



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 12:36 PM UTC

PDB ID : 1XWO / pdb_00001xwo
Title : crystal structure 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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

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 : 4-5-2 with Phenix2.0
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

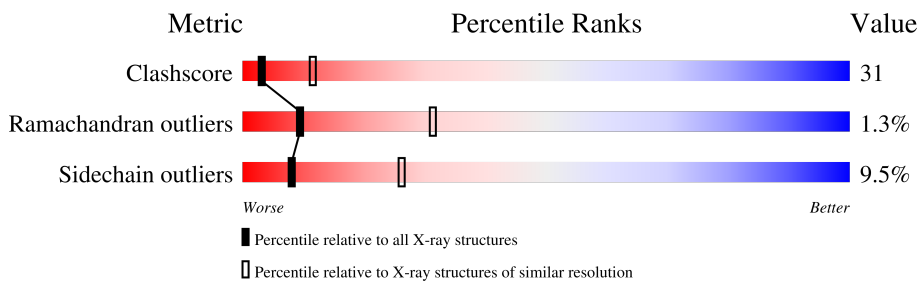
1 Overall quality at a glance

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	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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 $\leq 5\%$.

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			

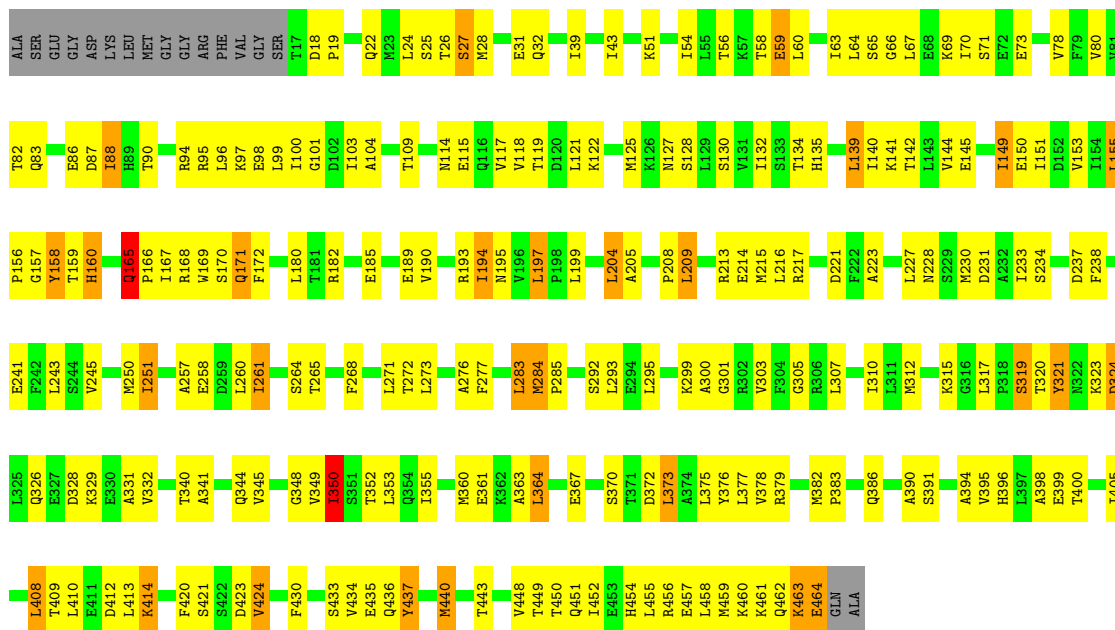
- Molecule 2 is water.

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		

Note EDS was not executed.

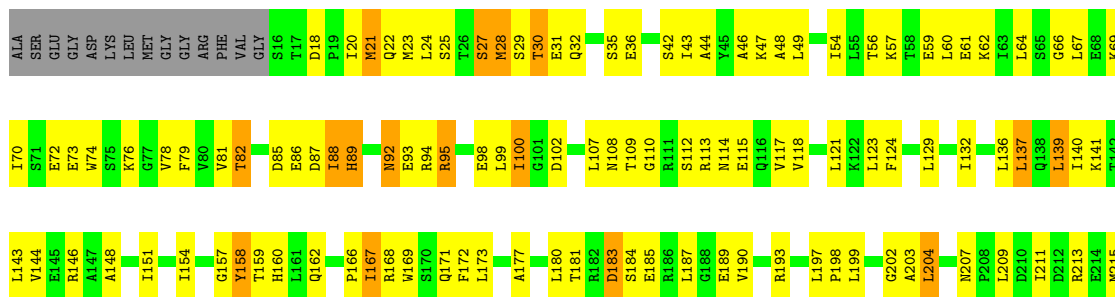
- Molecule 1: Delta crystallin

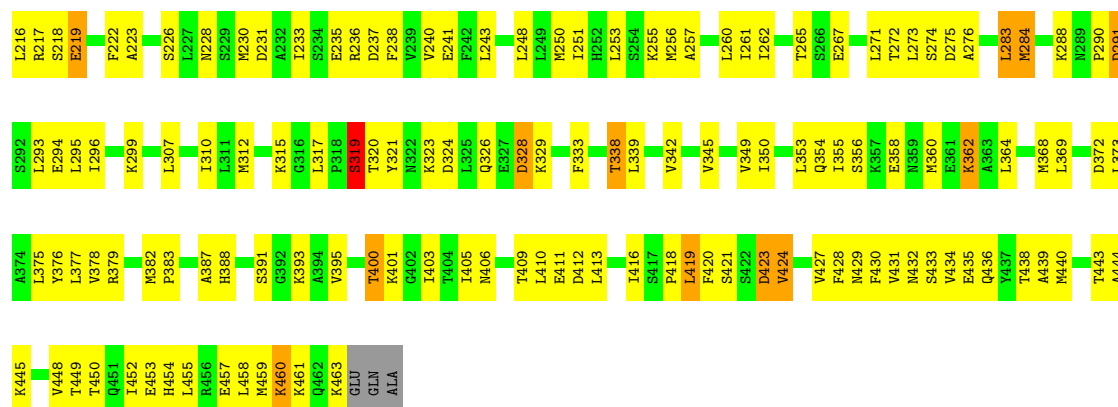
6%



- Molecule 1: Delta crystallin

6%





L377	V378	R379	K380	G381	M382	A387	H388	S391	G392	K393	A394	V395	E399	I403	T404	I405	N406	N407	I408	T409	D412	L413	K414	L419	F420	F428	N429	F430	V431	N432	Q436	M440	V448	T449	T450	Q451	I452	E453	H454	L455	M459	Q462	K463	E464	Q465	ALA				
R302	V303	R306	L307	A308	S309	I310	L311	M312	V313	L314	K315	G316	L317	P318	S319	T320	Y321	N322	K323	D324	L325	Q326	E327	D328	K329	E330	A331	V332	V335	V342	V345	V349	I350	L353	Q354	I355	S356	K357	E358	E361	K362	A363	L364	T365	P366	E367	M368	L369	L373	Y376
E219	L220	D221	S224	I225	N228	S229	M230	D231	S234	E235	R236	D237	F238	V239	L243	L249	M250	I251	H252	L253	S254	K255	M256	A257	L260	I261	I262	T265	S266	E267	F268	L271	T272	D275	S282	Q286	K287	K288	L293	E294	L295	I296	R297	S298	K299	A300	G301			

4 Data and refinement statistics

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

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	93.70Å 99.00Å 106.50Å 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	0.60	0/3517	1.03	10/4746 (0.2%)
1	B	0.62	0/3514	1.01	8/4742 (0.2%)
1	C	0.63	0/3523	1.01	11/4754 (0.2%)
1	D	0.59	1/3526 (0.0%)	0.98	7/4758 (0.1%)
All	All	0.61	1/14080 (0.0%)	1.01	36/19000 (0.2%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	26	THR	CA-CB	5.09	1.60	1.53

The worst 5 of 36 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	319	SER	N-CA-C	8.04	121.89	110.23
1	A	319	SER	N-CA-C	8.02	120.66	110.24
1	C	17	THR	N-CA-C	6.83	118.63	107.23
1	C	461	LYS	N-CA-C	-6.80	103.79	111.14
1	B	158	TYR	N-CA-C	6.72	120.19	109.24

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	221	0
1	B	3471	0	3589	255	0
1	C	3480	0	3595	222	0
1	D	3483	0	3598	266	0
2	A	82	0	0	10	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	883	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 31.

The worst 5 of 883 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%)	14 41
1	B	446/465 (96%)	398 (89%)	44 (10%)	4 (1%)	14 41
1	C	447/465 (96%)	400 (90%)	42 (9%)	5 (1%)	11 36
1	D	447/465 (96%)	392 (88%)	45 (10%)	10 (2%)	5 19

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	1786/1860 (96%)	1599 (90%)	164 (9%)	23 (1%)	9	31

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%)	355 (90%)	39 (10%)	7	24
1	B	394/405 (97%)	359 (91%)	35 (9%)	9	29
1	C	395/405 (98%)	355 (90%)	40 (10%)	7	23
1	D	395/405 (98%)	359 (91%)	36 (9%)	9	28
All	All	1578/1620 (97%)	1428 (90%)	150 (10%)	8	26

5 of 150 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	39	ILE
1	D	367	GLU
1	D	84	SER
1	D	199	LEU
1	B	95	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 65 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	326	GLN
1	D	354	GLN
1	B	354	GLN
1	B	326	GLN
1	D	406	ASN

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 oligosaccharides 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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates [i](#)

EDS was not executed - this section is therefore empty.

6.4 Ligands [i](#)

EDS was not executed - this section is therefore empty.

6.5 Other polymers [i](#)

EDS was not executed - this section is therefore empty.