



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 14, 2017 – 08:19 pm GMT

PDB ID : 1YGU
Title : Crystal structure of the tandem phosphatase domains of RPTP CD45 with a pTyr peptide
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Deposited on : 2005-01-05
Resolution : 2.90 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

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	recalc28949

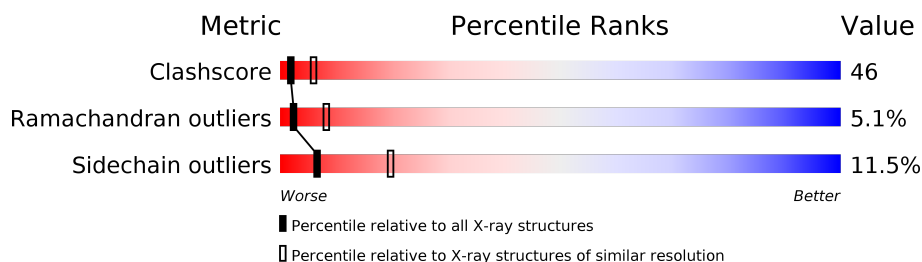
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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	112137	1807 (2.90-2.90)
Ramachandran outliers	110173	1768 (2.90-2.90)
Sidechain outliers	110143	1770 (2.90-2.90)

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. 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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	610	
1	B	610	
2	C	4	
2	D	4	

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	PTR	C	2004	X	-	-	-
2	PTR	D	2004	X	-	-	-

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 9529 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 Leukocyte common antigen.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	571	Total	C	N	O	S	Se	0	0	0
			4684	2983	815	866	7	13			
1	B	582	Total	C	N	O	S	Se	0	0	0
			4771	3033	835	883	7	13			

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	603	MSE	MET	MODIFIED RESIDUE	UNP P08575
A	627	PRO	LEU	VARIANT	UNP P08575
A	714	MSE	MET	MODIFIED RESIDUE	UNP P08575
A	725	MSE	MET	MODIFIED RESIDUE	UNP P08575
A	744	MSE	MET	MODIFIED RESIDUE	UNP P08575
A	828	SER	CYS	ENGINEERED	UNP P08575
A	844	MSE	MET	MODIFIED RESIDUE	UNP P08575
A	870	MSE	MET	MODIFIED RESIDUE	UNP P08575
A	907	MSE	MET	MODIFIED RESIDUE	UNP P08575
A	999	MSE	MET	MODIFIED RESIDUE	UNP P08575
A	1007	MSE	MET	MODIFIED RESIDUE	UNP P08575
A	1024	MSE	MET	MODIFIED RESIDUE	UNP P08575
A	1035	MSE	MET	MODIFIED RESIDUE	UNP P08575
A	1115	MSE	MET	MODIFIED RESIDUE	UNP P08575
A	1184	LEU	PRO	VARIANT	UNP P08575
A	1186	MSE	MET	MODIFIED RESIDUE	UNP P08575
B	603	MSE	MET	MODIFIED RESIDUE	UNP P08575
B	627	PRO	LEU	VARIANT	UNP P08575
B	714	MSE	MET	MODIFIED RESIDUE	UNP P08575
B	725	MSE	MET	MODIFIED RESIDUE	UNP P08575
B	744	MSE	MET	MODIFIED RESIDUE	UNP P08575
B	828	SER	CYS	ENGINEERED	UNP P08575
B	844	MSE	MET	MODIFIED RESIDUE	UNP P08575
B	870	MSE	MET	MODIFIED RESIDUE	UNP P08575
B	907	MSE	MET	MODIFIED RESIDUE	UNP P08575

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Chain	Residue	Modelled	Actual	Comment	Reference
B	999	MSE	MET	MODIFIED RESIDUE	UNP P08575
B	1007	MSE	MET	MODIFIED RESIDUE	UNP P08575
B	1024	MSE	MET	MODIFIED RESIDUE	UNP P08575
B	1035	MSE	MET	MODIFIED RESIDUE	UNP P08575
B	1115	MSE	MET	MODIFIED RESIDUE	UNP P08575
B	1184	LEU	PRO	VARIANT	UNP P08575
B	1186	MSE	MET	MODIFIED RESIDUE	UNP P08575

- Molecule 2 is a protein called Polyoma Middle T antigen.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	4	Total	C	N	O	P	0	0	0
			37	21	4	11	1			
2	D	4	Total	C	N	O	P	0	0	0
			37	21	4	11	1			

There are 2 discrepancies between the modelled and reference sequences:

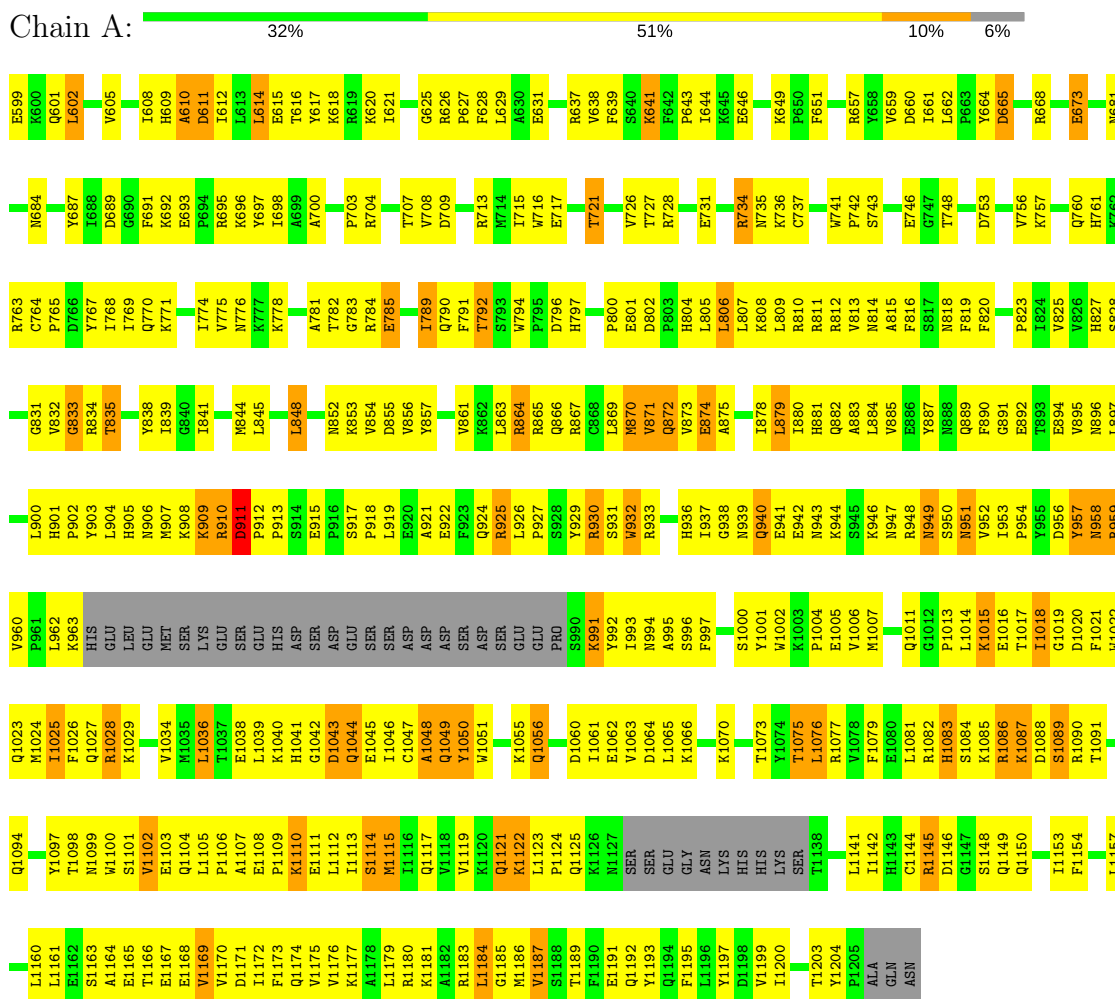
Chain	Residue	Modelled	Actual	Comment	Reference
C	2004	PTR	TYR	MODIFIED RESIDUE	UNP P03077
D	2004	PTR	TYR	MODIFIED RESIDUE	UNP P03077

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 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.

Note EDS was not executed.

- Molecule 1: Leukocyte common antigen



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	84.90Å 57.92Å 159.29Å 90.00° 98.66° 90.00°	Depositor
Resolution (Å)	29.16 – 2.90	Depositor
% Data completeness (in resolution range)	92.9 (29.16-2.90)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.262 , 0.305	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	9529	wwPDB-VP
Average B, all atoms (Å ²)	77.0	wwPDB-VP

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: PTR

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	0.52	0/4779	0.72	1/6440 (0.0%)
1	B	0.52	0/4870	0.73	2/6562 (0.0%)
2	C	0.77	0/20	1.20	0/23
2	D	0.92	0/20	1.25	0/23
All	All	0.52	0/9689	0.73	3/13048 (0.0%)

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
2	C	1	0
2	D	1	0
All	All	2	0

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1124	PRO	N-CA-C	5.53	126.47	112.10
1	B	602	LEU	N-CA-C	-5.19	96.99	111.00
1	A	781	ALA	N-CA-C	-5.09	97.25	111.00

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	C	2004	PTR	CA
2	D	2004	PTR	CA

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	4684	0	4645	419	0
1	B	4771	0	4723	446	0
2	C	37	0	25	1	0
2	D	37	0	25	1	0
All	All	9529	0	9418	866	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 46.

The worst 5 of 866 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:1179:LEU:HD22	1:A:1186:MSE:HE3	1.27	1.14
1:B:844:MSE:HE3	1:B:854:VAL:HB	1.28	1.11
1:A:874:GLU:CD	1:A:874:GLU:H	1.50	1.08
1:A:844:MSE:HE3	1:A:854:VAL:HB	1.34	1.08
1:B:912:PRO:HB2	1:B:915:GLU:HG2	1.35	1.05

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	565/610 (93%)	461 (82%)	80 (14%)	24 (4%)	3	12
1	B	578/610 (95%)	451 (78%)	93 (16%)	34 (6%)	2	6
2	C	1/4 (25%)	1 (100%)	0	0	100	100
2	D	1/4 (25%)	1 (100%)	0	0	100	100
All	All	1145/1228 (93%)	914 (80%)	173 (15%)	58 (5%)	2	8

5 of 58 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	819	PHE
1	A	870	MSE
1	A	871	VAL
1	A	911	ASP
1	A	930	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	514/538 (96%)	458 (89%)	56 (11%)	7	22
1	B	524/538 (97%)	461 (88%)	63 (12%)	6	17
2	C	3/3 (100%)	2 (67%)	1 (33%)	0	0
2	D	3/3 (100%)	3 (100%)	0	100	100
All	All	1044/1082 (96%)	924 (88%)	120 (12%)	6	20

5 of 120 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1180	ARG
1	B	782	THR
1	B	1124	PRO
1	A	1184	LEU
1	B	637	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 51 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1150	GLN
1	B	718	GLN
1	B	1121	GLN
1	B	633	GLN
1	B	761	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues 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	PTR	C	2004	2	15,16,17	1.61	5 (33%)	19,22,24	2.39	5 (26%)
2	PTR	D	2004	2	15,16,17	1.51	4 (26%)	19,22,24	2.85	7 (36%)

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	PTR	C	2004	2	1/1/2/3	0/9/11/13	0/1/1/1
2	PTR	D	2004	2	1/1/2/3	0/9/11/13	0/1/1/1

The worst 5 of 9 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	2004	PTR	P-O3P	-2.44	1.44	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	2004	PTR	P-O3P	-2.39	1.45	1.54
2	C	2004	PTR	CD2-CG	2.24	1.43	1.38
2	D	2004	PTR	CE2-CD2	2.28	1.42	1.38
2	D	2004	PTR	CD2-CG	2.29	1.43	1.38

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	2004	PTR	OH-CZ-CE1	-5.52	102.61	119.23
2	C	2004	PTR	OH-CZ-CE1	-4.25	106.43	119.23
2	D	2004	PTR	CE2-CD2-CG	-2.29	117.85	121.02
2	D	2004	PTR	CB-CG-CD1	-2.20	116.46	120.91
2	C	2004	PTR	CE2-CD2-CG	-2.11	118.10	121.02

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	D	2004	PTR	CA
2	C	2004	PTR	CA

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	2004	PTR	1	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

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 was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.