



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 14, 2017 – 03:24 am GMT

PDB ID : 1BLB
Title : CLOSE PACKING OF AN OLIGOMERIC EYE LENS BETA-CRYSTALLIN INDUCES LOSS OF SYMMETRY AND ORDERING OF SEQUENCE EXTENSIONS
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Deposited on : 1993-12-22
Resolution : 3.30 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
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : recalc28949

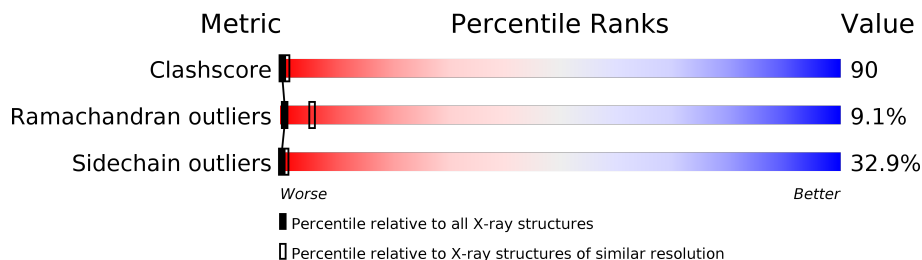
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.30 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	112137	1100 (3.36-3.24)
Ramachandran outliers	110173	1081 (3.36-3.24)
Sidechain outliers	110143	1080 (3.36-3.24)

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	204	
1	B	204	
1	C	204	
1	D	204	

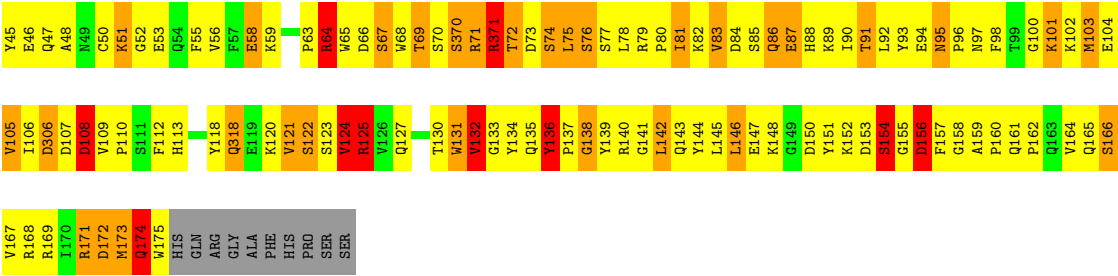
2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 5941 atoms, of which 0 are hydrogens and 0 are deuteriums.

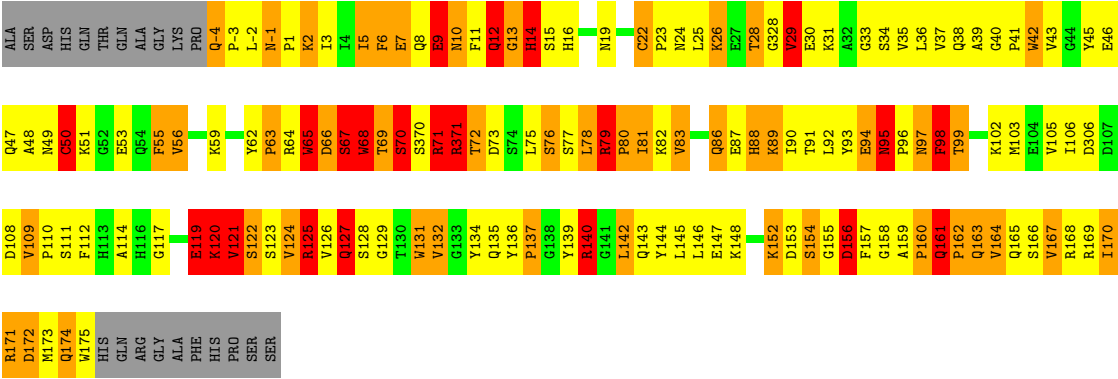
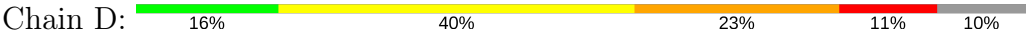
In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called BETA B2-CRYSTALLIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	185	Total	C	N	O	S	0	0	0
			1492	942	261	285	4			
1	B	181	Total	C	N	O	S	0	0	0
			1464	924	256	280	4			
1	C	187	Total	C	N	O	S	0	0	0
			1505	950	264	287	4			
1	D	183	Total	C	N	O	S	0	0	0
			1480	934	259	283	4			



● Molecule 1: BETA B2-CRYSTALLIN



4 Data and refinement statistics

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

Property	Value	Source
Space group	C 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	154.71Å 165.90Å 78.48Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	(Not available) – 3.30	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-3.30)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	RESTRAIN, X-PLOR	Depositor
R, R_{free}	(Not available) , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	5941	wwPDB-VP
Average B, all atoms (Å ²)	0.0	wwPDB-VP

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	1.31	6/1535 (0.4%)	1.83	34/2080 (1.6%)
1	B	1.30	6/1505 (0.4%)	1.77	38/2037 (1.9%)
1	C	1.28	6/1548 (0.4%)	1.80	29/2096 (1.4%)
1	D	1.30	7/1522 (0.5%)	1.80	39/2061 (1.9%)
All	All	1.30	25/6110 (0.4%)	1.80	140/8274 (1.7%)

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 outliers	#Planarity outliers
1	A	2	5
1	B	1	7
1	C	3	5
1	D	5	7
All	All	11	24

The worst 5 of 25 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	8	GLN	CD-OE1	5.69	1.36	1.24
1	B	12	GLN	CD-OE1	5.58	1.36	1.24
1	D	42	TRP	NE1-CE2	-5.51	1.30	1.37
1	B	131	TRP	NE1-CE2	-5.49	1.30	1.37
1	B	74	SER	N-CA	5.48	1.57	1.46

The worst 5 of 140 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	13	GLY	C-N-CA	16.12	162.01	121.70
1	C	132	VAL	CA-CB-CG2	11.88	128.71	110.90
1	A	167	VAL	CA-CB-CG1	11.19	127.68	110.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	167	VAL	CA-CB-CG2	11.00	127.40	110.90
1	D	109	VAL	CA-CB-CG2	10.44	126.57	110.90

5 of 11 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	-6	LYS	CA
1	A	67	SER	CA
1	B	86	GLN	CA
1	C	-5	PRO	CA
1	C	37	VAL	CA

5 of 24 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	140	ARG	Sidechain
1	A	168	ARG	Sidechain
1	A	169	ARG	Sidechain
1	A	71	ARG	Sidechain
1	A	79	ARG	Sidechain

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	1492	0	1416	270	2
1	B	1464	0	1391	274	0
1	C	1505	0	1435	286	1
1	D	1480	0	1406	270	1
All	All	5941	0	5648	1041	3

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 90.

The worst 5 of 1041 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:41:PRO:HB2	1:D:81:ILE:CD1	1.47	1.43
1:C:43:VAL:HG12	1:C:81:ILE:CD1	1.50	1.39
1:D:154:SER:HB2	1:D:159:ALA:CB	1.51	1.39
1:D:41:PRO:CB	1:D:81:ILE:HD11	1.55	1.36
1:D:154:SER:CB	1:D:159:ALA:HB3	1.61	1.31

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:19:ASN:ND2	1:D:-4:GLN:O[1_554]	1.99	0.21
1:A:67:SER:OG	1:A:136:TYR:CD2[3_555]	2.02	0.18
1:C:371:ARG:CD	1:C:371:ARG:CD[4_555]	2.03	0.17

5.3 Torsion angles

5.3.1 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	183/204 (90%)	144 (79%)	21 (12%)	18 (10%)	1	4
1	B	179/204 (88%)	130 (73%)	34 (19%)	15 (8%)	1	7
1	C	185/204 (91%)	137 (74%)	31 (17%)	17 (9%)	1	5
1	D	181/204 (89%)	136 (75%)	29 (16%)	16 (9%)	1	6
All	All	728/816 (89%)	547 (75%)	115 (16%)	66 (9%)	1	6

5 of 66 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	3	ILE
1	A	48	ALA
1	A	65	TRP
1	A	73	ASP

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Mol	Chain	Res	Type
1	A	96	PRO

5.3.2 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 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	162/177 (92%)	104 (64%)	58 (36%)	0	1
1	B	159/177 (90%)	104 (65%)	55 (35%)	0	1
1	C	163/177 (92%)	111 (68%)	52 (32%)	0	1
1	D	161/177 (91%)	114 (71%)	47 (29%)	0	1
All	All	645/708 (91%)	433 (67%)	212 (33%)	0	1

5 of 212 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	118	TYR
1	C	5	ILE
1	D	94	GLU
1	B	132	VAL
1	B	167	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 25 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	165	GLN
1	C	-4	GLN
1	D	95	ASN
1	B	174	GLN
1	C	-1	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 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 is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.