



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 9, 2026 – 11:54 AM UTC

PDB ID : 3CQF / pdb_00003cqf
Title : Crystal structure of anthrolysin O (ALO)
Authors : Bourdeau, R.W.; Malito, E.; Tang, W.J.
Deposited on : 2008-04-02
Resolution : 3.10 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) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

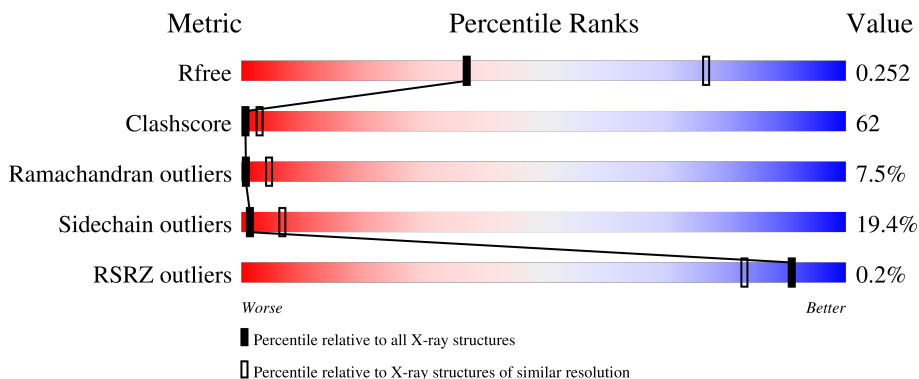
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

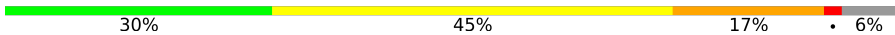
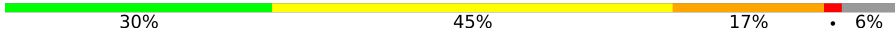
The reported resolution of this entry is 3.10 Å.

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}	180053	1456 (3.10-3.10)
Clashscore	190562	1539 (3.10-3.10)
Ramachandran outliers	187476	1467 (3.10-3.10)
Sidechain outliers	187428	1467 (3.10-3.10)
RSRZ outliers	180081	1456 (3.10-3.10)

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 $\leq 5\%$. 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.

Mol	Chain	Length	Quality of chain
1	A	489	 30% 45% 17% • 6%
1	B	489	 30% 45% 17% • 6%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 7101 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 Thiol-activated cytolysin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	462	Total	C	N	O	S	0	0	0
			3537	2229	588	714	6			
1	B	462	Total	C	N	O	S	0	0	0
			3537	2229	588	714	6			

There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	24	MET	-	expression tag	UNP Q81N62
A	25	HIS	-	expression tag	UNP Q81N62
A	26	HIS	-	expression tag	UNP Q81N62
A	27	HIS	-	expression tag	UNP Q81N62
A	28	HIS	-	expression tag	UNP Q81N62
A	29	HIS	-	expression tag	UNP Q81N62
A	30	HIS	-	expression tag	UNP Q81N62
A	31	ALA	-	expression tag	UNP Q81N62
A	32	ALA	-	expression tag	UNP Q81N62
A	33	ALA	-	expression tag	UNP Q81N62
A	34	MET	-	expression tag	UNP Q81N62
B	24	MET	-	expression tag	UNP Q81N62
B	25	HIS	-	expression tag	UNP Q81N62
B	26	HIS	-	expression tag	UNP Q81N62
B	27	HIS	-	expression tag	UNP Q81N62
B	28	HIS	-	expression tag	UNP Q81N62
B	29	HIS	-	expression tag	UNP Q81N62
B	30	HIS	-	expression tag	UNP Q81N62
B	31	ALA	-	expression tag	UNP Q81N62
B	32	ALA	-	expression tag	UNP Q81N62
B	33	ALA	-	expression tag	UNP Q81N62
B	34	MET	-	expression tag	UNP Q81N62

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	11	Total 11	O 11	0	0
2	B	16	Total 16	O 16	0	0

P506	V159	F224	E295	N368	V435	P506
T507	Q160	N225	T296	F369	I436	T507
T509	M161	A226	T297	A370	T437	A508
	P162	V227	S298	Y371		T509
	T163	A228	K299	P372	W441	
	Y164	N229	S300	I373	E442	
		G230	K301	S374	G443	
	V167	E231	D302	Y375	S444	
	A168	K232	V303	T376	G445	
		K233	Q304	S377	G445	
	V171	V234	A305	T378	T449	
	D172	M235	A306	F379		
	D173	V236	F307		T454	
	L174		K308	N383	V455	
		Y239	A309		I456	
	T177		L310	A386	P457	
	W178	V246		A387	L458	
	N179	S247	N314	Y388	P459	
	E180	A248	H389	N390	P460	
	K181	E249	S319	N391	N461	
	Y182	L250		T392	S462	
	S183	P251	D324	D393	K463	
	T184	N252	I325	Y394	N464	
	T185		F326	I395	I465	
	H186	S255	E327	E396	K466	
	T187	D256	E328	T397	I467	
	L188	F257	S329	T398	V468	
	P189	D259	T330	T399	A469	
		F331	F331	T400	R470	
	M192	N260	T332		E471	
	Q193	S261	A333	S403	C472	
	Y194	V262	V334		T473	
	T195	T263	V335	K406	G474	
	E196	F264	L336	M407	L475	
	M198	D265	G337	T408	A476	
	S197	E266	G338	L409	W477	
	V199	L267	D339	D410	E478	
	Y200	T268	ALA		W479	
	S201	R269	LYS	H411	W480	
	K202	K270	GLU	Y412		
	Q203	G271	HIS	G413	I484	
			ASN	A414	N485	
	I205	S275		Y415	E486	
	A206	A276	K345		Q487	
	S207	P277	V346	Q418		
	A208	P278	V347	F419	H488	
	L209	V279	T348	D420	V489	
	N210	M280		V421	P490	
	V211	V281	N352	S422	L491	
	N212	S282		W423	T492	
	A213	N283	R355	D424		
	Y215	V284	T358	E425	I495	
	L216	A285	K359	F426	K496	
		Y286	D360	T427	V497	
		G287	N361	F428	S498	
		R288		D429	I499	
	S219		L364	Q430		
	L220	Y291	S365		T502	
	N221		F366	K433	T503	
	I222		K367	E434	L504	
	D223	L294			Y505	

4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	141.74Å 141.75Å 294.10Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 3.10 30.00 – 3.10	Depositor EDS
% Data completeness (in resolution range)	98.4 (30.00-3.10) 98.4 (30.00-3.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.47 (at 3.11Å)	Xtriage
Refinement program	REFMAC 5.4.0067	Depositor
R, R_{free}	0.268 , 0.294 (Not available) , 0.252	Depositor DCC
R_{free} test set	2675 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å ²)	87.4	Xtriage
Anisotropy	0.041	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 96.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.487 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	7101	wwPDB-VP
Average B, all atoms (Å ²)	76.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.86% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

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	0.87	3/3606 (0.1%)	1.21	23/4922 (0.5%)
1	B	0.87	3/3606 (0.1%)	1.21	22/4922 (0.4%)
All	All	0.87	6/7212 (0.1%)	1.21	45/9844 (0.5%)

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	200	TYR	CA-C	5.96	1.57	1.52
1	A	200	TYR	CA-C	5.75	1.56	1.52
1	A	484	ILE	CA-CB	5.58	1.61	1.54
1	B	246	VAL	CA-CB	-5.33	1.48	1.54
1	B	484	ILE	CA-CB	5.16	1.61	1.54

The worst 5 of 45 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	388	VAL	N-CA-C	10.55	117.50	106.21
1	B	388	VAL	N-CA-C	10.24	117.17	106.21
1	A	140	LYS	CA-C-N	-8.12	112.35	120.31
1	A	140	LYS	C-N-CA	-8.12	112.35	120.31
1	B	153	LYS	N-CA-C	-7.71	103.70	113.72

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	3537	0	3406	435	0
1	B	3537	0	3406	432	0
2	A	11	0	0	1	0
2	B	16	0	0	1	0
All	All	7101	0	6812	864	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 62.

The worst 5 of 864 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:504:LEU:HD23	1:B:504:LEU:C	1.54	1.31
1:A:152:ARG:NH2	1:A:178:TRP:HB2	1.46	1.30
1:B:152:ARG:NH2	1:B:178:TRP:HB2	1.47	1.26
1:A:504:LEU:C	1:A:504:LEU:HD23	1.56	1.22
1:A:433:LYS:HA	1:A:433:LYS:CE	1.71	1.17

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	458/489 (94%)	358 (78%)	66 (14%)	34 (7%)	1 5
1	B	458/489 (94%)	357 (78%)	66 (14%)	35 (8%)	1 4
All	All	916/978 (94%)	715 (78%)	132 (14%)	69 (8%)	1 4

5 of 69 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	72	LYS

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Mol	Chain	Res	Type
1	A	73	VAL
1	A	74	GLU
1	A	100	THR
1	A	151	MET

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	387/423 (92%)	313 (81%)	74 (19%)	1	7
1	B	387/423 (92%)	311 (80%)	76 (20%)	1	6
All	All	774/846 (92%)	624 (81%)	150 (19%)	1	7

5 of 150 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	295	GLU
1	B	491	LEU
1	B	314	ASN
1	B	395	ILE
1	A	332	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 37 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	389	HIS
1	B	488	ASN
1	B	391	ASN
1	B	431	ASN
1	A	411	HIS

5.3.3 RNA ⓘ

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 [i](#)

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

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	462/489 (94%)	-1.01	1 (0%) 91 83	51, 76, 99, 105	0
1	B	462/489 (94%)	-1.03	1 (0%) 91 83	51, 76, 99, 105	0
All	All	924/978 (94%)	-1.02	2 (0%) 91 83	51, 76, 99, 105	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	366	PHE	2.1
1	A	339	ASP	2.1

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.