



## Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 03:38 pm BST

PDB ID : 6ETA  
Title : Crystal Structure of Human Gamma-D crystallin Mutant P23T+R36S at Room Temperature  
Authors : James, S.; McManus, J.; Khan, A.R.  
Deposited on : 2017-10-25  
Resolution : 2.20 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto: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.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

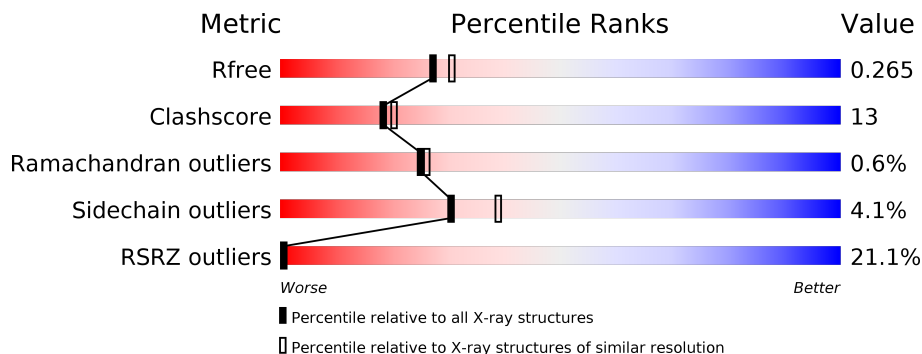
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.20 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))
$R_{free}$	130704	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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  $\geq 3$ , 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	174	
1	B	174	

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 2888 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 Gamma-crystallin D.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	171	1395	866	257	262	10	0	0	0
1	B	170	1381	859	253	259	10	0	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	23	THR	PRO	engineered mutation	UNP P07320
A	36	SER	ARG	engineered mutation	UNP P07320
B	23	THR	PRO	engineered mutation	UNP P07320
B	36	SER	ARG	engineered mutation	UNP P07320

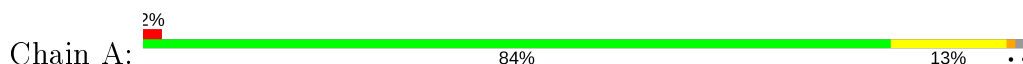
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	73	Total	O	0	0
			73	73		
2	B	39	Total	O	0	0
			39	39		

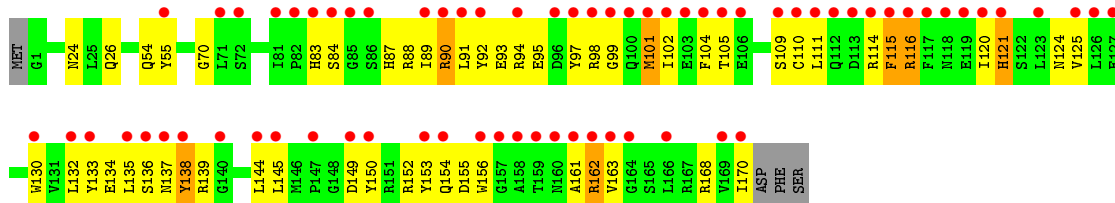
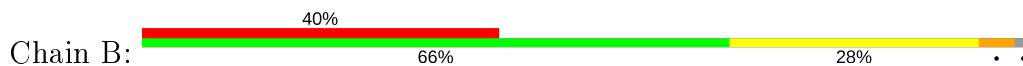
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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.

- Molecule 1: Gamma-crystallin D



- Molecule 1: Gamma-crystallin D



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	54.04Å 82.10Å 106.25Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.16 – 2.20 48.16 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.6 (48.16-2.20) 99.6 (48.16-2.20)	Depositor EDS
$R_{merge}$	0.13	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.29 (at 2.20Å)	Xtrriage
Refinement program	PHENIX (1.11.1_2575: ???)	Depositor
R, $R_{free}$	0.233 , 0.265 0.233 , 0.265	Depositor DCC
$R_{free}$ test set	1233 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	38.7	Xtrriage
Anisotropy	0.541	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 45.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	2888	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	59.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.34% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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 [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	0.25	0/1430	0.48	0/1931
1	B	0.29	0/1416	0.56	0/1913
All	All	0.27	0/2846	0.52	0/3844

There are no bond length outliers.

There are no bond angle outliers.

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	1395	0	1282	13	0
1	B	1381	0	1267	58	0
2	A	73	0	0	1	0
2	B	39	0	0	1	0
All	All	2888	0	2549	71	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 13.

All (71) 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:B:89:ILE:HD11	1:B:130:TRP:CH2	2.07	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:89:ILE:HD11	1:B:130:TRP:CZ2	2.11	0.85
1:B:104:PHE:HZ	1:B:111:LEU:HD21	1.41	0.83
1:B:87:HIS:HB3	1:B:130:TRP:CZ2	2.20	0.77
1:B:104:PHE:CZ	1:B:111:LEU:HD21	2.20	0.77
1:B:87:HIS:ND1	1:B:168:ARG:HG2	2.07	0.68
1:B:94:ARG:NH1	1:B:95:GLU:OE1	2.27	0.68
1:B:152:ARG:HD2	1:B:153:TYR:H	1.58	0.67
1:B:111:LEU:HD23	1:B:114:ARG:HB2	1.77	0.67
1:B:89:ILE:HD11	1:B:130:TRP:CZ3	2.31	0.65
1:B:132:LEU:HD21	1:B:163:VAL:HG22	1.79	0.64
1:B:24:ASN:HD21	1:B:26:GLN:HE21	1.45	0.63
1:B:92:TYR:CG	1:B:97:TYR:HA	2.35	0.62
1:B:89:ILE:HD11	1:B:130:TRP:CE2	2.35	0.61
1:A:134:GLU:HG2	1:A:135:LEU:HD13	1.83	0.61
1:B:134:GLU:HG2	1:B:135:LEU:HD13	1.82	0.60
1:B:89:ILE:HG22	1:B:90:ARG:N	2.19	0.58
1:B:130:TRP:CZ3	1:B:168:ARG:HG3	2.38	0.58
1:B:89:ILE:CD1	1:B:130:TRP:CZ2	2.87	0.56
1:B:153:TYR:CE1	1:B:154:GLN:HG2	2.40	0.56
1:B:93:GLU:HG2	1:B:99:GLY:HA3	1.88	0.55
1:B:24:ASN:ND2	1:B:26:GLN:HE21	2.04	0.54
1:B:136:SER:O	1:B:139:ARG:HG2	2.07	0.54
1:B:134:GLU:HG2	1:B:135:LEU:CD1	2.38	0.54
1:B:88:ARG:HG3	1:B:88:ARG:HH11	1.72	0.53
1:B:135:LEU:HD23	1:B:139:ARG:NE	2.24	0.53
1:B:111:LEU:CD2	1:B:114:ARG:HB2	2.39	0.53
1:B:90:ARG:N	1:B:124:ASN:O	2.39	0.52
1:B:135:LEU:HD23	1:B:139:ARG:HE	1.74	0.52
1:B:115:PHE:O	1:B:116:ARG:HB3	2.11	0.51
1:A:87:HIS:HB3	1:A:130:TRP:CZ2	2.46	0.51
1:A:43:MET:HE3	1:A:144:LEU:HD13	1.92	0.51
1:B:54:GLN:HE22	1:B:144:LEU:H	1.58	0.51
1:B:136:SER:O	1:B:139:ARG:NH1	2.43	0.51
1:B:102:ILE:HD11	1:B:115:PHE:CG	2.46	0.50
1:B:91:LEU:HB3	1:B:120:ILE:HD12	1.94	0.50
1:A:38:ASP:O	1:A:59:ARG:NH1	2.44	0.50
1:B:125:VAL:O	1:B:125:VAL:HG13	2.12	0.50
1:B:83:HIS:ND1	1:B:170:ILE:O	2.41	0.49
1:A:67:GLN:NE2	2:A:206:HOH:O	2.45	0.49
1:B:89:ILE:CD1	1:B:130:TRP:CH2	2.91	0.48
1:A:46:GLU:O	1:A:76:ARG:HG3	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:137:ASN:OD1	2:B:201:HOH:O	2.20	0.48
1:B:150:TYR:HB3	1:B:155:ASP:HB3	1.96	0.48
1:B:120:ILE:HB	1:B:163:VAL:HG21	1.96	0.47
1:B:87:HIS:HB3	1:B:130:TRP:HZ2	1.76	0.47
1:B:93:GLU:HG3	1:B:94:ARG:HG2	1.95	0.47
1:B:89:ILE:HD13	1:B:104:PHE:HB2	1.96	0.47
1:B:134:GLU:HG3	1:B:162:ARG:HB3	1.97	0.47
1:B:149:ASP:OD1	1:B:149:ASP:N	2.48	0.47
1:B:121:HIS:CD2	1:B:161:ALA:CB	2.99	0.45
1:B:88:ARG:HG3	1:B:88:ARG:NH1	2.31	0.45
1:B:135:LEU:HB2	1:B:139:ARG:HG3	1.99	0.44
1:B:102:ILE:HD11	1:B:115:PHE:CD2	2.52	0.44
1:A:23:THR:OG1	1:A:49:ASN:HA	2.17	0.44
1:B:121:HIS:HD2	1:B:161:ALA:CB	2.30	0.44
1:A:95:GLU:HA	1:A:122:SER:HB3	2.00	0.43
1:A:6:TYR:HB2	1:A:34:SER:OG	2.20	0.42
1:B:135:LEU:CB	1:B:139:ARG:HG3	2.49	0.42
1:A:134:GLU:OE2	1:A:162:ARG:NH1	2.52	0.42
1:B:55:TYR:CZ	1:B:70:GLY:HA2	2.55	0.42
1:A:111:LEU:HD21	1:A:120:ILE:HD11	2.02	0.41
1:B:135:LEU:HB3	1:B:139:ARG:CZ	2.51	0.41
1:A:43:MET:HE1	1:A:131:VAL:HG22	2.03	0.41
1:A:93:GLU:HG2	1:A:94:ARG:HG3	2.01	0.41
1:B:121:HIS:CD2	1:B:161:ALA:HB2	2.56	0.41
1:B:101:MET:HG2	1:B:102:ILE:N	2.36	0.41
1:B:111:LEU:HA	1:B:111:LEU:HD23	1.69	0.40
1:B:133:TYR:CD2	1:B:138:TYR:HB2	2.56	0.40
1:B:132:LEU:HB2	1:B:145:LEU:HD11	2.04	0.40
1:B:153:TYR:HA	1:B:156:TRP:CZ2	2.57	0.40

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	169/174 (97%)	166 (98%)	3 (2%)	0	100	100
1	B	168/174 (97%)	159 (95%)	7 (4%)	2 (1%)	13	10
All	All	337/348 (97%)	325 (96%)	10 (3%)	2 (1%)	25	26

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	116	ARG
1	B	138	TYR

### 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	146/156 (94%)	144 (99%)	2 (1%)	67	80
1	B	144/156 (92%)	134 (93%)	10 (7%)	15	16
All	All	290/312 (93%)	278 (96%)	12 (4%)	30	39

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	101	MET
1	A	135	LEU
1	B	84	SER
1	B	90	ARG
1	B	98	ARG
1	B	101	MET
1	B	105	THR
1	B	109	SER
1	B	110	CYS
1	B	115	PHE
1	B	121	HIS
1	B	162	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such

sidechains are listed below:

Mol	Chain	Res	Type
1	A	33	ASN
1	B	24	ASN
1	B	54	GLN

### 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

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	171/174 (98%)	0.48	3 (1%) 68 66	27, 38, 57, 114	0
1	B	170/174 (97%)	1.82	69 (40%) 0 0	30, 72, 130, 146	0
All	All	341/348 (97%)	1.15	72 (21%) 1 1	27, 47, 120, 146	0

All (72) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	163	VAL	9.3
1	B	111	LEU	8.8
1	B	120	ILE	7.7
1	B	117	PHE	7.7
1	B	115	PHE	7.5
1	B	83	HIS	7.0
1	B	132	LEU	5.9
1	B	100	GLN	5.9
1	B	161	ALA	5.4
1	B	105	THR	5.2
1	B	158	ALA	5.1
1	B	156	TRP	4.7
1	B	130	TRP	4.7
1	B	137	ASN	4.5
1	A	171	ASP	4.4
1	B	113	ASP	4.4
1	B	109	SER	4.3
1	B	91	LEU	4.1
1	B	101	MET	4.1
1	B	125	VAL	4.1
1	B	138	TYR	4.1
1	B	102	ILE	4.0
1	B	144	LEU	3.9
1	B	164	GLY	3.9

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	B	97	TYR	3.9
1	B	133	TYR	3.7
1	B	118	ASN	3.7
1	B	126	LEU	3.6
1	B	85	GLY	3.6
1	B	149	ASP	3.6
1	B	104	PHE	3.4
1	B	90	ARG	3.3
1	B	153	TYR	3.3
1	B	121	HIS	3.2
1	B	150	TYR	3.1
1	B	116	ARG	3.1
1	B	86	SER	3.1
1	B	140	GLY	3.0
1	B	159	THR	3.0
1	B	71	LEU	3.0
1	B	84	SER	2.9
1	B	110	CYS	2.9
1	B	94	ARG	2.9
1	B	103	GLU	2.9
1	B	106	GLU	2.9
1	B	119	GLU	2.9
1	B	55	TYR	2.8
1	B	166	LEU	2.7
1	B	157	GLY	2.7
1	B	136	SER	2.7
1	B	92	TYR	2.6
1	B	169	VAL	2.6
1	B	162	ARG	2.6
1	B	127	GLU	2.6
1	A	43	MET	2.6
1	B	82	PRO	2.5
1	B	114	ARG	2.5
1	B	123	LEU	2.5
1	B	98	ARG	2.5
1	B	154	GLN	2.5
1	B	170	ILE	2.4
1	B	135	LEU	2.4
1	A	115	PHE	2.4
1	B	160	ASN	2.4
1	B	96	ASP	2.4
1	B	81	ILE	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	112	GLN	2.3
1	B	147	PRO	2.3
1	B	99	GLY	2.3
1	B	72	SER	2.2
1	B	89	ILE	2.2
1	B	145	LEU	2.1

## 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 carbohydrates 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.