Full wwPDB X-ray Structure Validation Report (i)

May 29, 2024 – 03:47 PM EDT

PDB ID	:	1ALC
Title	:	REFINED STRUCTURE OF BABOON ALPHA-LACTALBUMIN AT 1.7 ANGSTROMS RESOLUTION. COMPARISON WITH C-TYPE LYSOZYME
Authors	:	Acharya, K.R.; Stuart, D.I.; Phillips, D.C.
Deposited on	:	1989-08-14
Resolution	:	1.70 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 (i) 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 (i)) were used in the production of this report:

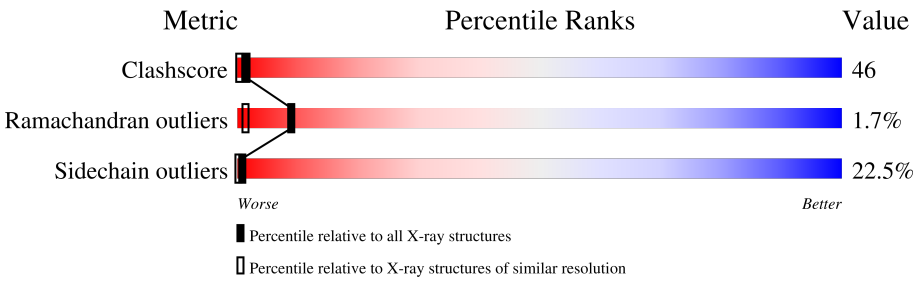
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.70 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	141614	4695 (1.70-1.70)
Ramachandran outliers	138981	4610 (1.70-1.70)
Sidechain outliers	138945	4610 (1.70-1.70)

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 <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	123	42% 37% 15% 5% •

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 1131 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 ALPHA-LACTALBUMIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	122	980	618	156	196	10	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	45	ASP	ASN	conflict	UNP P12065

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Ca		
2	A	1	1	1	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	150	150	150	0	0

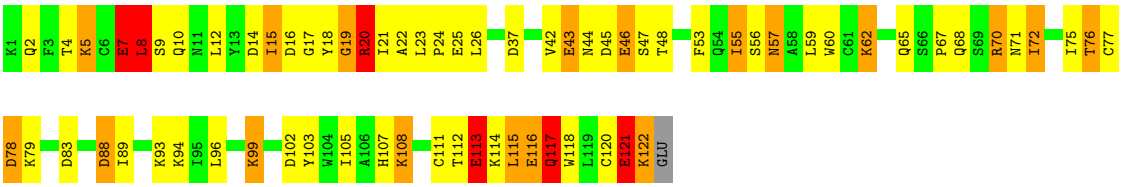
3 Residue-property plots (i)

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: ALPHA-LACTALBUMIN

Chain A: 42% 37% 15% 5%



4 Data and refinement statistics (i)

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	35.50Å 69.10Å 46.10Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	(Not available) – 1.70	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-1.70)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROLSQ	Depositor
R, R_{free}	0.220 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	1131	wwPDB-VP
Average B, all atoms ($Å^2$)	29.0	wwPDB-VP

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: CA

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	1.09	2/998 (0.2%)	1.60	16/1348 (1.2%)

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	1	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	121	GLU	CG-CD	11.45	1.69	1.51
1	A	19	GLY	CA-C	6.97	1.63	1.51

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	121	GLU	CB-CG-CD	8.96	138.40	114.20
1	A	122	LYS	CA-C-O	-8.47	102.31	120.10
1	A	121	GLU	CA-CB-CG	-8.45	94.81	113.40
1	A	122	LYS	CA-CB-CG	8.07	131.15	113.40
1	A	122	LYS	N-CA-CB	7.94	124.90	110.60
1	A	19	GLY	N-CA-C	7.19	131.08	113.10
1	A	19	GLY	CA-C-N	-7.18	101.40	117.20
1	A	20	ARG	NE-CZ-NH2	6.99	123.79	120.30
1	A	70	ARG	NE-CZ-NH1	6.93	123.77	120.30
1	A	19	GLY	O-C-N	6.41	132.95	122.70
1	A	83	ASP	CB-CG-OD2	6.39	124.05	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	77	CYS	O-C-N	6.30	132.77	122.70
1	A	121	GLU	O-C-N	6.26	132.72	122.70
1	A	8	LEU	CA-CB-CG	6.18	129.51	115.30
1	A	113	GLU	CA-CB-CG	6.18	126.99	113.40
1	A	7	GLU	CB-CA-C	5.64	121.67	110.40

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	122	LYS	CA

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	121	GLU	Peptide

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	980	0	941	89	3
2	A	1	0	0	0	0
3	A	150	0	0	22	8
All	All	1131	0	941	89	9

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 46.

All (89) 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:26:LEU:HD11	3:A:349:HOH:O	1.18	1.33
1:A:122:LYS:HG3	3:A:328:HOH:O	1.39	1.23
1:A:55:ILE:HD13	1:A:60:TRP:HB2	1.23	1.14
1:A:55:ILE:C	1:A:55:ILE:HD12	1.66	1.14
1:A:105:ILE:HB	3:A:340:HOH:O	1.45	1.13

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:18:TYR:HD1	3:A:294:HOH:O	1.31	1.10
1:A:70:ARG:HB3	1:A:72:ILE:HD11	1.33	1.10
1:A:43:GLU:HG3	3:A:317:HOH:O	0.92	1.09
1:A:12:LEU:HB3	1:A:15:ILE:HD13	1.09	1.08
1:A:55:ILE:CD1	1:A:60:TRP:HB2	1.88	1.03
1:A:114:LYS:HA	3:A:269:HOH:O	1.59	1.02
1:A:26:LEU:CD1	3:A:349:HOH:O	1.80	1.02
1:A:19:GLY:O	1:A:20:ARG:HG3	1.60	1.01
1:A:4:THR:HG22	1:A:7:GLU:HB3	1.42	1.01
1:A:12:LEU:HB3	1:A:15:ILE:CD1	1.98	0.93
1:A:9:SER:HB3	3:A:309:HOH:O	1.75	0.87
1:A:105:ILE:HG21	3:A:342:HOH:O	1.74	0.84
1:A:55:ILE:C	1:A:55:ILE:CD1	2.45	0.84
1:A:72:ILE:N	1:A:72:ILE:HD13	1.93	0.82
1:A:105:ILE:CG2	3:A:342:HOH:O	2.28	0.80
1:A:12:LEU:CB	1:A:15:ILE:HD13	2.03	0.80
1:A:120:CYS:SG	3:A:220:HOH:O	2.40	0.79
1:A:55:ILE:HD13	1:A:60:TRP:CB	2.09	0.79
1:A:55:ILE:HD12	1:A:56:SER:N	1.97	0.79
1:A:9:SER:CB	3:A:309:HOH:O	2.31	0.75
1:A:18:TYR:CD1	3:A:294:HOH:O	2.14	0.74
1:A:105:ILE:HG12	1:A:105:ILE:O	1.87	0.74
1:A:48:THR:H	1:A:57:ASN:HD21	1.36	0.74
1:A:99:LYS:HG2	1:A:103:TYR:HB2	1.68	0.73
1:A:25:GLU:CG	1:A:107:HIS:NE2	2.51	0.73
1:A:70:ARG:HB3	1:A:72:ILE:CD1	2.15	0.73
1:A:114:LYS:O	1:A:114:LYS:CG	2.36	0.71
1:A:25:GLU:HG3	1:A:107:HIS:NE2	2.05	0.70
1:A:76:THR:HG23	1:A:79:LYS:HG2	1.74	0.69
1:A:115:LEU:HA	1:A:118:TRP:HD1	1.57	0.69
1:A:62:LYS:HD2	1:A:76:THR:HA	1.75	0.67
1:A:19:GLY:C	1:A:20:ARG:HG3	2.13	0.67
1:A:16:ASP:OD2	3:A:311:HOH:O	2.13	0.67
1:A:2:GLN:HE21	1:A:37:ASP:HB2	1.60	0.66
1:A:114:LYS:O	1:A:114:LYS:HG3	1.94	0.66
1:A:4:THR:CG2	1:A:7:GLU:H	2.09	0.65
1:A:55:ILE:HD12	1:A:55:ILE:O	1.97	0.64
1:A:4:THR:CG2	1:A:7:GLU:HB3	2.23	0.64
1:A:22:ALA:O	1:A:25:GLU:HB3	2.00	0.61
1:A:46:GLU:HB2	3:A:350:HOH:O	2.02	0.60
1:A:122:LYS:CG	3:A:328:HOH:O	2.17	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:72:ILE:N	1:A:72:ILE:CD1	2.65	0.60
1:A:48:THR:H	1:A:57:ASN:ND2	1.99	0.59
1:A:4:THR:HG23	1:A:7:GLU:H	1.66	0.59
1:A:59:LEU:HD23	1:A:60:TRP:CE2	2.38	0.59
1:A:71:ASN:HD21	1:A:75:ILE:H	1.54	0.56
1:A:4:THR:HG22	1:A:7:GLU:CB	2.28	0.56
1:A:113:GLU:O	1:A:114:LYS:HG2	2.06	0.56
1:A:9:SER:OG	1:A:23:LEU:HD21	2.07	0.55
1:A:102:ASP:HB2	3:A:242:HOH:O	2.06	0.55
1:A:18:TYR:O	1:A:21:ILE:HG12	2.07	0.54
1:A:42:VAL:O	1:A:44:ASN:ND2	2.41	0.54
1:A:117:GLN:HG3	1:A:118:TRP:CD1	2.43	0.53
1:A:96:LEU:HD11	3:A:349:HOH:O	2.09	0.53
1:A:46:GLU:CB	3:A:350:HOH:O	2.56	0.52
1:A:44:ASN:ND2	1:A:44:ASN:N	2.57	0.51
1:A:75:ILE:HD11	1:A:79:LYS:CB	2.40	0.51
1:A:4:THR:HG21	3:A:209:HOH:O	2.11	0.51
1:A:111:CYS:O	1:A:112:THR:HG23	2.12	0.49
1:A:121:GLU:O	1:A:121:GLU:HG3	2.12	0.49
1:A:47:SER:HA	1:A:65:GLN:NE2	2.27	0.48
1:A:23:LEU:N	1:A:24:PRO:CD	2.77	0.48
1:A:17:GLY:N	1:A:21:ILE:O	2.45	0.47
1:A:55:ILE:HD11	1:A:60:TRP:HB2	1.86	0.47
1:A:70:ARG:C	1:A:72:ILE:HD13	2.35	0.47
1:A:67:PRO:HB3	3:A:248:HOH:O	2.15	0.46
1:A:55:ILE:CD1	1:A:56:SER:O	2.64	0.46
1:A:102:ASP:OD1	1:A:108:LYS:HG2	2.16	0.46
1:A:55:ILE:CD1	1:A:56:SER:N	2.73	0.46
1:A:120:CYS:SG	1:A:121:GLU:N	2.89	0.46
1:A:5:LYS:HE2	1:A:5:LYS:HB3	1.66	0.46
1:A:12:LEU:CD2	1:A:89:ILE:HD11	2.47	0.45
1:A:105:ILE:O	1:A:105:ILE:CG1	2.63	0.45
1:A:10:GLN:NE2	3:A:346:HOH:O	2.50	0.44
1:A:15:ILE:CD1	1:A:26:LEU:HD22	2.49	0.43
1:A:2:GLN:NE2	1:A:37:ASP:HB2	2.30	0.42
1:A:8:LEU:HD13	1:A:12:LEU:CD1	2.49	0.42
1:A:115:LEU:HA	1:A:118:TRP:CD1	2.47	0.42
1:A:120:CYS:O	1:A:121:GLU:CB	2.69	0.41
1:A:111:CYS:O	1:A:112:THR:CG2	2.69	0.41
1:A:116:GLU:C	1:A:118:TRP:H	2.25	0.41
1:A:117:GLN:OE1	1:A:118:TRP:CZ2	2.74	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:53:PHE:CD2	1:A:88:ASP:HB3	2.56	0.40
1:A:70:ARG:O	1:A:72:ILE:HD13	2.21	0.40

All (9) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:285:HOH:O	3:A:285:HOH:O[2_765]	1.03	1.17
3:A:307:HOH:O	3:A:307:HOH:O[2_765]	1.72	0.48
3:A:339:HOH:O	3:A:339:HOH:O[2_655]	1.77	0.43
1:A:70:ARG:NH1	3:A:272:HOH:O[2_655]	1.79	0.41
1:A:78:ASP:OD2	1:A:93:LYS:NZ[4_456]	1.79	0.41
3:A:233:HOH:O	3:A:322:HOH:O[1_455]	1.93	0.27
3:A:275:HOH:O	3:A:275:HOH:O[2_655]	1.97	0.23
1:A:43:GLU:OE1	3:A:312:HOH:O[1_455]	2.07	0.13
3:A:210:HOH:O	3:A:330:HOH:O[4_556]	2.11	0.09

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	120/123 (98%)	105 (88%)	13 (11%)	2 (2%)	9 1

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	121	GLU
1	A	117	GLN

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	111/112 (99%)	86 (78%)	25 (22%)	1 0

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	LYS
1	A	7	GLU
1	A	8	LEU
1	A	14	ASP
1	A	15	ILE
1	A	20	ARG
1	A	43	GLU
1	A	45	ASP
1	A	46	GLU
1	A	55	ILE
1	A	57	ASN
1	A	62	LYS
1	A	68	GLN
1	A	72	ILE
1	A	76	THR
1	A	78	ASP
1	A	88	ASP
1	A	94	LYS
1	A	99	LYS
1	A	108	LYS
1	A	113	GLU
1	A	115	LEU
1	A	116	GLU
1	A	117	GLN
1	A	121	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	2	GLN
1	A	44	ASN
1	A	57	ASN
1	A	65	GLN
1	A	68	GLN
1	A	71	ASN

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 1 ligands modelled in this entry, 1 is 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)

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates (i)

EDS was not executed - this section is therefore empty.

6.4 Ligands (i)

EDS was not executed - this section is therefore empty.

6.5 Other polymers (i)

EDS was not executed - this section is therefore empty.