



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 27, 2014 – 11:10 AM GMT

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 : 2005-05-27
Resolution : 2.50 Å(reported)

This is a full wwPDB validation 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/ValidationPDFNotes.html>

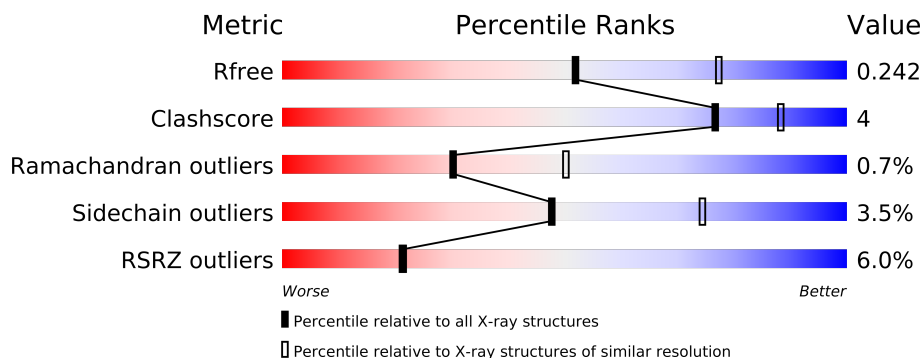
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

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}	66092	2784 (2.50-2.50)
Clashscore	79885	3562 (2.50-2.50)
Ramachandran outliers	78287	3480 (2.50-2.50)
Sidechain outliers	78261	3482 (2.50-2.50)
RSRZ outliers	66119	2785 (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 ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	251	
1	B	251	
1	C	251	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 5516 atoms, of which 0 are hydrogen and 0 are deuterium.

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.

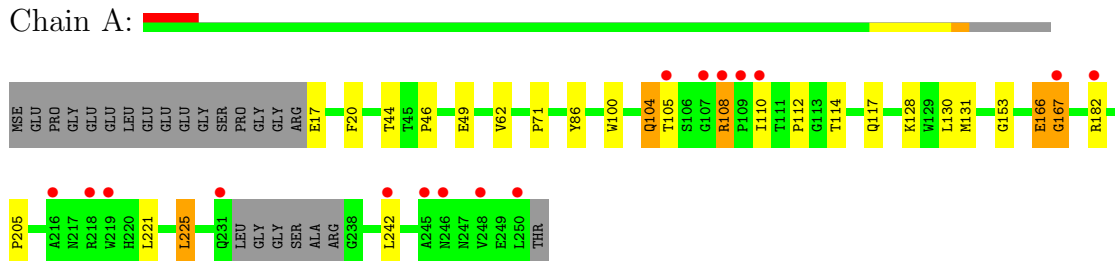
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	56	Total	O	0	0
			56	56		
2	B	87	Total	O	0	0
			87	87		
2	C	74	Total	O	0	0
			74	74		

3 Residue-property plots

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 ($RSRZ > 2$). 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.

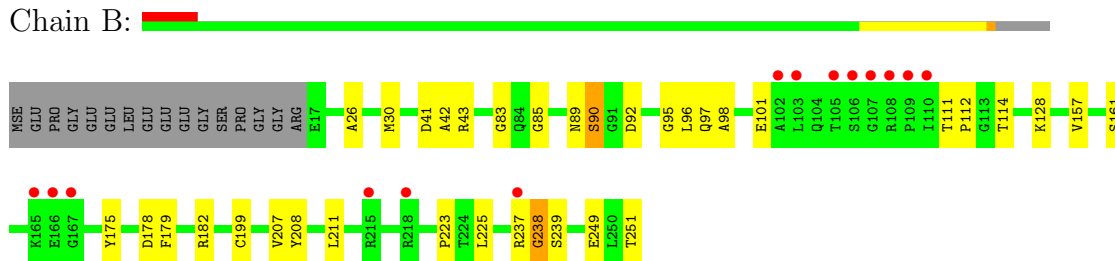
- Molecule 1: Basophilic leukemia expressed protein BLES03

Chain A:



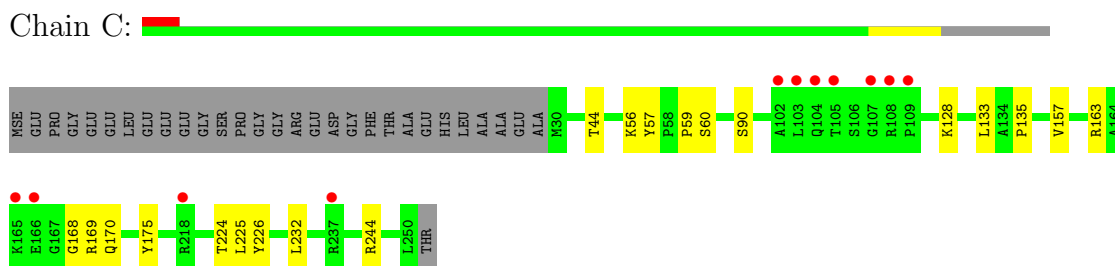
- Molecule 1: Basophilic leukemia expressed protein BLES03

Chain B:



- Molecule 1: Basophilic leukemia expressed protein BLES03

Chain C:



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	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
$\langle I/\sigma(I) \rangle$ ¹	2.79 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.188 , 0.245 0.188 , 0.242	Depositor DCC
R_{free} test set	1605 reflections (5.10%)	DCC
Wilson B-factor (Å ²)	38.7	Xtriage
Anisotropy	0.270	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 30.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 31489 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	5516	wwPDB-VP
Average B, all atoms (Å ²)	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.*

¹Intensities estimated from amplitudes.

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 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

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

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 4.

All (40) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(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:17:GLU:HB3	1:A:20:PHE:HD2	1.80	0.47
1:A:114:THR:HA	1:A:117:GLN:OE1	2.14	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:42:ALA:HB3	1:B:83:GLY:HA2	2.02	0.42
1:B:179:PHE:CD1	1:B:179:PHE:C	2.93	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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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	Distance(Å)	Clash(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%)	25	42
1	B	234/251 (93%)	223 (95%)	9 (4%)	2 (1%)	25	42
1	C	219/251 (87%)	212 (97%)	6 (3%)	1 (0%)	38	60
All	All	677/753 (90%)	648 (96%)	24 (4%)	5 (1%)	30	50

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%)	34	58
1	B	185/192 (96%)	177 (96%)	8 (4%)	40	65
1	C	175/192 (91%)	173 (99%)	2 (1%)	84	96
All	All	540/576 (94%)	521 (96%)	19 (4%)	48	74

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 ⓘ

There are no RNA chains in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

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, 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	228/251 (90%)	0.22	16 (7%) 16 15	18, 41, 74, 92	0
1	B	235/251 (93%)	0.09	14 (5%) 21 21	18, 35, 69, 85	0
1	C	221/251 (88%)	-0.07	11 (4%) 28 28	12, 31, 68, 86	0
All	All	684/753 (90%)	0.08	41 (5%) 21 21	12, 36, 72, 92	0

All (41) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	110	ILE	4.2
1	B	105	THR	4.1
1	A	107	GLY	4.0
1	B	106	SER	3.9
1	A	246	ASN	3.7
1	B	166	GLU	3.5
1	C	105	THR	3.5
1	A	108	ARG	3.2
1	C	237	ARG	3.2
1	A	219	TRP	3.2
1	B	107	GLY	3.1
1	B	109	PRO	3.0
1	B	165	LYS	3.0
1	A	245	ALA	2.9
1	B	103	LEU	2.9
1	C	108	ARG	2.9
1	B	108	ARG	2.8
1	A	218	ARG	2.8
1	C	166	GLU	2.7
1	C	107	GLY	2.6
1	C	218	ARG	2.6
1	C	103	LEU	2.6
1	B	110	ILE	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	102	ALA	2.5
1	A	250	LEU	2.5
1	A	242	LEU	2.5
1	A	182	ARG	2.5
1	B	237	ARG	2.5
1	C	165	LYS	2.5
1	A	105	THR	2.4
1	B	102	ALA	2.4
1	A	248	VAL	2.3
1	B	218	ARG	2.3
1	A	109	PRO	2.2
1	B	167	GLY	2.2
1	C	109	PRO	2.2
1	A	216	ALA	2.2
1	A	231	GLN	2.1
1	C	104	GLN	2.1
1	B	215	ARG	2.1
1	A	167	GLY	2.0

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.