Full wwPDB X-ray Structure Validation Report (i)

Aug 22, 2022 – 10:03 PM EDT

PDB ID	:	3W36
Title	:	Crystal structure of holo-type bacterial Vanadium-dependent chloroperoxidase
Authors	:	Liscombe, D.K.; Miyanaga, A.; Fielding, E.; Bernhardt, P.; Li, A.; Winter, J.M.; Gilson, M.K.; Noel, J.P.; Moore, B.S.
Deposited on	:	2012-12-11
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:

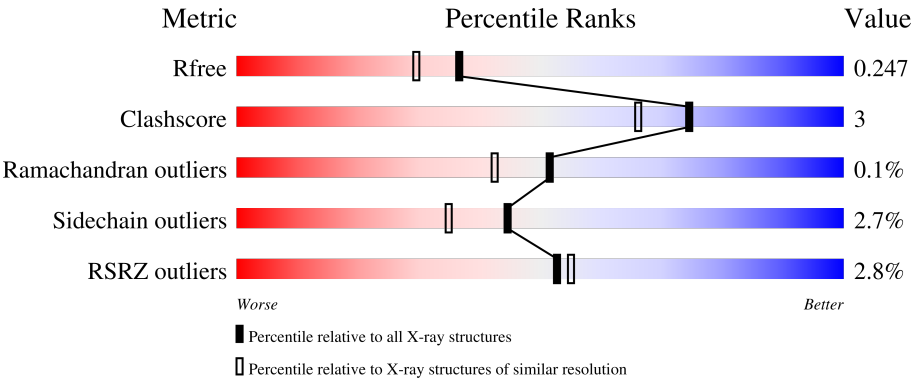
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.29
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.29

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}	130704	11647 (2.00-1.96)
Clashscore	141614	1014 (1.98-1.98)
Ramachandran outliers	138981	1006 (1.98-1.98)
Sidechain outliers	138945	1006 (1.98-1.98)
RSRZ outliers	127900	11410 (2.00-1.96)

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	531	5% 78% 10% • 11%
1	B	531	80% 8% • 11%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 8096 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.

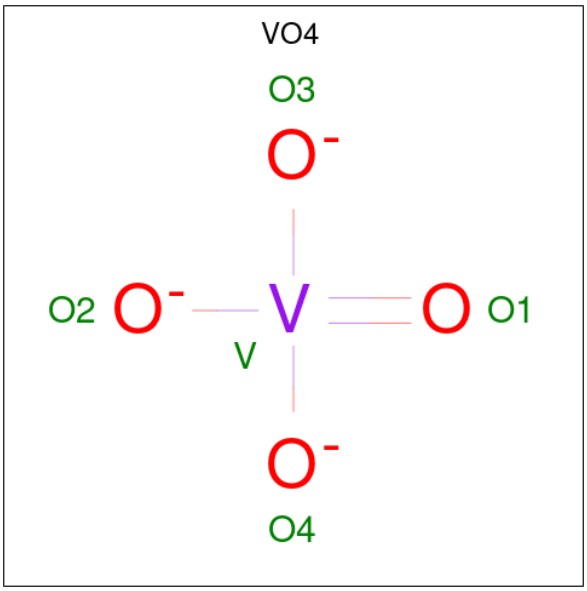
- Molecule 1 is a protein called NapH1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	470	Total	C	N	O	S	0	0	0
			3726	2352	675	689	10			
1	B	471	Total	C	N	O	S	0	0	0
			3733	2355	676	692	10			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	GLY	-	expression tag	UNP A7KH27
A	-2	SER	-	expression tag	UNP A7KH27
A	-1	HIS	-	expression tag	UNP A7KH27
A	0	GLY	-	expression tag	UNP A7KH27
B	-3	GLY	-	expression tag	UNP A7KH27
B	-2	SER	-	expression tag	UNP A7KH27
B	-1	HIS	-	expression tag	UNP A7KH27
B	0	GLY	-	expression tag	UNP A7KH27

- Molecule 2 is VANADATE ION (three-letter code: VO4) (formula: O_4V).



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

- Molecule 3 is water.

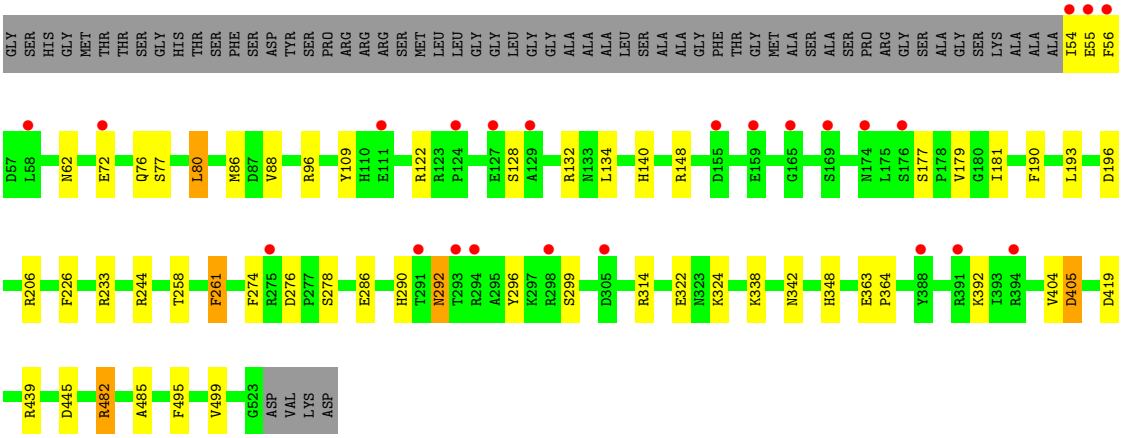
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	234	Total O 234 234	0	0
3	B	393	Total O 393 393	0	0

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.

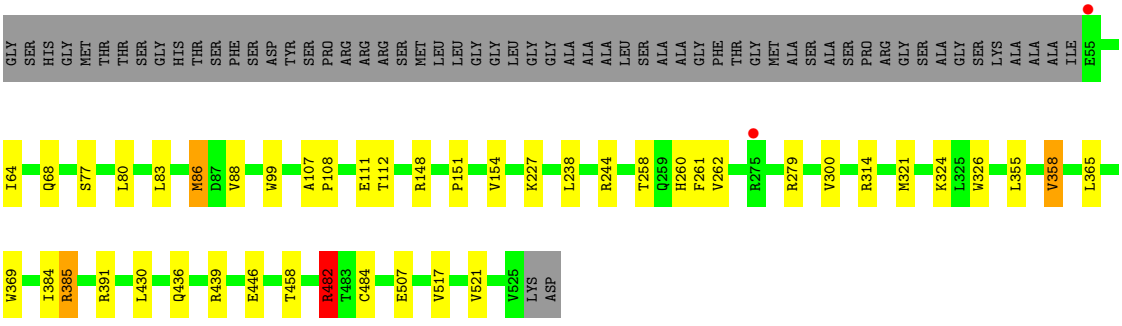
• Molecule 1: NapH1

Chain A:



• Molecule 1: NapH1

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	57.53Å 135.09Å 159.37Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	38.41 – 1.97 38.38 – 1.76	Depositor EDS
% Data completeness (in resolution range)	98.8 (38.41-1.97) 90.5 (38.38-1.76)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.46 (at 1.76Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.205 , 0.243 0.211 , 0.247	Depositor DCC
R_{free} test set	5582 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å^2)	25.4	Xtriage
Anisotropy	0.722	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 46.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	8096	wwPDB-VP
Average B, all atoms (Å^2)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.66% 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

Bond lengths and bond angles in the following residue types are not validated in this section: VO4

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	0.92	1/3835 (0.0%)	0.93	13/5231 (0.2%)
1	B	1.00	5/3842 (0.1%)	0.96	13/5241 (0.2%)
All	All	0.96	6/7677 (0.1%)	0.94	26/10472 (0.2%)

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	99	TRP	CB-CG	-6.58	1.38	1.50
1	A	322	GLU	CD-OE1	6.27	1.32	1.25
1	B	326	TRP	CZ3-CH2	5.08	1.48	1.40
1	B	458	THR	N-CA	5.08	1.56	1.46
1	B	238	LEU	C-O	-5.08	1.13	1.23
1	B	326	TRP	CD2-CE2	5.07	1.47	1.41

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	385	ARG	NE-CZ-NH2	-10.10	115.25	120.30
1	B	391	ARG	NE-CZ-NH2	-9.11	115.75	120.30
1	A	206	ARG	NE-CZ-NH1	8.40	124.50	120.30
1	B	482	ARG	NE-CZ-NH2	-7.68	116.46	120.30
1	A	445	ASP	CB-CG-OD2	7.24	124.82	118.30
1	B	391	ARG	NE-CZ-NH1	7.15	123.88	120.30
1	B	244	ARG	NE-CZ-NH2	-6.48	117.06	120.30
1	A	206	ARG	NE-CZ-NH2	-6.26	117.17	120.30
1	A	419	ASP	CB-CG-OD1	6.19	123.87	118.30
1	B	314	ARG	NE-CZ-NH1	6.15	123.38	120.30
1	A	405	ASP	CB-CG-OD1	6.00	123.70	118.30
1	B	86	MET	CG-SD-CE	-5.89	90.77	100.20
1	B	482	ARG	NE-CZ-NH1	5.78	123.19	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	148	ARG	NE-CZ-NH2	-5.66	117.47	120.30
1	A	233	ARG	NE-CZ-NH2	-5.47	117.56	120.30
1	A	96	ARG	NE-CZ-NH1	5.41	123.00	120.30
1	A	482	ARG	NE-CZ-NH1	5.40	123.00	120.30
1	B	314	ARG	NE-CZ-NH2	-5.40	117.60	120.30
1	B	358	VAL	CG1-CB-CG2	-5.34	102.36	110.90
1	A	314	ARG	NE-CZ-NH1	5.29	122.95	120.30
1	A	244	ARG	NE-CZ-NH1	5.29	122.94	120.30
1	A	439	ARG	NE-CZ-NH1	5.22	122.91	120.30
1	B	391	ARG	CG-CD-NE	-5.14	101.00	111.80
1	A	482	ARG	NE-CZ-NH2	-5.04	117.78	120.30
1	B	439	ARG	NE-CZ-NH1	5.03	122.81	120.30
1	A	261	PHE	CB-CG-CD1	5.02	124.31	120.80

There are no chirality outliers.

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	3726	0	3568	27	0
1	B	3733	0	3570	21	0
2	A	5	0	0	1	0
2	B	5	0	0	0	0
3	A	234	0	0	5	0
3	B	393	0	0	3	0
All	All	8096	0	7138	47	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 3.

All (47) 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)
2:A:600:VO4:O4	3:A:812:HOH:O	1.70	1.09

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:385:ARG:HD2	3:B:963:HOH:O	1.85	0.76
1:B:385:ARG:CD	3:B:963:HOH:O	2.39	0.69
1:A:140:HIS:CE1	1:A:179:VAL:HG13	2.28	0.68
1:B:88:VAL:CG1	1:B:324:LYS:HG2	2.25	0.65
1:B:482:ARG:O	1:B:482:ARG:HD3	1.95	0.65
1:B:279:ARG:HB3	3:B:1051:HOH:O	1.97	0.65
1:B:88:VAL:HG11	1:B:324:LYS:HG2	1.79	0.63
1:A:258:THR:HG1	1:B:258:THR:HG1	1.48	0.61
1:A:148:ARG:HD3	1:A:190:PHE:CD2	2.40	0.56
1:A:348:HIS:HD2	3:A:844:HOH:O	1.89	0.56
1:A:88:VAL:CG1	1:A:324:LYS:HG2	2.37	0.55
1:A:342:ASN:HA	3:A:923:HOH:O	2.08	0.53
1:A:348:HIS:CD2	3:A:844:HOH:O	2.61	0.52
1:A:148:ARG:HD3	1:A:190:PHE:CG	2.46	0.51
1:B:517:VAL:O	1:B:521:VAL:HG23	2.11	0.50
1:A:54:ILE:HG23	1:A:54:ILE:O	2.11	0.50
1:A:122:ARG:NH1	1:A:122:ARG:HB2	2.28	0.49
1:A:88:VAL:HG12	1:A:324:LYS:HG2	1.96	0.48
1:B:324:LYS:N	1:B:324:LYS:HD2	2.28	0.47
1:B:300:VAL:HG13	1:B:384:ILE:HG12	1.96	0.47
1:B:111:GLU:HG2	1:B:112:THR:HG23	1.96	0.47
1:A:128:SER:HB3	3:A:890:HOH:O	2.13	0.47
1:A:177:SER:O	1:A:181:ILE:HG13	2.16	0.45
1:A:62:ASN:OD1	1:A:62:ASN:C	2.55	0.45
1:A:226:PHE:CZ	1:B:260:HIS:CE1	3.05	0.45
1:B:64:ILE:O	1:B:68:GLN:HG2	2.16	0.45
1:A:109:TYR:HB3	1:A:134:LEU:HD11	1.98	0.45
1:A:276:ASP:OD2	1:A:278:SER:OG	2.36	0.44
1:A:193:LEU:HA	1:A:196:ASP:HB3	2.00	0.44
1:B:482:ARG:HD3	1:B:482:ARG:C	2.32	0.44
1:A:290:HIS:HA	1:A:296:TYR:CD1	2.53	0.44
1:A:485:ALA:HB1	1:A:499:VAL:HB	1.99	0.43
1:B:365:LEU:CD2	1:B:430:LEU:HD21	2.49	0.43
1:B:355:LEU:HA	1:B:358:VAL:HG12	2.00	0.43
1:A:80:LEU:HD12	1:A:80:LEU:HA	1.89	0.43
1:B:151:PRO:O	1:B:154:VAL:HG12	2.19	0.42
1:A:55:GLU:OE2	1:A:55:GLU:HA	2.19	0.42
1:B:262:VAL:O	1:B:262:VAL:HG13	2.18	0.42
1:A:274:PHE:CD1	1:A:274:PHE:C	2.94	0.42
1:A:292:ASN:N	1:A:292:ASN:OD1	2.54	0.41
1:A:299:SER:HB3	1:A:495:PHE:CD1	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:404:VAL:HG23	1:A:405:ASP:N	2.35	0.41
1:A:363:GLU:N	1:A:364:PRO:CD	2.84	0.41
1:B:436:GLN:HB2	1:B:507:GLU:HG3	2.03	0.40
1:B:107:ALA:N	1:B:108:PRO:HD2	2.36	0.40
1:B:321:MET:HG3	1:B:484:CYS:HA	2.04	0.40

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	468/531 (88%)	455 (97%)	12 (3%)	1 (0%)	47 38
1	B	469/531 (88%)	461 (98%)	8 (2%)	0	100 100
All	All	937/1062 (88%)	916 (98%)	20 (2%)	1 (0%)	51 42

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	56	PHE

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.

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	391/430 (91%)	379 (97%)	12 (3%)	40	28
1	B	392/430 (91%)	383 (98%)	9 (2%)	50	44
All	All	783/860 (91%)	762 (97%)	21 (3%)	44	35

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	72	GLU
1	A	76	GLN
1	A	77	SER
1	A	80	LEU
1	A	86	MET
1	A	132	ARG
1	A	261	PHE
1	A	286	GLU
1	A	292	ASN
1	A	338	LYS
1	A	392	LYS
1	A	482	ARG
1	B	77	SER
1	B	80	LEU
1	B	83	LEU
1	B	86	MET
1	B	227	LYS
1	B	261	PHE
1	B	369	TRP
1	B	446	GLU
1	B	482	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	95	ASN

5.3.3 RNA

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 monosaccharides in this entry.

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	$\#\|Z\| > 2$
2	VO4	A	600	1	1,4,4	4.19	1 (100%)	-		
2	VO4	B	600	1	1,4,4	4.23	1 (100%)	-		

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	600	VO4	O1-V	4.23	1.87	1.63
2	A	600	VO4	O1-V	4.19	1.87	1.63

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	600	VO4	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^{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	470/531 (88%)	0.30	24 (5%) 28 30	16, 35, 58, 83	0
1	B	471/531 (88%)	-0.03	2 (0%) 92 93	16, 25, 43, 63	0
All	All	941/1062 (88%)	0.13	26 (2%) 53 55	16, 30, 53, 83	0

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	54	ILE	5.4
1	A	111	GLU	3.8
1	A	294	ARG	3.7
1	A	298	ARG	3.7
1	A	169	SER	3.6
1	A	55	GLU	3.1
1	A	275	ARG	3.0
1	A	124	PRO	2.7
1	A	291	THR	2.7
1	A	176	SER	2.7
1	A	293	THR	2.6
1	B	55	GLU	2.6
1	A	127	GLU	2.5
1	A	56	PHE	2.5
1	A	159	GLU	2.4
1	A	155	ASP	2.3
1	A	394	ARG	2.3
1	A	58	LEU	2.2
1	A	129	ALA	2.2
1	A	388	TYR	2.2
1	A	165	GLY	2.1
1	B	275	ARG	2.1
1	A	391	ARG	2.0
1	A	72	GLU	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	305	ASP	2.0
1	A	174	ASN	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 monosaccharides 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. The B-factors column lists the minimum, median, 95^{th} 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	B-factors(Å^2)	Q<0.9
2	VO4	B	600	5/5	0.98	0.13	17,17,18,18	0
2	VO4	A	600	5/5	0.99	0.11	26,27,27,27	0

6.5 Other polymers (i)

There are no such residues in this entry.