Full wwPDB X-ray Structure Validation Report (i)

Apr 25, 2026 – 11:50 AM EDT

PDB ID	:	4YFE / pdb_00004yfe
Title	:	Crystal structure of PTP delta Fn1-Fn2
Authors	:	Yamagata, A.; Fukai, S.
Deposited on	:	2015-02-25
Resolution	:	1.97 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*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

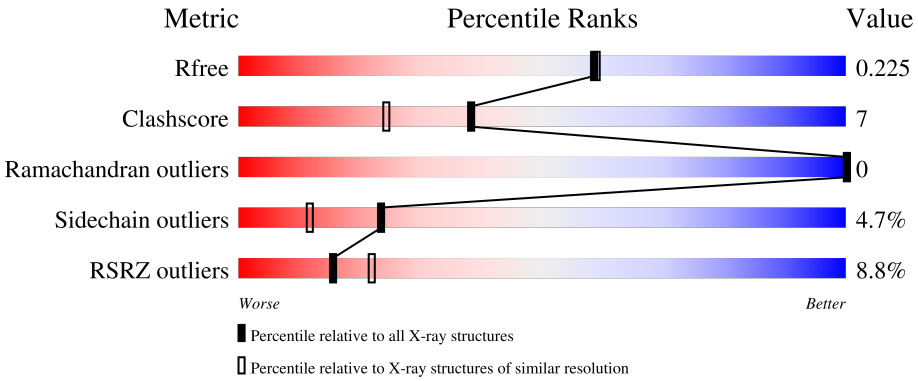
MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.97 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}	180053	1506 (1.98-1.98)
Clashscore	190562	1534 (1.98-1.98)
Ramachandran outliers	187476	1518 (1.98-1.98)
Sidechain outliers	187428	1518 (1.98-1.98)
RSRZ outliers	180081	1506 (1.98-1.98)

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 of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. 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 <=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	200	2% 82% 14%
1	B	200	14% 78% 18%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 3296 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 Receptor-type tyrosine-protein phosphatase delta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	193	Total	C	N	O	S	0	0	0
			1494	942	248	301	3			
1	B	193	Total	C	N	O	S	0	0	0
			1494	942	248	301	3			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	327	MET	-	expression tag	UNP Q64487
A	519	LEU	-	expression tag	UNP Q64487
A	520	GLU	-	expression tag	UNP Q64487
A	521	HIS	-	expression tag	UNP Q64487
A	522	HIS	-	expression tag	UNP Q64487
A	523	HIS	-	expression tag	UNP Q64487
A	524	HIS	-	expression tag	UNP Q64487
A	525	HIS	-	expression tag	UNP Q64487
A	526	HIS	-	expression tag	UNP Q64487
B	327	MET	-	expression tag	UNP Q64487
B	519	LEU	-	expression tag	UNP Q64487
B	520	GLU	-	expression tag	UNP Q64487
B	521	HIS	-	expression tag	UNP Q64487
B	522	HIS	-	expression tag	UNP Q64487
B	523	HIS	-	expression tag	UNP Q64487
B	524	HIS	-	expression tag	UNP Q64487
B	525	HIS	-	expression tag	UNP Q64487
B	526	HIS	-	expression tag	UNP Q64487

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	194	Total	O	0	0
			194	194		

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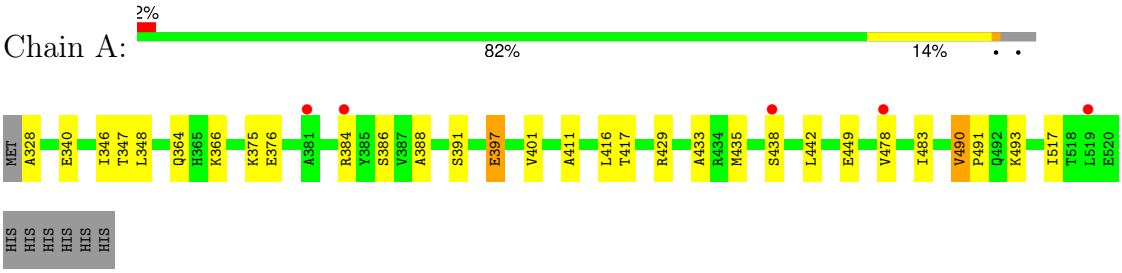
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	114	Total	O	0	0
			114	114		

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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.

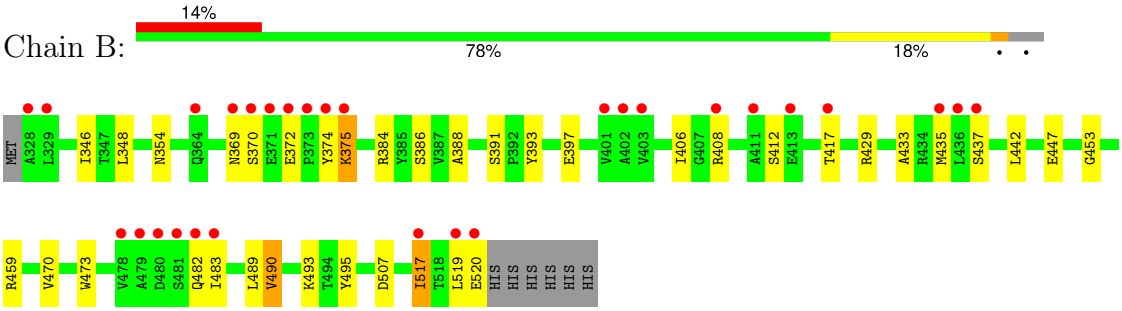
• Molecule 1: Receptor-type tyrosine-protein phosphatase delta

Chain A:



• Molecule 1: Receptor-type tyrosine-protein phosphatase delta

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	51.91Å 65.08Å 134.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.40 – 1.97 48.40 – 1.97	Depositor EDS
% Data completeness (in resolution range)	99.8 (48.40-1.97) 99.8 (48.40-1.97)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.12	Depositor
$< I/\sigma(I) >$ [1]	4.26 (at 1.97Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.9_1692)	Depositor
R, R_{free}	0.204 , 0.223 0.205 , 0.225	Depositor DCC
R_{free} test set	1660 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å^2)	20.8	Xtriage
Anisotropy	0.551	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 45.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	3296	wwPDB-VP
Average B, all atoms (Å^2)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.41% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

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	0.41	0/1532	0.85	0/2101
1	B	0.42	0/1532	0.93	5/2101 (0.2%)
All	All	0.41	0/3064	0.89	5/4202 (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	1
All	All	0	2

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	370	SER	N-CA-C	5.88	119.49	110.20
1	B	406	ILE	N-CA-C	-5.73	105.14	110.53
1	B	372	GLU	N-CA-C	-5.59	102.37	110.08
1	B	354	ASN	CA-C-N	5.04	124.65	119.05
1	B	354	ASN	C-N-CA	5.04	124.65	119.05

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	388	ALA	Peptide
1	B	388	ALA	Peptide

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	1494	0	1461	19	0
1	B	1494	0	1461	24	0
2	A	194	0	0	5	3
2	B	114	0	0	7	1
All	All	3296	0	2922	41	3

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 7.

All (41) 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:A:429:ARG:NH1	1:A:449:GLU:OE1	2.06	0.89
1:B:375:LYS:NZ	2:B:708:HOH:O	2.23	0.69
1:B:369:ASN:OD1	2:B:661:HOH:O	2.10	0.68
1:B:519:LEU:O	1:B:520:GLU:HB2	1.96	0.66
1:A:366:LYS:HE2	2:A:623:HOH:O	2.00	0.62
1:A:490:VAL:HG22	1:A:493:LYS:HG3	1.82	0.61
1:A:340:GLU:HB2	1:A:347:THR:HB	1.86	0.57
1:B:408:ARG:NH1	2:B:672:HOH:O	2.30	0.57
1:A:384:ARG:NH1	1:B:384:ARG:HB3	2.19	0.56
1:B:470:VAL:HA	1:B:473:TRP:CD1	2.41	0.56
1:B:490:VAL:HG22	1:B:493:LYS:HG3	1.88	0.55
1:B:384:ARG:NH2	2:B:700:HOH:O	2.40	0.54
1:B:447:GLU:OE1	2:B:679:HOH:O	2.18	0.54
1:B:517:ILE:HG12	1:B:519:LEU:HD22	1.90	0.54
1:A:384:ARG:NH2	2:A:738:HOH:O	2.42	0.52
1:A:384:ARG:CZ	2:A:738:HOH:O	2.56	0.52
1:A:384:ARG:HH11	1:B:384:ARG:HB3	1.75	0.52
1:A:478:VAL:HG11	2:A:604:HOH:O	2.11	0.50
1:B:489:LEU:HD22	1:B:495:TYR:CE1	2.49	0.48
1:A:328:ALA:N	2:A:606:HOH:O	2.47	0.47
1:B:412:SER:HB2	2:B:629:HOH:O	2.13	0.47
1:B:346:ILE:HD13	1:B:417:THR:HG23	1.95	0.47
1:A:438:SER:HB2	1:A:491:PRO:HB3	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:517:ILE:CG1	1:B:519:LEU:HB2	2.46	0.46
1:B:433:ALA:HA	1:B:442:LEU:O	2.15	0.46
1:B:517:ILE:HG13	1:B:519:LEU:HB2	1.97	0.46
1:A:401:VAL:HG22	1:A:411:ALA:HA	1.98	0.45
1:B:459:ARG:HH12	1:B:507:ASP:CG	2.24	0.45
1:A:397:GLU:HG3	1:A:416:LEU:CD2	2.46	0.45
1:A:442:LEU:HD21	1:A:483:ILE:HD11	1.98	0.45
1:B:346:ILE:HD13	1:B:417:THR:CG2	2.49	0.43
1:B:442:LEU:HD21	1:B:483:ILE:HD11	2.01	0.42
1:A:397:GLU:HG3	1:A:416:LEU:HD23	2.02	0.42
1:A:346:ILE:HD13	1:A:417:THR:CG2	2.50	0.42
1:A:490:VAL:HG22	1:A:493:LYS:CG	2.49	0.41
1:A:433:ALA:HA	1:A:442:LEU:O	2.20	0.41
1:B:393:TYR:CG	1:B:453:GLY:HA2	2.56	0.41
1:B:429:ARG:HE	1:B:429:ARG:HB2	1.64	0.41
1:A:364:GLN:HG2	1:A:376:GLU:HG2	2.03	0.40
1:B:482:GLN:NE2	2:B:680:HOH:O	2.55	0.40
1:B:374:TYR:OH	1:B:397:GLU:OE2	2.34	0.40

All (3) 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:A:602:HOH:O	2:A:614:HOH:O[3_555]	1.87	0.33
2:A:662:HOH:O	2:B:632:HOH:O[2_455]	2.14	0.06
2:A:655:HOH:O	2:A:682:HOH:O[2_455]	2.17	0.03

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	191/200 (96%)	189 (99%)	2 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	191/200 (96%)	189 (99%)	2 (1%)	0	100	100
All	All	382/400 (96%)	378 (99%)	4 (1%)	0	100	100

There are no Ramachandran outliers to report.

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	171/178 (96%)	163 (95%)	8 (5%)	23	12
1	B	171/178 (96%)	163 (95%)	8 (5%)	23	12
All	All	342/356 (96%)	326 (95%)	16 (5%)	23	12

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	348	LEU
1	A	375	LYS
1	A	386	SER
1	A	391	SER
1	A	397	GLU
1	A	435	MET
1	A	490	VAL
1	A	517	ILE
1	B	348	LEU
1	B	375	LYS
1	B	386	SER
1	B	391	SER
1	B	435	MET
1	B	437	SER
1	B	490	VAL
1	B	517	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	482	GLN
1	B	468	GLN

5.3.3 RNA

There are no RNA molecules 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 oligosaccharides 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^{th} 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	193/200 (96%)	-0.04	5 (2%) 57 67	10, 19, 38, 51	0
1	B	193/200 (96%)	0.92	29 (15%) 5 7	16, 34, 63, 78	0
All	All	386/400 (96%)	0.44	34 (8%) 15 22	10, 26, 54, 78	0

All (34) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	481	SER	5.0
1	B	479	ALA	4.8
1	B	436	LEU	4.2
1	B	519	LEU	4.0
1	B	413	GLU	3.4
1	B	520	GLU	3.2
1	B	483	ILE	3.0
1	B	517	ILE	3.0
1	B	374	TYR	2.9
1	B	372	GLU	2.7
1	B	435	MET	2.7
1	B	437	SER	2.7
1	B	480	ASP	2.7
1	A	519	LEU	2.6
1	B	411	ALA	2.6
1	B	329	LEU	2.6
1	A	381	ALA	2.6
1	B	373	PRO	2.5
1	B	371	GLU	2.5
1	B	364	GLN	2.4
1	B	401	VAL	2.4
1	B	369	ASN	2.4
1	B	328	ALA	2.4
1	B	408	ARG	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	370	SER	2.3
1	B	403	VAL	2.2
1	B	417	THR	2.2
1	B	478	VAL	2.1
1	B	375	LYS	2.1
1	A	438	SER	2.1
1	B	402	ALA	2.1
1	B	482	GLN	2.1
1	A	384	ARG	2.1
1	A	478	VAL	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 oligosaccharides in this entry.

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.