



# wwPDB X-ray Structure Validation Summary Report i

Feb 27, 2014 – 12:39 PM GMT

PDB ID : 3HM6  
Title : Crystal structure of the cytoplasmic domain of human plexin B1  
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Genomics Consortium (SGC)  
Deposited on : 2009-05-28  
Resolution : 2.40 Å(reported)

This is a wwPDB validation summary 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/ValidationPDFNotes.html>

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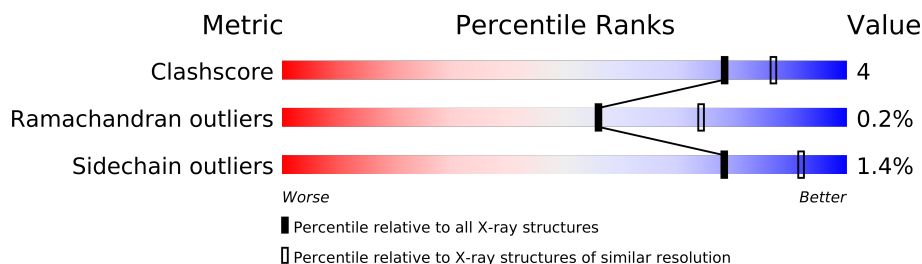
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.15 2013
Xtriage (Phenix)	:	dev-1323
EDS	:	<b>FAILED</b>
Percentile statistics	:	21963
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 2.40 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	79885	2789 (2.40-2.40)
Ramachandran outliers	78287	2736 (2.40-2.40)
Sidechain outliers	78261	2737 (2.40-2.40)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Note EDS failed to run properly.

Mol	Chain	Length	Quality of chain
1	X	644	
2	C	27	

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 4134 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 Plexin-B1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	X	503	Total	C	N	O	S	0	0	0
			3943	2543	663	724	13			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
X	1492	MET	-	EXPRESSION TAG	UNP O43157
X	1493	GLY	-	EXPRESSION TAG	UNP O43157
X	1494	SER	-	EXPRESSION TAG	UNP O43157
X	1495	SER	-	EXPRESSION TAG	UNP O43157
X	1496	HIS	-	EXPRESSION TAG	UNP O43157
X	1497	HIS	-	EXPRESSION TAG	UNP O43157
X	1498	HIS	-	EXPRESSION TAG	UNP O43157
X	1499	HIS	-	EXPRESSION TAG	UNP O43157
X	1500	HIS	-	EXPRESSION TAG	UNP O43157
X	1501	HIS	-	EXPRESSION TAG	UNP O43157
X	1502	SER	-	EXPRESSION TAG	UNP O43157
X	1503	SER	-	EXPRESSION TAG	UNP O43157
X	1504	GLY	-	EXPRESSION TAG	UNP O43157
X	1505	LEU	-	EXPRESSION TAG	UNP O43157
X	1506	VAL	-	EXPRESSION TAG	UNP O43157
X	1507	PRO	-	EXPRESSION TAG	UNP O43157
X	1508	ARG	-	EXPRESSION TAG	UNP O43157
X	1509	GLY	-	EXPRESSION TAG	UNP O43157
X	1510	SER	-	EXPRESSION TAG	UNP O43157
X	1625	THR	SER	ENGINEERED	UNP O43157

- Molecule 2 is a protein called Unknown peptide.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	27	Total	C	N	O	0	0	0
			135	81	27	27			

- Molecule 3 is UNKNOWN ATOM OR ION (three-letter code: UNX) (formula: X).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	X	19	Total	X	0	0
			19	19		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	X	37	Total	O	0	0
			37	37		



## 4 Data and refinement statistics i

EDS failed to run properly - this section will therefore be incomplete.

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	74.35Å 74.35Å 214.40Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	28.08 – 2.40	Depositor
% Data completeness (in resolution range)	99.8 (28.08-2.40)	Depositor
$R_{merge}$	0.04	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.12 (at 2.42Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.227 , 0.262	Depositor
Wilson B-factor (Å <sup>2</sup> )	52.3	Xtriage
Anisotropy	0.024	Xtriage
Estimated twinning fraction	0.027 for -h,-k,l	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 27598 reflections	Xtriage
Total number of atoms	4134	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.82% of the height of the origin peak. No significant pseudotranslation is detected.*

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

## 5 Model quality

### 5.1 Standard geometry

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

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	X	0.61	0/4025	0.64	0/5475

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 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 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	X	3943	0	3903	29	0
2	C	135	0	29	0	0
3	X	19	0	0	0	0
4	X	37	0	0	0	0
All	All	4134	0	3932	29	0

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.

The worst 5 of 29 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:X:2055:ASP:O	1:X:2059:THR:HG23	1.71	0.89
1:X:1983:LEU:HD21	1:X:2017:MET:HA	1.59	0.84
1:X:1668:VAL:HG22	1:X:1967:ILE:HD11	1.76	0.68
1:X:1736:ASP:OD1	1:X:2033:ILE:HG13	1.93	0.68
1:X:2128:VAL:HG12	1:X:2128:VAL:O	1.99	0.62

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	X	491/644 (76%)	468 (95%)	22 (4%)	1 (0%)	56 74

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	X	1981	LEU

### 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	X	416/572 (73%)	410 (99%)	6 (1%)	78 92

5 of 6 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	X	1702	SER
1	X	1968	SER
1	X	1705	GLU

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Mol	Chain	Res	Type
1	X	1612	SER
1	X	1808	ARG

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 ⓘ

Of 19 ligands modelled in this entry, 19 are unknown - leaving 0 for Mogul analysis.

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.

## 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 ⓘ

EDS failed to run properly - this section will therefore be empty.

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

EDS failed to run properly - this section will therefore be empty.

### 6.3 Carbohydrates ⓘ

EDS failed to run properly - this section will therefore be empty.

### 6.4 Ligands ⓘ

EDS failed to run properly - this section will therefore be empty.

### 6.5 Other polymers ⓘ

EDS failed to run properly - this section will therefore be empty.