



# wwPDB X-ray Structure Validation Summary Report

Feb 13, 2017 – 02:50 pm GMT

PDB ID : 2E2X  
Title : Sec14 Homology Module of Neurofibromin in complex with phosphatidyethanolamine  
Authors : D'Angelo, I.; Welti, S.; Scheffzek, K.  
Deposited on : 2006-11-18  
Resolution : 2.50 Å (reported)

This is a wwPDB X-ray Structure 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/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  
Mogul : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : trunk28620  
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) : recalc28949

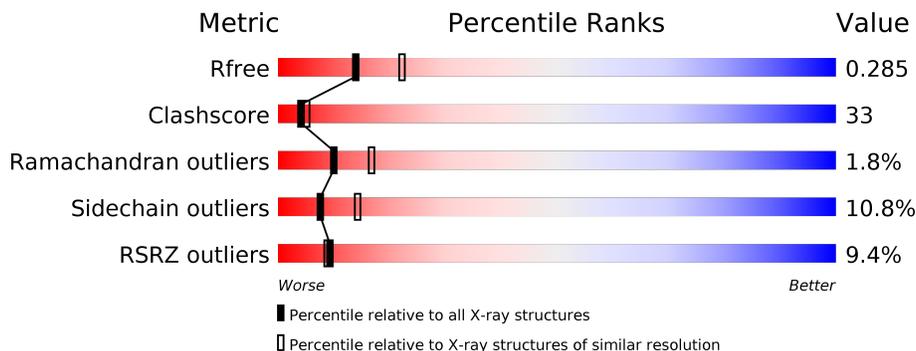
# 1 Overall quality at a glance

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	277	
1	B	277	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	PEV	A	400	X	-	-	X
2	PEV	B	500	X	-	X	X

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 4218 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.

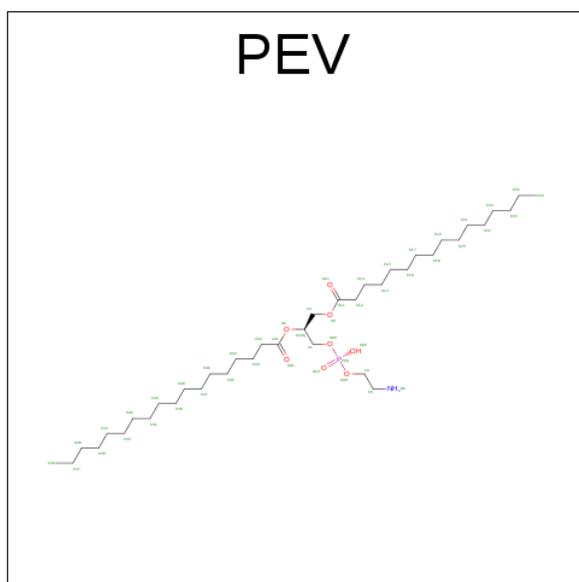
- Molecule 1 is a protein called Neurofibromin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	250	2013	1302	336	370	5	0	0	0
1	B	250	2015	1303	336	371	5	0	0	0

There are 10 discrepancies between the modelled and reference sequences:

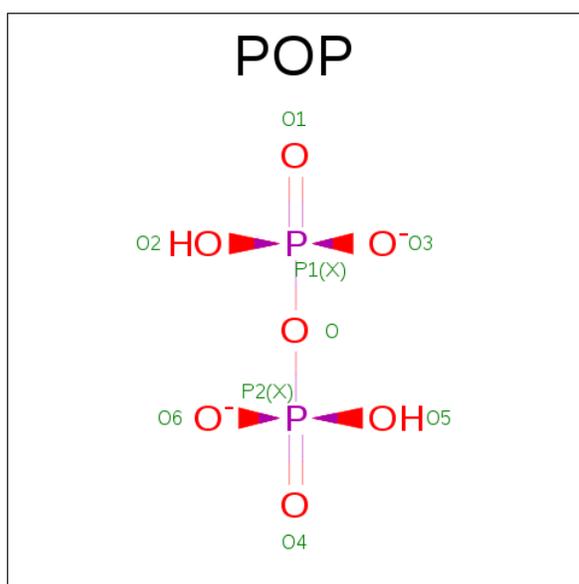
Chain	Residue	Modelled	Actual	Comment	Reference
A	1540	GLY	-	EXPRESSION TAG	UNP P21359
A	1541	ALA	-	EXPRESSION TAG	UNP P21359
A	1542	MET	-	EXPRESSION TAG	UNP P21359
A	1543	THR	-	EXPRESSION TAG	UNP P21359
A	1544	GLY	-	EXPRESSION TAG	UNP P21359
B	1540	GLY	-	EXPRESSION TAG	UNP P21359
B	1541	ALA	-	EXPRESSION TAG	UNP P21359
B	1542	MET	-	EXPRESSION TAG	UNP P21359
B	1543	THR	-	EXPRESSION TAG	UNP P21359
B	1544	GLY	-	EXPRESSION TAG	UNP P21359

- Molecule 2 is (1S)-2-[[[(2-AMINOETHOXY)(HYDROXY)PHOSPHORYL]OXY]-1-[(PALMITOYLOXY)METHYL]ETHYL STEARATE (three-letter code: PEV) (formula: C<sub>39</sub>H<sub>78</sub>NO<sub>8</sub>P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	3	0
			49	39	1	8	1		
2	B	1	Total	C	N	O	P	3	0
			49	39	1	8	1		

- Molecule 3 is PYROPHOSPHATE 2- (three-letter code: POP) (formula:  $H_2O_7P_2$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	O	P	0	0
			9	7	2		
3	B	1	Total	O	P	0	0
			9	7	2		

- Molecule 4 is water.

<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>		<b>ZeroOcc</b>	<b>AltConf</b>
4	A	30	Total 30	O 30	0	0
4	B	44	Total 44	O 44	0	0



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	110.10Å 110.10Å 121.90Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.00 – 2.50 19.46 – 2.50	Depositor EDS
% Data completeness (in resolution range)	(Not available) (15.00-2.50) 99.6 (19.46-2.50)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	0.15	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.57 (at 2.50Å)	Xtrriage
Refinement program	REFMAC 5.0	Depositor
R, $R_{free}$	0.254 , 0.283 0.267 , 0.285	Depositor DCC
$R_{free}$ test set	1293 reflections (5.16%)	DCC
Wilson B-factor (Å <sup>2</sup> )	49.0	Xtrriage
Anisotropy	0.175	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 33.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	4218	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	54.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.24% 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](#)

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

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	0.49	0/2063	0.75	2/2801 (0.1%)
1	B	0.60	1/2065 (0.0%)	0.89	5/2804 (0.2%)
All	All	0.55	1/4128 (0.0%)	0.82	7/5605 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	1596	GLN	CG-CD	6.31	1.65	1.51

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1599	GLY	C-N-CA	-8.78	99.76	121.70
1	B	1595	GLY	CA-C-N	-6.49	102.91	117.20
1	A	1595	GLY	N-CA-C	-5.88	98.40	113.10
1	A	1646	PRO	N-CA-C	-5.59	97.57	112.10
1	B	1597	ILE	C-N-CA	-5.40	108.20	121.70

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	2013	0	1994	118	0
1	B	2015	0	1999	138	0
2	A	49	0	77	17	0
2	B	49	0	77	49	0
3	B	18	0	0	2	0
4	A	30	0	0	4	0
4	B	44	0	0	3	0
All	All	4218	0	4147	271	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 33.

The worst 5 of 271 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:1620:ILE:CD1	2:B:500:PEV:H131	1.47	1.43
1:B:1620:ILE:CD1	2:B:500:PEV:C13	2.13	1.26
1:B:1620:ILE:CD1	2:B:500:PEV:C12	2.34	1.06
1:B:1679:LEU:CD2	2:B:500:PEV:H322	1.84	1.05
1:A:1634:LYS:HE3	1:A:1634:LYS:H	1.23	1.04

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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	248/277 (90%)	232 (94%)	11 (4%)	5 (2%)	<a href="#">9</a> <a href="#">14</a>
1	B	248/277 (90%)	229 (92%)	15 (6%)	4 (2%)	<a href="#">11</a> <a href="#">19</a>
All	All	496/554 (90%)	461 (93%)	26 (5%)	9 (2%)	<a href="#">10</a> <a href="#">17</a>

5 of 9 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1597	ILE
1	B	1596	GLN
1	B	1691	PRO
1	A	1596	GLN
1	A	1699	GLU

### 5.3.2 Protein sidechains [i](#)

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	218/244 (89%)	197 (90%)	21 (10%)	10	18
1	B	219/244 (90%)	193 (88%)	26 (12%)	6	11
All	All	437/488 (90%)	390 (89%)	47 (11%)	7	14

5 of 47 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	1594	THR
1	B	1614	TYR
1	B	1801	GLN
1	B	1597	ILE
1	B	1638	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 20 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1805	HIS
1	A	1814	GLN
1	B	1777	GLN
1	A	1794	GLN
1	A	1801	GLN

### 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
2	PEV	A	400	-	48,48,48	0.52	0	50,53,53	1.23	4 (8%)
2	PEV	B	500	-	48,48,48	0.52	0	50,53,53	1.23	4 (8%)
3	POP	B	601	-	8,8,8	0.74	0	8,13,13	0.56	0
3	POP	B	602	-	8,8,8	0.97	0	8,13,13	0.50	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
2	PEV	A	400	-	1/1/4/4	0/52/52/52	0/0/0/0
2	PEV	B	500	-	1/1/4/4	0/52/52/52	0/0/0/0
3	POP	B	601	-	-	0/6/6/6	0/0/0/0
3	POP	B	602	-	-	0/6/6/6	0/0/0/0

There are no bond length outliers.

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	500	PEV	C3-C2-C1	-2.90	105.32	111.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	400	PEV	C3-C2-C1	-2.89	105.33	111.86
2	A	400	PEV	O3-C11-C12	2.73	119.83	111.90
2	B	500	PEV	O3-C11-C12	2.74	119.87	111.90
2	A	400	PEV	O2-C31-C32	3.26	118.32	111.55

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	400	PEV	C2
2	B	500	PEV	C2

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 68 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	400	PEV	17	0
2	B	500	PEV	49	0
3	B	602	POP	2	0

## 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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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	250/277 (90%)	0.63	26 (10%) <b>7</b> <b>6</b>	33, 57, 84, 95	0
1	B	250/277 (90%)	0.54	21 (8%) <b>12</b> <b>11</b>	25, 50, 71, 79	0
All	All	500/554 (90%)	0.58	47 (9%) <b>9</b> <b>9</b>	25, 53, 79, 95	0

The worst 5 of 47 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1595	GLY	10.7
1	A	1596	GLN	6.7
1	A	1604	TYR	5.0
1	A	1700	HIS	4.5
1	A	1815	PRO	4.4

### 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](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	PEV	B	500	49/49	0.67	0.42	4.48	20,71,84,86	3
2	PEV	A	400	49/49	0.73	0.38	4.47	20,71,84,86	3
3	POP	B	602	9/9	0.91	0.27	1.72	83,94,101,104	0
3	POP	B	601	9/9	0.66	0.20	-0.20	145,147,151,151	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.