



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 9, 2026 – 12:48 PM UTC

PDB ID : 1I0A / pdb_00001i0a
Title : CRYSTAL STRUCTURE OF WILD TYPE TURKEY DELTA 1 CRYSTALLIN (EYE LENS PROTEIN)
Authors : Sampaleanu, L.M.; Vallee, F.; Slingsby, C.; Howell, P.L.
Deposited on : 2001-01-29
Resolution : 2.50 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)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

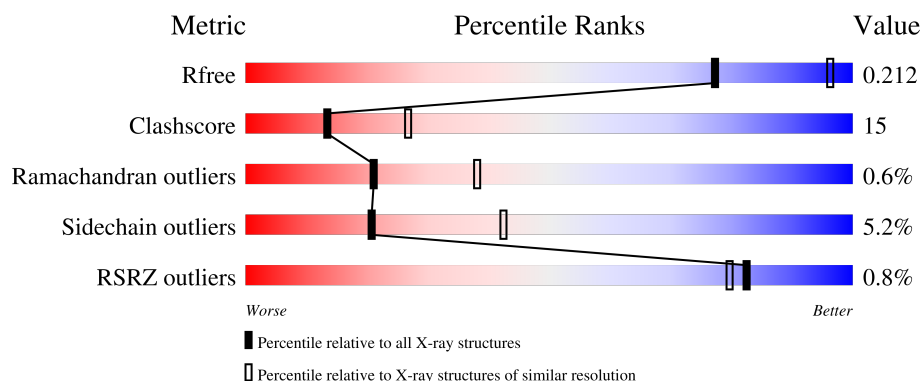
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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))
R_{free}	180053	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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 $\leq 5\%$. 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.

Mol	Chain	Length	Quality of chain
1	A	466	% 68% 27% • •
1	B	466	% 64% 29% • 5%
1	C	466	68% 26% • 5%
1	D	466	% 69% 23% • 5%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 14263 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 I.

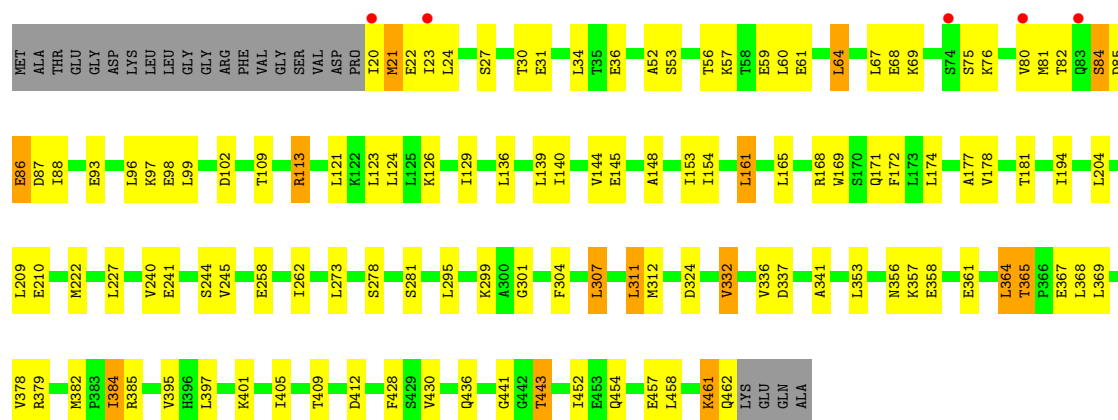
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	453	Total	C	N	O	S	0	0	0
			3461	2192	581	679	9			
1	B	444	Total	C	N	O	S	0	0	0
			3407	2156	572	670	9			
1	C	445	Total	C	N	O	S	0	0	0
			3413	2159	572	673	9			
1	D	443	Total	C	N	O	S	0	0	0
			3394	2148	569	668	9			

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	146	Total	O	0	0
			146	146		
2	B	156	Total	O	0	0
			156	156		
2	C	142	Total	O	0	0
			142	142		
2	D	144	Total	O	0	0
			144	144		

T371	T233	SL12	MET
L375	R236	THR	ALA
R379	D237	GLY	THR
M382	F238	GLY	GLY
I384	V239	ASP	GLY
R385	V240	LYS	LYS
Q386	E241	LEU	LEU
S391	L242	GLY	GLY
G392	L245	GLY	GLY
K393	V248	ARG	ARG
A394	L248	PHE	PHE
V395	I251	VAL	VAL
R396	K255	GLY	GLY
L397	L260	SER	SER
A398	L283	VAL	VAL
E399	K287	D18	D18
T400	G298	P19	P19
K401	I403	I20	I20
G402	T404	I23	I23
I405	A309	L24	L24
M406	L161	L34	L34
M407	L165	T35	T35
I416	M312	E50	E50
L419	V313	L55	L55
A421	G316	T56	T56
S422	L325	K57	K57
D423	E327	T58	T58
V430	D328	E59	E59
V431	K329	L60	L60
E435	V332	E61	E61
Q436	V336	L64	L64
Y437	L339	M81	M81
T443	T340	D85	D85
I452	A341	L88	L88
R456	L353	A91	A91
K460	K357	T92	T92
K461	E358	E93	E93
Q462	L363	R94	R94
LYS	R213	L96	L96
GLU	E361	L99	L99
GLN	K362	T100	T100
ALA	A363	G101	G101
	L364	D102	D102
	L365	M222	M222
	P366	G105	G105
	E367	L227	L227
	L369	G109	G109

Chain D: 69% 23% 5%



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	89.42Å 146.55Å 152.90Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.78 – 2.50 19.78 – 2.50	Depositor EDS
% Data completeness (in resolution range)	95.1 (19.78-2.50) 95.0 (19.78-2.50)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	0.05	Depositor
$\langle I/\sigma(I) \rangle$ ¹	7.09 (at 2.51Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.156 , 0.213 0.156 , 0.212	Depositor DCC
R_{free} test set	6641 reflections (9.94%)	wwPDB-VP
Wilson B-factor (Å ²)	33.2	Xtriage
Anisotropy	0.066	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 73.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.004 for -h,l,k	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	14263	wwPDB-VP
Average B, all atoms (Å ²)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.96% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 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	0.40	0/3493	0.87	3/4722 (0.1%)
1	B	0.42	0/3437	0.86	2/4644 (0.0%)
1	C	0.40	0/3444	0.91	4/4656 (0.1%)
1	D	0.41	0/3424	0.87	5/4628 (0.1%)
All	All	0.41	0/13798	0.88	14/18650 (0.1%)

There are no bond length outliers.

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	85	ASP	N-CA-C	-12.03	92.48	110.28
1	A	85	ASP	N-CA-C	-7.01	96.17	108.23
1	C	365	THR	CA-C-N	6.45	126.67	119.32
1	C	365	THR	C-N-CA	6.45	126.67	119.32
1	D	384	ILE	N-CA-C	6.11	116.78	110.36

There are no chirality outliers.

There are no planarity outliers.

5.2 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	3461	0	3651	105	0
1	B	3407	0	3607	128	0
1	C	3413	0	3605	103	0
1	D	3394	0	3588	101	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	146	0	0	5	0
2	B	156	0	0	6	0
2	C	142	0	0	4	0
2	D	144	0	0	6	0
All	All	14263	0	14451	412	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 15.

The worst 5 of 412 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:126:LYS:HD2	1:A:222:MET:HE1	1.49	0.93
1:B:32:GLN:HE21	1:B:81:MET:HG2	1.34	0.92
1:C:382:MET:HE3	1:C:419:LEU:HD12	1.53	0.90
1:C:194:ILE:HD13	1:C:238:PHE:HB2	1.56	0.88
1:B:126:LYS:HD2	1:B:222:MET:HE1	1.56	0.85

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	451/466 (97%)	435 (96%)	12 (3%)	4 (1%)	14	27
1	B	442/466 (95%)	427 (97%)	14 (3%)	1 (0%)	43	63
1	C	443/466 (95%)	427 (96%)	12 (3%)	4 (1%)	14	27
1	D	441/466 (95%)	426 (97%)	13 (3%)	2 (0%)	24	43
All	All	1777/1864 (95%)	1715 (96%)	51 (3%)	11 (1%)	21	38

5 of 11 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	204	LEU
1	D	204	LEU
1	C	204	LEU
1	C	400	THR
1	A	204	LEU

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	394/406 (97%)	373 (95%)	21 (5%)	20	42
1	B	390/406 (96%)	367 (94%)	23 (6%)	18	37
1	C	391/406 (96%)	373 (95%)	18 (5%)	24	48
1	D	388/406 (96%)	368 (95%)	20 (5%)	21	42
All	All	1563/1624 (96%)	1481 (95%)	82 (5%)	21	42

5 of 82 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	357	LYS
1	D	121	LEU
1	C	407	ASN
1	D	67	LEU
1	D	161	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 43 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	359	ASN
1	D	108	GLN
1	C	388	GLN
1	C	432	ASN
1	D	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 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](#)

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	453/466 (97%)	-0.45	3 (0%) 84 81	18, 36, 83, 98	0
1	B	444/466 (95%)	-0.46	5 (1%) 78 75	17, 37, 80, 100	0
1	C	445/466 (95%)	-0.49	1 (0%) 91 89	18, 37, 76, 93	0
1	D	443/466 (95%)	-0.60	5 (1%) 78 75	16, 34, 76, 100	0
All	All	1785/1864 (95%)	-0.50	14 (0%) 82 80	16, 36, 80, 100	0

The worst 5 of 14 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	82	THR	4.0
1	D	80	VAL	3.5
1	B	80	VAL	3.5
1	A	17	VAL	3.4
1	A	462	GLN	3.2

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.