



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 8, 2026 – 04:03 PM UTC

PDB ID : 1M3J / pdb_00001m3j
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

<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

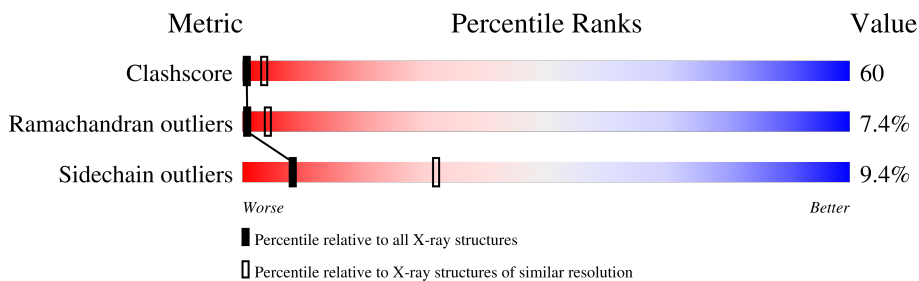
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 Å.

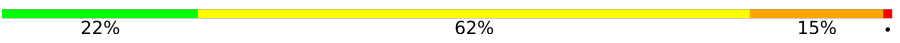
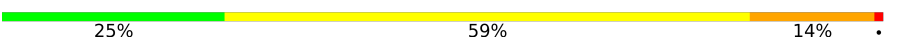
Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (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 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	

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.

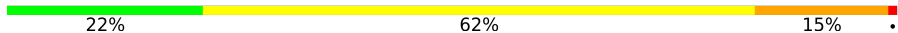
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	26	Total	O	0	0
			26	26		
2	B	31	Total	O	0	0
			31	31		

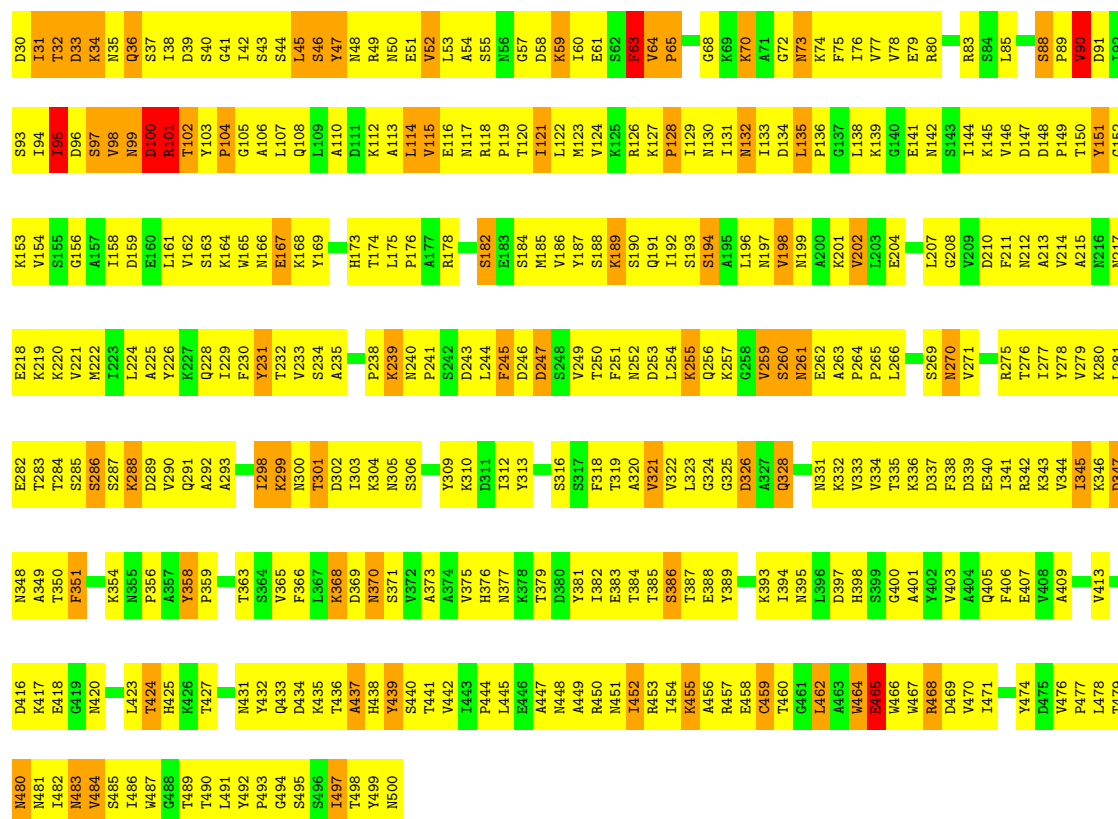
3 Residue-property plots

These plots are drawn for all protein, RNA, 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.

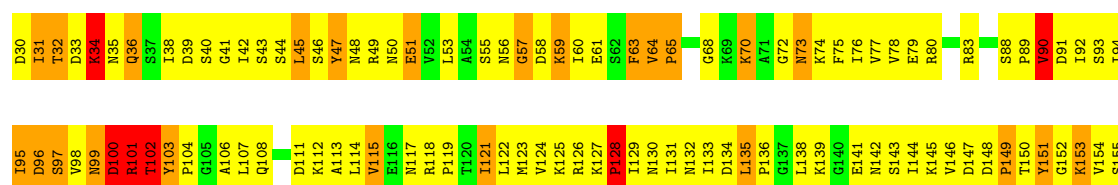
- Molecule 1: perfringolysin o

Chain A: 



- Molecule 1: perfringolysin o

Chain B: 



G156	A225	V290	K354	E418	W487	G156
A157	Y226	Q291	N355	G419	G488	A157
I158	K227	A292	P356	N420	T489	I158
D159	Q228	A293	A357	H425	L491	D159
E160	I229	F294	Y358	K426	Y492	E160
L161	F230	K295	P359	T427	P493	L161
V162	Y231	A296	I360	N431	G494	V162
S163	T232	L297	S361	Y432	I497	S163
K164	V233	K298	T362	Q433	T498	K164
W165	S234	T299	K363	D434	Y499	W165
V166	A235	N300	S364	N434	N500	V166
E167	D236	T301	V365			E167
K168	K239	D302	F366	K435		K168
Y169	N240	I303	L367	T436		Y169
T172	P241	K304	K368	A437		T172
H173	F245	N305	D369	H438		H173
R178	D246	S306	N370	Y439		R178
S182	D247	Q307	S371	S440		S182
E183	T250	G308	V372	T441		E183
S184	F251	Y309	A373	V442		S184
M185	N252	K310	A374	E446		M185
Y187	D253	D311	V375	A447		Y187
K189	L254	I312	T379	N448		K189
S190	K255	Y313	D380	A449		S190
Q191	K256	E314	Y381	A450		Q191
I192	Q257	N315	I382	R451		I192
L196	G258	S316	K382	M451		L196
N197	V259	S317	E383	I452		N197
V198	S260	F318	T384	R453		V198
M199	P265	T319	T385	I454		M199
V202	L266	A320	S386	A456		V202
L203	R261	V321	T387	R457		L203
E204	E262	L322	E388	E458		E204
L207	A263	G324	Y389	C459		L207
G208	P264	G325	S390	T460		G208
V209	P265	D326	K391	G461		V209
D210	L266	A327	G392	L462		D210
F211	S269	Q328	I394	W464		F211
N212	N270	N331	N395	E465		N212
A213	V271	K332	L396	W466		A213
V214	A272	V333	D397	W467		V214
A215	Y273	V334	H398	R468		A215
N216	G274	T335	S399	D469		N216
N217	R275	K336	G400	V470		N217
E218	T276	D337	A401	I471		E218
K219	I277	F338	Y402			K219
K220	Y278	D339	V403	D475		K220
V221	V279	E340	A404	W476		V221
M222	K280	I341	Q405	P477		M222
I223	L281	K342	F406	L478		I223
L224	E282	K343	E407	T479		L224
	T283	V344	V408	M480		
	T284	I345	A409	M481		
	S285	K346	E412	I482		
	S286	D347	V413	M483		
	S287	N348	E414	W484		
	K288			S485		
	D289			I486		

4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore 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 [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	0.55	0/3776	1.07	32/5127 (0.6%)
1	B	0.55	0/3776	1.09	33/5127 (0.6%)
All	All	0.55	0/7552	1.08	65/10254 (0.6%)

There are no bond length outliers.

The worst 5 of 65 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	90	VAL	N-CA-C	-11.26	102.66	112.12
1	A	135	LEU	CA-C-N	9.59	129.64	119.76
1	A	135	LEU	C-N-CA	9.59	129.64	119.76
1	B	64	VAL	CA-C-N	7.86	129.66	119.84
1	B	64	VAL	C-N-CA	7.86	129.66	119.84

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	3705	0	3656	450	0
1	B	3705	0	3656	440	0
2	A	26	0	0	3	0
2	B	31	0	0	0	0
All	All	7467	0	7312	890	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 60.

The worst 5 of 890 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
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:H	1:A:70:LYS:HD3	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	4
1	B	469/471 (100%)	358 (76%)	76 (16%)	35 (8%)	1	4
All	All	938/942 (100%)	716 (76%)	153 (16%)	69 (7%)	1	4

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 ⓘ

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%)	375 (90%)	43 (10%)	7	28
1	B	418/418 (100%)	382 (91%)	36 (9%)	10	36
All	All	836/836 (100%)	757 (91%)	79 (9%)	8	32

5 of 79 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	184	SER
1	B	453	ARG
1	B	239	LYS
1	B	351	PHE
1	B	475	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 34 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	300	ASN
1	B	405	GLN
1	B	451	ASN
1	A	420	ASN
1	A	291	GLN

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 [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.