



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 13, 2017 – 09:10 pm GMT

PDB ID : 3V0F  
Title : Crystal structure of *Ciona intestinalis* voltage sensor-containing phosphatase (Ci-VSP), residues 241-576(C363S), form II  
Authors : Liu, L.; Kohout, S.C.; Xu, Q.; Muller, S.; Kimberlin, C.; Isacoff, E.Y.; Minor, D.L.  
Deposited on : 2011-12-07  
Resolution : 1.30 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](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

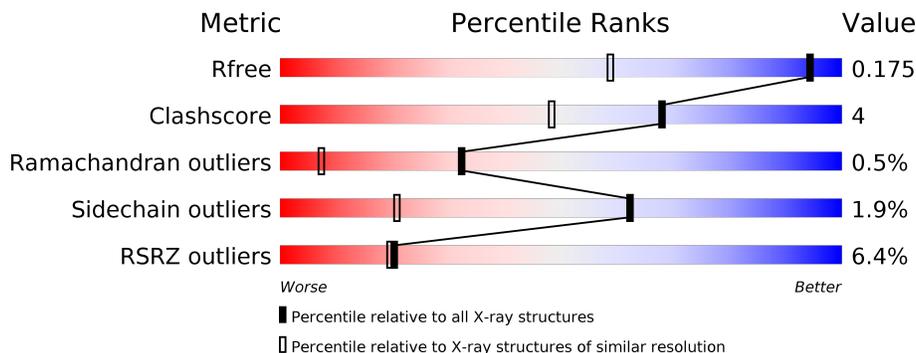
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

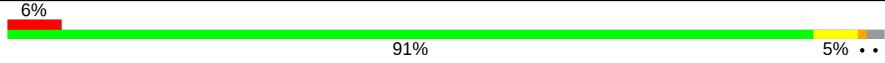
The reported resolution of this entry is 1.30 Å.

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	1131 (1.32-1.28)
Clashscore	112137	1185 (1.32-1.28)
Ramachandran outliers	110173	1138 (1.32-1.28)
Sidechain outliers	110143	1138 (1.32-1.28)
RSRZ outliers	101464	1133 (1.32-1.28)

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	339	 6% 91% 5% ..
1	B	339	 6% 87% 9% 5%

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 6488 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.

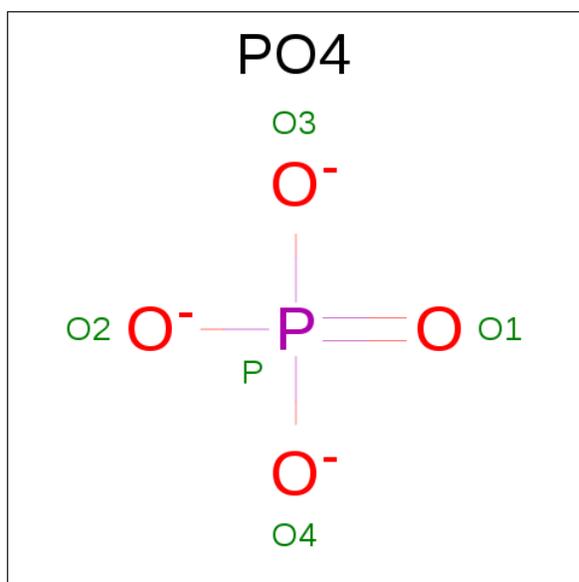
- Molecule 1 is a protein called Voltage-sensor containing phosphatase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	331	2784	1772	479	515	18	0	27	0
1	B	323	2811	1798	478	516	19	0	43	0

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	238	GLY	-	EXPRESSION TAG	UNP Q4W8A1
A	239	HIS	-	EXPRESSION TAG	UNP Q4W8A1
A	240	MET	-	EXPRESSION TAG	UNP Q4W8A1
A	363	SER	CYS	ENGINEERED MUTATION	UNP Q4W8A1
B	238	GLY	-	EXPRESSION TAG	UNP Q4W8A1
B	239	HIS	-	EXPRESSION TAG	UNP Q4W8A1
B	240	MET	-	EXPRESSION TAG	UNP Q4W8A1
B	363	SER	CYS	ENGINEERED MUTATION	UNP Q4W8A1

- Molecule 2 is PHOSPHATE ION (three-letter code: PO4) (formula: O<sub>4</sub>P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	P	0	1
			10	8	2		
2	B	1	Total	O	P	0	1
			10	8	2		

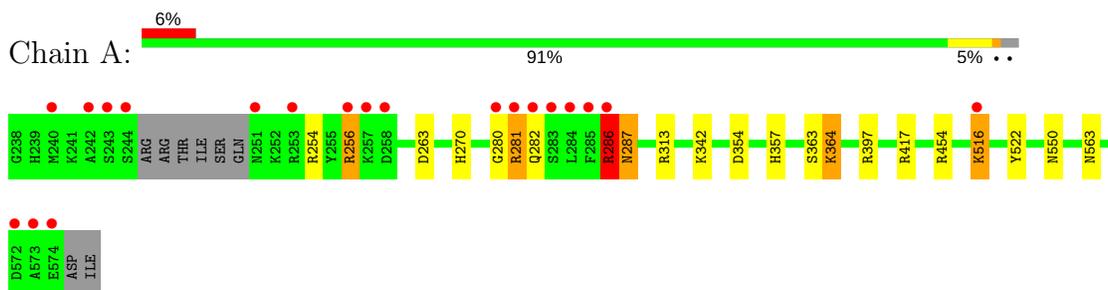
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	429	Total	O	0	0
			429	429		
3	B	441	Total	O	0	4
			444	444		

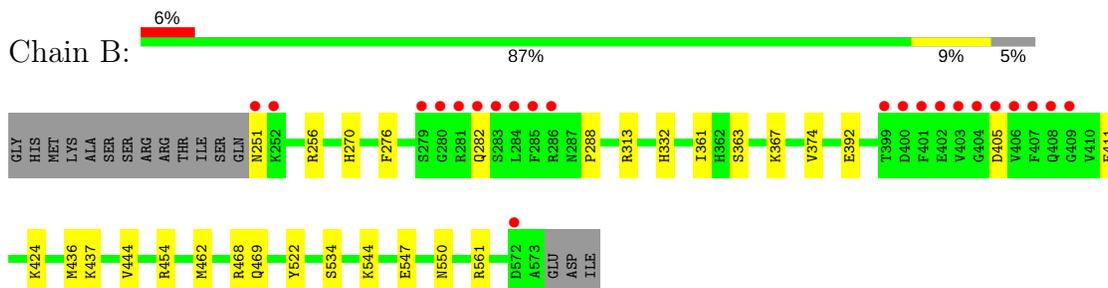
### 3 Residue-property plots [i](#)

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.

- Molecule 1: Voltage-sensor containing phosphatase



- Molecule 1: Voltage-sensor containing phosphatase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	50.75Å 80.38Å 83.64Å 90.00° 93.12° 90.00°	Depositor
Resolution (Å)	83.51 – 1.30 42.31 – 1.30	Depositor EDS
% Data completeness (in resolution range)	93.9 (83.51-1.30) 93.8 (42.31-1.30)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.57 (at 1.30Å)	Xtrriage
Refinement program	REFMAC 5.5.0109	Depositor
R, $R_{free}$	0.140 , 0.175 0.141 , 0.175	Depositor DCC
$R_{free}$ test set	7732 reflections (5.29%)	DCC
Wilson B-factor (Å <sup>2</sup> )	14.5	Xtrriage
Anisotropy	0.107	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 50.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.98	EDS
Total number of atoms	6488	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	22.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.48% 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: PO4

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	0.48	0/2906	0.68	3/3904 (0.1%)
1	B	0.50	0/2964	0.71	2/3982 (0.1%)
All	All	0.49	0/5870	0.69	5/7886 (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

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	A	417	ARG	NE-CZ-NH2	-7.43	116.58	120.30
1	B	454	ARG	NE-CZ-NH1	5.26	122.93	120.30
1	A	417	ARG	NE-CZ-NH1	5.21	122.91	120.30
1	B	454	ARG	NE-CZ-NH2	-5.20	117.70	120.30
1	A	454	ARG	NE-CZ-NH1	5.17	122.88	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	286	ARG	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	2784	0	2801	25	0
1	B	2811	0	2870	25	0
2	A	10	0	0	1	0
2	B	10	0	0	0	0
3	A	429	0	0	6	0
3	B	444	0	0	6	0
All	All	6488	0	5671	50	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 4.

All (50) 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:561[B]:ARG:CG	1:B:561[B]:ARG:HH11	1.70	1.04
1:A:263:ASP:H	1:A:287:ASN:HD21	1.04	1.01
1:B:561[B]:ARG:CB	1:B:561[B]:ARG:HH11	1.74	1.00
1:A:263:ASP:H	1:A:287:ASN:ND2	1.60	0.98
1:A:516[B]:LYS:H	1:A:516[B]:LYS:HD2	1.25	0.97
1:B:561[B]:ARG:HH11	1:B:561[B]:ARG:HG3	1.35	0.88
1:A:263:ASP:N	1:A:287:ASN:HD21	1.72	0.87
1:A:516[A]:LYS:H	1:A:516[A]:LYS:HD2	1.44	0.81
1:B:561[B]:ARG:NH1	1:B:561[B]:ARG:HG3	1.93	0.80
1:B:561[B]:ARG:CB	1:B:561[B]:ARG:NH1	2.51	0.72
1:A:563[B]:ASN:ND2	3:A:869:HOH:O	2.24	0.69
1:B:561[B]:ARG:CZ	1:B:561[B]:ARG:HA	2.24	0.67
1:B:561[B]:ARG:HB3	1:B:561[B]:ARG:HH11	1.59	0.67
1:B:468[A]:ARG:NH2	3:B:843:HOH:O	2.28	0.67
1:B:561[B]:ARG:NH1	1:B:561[B]:ARG:HA	2.11	0.66
1:B:561[B]:ARG:HD2	1:B:561[B]:ARG:N	2.10	0.65
1:A:281[A]:ARG:H	1:A:281[A]:ARG:NE	1.96	0.63
1:A:286:ARG:HH21	1:A:313:ARG:HH22	1.46	0.63
1:B:561[B]:ARG:NH1	1:B:561[B]:ARG:CA	2.67	0.57
1:A:522:TYR:HD2	3:A:140:HOH:O	1.88	0.55
1:B:282[A]:GLN:HE22	1:B:288:PRO:HG3	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:444[B]:VAL:HG21	1:B:462:MET:SD	2.48	0.53
1:A:286:ARG:HH21	1:A:313:ARG:NH2	2.06	0.53
1:A:516[A]:LYS:HG2	3:A:839:HOH:O	2.07	0.53
1:A:270:HIS:HD2	3:A:580:HOH:O	1.93	0.52
1:A:254:ARG:HB3	1:A:256[A]:ARG:HD2	1.92	0.52
1:B:522:TYR:HD2	3:B:828:HOH:O	1.94	0.51
1:A:286:ARG:HH22	1:A:364:LYS:HG3	1.75	0.49
1:A:270:HIS:HE1	3:A:612:HOH:O	1.95	0.49
1:B:270:HIS:HD2	3:B:602:HOH:O	1.98	0.47
1:B:367[B]:LYS:HE3	1:B:367[B]:LYS:HB2	1.55	0.47
1:B:392:GLU:HG3	3:B:709:HOH:O	2.15	0.46
1:B:276:PHE:CZ	1:B:313[B]:ARG:HG3	2.50	0.46
1:B:332:HIS:CD2	1:B:411[B]:GLU:OE1	2.69	0.46
1:A:342[B]:LYS:HB2	1:A:342[B]:LYS:HE3	1.39	0.45
1:B:544[B]:LYS:HG3	1:B:547[B]:GLU:OE2	2.17	0.44
1:A:281[A]:ARG:H	1:A:281[A]:ARG:HE	1.66	0.43
1:A:516[B]:LYS:HG2	3:A:839:HOH:O	2.18	0.43
1:B:361:ILE:HD12	1:B:374:VAL:HG22	1.99	0.43
1:B:437[A]:LYS:HB2	1:B:534[A]:SER:HA	2.00	0.43
1:A:254:ARG:CB	1:A:256[A]:ARG:HD2	2.49	0.43
1:A:363[A]:SER:OG	2:A:1[A]:PO4:O1	2.24	0.42
1:B:270:HIS:HE1	3:B:842:HOH:O	2.02	0.41
1:A:354:ASP:HB3	1:A:357:HIS:CD2	2.55	0.41
1:B:436[A]:MET:HE2	3:B:833:HOH:O	2.21	0.41
1:A:516[B]:LYS:CD	1:A:516[B]:LYS:H	2.01	0.41
1:A:280[A]:GLY:HA3	1:A:281[A]:ARG:HH21	1.87	0.40

There are no symmetry-related clashes.

## 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	350/339 (103%)	336 (96%)	12 (3%)	2 (1%)	28	5
1	B	358/339 (106%)	348 (97%)	9 (2%)	1 (0%)	44	17
All	All	708/678 (104%)	684 (97%)	21 (3%)	3 (0%)	32	11

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	550	ASN
1	B	550	ASN
1	A	364	LYS

### 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	315/301 (105%)	307 (98%)	8 (2%)	53	11
1	B	324/301 (108%)	319 (98%)	5 (2%)	70	31
All	All	639/602 (106%)	626 (98%)	13 (2%)	62	18

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	256[A]	ARG
1	A	256[B]	ARG
1	A	281[A]	ARG
1	A	282[A]	GLN
1	A	286	ARG
1	A	287	ASN
1	A	516[A]	LYS
1	A	516[B]	LYS
1	B	251	ASN
1	B	256	ARG
1	B	405	ASP
1	B	424	LYS
1	B	469	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	270	HIS
1	A	282[A]	GLN
1	A	287	ASN
1	B	270	HIS
1	B	282[A]	GLN
1	B	469	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	PO4	A	1[A]	-	4,4,4	0.98	0	6,6,6	0.92	0
2	PO4	A	1[B]	-	4,4,4	0.84	0	6,6,6	0.60	0
2	PO4	B	2[A]	-	4,4,4	1.04	0	6,6,6	0.99	0
2	PO4	B	2[B]	-	4,4,4	0.69	0	6,6,6	0.38	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	PO4	A	1[A]	-	-	0/0/0/0	0/0/0/0
2	PO4	A	1[B]	-	-	0/0/0/0	0/0/0/0
2	PO4	B	2[A]	-	-	0/0/0/0	0/0/0/0
2	PO4	B	2[B]	-	-	0/0/0/0	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

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	A	1[A]	PO4	1	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

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	331/339 (97%)	-0.00	20 (6%) 23 22	11, 19, 42, 54	6 (1%)
1	B	323/339 (95%)	-0.01	22 (6%) 18 18	10, 17, 36, 55	7 (2%)
All	All	654/678 (96%)	-0.01	42 (6%) 20 19	10, 18, 38, 55	13 (1%)

All (42) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	284[A]	LEU	14.2
1	B	281[A]	ARG	10.6
1	A	285[A]	PHE	9.5
1	B	406	VAL	8.2
1	A	283[A]	SER	7.9
1	B	404	GLY	7.5
1	A	244	SER	7.4
1	A	286	ARG	7.1
1	B	285[A]	PHE	7.0
1	B	407	PHE	6.6
1	B	405	ASP	6.5
1	A	281[A]	ARG	6.4
1	B	401	PHE	5.9
1	B	400	ASP	5.7
1	A	280[A]	GLY	5.1
1	B	403	VAL	4.8
1	B	280[A]	GLY	4.8
1	B	251	ASN	4.5
1	B	282[A]	GLN	4.3
1	A	243	SER	4.2
1	A	572	ASP	4.2
1	A	282[A]	GLN	3.9
1	A	574	GLU	3.7
1	B	252	LYS	3.7

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Mol	Chain	Res	Type	RSRZ
1	A	253	ARG	3.6
1	A	573	ALA	3.6
1	B	402	GLU	3.4
1	B	408	GLN	3.4
1	A	242	ALA	2.9
1	B	572	ASP	2.9
1	B	283[A]	SER	2.8
1	A	516[A]	LYS	2.8
1	A	257	LYS	2.5
1	B	279	SER	2.5
1	B	286[A]	ARG	2.5
1	A	256[A]	ARG	2.4
1	A	251	ASN	2.4
1	A	240	MET	2.2
1	B	399	THR	2.2
1	B	409	GLY	2.2
1	B	284[A]	LEU	2.1
1	A	258	ASP	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 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(Å <sup>2</sup> )	Q < 0.9
2	PO4	A	1[A]	5/5	0.99	0.07	0.33	15,17,21,22	5
2	PO4	A	1[B]	5/5	0.99	0.07	0.33	9,10,11,12	5
2	PO4	B	2[A]	5/5	0.99	0.06	-0.84	14,16,19,20	5
2	PO4	B	2[B]	5/5	0.99	0.06	-0.84	8,9,11,11	5

## 6.5 Other polymers [i](#)

There are no such residues in this entry.