



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 4, 2017 – 05:16 PM EDT

PDB ID : 1ZTP  
Title : X-ray structure of gene product from homo sapiens Hs.433573  
Authors : Wesenberg, G.E.; Phillips Jr., G.N.; Bitto, E.; Bingman, C.A.; Allard, S.T.M.;  
Center for Eukaryotic Structural Genomics (CESG)  
Deposited on : unknown  
Resolution : 2.50 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.

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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) : 1.9-1692  
EDS : rb-20030345  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20030345

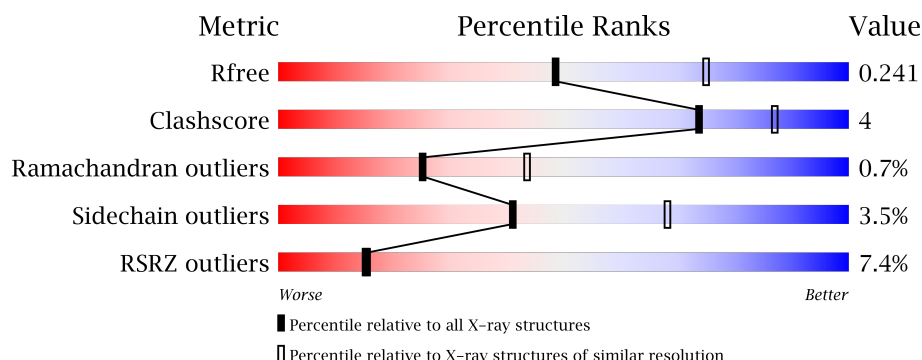
# 1 Overall quality at a glance

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))
$R_{free}$	100719	3846 (2.50-2.50)
Clashscore	112137	4554 (2.50-2.50)
Ramachandran outliers	110173	4463 (2.50-2.50)
Sidechain outliers	110143	4465 (2.50-2.50)
RSRZ outliers	101464	3876 (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 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.

Mol	Chain	Length	Quality of chain
1	A	251	<div> <div>8%</div> <div>80%</div> <div>9%</div> <div>9%</div> </div>
1	B	251	<div> <div>8%</div> <div>79%</div> <div>14%</div> <div>6%</div> </div>
1	C	251	<div> <div>4%</div> <div>80%</div> <div>8%</div> <div>12%</div> </div>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 5516 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 Basophilic leukemia expressed protein BLES03.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	228	Total	C	N	O	S	Se	0	0	0
			1769	1123	313	327	3	3			
1	B	235	Total	C	N	O	S	Se	0	1	0
			1818	1151	323	337	3	4			
1	C	221	Total	C	N	O	S	Se	0	0	0
			1712	1087	307	312	3	3			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MSE	MET	modified residue	UNP Q9H3H3
A	30	MSE	MET	modified residue	UNP Q9H3H3
A	34	MSE	MET	modified residue	UNP Q9H3H3
A	131	MSE	MET	modified residue	UNP Q9H3H3
B	1	MSE	MET	modified residue	UNP Q9H3H3
B	30	MSE	MET	modified residue	UNP Q9H3H3
B	34	MSE	MET	modified residue	UNP Q9H3H3
B	131	MSE	MET	modified residue	UNP Q9H3H3
C	1	MSE	MET	modified residue	UNP Q9H3H3
C	30	MSE	MET	modified residue	UNP Q9H3H3
C	34	MSE	MET	modified residue	UNP Q9H3H3
C	131	MSE	MET	modified residue	UNP Q9H3H3

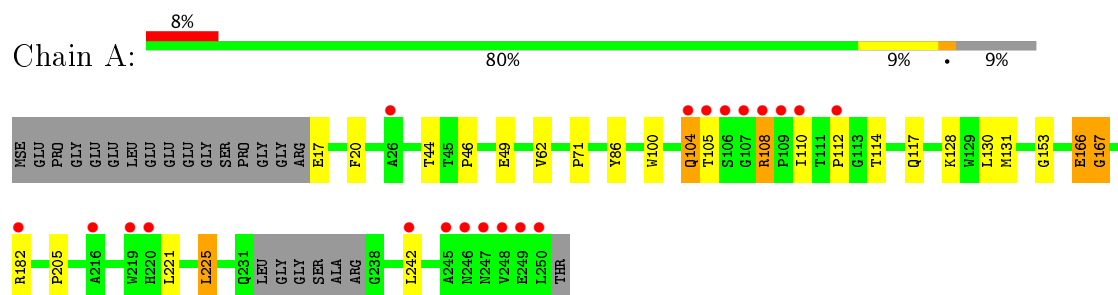
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	56	Total	O	0	0
			56	56		
2	B	87	Total	O	0	0
			87	87		
2	C	74	Total	O	0	0
			74	74		

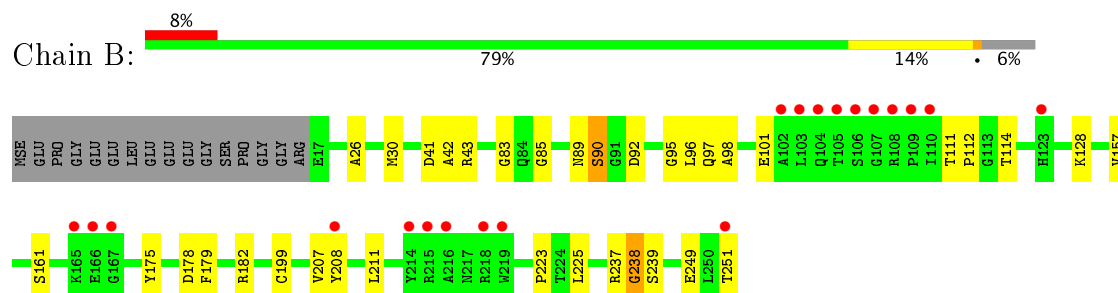
### 3 Residue-property plots [i](#)

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.

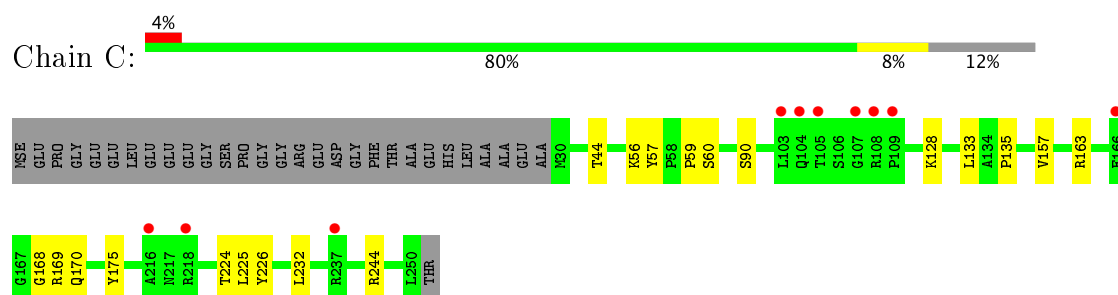
- Molecule 1: Basophilic leukemia expressed protein BLES03



- Molecule 1: Basophilic leukemia expressed protein BLES03



- Molecule 1: Basophilic leukemia expressed protein BLES03



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	62.55Å 116.81Å 123.64Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.50 43.97 – 2.50	Depositor EDS
% Data completeness (in resolution range)	97.8 (50.00-2.50) 97.8 (43.97-2.50)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.79 (at 2.51Å)	Xtriage
Refinement program	REFMAC refmac_5.2.0005	Depositor
R, $R_{free}$	0.188 , 0.245 0.186 , 0.241	Depositor DCC
$R_{free}$ test set	1604 reflections (5.10%)	DCC
Wilson B-factor (Å <sup>2</sup> )	38.7	Xtriage
Anisotropy	0.270	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 54.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	5516	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.51% 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	0.58	0/1813	0.68	0/2468
1	B	0.63	0/1868	0.74	1/2541 (0.0%)
1	C	0.64	0/1756	0.68	1/2392 (0.0%)
All	All	0.62	0/5437	0.70	2/7401 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	178	ASP	CB-CG-OD1	5.05	122.84	118.30
1	C	232	LEU	CA-CB-CG	5.04	126.88	115.30

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	1769	0	1722	13	0
1	B	1818	0	1775	18	0
1	C	1712	0	1684	9	0
2	A	56	0	0	2	0
2	B	87	0	0	1	1
2	C	74	0	0	0	1
All	All	5516	0	5181	40	1

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 4.

All (40) 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:ASN:O	1:B:90:SER:HB2	1.96	0.65
1:B:208:TYR:CD2	1:B:223:PRO:HA	2.32	0.63
1:A:46:PRO:HD2	1:A:49:GLU:OE1	1.98	0.63
1:B:26:ALA:O	1:B:30:MSE:HG3	2.00	0.62
1:C:157:VAL:HG13	1:C:175:TYR:HB2	1.83	0.60
1:B:98:ALA:O	1:B:101:GLU:HB3	2.05	0.57
1:A:205:PRO:HG3	1:A:225:LEU:HD12	1.88	0.55
1:C:225:LEU:HD23	1:C:226:TYR:CE2	2.42	0.54
1:A:153:GLY:HA2	2:A:266:HOH:O	2.08	0.52
1:B:237:ARG:O	1:B:238:GLY:C	2.46	0.52
1:B:249:GLU:C	1:B:251:THR:H	2.14	0.51
1:A:166:GLU:O	1:A:167:GLY:C	2.48	0.51
1:A:112:PRO:HD3	1:A:221:LEU:HD22	1.93	0.51
1:B:157:VAL:HG13	1:B:175:TYR:HB2	1.92	0.50
1:A:86:TYR:HA	2:A:271:HOH:O	2.10	0.49
1:B:208:TYR:HD2	1:B:223:PRO:HA	1.74	0.49
1:A:62:VAL:HG22	1:A:71:PRO:HG2	1.95	0.48
1:A:110:ILE:HG22	1:A:221:LEU:HD11	1.95	0.48
1:A:100:TRP:O	1:A:104:GLN:NE2	2.46	0.48
1:B:208:TYR:CE2	1:B:223:PRO:HA	2.48	0.48
1:A:114:THR:HA	1:A:117:GLN:OE1	2.14	0.47
1:A:17:GLU:HB3	1:A:20:PHE:HD2	1.80	0.47
1:A:128:LYS:HG3	1:A:130:LEU:HD21	1.96	0.47
1:B:43:ARG:HB2	1:B:43:ARG:HE	1.60	0.46
1:B:207:VAL:O	1:B:211:LEU:HG	2.16	0.46
1:B:111:THR:HB	1:B:112:PRO:HD2	1.99	0.45
1:B:96:LEU:HG	1:B:211:LEU:HD21	2.00	0.44
1:C:157:VAL:CG1	1:C:175:TYR:HB2	2.48	0.43
1:A:205:PRO:CG	1:A:225:LEU:HD12	2.48	0.43
1:B:41:ASP:OD1	1:B:43:ARG:HB2	2.18	0.43
1:C:56:LYS:HE3	1:C:57:TYR:OH	2.18	0.43
1:C:224:THR:HG22	1:C:244:ARG:HD2	2.01	0.42
1:C:133:LEU:O	1:C:169:ARG:HG2	2.19	0.42
1:B:179:PHE:CD1	1:B:179:PHE:C	2.93	0.42
1:B:42:ALA:HB3	1:B:83:GLY:HA2	2.02	0.42
1:B:92:ASP:OD2	1:B:95:GLY:HA3	2.20	0.41
1:C:59:PRO:O	1:C:170:GLN:NE2	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:135:PRO:HG3	1:C:168:GLY:O	2.20	0.41
1:B:182:ARG:NH1	2:B:323:HOH:O	2.52	0.40
1:C:60:SER:O	1:C:163:ARG:HD3	2.21	0.40

All (1) 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)
2:B:334:HOH:O	2:C:324:HOH:O[1_455]	2.16	0.04

## 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	224/251 (89%)	213 (95%)	9 (4%)	2 (1%)	20	36
1	B	234/251 (93%)	223 (95%)	9 (4%)	2 (1%)	20	36
1	C	219/251 (87%)	212 (97%)	6 (3%)	1 (0%)	32	53
All	All	677/753 (90%)	648 (96%)	24 (4%)	5 (1%)	25	43

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	90	SER
1	A	167	GLY
1	B	238	GLY
1	B	85	GLY
1	A	108	ARG

### 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	180/192 (94%)	171 (95%)	9 (5%)	28	51
1	B	185/192 (96%)	177 (96%)	8 (4%)	33	58
1	C	175/192 (91%)	173 (99%)	2 (1%)	78	92
All	All	540/576 (94%)	521 (96%)	19 (4%)	41	68

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	44	THR
1	A	104	GLN
1	A	105	THR
1	A	108	ARG
1	A	131	MSE
1	A	166	GLU
1	A	182	ARG
1	A	225	LEU
1	A	242	LEU
1	B	90	SER
1	B	97	GLN
1	B	114	THR
1	B	128	LYS
1	B	161	SER
1	B	199	CYS
1	B	225	LEU
1	B	239	SER
1	C	44	THR
1	C	128	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 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	225/251 (89%)	0.55	20 (8%)	10 10	18, 41, 74, 92	0
1	B	232/251 (92%)	0.29	20 (8%)	11 11	18, 35, 69, 85	0
1	C	218/251 (86%)	0.36	10 (4%)	33 35	12, 31, 68, 86	0
All	All	675/753 (89%)	0.40	50 (7%)	15 15	12, 36, 71, 92	0

All (50) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	105	THR	4.6
1	A	110	ILE	4.6
1	B	107	GLY	4.5
1	B	166	GLU	4.5
1	B	105	THR	4.5
1	C	237	ARG	4.4
1	B	106	SER	4.3
1	A	246	ASN	4.2
1	A	108	ARG	3.9
1	A	107	GLY	3.9
1	A	182	ARG	3.5
1	C	107	GLY	3.5
1	C	218	ARG	3.4
1	C	108	ARG	3.4
1	B	109	PRO	3.1
1	B	103	LEU	3.1
1	B	218	ARG	3.1
1	A	242	LEU	3.1
1	C	103	LEU	3.0
1	C	109	PRO	3.0
1	A	245	ALA	3.0
1	A	250	LEU	2.8
1	B	215	ARG	2.8

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Mol	Chain	Res	Type	RSRZ
1	C	166	GLU	2.8
1	B	219	TRP	2.8
1	B	165	LYS	2.8
1	B	108	ARG	2.7
1	B	102	ALA	2.7
1	A	105	THR	2.7
1	C	104	GLN	2.7
1	C	216	ALA	2.7
1	A	219	TRP	2.7
1	B	167	GLY	2.6
1	A	248	VAL	2.5
1	A	249	GLU	2.5
1	A	247	ASN	2.5
1	B	208	TYR	2.4
1	A	112	PRO	2.4
1	B	214	TYR	2.4
1	A	109	PRO	2.3
1	B	216	ALA	2.3
1	B	110	ILE	2.2
1	B	123	HIS	2.2
1	A	26	ALA	2.2
1	A	104	GLN	2.2
1	B	251	THR	2.2
1	B	104	GLN	2.1
1	A	106	SER	2.1
1	A	216	ALA	2.1
1	A	220	HIS	2.0

## 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 ⓘ

There are no such residues in this entry.