



wwPDB NMR Structure Validation Summary Report ⓘ

Apr 20, 2024 – 10:06 PM EDT

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

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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 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 : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
wwPDB-RCI : v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV : Wang et al. (2010)
wwPDB-ShiftChecker : v1.2
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36.2

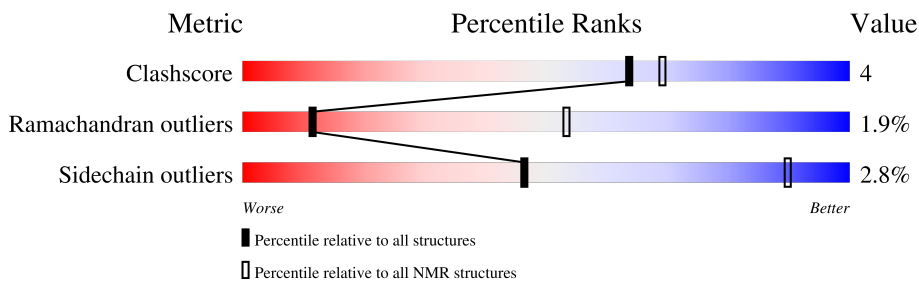
1 Overall quality at a glance

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	42% 53%
1	B	175	43% 53%

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)	1.38	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

4 Residue-property plots [i](#)

4.1 Average score per residue in the NMR ensemble

These plots are provided for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic is the same as shown in the summary in section 1 of this report. The second graphic shows the sequence where residues are colour-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 outliers are shown as green connectors. Residues which are classified as ill-defined in the NMR ensemble, are shown in cyan with an underline colour-coded according to the previous scheme. Residues which were present in the experimental sample, but not modelled in the final structure are shown in grey.

- Molecule 1: Alpha-crystallin B chain

Chain A:  42% .. 53%

MET ASP ILE ILE ILE ILE HIS HIS PRO TRP TRP ILE ARG ARG ARG PHE PHE PHE PHE HIS HIS SER SER PRO SER ARG ARG LEU LEU PHE ASP ASP GLN PHE PHE PHE GLY GLY GLU HIS LEU LEU LEU LEU GLU SER SER ASP ASP PHE PHE PRO THR THR THR SER SER LEU LEU SER SER PHE PHE TYR TYR LEU ARG ARG PRO PRO PHE PHE LEU LEU ARG ARG ALA ALA PRO PRO SER SER TRP

PHE ASP THR GLY LEU LEU SER SER MET R69 L70 E71 K72 I124 P125 V128 I133 K150 GLN VAL SER SER GLY PRO GLU THR ARG THR ILE ILE PRO THR THR ARG GLU LYS LYS PRO ALA VAL THR ALA THR THR SER SER LEU LEU SER SER LYS LYS

- Molecule 1: Alpha-crystallin B chain

Chain B:  43% .. 53%

MET ASP ILE ILE ILE ILE HIS HIS PRO TRP TRP ILE ARG ARG ARG PHE PHE PHE PHE HIS HIS SER SER PRO SER ARG ARG LEU LEU PHE ASP ASP GLN PHE PHE PHE GLY GLY GLU HIS LEU LEU LEU LEU GLU SER SER ASP ASP PHE PHE PRO THR THR THR SER SER LEU LEU SER SER PHE PHE TYR TYR LEU ARG ARG PRO PRO PHE PHE LEU LEU ARG ARG ALA ALA PRO PRO SER SER TRP

PHE ASP THR GLY LEU LEU SER SER MET R69 L70 E71 K72 P125 I133 K150 GLN VAL SER SER GLY PRO GLU THR THR ARG THR ILE ILE PRO THR THR ARG GLU LYS LYS PRO ALA VAL THR THR SER SER LEU LEU SER SER LYS LYS

4.2 Residue scores for the representative (medoid) model from the NMR ensemble

The representative model is number 10. Colouring as in section 4.1 above.

- Molecule 1: Alpha-crystallin B chain

Chain A:  40% ... 53%

MET ASP ILE ILE ILE ILE HIS HIS PRO TRP TRP ILE ARG ARG ARG PHE PHE PHE PHE HIS HIS SER SER PRO SER ARG ARG LEU LEU PHE ASP ASP GLN PHE PHE PHE GLY GLY GLU HIS LEU LEU LEU LEU GLU SER SER ASP ASP PHE PHE PRO THR THR THR SER SER LEU LEU SER SER PHE PHE TYR TYR LEU ARG ARG PRO PRO PHE PHE LEU LEU ARG ARG ALA ALA PRO PRO SER SER TRP

PHE ASP THR GLY LEU LEU SER SER MET R69 L70 E71 K72 W81 F84 K103 G112 P125 I133 L143 I144 K150 GLN VAL SER SER GLY PRO GLU THR THR ARG THR ILE ILE ILE THR THR ARG ARG GLU LYS LYS PRO ALA VAL THR THR ALA ALA PRO PRO SER SER LYS LYS

- Molecule 1: Alpha-crystallin B chain



MET ASP ILE ILE ILE HIS HIS TRP TRP ILE ARG ARG PRO PHE PHE PRO PRO HIS HIS SER PRO SER ARG LEU LEU ASP GLN PHE PHE GLY GLU HIS LEU LEU LEU GLU SER SER ASP LEU LEU PHE PRO THR THR THR THR SER SER LEU SER PRO PHE TYR TYR ARG ARG PRO PRO PHE PHE LEU ARG ALA PRO SER TRP

PHE ASP THR GLY LEU SER GLU MET R69 L70 E71 K72 V61 F84 K103 K121 P125 I133 L143 T144 K150 VAL SER GLY PRO GLU ARG THR ILE ILE THR ARG GLU LYS PRO ALA VAL THR ALA ALA PRO LYS

5 Refinement protocol and experimental data overview

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.

6 Model quality i

6.1 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 (average) 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	0.97±0.04	0±0/642 (0.0± 0.0%)	0.76±0.03	0±0/865 (0.0± 0.0%)
1	B	0.97±0.05	0±0/642 (0.0± 0.0%)	0.76±0.03	0±0/865 (0.0± 0.0%)
All	All	0.97	2/12840 (0.0%)	0.76	0/17300 (0.0%)

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	Planarity
1	A	0.0±0.0	0.3±0.5
1	B	0.0±0.0	0.4±0.7
All	All	0	7

All unique bond outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	112	GLY	N-CA	-5.79	1.37	1.46	2	1
1	B	112	GLY	N-CA	-5.76	1.37	1.46	2	1

There are no bond-angle outliers.

There are no chirality outliers.

5 of 6 unique planar outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Group	Models (Total)
1	B	116	ARG	Sidechain	2
1	A	120	ARG	Sidechain	1
1	B	120	ARG	Sidechain	1
1	A	116	ARG	Sidechain	1

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Mol	Chain	Res	Type	Group	Models (Total)
1	A	107	ARG	Sidechain	1

6.2 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 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.

5 of 79 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

6.3 Torsion angles [i](#)

6.3.1 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 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

5 of 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	A	125	PRO	8
1	B	125	PRO	8
1	A	110	GLU	4
1	B	110	GLU	3
1	A	106	GLU	1

6.3.2 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 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

5 of 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	A	84	PHE	3
1	B	84	PHE	3
1	A	103	LYS	3
1	B	103	LYS	3
1	A	80	ASP	2

6.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.6 Ligand geometry [i](#)

There are no ligands in this entry.

6.7 Other polymers [i](#)

There are no such molecules in this entry.

6.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

7 Chemical shift validation

No chemical shift data were provided