



wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 31, 2016 – 11:38 PM GMT

PDB ID : 1XWO
Title : crystal structrue of goose delta crystallin
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Deposited on : 2004-11-02
Resolution : 2.80 Å(reported)

This is a wwPDB X-ray 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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
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:

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

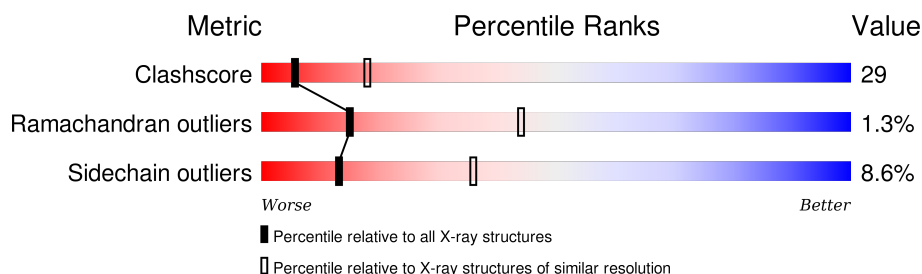
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	465	
1	B	465	
1	C	465	
1	D	465	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 14142 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 Delta crystallin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	448	Total	C	N	O	S	0	0	0
			3474	2193	588	678	15			
1	B	448	Total	C	N	O	S	0	0	0
			3471	2191	588	677	15			
1	C	449	Total	C	N	O	S	0	0	0
			3480	2196	589	680	15			
1	D	449	Total	C	N	O	S	0	0	0
			3483	2198	590	680	15			

- Molecule 2 is water.

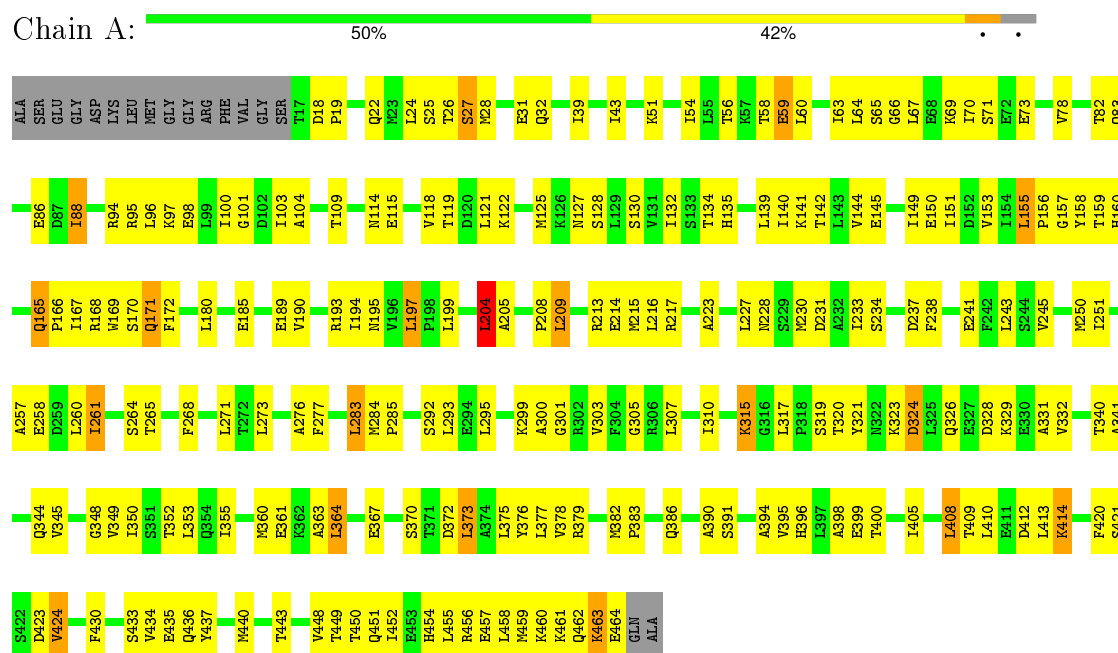
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	82	Total	O	0	0
			82	82		
2	B	53	Total	O	0	0
			53	53		
2	C	59	Total	O	0	0
			59	59		
2	D	40	Total	O	0	0
			40	40		

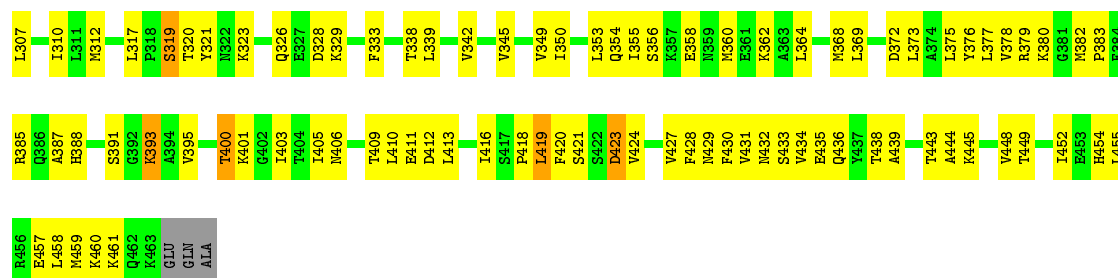
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-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. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

Note EDS was not executed.

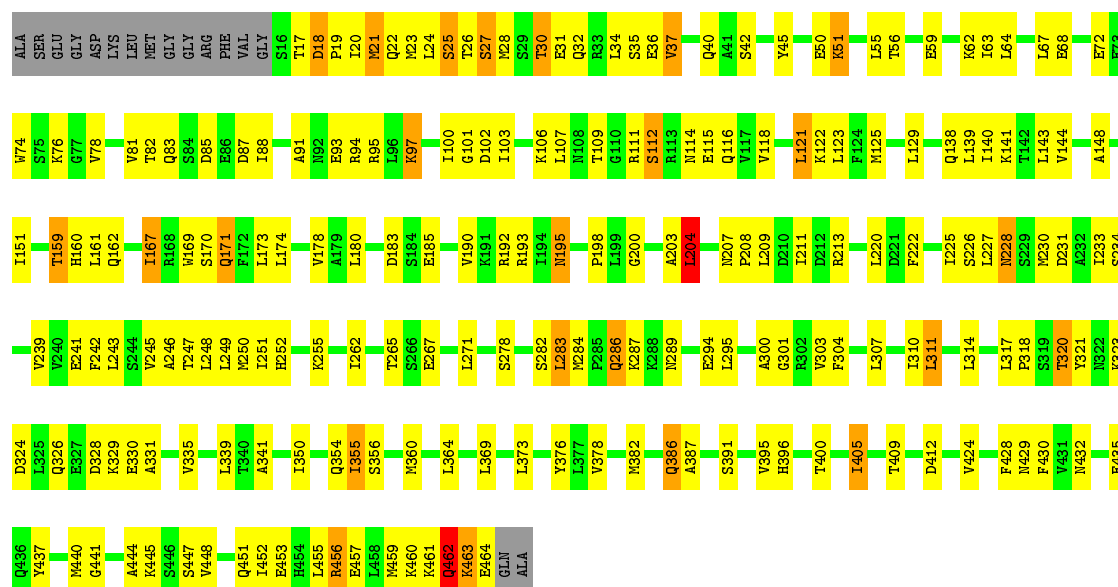
- Molecule 1: Delta crystallin





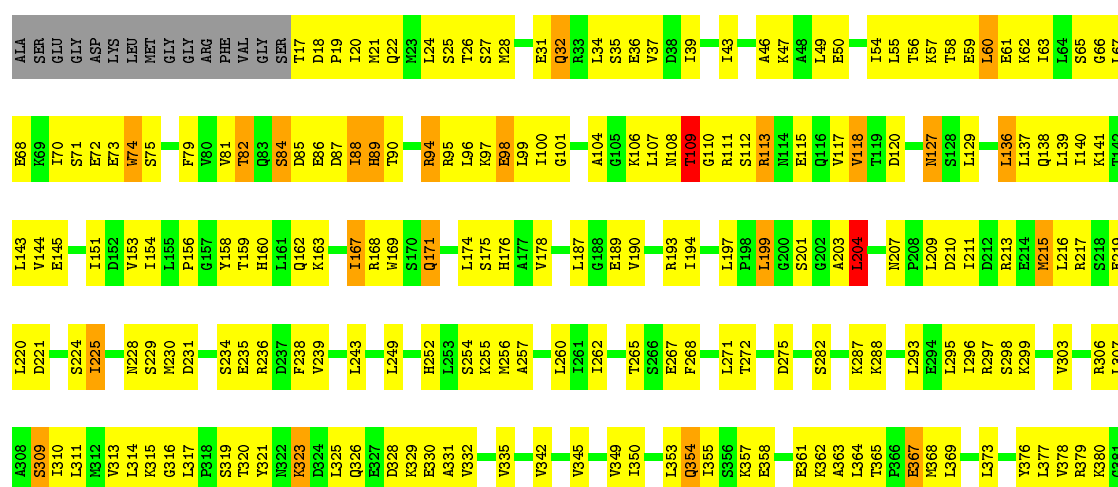
• Molecule 1: Delta crystallin

Chain C: 53% 38% 5% .



• Molecule 1: Delta crystallin

Chain D: 46% 45% 5% .



H382	
A387	
H388	
S391	
H392	
K393	
A394	
V395	
E399	
I403	
T404	
I405	
H406	
H407	
L408	
T409	
D412	
L413	
K414	
L419	
F420	
F428	
H429	
H432	
Q436	
V448	
T449	
T450	
Q451	
I452	
E453	
H454	
L455	
Q462	
K463	
E464	
Q465	
ALA	

4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	93.70 Å 99.00 Å 106.50 Å 90.00° 101.40° 90.00°	Depositor
Resolution (Å)	20.00 – 2.80	Depositor
% Data completeness (in resolution range)	(Not available) (20.00-2.80)	Depositor
R_{merge}	0.14	Depositor
R_{sym}	0.14	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.210 , 0.289	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	14142	wwPDB-VP
Average B, all atoms (Å ²)	34.0	wwPDB-VP

5 Model quality [i](#)

5.1 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 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	0.48	0/3517	0.70	0/4746
1	B	0.48	0/3514	0.66	0/4742
1	C	0.51	2/3523 (0.1%)	0.70	1/4754 (0.0%)
1	D	0.46	0/3526	0.66	0/4758
All	All	0.48	2/14080 (0.0%)	0.68	1/19000 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	464	GLU	CG-CD	-7.96	1.40	1.51
1	C	464	GLU	CB-CG	-7.51	1.37	1.52

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	464	GLU	OE1-CD-OE2	5.80	130.26	123.30

There are no chirality outliers.

There are no planarity outliers.

5.2 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 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	3474	0	3590	211	0
1	B	3471	0	3589	237	0
1	C	3480	0	3595	203	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	3483	0	3598	246	0
2	A	82	0	0	9	0
2	B	53	0	0	5	0
2	C	59	0	0	8	0
2	D	40	0	0	4	0
All	All	14142	0	14372	826	0

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 29.

The worst 5 of 826 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:D:320:THR:HG22	1:D:321:TYR:H	1.16	1.09
1:D:194:ILE:HG12	2:D:498:HOH:O	1.52	1.08
1:A:310:ILE:HG12	2:A:531:HOH:O	1.54	1.06
1:C:283:LEU:H	1:C:283:LEU:HD22	1.19	1.02
1:C:243:LEU:HD11	1:C:310:ILE:HD12	1.37	1.02

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 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 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	446/465 (96%)	409 (92%)	33 (7%)	4 (1%)	21	55
1	B	446/465 (96%)	398 (89%)	44 (10%)	4 (1%)	21	55
1	C	447/465 (96%)	400 (90%)	42 (9%)	5 (1%)	17	50
1	D	447/465 (96%)	392 (88%)	45 (10%)	10 (2%)	8	28
All	All	1786/1860 (96%)	1599 (90%)	164 (9%)	23 (1%)	15	44

5 of 23 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	204	LEU
1	B	204	LEU
1	B	419	LEU
1	D	109	THR
1	A	462	GLN

5.3.2 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	394/405 (97%)	362 (92%)	32 (8%)	15	39
1	B	394/405 (97%)	366 (93%)	28 (7%)	18	46
1	C	395/405 (98%)	355 (90%)	40 (10%)	9	27
1	D	395/405 (98%)	360 (91%)	35 (9%)	12	34
All	All	1578/1620 (97%)	1443 (91%)	135 (9%)	13	36

5 of 135 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	21	MET
1	C	121	LEU
1	D	309	SER
1	C	27	SER
1	C	81	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 59 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	451	GLN
1	C	207	ASN
1	D	406	ASN
1	C	22	GLN
1	C	135	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section will therefore be empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates

EDS was not executed - this section will therefore be empty.

6.4 Ligands

EDS was not executed - this section will therefore be empty.

6.5 Other polymers

EDS was not executed - this section will therefore be empty.