



Full wwPDB NMR Structure Validation Report ⓘ

May 28, 2020 – 10:34 pm BST

PDB ID : 2KLR
Title : Solid-state NMR structure of the alpha-crystallin domain in alphaB-crystallin oligomers
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Deposited on : 2009-07-08

This is a Full wwPDB NMR 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/NMRValidationReportHelp>

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:

Cyrange : Kirchner and Güntert (2011)
NmrClust : Kelley et al. (1996)
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
RCI : v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV : Wang et al. (2010)
ShiftChecker : 2.11
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

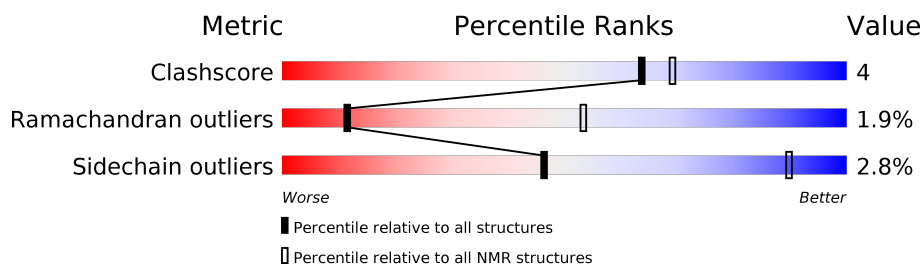
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLID-STATE NMR

The overall completeness of chemical shifts assignment was not calculated.

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)	NMR archive (#Entries)
Clashscore	158937	12864
Ramachandran outliers	154571	11451
Sidechain outliers	154315	11428

The table below summarises the geometric issues observed across the polymeric chains and their fit to the experimental data. The red, orange, yellow and green segments indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A cyan segment indicates the fraction of residues that are not part of the well-defined cores, and 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 $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	175	
1	B	175	

2 Ensemble composition and analysis i

This entry contains 10 models. Model 10 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *lowest energy*.

The following residues are included in the computation of the global validation metrics.

Well-defined (core) protein residues			
Well-defined core	Residue range (total)	Backbone RMSD (Å)	Medoid model
1	A:73-A:150, B:73-B:150 (156)	0.80	10

Ill-defined regions of proteins are excluded from the global statistics.

Ligands and non-protein polymers are included in the analysis.

The models can be grouped into 2 clusters and 2 single-model clusters were found.

Cluster number	Models
1	2, 4, 8, 10
2	1, 3, 6, 9
Single-model clusters	5; 7

3 Entry composition

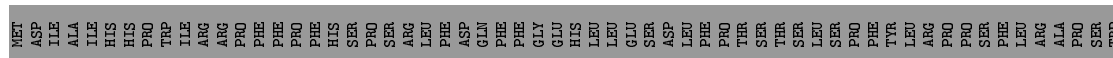
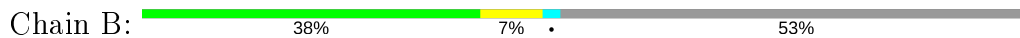
There is only 1 type of molecule in this entry. The entry contains 2670 atoms, of which 1338 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Alpha-crystallin B chain.

Mol	Chain	Residues	Atoms					Trace
			Total	C	H	N	O	
1	A	82	1335	417	669	123	126	0
1	B	82	1335	417	669	123	126	0

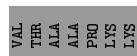
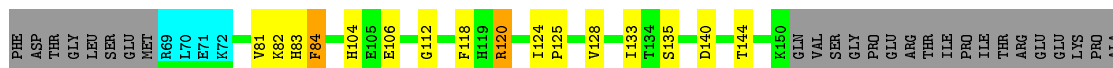
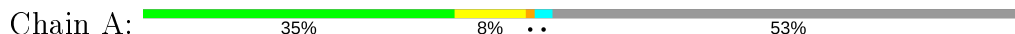


- Molecule 1: Alpha-crystallin B chain

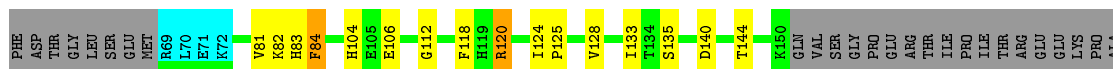


4.2.2 Score per residue for model 2

- Molecule 1: Alpha-crystallin B chain

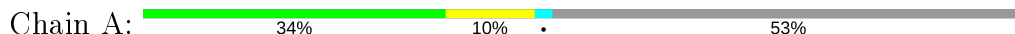


- Molecule 1: Alpha-crystallin B chain



4.2.3 Score per residue for model 3

- Molecule 1: Alpha-crystallin B chain



5 Refinement protocol and experimental data overview i

The models were refined using the following method: *simulated annealing, molecular dynamics, torsion angle dynamics*.

Of the 200 calculated structures, 10 were deposited, based on the following criterion: *structures with the lowest energy*.

The following table shows the software used for structure solution, optimisation and refinement.

Software name	Classification	Version
X-PLOR NIH	structure solution	
ARIA	structure solution	2.2
ARIA	refinement	2.2
CNS	structure solution	1.2
CNS	refinement	1.2
SOLARIA	structure solution	1

No chemical shift data was provided. Note: This is a solid-state NMR structure, where hydrogen atoms are typically not assigned a chemical shift value, which may lead to lower completeness of assignment measure.

No validations of the models with respect to experimental NMR restraints is performed at this time.

COVALENT-GEOMETRY INFOmissingINFO

5.1 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 each 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 averaged over the ensemble.

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	629	626	621	6±2
1	B	629	626	621	6±2
All	All	12580	12520	12420	108

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 4.

All unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:83:HIS:HA	1:B:140:ASP:O	0.66	1.91	8	4
1:A:83:HIS:HA	1:A:140:ASP:O	0.64	1.91	8	4
1:A:122:TYR:CD2	1:B:112:GLY:HA3	0.59	2.33	3	3
1:B:98:ILE:HG23	1:B:122:TYR:HB2	0.58	1.75	5	1
1:A:98:ILE:HG23	1:A:122:TYR:HB2	0.58	1.75	5	1
1:A:73:ASP:O	1:A:148:PRO:HA	0.56	2.00	1	2
1:A:129:ASP:H	1:A:148:PRO:HB3	0.56	1.61	3	1
1:B:129:ASP:H	1:B:148:PRO:HB3	0.55	1.61	3	1
1:B:73:ASP:O	1:B:148:PRO:HA	0.55	2.01	1	1
1:B:79:LEU:HD22	1:B:122:TYR:CE1	0.55	2.37	6	1
1:A:112:GLY:HA3	1:B:122:TYR:CD2	0.54	2.38	3	2
1:A:81:VAL:HG12	1:A:82:LYS:O	0.54	2.02	2	1
1:A:79:LEU:HD22	1:A:122:TYR:CZ	0.54	2.38	8	1
1:B:81:VAL:HG12	1:B:82:LYS:O	0.54	2.02	2	1
1:B:133:ILE:HA	1:B:146:ASN:O	0.54	2.03	8	3
1:B:81:VAL:HB	1:B:141:GLY:O	0.54	2.02	5	1
1:A:133:ILE:HA	1:A:146:ASN:O	0.53	2.02	8	3
1:B:77:VAL:HB	1:B:145:VAL:CG2	0.53	2.33	1	2
1:A:79:LEU:HD22	1:A:122:TYR:CE1	0.53	2.37	6	1
1:A:112:GLY:HA2	1:B:121:LYS:O	0.53	2.04	3	2
1:B:79:LEU:HD22	1:B:122:TYR:CZ	0.53	2.38	8	1
1:A:77:VAL:HB	1:A:145:VAL:CG2	0.52	2.33	1	2
1:B:124:ILE:O	1:B:128:VAL:HB	0.52	2.04	2	5
1:A:81:VAL:HB	1:A:141:GLY:O	0.52	2.03	5	1
1:A:124:ILE:O	1:A:128:VAL:HB	0.52	2.03	2	6
1:A:121:LYS:O	1:B:112:GLY:HA2	0.52	2.03	3	1
1:A:106:GLU:HB3	1:A:107:ARG:NH1	0.50	2.21	4	1
1:A:81:VAL:HA	1:A:120:ARG:CZ	0.50	2.37	2	1
1:B:106:GLU:HB3	1:B:107:ARG:NH1	0.50	2.22	4	1
1:B:81:VAL:HA	1:B:120:ARG:CZ	0.49	2.38	2	1
1:A:79:LEU:HD13	1:A:100:VAL:HB	0.48	1.85	7	1
1:B:107:ARG:HG2	1:B:114:ILE:HD11	0.48	1.85	5	1
1:A:79:LEU:HA	1:A:120:ARG:HD2	0.48	1.86	7	1
1:A:84:PHE:HA	1:A:104:HIS:HB2	0.47	1.86	2	1
1:B:79:LEU:HD13	1:B:100:VAL:HB	0.47	1.86	7	1
1:B:79:LEU:HA	1:B:120:ARG:HD2	0.47	1.86	7	1
1:A:107:ARG:HG2	1:A:114:ILE:HD11	0.47	1.85	5	1
1:B:84:PHE:HA	1:B:104:HIS:HB2	0.47	1.86	2	1
1:A:143:LEU:HD12	1:A:144:THR:N	0.47	2.24	10	1
1:B:143:LEU:HD12	1:B:144:THR:N	0.46	2.25	10	1
1:A:126:ALA:O	1:A:150:LYS:HA	0.44	2.13	3	1
1:A:147:GLY:N	1:A:148:PRO:HD2	0.44	2.28	3	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:126:ALA:O	1:B:150:LYS:HA	0.44	2.12	3	1
1:A:130:PRO:HA	1:A:133:ILE:CG2	0.44	2.43	3	1
1:A:128:VAL:HG13	1:A:133:ILE:CD1	0.44	2.43	2	1
1:B:106:GLU:HB3	1:B:107:ARG:CZ	0.44	2.42	4	1
1:B:128:VAL:HG13	1:B:133:ILE:CD1	0.43	2.43	2	1
1:A:110:GLU:CD	1:A:110:GLU:H	0.43	2.16	4	1
1:A:106:GLU:HB3	1:A:107:ARG:CZ	0.43	2.43	4	1
1:A:81:VAL:HB	1:A:120:ARG:NH1	0.43	2.29	9	1
1:B:81:VAL:HB	1:B:120:ARG:NH1	0.43	2.28	9	1
1:B:110:GLU:H	1:B:110:GLU:CD	0.43	2.16	4	1
1:B:135:SER:HA	1:B:144:THR:O	0.43	2.13	2	1
1:B:147:GLY:N	1:B:148:PRO:HD2	0.43	2.28	3	1
1:A:135:SER:HA	1:A:144:THR:O	0.43	2.14	2	2
1:B:134:THR:O	1:B:145:VAL:HA	0.42	2.14	3	2
1:B:88:GLU:HB3	1:B:103:LYS:O	0.42	2.15	6	1
1:B:130:PRO:HA	1:B:133:ILE:CG2	0.42	2.44	3	1
1:A:88:GLU:HB3	1:A:103:LYS:O	0.42	2.15	6	1
1:A:120:ARG:NH2	1:B:114:ILE:HD12	0.42	2.30	5	1
1:A:134:THR:O	1:A:145:VAL:HA	0.42	2.15	3	2
1:A:88:GLU:HB3	1:A:103:LYS:HG3	0.42	1.91	8	1
1:B:88:GLU:HB3	1:B:103:LYS:HG3	0.42	1.91	8	1
1:A:121:LYS:O	1:A:121:LYS:HD2	0.41	2.15	5	1
1:B:121:LYS:HD2	1:B:121:LYS:O	0.41	2.15	5	1
1:B:135:SER:HB2	1:B:143:LEU:HD11	0.41	1.92	4	1
1:B:77:VAL:HB	1:B:145:VAL:HG23	0.41	1.91	1	1
1:A:114:ILE:HD12	1:B:120:ARG:NH2	0.41	2.31	5	1
1:B:84:PHE:HB3	1:B:118:PHE:CE1	0.41	2.51	2	1
1:A:150:LYS:HB2	1:A:150:LYS:NZ	0.41	2.30	9	1
1:A:84:PHE:HB3	1:A:118:PHE:CE1	0.41	2.51	2	1
1:B:85:SER:OG	1:B:104:HIS:HB2	0.41	2.16	7	1
1:A:120:ARG:HG2	1:B:114:ILE:CB	0.40	2.47	5	1
1:B:109:ASP:HB3	1:B:112:GLY:O	0.40	2.16	6	1
1:A:135:SER:HB2	1:A:143:LEU:HD11	0.40	1.93	4	1
1:A:85:SER:OG	1:A:104:HIS:HB2	0.40	2.16	7	1
1:A:109:ASP:HB3	1:A:112:GLY:O	0.40	2.16	6	1
1:A:133:ILE:HG12	1:A:147:GLY:HA3	0.40	1.94	8	1
1:A:130:PRO:HA	1:A:133:ILE:CG1	0.40	2.47	9	1

5.2 Torsion angles [i](#)

5.2.1 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 PDB entries followed by that with respect to all NMR entries. 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	77/175 (44%)	70±1 (91±2%)	5±2 (7±2%)	2±1 (2±1%)	11	53
1	B	77/175 (44%)	70±1 (91±2%)	5±2 (7±2%)	1±1 (2±1%)	12	54
All	All	1540/3500 (44%)	1407 (91%)	104 (7%)	29 (2%)	11	53

All 10 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	B	125	PRO	8
1	A	125	PRO	8
1	A	110	GLU	4
1	B	110	GLU	3
1	A	81	VAL	1
1	A	106	GLU	1
1	B	106	GLU	1
1	B	81	VAL	1
1	A	73	ASP	1
1	B	73	ASP	1

5.2.2 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 PDB entries followed by that with respect to all NMR entries. 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	72/161 (45%)	70±2 (97±2%)	2±2 (3±2%)	46	90
1	B	72/161 (45%)	70±2 (97±2%)	2±2 (3±2%)	46	90
All	All	1440/3220 (45%)	1400 (97%)	40 (3%)	46	90

All 26 unique residues with a non-rotameric sidechain are listed below. They are sorted by the

frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	B	103	LYS	3
1	A	103	LYS	3
1	B	84	PHE	3
1	A	84	PHE	3
1	A	134	THR	2
1	B	134	THR	2
1	A	137	LEU	2
1	B	137	LEU	2
1	A	80	ASP	2
1	B	80	ASP	2
1	A	81	VAL	1
1	A	125	PRO	1
1	A	90	LYS	1
1	B	81	VAL	1
1	A	107	ARG	1
1	B	92	LYS	1
1	B	121	LYS	1
1	B	90	LYS	1
1	B	107	ARG	1
1	A	92	LYS	1
1	A	133	ILE	1
1	B	125	PRO	1
1	A	121	LYS	1
1	B	143	LEU	1
1	B	133	ILE	1
1	A	143	LEU	1

5.2.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.4 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.5 Ligand geometry [i](#)

There are no ligands in this entry.

5.6 Other polymers [i](#)

There are no such molecules in this entry.

5.7 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Chemical shift validation

No chemical shift data were provided