



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 07:55 AM UTC

PDB ID : 3PAL / pdb_00003pal
Title : IONIC INTERACTIONS WITH PARVALBUMINS. CRYSTAL STRUCTURE DETERMINATION OF PIKE 4.10 PARVALBUMIN IN FOUR DIFFERENT IONIC ENVIRONMENTS
Authors : Declercq, J.P.; Tinant, B.; Parello, J.; Rambaud, J.
Deposited on : 1990-11-08
Resolution : 2.40 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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

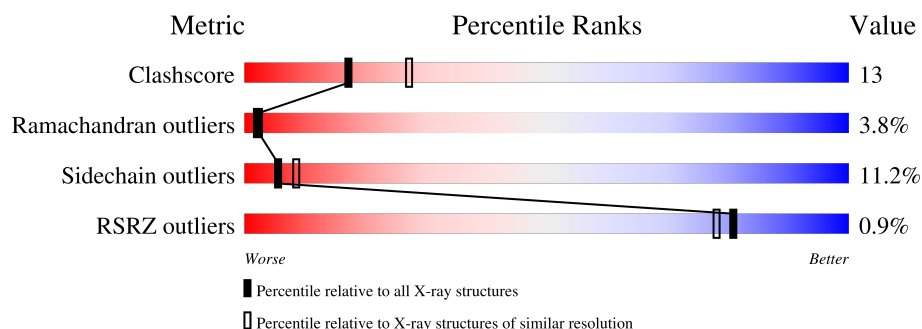
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

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	108	40% 42% 17% .

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 903 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 PARVALBUMIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	108	Total	C	N	O	S	3	0	0
			805	512	127	163	3			

- Molecule 2 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Ca	0	0
			2	2		

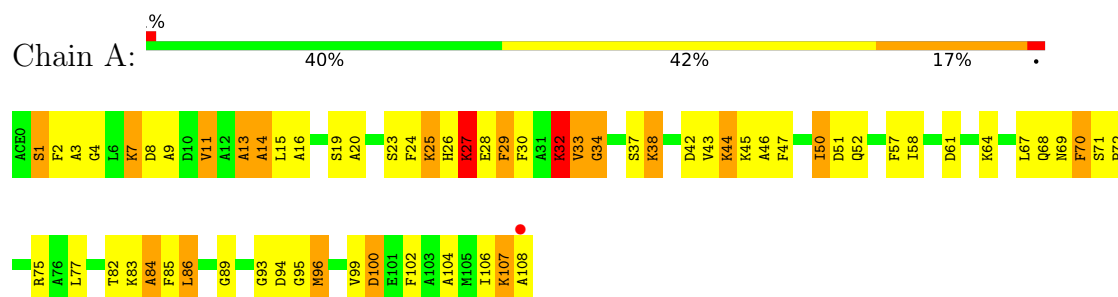
- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Mg	0	0
			1	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	95	Total	O	0	0
			95	95		

- Molecule 1: PARVALBUMIN



4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	57.80Å 57.80Å 90.10Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	(Not available) – 2.40 48.65 – 2.40	Depositor EDS
% Data completeness (in resolution range)	(Not available) ((Not available)-2.40) 71.6 (48.65-2.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$	-	Xtriage
Refinement program	EREF	Depositor
R, R_{free}	0.167 , (Not available) 0.174 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	14.9	Xtriage
Anisotropy	0.182	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 85.0	EDS
L-test for twinning ¹	$\langle L \rangle = 0.36$, $\langle L^2 \rangle = 0.19$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	903	wwPDB-VP
Average B, all atoms (Å ²)	14.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.55% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Theoretical 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, CA, ACE

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	1.46	4/815 (0.5%)	2.38	51/1091 (4.7%)

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	15

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	26	HIS	CE1-NE2	13.06	1.45	1.32
1	A	26	HIS	ND1-CE1	8.18	1.40	1.32
1	A	58	ILE	N-CA	5.73	1.52	1.46
1	A	26	HIS	CG-ND1	5.58	1.44	1.38

All (51) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	44	LYS	CA-C-N	-9.79	107.16	120.28
1	A	44	LYS	C-N-CA	-9.79	107.16	120.28
1	A	85	PHE	CA-CB-CG	8.31	122.11	113.80
1	A	52	GLN	CA-C-N	-7.50	110.65	122.65
1	A	52	GLN	C-N-CA	-7.50	110.65	122.65
1	A	33	VAL	N-CA-C	-7.39	103.01	113.07
1	A	86	LEU	N-CA-C	-7.03	104.17	112.89
1	A	26	HIS	N-CA-C	6.84	119.37	111.02
1	A	100	ASP	CA-CB-CG	-6.67	105.93	112.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	7	LYS	CA-C-N	6.66	134.26	121.54
1	A	7	LYS	C-N-CA	6.66	134.26	121.54
1	A	57	PHE	CA-CB-CG	6.63	120.43	113.80
1	A	9	ALA	O-C-N	6.58	129.20	122.09
1	A	45	LYS	O-C-N	6.40	128.91	122.12
1	A	96	MET	CA-C-O	-6.32	114.50	121.33
1	A	94	ASP	O-C-N	6.18	130.06	122.34
1	A	70	PHE	CA-CB-CG	-6.15	107.65	113.80
1	A	86	LEU	N-CA-CB	-6.11	100.45	110.40
1	A	13	ALA	CB-CA-C	-6.05	101.64	110.96
1	A	70	PHE	CA-C-N	-6.03	110.45	122.40
1	A	70	PHE	C-N-CA	-6.03	110.45	122.40
1	A	7	LYS	O-C-N	6.02	130.39	123.29
1	A	14	ALA	CB-CA-C	-5.98	101.42	110.92
1	A	47	PHE	N-CA-C	-5.90	104.85	111.28
1	A	27	LYS	O-C-N	5.75	129.35	122.27
1	A	84	ALA	N-CA-CB	-5.68	101.56	110.30
1	A	102	PHE	O-C-N	5.63	128.11	122.08
1	A	96	MET	O-C-N	5.58	129.61	123.25
1	A	16	ALA	N-CA-CB	5.57	118.40	110.16
1	A	24	PHE	N-CA-CB	5.55	118.12	109.85
1	A	50	ILE	N-CA-C	-5.50	104.86	112.50
1	A	9	ALA	CB-CA-C	-5.47	102.26	110.90
1	A	28	GLU	CA-CB-CG	-5.46	103.19	114.10
1	A	11	VAL	CA-C-O	-5.43	114.89	120.71
1	A	37	SER	N-CA-CB	-5.42	103.68	111.54
1	A	19	SER	CA-C-N	-5.33	112.54	121.39
1	A	19	SER	C-N-CA	-5.33	112.54	121.39
1	A	77	LEU	O-C-N	-5.29	116.77	123.01
1	A	104	ALA	N-CA-C	5.25	117.41	111.11
1	A	69	ASN	N-CA-C	-5.24	106.15	112.54
1	A	72	PRO	CB-CA-C	-5.18	104.44	113.20
1	A	70	PHE	N-CA-C	-5.16	105.81	112.68
1	A	47	PHE	CB-CA-C	-5.16	102.23	110.79
1	A	94	ASP	N-CA-CB	5.14	118.09	110.49
1	A	93	GLY	CA-C-N	-5.11	114.11	122.54
1	A	93	GLY	C-N-CA	-5.11	114.11	122.54
1	A	82	THR	CA-C-N	-5.11	112.67	121.66
1	A	82	THR	C-N-CA	-5.11	112.67	121.66
1	A	32	LYS	N-CA-CB	-5.10	102.07	109.82
1	A	33	VAL	CA-CB-CG2	5.07	119.03	110.40
1	A	42	ASP	O-C-N	5.01	128.44	122.27

There are no chirality outliers.

All (15) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	100	ASP	Mainchain
1	A	107	LYS	Mainchain
1	A	13	ALA	Mainchain
1	A	29	PHE	Mainchain
1	A	32	LYS	Mainchain
1	A	34	GLY	Mainchain
1	A	43	VAL	Mainchain
1	A	44	LYS	Mainchain
1	A	51	ASP	Mainchain
1	A	61	ASP	Mainchain
1	A	70	PHE	Mainchain
1	A	84	ALA	Mainchain
1	A	86	LEU	Mainchain
1	A	89	GLY	Mainchain
1	A	95	GLY	Mainchain

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	805	0	784	20	0
2	A	2	0	0	0	0
3	A	1	0	0	0	0
4	A	95	0	0	1	0
All	All	903	0	784	20	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 13.

All (20) 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:3:ALA:O	1:A:38:LYS:HE2	1.94	0.68
1:A:27:LYS:HE3	1:A:30:PHE:HB2	1.77	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:11:VAL:HG22	1:A:33:VAL:HG22	1.83	0.61
1:A:14:ALA:HA	1:A:32:LYS:HD3	1.85	0.58
1:A:14:ALA:HA	1:A:32:LYS:CD	2.37	0.55
1:A:106:ILE:HG22	1:A:108:ALA:H	1.70	0.55
1:A:29:PHE:O	1:A:32:LYS:HB2	2.12	0.50
1:A:25:LYS:HD2	4:A:287:HOH:O	2.13	0.48
1:A:34:GLY:O	1:A:38:LYS:HG2	2.15	0.47
1:A:68:GLN:HA	1:A:71:SER:O	2.15	0.46
1:A:1:SER:O	1:A:4:GLY:N	2.47	0.45
1:A:83:LYS:HE2	1:A:83:LYS:HB3	1.47	0.44
1:A:38:LYS:HD2	1:A:38:LYS:HA	1.62	0.44
1:A:67:LEU:HD23	1:A:67:LEU:HA	1.78	0.43
1:A:75:ARG:HH11	1:A:75:ARG:HD2	1.71	0.43
1:A:27:LYS:HE3	1:A:27:LYS:HA	2.02	0.42
1:A:20:ALA:HB3	1:A:23:SER:HB3	2.02	0.42
1:A:27:LYS:HE3	1:A:30:PHE:CB	2.48	0.42
1:A:46:ALA:O	1:A:50:ILE:HG13	2.20	0.41
1:A:27:LYS:HD3	1:A:27:LYS:O	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	106/108 (98%)	101 (95%)	1 (1%)	4 (4%)	2 2

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	2	PHE
1	A	8	ASP
1	A	1	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	107	LYS

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	80/80 (100%)	71 (89%)	9 (11%)	5 8

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	LYS
1	A	15	LEU
1	A	25	LYS
1	A	27	LYS
1	A	32	LYS
1	A	38	LYS
1	A	64	LYS
1	A	96	MET
1	A	99	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	52	GLN

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](#)

Of 3 ligands modelled in this entry, 3 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	107/108 (99%)	-0.73	1 (0%) 81 78	5, 10, 28, 60	1 (0%)

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	108	ALA	4.2

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(Å ²)	Q<0.9
2	CA	A	110	1/1	0.98	0.02	6,6,6,6	0
2	CA	A	111	1/1	1.00	0.03	7,7,7,7	0
3	MG	A	223	1/1	1.00	0.05	5,5,5,5	0

6.5 Other polymers [i](#)

There are no such residues in this entry.