



Full wwPDB X-ray Structure Validation Report

Feb 27, 2014 – 05:41 AM GMT

PDB ID : 2D1G
Title : Structure of Francisella tularensis Acid Phosphatase A (AcpA) bound to orthovanadate
Authors : Felts, R.L.; Reilly, T.J.; Tanner, J.J.
Deposited on : 2005-08-20
Resolution : 1.75 Å(reported)

This is a full wwPDB validation 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/ValidationPDFNotes.html>

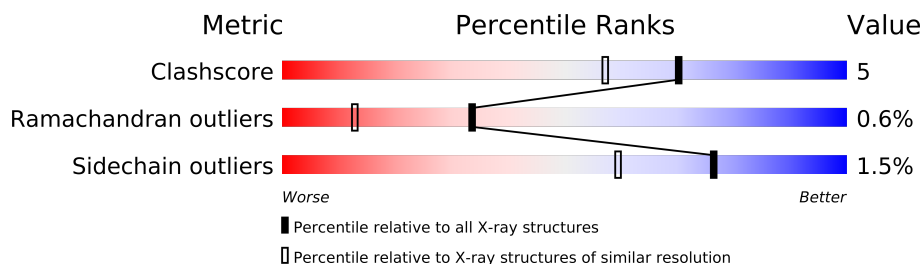
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : **FAILED**
Percentile statistics : 21963
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 1.75 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	79885	1304 (1.76-1.76)
Ramachandran outliers	78287	1288 (1.76-1.76)
Sidechain outliers	78261	1288 (1.76-1.76)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Note EDS failed to run properly.

Mol	Chain	Length	Quality of chain
1	A	498	
1	B	498	

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 8182 atoms, of which 0 are hydrogen and 0 are deuterium.

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.

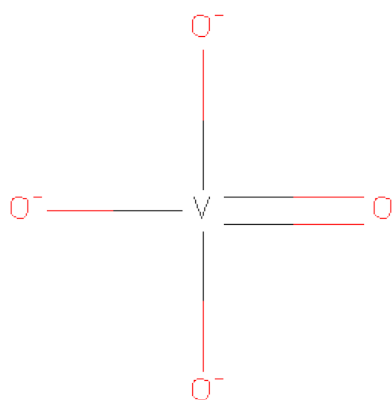
- Molecule 1 is a protein called acid phosphatase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	481	Total	C	N	O	S	0	5	0
			3817	2413	644	746	14			
1	B	472	Total	C	N	O	S	0	1	0
			3725	2352	630	730	13			

There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	INITIATING METHIONINE	UNP Q2A5P7
A	375	ASP	ALA	SEE REMARK 999	UNP Q2A5P7
A	376	TRP	GLY	SEE REMARK 999	UNP Q2A5P7
A	377	ASP	ILE	SEE REMARK 999	UNP Q2A5P7
A	378	SER	ALA	SEE REMARK 999	UNP Q2A5P7
A	379	THR	HIS	SEE REMARK 999	UNP Q2A5P7
A	494	HIS	-	EXPRESSION TAG	UNP Q2A5P7
A	495	HIS	-	EXPRESSION TAG	UNP Q2A5P7
A	496	HIS	-	EXPRESSION TAG	UNP Q2A5P7
A	497	HIS	-	EXPRESSION TAG	UNP Q2A5P7
A	498	HIS	-	EXPRESSION TAG	UNP Q2A5P7
B	1	MET	-	INITIATING METHIONINE	UNP Q2A5P7
B	375	ASP	ALA	SEE REMARK 999	UNP Q2A5P7
B	376	TRP	GLY	SEE REMARK 999	UNP Q2A5P7
B	377	ASP	ILE	SEE REMARK 999	UNP Q2A5P7
B	378	SER	ALA	SEE REMARK 999	UNP Q2A5P7
B	379	THR	HIS	SEE REMARK 999	UNP Q2A5P7
B	494	HIS	-	EXPRESSION TAG	UNP Q2A5P7
B	495	HIS	-	EXPRESSION TAG	UNP Q2A5P7
B	496	HIS	-	EXPRESSION TAG	UNP Q2A5P7
B	497	HIS	-	EXPRESSION TAG	UNP Q2A5P7
B	498	HIS	-	EXPRESSION TAG	UNP Q2A5P7

- Molecule 2 is VANADATE ION (three-letter code: VO4) (formula: O₄V).

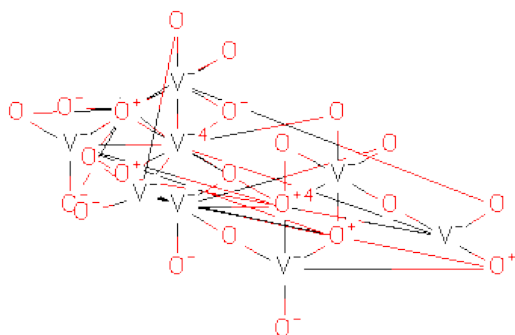


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	V	0	0
			5	4	1		
2	B	1	Total	O	V	0	0
			5	4	1		

- Molecule 3 is UNKNOWN ATOM OR ION (three-letter code: UNX) (formula: X).

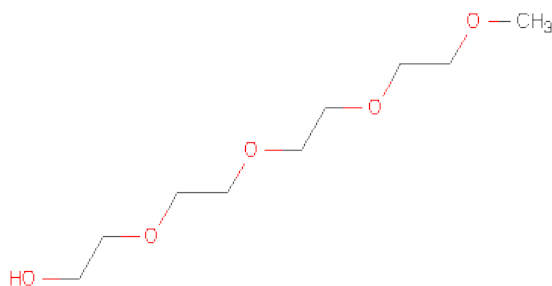
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	X	0	0
			1	1		
3	A	1	Total	X	0	0
			1	1		

- Molecule 4 is DECAVANADATE (three-letter code: DVT) (formula: O₂₈V₁₀).



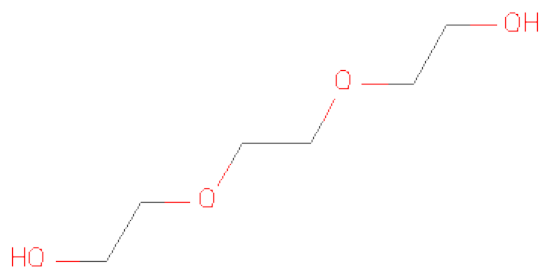
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	O	V	0	0
			38	28	10		

- Molecule 5 is 2-{2-[2-2-(METHOXY-ETHOXY)-ETHOXY]-ETHOXY}-ETHANOL (three-letter code: ETE) (formula: C₉H₂₀O₅).



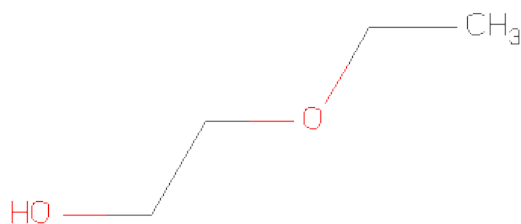
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			14	9	5		

- Molecule 6 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: C₆H₁₄O₄).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total	C	O	0	0
			10	6	4		
6	B	1	Total	C	O	0	0
			10	6	4		

- Molecule 7 is 2-ETHOXYETHANOL (three-letter code: ETX) (formula: $C_4H_{10}O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			6	4	2		

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	345	Total 345	O 345	0	0
8	B	205	Total 205	O 205	0	0

4 Data and refinement statistics

EDS failed to run properly - this section will therefore be incomplete.

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	112.08Å 144.40Å 123.86Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	44.28 – 1.75	Depositor
% Data completeness (in resolution range)	100.0 (44.28-1.75)	Depositor
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.79 (at 1.75Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.198 , 0.231	Depositor
Wilson B-factor (Å ²)	19.7	Xtriage
Anisotropy	0.140	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	0 of 98094 reflections	Xtriage
Total number of atoms	8182	wwPDB-VP
Average B, all atoms (Å ²)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.56% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PGE, UNX, ETX, VO4, ETE, DVT

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	0.56	0/3941	0.64	1/5362 (0.0%)
1	B	0.68	9/3836 (0.2%)	0.61	1/5224 (0.0%)
All	All	0.62	9/7777 (0.1%)	0.62	2/10586 (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
1	A	0	4
1	B	0	1
All	All	0	5

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	223	SER	CB-OG	8.94	1.53	1.42
1	B	11	TYR	CE1-CZ	8.81	1.50	1.38
1	B	11	TYR	CG-CD2	8.79	1.50	1.39
1	B	215	ASP	CG-OD2	7.13	1.41	1.25
1	B	215	ASP	CG-OD1	6.73	1.40	1.25
1	B	11	TYR	CE2-CZ	5.40	1.45	1.38
1	B	6	SER	CB-OG	5.40	1.49	1.42
1	B	11	TYR	CG-CD1	5.38	1.46	1.39
1	B	263	SER	C-N	5.22	1.42	1.33

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	67	VAL	N-CA-C	7.03	129.99	111.00
1	B	215	ASP	CB-CG-OD2	-5.28	113.55	118.30

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	130	ASP	Peptide
1	A	132	ASP	Peptide
1	A	43	GLU	Peptide
1	A	66	PHE	Peptide
1	B	495	HIS	Peptide

5.2 Close contacts ⓘ

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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3817	0	3537	31	0
1	B	3725	0	3413	37	0
2	A	5	0	0	1	0
2	B	5	0	0	2	0
3	A	1	0	0	0	0
3	B	1	0	0	1	0
4	B	38	0	0	1	0
5	A	14	0	20	1	0
6	B	20	0	28	0	0
7	A	6	0	10	4	0
8	A	345	0	0	3	0
8	B	205	0	0	4	0
All	All	8182	0	7008	67	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 5.

All (67) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:175:SER:OG	1:B:386:ASP:OD2	1.61	1.14
1:B:254:GLN:HG2	8:B:2162:HOH:O	1.74	0.85
1:A:401:GLN:HE22	1:B:431:HIS:H	1.27	0.82
1:B:26:ASN:HD21	1:B:36:HIS:HE1	1.30	0.78
1:B:214:ASP:OD1	1:B:302:HIS:HE1	1.71	0.71
1:A:131:ASN:ND2	1:A:133:THR:CB	2.53	0.71
1:A:26:ASN:HD21	1:A:36:HIS:HE1	1.39	0.71
1:B:175:SER:OG	3:B:701:UNX:UNK	1.72	0.70
1:A:257:PHE:O	1:A:302:HIS:HD2	1.75	0.70
1:B:53:MET:HG3	1:B:145:TYR:CE1	2.31	0.66
1:B:153:ALA:H	1:B:360:GLN:HE21	1.44	0.65
1:B:25:ALA:HA	1:B:28:LEU:HD22	1.79	0.65
1:A:365:ASN:HD22	7:A:1006:ETX:H12	1.61	0.64
1:A:131:ASN:HD22	1:A:133:THR:CB	2.11	0.63
1:A:372:GLN:HE22	1:A:480:ILE:HD12	1.63	0.63
1:B:175:SER:HB2	2:B:901:VO4:O1	2.02	0.59
1:A:214:ASP:OD1	1:A:302:HIS:HE1	1.86	0.58
1:B:372:GLN:HE21	1:B:372:GLN:HA	1.69	0.57
1:B:257:PHE:O	1:B:302:HIS:HD2	1.87	0.56
1:B:284:TYR:HD1	8:B:2162:HOH:O	1.88	0.55
1:B:26:ASN:ND2	1:B:36:HIS:HE1	2.01	0.54
1:B:478:LYS:HG3	8:B:2165:HOH:O	2.07	0.54
1:A:100:GLN:NE2	1:A:275:ASN:HD21	2.05	0.54
1:B:175:SER:CB	1:B:386:ASP:OD2	2.55	0.54
1:A:401:GLN:NE2	1:B:431:HIS:H	2.01	0.53
1:B:26:ASN:HD21	1:B:36:HIS:CE1	2.19	0.53
1:A:153:ALA:H	1:A:360:GLN:NE2	2.07	0.53
1:B:153:ALA:H	1:B:360:GLN:NE2	2.05	0.52
1:A:365:ASN:HD22	7:A:1006:ETX:C1	2.22	0.52
1:B:26:ASN:ND2	1:B:36:HIS:CE1	2.78	0.51
1:A:174:PRO:HB2	2:A:801:VO4:O3	2.10	0.51
1:A:445:TYR:HD1	5:A:1001:ETE:H222	1.75	0.51
1:B:495:HIS:ND1	4:B:2001:DVT:O18	2.44	0.51
1:B:215:ASP:OD2	1:B:301:HIS:HA	2.11	0.51
1:A:55:PRO:HB2	1:A:68:ALA:HB2	1.93	0.50
1:B:495:HIS:HB3	1:B:497:HIS:O	2.12	0.49
1:A:459:LYS:HD2	8:A:1065:HOH:O	2.13	0.49
1:A:26:ASN:ND2	1:A:36:HIS:HE1	2.09	0.48
1:A:97:ARG:NH1	8:A:1279:HOH:O	2.35	0.48
1:A:239:ILE:HB	1:A:440:LEU:CD1	2.44	0.48
1:A:257:PHE:HB3	1:A:322:ASP:HA	1.94	0.48
1:B:97:ARG:HB3	1:B:150:THR:OG1	2.13	0.48
1:B:257:PHE:HB3	1:B:322:ASP:HA	1.95	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:131:ASN:HD22	1:A:134:TYR:H	1.62	0.46
1:B:198:GLU:OE2	1:B:198:GLU:HA	2.15	0.46
1:A:26:ASN:HD21	1:A:36:HIS:CE1	2.28	0.46
1:B:214:ASP:OD1	1:B:302:HIS:CE1	2.61	0.46
1:B:403:SER:HB2	1:B:409:GLN:OE1	2.15	0.45
1:A:100:GLN:HE22	1:A:275:ASN:HD21	1.63	0.45
7:A:1006:ETX:C2	8:A:1307:HOH:O	2.65	0.45
1:B:55:PRO:HB2	1:B:68:ALA:HB2	1.99	0.44
1:B:44:ASN:ND2	2:B:901:VO4:O2	2.43	0.44
1:B:257:PHE:N	8:B:2162:HOH:O	2.50	0.44
1:B:53:MET:HG3	1:B:145:TYR:CD1	2.54	0.43
1:A:372:GLN:HE22	1:A:480:ILE:CD1	2.29	0.43
1:B:355:ASN:HB2	1:B:356:PRO:HD2	2.00	0.43
1:A:26:ASN:ND2	1:A:36:HIS:CE1	2.87	0.42
1:A:365:ASN:HB3	7:A:1006:ETX:H31	2.02	0.42
1:A:239:ILE:HB	1:A:440:LEU:HD11	2.02	0.42
1:B:264:GLY:C	1:B:266:THR:H	2.21	0.42
1:A:53:MET:HE1	1:A:83:LEU:HD21	2.02	0.42
1:B:100:GLN:NE2	1:B:275:ASN:HD21	2.17	0.42
1:A:132:ASP:N	1:A:133:THR:CB	2.82	0.42
1:B:239:ILE:HB	1:B:440:LEU:CD1	2.51	0.41
1:B:257:PHE:O	1:B:302:HIS:CD2	2.73	0.40
1:A:250:TRP:HA	1:A:338:VAL:O	2.22	0.40
1:A:153:ALA:H	1:A:360:GLN:HE21	1.68	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	482/498 (97%)	468 (97%)	12 (2%)	2 (0%)	43	21
1	B	465/498 (93%)	449 (97%)	12 (3%)	4 (1%)	25	7
All	All	947/996 (95%)	917 (97%)	24 (2%)	6 (1%)	33	13

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	133	THR
1	B	264	GLY
1	B	496	HIS
1	A	174	PRO
1	B	265	LYS
1	B	174	PRO

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	411/436 (94%)	405 (98%)	6 (2%)	76	59
1	B	399/436 (92%)	392 (98%)	7 (2%)	71	50
All	All	810/872 (93%)	797 (98%)	13 (2%)	76	55

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

Mol	Chain	Res	Type
1	A	67	VAL
1	A	191	MET
1	A	289	GLU
1	A	341	LEU
1	A	372	GLN
1	A	377	ASP
1	B	28	LEU
1	B	289	GLU
1	B	341	LEU
1	B	377	ASP
1	B	417[A]	MET
1	B	417[B]	MET
1	B	495	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	5	ASN
1	A	23	ASN
1	A	26	ASN
1	A	36	HIS
1	A	71	ASN
1	A	100	GLN
1	A	104	GLN
1	A	131	ASN
1	A	302	HIS
1	A	316	GLN
1	A	347	GLN
1	A	360	GLN
1	A	365	ASN
1	A	372	GLN
1	A	401	GLN
1	B	19	GLN
1	B	23	ASN
1	B	26	ASN
1	B	36	HIS
1	B	98	ASN
1	B	100	GLN
1	B	302	HIS
1	B	316	GLN
1	B	360	GLN
1	B	372	GLN

5.3.3 RNA ⓘ

There are no RNA chains 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 carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 9 ligands modelled in this entry, 2 are unknown - leaving 7 for Mogul analysis.

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$
5	ETE	A	1001	-	13,13,13	0.54	0	12,12,12	0.18	0
7	ETX	A	1006	-	5,5,5	0.45	0	4,4,4	0.34	0
2	VO4	A	801	-	4,4,4	6.45	1 (25%)	0,6,6	0.00	-
6	PGE	B	1002	-	9,9,9	0.42	0	8,8,8	0.29	0
6	PGE	B	1004	-	9,9,9	0.48	0	8,8,8	0.40	0
4	DVT	B	2001	-	60,60,60	12.20	10 (16%)	0,206,206	0.00	-
2	VO4	B	901	-	4,4,4	6.27	4 (100%)	0,6,6	0.00	-

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
5	ETE	A	1001	-	-	0/11/11/11	0/0/0/0
7	ETX	A	1006	-	-	0/3/3/3	0/0/0/0
2	VO4	A	801	-	-	0/0/0/0	0/0/0/0
6	PGE	B	1002	-	-	0/7/7/7	0/0/0/0
6	PGE	B	1004	-	-	0/7/7/7	0/0/0/0
4	DVT	B	2001	-	-	0/0/560/560	0/0/23/23
2	VO4	B	901	-	-	0/0/0/0	0/0/0/0

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	2001	DVT	O7-V8	72.83	4.40	2.11
4	B	2001	DVT	O7-V6	42.69	4.60	2.28
4	B	2001	DVT	O16-V2	25.13	2.08	1.68
4	B	2001	DVT	O7-V4	21.78	3.46	2.28
4	B	2001	DVT	O7-V7	21.30	3.44	2.28
4	B	2001	DVT	O7-V2	-13.61	1.68	2.11
2	A	801	VO4	O1-V	12.60	1.92	1.62
2	B	901	VO4	O1-V	11.94	1.91	1.62
4	B	2001	DVT	O7-V5	-3.87	2.07	2.28

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	2001	DVT	O16-V5	2.49	2.26	1.98
2	B	901	VO4	O4-V	2.37	1.92	1.71
2	B	901	VO4	O3-V	2.18	1.91	1.71
2	B	901	VO4	O2-V	2.07	1.90	1.71
4	B	2001	DVT	O17-V3	2.06	2.05	2.00
4	B	2001	DVT	O1-V2	2.06	1.72	1.68

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

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 ⓘ

EDS failed to run properly - this section will therefore be empty.

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

EDS failed to run properly - this section will therefore be empty.

6.3 Carbohydrates ⓘ

EDS failed to run properly - this section will therefore be empty.

6.4 Ligands ⓘ

EDS failed to run properly - this section will therefore be empty.

6.5 Other polymers ⓘ

EDS failed to run properly - this section will therefore be empty.