



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 02:56 PM UTC

PDB ID : 3W36 / pdb_00003w36
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 ⓘ 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 ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

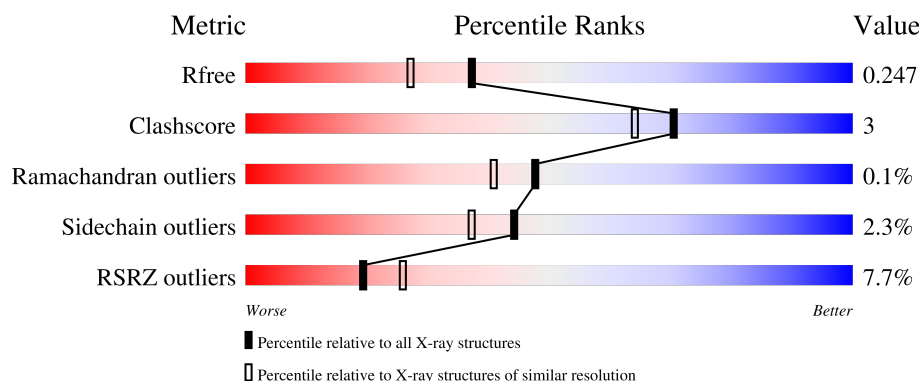
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.97 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}	180053	1506 (1.98-1.98)
Clashscore	190562	1534 (1.98-1.98)
Ramachandran outliers	187476	1518 (1.98-1.98)
Sidechain outliers	187428	1518 (1.98-1.98)
RSRZ outliers	180081	1506 (1.98-1.98)

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 $\leq 5\%$. 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	531	12% 76% 11% • 11%
1	B	531	2% 78% 10% 11%

2 Entry composition

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.

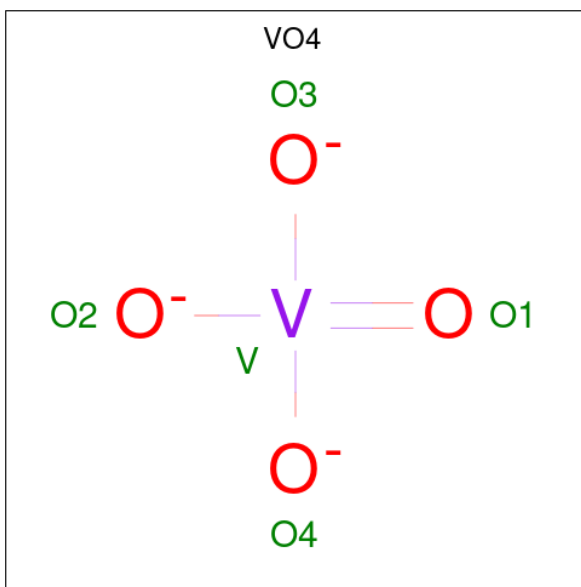
- Molecule 1 is a protein called NapH1.

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 (CCD ID: 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 water.

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

4 Data and refinement statistics

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 38.41 – 1.97	Depositor EDS
% Data completeness (in resolution range)	98.8 (38.41-1.97) 98.8 (38.41-1.97)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ 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 (4.51%)	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)	0.35 , 51.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	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.*

¹Intensities estimated from amplitudes.

²Theoretical 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

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	1.25	6/3835 (0.2%)	1.15	14/5231 (0.3%)
1	B	1.34	13/3842 (0.3%)	1.20	14/5241 (0.3%)
All	All	1.29	19/7677 (0.2%)	1.17	28/10472 (0.3%)

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	238	LEU	C-O	-8.47	1.13	1.24
1	B	458	THR	N-CA	8.39	1.56	1.46
1	B	250	PRO	CA-C	7.33	1.61	1.52
1	A	223	ASN	CA-C	7.13	1.61	1.52
1	B	285	PRO	CA-C	6.85	1.59	1.52
1	B	262	VAL	CA-CB	6.71	1.61	1.54
1	B	423	TYR	CA-C	-6.24	1.47	1.52
1	B	379	ARG	N-CA	5.76	1.53	1.45
1	A	134	LEU	N-CA	5.63	1.53	1.46
1	B	314	ARG	C-O	-5.60	1.17	1.24
1	A	420	HIS	N-CA	-5.50	1.40	1.46
1	B	418	GLY	CA-C	5.50	1.57	1.52
1	A	413	SER	C-O	5.34	1.30	1.23
1	B	427	SER	N-CA	5.20	1.52	1.46
1	A	189	ALA	CA-C	5.10	1.59	1.52
1	B	414	TYR	CA-C	5.10	1.59	1.52
1	B	89	THR	CA-C	-5.07	1.45	1.52
1	A	197	GLY	N-CA	5.01	1.52	1.45
1	B	454	PRO	C-O	5.01	1.29	1.23

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	150	LEU	CA-C-N	-7.71	111.69	119.56
1	B	150	LEU	C-N-CA	-7.71	111.69	119.56
1	A	378	VAL	N-CA-C	7.37	119.08	109.58
1	A	282	ILE	CA-C-N	-7.35	113.11	120.31
1	A	282	ILE	C-N-CA	-7.35	113.11	120.31
1	B	318	ALA	N-CA-C	-7.28	103.34	111.28
1	A	328	ILE	N-CA-C	6.26	116.42	110.53
1	B	367	ALA	N-CA-C	6.16	117.66	111.07
1	B	95	ASN	N-CA-C	6.09	118.70	111.33
1	B	328	ILE	N-CA-C	6.09	116.20	110.30
1	B	259	GLN	N-CA-C	5.90	118.38	110.35
1	B	366	ILE	N-CA-C	-5.86	104.79	110.42
1	B	188	ASN	N-CA-C	5.84	117.64	111.28
1	B	82	ILE	CB-CA-C	-5.53	104.65	110.62
1	B	230	ASN	CA-C-N	5.51	125.60	119.87
1	B	230	ASN	C-N-CA	5.51	125.60	119.87
1	A	366	ILE	N-CA-C	-5.49	105.15	110.42
1	A	286	GLU	N-CA-C	5.45	117.93	111.33
1	A	287	PHE	N-CA-C	5.31	119.24	112.87
1	A	367	ALA	N-CA-C	5.25	117.09	111.36
1	A	77	SER	CA-C-N	5.25	125.95	120.12
1	A	77	SER	C-N-CA	5.25	125.95	120.12
1	A	235	GLN	CB-CA-C	-5.20	104.39	110.17
1	B	235	GLN	CA-C-N	-5.14	114.47	119.76
1	B	235	GLN	C-N-CA	-5.14	114.47	119.76
1	A	350	TRP	N-CA-C	-5.12	105.61	111.14
1	A	493	VAL	N-CA-C	5.12	119.40	113.42
1	A	387	VAL	N-CA-C	5.11	115.33	110.53

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-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 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	29	0
1	B	3733	0	3570	22	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	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 3.

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)
2:A:600:VO4:O4	3:A:812:HOH:O	1.70	1.09
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:B:354:MET:HA	1:B:354:MET:HE2	1.81	0.62
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:B:482:ARG:HD3	1:B:482:ARG:C	2.32	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:A:62:ASN:OD1	1:A:62:ASN:C	2.55	0.50
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:274:PHE:C	1:A:274:PHE:CD1	2.94	0.46
1:A:177:SER:O	1:A:181:ILE:HG13	2.16	0.45
1:A:226:PHE:CZ	1:B:260:HIS:CE1	3.05	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:CG	1:A:278:SER:HG	2.25	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: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:A:369:TRP:O	1:A:370:HIS:C	2.61	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: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
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 ⓘ

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	468/531 (88%)	455 (97%)	12 (3%)	1 (0%)	43	35
1	B	469/531 (88%)	461 (98%)	8 (2%)	0	100	100
All	All	937/1062 (88%)	916 (98%)	20 (2%)	1 (0%)	48	41

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	56	PHE

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	391/430 (91%)	379 (97%)	12 (3%)	35	26
1	B	392/430 (91%)	386 (98%)	6 (2%)	57	52
All	All	783/860 (91%)	765 (98%)	18 (2%)	44	37

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	76	GLN
1	A	77	SER
1	A	80	LEU
1	A	83	LEU
1	A	132	ARG
1	A	152	GLN
1	A	286	GLU
1	A	292	ASN
1	A	300	VAL
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	227	LYS
1	B	446	GLU
1	B	482	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	508	GLN
1	B	76	GLN
1	B	95	ASN
1	B	337	ASN

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 oligosaccharides 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	0,4,4	-	-	-		
2	VO4	B	600	1	0,4,4	-	-	-		

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	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, 95th 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%)	1.06	62 (13%) 7 10	16, 35, 58, 83	0
1	B	471/531 (88%)	0.26	10 (2%) 63 72	16, 25, 43, 63	0
All	All	941/1062 (88%)	0.66	72 (7%) 19 26	16, 30, 53, 83	0

All (72) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	54	ILE	7.8
1	A	169	SER	4.4
1	A	163	ALA	4.2
1	B	71	ASP	3.7
1	B	525	VAL	3.6
1	A	298	ARG	3.6
1	A	295	ALA	3.5
1	A	174	ASN	3.5
1	A	70	THR	3.3
1	A	122	ARG	3.2
1	A	523	GLY	3.1
1	A	166	LEU	3.1
1	B	70	THR	3.1
1	A	479	ASP	3.0
1	A	109	TYR	2.9
1	A	291	THR	2.9
1	A	292	ASN	2.9
1	B	279	ARG	2.9
1	A	159	GLU	2.8
1	A	155	ASP	2.8
1	A	160	LEU	2.8
1	A	162	THR	2.8
1	A	293	THR	2.7
1	A	164	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	391	ARG	2.7
1	A	172	THR	2.7
1	A	521	VAL	2.7
1	A	389	GLY	2.6
1	B	155	ASP	2.6
1	A	294	ARG	2.6
1	A	111	GLU	2.6
1	A	168	PRO	2.6
1	A	154	VAL	2.6
1	A	176	SER	2.6
1	A	146	TRP	2.6
1	A	179	VAL	2.6
1	B	125	SER	2.5
1	A	395	ALA	2.5
1	A	275	ARG	2.5
1	A	472	ILE	2.5
1	A	286	GLU	2.5
1	A	175	LEU	2.4
1	A	289	ASP	2.4
1	A	66	TRP	2.4
1	B	479	ASP	2.4
1	A	127	GLU	2.3
1	A	102	ALA	2.3
1	A	59	ASP	2.3
1	A	55	GLU	2.2
1	A	57	ASP	2.2
1	A	511	ASP	2.2
1	A	279	ARG	2.2
1	A	276	ASP	2.2
1	A	124	PRO	2.2
1	A	74	ALA	2.2
1	A	136	ILE	2.2
1	A	464	ILE	2.1
1	A	280	PHE	2.1
1	A	177	SER	2.1
1	A	278	SER	2.1
1	B	76	GLN	2.1
1	A	267	ALA	2.1
1	A	71	ASP	2.1
1	A	405	ASP	2.1
1	A	128	SER	2.0
1	B	154	VAL	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	134	LEU	2.0
1	B	56	PHE	2.0
1	A	119	GLN	2.0
1	A	156	GLN	2.0
1	A	180	GLY	2.0
1	A	123	ARG	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 oligosaccharides 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, 95th 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	0.06	17,17,18,18	0
2	VO4	A	600	5/5	0.99	0.06	26,27,27,27	0

6.5 Other polymers [i](#)

There are no such residues in this entry.