



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 1, 2026 – 08:16 PM UTC

PDB ID : 2X2Z / pdb_00002x2z
Title : Crystal structure AMA1 from Toxoplasma gondii
Authors : Crawford, J.; Tonkin, M.L.; Grujic, O.; Boulanger, M.J.
Deposited on : 2010-01-18
Resolution : 2.00 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
Mogul : 2022.3.0, CSD as543be (2022)
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

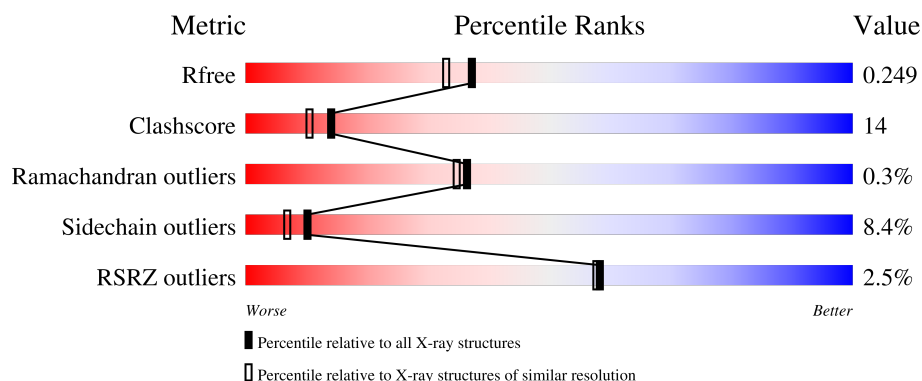
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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))
R_{free}	180053	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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 $\leq 5\%$. 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	456	
1	B	456	
1	D	456	
1	E	456	

2 Entry composition [i](#)

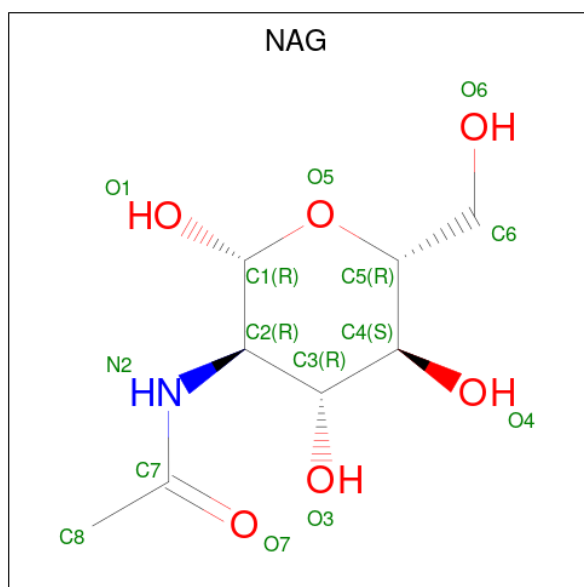
There are 4 unique types of molecules in this entry. The entry contains 13675 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 APICAL MEMBRANE ANTIGEN 1, PUTATIVE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	407	Total	C	N	O	S	0	1	0
			3218	2022	550	624	22			
1	B	401	Total	C	N	O	S	0	0	0
			3173	1999	540	612	22			
1	D	367	Total	C	N	O	S	0	0	0
			2909	1836	497	556	20			
1	E	396	Total	C	N	O	S	0	1	0
			3143	1978	537	606	22			

- Molecule 2 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



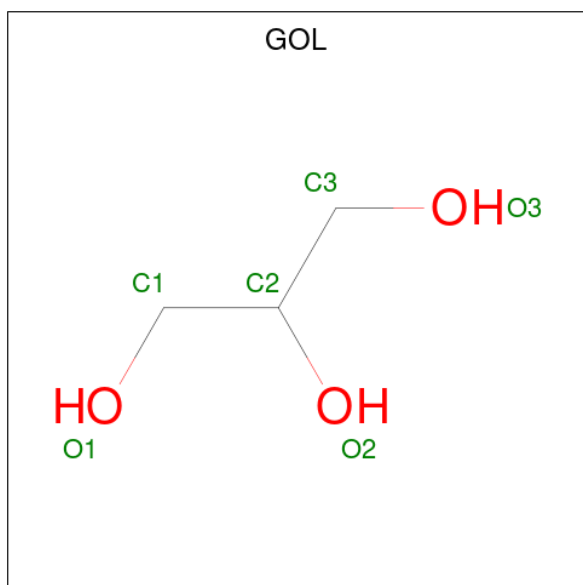
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	D	1	Total	C	N	O	0	0
			14	8	1	5		
2	E	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	D	1	Total	C	O	0	0
			6	3	3		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	316	Total	O	0	0
			316	316		
4	B	294	Total	O	0	0
			294	294		
4	D	276	Total	O	0	0
			276	276		
4	E	284	Total	O	0	0
			284	284		

- Molecule 1: APICAL MEMBRANE ANTIGEN 1, PUTATIVE





4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	66.15Å 76.07Å 88.25Å 72.19° 71.44° 72.90°	Depositor
Resolution (Å)	43.90 – 2.00 43.90 – 2.00	Depositor EDS
% Data completeness (in resolution range)	96.4 (43.90-2.00) 96.4 (43.90-2.00)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.00 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.5.0088	Depositor
R, R_{free}	0.180 , 0.248 0.179 , 0.249	Depositor DCC
R_{free} test set	4915 reflections (4.80%)	wwPDB-VP
Wilson B-factor (Å ²)	23.1	Xtriage
Anisotropy	0.040	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 49.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	13675	wwPDB-VP
Average B, all atoms (Å ²)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.37% 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](#)

Bond lengths and bond angles in the following residue types are not validated in this section: NAG, GOL

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	1.22	3/3308 (0.1%)	1.16	5/4491 (0.1%)
1	B	1.28	10/3258 (0.3%)	1.22	13/4418 (0.3%)
1	D	1.33	11/2985 (0.4%)	1.21	17/4039 (0.4%)
1	E	1.21	4/3228 (0.1%)	1.18	8/4375 (0.2%)
All	All	1.26	28/12779 (0.2%)	1.19	43/17323 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	2
1	D	0	2
1	E	0	1
All	All	0	6

The worst 5 of 28 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	242	CYS	CA-CB	9.13	1.69	1.53
1	D	255	CYS	CB-SG	-8.67	1.52	1.81
1	B	242	CYS	CA-CB	8.58	1.68	1.53
1	B	255	CYS	CB-SG	-8.42	1.53	1.81
1	D	290	ALA	CA-CB	8.01	1.66	1.53

The worst 5 of 43 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	199	PHE	CA-C-N	-10.24	108.33	126.45
1	E	199	PHE	C-N-CA	-10.24	108.33	126.45
1	D	255	CYS	N-CA-C	9.11	123.79	110.59
1	E	351	ASN	N-CA-C	8.54	123.06	112.47
1	B	242	CYS	N-CA-C	-8.42	93.32	108.48

There are no chirality outliers.

5 of 6 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	429	PRO	Peptide
1	B	241	TYR	Peptide
1	B	430	GLU	Peptide
1	D	241	TYR	Peptide
1	D	259	ARG	Peptide

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	3218	0	3039	76	0
1	B	3173	0	3002	96	0
1	D	2909	0	2756	79	0
1	E	3143	0	2971	105	0
2	A	14	0	13	0	0
2	B	14	0	13	0	0
2	D	14	0	13	3	0
2	E	14	0	13	2	0
3	D	6	0	8	0	0
4	A	316	0	0	10	0
4	B	294	0	0	18	0
4	D	276	0	0	19	0
4	E	284	0	0	20	0
All	All	13675	0	11828	349	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 14.

The worst 5 of 349 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:242:CYS:CB	1:B:242:CYS:SG	2.02	1.48
1:D:242:CYS:SG	1:D:242:CYS:CB	2.04	1.44
1:D:398:SER:HB2	4:D:2254:HOH:O	1.25	1.30
1:E:119:ILE:HG13	4:E:2041:HOH:O	0.99	1.15
1:D:435:CYS:HB2	1:D:459:CYS:SG	1.88	1.14

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	402/456 (88%)	387 (96%)	14 (4%)	1 (0%)	43	42
1	B	391/456 (86%)	378 (97%)	12 (3%)	1 (0%)	36	35
1	D	352/456 (77%)	337 (96%)	14 (4%)	1 (0%)	36	35
1	E	387/456 (85%)	370 (96%)	16 (4%)	1 (0%)	36	35
All	All	1532/1824 (84%)	1472 (96%)	56 (4%)	4 (0%)	36	35

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	208	ASN
1	B	427	PRO
1	E	208	ASN
1	D	332	ASP

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	356/388 (92%)	327 (92%)	29 (8%)	11	7
1	B	351/388 (90%)	317 (90%)	34 (10%)	8	5
1	D	321/388 (83%)	294 (92%)	27 (8%)	10	7
1	E	347/388 (89%)	321 (92%)	26 (8%)	12	9
All	All	1375/1552 (89%)	1259 (92%)	116 (8%)	10	7

5 of 116 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	426	PRO
1	E	411	GLU
1	D	171	ILE
1	E	408	SER
1	E	207	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 62 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	455	GLN
1	E	340	HIS
1	D	289	GLN
1	E	323	GLN
1	E	434	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 ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

5 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	E	1001	1	14,14,15	0.69	0	17,19,21	1.39	3 (17%)
2	NAG	B	1001	1	14,14,15	1.09	1 (7%)	17,19,21	1.12	1 (5%)
2	NAG	A	1001	1	14,14,15	0.82	0	17,19,21	1.94	3 (17%)
2	NAG	D	1001	1	14,14,15	0.65	0	17,19,21	2.22	5 (29%)
3	GOL	D	1472	-	5,5,5	0.39	0	5,5,5	0.52	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	E	1001	1	-	3/6/23/26	0/1/1/1
2	NAG	B	1001	1	-	2/6/23/26	0/1/1/1
2	NAG	A	1001	1	-	2/6/23/26	0/1/1/1
2	NAG	D	1001	1	-	4/6/23/26	0/1/1/1
3	GOL	D	1472	-	-	0/4/4/4	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1001	NAG	O5-C1	-3.08	1.38	1.43

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1001	NAG	C2-N2-C7	5.66	130.48	122.90
2	D	1001	NAG	O7-C7-C8	-4.34	114.33	122.05
2	D	1001	NAG	C8-C7-N2	4.21	123.11	116.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	1001	NAG	O5-C5-C6	3.65	114.77	107.66
2	D	1001	NAG	C4-C3-C2	3.55	116.22	111.02

There are no chirality outliers.

5 of 11 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1001	NAG	C8-C7-N2-C2
2	A	1001	NAG	O7-C7-N2-C2
2	B	1001	NAG	C8-C7-N2-C2
2	B	1001	NAG	O7-C7-N2-C2
2	D	1001	NAG	C8-C7-N2-C2

There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	1001	NAG	2	0
2	D	1001	NAG	3	0

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	407/456 (89%)	-0.22	9 (2%) 62 61	9, 22, 45, 57	1 (0%)
1	B	401/456 (87%)	-0.18	6 (1%) 72 71	10, 23, 46, 56	0
1	D	367/456 (80%)	-0.06	17 (4%) 37 36	12, 22, 56, 67	0
1	E	396/456 (86%)	-0.13	7 (1%) 67 67	12, 24, 42, 59	1 (0%)
All	All	1571/1824 (86%)	-0.15	39 (2%) 58 58	9, 23, 46, 67	2 (0%)

The worst 5 of 39 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	441	PRO	4.3
1	D	444	PHE	4.0
1	B	166	PRO	3.6
1	D	471	CYS	3.2
1	D	461	GLY	3.2

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 oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q < 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	NAG	D	1001	14/15	0.82	0.12	35,38,42,43	0
2	NAG	E	1001	14/15	0.84	0.10	28,32,37,37	0
2	NAG	B	1001	14/15	0.88	0.09	22,27,34,38	0
3	GOL	D	1472	6/6	0.94	0.07	20,25,26,26	0
2	NAG	A	1001	14/15	0.95	0.07	18,24,28,30	0

6.5 Other polymers [i](#)

There are no such residues in this entry.