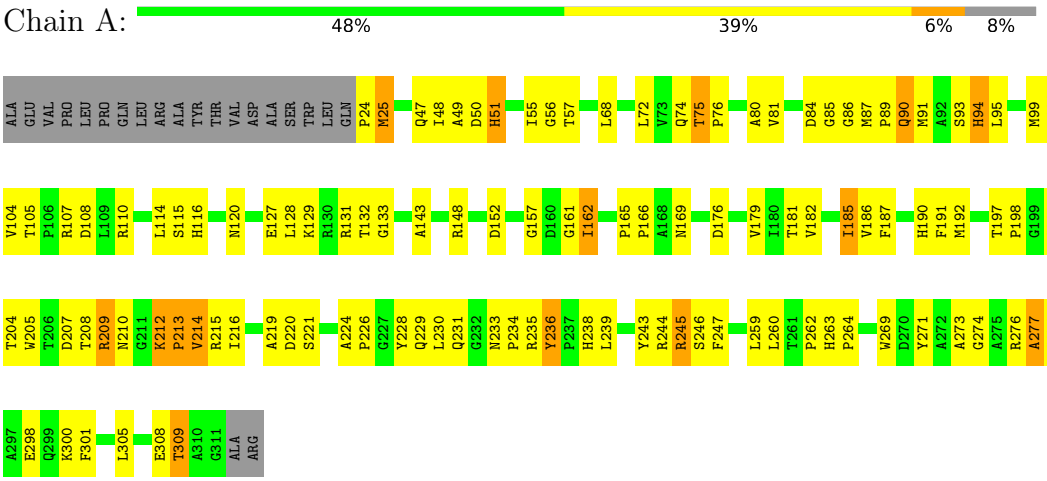
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	109	Total O 109 109	0	0
3	B	94	Total O 94 94	0	0
3	C	88	Total O 88 88	0	0
3	D	105	Total O 105 105	0	0

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.

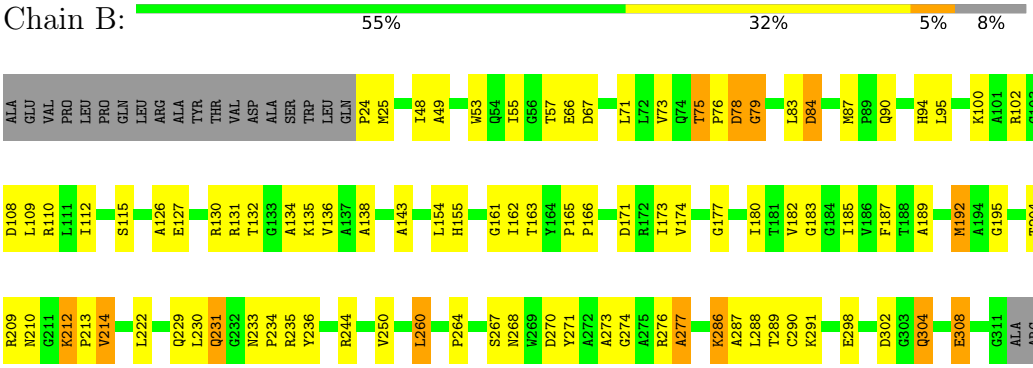
• Molecule 1: Metallo-beta-lactamase L1

Chain A:



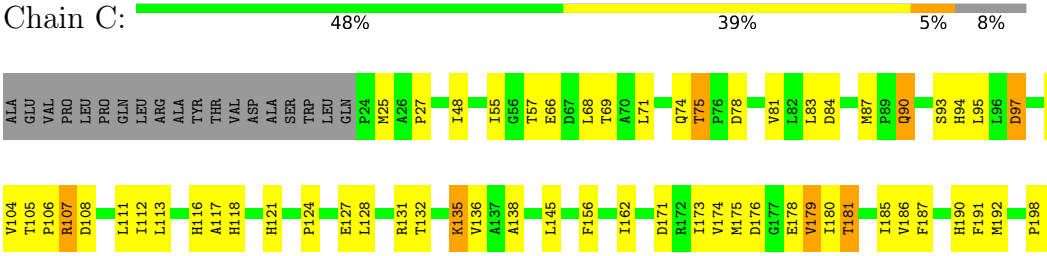
• Molecule 1: Metallo-beta-lactamase L1

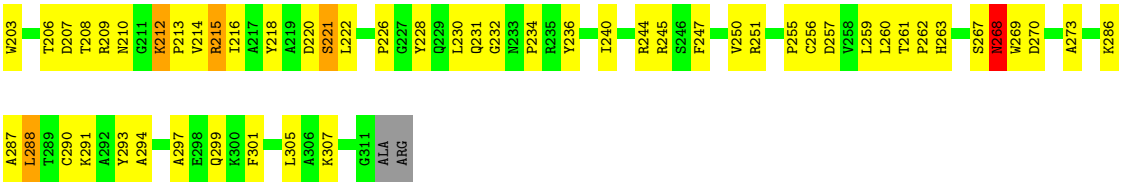
Chain B:



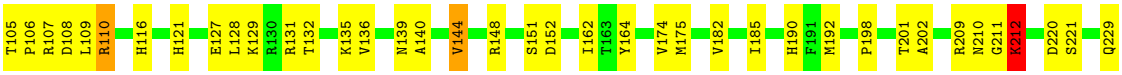
• Molecule 1: Metallo-beta-lactamase L1

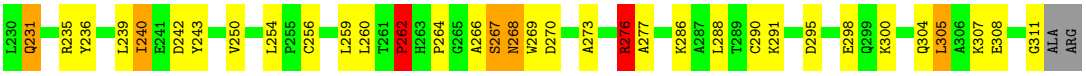
Chain C:





• Molecule 1: Metallo-beta-lactamase L1





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α, β, γ	86.38Å 86.38Å 227.36Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	10.00 – 2.25 28.06 – 2.25	Depositor EDS
% Data completeness (in resolution range)	(Not available) (10.00-2.25) 98.9 (28.06-2.25)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.91 (at 2.24Å)	Xtriage
Refinement program	SHELX, SHELXL-97	Depositor
R, R_{free}	0.253 , 0.283 0.244 , 0.287	Depositor DCC
R_{free} test set	2382 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å^2)	49.8	Xtriage
Anisotropy	0.184	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 54.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.478 for -h,-k,l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	7820	wwPDB-VP
Average B, all atoms (Å^2)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.14% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

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: ZN

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	0.50	0/1899	0.75	1/2589 (0.0%)
1	B	0.57	1/1899 (0.1%)	0.76	1/2589 (0.0%)
1	C	0.58	0/1899	0.78	3/2589 (0.1%)
1	D	0.69	6/1899 (0.3%)	0.81	4/2589 (0.2%)
All	All	0.59	7/7596 (0.1%)	0.77	9/10356 (0.1%)

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	276	ARG	CZ-NH2	9.63	1.45	1.33
1	D	286	LYS	CE-NZ	6.66	1.65	1.49
1	D	311	GLY	C-O	6.54	1.34	1.23
1	D	212	LYS	CD-CE	5.92	1.66	1.51
1	B	308	GLU	CD-OE2	5.53	1.31	1.25

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	110	ARG	NE-CZ-NH1	8.81	124.71	120.30
1	C	107	ARG	NE-CZ-NH1	8.40	124.50	120.30
1	D	276	ARG	NE-CZ-NH2	-7.14	116.73	120.30
1	D	276	ARG	NE-CZ-NH1	5.98	123.29	120.30
1	D	110	ARG	NE-CZ-NH2	-5.95	117.33	120.30

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	1854	0	1816	97	0
1	B	1854	0	1816	95	0
1	C	1854	0	1816	124	0
1	D	1854	0	1816	101	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
3	A	109	0	0	9	0
3	B	94	0	0	13	0
3	C	88	0	0	13	1
3	D	105	0	0	21	0
All	All	7820	0	7264	404	1

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 28.

The worst 5 of 404 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:D:96:LEU:HD12	1:D:131:ARG:HH21	1.13	1.06
1:C:107:ARG:HG2	3:C:2080:HOH:O	1.64	0.95
1:C:212:LYS:HD2	1:C:213:PRO:HD2	1.50	0.93
1:A:245:ARG:HH22	1:C:245:ARG:NH1	1.68	0.92
1:D:104:VAL:HG13	1:D:108:ASP:HB2	1.52	0.92

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:2018:HOH:O	3:C:2018:HOH:O[4_556]	1.93	0.27

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	246/269 (91%)	215 (87%)	26 (11%)	5 (2%)	7 4
1	B	246/269 (91%)	218 (89%)	23 (9%)	5 (2%)	7 4
1	C	246/269 (91%)	221 (90%)	21 (8%)	4 (2%)	9 5
1	D	246/269 (91%)	220 (89%)	24 (10%)	2 (1%)	19 17
All	All	984/1076 (91%)	874 (89%)	94 (10%)	16 (2%)	9 5

5 of 16 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	274	GLY
1	A	309	THR
1	B	277	ALA
1	D	57	THR
1	A	277	ALA

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	185/202 (92%)	167 (90%)	18 (10%)	8 6
1	B	185/202 (92%)	174 (94%)	11 (6%)	19 19
1	C	185/202 (92%)	166 (90%)	19 (10%)	7 5
1	D	185/202 (92%)	167 (90%)	18 (10%)	8 6
All	All	740/808 (92%)	674 (91%)	66 (9%)	9 8

5 of 66 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	240	ILE
1	D	262	PRO
1	D	307	LYS
1	B	231	GLN
1	B	214	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 8 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	98	ASN
1	C	90	GLN
1	B	90	GLN
1	A	268	ASN
1	C	47	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 8 ligands modelled in this entry, 8 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.

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

6.1 Protein, DNA and RNA chains

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates

Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands

Unable to reproduce the depositors R factor - this section is therefore empty.

6.5 Other polymers

Unable to reproduce the depositors R factor - this section is therefore empty.