wwPDB X-ray Structure Validation Summary Report ⓘ

Dec 3, 2023 – 07:38 am GMT

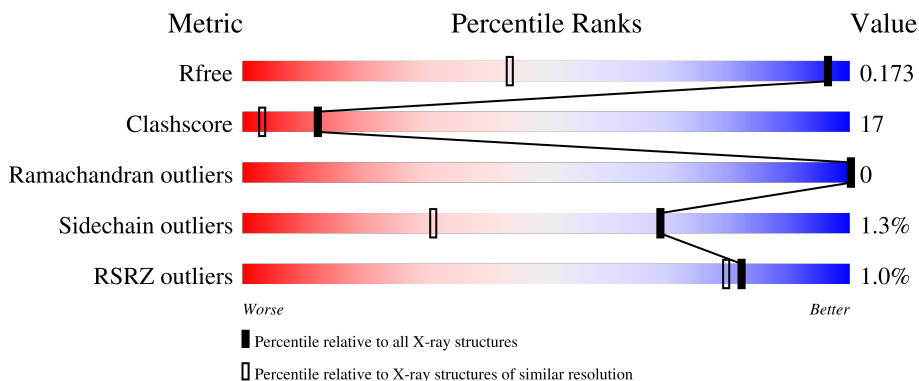|		
PDB ID	:	2WJ5
Title	:	Rat alpha crystallin domain
Authors	:	Naylor, C.E.; Bagneris, C.; Bateman, O.A.; Cronin, N.; Keep, N.H.; Slingsby, C.
Deposited on	:	2009-05-22
Resolution	:	1.12 Å(reported)

1 Overall quality at a glance ⓘ

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

The reported resolution of this entry is 1.12 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	Percentile Ranks	Value
Rfree		0.173
Clashscore		17
Ramachandran outliers		0
Sidechain outliers		1.3%
RSRZ outliers		1.0%

Worse   *Better*

▌ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R$_{free}$	130704	1168 (1.14-1.10)
Clashscore	141614	1205 (1.14-1.10)
Ramachandran outliers	138981	1168 (1.14-1.10)
Sidechain outliers	138945	1165 (1.14-1.10)
RSRZ outliers	127900	1146 (1.14-1.10)

2 Entry composition ⓘ

There are 2 unique types of molecules in this entry. The entry contains 1061 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 HEAT SHOCK PROTEIN BETA-6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	96	834	528	148	156	2	0	14	0

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
2	A	227	227	227	0	0

SEQUENCE-PLOTS INFOmissingINFO

3 Data and refinement statistics ⓘ

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	105.48Å 37.96Å 28.08Å 90.00° 91.55° 90.00°	Depositor
Resolution (Å)	28.07 – 1.12 28.07 – 1.12	Depositor EDS
% Data completeness (in resolution range)	91.5 (28.07-1.12) 91.6 (28.07-1.12)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.71 (at 1.12Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.152 , 0.180 0.144 , 0.173	Depositor DCC
R_{free} test set	1968 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	10.3	Xtriage
Anisotropy	0.523	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 70.2	EDS
L-test for twinning[2]	$< |L| > = 0.49, < L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.034 for -h,-k,l	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	1061	wwPDB-VP
Average B, all atoms (Å^2)	18.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 12.59% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

4 Model quality ⓘ

4.1 Standard geometry ⓘ

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	1.21	2/879 (0.2%)	1.19	4/1196 (0.3%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	20	LYS	CB-CG	-7.41	1.32	1.52
1	A	14	SER	CA-CB	5.14	1.60	1.52

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	41[A]	ARG	NE-CZ-NH1	7.60	124.10	120.30
1	A	41[B]	ARG	NE-CZ-NH1	7.60	124.10	120.30
1	A	45	ARG	NE-CZ-NH2	-6.21	117.20	120.30
1	A	58	ARG	NE-CZ-NH2	-5.22	117.69	120.30

There are no chirality outliers.

There are no planarity outliers.

4.2 Too-close contacts ⓘ

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	834	0	814	28	0
2	A	227	0	0	8	0
All	All	1061	0	814	28	0

WORLDWIDE wwPDB
PROTEIN DATA BANK

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 17.

The worst 5 of 28 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:43[B]:GLU:CD	1:A:51[B]:PHE:CE2	2.11	1.24
1:A:48[B]:GLU:HB2	2:A:2158:HOH:O	1.54	1.07
1:A:43[B]:GLU:CD	1:A:51[B]:PHE:HE2	1.55	1.02
1:A:43[B]:GLU:OE2	1:A:51[B]:PHE:HE2	1.55	0.90
1:A:5:GLN:NE2	2:A:2037:HOH:O	2.04	0.89

There are no symmetry-related clashes.

4.3 Torsion angles ⓘ

4.3.1 Protein backbone ⓘ

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	108/101 (107%)	107 (99%)	1 (1%)	0	100 100

There are no Ramachandran outliers to report.

4.3.2 Protein sidechains ⓘ

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	93/82 (113%)	92 (99%)	1 (1%)	73 38

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	20	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

4.3.3 RNA ⓘ

There are no RNA molecules in this entry.

4.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

4.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

4.6 Ligand geometry ⓘ

There are no ligands in this entry.

4.7 Other polymers ⓘ

There are no such residues in this entry.

4.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

5 Fit of model and data ⓘ

5.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	96/101 (95%)	0.42	1 (1%)	82	79	10, 14, 25, 34	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	96	SER	6.5

5.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.4 Ligands ⓘ

There are no ligands in this entry.

5.5 Other polymers ⓘ

There are no such residues in this entry.