



Full wwPDB X-ray Structure Validation Report

Feb 27, 2014 – 04:43 AM GMT

PDB ID : 3C0N
Title : Crystal structure of the proaerolysin mutant Y221G at 2.2 Å
Authors : Pernot, L.; Schiltz, M.; Thurnheer, S.; Burr, S.E.; van der Goot, G.
Deposited on : 2008-01-21
Resolution : 2.20 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>

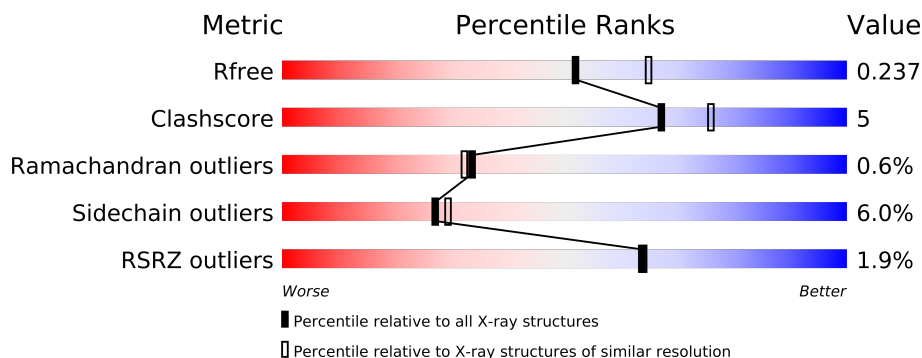
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 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 2.20 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	2938 (2.20-2.20)
Clashscore	79885	3751 (2.20-2.20)
Ramachandran outliers	78287	3681 (2.20-2.20)
Sidechain outliers	78261	3682 (2.20-2.20)
RSRZ outliers	66119	2939 (2.20-2.20)

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	470	
1	B	470	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 7456 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 Aerolysin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	450	Total	C	N	O	S	0	0	0
			3519	2223	606	681	9			
1	B	450	Total	C	N	O	S	0	0	0
			3520	2224	606	681	9			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	221	GLY	TYR	ENGINEERED	UNP P09167
B	221	GLY	TYR	ENGINEERED	UNP P09167

- Molecule 2 is water.

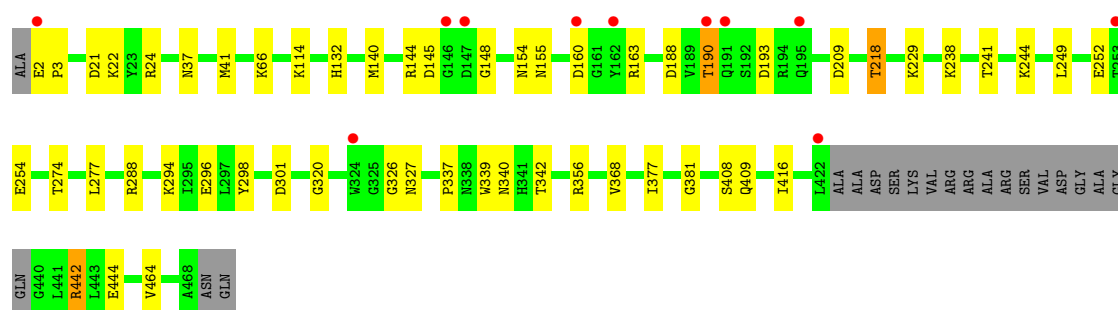
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	177	Total	O	0	0
			177	177		
2	B	240	Total	O	0	0
			240	240		

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.

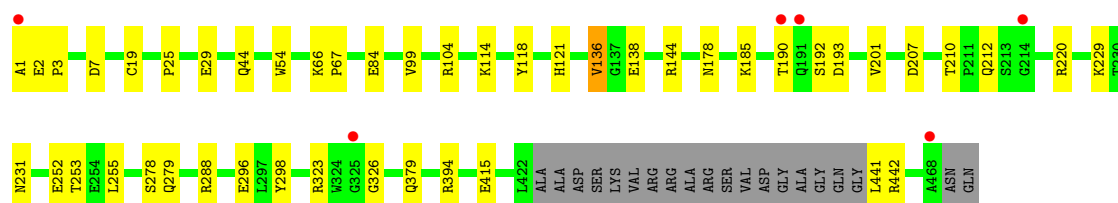
• Molecule 1: Aerolysin

Chain A: 



• Molecule 1: Aerolysin

Chain B: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	70.36Å 89.77Å 166.62Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	64.82 – 2.20 64.82 – 2.20	Depositor EDS
% Data completeness (in resolution range)	100.0 (64.82-2.20) 100.0 (64.82-2.20)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	0.11	Depositor
$\langle I/\sigma(I) \rangle$ ¹	6.23 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.3.0008	Depositor
R, R_{free}	0.189 , 0.238 0.197 , 0.237	Depositor DCC
R_{free} test set	2755 reflections (5.34%)	DCC
Wilson B-factor (Å ²)	31.5	Xtriage
Anisotropy	0.113	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 22.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 54335 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	7456	wwPDB-VP
Average B, all atoms (Å ²)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.08% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

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	0.57	0/3616	0.86	0/4935
1	B	0.58	0/3617	0.86	0/4937
All	All	0.57	0/7233	0.86	0/9872

There are no bond length outliers.

There are no bond angle outliers.

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	3519	0	0	18	0
1	B	3520	0	0	19	0
2	A	177	0	0	3	0
2	B	240	0	0	4	0
All	All	7456	0	0	34	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 5.

All (34) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:2:GLU:N	1:B:3:PRO:CD	2.41	0.83

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:249:LEU:CD2	1:B:394:ARG:NH2	2.58	0.67
1:A:37:ASN:ND2	2:A:626:HOH:O	2.30	0.63
1:A:41:MET:CE	2:B:595:HOH:O	2.48	0.61
1:B:207:ASP:OD2	1:B:442:ARG:NH1	2.37	0.57
1:B:1:ALA:C	1:B:3:PRO:CD	2.73	0.56
1:A:296:GLU:OE1	1:A:298:TYR:OH	2.24	0.56
1:A:2:GLU:O	1:A:2:GLU:CG	2.54	0.56
1:A:218:THR:CG2	2:A:560:HOH:O	2.54	0.56
1:A:2:GLU:N	1:A:3:PRO:CD	2.69	0.56
1:B:99:VAL:CG2	1:B:144:ARG:NH2	2.71	0.54
1:A:114:LYS:NZ	1:B:415:GLU:OE1	2.41	0.53
1:B:296:GLU:OE1	1:B:298:TYR:OH	2.28	0.52
1:B:229:LYS:NZ	1:B:231:ASN:ND2	2.58	0.51
1:B:1:ALA:N	2:B:663:HOH:O	2.45	0.50
1:B:7:ASP:OD1	1:B:84:GLU:OE2	2.30	0.50
1:A:209:ASP:OD1	1:A:288:ARG:NH1	2.45	0.49
1:B:212:GLN:OE1	1:B:441:LEU:N	2.45	0.49
1:A:144:ARG:NH2	2:A:544:HOH:O	2.46	0.49
1:A:442:ARG:NH2	1:A:444:GLU:OE2	2.47	0.48
1:A:145:ASP:N	1:A:148:GLY:O	2.47	0.47
1:A:368:VAL:CG1	1:A:368:VAL:O	2.63	0.47
1:B:19:CYS:SG	1:B:25:PRO:CD	3.04	0.46
1:A:132:HIS:CE1	1:A:154:ASN:OD1	2.68	0.46
1:B:178:ASN:ND2	2:B:632:HOH:O	2.48	0.45
1:B:121:HIS:O	1:B:323:ARG:NH2	2.50	0.44
1:B:114:LYS:NZ	1:B:138:GLU:OE2	2.51	0.43
1:A:294:LYS:NZ	1:B:138:GLU:OE2	2.52	0.43
1:A:377:ILE:O	1:A:381:GLY:N	2.52	0.43
1:A:188:ASP:O	1:A:190:THR:N	2.52	0.42
1:B:54:TRP:CZ3	1:B:67:PRO:CD	3.02	0.42
1:A:320:GLY:O	1:A:339:TRP:N	2.53	0.42
1:B:118:TYR:CE1	1:B:136:VAL:CG1	3.03	0.41
1:B:379:GLN:NE2	2:B:580:HOH: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	446/470 (95%)	425 (95%)	18 (4%)	3 (1%)	30	28
1	B	446/470 (95%)	427 (96%)	17 (4%)	2 (0%)	43	45
All	All	892/940 (95%)	852 (96%)	35 (4%)	5 (1%)	33	32

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	190	THR
1	B	193	ASP
1	B	326	GLY
1	A	193	ASP
1	A	326	GLY

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	378/391 (97%)	350 (93%)	28 (7%)	20	19
1	B	378/391 (97%)	361 (96%)	17 (4%)	38	44
All	All	756/782 (97%)	711 (94%)	45 (6%)	27	29

All (45) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	21	ASP
1	A	22	LYS
1	A	24	ARG
1	A	66	LYS
1	A	140	MET
1	A	155	ASN
1	A	160	ASP
1	A	163	ARG
1	A	218	THR
1	A	229	LYS

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Mol	Chain	Res	Type
1	A	238	LYS
1	A	241	THR
1	A	244	LYS
1	A	252	GLU
1	A	254	GLU
1	A	274	THR
1	A	277	LEU
1	A	301	ASP
1	A	327	ASN
1	A	337	PRO
1	A	340	ASN
1	A	342	THR
1	A	356	ARG
1	A	408	SER
1	A	409	GLN
1	A	416	ILE
1	A	442	ARG
1	A	464	VAL
1	B	29	GLU
1	B	44	GLN
1	B	66	LYS
1	B	104	ARG
1	B	136	VAL
1	B	185	LYS
1	B	190	THR
1	B	192	SER
1	B	201	VAL
1	B	210	THR
1	B	220	ARG
1	B	252	GLU
1	B	253	THR
1	B	255	LEU
1	B	278	SER
1	B	279	GLN
1	B	288	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 ⓘ

There are no ligands in this entry.

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	450/470 (95%)	-0.23	11 (2%) 56 56	15, 30, 61, 76	0
1	B	450/470 (95%)	-0.25	6 (1%) 74 74	13, 27, 61, 85	0
All	All	900/940 (95%)	-0.24	17 (1%) 64 64	13, 29, 61, 85	0

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	147	ASP	4.5
1	A	190	THR	4.2
1	B	468	ALA	4.1
1	A	146	GLY	4.1
1	A	324	TRP	3.6
1	A	422	LEU	3.5
1	B	191	GLN	3.4
1	A	191	GLN	3.1
1	B	1	ALA	2.7
1	A	195	GLN	2.6
1	A	2	GLU	2.5
1	A	253	THR	2.4
1	B	325	GLY	2.4
1	A	160	ASP	2.3
1	B	190	THR	2.2
1	B	214	GLY	2.1
1	A	162	TYR	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

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.