W O R L D W I D E
wwPDB
PROTEIN DATA BANK

wwPDB X-ray Structure Validation Summary Report (i)

Jan 31, 2016 – 10:01 PM GMT

PDB ID : 1RPT
Title : CRYSTAL STRUCTURES OF RAT ACID PHOSPHATASE COMPLEXED
WITH THE TRANSITIONS STATE ANALOGS VANADATE AND MOLYB-
DATE: IMPLICATIONS FOR THE REACTION MECHANISM
Authors : Lindqvist, Y.; Schneider, G.
Deposited on : 1993-11-29
Resolution : 3.00 Å(reported)

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : NOT EXECUTED
EDS : NOT EXECUTED
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

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 3.00 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	Percentile Ranks	Value
Clashscore		17
Ramachandran outliers		3.8%
Sidechain outliers		18.3%

Worse .... *Better*

■ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution
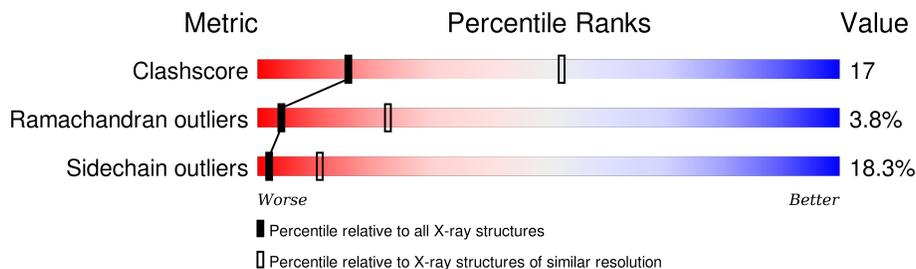
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	102246	1912 (3.00-3.00)
Ramachandran outliers	100387	1853 (3.00-3.00)
Sidechain outliers	100360	1856 (3.00-3.00)

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 >=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 <=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	342	44%　　　　37%　　　15%　•

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
4	VO4	A	343	-	-	X	-

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 2852 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 PROSTATIC ACID PHOSPHATASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	342	2794	1793	468	517	16	0	0	0

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	97	ASN	ILE	CONFLICT	UNP P20646
A	191	LEU	PHE	CONFLICT	UNP P20646
A	192	PRO	ARG	CONFLICT	UNP P20646
A	257	HIS	TYR	CONFLICT	UNP P20646
A	269	ASP	GLU	CONFLICT	UNP P20646
A	270	VAL	LEU	CONFLICT	UNP P20646
A	293	HIS	THR	CONFLICT	UNP P20646

- Molecule 2 is a polymer of unknown type called SUGAR (3-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
2	A	3	39	22	2	15	0	0

- Molecule 3 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 4 is VANADATE ION (three-letter code: VO4) (formula: O_4V).
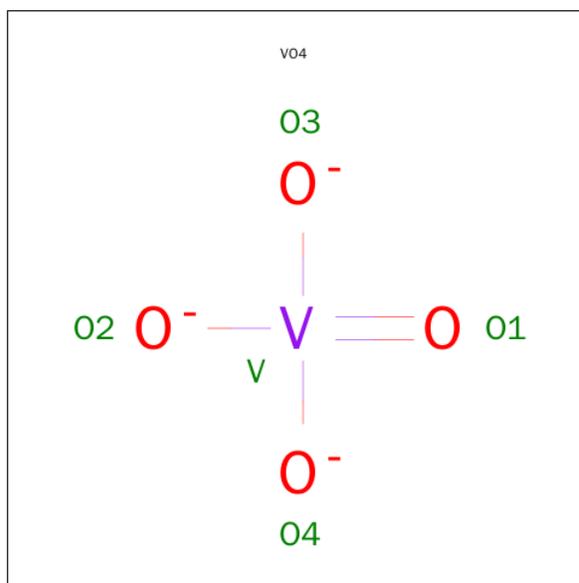
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	V	0	0
			5	4	1		

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 errors 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: PROSTATIC ACID PHOSPHATASE

Chain A:
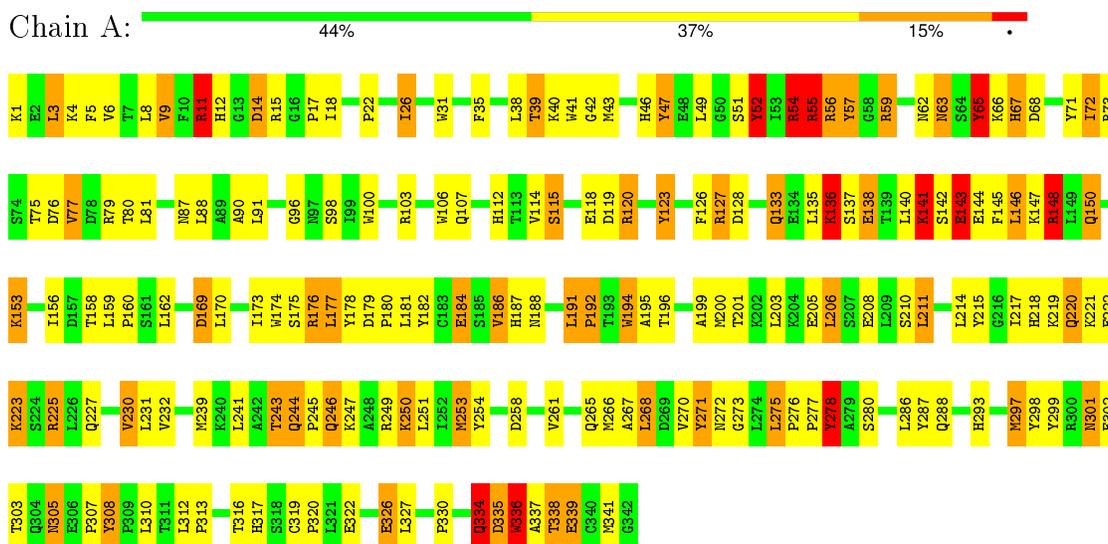
4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α, β, γ	89.40Å　　89.40Å　　152.00Å 90.00°　　90.00°　　120.00°	Depositor
Resolution (Å)	(Not available)　－　3.00	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-3.00)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.215　　,　　(Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2852	wwPDB-VP
Average B, all atoms (Å²)	16.0	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: VO4, BMA, NAG

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	1.26	5/2873 (0.2%)	2.10	108/3898 (2.8%)

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	6

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	31	TRP	CG-CD2	-5.73	1.33	1.43
1	A	127	ARG	NE-CZ	5.71	1.40	1.33
1	A	59	ARG	CZ-NH1	5.50	1.40	1.33
1	A	51	SER	CA-CB	-5.41	1.44	1.52
1	A	31	TRP	CD1-NE1	-5.11	1.29	1.38

The worst 5 of 108 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	127	ARG	NE-CZ-NH1	15.47	128.03	120.30
1	A	47	TYR	CB-CG-CD1	-14.15	112.51	121.00
1	A	55	ARG	NE-CZ-NH1	13.38	126.99	120.30
1	A	31	TRP	CD1-CG-CD2	11.89	115.81	106.30
1	A	103	ARG	NE-CZ-NH1	11.15	125.87	120.30

There are no chirality outliers.

5 of 6 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	128	ASP	Mainchain
1	A	182	TYR	Sidechain
1	A	278	TYR	Sidechain
1	A	52	TYR	Sidechain
1	A	65	TYR	Sidechain

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	2794	0	2736	94	0
2	A	39	0	34	2	0
3	A	14	0	13	2	0
4	A	5	0	0	4	0
All	All	2852	0	2783	97	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 17.

The worst 5 of 97 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:266:MET:SD	1:A:271:TYR:HD2	1.95	0.89
1:A:55:ARG:HH11	1:A:55:ARG:HG2	1.44	0.81
1:A:338:THR:HA	1:A:341:MET:SD	2.19	0.81
1:A:258:ASP:HB2	1:A:276:PRO:HG2	1.68	0.76
1:A:211:LEU:HD23	1:A:275:LEU:HD23	1.71	0.71

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	340/342 (99%)	283 (83%)	44 (13%)	13 (4%)	4	22

5 of 13 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	67	HIS
1	A	127	ARG
1	A	337	ALA
1	A	62	ASN
1	A	143	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	311/311 (100%)	254 (82%)	57 (18%)	2	11

5 of 57 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	120	ARG
1	A	146	LEU
1	A	316	THR
1	A	133	GLN
1	A	140	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	87	ASN
1	A	107	GLN
1	A	265	GLN
1	A	304	GLN

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Mol	Chain	Res	Type
1	A	305	ASN

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 ⓘ

3 carbohydrates 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	NAG	A	344	1,2	14,14,15	1.56	2 (14%)	15,19,21	1.10	1 (6%)
2	NAG	A	345	2	14,14,15	1.17	1 (7%)	15,19,21	2.66	4 (26%)
2	BMA	A	346	2	11,11,12	1.99	2 (18%)	14,15,17	3.13	8 (57%)

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	NAG	A	344	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	345	2	-	0/6/23/26	0/1/1/1
2	BMA	A	346	2	-	0/2/19/22	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	344	NAG	C4-C5	-4.08	1.44	1.53
2	A	346	BMA	C2-C3	-3.57	1.47	1.52
2	A	344	NAG	O3-C3	-2.32	1.37	1.43
2	A	345	NAG	O5-C1	2.77	1.48	1.43
2	A	346	BMA	C4-C5	4.79	1.63	1.53

The worst 5 of 13 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	346	BMA	C1-C2-C3	-8.38	99.63	109.54
2	A	345	NAG	C2-N2-C7	-6.64	114.51	123.04
2	A	346	BMA	C2-C3-C4	-3.83	104.53	111.04
2	A	346	BMA	O5-C5-C6	-2.81	101.26	107.35
2	A	346	BMA	O4-C4-C3	-2.26	105.25	110.34

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	344	NAG	1	0
2	A	345	NAG	1	0

5.6 Ligand geometry (i)

2 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	#$|Z| > 2$
4	VO4	A	343	1	1,4,4	0.41	0	0,6,6	0.00	-
3	NAG	A	347	1	14,14,15	1.93	5 (35%)	15,19,21	1.88	3 (20%)

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
4	VO4	A	343	1	-	0/0/0/0	0/0/0/0
3	NAG	A	347	1	-	0/6/23/26	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	347	NAG	C8-C7	2.06	1.54	1.50
3	A	347	NAG	O5-C5	2.18	1.48	1.43
3	A	347	NAG	C6-C5	2.20	1.59	1.51
3	A	347	NAG	C4-C5	3.56	1.60	1.53
3	A	347	NAG	C4-C3	4.11	1.63	1.52

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	347	NAG	C1-O5-C5	-4.43	106.63	112.25
3	A	347	NAG	C8-C7-N2	-2.21	111.87	116.11
3	A	347	NAG	C6-C5-C4	4.74	124.71	113.02

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	343	VO4	4	0
3	A	347	NAG	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　ⓘ

6.1　Protein, DNA and RNA chains　ⓘ

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3　Carbohydrates　ⓘ

EDS was not executed - this section will therefore be empty.

6.4　Ligands　ⓘ

EDS was not executed - this section will therefore be empty.

6.5　Other polymers　ⓘ

EDS was not executed - this section will therefore be empty.