



wwPDB X-ray Structure Validation Summary Report ⓘ

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PDB ID : 3CQF
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
<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) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

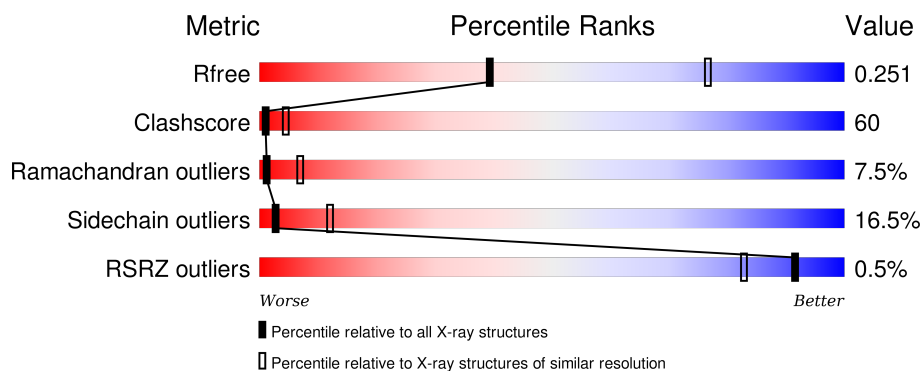
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

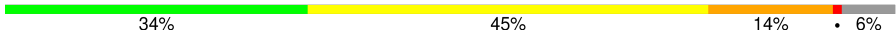

The reported resolution of this entry is 3.10 Å.

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}	91344	1114 (3.14-3.06)
Clashscore	102246	1222 (3.14-3.06)
Ramachandran outliers	100387	1174 (3.14-3.06)
Sidechain outliers	100360	1174 (3.14-3.06)
RSRZ outliers	91569	1119 (3.14-3.06)

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.

Mol	Chain	Length	Quality of chain
1	A	489	 34% 45% 14% • 6%
1	B	489	 34% 46% 14% • 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

S444	G445	T449	T454	Y455	I456	P457	L458	P459	P460	M461	S462	K463	M464	K465	K466	I467	V468	A469	R470	E471	C472	T473	W477	E478	W479	W480	R481	I484	M485	E486	Q487	M488	V489	P490	L491	T492	I495	K496	V497	S498	I499	T502	T503	L504	Y505	P506	T507	A508	T509	H512	S231	K232	K233	V234	M235	V236	Y239	I242	V246	S247	A248	E249	L250	P251	N252	S255	D256	L257	F258	N259	N260	S261	V262	D265	E266	L267	T268	R269	K270	G271	S275	A276	P277	P278	V279	M280	V281	S282	N283	V284	A285	Y286	G287	R288	Y291	L294	E295	T296	T297	S298	K299	S300			
S374	T375	T376	S377	T378	F379	N383	A386	A387	V388	R389	N390	N391	T392	D393	Y394	I395	E396	T397	T398	T399	T400	S403	K406	W407	T408	L409	D410	H411	Y412	G413	A414	Y415	Q418	F419	D420	V421	S422	H423	D424	E425	F426	T427	F428	D429	K433	E434	V435	L436	T437	W441	E442	G443	K301	D302	V303	Q304	A305	A306	F307	K308	A309	L310	N314	S319	D324	I325	F326	E327	E328	S329	T330	F331	T332	A333	V334	V335	L336	G337	G338	D339	A340	L341	G342	H343	A344	K345	V346	V347	T348	N352	R355	T358	K359	D360	N361	L364	S365	F366	K367	N368	P369	A370	Y371	P372	I373

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 30.65 – 3.10	Depositor EDS
% Data completeness (in resolution range)	98.4 (30.00-3.10) 98.4 (30.65-3.10)	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 0.256 , 0.251	Depositor DCC
R_{free} test set	2675 reflections (5.33%)	DCC
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 , 44.9	EDS
Estimated twinning fraction	0.487 for -k,-h,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 52860 reflections	Xtriage
F_o, F_c correlation	0.91	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, 0.375 respectively for untwinned datasets, and 0.333, 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	0.66	0/3606	0.81	2/4922 (0.0%)
1	B	0.66	0/3606	0.81	2/4922 (0.0%)
All	All	0.66	0/7212	0.81	4/9844 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	481	ARG	NE-CZ-NH1	-5.58	117.51	120.30
1	B	481	ARG	NE-CZ-NH1	-5.51	117.55	120.30
1	B	149	PRO	N-CA-CB	5.34	109.71	103.30
1	A	149	PRO	N-CA-CB	5.20	109.54	103.30

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	3537	0	3406	413	0
1	B	3537	0	3406	416	0
2	A	11	0	0	1	0
2	B	16	0	0	1	0
All	All	7101	0	6812	827	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 827 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:152:ARG:NH2	1:A:178:TRP:HB2	1.46	1.30
1:B:504:LEU:C	1:B:504:LEU:HD23	1.54	1.26
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	1.18
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	7
1	B	458/489 (94%)	357 (78%)	66 (14%)	35 (8%)	1	7
All	All	916/978 (94%)	715 (78%)	132 (14%)	69 (8%)	1	7

5 of 69 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	72	LYS
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%)	323 (84%)	64 (16%)	3	12
1	B	387/423 (92%)	323 (84%)	64 (16%)	3	12
All	All	774/846 (92%)	646 (84%)	128 (16%)	3	12

5 of 128 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	468	VAL
1	B	106	LEU
1	B	436	LEU
1	A	492	THR
1	B	61	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 26 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	418	GLN
1	B	113	ASN
1	B	418	GLN
1	A	512	HIS
1	B	83	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 [i](#)

There are no carbohydrates 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%)	0.25	2 (0%) 93 85	51, 76, 99, 105	0
1	B	462/489 (94%)	0.25	3 (0%) 90 80	51, 76, 99, 105	0
All	All	924/978 (94%)	0.25	5 (0%) 91 83	51, 76, 99, 105	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	79	LYS	2.9
1	B	79	LYS	2.6
1	B	242	ILE	2.6
1	A	230	GLY	2.5
1	B	144	ILE	2.2

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 carbohydrates 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.