



# wwPDB X-ray Structure Validation Summary Report

Feb 28, 2014 – 12:37 PM GMT

PDB ID : 2CE8  
Title : AN EH1 PEPTIDE BOUND TO THE GROUCHO-TLE WD40 DOMAIN.  
Authors : Pickles, L.M.; Roe, S.M.; Pearl, L.H.  
Deposited on : 2006-02-03  
Resolution : 2.03 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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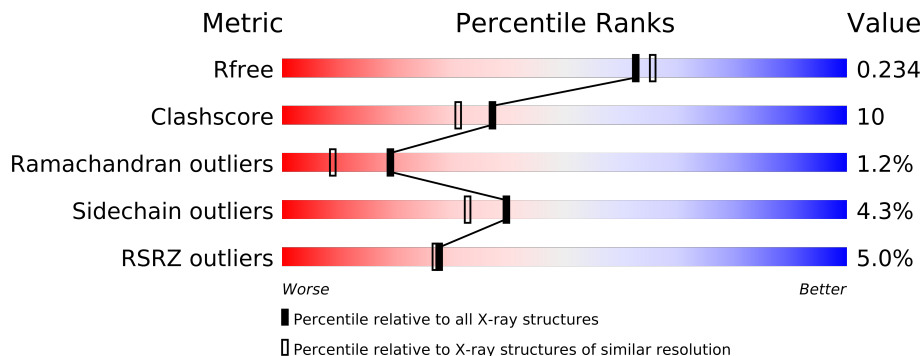
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : 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 2.03 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	6003 (2.04-2.00)
Clashscore	79885	7467 (2.04-2.00)
Ramachandran outliers	78287	7370 (2.04-2.00)
Sidechain outliers	78261	7368 (2.04-2.00)
RSRZ outliers	66119	6006 (2.04-2.00)

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.

Mol	Chain	Length	Quality of chain
1	A	337	
1	B	337	
1	C	337	
1	D	337	
2	X	9	
2	Y	9	

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 11565 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 TRANSDUCIN-LIKE ENHANCER PROTEIN 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	337	Total	C	N	O	S	0	0	0
			2587	1628	445	497	17			
1	B	337	Total	C	N	O	S	0	0	0
			2587	1628	445	497	17			
1	C	337	Total	C	N	O	S	0	0	0
			2587	1628	445	497	17			
1	D	337	Total	C	N	O	S	0	0	0
			2587	1628	445	497	17			

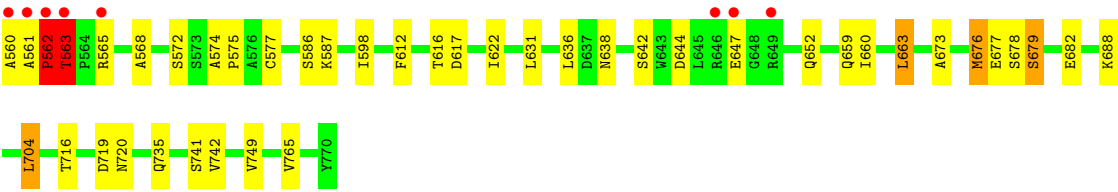
- Molecule 2 is a protein called EH1 PEPTIDE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	X	9	Total	C	N	O	S	0	0	0
			70	46	10	13	1			
2	Y	9	Total	C	N	O	S	0	0	0
			70	46	10	13	1			

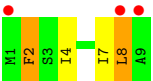
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	291	Total	O	0	0
			291	291		
3	B	279	Total	O	0	0
			279	279		
3	C	265	Total	O	0	0
			265	265		
3	D	235	Total	O	0	0
			235	235		
3	X	4	Total	O	0	0
			4	4		
3	Y	3	Total	O	0	0
			3	3		

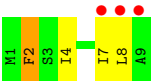




• Molecule 2: EH1 PEPTIDE



• Molecule 2: EH1 PEPTIDE



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	107.58Å 56.35Å 125.25Å 90.00° 112.32° 90.00°	Depositor
Resolution (Å)	116.25 – 2.03 31.84 – 2.03	Depositor EDS
% Data completeness (in resolution range)	96.4 (116.25-2.03) 96.4 (31.84-2.03)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.82 (at 2.03Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, $R_{free}$	0.179 , 0.238 0.179 , 0.234	Depositor DCC
$R_{free}$ test set	4380 reflections (5.26%)	DCC
Wilson B-factor (Å <sup>2</sup> )	18.8	Xtriage
Anisotropy	0.298	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 36.2	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	7 of 87638 reflections (0.008%)	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	11565	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 82.34 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 2.8585e-07. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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

## 5 Model quality

### 5.1 Standard geometry

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	0.88	0/2653	0.84	1/3612 (0.0%)
1	B	0.90	1/2653 (0.0%)	0.90	6/3612 (0.2%)
1	C	0.83	0/2653	0.80	1/3612 (0.0%)
1	D	0.83	0/2653	0.90	6/3612 (0.2%)
2	X	0.75	0/70	0.93	0/93
2	Y	0.69	0/70	0.83	0/93
All	All	0.86	1/10752 (0.0%)	0.86	14/14634 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	2
1	D	0	3
All	All	0	6

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	677	GLU	CG-CD	5.46	1.60	1.51

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	663	LEU	CA-CB-CG	9.15	136.35	115.30
1	D	704	LEU	CA-CB-CG	7.56	132.70	115.30
1	B	663	LEU	CA-CB-CG	7.38	132.27	115.30
1	C	704	LEU	CA-CB-CG	6.85	131.05	115.30
1	A	663	LEU	CA-CB-CG	6.69	130.69	115.30

There are no chirality outliers.

5 of 6 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	562	PRO	Peptide
1	B	514	HIS	Peptide
1	B	516	GLY	Peptide
1	D	518	LYS	Peptide
1	D	559	LEU	Peptide

## 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	A	2587	0	2503	42	0
1	B	2587	0	2503	51	0
1	C	2587	0	2503	49	0
1	D	2587	0	2503	65	0
2	X	70	0	73	5	0
2	Y	70	0	73	6	0
3	A	291	0	0	13	0
3	B	279	0	0	11	0
3	C	265	0	0	10	0
3	D	235	0	0	12	1
3	X	4	0	0	0	0
3	Y	3	0	0	0	0
All	All	11565	0	10158	208	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 10.

The worst 5 of 208 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:518:LYS:CB	1:D:519:SER:HB2	1.51	1.39
1:D:518:LYS:HB3	1:D:519:SER:CB	1.78	1.11
1:B:649:ARG:HD3	3:B:2140:HOH:O	1.54	1.06
1:A:562:PRO:HB2	1:A:563:THR:CB	1.91	1.01

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:562:PRO:CB	1:A:563:THR:HB	1.90	1.00

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)
3:D:2052:HOH:O	3:D:2220:HOH:O[2_645]	1.84	0.36

## 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	335/337 (99%)	322 (96%)	12 (4%)	1 (0%)	50	43
1	B	335/337 (99%)	311 (93%)	16 (5%)	8 (2%)	9	2
1	C	335/337 (99%)	318 (95%)	16 (5%)	1 (0%)	50	43
1	D	335/337 (99%)	313 (93%)	16 (5%)	6 (2%)	13	4
2	X	7/9 (78%)	7 (100%)	0	0	100	100
2	Y	7/9 (78%)	6 (86%)	1 (14%)	0	100	100
All	All	1354/1366 (99%)	1277 (94%)	61 (4%)	16 (1%)	19	9

5 of 16 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	562	PRO
1	B	514	HIS
1	B	515	PRO
1	B	517	ASN
1	B	518	LYS

### 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	288/288 (100%)	279 (97%)	9 (3%)	52	48
1	B	288/288 (100%)	277 (96%)	11 (4%)	44	38
1	C	288/288 (100%)	275 (96%)	13 (4%)	38	31
1	D	288/288 (100%)	274 (95%)	14 (5%)	35	27
2	X	8/8 (100%)	6 (75%)	2 (25%)	1	0
2	Y	8/8 (100%)	7 (88%)	1 (12%)	7	3
All	All	1168/1168 (100%)	1118 (96%)	50 (4%)	40	33

5 of 50 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	519	SER
1	C	646	ARG
1	D	741	SER
1	C	522	SER
1	C	563	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 41 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	723	ASN
1	C	613	GLN
1	D	659	GLN
1	B	735	GLN
1	C	483	HIS

### 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, 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	337/337 (100%)	-0.25	10 (2%) 48 48	7, 14, 36, 52	0
1	B	337/337 (100%)	-0.07	16 (4%) 30 29	8, 16, 39, 52	0
1	C	337/337 (100%)	-0.16	14 (4%) 35 34	9, 16, 38, 56	0
1	D	337/337 (100%)	0.03	22 (6%) 18 17	9, 18, 44, 54	0
2	X	9/9 (100%)	1.75	3 (33%) 1 1	37, 42, 51, 54	0
2	Y	9/9 (100%)	1.92	3 (33%) 1 1	39, 41, 57, 59	0
All	All	1366/1366 (100%)	-0.09	68 (4%) 28 27	7, 16, 41, 59	0

The worst 5 of 68 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	454	GLY	7.7
1	C	561	ALA	7.7
2	Y	9	ALA	7.4
1	C	562	PRO	7.3
1	A	561	ALA	7.0

### 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.