wwPDB NMR Structure Validation Summary Report (i)

Apr 20, 2024 – 10:27 AM EDT

PDB ID	:	3J07
EMDB ID	:	EMD-1776
BMRB ID	:	16391
Title	:	Model of a 24mer alphaB-crystallin multimer
Authors	:	Jehle, S.; Vollmar, B.; Bardiaux, B.; Dove, K.K.; Rajagopal, P.; Gonen, T.; Oschkinat, H.; Klevit, R.E.
Deposited on	:	2011-04-27
Based on initial model	:	2KLR

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 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:

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

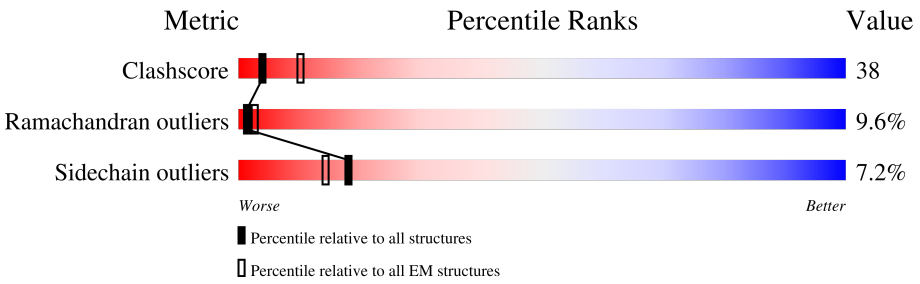
1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
SOLID-STATE NMR, SOLUTION SCATTERING, ELECTRON MICROSCOPY

The reported resolution of this entry is 20.00 Å.

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	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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	175	45% 43% 12%
1	B	175	46% 45% 9%
1	C	175	43% 44% 11% •
1	D	175	41% 46% 11% •
1	E	175	47% 41% 13%
1	F	175	42% 47% 10% •
1	G	175	44% 43% 11% •
1	H	175	45% 44% 10% •

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Mol	Chain	Length	Quality of chain
1	I	175	43% 45% 9% •
1	J	175	41% 49% 10%
1	K	175	46% 40% 10% •
1	L	175	45% 43% 10% •
1	M	175	45% 41% 13% •
1	N	175	44% 49% 7%
1	O	175	44% 42% 11% •
1	P	175	42% 46% 11% •
1	Q	175	47% 41% 10% •
1	R	175	47% 42% 11%
1	S	175	45% 43% 10% •
1	T	175	46% 44% 10% •
1	U	175	43% 45% 11% •
1	V	175	43% 46% 10% •
1	W	175	42% 45% 11% •
1	X	175	43% 43% 11% •

2 Ensemble composition and analysis (i)

This entry contains 1 models. Identification of well-defined residues and clustering analysis are not possible.

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 42144 atoms, of which 8232 are hydrogens and 0 are deuteriums.

In the tables below, 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-crystallin B chain.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
1	A	175	1756	916	343	236	259	2	0	
1	B	175	1756	916	343	236	259	2	0	
1	C	175	1756	916	343	236	259	2	0	
1	D	175	1756	916	343	236	259	2	0	
1	E	175	1756	916	343	236	259	2	0	
1	F	175	1756	916	343	236	259	2	0	
1	G	175	1756	916	343	236	259	2	0	
1	H	175	1756	916	343	236	259	2	0	
1	I	175	1756	916	343	236	259	2	0	
1	J	175	1756	916	343	236	259	2	0	
1	K	175	1756	916	343	236	259	2	0	
1	L	175	1756	916	343	236	259	2	0	
1	M	175	1756	916	343	236	259	2	0	
1	N	175	1756	916	343	236	259	2	0	
1	O	175	1756	916	343	236	259	2	0	
1	P	175	1756	916	343	236	259	2	0	
1	Q	175	1756	916	343	236	259	2	0	

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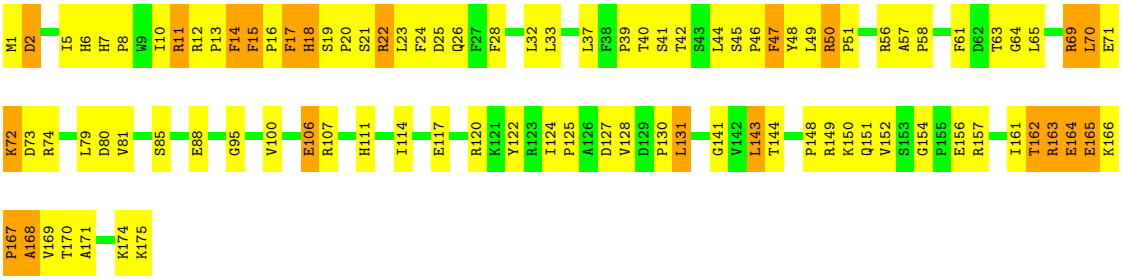
Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
1	R	175	1756	916	343	236	259	2	0	
			Total	C	H	N	O	S		
1	S	175	1756	916	343	236	259	2	0	
			Total	C	H	N	O	S		
1	T	175	1756	916	343	236	259	2	0	
			Total	C	H	N	O	S		
1	U	175	1756	916	343	236	259	2	0	
			Total	C	H	N	O	S		
1	V	175	1756	916	343	236	259	2	0	
			Total	C	H	N	O	S		
1	W	175	1756	916	343	236	259	2	0	
			Total	C	H	N	O	S		
1	X	175	1756	916	343	236	259	2	0	

4 Residue-property plots (i)

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.

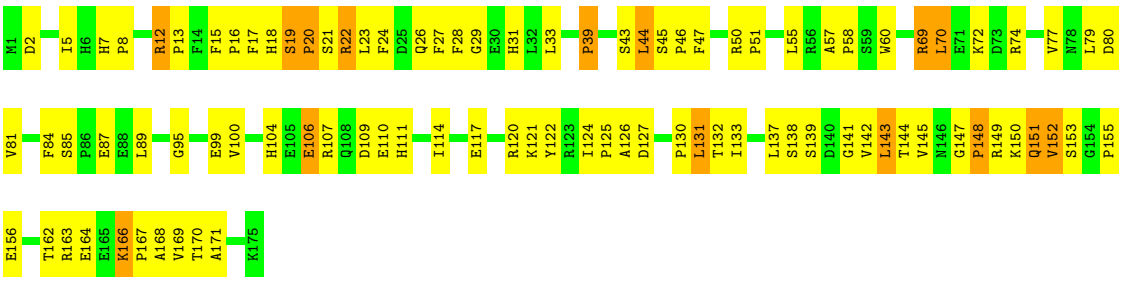
• Molecule 1: Alpha-crystallin B chain

Chain A: 45% 43% 12%



• Molecule 1: Alpha-crystallin B chain

Chain B: 46% 45% 9%

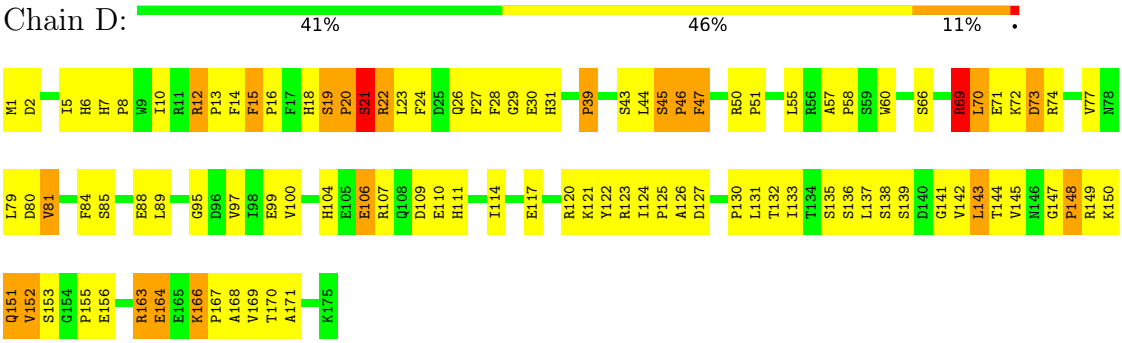


• Molecule 1: Alpha-crystallin B chain

Chain C: 43% 44% 11%

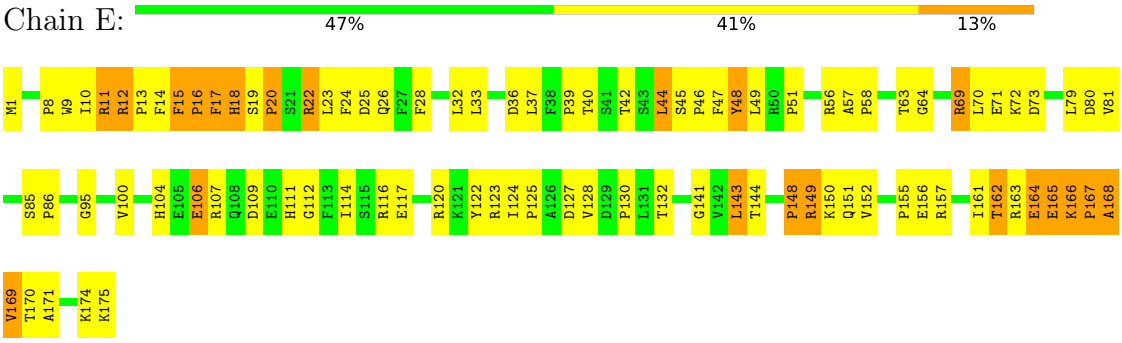
• Molecule 1: Alpha-crystallin B chain

Chain D:



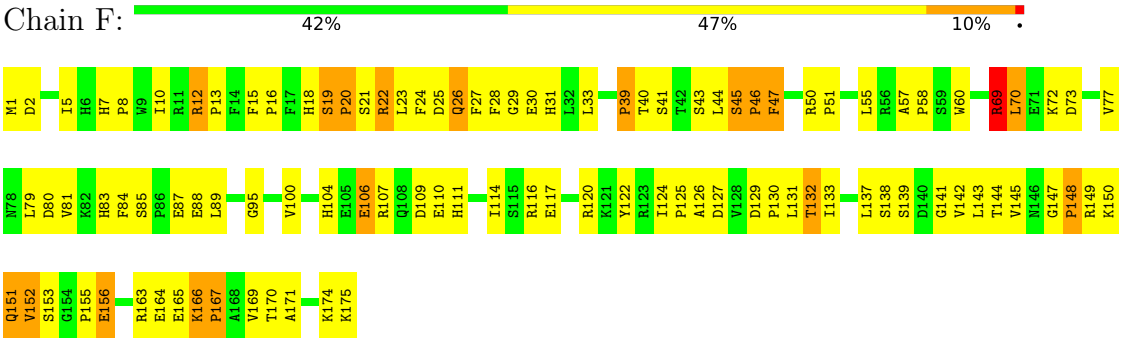
- Molecule 1: Alpha-crystallin B chain

Chain E:



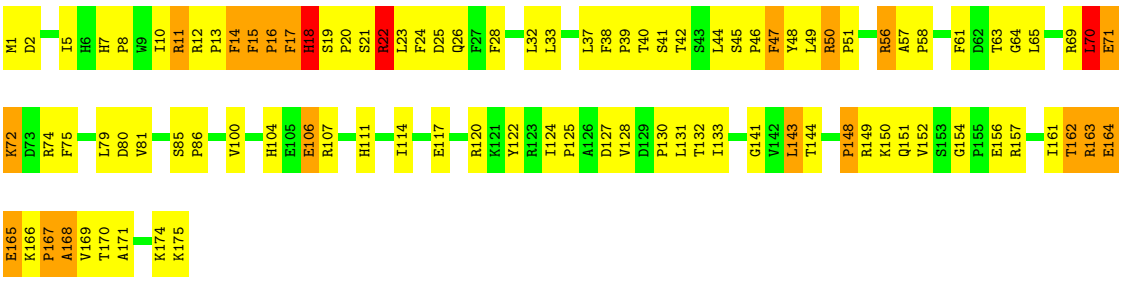
- Molecule 1: Alpha-crystallin B chain

Chain F:



- Molecule 1: Alpha-crystallin B chain

Chain G:



- Molecule 1: Alpha-crystallin B chain

Chain H: 45% 44% 10%

M1 D2 I5 H6 H7 P8 W9 I10 R11 R12 P13 F14 F15 P16 F17 H18 S19 P20 S21 R22 L23 F24 D25 Q26 F27 F28 G29 E30 H31 L32 L33 P39 T40 S41 L44 S45 P46 F47 R50 P51 L55 R56 A57 P58 S59 W60 R69 L70 E71 K72 D73 R74 V77

N78 L79 D80 V81 F84 S85 P86 E87 E88 G95 V100 H104 E105 E106 R107 Q108 D109 E110 H111 I114 E117 R120 K121 Y122 R123 I124 P125 A126 D127 P130 L131 T132 I133 L137 S138 S139 D140 G141 V142 L143 T144 V145 N146 G147 P148 R149 K150 Q151 V152 S153 G154

P155 E156 T162 R163 E164 E165 K166 P167 A168 V169 T170 A171 K174 K175

- Molecule 1: Alpha-crystallin B chain

Chain I: 43% 45% 9%

M1 D2 I5 W9 I10 R11 R12 P13 F14 F15 P16 F17 H18 S19 P20 S21 R22 L23 F24 D25 Q26 F27 F28 G29 E30 H31 L32 L33 L37 F38 P39 T40 S41 T42 S43 L44 S45 P46 F47 Y48 L49 R56 A57 P58 T63 G64 L65 R69 L70 E71 K72 D73 R74 F75

S76 V77 N78 L79 D80 V81 S85 P86 G95 V100 H104 E105 E106 R107 Q108 D109 E110 H111 G112 F113 I114 E117 R120 K121 Y122 R123 I124 P125 A126 D127 V128 D129 P130 L131 T132 I133 G141 V142 L143 T144 P148 R149 K150 Q151 V152 S153 G154 P155 E156 I161 T162

R163 E164 E165 K166 P167 A168 V169 T170 A171 K174 K175

- Molecule 1: Alpha-crystallin B chain

Chain J: 41% 49% 10%

M1 D2 I5 H6 H7 P8 R12 P13 F14 F15 P16 F17 H18 S19 P20 S21 R22 L23 F24 D25 Q26 F27 F28 G29 E30 H31 P39 T40 S41 T42 S43 L44 S45 P46 F47 R50 P51 L55 R56 A57 P58 S59 W60 R69 L70 E71 K72 D73 R74 V77 N78 L79 D80

V81 F84 S85 P86 E87 E88 L89 G95 D96 V97 I98 E99 V100 H104 E105 E106 R107 E110 H111 I114 E117 R120 K121 Y122 R123 I124 P125 A126 D127 P130 L131 T132 I133 S136 L137 S138 S139 D140 G141 V142 L143 T144 V145 N146 G147 P148 R149 K150 Q151 V152 S153

G154 P155 E156 R157 T158 T162 R163 E164 E165 K166 P167 A168 V169 T170 K174 K175

- Molecule 1: Alpha-crystallin B chain

Chain K: 46% 40% 10%

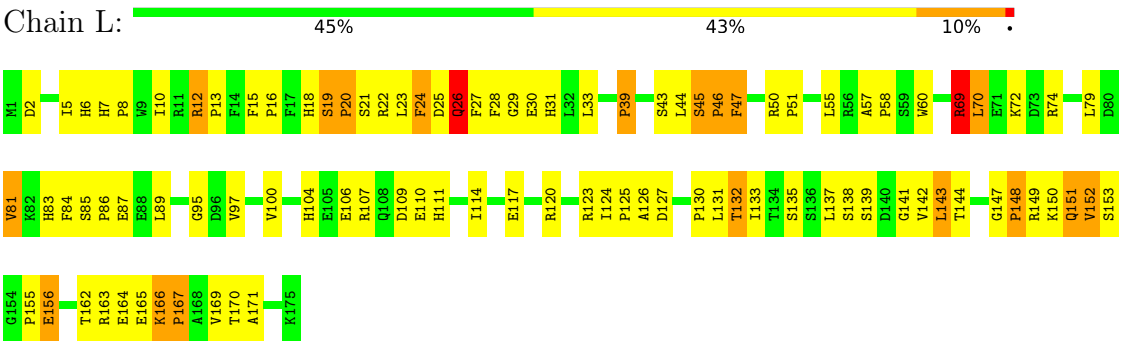
M1 R11 R12 P13 F14 F15 P16 F17 H18 S19 P20 S21 R22 L23 F24 D25 Q26 F27 F28 G29 E30 H31 L32 L33 L37 F38 P39 T40 S41 T42 S43 L44 S45 P46 F47 Y48 L49 R56 A57 P58 T63 G64 L65 S66 R69 L70 E71 K72 D73 R74 F75 S76 V77 N78 L79

D80 V81 S85 P86 G95 V100 H104 E105 E106 R107 H111 I114 E117 R120 K121 Y122 R123 I124 P125 A126 D127 V128 D129 P130 L131 G141 V142 L143 T144 P148 R149 K150 Q151 V152 P155 E156 R157 I161 T162 R163 E164 E165 K166 P167 A168 V169 T170 A171

K174 K175

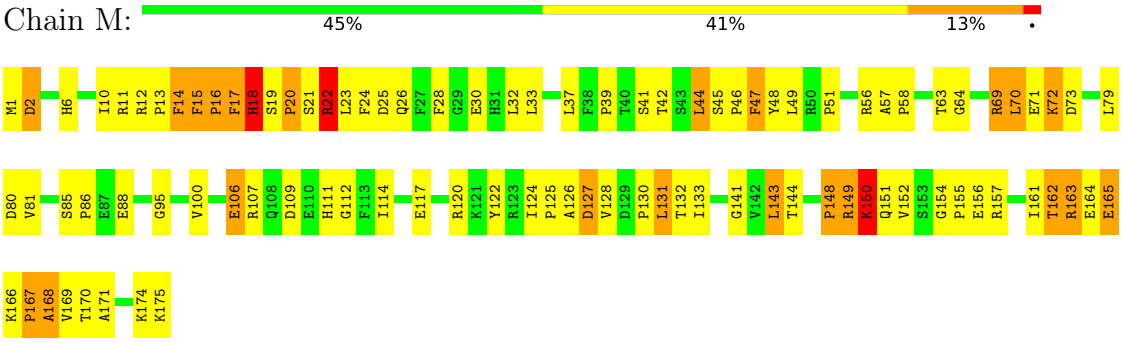
- Molecule 1: Alpha-crystallin B chain

Chain L:



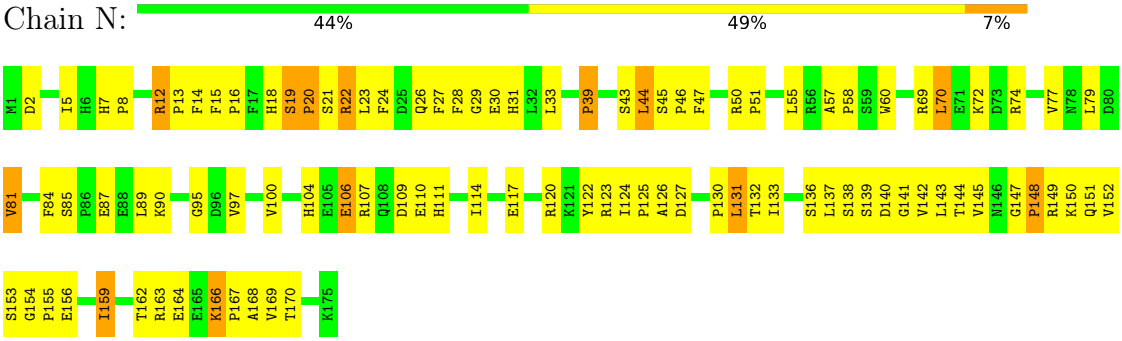
- Molecule 1: Alpha-crystallin B chain

Chain M:



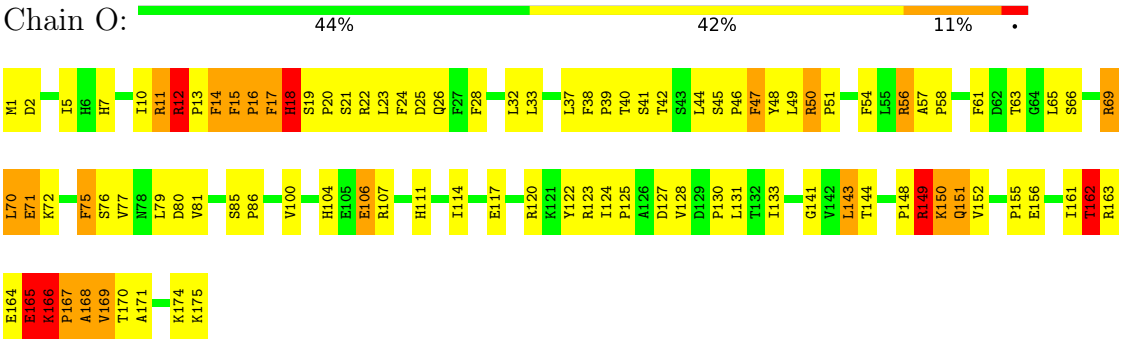
- Molecule 1: Alpha-crystallin B chain

Chain N:



- Molecule 1: Alpha-crystallin B chain

Chain O:



- Molecule 1: Alpha-crystallin B chain

Chain P: 42% 46% 11%

M1 D2 I5 H6 I10 R11 R12 P13 F14 F15 P16 F17 H18 S19 P20 S21 R22 L23 F24 D25 Q26 F27 F28 G29 E30 H31 P39 T40 S41 L44 S45 P46 F47 R50 P51 L55 R56 A57 P58 S59 W60 R69 L70 E71 K72 D73 R74 V77 N78 L79 D80 V81

F84 S85 P86 E87 E88 L89 G95 D96 V97 I98 E99 V100 H104 E105 E106 R107 Q108 D109 E110 H111 I114 E117 R120 K121 Y122 R123 I124 P125 A126 D127 P130 L131 T132 I133 T134 S135 S136 L137 S138 S139 D140 G141 V142 L143 T144 V145 N146 G147 P148 R149 K150 Q151 V152

S153 G154 P155 E156 T162 R163 E164 E165 K166 P167 A168 V169 T170 A171 K175

- Molecule 1: Alpha-crystallin B chain

Chain Q: 47% 41% 10%

M1 I5 R11 R12 P13 F14 F15 P16 F17 H18 S19 P20 S21 R22 L23 F24 D25 Q26 F27 F28 G29 E30 H31 L32 L33 L37 F38 P39 T40 S41 T42 S43 L44 S45 P46 F47 Y48 L49 R50 P51 R56 A57 P58 T63 G64 R69 L70 E71 K72 D73 R74 F75 S76 V77

N78 L79 D80 V81 S85 P86 G95 V100 H104 E105 E106 R107 H111 I114 E117 R120 K121 Y122 R123 I124 P125 A126 D127 P130 L131 G141 V142 L143 T144 V145 P148 R149 K150 Q151 V152 P155 E156 R157 T158 I161 T162 R163 E164 E165 K166 P167 A168

V169 T170 P173 K174 K175

- Molecule 1: Alpha-crystallin B chain

Chain R: 47% 42% 11%

M1 D2 I5 H6 I10 R11 R12 P13 F14 F15 P16 F17 H18 S19 P20 S21 R22 L23 F24 D25 Q26 F27 F28 G29 E30 H31 P39 L44 S45 P46 F47 R50 P51 L55 R56 A57 P58 S59 W60 R69 L70 E71 K72 V77 N78 L79 D80 V81 F84 S85 P86

E87 E88 L89 G95 E99 V100 H104 E105 E106 R107 Q108 D109 E110 H111 I114 E117 R120 K121 Y122 R123 I124 P125 A126 D127 V128 D129 P130 L131 T132 I133 L137 S138 S139 D140 G141 V142 L143 T144 V145 N146 G147 P148 R149 K150 Q151 V152 S153 G154 P155 E156 T162 R163

E164 E165 K166 P167 A168 V169 T170 A171 K175

- Molecule 1: Alpha-crystallin B chain

Chain S: 45% 43% 10%

M1 I5 I10 R11 R12 P13 F14 F15 P16 F17 H18 S19 P20 S21 R22 L23 F24 D25 Q26 F27 F28 L32 L33 L37 F38 P39 T40 S41 T42 S43 L44 S45 P46 F47 Y48 L49 R50 P51 F54 L55 R56 A57 P58 T63 G64 R69 L70 E71 K72 D73 R74 F75

N78 L79 D80 V81 S85 P86 G95 V100 H104 E105 E106 R107 Q108 D109 E110 H111 G112 F113 I114 E117 R120 K121 Y122 R123 I124 P125 A126 D127 V128 D129 P130 L131 G141 V142 L143 T144 P148 R149 K150 Q151 V152 S153 G154 P155 E156 R157 T162 R163 E164 E165 K166

P167 A168 V169 T170 A171 K174 K175

- Molecule 1: Alpha-crystallin B chain

Chain T: 46% 44% 10% •

M1 D2 I5 I10 R11 R12 P13 F14 F15 P16 F17 H18 S19 P20 S21 R22 L23 F24 D25 Q26 F27 F28 G29 E30 H31 L32 L33 P39 T40 S41 L44 S45 P46 F47 R50 P51 L55 R56 A57 P58 S59 W60 R69 L70 E71 K72 D73 R74 V77 N78 L79 D80

V81 F84 S85 E88 L89 G95 V100 H104 E105 E106 R107 Q108 D109 E110 H111 I114 E117 R120 K121 Y122 R123 I124 P125 A126 D127 V128 D129 P130 L131 T132 I133 L137 S138 S139 D140 G141 V142 L143 T144 V145 N146 G147 P148 R149 K150 Q151 V152 S153 G154 P155 E156

R163 E164 E165 K166 P167 A168 V169 T170 A171 K174 K175

• Molecule 1: Alpha-crystallin B chain

Chain U: 43% 45% 11% •

M1 I5 H6 H7 P8 W9 I10 R11 R12 P13 F14 F15 P16 F17 H18 S19 P20 S21 R22 L23 F24 D25 Q26 F27 F28 L32 L33 L37 F38 P39 T40 S41 T42 S43 L44 S45 P46 F47 Y48 L49 R50 P51 F54 L55 R56 A57 P58 F61 D62 T63 G64 R69 L70 E71

K72 D73 R74 F75 S76 V77 N78 L79 D80 V81 S85 P86 V100 H104 E105 E106 R107 Q108 D109 G112 F113 I114 E117 R120 K121 Y122 R123 I124 P125 A126 D127 V128 D129 P130 I133 G141 V142 L143 T144 V145 P148 R149 K150 Q151 V152 S153 G154 P155 E156 R157

I161 T162 R163 E164 E165 K166 P167 A168 V169 T170 A171 K174 K175

• Molecule 1: Alpha-crystallin B chain

Chain V: 43% 46% 10% •

M1 D2 I5 H6 I10 R11 R12 P13 F14 F15 P16 F17 H18 S19 P20 S21 R22 L23 F24 D25 Q26 F27 F28 G29 E30 H31 P39 T40 S41 L44 S45 P46 F47 R50 P51 L55 R56 A57 P58 S59 W60 R69 L70 E71 K72 D73 R74 V77 N78 L79 D80 V81

F84 S85 P86 E87 G95 V100 H104 E105 E106 R107 Q108 D109 E110 H111 I114 E117 R120 K121 Y122 R123 I124 P125 A126 D127 P130 L131 T132 I133 T134 L137 S138 S139 D140 G141 V142 L143 T144 V145 N146 G147 P148 R149 K150 Q151 V152 S153 G154 P155 E156 R157

T162 R163 E164 E165 K166 P167 A168 V169 T170 A171 K174 K175

• Molecule 1: Alpha-crystallin B chain

Chain W: 42% 45% 11% •

M1 P8 W9 I10 R11 R12 P13 F14 F15 P16 F17 H18 S19 P20 S21 R22 L23 F24 D25 Q26 F27 F28 G29 E30 H31 L32 L33 E34 L37 F38 P39 T40 S41 T42 S43 L44 S45 P46 F47 Y48 L49 R50 P51 F54 L55 R56 A57 P58 F61 D62 T63 G64 L65 S66 R69

L70 E71 K72 D73 R74 F75 S76 V77 N78 L79 D80 V81 S85 G95 V100 H104 E105 E106 R107 Q108 D109 E110 H111 G112 F113 I114 E117 R120 K121 Y122 R123 I124 P125 A126 D127 V128 D129 P130 L131 T132 I133 G141 V142 L143 T144 P148 R149 K150 Q151 V152 P155

E156 R157 T158 I161 T162 R163 E164 E165 K166 P167 A168 V169 T170 K174 K175

• Molecule 1: Alpha-crystallin B chain

Chain X: 43% 43% 11%

M1 D2 I5 H6 I10 R11 R12 P13 F14 F15 P16 F17 H18 S19 P20 S21 R22 L23 F24 D25 Q26 F27 F28 G29 E30 H31 P39 T40 S41 T42 S43 L44 S45 P46 F47 R50 P51 L55 R56 A57 P58 S59 W60 R69 L70 E71 K72 D73 R74 V77 N78 L79 D80

V81 F84 S85 P86 E87 E88 L89 G95 D96 V97 V100 H104 E105 E106 R107 Q108 D109 E110 H111 I114 E117 R120 K121 Y122 R123 I124 P125 A126 D127 V128 D129 P130 L131 T132 I133 L137 S138 S139 D140 G141 V142 L143 T144 V145 N146 G147 P148 R149 K150 Q151 V152 S153

G154 P155 E156 I159 R163 E164 E165 K166 P167 A168 V169 T170 A171 K174 K175

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, 1 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)

There are no covalent bond-length or bond-angle outliers.

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	1	4
1	B	0	4
1	C	0	2
1	D	0	4
1	E	0	3
1	F	0	4
1	G	1	5
1	H	1	3
1	I	1	3
1	J	0	4
1	K	2	3
1	L	0	3
1	M	0	3
1	N	0	4
1	O	0	5
1	P	0	3
1	Q	2	3
1	R	0	4
1	S	0	4
1	T	0	4
1	U	0	1
1	V	0	3
1	W	2	5
1	X	0	4
All	All	10	85

There are no bond-length outliers.

There are no bond-angle outliers.

5 of 10 chiral outliers are listed below.

Mol	Chain	Res	Type	Atoms
1	A	162	THR	CB

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
1	G	162	THR	CB
1	H	42	THR	CB
1	I	162	THR	CB
1	K	3	ILE	CB

5 of 85 planar outliers are listed below.

Mol	Chain	Res	Type	Group
1	A	11	ARG	Sidechain
1	A	22	ARG	Sidechain
1	A	50	ARG	Sidechain
1	A	69	ARG	Sidechain
1	B	12	ARG	Sidechain

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	1413	343	1375	190
1	B	1413	343	1375	101
1	C	1413	343	1375	191
1	D	1413	343	1375	127
1	E	1413	343	1375	198
1	F	1413	343	1375	122
1	G	1413	343	1375	198
1	H	1413	343	1375	124
1	I	1413	343	1375	178
1	J	1413	343	1375	114
1	K	1413	343	1375	185
1	L	1413	343	1375	119
1	M	1413	343	1375	179
1	N	1413	343	1375	108
1	O	1413	343	1375	182
1	P	1413	343	1375	116
1	Q	1413	343	1375	193
1	R	1413	343	1375	117
1	S	1413	343	1375	193

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Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	T	1413	343	1375	105
1	U	1413	343	1375	189
1	V	1413	343	1375	119
1	W	1413	343	1375	198
1	X	1413	343	1375	130
All	All	33912	8232	33000	2512

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 38.

5 of 2512 clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)
1:B:26:GLN:HB2	1:C:163:ARG:HB3	1.09	1.23
1:T:26:GLN:HB2	1:U:163:ARG:HB3	1.04	1.27
1:J:26:GLN:HB3	1:K:163:ARG:HB3	1.03	1.25
1:W:15:PHE:HB3	1:W:16:PRO:HD3	0.98	1.36
1:C:15:PHE:HB3	1:C:16:PRO:CD	0.96	1.90

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	173/175 (99%)	115 (66%)	45 (26%)	13 (8%)	2 15
1	B	173/175 (99%)	122 (71%)	36 (21%)	15 (9%)	1 12
1	C	173/175 (99%)	119 (69%)	36 (21%)	18 (10%)	1 9
1	D	173/175 (99%)	121 (70%)	31 (18%)	21 (12%)	1 7
1	E	173/175 (99%)	120 (69%)	40 (23%)	13 (8%)	2 15
1	F	173/175 (99%)	121 (70%)	36 (21%)	16 (9%)	1 11
1	G	173/175 (99%)	115 (66%)	44 (25%)	14 (8%)	2 14
1	H	173/175 (99%)	118 (68%)	39 (23%)	16 (9%)	1 11
1	I	173/175 (99%)	120 (69%)	35 (20%)	18 (10%)	1 9
1	J	173/175 (99%)	124 (72%)	32 (18%)	17 (10%)	1 10

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	K	173/175 (99%)	117 (68%)	38 (22%)	18 (10%)	1 9
1	L	173/175 (99%)	120 (69%)	35 (20%)	18 (10%)	1 9
1	M	173/175 (99%)	116 (67%)	42 (24%)	15 (9%)	1 12
1	N	173/175 (99%)	120 (69%)	37 (21%)	16 (9%)	1 11
1	O	173/175 (99%)	119 (69%)	32 (18%)	22 (13%)	1 6
1	P	173/175 (99%)	120 (69%)	32 (18%)	21 (12%)	1 7
1	Q	173/175 (99%)	116 (67%)	42 (24%)	15 (9%)	1 12
1	R	173/175 (99%)	121 (70%)	36 (21%)	16 (9%)	1 11
1	S	173/175 (99%)	122 (71%)	37 (21%)	14 (8%)	2 14
1	T	173/175 (99%)	119 (69%)	36 (21%)	18 (10%)	1 9
1	U	173/175 (99%)	116 (67%)	41 (24%)	16 (9%)	1 11
1	V	173/175 (99%)	118 (68%)	39 (23%)	16 (9%)	1 11
1	W	173/175 (99%)	117 (68%)	42 (24%)	14 (8%)	2 14
1	X	173/175 (99%)	120 (69%)	34 (20%)	19 (11%)	1 8
All	All	4152/4200 (99%)	2856 (69%)	897 (22%)	399 (10%)	1 10

5 of 399 Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type
1	A	2	ASP
1	A	18	HIS
1	A	21	SER
1	A	39	PRO
1	A	41	SER

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	161/161 (100%)	148 (92%)	13 (8%)	15 63
1	B	161/161 (100%)	153 (95%)	8 (5%)	28 77

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	161/161 (100%)	146 (91%)	15 (9%)	12	59
1	D	161/161 (100%)	151 (94%)	10 (6%)	22	71
1	E	161/161 (100%)	149 (93%)	12 (7%)	17	65
1	F	161/161 (100%)	154 (96%)	7 (4%)	33	81
1	G	161/161 (100%)	144 (89%)	17 (11%)	10	55
1	H	161/161 (100%)	154 (96%)	7 (4%)	33	81
1	I	161/161 (100%)	148 (92%)	13 (8%)	15	63
1	J	161/161 (100%)	155 (96%)	6 (4%)	37	85
1	K	161/161 (100%)	141 (88%)	20 (12%)	8	50
1	L	161/161 (100%)	155 (96%)	6 (4%)	37	85
1	M	161/161 (100%)	145 (90%)	16 (10%)	11	57
1	N	161/161 (100%)	154 (96%)	7 (4%)	33	81
1	O	161/161 (100%)	143 (89%)	18 (11%)	9	53
1	P	161/161 (100%)	151 (94%)	10 (6%)	22	71
1	Q	161/161 (100%)	147 (91%)	14 (9%)	14	60
1	R	161/161 (100%)	154 (96%)	7 (4%)	33	81
1	S	161/161 (100%)	147 (91%)	14 (9%)	14	60
1	T	161/161 (100%)	157 (98%)	4 (2%)	50	91
1	U	161/161 (100%)	146 (91%)	15 (9%)	12	59
1	V	161/161 (100%)	149 (93%)	12 (7%)	17	65
1	W	161/161 (100%)	143 (89%)	18 (11%)	9	53
1	X	161/161 (100%)	152 (94%)	9 (6%)	25	74
All	All	3864/3864 (100%)	3586 (93%)	278 (7%)	18	66

5 of 278 residues with a non-rotameric sidechain are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type
1	A	14	PHE
1	A	15	PHE
1	A	17	PHE
1	A	22	ARG
1	A	25	ASP

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 (i)

No chemical shift data were provided