



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 8, 2026 – 12:20 PM UTC

PDB ID : 1M3I / pdb_00001m3i
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 ⓘ 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 ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

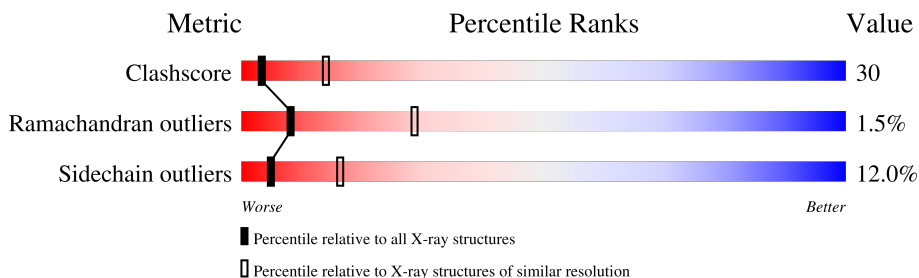
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (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 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 $\leq 5\%$

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	471	
1	B	471	
1	C	471	
1	D	471	

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.

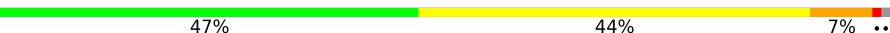
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	70	Total	O	0	0
			70	70		
2	B	88	Total	O	0	0
			88	88		
2	C	58	Total	O	0	0
			58	58		
2	D	76	Total	O	0	0
			76	76		

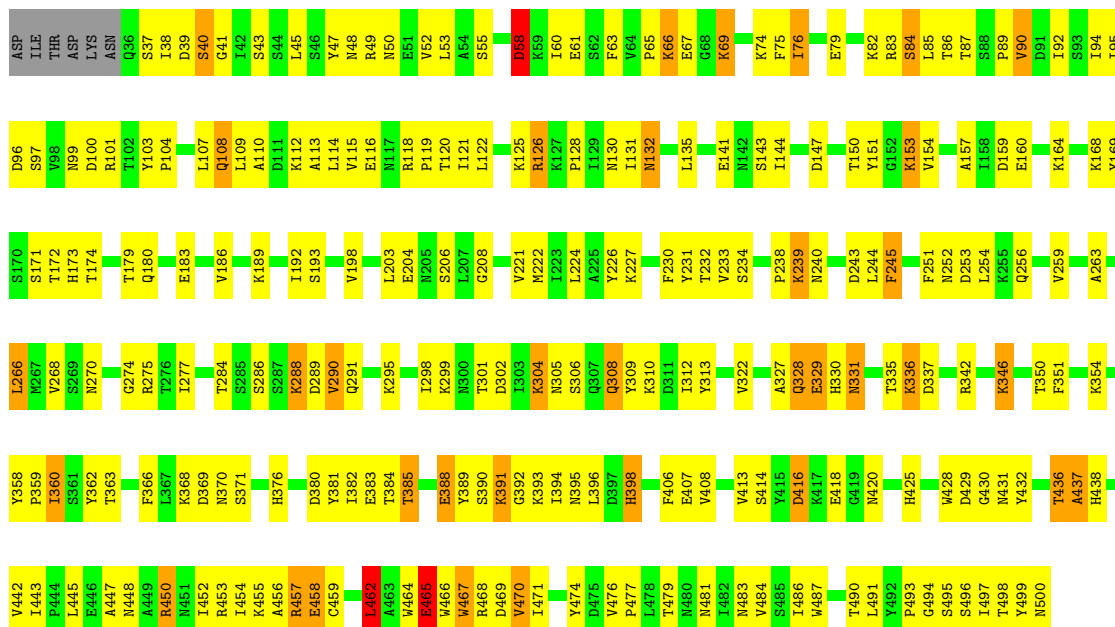
3 Residue-property plots

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.

Note EDS was not executed.

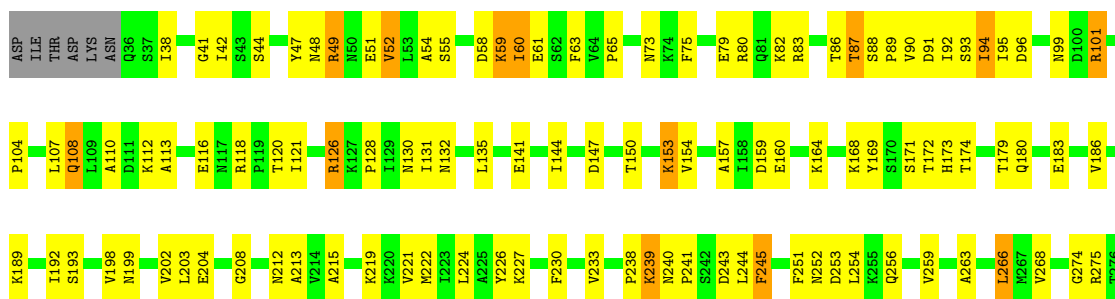
• Molecule 1: perfringolysin O

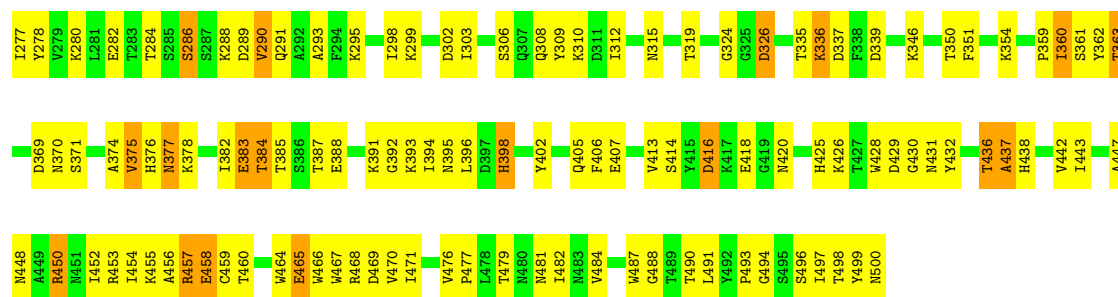
Chain A: 



• Molecule 1: perfringolysin O

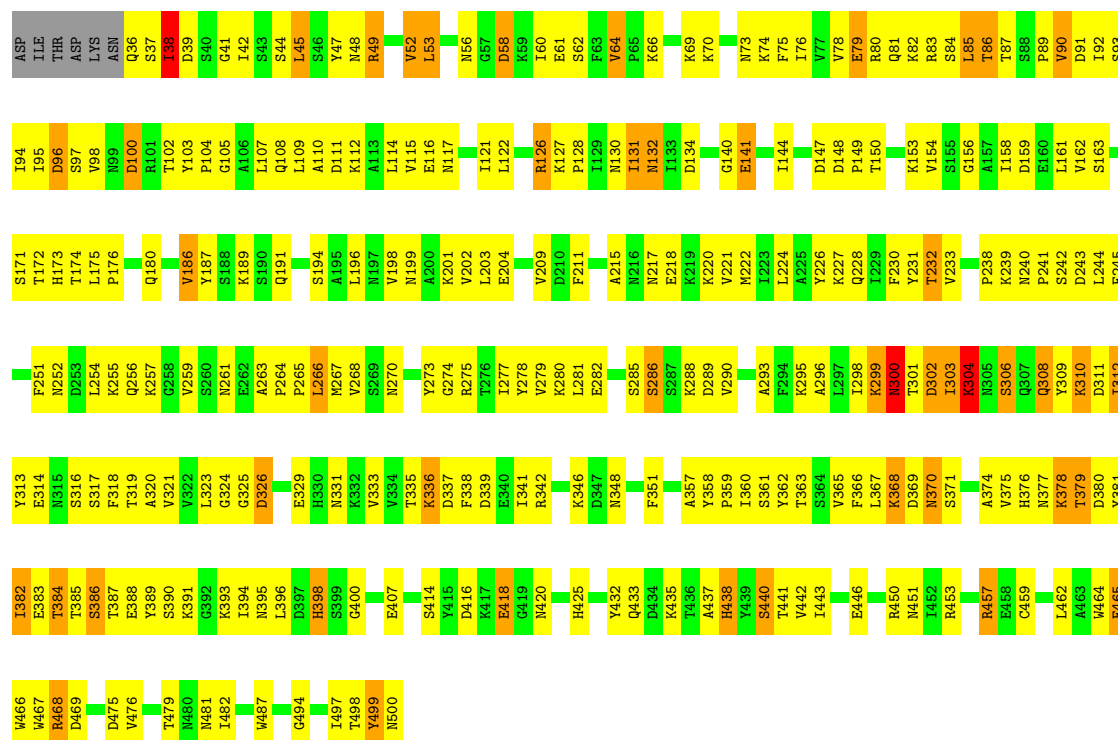
Chain B: 





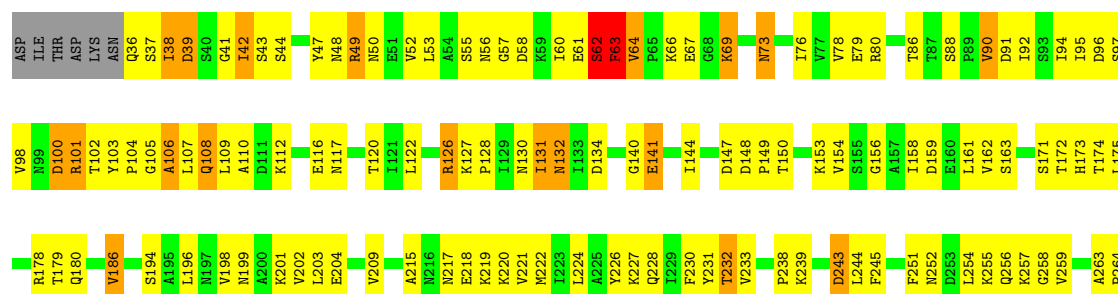
• Molecule 1: perfringolysin O

Chain C: 40% 48% 9% ..



• Molecule 1: perfringolysin O

Chain D: 43% 47% 8% .



S495	S496	T497	T498	Y499	M500	S414	Y415	D416	K417	E418	G419	M420	E421	H425	D429	Q433	D434	K435	T436	A437	H438	Y439	S440	T441	V442	I443	P444	L445	E446	A449	R450	M451	I452	R453	R457	E458	C459	W464	E465	W466	W467	R468	D469	V470	Y474	D475	W476	F477	L478	T479	R480	N481	I482	W487	G494	P265	L266	M267	V268	S269	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	R315	S316	S317	F318	T319	A320	V321	V322	L323	D326	A327	Q328	E329	H330	N331	K332	Y333	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
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4 Data and refinement statistics

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	130.41 Å 130.41 Å 129.90 Å 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 [i](#)

5.1 Standard geometry [i](#)

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	0.40	0/3728	0.88	13/5062 (0.3%)
1	B	0.42	0/3728	0.87	9/5062 (0.2%)
1	C	0.44	0/3728	0.88	8/5062 (0.2%)
1	D	0.41	0/3728	0.88	10/5062 (0.2%)
All	All	0.42	0/14912	0.88	40/20248 (0.2%)

There are no bond length outliers.

The worst 5 of 40 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	300	ASN	N-CA-C	12.48	128.45	113.23
1	A	95	ILE	N-CA-C	8.08	118.09	110.74
1	D	63	PHE	N-CA-C	-6.76	98.80	109.07
1	A	383	GLU	N-CA-C	-6.73	101.64	110.53
1	B	336	LYS	N-CA-C	-6.69	104.33	113.30

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	3657	0	3611	210	0
1	B	3657	0	3611	185	0
1	C	3657	0	3611	282	0
1	D	3657	0	3611	219	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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
All	All	14920	0	14444	882	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 882 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%)	8	28
1	B	463/471 (98%)	417 (90%)	39 (8%)	7 (2%)	8	28
1	C	463/471 (98%)	416 (90%)	41 (9%)	6 (1%)	9	32
1	D	463/471 (98%)	424 (92%)	31 (7%)	8 (2%)	7	26
All	All	1852/1884 (98%)	1678 (91%)	146 (8%)	28 (2%)	8	28

5 of 28 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	462	LEU
1	B	58	ASP
1	D	38	ILE
1	D	62	SER
1	A	465	GLU

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	412/418 (99%)	367 (89%)	45 (11%)	6	20
1	B	412/418 (99%)	371 (90%)	41 (10%)	7	24
1	C	412/418 (99%)	349 (85%)	63 (15%)	3	9
1	D	412/418 (99%)	363 (88%)	49 (12%)	5	16
All	All	1648/1672 (99%)	1450 (88%)	198 (12%)	5	16

5 of 198 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	239	LYS
1	C	440	SER
1	C	299	LYS
1	C	346	LYS
1	D	43	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 71 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	108	GLN
1	D	180	GLN
1	D	331	ASN
1	B	166	ASN
1	B	132	ASN

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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

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.