wwPDB NMR Structure Validation Summary Report (i)

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PDB ID	:	2K1W
Title	:	NMR solution structure of M-crystallin in calcium loaded form(holo).
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This is a wwPDB NMR 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/NMRValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (i)) were used in the production of this report:

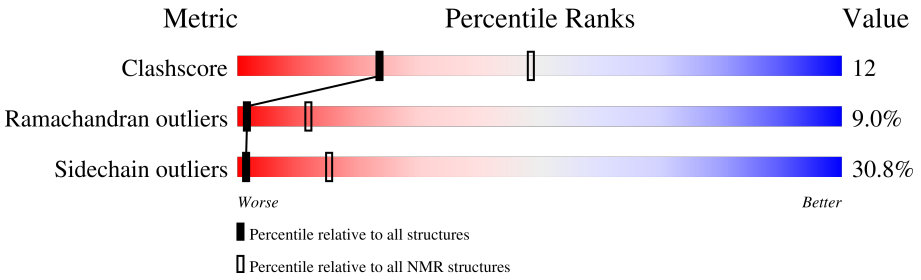
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	2.27
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.27

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
SOLUTION 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 <=5%

Mol	Chain	Length	Quality of chain
1	A	85	39% 35% • • 21%

2 Ensemble composition and analysis (i)

This entry contains 20 models. Model 1 is the overall representative, medoid model (most similar to other models).

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:5-A:19, A:34-A:85 (67)	0.28	1

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	1, 2, 3, 4, 5, 6, 7, 8, 9, 11, 13, 14, 16
2	15, 17, 18, 19, 20
Single-model clusters	10; 12

3 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 1277 atoms, of which 612 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Beta/gama crystallin family protein.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	85	1275	418	612	110	134	1	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	expression tag	UNP Q8TMX3

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

Mol	Chain	Residues	Atoms	
			Total	Ca
2	A	2	2	2

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: Beta/gama crystallin family protein

Chain A: 39% 35% • • 21%

M1 N2 A3 A4 E5 V6 H11 V12 N13 F14 G15 G16 K17 S18 F19 D20 A21 T22 S23 D24 Q25 P26 G27 A28 G29 D30 N31 L32 N33 D34 K35 I36 S37 S38 I39 K40 V41 K42 W46 R47 Y51 I52 N53 Y54 G55 L61 G62 Y66 V69 E70 G73 I74 P75

D76 N77 S81 Q84 I85

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

The representative model is number 1. Colouring as in section 4.1 above.

- Molecule 1: Beta/gama crystallin family protein

Chain A: 35% 38% 5% • 21%

M1 N2 A3 A4 E5 V6 I7 V8 H11 V12 N13 F14 G15 G16 K17 S18 F19 D20 A21 T22 S23 D24 Q25 P26 G27 A28 G29 D30 N31 L32 N33 D34 K35 I36 S37 S38 V41 K42 S43 W46 R47 Y51 I52 N53 Y54 G55 G56 R57 L61 G62 E65 Y66 V69

E70 G73 I74 P75 D76 N77 S81 F82 R83 Q84 I85

5 Refinement protocol and experimental data overview (i)

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

Of the 400 calculated structures, 20 were deposited, based on the following criterion: *target function.*

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

Software name	Classification	Version
CYANA	structure solution	3.0
CYANA	refinement	3.0

No chemical shift data was provided.

6 Model quality (i)

6.1 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 (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	0.43±0.01	1±0/558 (0.2± 0.0%)	0.49±0.01	1±0/753 (0.1± 0.0%)
All	All	0.43	20/11160 (0.2%)	0.49	20/15060 (0.1%)

All unique bond outliers are listed below.

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	75	PRO	CG-CD	9.36	1.81	1.50	16	20

All unique angle outliers are listed below.

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
1	A	75	PRO	N-CD-CG	-10.64	87.23	103.20	2	20

There are no chirality outliers.

There are no planarity outliers.

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	542	509	508	13±2
All	All	10880	10180	10170	256

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 12.

5 of 56 unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:75:PRO:CD	1:A:75:PRO:CG	1.55	1.79	3	20
1:A:34:ASP:O	1:A:74:ILE:HG23	0.65	1.91	11	17
1:A:66:TYR:OH	1:A:72:ALA:HB2	0.65	1.92	2	2
1:A:34:ASP:OD2	1:A:75:PRO:HD2	0.62	1.93	11	6
1:A:73:GLY:C	1:A:75:PRO:HD3	0.61	2.16	2	14

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	66/85 (78%)	47±2 (72±3%)	13±2 (19±3%)	6±1 (9±2%)	1	12
All	All	1320/1700 (78%)	946 (72%)	255 (19%)	119 (9%)	1	12

5 of 12 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	70	GLU	20
1	A	75	PRO	20
1	A	15	GLY	17
1	A	73	GLY	16
1	A	69	VAL	15

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	58/70 (83%)	40±2 (69±3%)	18±2 (31±3%)	1 15
All	All	1160/1400 (83%)	803 (69%)	357 (31%)	1 15

5 of 36 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	46	TRP	20
1	A	51	TYR	20
1	A	61	LEU	20
1	A	81	SER	20
1	A	11	HIS	19

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)

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

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 (i)

No chemical shift data were provided