



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 9, 2017 – 01:04 PM EST

PDB ID : 5LUM  
Title : Alpha-crystallin domain of human HSPB6 patched with its N-terminal peptide  
Authors : Sluchanko, N.N.; Beelen, S.; Kulikova, A.A.; Weeks, S.D.; Antson, A.A.; Gusev, N.B.; Strelkov, S.V.  
Deposited on : 2016-09-09  
Resolution : 2.60 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

<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 : 1.7.1 (RC1), CSD as537be (2016)  
Xtriage (Phenix) : 1.9-1692  
EDS : **FAILED**  
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) : rb-20028442

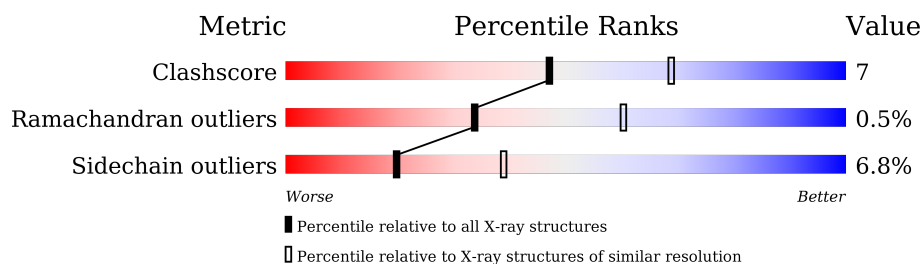
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.60 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	2679 (2.60-2.60)
Ramachandran outliers	100387	2635 (2.60-2.60)
Sidechain outliers	100360	2635 (2.60-2.60)




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. 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 failed to run properly.

Mol	Chain	Length	Quality of chain
1	F	9	
1	G	9	
1	H	9	
1	I	9	
1	J	9	
2	A	78	
2	B	78	

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Length	Quality of chain
2	C	78	 68% 29% •
2	D	78	 85% 13% •
2	E	78	 90% 10%

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 3416 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 Heat shock protein beta-6.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
1	F	9	Total	C	N	O	0	0	0
			67	44	10	13			
1	G	9	Total	C	N	O	0	0	0
			67	44	10	13			
1	H	9	Total	C	N	O	0	0	0
			67	44	10	13			
1	I	9	Total	C	N	O	0	0	0
			67	44	10	13			
1	J	9	Total	C	N	O	0	0	0
			67	44	10	13			

- Molecule 2 is a protein called Heat shock protein beta-6.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	A	78	Total	C	N	O	0	1	0
			615	390	115	110			
2	B	78	Total	C	N	O	0	0	0
			608	385	113	110			
2	C	78	Total	C	N	O	0	0	0
			608	385	113	110			
2	D	78	Total	C	N	O	0	0	0
			608	385	113	110			
2	E	78	Total	C	N	O	0	0	0
			608	385	113	110			

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		
3	E	1	Total	O	S	0	0
			5	4	1		

- Molecule 4 is water.


Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	3	Total	O	0	0
			3	3		
4	G	2	Total	O	0	0
			2	2		
4	B	3	Total	O	0	0
			3	3		
4	C	2	Total	O	0	0
			2	2		
4	D	1	Total	O	0	0
			1	1		
4	E	3	Total	O	0	0
			3	3		

### 3 Residue-property plots

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 ( $\text{RSRZ} > 2$ ). 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 failed to run properly.

- Molecule 1: Heat shock protein beta-6

Chain F: 




- Molecule 1: Heat shock protein beta-6

Chain G: 



- Molecule 1: Heat shock protein beta-6

Chain H: 



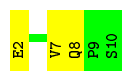
- Molecule 1: Heat shock protein beta-6

Chain I: 




- Molecule 1: Heat shock protein beta-6

Chain J: 



- Molecule 2: Heat shock protein beta-6

Chain A: 



- Molecule 2: Heat shock protein beta-6

Chain B: 62% 37%



- Molecule 2: Heat shock protein beta-6

Chain C: 68% 29%



- Molecule 2: Heat shock protein beta-6

Chain D: 85% 13%



- Molecule 2: Heat shock protein beta-6

Chain E: 90% 10%



## 4 Data and refinement statistics

EDS failed to run properly - this section is therefore incomplete.

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	105.69Å 105.69Å 111.95Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	28.61 – 2.60	Depositor
% Data completeness (in resolution range)	100.0 (28.61-2.60)	Depositor
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.26 (at 2.61Å)	Xtriage
Refinement program	BUSTER-TNT	Depositor
R, $R_{free}$	0.207 , 0.227	Depositor
Wilson B-factor (Å <sup>2</sup> )	82.5	Xtriage
Anisotropy	0.357	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.036 for -h,-k,l	Xtriage
Total number of atoms	3416	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	100.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.19% 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SO4

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	F	0.55	0/69	0.77	0/96
1	G	0.69	0/69	1.01	0/96
1	H	0.57	0/69	0.94	0/96
1	I	0.57	0/69	0.78	0/96
1	J	0.58	0/69	0.77	0/96
2	A	0.54	0/637	0.80	0/867
2	B	0.53	0/626	0.78	0/852
2	C	0.53	0/626	0.76	0/852
2	D	0.48	0/626	0.75	0/852
2	E	0.45	0/626	0.72	0/852
All	All	0.52	0/3486	0.77	0/4755

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

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	F	67	0	68	1	0
1	G	67	0	68	3	0
1	H	67	0	68	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	I	67	0	68	1	0
1	J	67	0	68	0	0
2	A	615	0	595	4	0
2	B	608	0	588	18	0
2	C	608	0	588	23	0
2	D	608	0	588	7	0
2	E	608	0	588	3	0
3	A	10	0	0	0	0
3	D	5	0	0	0	0
3	E	5	0	0	0	0
4	A	3	0	0	0	0
4	B	3	0	0	0	0
4	C	2	0	0	0	0
4	D	1	0	0	0	0
4	E	3	0	0	0	0
4	G	2	0	0	0	0
All	All	3416	0	3287	50	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 7.

All (50) 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)
2:B:130:ALA:HB2	2:D:138:PRO:HB3	1.61	0.81
2:C:92:VAL:HG11	2:C:129:PRO:HB3	1.71	0.72
2:B:74:PHE:HB3	2:B:146:ALA:HB3	1.72	0.72
2:D:78:LEU:HD11	2:D:119:ARG:HD2	1.75	0.68
1:F:7:VAL:H	1:G:8:GLN:HE22	1.39	0.68
2:B:100:HIS:HD2	2:B:118:HIS:ND1	1.94	0.66
2:C:119:ARG:HG3	2:C:119:ARG:HH11	1.61	0.65
2:B:116:GLU:HG2	2:C:116:GLU:HG2	1.77	0.64
2:C:110:HIS:CD2	2:C:111:GLY:H	2.16	0.64
2:C:128:ASP:HB2	2:C:149:ALA:HB2	1.79	0.64
2:B:122:ARG:HE	2:C:110:HIS:HB2	1.64	0.63
2:C:110:HIS:HD2	2:C:111:GLY:H	1.46	0.63
2:C:78:LEU:HD23	2:C:117:PHE:HE2	1.66	0.60
2:E:92:VAL:HG11	2:E:129:PRO:HB3	1.84	0.58
2:D:92:VAL:HG11	2:D:129:PRO:HB3	1.84	0.58
2:C:78:LEU:HD23	2:C:117:PHE:CE2	2.38	0.58
2:B:97:VAL:HG23	2:B:123:LEU:HG	1.86	0.58

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:126:GLY:O	2:B:127:VAL:HG23	2.05	0.56
2:B:106:ARG:HH21	2:E:95:GLU:H	1.52	0.55
2:C:106:ARG:HG3	2:C:112:PHE:HD1	1.72	0.54
2:B:122:ARG:HE	2:C:110:HIS:CB	2.22	0.52
2:B:76:VAL:HG11	2:B:121:TYR:CE1	2.45	0.52
2:D:108:ASP:HB3	2:D:111:GLY:H	1.76	0.51
2:A:100[B]:HIS:CE1	2:A:118:HIS:CE1	3.00	0.49
2:D:74:PHE:HB3	2:D:146:ALA:HB3	1.94	0.49
2:E:97:VAL:HG23	2:E:123:LEU:HG	1.94	0.49
2:C:119:ARG:HD3	2:C:120:ARG:H	1.77	0.48
2:C:119:ARG:CG	2:C:119:ARG:HH11	2.26	0.48
1:G:2:GLU:HG3	2:D:81:LYS:HB2	1.95	0.48
2:D:85:PRO:HG3	2:D:136:LEU:HD23	1.95	0.48
2:A:92:VAL:HG11	2:A:129:PRO:HB3	1.96	0.47
2:C:131:ALA:HB1	2:C:147:ALA:HB3	1.97	0.47
2:A:105:GLU:HG3	2:A:112:PHE:HB3	1.97	0.46
2:C:106:ARG:HG3	2:C:112:PHE:CD1	2.49	0.46
2:B:92:VAL:HG11	2:B:129:PRO:HB3	1.98	0.46
1:G:10:SER:HB2	2:B:135:ALA:HB1	1.98	0.45
2:A:85:PRO:HG3	2:A:136:LEU:HD23	1.99	0.44
2:B:91:LYS:HE3	2:B:93:VAL:HG21	2.00	0.44
2:C:87:GLU:O	2:C:101:ALA:HA	2.18	0.43
2:B:115:ARG:HG2	2:C:117:PHE:HD1	1.82	0.43
2:C:119:ARG:HD2	2:C:121:TYR:CZ	2.54	0.43
2:B:87:GLU:O	2:B:101:ALA:HA	2.18	0.42
2:B:110:HIS:HA	2:B:111:GLY:HA2	1.93	0.41
2:B:78:LEU:HD23	2:B:117:PHE:CE2	2.55	0.41
2:C:119:ARG:HD3	2:C:120:ARG:N	2.35	0.41
2:C:123:LEU:HD22	2:C:127:VAL:HG11	2.03	0.41
2:B:122:ARG:HH21	2:C:110:HIS:HB2	1.86	0.40
2:C:72:GLY:O	2:C:148:PRO:HG3	2.22	0.40
1:I:2:GLU:O	1:I:3:ILE:HG13	2.22	0.40
2:C:75:SER:OG	2:C:145:GLN:HG2	2.20	0.40

There are no symmetry-related clashes.

## 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	F	7/9 (78%)	7 (100%)	0	0	100	100
1	G	7/9 (78%)	7 (100%)	0	0	100	100
1	H	7/9 (78%)	7 (100%)	0	0	100	100
1	I	7/9 (78%)	7 (100%)	0	0	100	100
1	J	7/9 (78%)	7 (100%)	0	0	100	100
2	A	77/78 (99%)	75 (97%)	2 (3%)	0	100	100
2	B	76/78 (97%)	71 (93%)	4 (5%)	1 (1%)	15	30
2	C	76/78 (97%)	72 (95%)	4 (5%)	0	100	100
2	D	76/78 (97%)	72 (95%)	4 (5%)	0	100	100
2	E	76/78 (97%)	72 (95%)	3 (4%)	1 (1%)	15	30
All	All	416/435 (96%)	397 (95%)	17 (4%)	2 (0%)	34	60

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	E	109	GLU
2	B	108	ASP

### 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	F	9/9 (100%)	8 (89%)	1 (11%)	8	13

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	G	9/9 (100%)	6 (67%)	3 (33%)	0	0
1	H	9/9 (100%)	7 (78%)	2 (22%)	1	2
1	I	9/9 (100%)	7 (78%)	2 (22%)	1	2
1	J	9/9 (100%)	6 (67%)	3 (33%)	0	0
2	A	65/64 (102%)	62 (95%)	3 (5%)	33	61
2	B	64/64 (100%)	60 (94%)	4 (6%)	22	44
2	C	64/64 (100%)	61 (95%)	3 (5%)	32	59
2	D	64/64 (100%)	62 (97%)	2 (3%)	47	76
2	E	64/64 (100%)	62 (97%)	2 (3%)	47	76
All	All	366/365 (100%)	341 (93%)	25 (7%)	20	39

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	3	ILE
2	A	78	LEU
2	A	104	GLU
2	A	123	LEU
1	G	3	ILE
1	G	7	VAL
1	G	10	SER
2	B	104	GLU
2	B	110	HIS
2	B	119	ARG
2	B	120	ARG
1	H	7	VAL
1	H	10	SER
2	C	106	ARG
2	C	115	ARG
2	C	119	ARG
1	I	7	VAL
1	I	8	GLN
2	D	78	LEU
2	D	108	ASP
1	J	2	GLU
1	J	7	VAL
1	J	8	GLN
2	E	103	HIS
2	E	110	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	F	8	GLN
1	G	8	GLN
2	B	100	HIS
2	B	103	HIS
1	H	8	GLN
2	C	103	HIS
2	C	110	HIS
2	D	100	HIS
2	D	118	HIS
2	E	100	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](#)

4 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. 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  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
3	SO4	A	201	-	4,4,4	0.26	0	6,6,6	0.23	0
3	SO4	A	202	-	4,4,4	0.27	0	6,6,6	0.14	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
3	SO4	D	201	-	4,4,4	0.28	0	6,6,6	0.38	0
3	SO4	E	201	-	4,4,4	0.20	0	6,6,6	0.17	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	SO4	A	201	-	-	0/0/0/0	0/0/0/0
3	SO4	A	202	-	-	0/0/0/0	0/0/0/0
3	SO4	D	201	-	-	0/0/0/0	0/0/0/0
3	SO4	E	201	-	-	0/0/0/0	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 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 failed to run properly - this section is therefore empty.

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

EDS failed to run properly - this section is therefore empty.

### 6.3 Carbohydrates

EDS failed to run properly - this section is therefore empty.

### 6.4 Ligands

EDS failed to run properly - this section is therefore empty.

### 6.5 Other polymers

EDS failed to run properly - this section is therefore empty.