wwPDB X-ray Structure Validation Summary Report (i)

May 16, 2020 – 07:39 pm BST

PDB ID	:	1M3I
Title	:	Perfringolysin O, new crystal form
Authors	:	Rossjohn, J.; Parker, M.; Polekhina, G.; Feil, S.; Tweten, R.
Deposited on	:	2002-06-28
Resolution	:	2.90 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 following versions of software and data (see references (1)) were used in the production of this report:

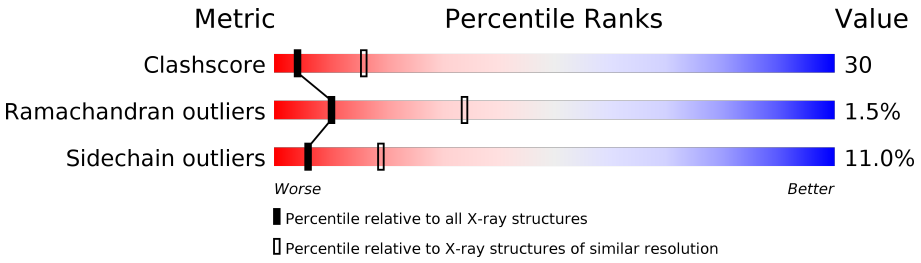
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 2.90 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))
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)

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 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%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	471	49% 44% 6%
1	B	471	54% 39% 6%
1	C	471	41% 49% 8%
1	D	471	45% 47% 6%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 14920 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	465	Total	C	N	O	S	0	0	0
			3657	2304	614	734	5			
1	B	465	Total	C	N	O	S	0	0	0
			3657	2304	614	734	5			
1	C	465	Total	C	N	O	S	0	0	0
			3657	2304	614	734	5			
1	D	465	Total	C	N	O	S	0	0	0
			3657	2304	614	734	5			

There are 4 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
C	114	LEU	PHE	see remark 999	UNP P19995
D	114	LEU	PHE	see remark 999	UNP P19995

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	70	Total	O	0	0
			70	70		
2	B	88	Total	O	0	0
			88	88		
2	C	58	Total	O	0	0
			58	58		
2	D	76	Total	O	0	0
			76	76		

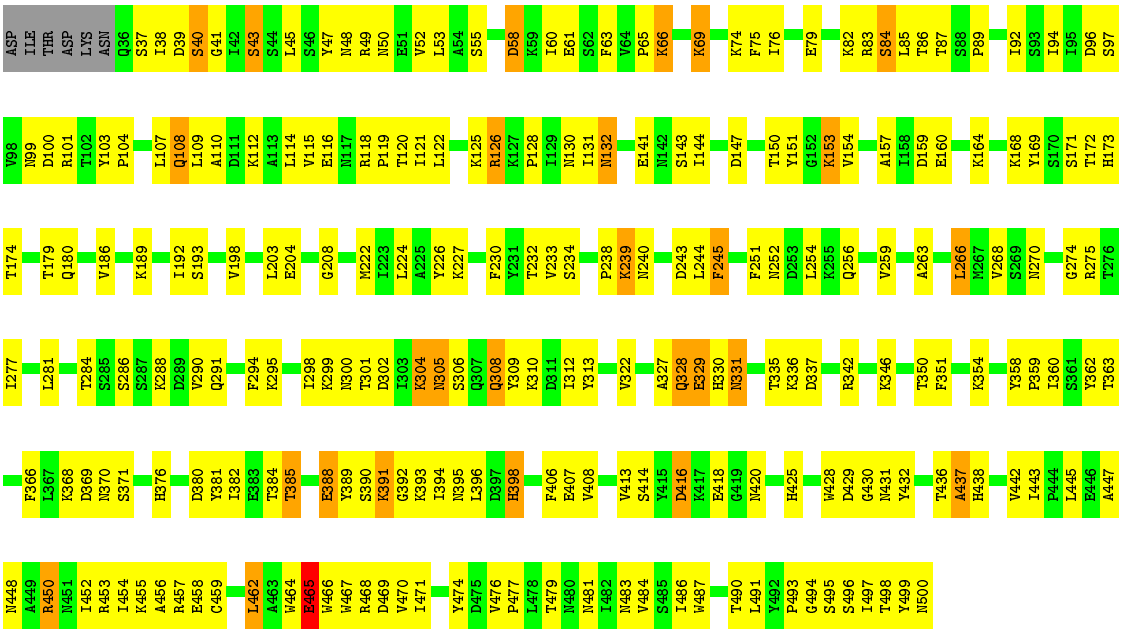
3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA 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.

Note EDS was not executed.

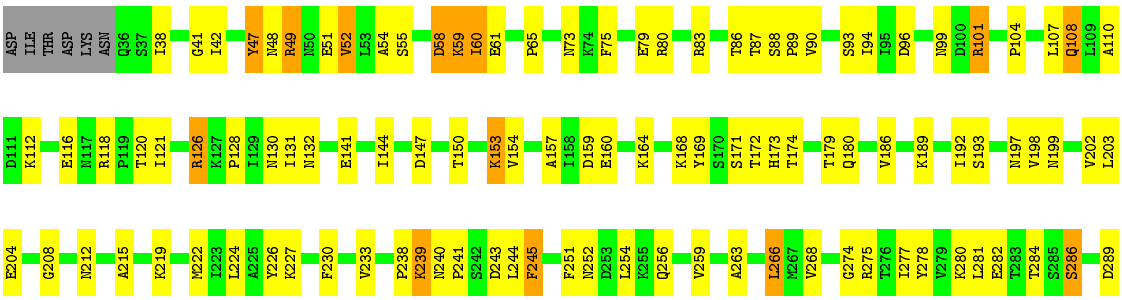
- Molecule 1: perfringolysin O

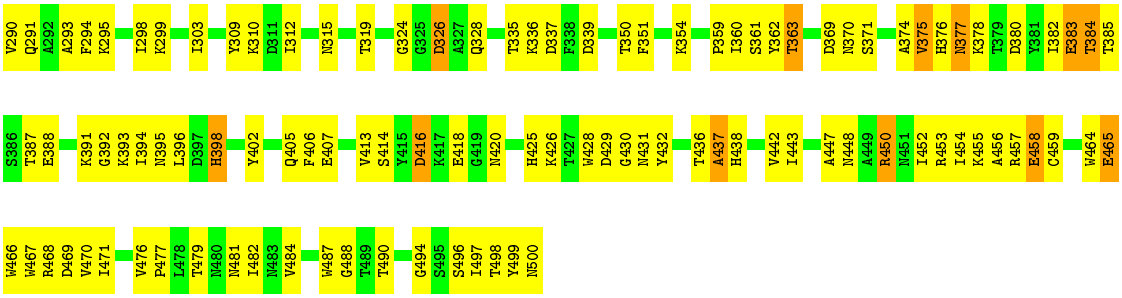
Chain A:



- Molecule 1: perfringolysin O

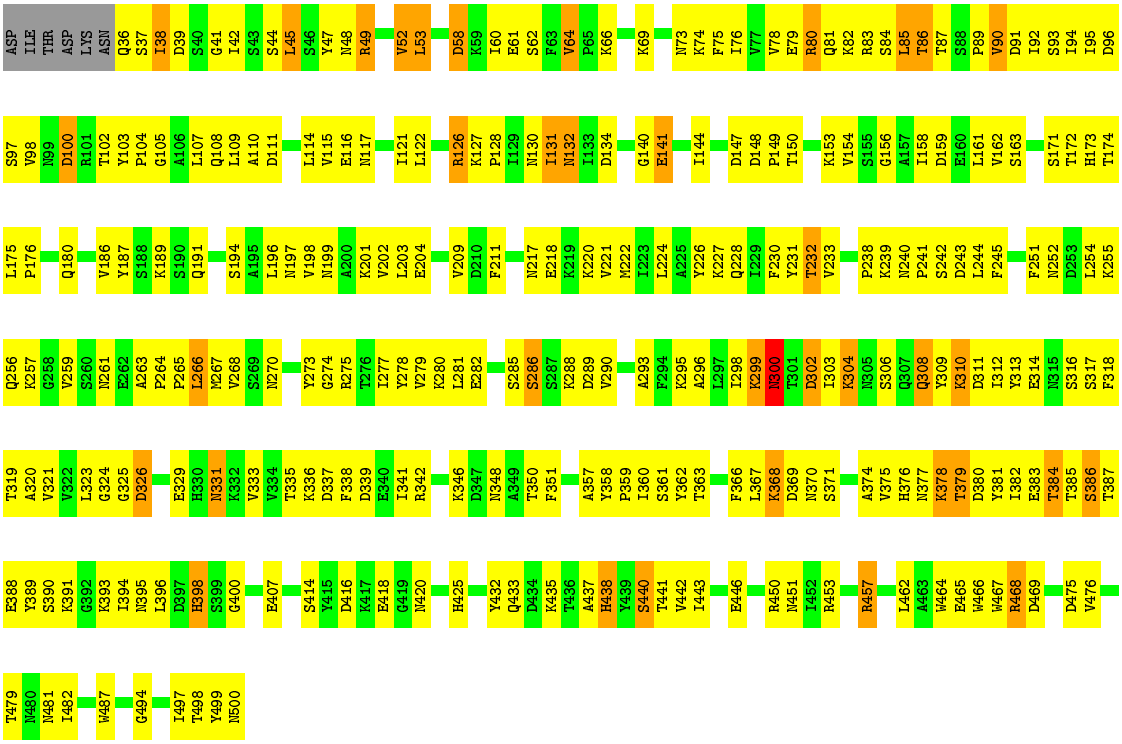
Chain B:





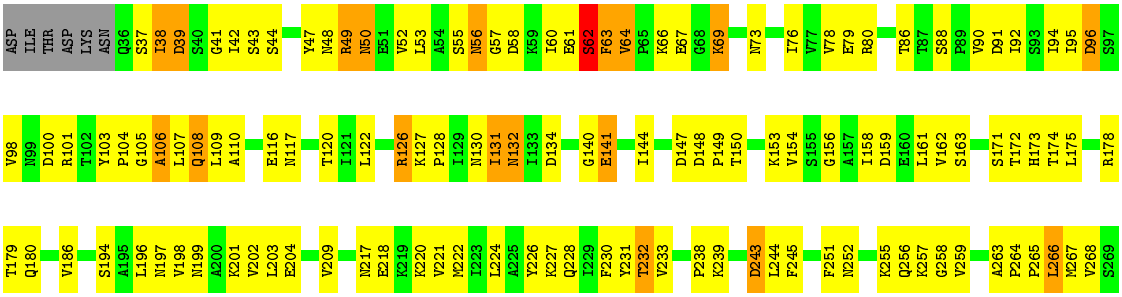
• Molecule 1: perfringolysin O

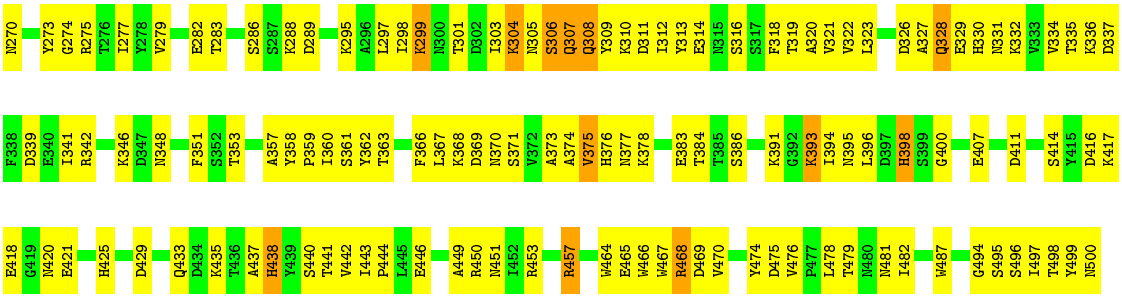
Chain C:



• Molecule 1: perfringolysin O

Chain D:




N270
Y273
G274
R275
T276
I277
Y278
V279
E282
T283
S286
S287
K288
D289
K295
A296
L297
I298
K299
N300
T301
D302
I303
K304
N305
S306
Q307
Q308
Y309
K310
D311
I312
Y313
E314
N315
S316
S317
F318
T319
A320
V321
V322
L323
D326
A327
Q328
E329
H330
N331
K332
V333
V334
T335
K336
D337
F338
D339
E340
I341
R342
K346
D347
N348
F351
S352
T353
A357
Y358
P359
I360
S361
Y362
T363
F366
L367
K368
D369
N370
S371
V372
A373
A374
V375
H376
N377
K378
E383
T384
T385
S386
K391
G392
K393
I394
N395
L396
D397
H398
S399
G400
E407
D411
S414
Y415
D416
K417
E418
G419
N420
E421
H425
D429
Q433
D434
K435
T436
A437
H438
Y439
S440
T441
V442
I443
P444
L445
E446
A449
R450
N451
I452
R453
R457
W464
E465
W466
W467
R468
D469
V470
Y474
D475
V476
P477
L478
T479
N480
N481
I482
W487
G494
S495
S496
I497
T498
Y499
N500

4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	P 31	Depositor
Cell constants a, b, c, α, β, γ	130.41Å 130.41Å 129.90Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 2.90	Depositor
% Data completeness (in resolution range)	95.2 (20.00-2.90)	Depositor
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.233 , 0.280	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	14920	wwPDB-VP
Average B, all atoms (Å^2)	67.0	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	0.35	0/3728	0.57	0/5062
1	B	0.36	0/3728	0.56	0/5062
1	C	0.37	0/3728	0.57	1/5062 (0.0%)
1	D	0.35	0/3728	0.56	0/5062
All	All	0.36	0/14912	0.57	1/20248 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	300	ASN	N-CA-C	6.46	128.45	111.00

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	3657	0	3611	211	0
1	B	3657	0	3611	174	0
1	C	3657	0	3611	275	0
1	D	3657	0	3611	214	0
2	A	70	0	0	14	0
2	B	88	0	0	6	0
2	C	58	0	0	4	0
2	D	76	0	0	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	14920	0	14444	860	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 30.

The worst 5 of 860 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:A:335:THR:HG22	1:A:337:ASP:H	1.27	0.99
1:B:335:THR:HG22	1:B:337:ASP:H	1.28	0.98
1:A:87:THR:HG22	1:A:89:PRO:HD3	1.45	0.97
1:C:289:ASP:HB3	1:C:309:TYR:HE1	1.25	0.94
1:A:301:THR:O	1:A:304:LYS:HG3	1.68	0.94

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	463/471 (98%)	421 (91%)	35 (8%)	7 (2%)	10	34
1	B	463/471 (98%)	417 (90%)	39 (8%)	7 (2%)	10	34
1	C	463/471 (98%)	416 (90%)	41 (9%)	6 (1%)	12	37
1	D	463/471 (98%)	424 (92%)	31 (7%)	8 (2%)	9	31
All	All	1852/1884 (98%)	1678 (91%)	146 (8%)	28 (2%)	10	34

5 of 28 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	462	LEU
1	B	58	ASP

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Mol	Chain	Res	Type
1	D	38	ILE
1	D	62	SER
1	A	465	GLU

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	412/418 (99%)	374 (91%)	38 (9%)	9 27
1	B	412/418 (99%)	372 (90%)	40 (10%)	8 25
1	C	412/418 (99%)	357 (87%)	55 (13%)	4 11
1	D	412/418 (99%)	364 (88%)	48 (12%)	5 16
All	All	1648/1672 (99%)	1467 (89%)	181 (11%)	6 19

5 of 181 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	53	LEU
1	C	232	THR
1	D	328	GLN
1	C	69	LYS
1	C	100	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 55 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	48	ASN
1	C	217	ASN
1	D	330	HIS
1	C	99	ASN
1	C	117	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

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

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.