



wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 31, 2016 – 08:47 PM GMT

PDB ID : 1M3J
Title : CRYSTAL form II of perfringolysin O
Authors : Rossjohn, J.; Parker, M.; Polekhina, G.; Feil, S.; Tweten, R.
Deposited on : 2002-06-28
Resolution : 3.00 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
<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

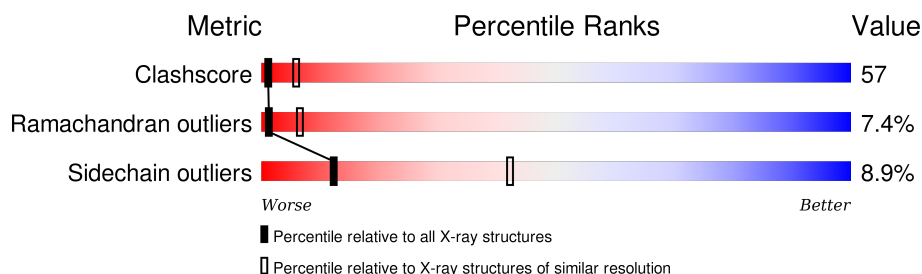
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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	1912 (3.00-3.00)
Ramachandran outliers	100387	1853 (3.00-3.00)
Sidechain outliers	100360	1856 (3.00-3.00)

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	471	<div> <div>25%</div> <div>64%</div> <div>11%</div> </div>
1	B	471	<div> <div>27%</div> <div>61%</div> <div>11%</div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 7467 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 perfringolysin o.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	471	Total	C	N	O	S	0	0	0
			3705	2332	622	746	5			
1	B	471	Total	C	N	O	S	0	0	0
			3705	2332	622	746	5			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	114	LEU	PHE	see remark 999	UNP P19995
B	114	LEU	PHE	see remark 999	UNP P19995

- Molecule 2 is water.

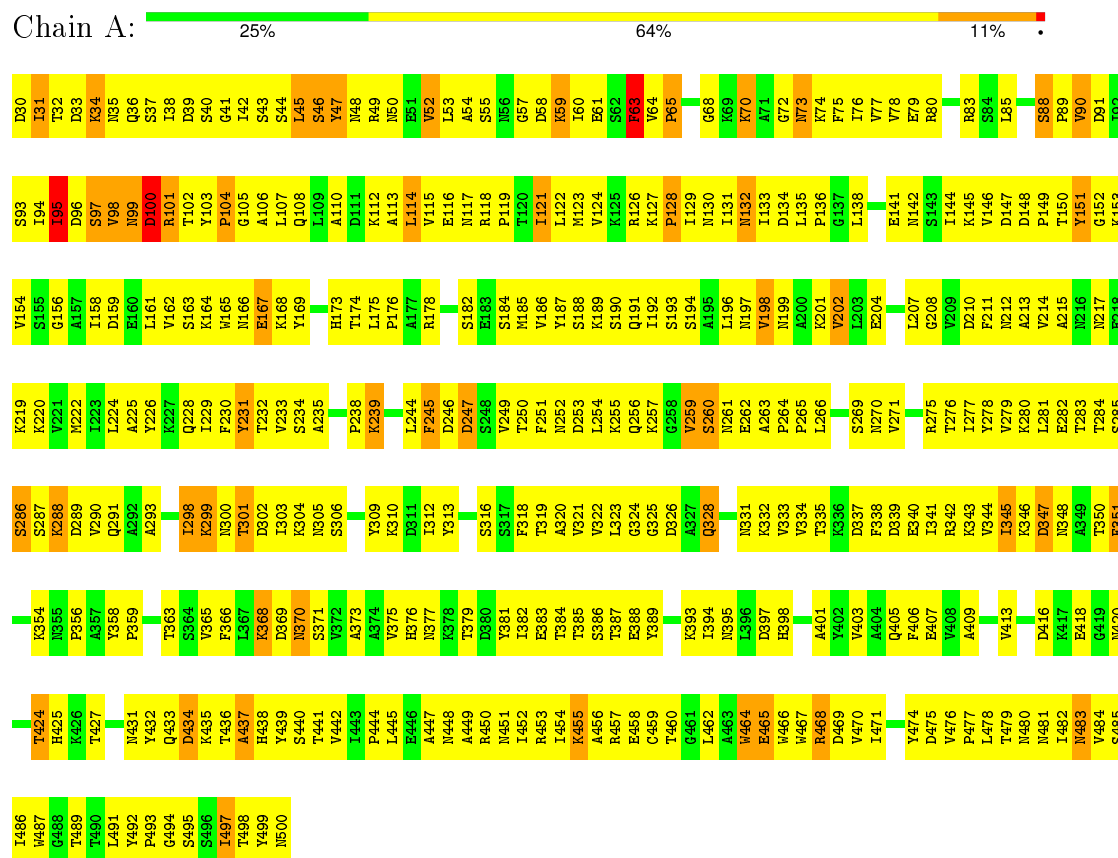
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	26	Total	O	0	0
			26	26		
2	B	31	Total	O	0	0
			31	31		

3 Residue-property plots

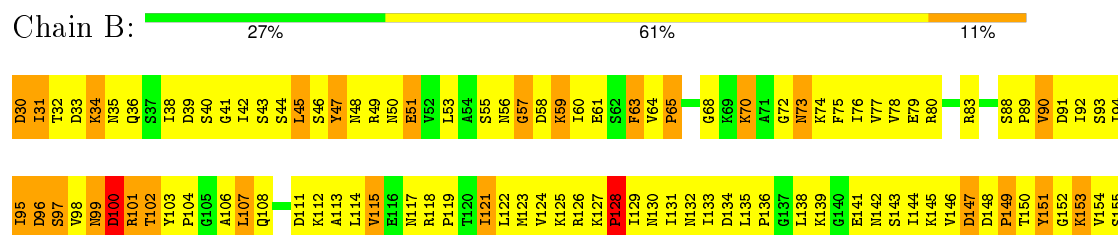
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according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



- Molecule 1: perfringolysin o



T490	G494	H425	N355	A293	Y226	G156
L491		F294	P356	F294	K227	A157
Y492		K295	A357	K295	Q228	I158
P493		A296	Y358	A296	I229	D159
G494		L297	P359	L297	F230	
		I360	I360	I298	Y231	V162
		S361	S361	K299	T232	S163
I497		Y362	Y362	N300	V233	K164
T498		T363	T363	T301	S234	V165
Y499		S364	S364	A302	A235	N166
N500		T436	V365	I303	D236	E167
		A437	F366	K304		K168
		H438	L367	N305	K239	Y169
		Y439	K368	S306	N240	
		S440	D369	Q307	P241	T172
		T441	N370	Q308		H173
		V442	S371	Y309	F245	
			V372	K310	D246	R178
			A373	D311		
			A374	I312	T250	S182
			V375	I313	F251	E183
				E314	N252	S184
			T379	N315	D253	M185
			D380	S316	L254	V186
			Y381	S317	K255	Y187
			I382	F318	Q256	S188
			E383	T319	K257	K189
			T384	A320	G258	S190
			T385	V321	V259	Q191
			S386	V322	S260	I192
			T387	L323		S193
			E388	G324	A263	
			Y389	G325	P263	L196
			S390	D326	P265	N197
			K391	A327	L266	V198
			G392	Q328		N199
			K393	E329	S269	
			I394	H330	N270	V202
			N395	N331	V271	L203
			L396	K332	A272	E204
			D397	V333	Y273	
			H398	V334	G274	L207
				T335	R275	G208
			A401	K336	T276	V209
			Y402	D337	I277	D210
			V403	F338	Y278	F211
			A404	D339	V279	N212
			Q405	E340	K280	A213
			F406	I341	L281	V214
			E407	R342	E282	A215
			V408	K343	T283	N216
			A409	T344	T284	N217
				I345	S285	E218
			E412	K346	S286	K219
			V413	D347	S287	K220
				N348	K288	V221
			K417		D289	N222
			E418	F351	V290	I223
			G419		Q291	L224
			N420	K354	A292	A225

4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	167.00Å 214.11Å 47.07Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 3.00	Depositor
% Data completeness (in resolution range)	(Not available) (20.00-3.00)	Depositor
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.247 , 0.337	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	7467	wwPDB-VP
Average B, all atoms (Å ²)	52.0	wwPDB-VP

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	0.46	0/3776	0.70	0/5127
1	B	0.48	0/3776	0.70	0/5127
All	All	0.47	0/7552	0.70	0/10254

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-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 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	3705	0	3656	427	0
1	B	3705	0	3656	418	0
2	A	26	0	0	3	0
2	B	31	0	0	0	0
All	All	7467	0	7312	845	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 57.

The worst 5 of 845 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:B:96:ASP:HB2	1:B:100:ASP:HB2	1.22	1.17

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:96:ASP:HB2	1:A:100:ASP:HB2	1.23	1.16
1:A:481:ASN:HB2	1:A:500:ASN:ND2	1.62	1.12
1:B:70:LYS:H	1:B:70:LYS:HD3	1.08	1.10
1:A:70:LYS:HD3	1:A:70:LYS:H	1.15	1.09

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	469/471 (100%)	358 (76%)	77 (16%)	34 (7%)	1	7
1	B	469/471 (100%)	358 (76%)	76 (16%)	35 (8%)	1	6
All	All	938/942 (100%)	716 (76%)	153 (16%)	69 (7%)	1	6

5 of 69 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	298	ILE
1	B	288	LYS
1	B	438	HIS
1	A	151	TYR
1	A	259	VAL

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	418/418 (100%)	379 (91%)	39 (9%)	11	39
1	B	418/418 (100%)	383 (92%)	35 (8%)	14	45
All	All	836/836 (100%)	762 (91%)	74 (9%)	12	42

5 of 74 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	424	THR
1	B	34	LYS
1	B	395	ASN
1	A	434	ASP
1	A	475	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 32 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	451	ASN
1	B	50	ASN
1	B	433	GLN
1	B	48	ASN
1	B	56	ASN

5.3.3 RNA ⓘ

There are no RNA molecules 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 [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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

EDS was not executed - this section will therefore be empty.

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates [i](#)

EDS was not executed - this section will therefore be empty.

6.4 Ligands [i](#)

EDS was not executed - this section will therefore be empty.

6.5 Other polymers [i](#)

EDS was not executed - this section will therefore be empty.