



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 05:53 PM UTC

PDB ID : 1VNC / pdb_00001vnc
Title : CHLOROPEROXIDASE FROM THE FUNGUS CURVULARIA INAEQUALIS
Authors : Messerschmidt, A.; Wever, R.
Deposited on : 1995-09-01
Resolution : 2.10 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)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

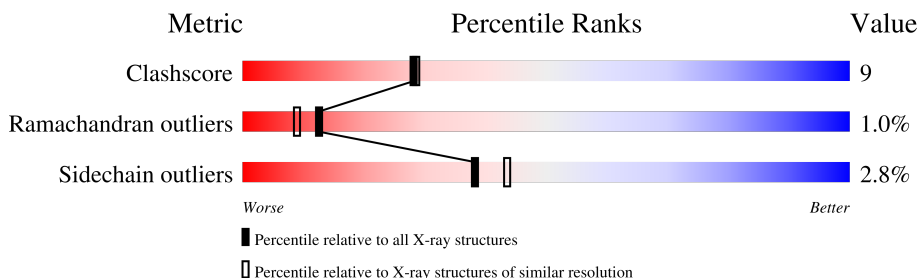
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)

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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	609	

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
2	VO4	A	610	-	-	X	-
3	AZI	A	611	-	X	-	-

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 4920 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.

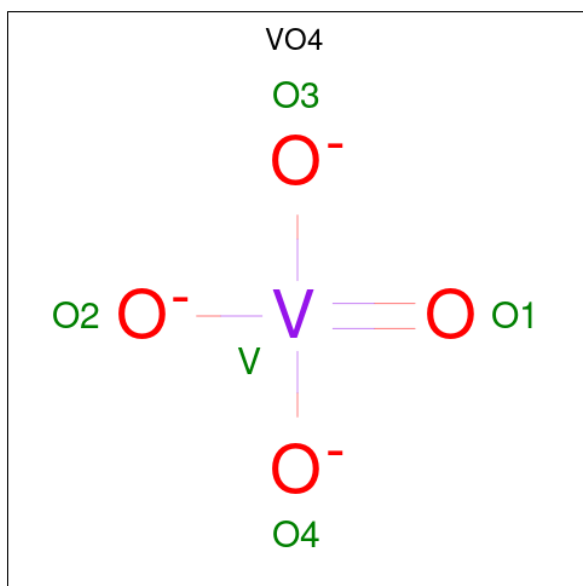
- Molecule 1 is a protein called VANADIUM-CONTAINING CHLOROPEROXIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	576	4484	2854	771	847	12	51	0	0

There is a discrepancy between the modelled and reference sequences:

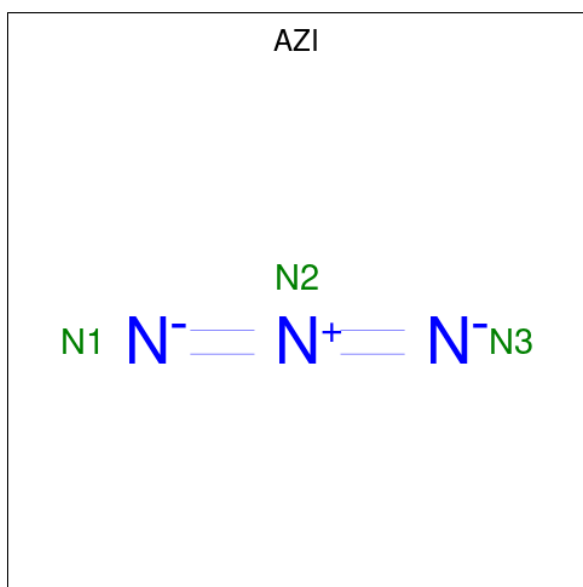
Chain	Residue	Modelled	Actual	Comment	Reference
A	544	GLU	PRO	conflict	UNP P49053

- Molecule 2 is VANADATE ION (CCD ID: VO4) (formula: O₄V).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	V		
2	A	1	4	3	1	0	0

- Molecule 3 is AZIDE ION (CCD ID: AZI) (formula: N₃).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total N 3 3	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	429	Total O 429 429	0	0

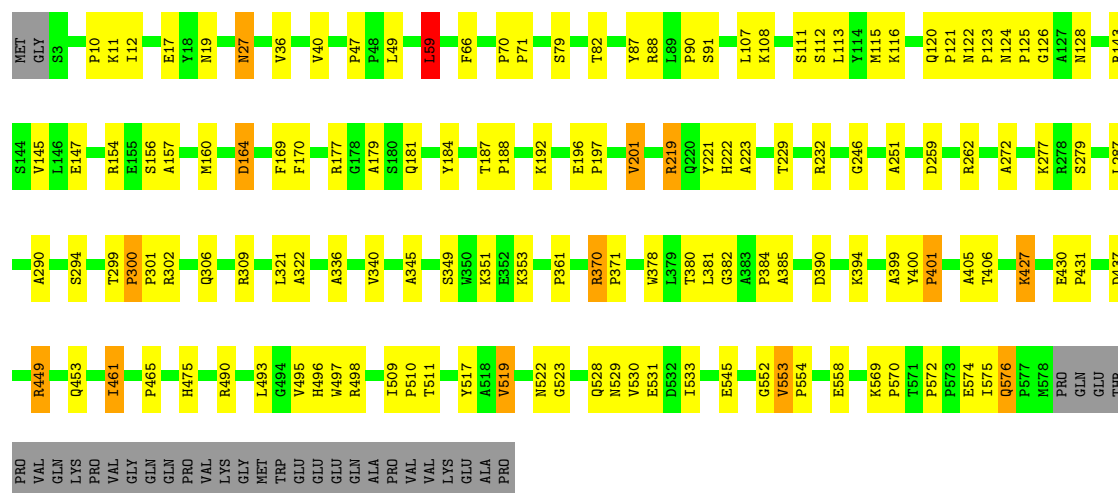
3 Residue-property plots

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. 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. 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: VANADIUM-CONTAINING CHLOROPEROXIDASE

Chain A:  72% 21% 5%



4 Data and refinement statistics

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

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, α , β , γ	131.69Å 131.69Å 112.97Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	8.00 – 2.10	Depositor
% Data completeness (in resolution range)	98.5 (8.00-2.10)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.200 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	4920	wwPDB-VP
Average B, all atoms (Å ²)	23.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

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

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	0.73	3/4617 (0.1%)	1.15	36/6313 (0.6%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	223	ALA	CA-CB	10.06	1.59	1.52
1	A	201	VAL	CA-CB	8.21	1.64	1.55
1	A	553	VAL	CA-CB	5.74	1.57	1.54

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	370	ARG	CA-C-N	8.63	129.16	119.32
1	A	370	ARG	C-N-CA	8.63	129.16	119.32
1	A	47	PRO	N-CA-C	8.42	120.98	110.70
1	A	381	LEU	N-CA-C	-7.75	102.83	111.28
1	A	222	HIS	N-CA-C	7.75	120.31	109.15
1	A	229	THR	N-CA-C	7.65	122.75	113.41
1	A	552	GLY	N-CA-C	7.62	121.71	112.49
1	A	399	ALA	N-CA-C	7.06	120.38	111.69
1	A	322	ALA	N-CA-C	6.75	120.00	111.69
1	A	116	LYS	CA-C-N	6.40	127.84	119.84
1	A	116	LYS	C-N-CA	6.40	127.84	119.84
1	A	121	PRO	N-CA-CB	6.29	109.86	103.25
1	A	123	PRO	N-CA-CB	6.25	109.82	103.25
1	A	384	PRO	N-CA-C	6.25	120.24	110.80
1	A	192	LYS	N-CA-C	6.22	119.38	109.24
1	A	272	ALA	N-CA-C	6.21	120.69	113.18
1	A	91	SER	CA-C-N	6.21	127.60	119.84
1	A	91	SER	C-N-CA	6.21	127.60	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	294	SER	N-CA-C	6.16	118.86	110.55
1	A	59	LEU	N-CA-C	-6.14	104.51	111.14
1	A	427	LYS	N-CA-C	-5.95	101.47	110.28
1	A	197	PRO	N-CA-C	5.86	121.54	113.98
1	A	27	ASN	N-CA-C	-5.85	104.81	111.07
1	A	125	PRO	N-CA-CB	5.81	109.81	103.30
1	A	300	PRO	N-CA-C	5.75	117.72	110.70
1	A	70	PRO	CA-C-N	5.52	125.72	120.31
1	A	70	PRO	C-N-CA	5.52	125.72	120.31
1	A	157	ALA	N-CA-C	-5.41	104.80	111.40
1	A	382	GLY	N-CA-C	5.35	119.60	112.65
1	A	517	TYR	N-CA-C	5.31	118.37	110.14
1	A	510	PRO	N-CA-C	5.28	119.33	111.41
1	A	19	ASN	N-CA-C	5.21	119.35	113.15
1	A	449	ARG	N-CA-C	5.21	116.05	108.14
1	A	279	SER	CA-C-N	5.13	124.74	119.05
1	A	279	SER	C-N-CA	5.13	124.74	119.05
1	A	70	PRO	N-CA-C	5.00	116.80	110.70

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	4484	0	4256	75	0
2	A	4	0	0	2	0
3	A	3	0	0	1	0
4	A	429	0	0	12	0
All	All	4920	0	4256	77	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 9.

All (77) 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:232:ARG:H	1:A:576:GLN:HE22	1.16	0.92
1:A:27:ASN:HD22	1:A:309:ARG:HH11	1.26	0.82
1:A:390:ASP:HB3	4:A:4041:HOH:O	1.83	0.77
1:A:17:GLU:HG2	1:A:321:LEU:HD12	1.67	0.76
1:A:219:ARG:HH11	1:A:219:ARG:HG2	1.51	0.75
1:A:112:SER:HA	1:A:115:MET:HE2	1.69	0.75
1:A:453:GLN:OE1	1:A:465:PRO:HG2	1.88	0.73
1:A:394:LYS:NZ	1:A:495:VAL:HA	2.04	0.72
1:A:351:LYS:HD3	4:A:5009:HOH:O	1.91	0.70
1:A:385:ALA:HB3	4:A:4044:HOH:O	1.93	0.69
1:A:111:SER:O	1:A:115:MET:HB3	1.93	0.68
2:A:610:VO4:O1	2:A:610:VO4:V	1.54	0.63
1:A:394:LYS:HZ2	1:A:495:VAL:HA	1.66	0.60
1:A:576:GLN:HE21	1:A:576:GLN:HA	1.69	0.58
1:A:156:SER:O	1:A:160:MET:HG3	2.05	0.57
1:A:287:LEU:HD23	1:A:493:LEU:HD21	1.86	0.56
1:A:10:PRO:HB3	1:A:461:ILE:HD11	1.87	0.56
1:A:336:ALA:O	1:A:340:VAL:HG23	2.06	0.55
1:A:530:VAL:HA	1:A:533:ILE:HD12	1.88	0.54
1:A:531:GLU:H	1:A:531:GLU:CD	2.17	0.53
1:A:177:ARG:HB2	4:A:4099:HOH:O	2.07	0.53
1:A:90:PRO:HG2	1:A:164:ASP:HB3	1.91	0.53
1:A:349:SER:HB3	1:A:406:THR:HG21	1.91	0.53
1:A:49:LEU:CD1	1:A:179:ALA:HB2	2.39	0.53
1:A:299:THR:HB	1:A:300:PRO:CD	2.39	0.52
1:A:27:ASN:ND2	1:A:309:ARG:HD2	2.23	0.52
1:A:201:VAL:HG13	4:A:4082:HOH:O	2.08	0.52
1:A:219:ARG:HH11	1:A:219:ARG:CG	2.21	0.52
1:A:437:ASP:HA	1:A:475:HIS:HA	1.93	0.50
1:A:511:THR:HB	4:A:2172:HOH:O	2.11	0.49
1:A:59:LEU:HG	1:A:169:PHE:CE1	2.48	0.49
1:A:554:PRO:O	1:A:558:GLU:HG3	2.12	0.49
1:A:82:THR:HG21	1:A:87:TYR:O	2.14	0.48
1:A:519:VAL:CG1	1:A:523:GLY:HA2	2.44	0.48
1:A:519:VAL:HG13	1:A:523:GLY:HA2	1.96	0.48
1:A:107:LEU:HD11	1:A:145:VAL:HG22	1.96	0.48
1:A:143:ARG:O	1:A:147:GLU:HG3	2.14	0.48
1:A:36:VAL:O	1:A:40:VAL:HG22	2.15	0.47
1:A:66:PHE:HB3	1:A:71:PRO:HD3	1.97	0.47
1:A:188:PRO:HB3	4:A:2081:HOH:O	2.14	0.47
1:A:545:GLU:HG2	4:A:2185:HOH:O	2.15	0.47
1:A:17:GLU:CG	1:A:321:LEU:HD12	2.41	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:246:GLY:C	1:A:251:ALA:HA	2.41	0.46
1:A:529:ASN:HB3	1:A:531:GLU:OE1	2.16	0.46
1:A:259:ASP:HB3	1:A:498:ARG:HH22	1.81	0.46
1:A:17:GLU:HB2	4:A:2002:HOH:O	2.16	0.45
2:A:610:VO4:O1	3:A:611:AZI:N1	2.51	0.44
1:A:79:SER:O	1:A:82:THR:HG22	2.17	0.44
1:A:277:LYS:HD2	1:A:522:ASN:O	2.18	0.44
1:A:394:LYS:HE3	1:A:394:LYS:HB3	1.80	0.44
1:A:427:LYS:NZ	4:A:5046:HOH:O	2.50	0.44
1:A:113:LEU:HD23	1:A:170:PHE:HE1	1.83	0.44
1:A:553:VAL:HB	1:A:554:PRO:HD3	1.99	0.44
1:A:572:PRO:HG2	1:A:575:ILE:HG12	2.00	0.44
1:A:361:PRO:HA	1:A:497:TRP:CZ2	2.52	0.43
1:A:378:TRP:CH2	1:A:380:THR:HG22	2.52	0.43
1:A:262:ARG:HG2	4:A:4062:HOH:O	2.17	0.43
1:A:394:LYS:HZ1	1:A:495:VAL:HA	1.78	0.43
1:A:509:ILE:HD13	1:A:528:GLN:HG2	2.00	0.43
1:A:17:GLU:HG2	1:A:321:LEU:CD1	2.44	0.43
1:A:287:LEU:HD23	1:A:493:LEU:CD2	2.49	0.43
1:A:370:ARG:HA	1:A:371:PRO:HD3	1.82	0.43
1:A:11:LYS:HE3	1:A:12:ILE:O	2.19	0.43
1:A:184:TYR:HD2	4:A:2079:HOH:O	2.02	0.43
1:A:302:ARG:O	1:A:306:GLN:HG3	2.19	0.42
1:A:490:ARG:HB3	1:A:496:HIS:HD2	1.84	0.42
1:A:145:VAL:HG21	1:A:154:ARG:NH2	2.34	0.42
1:A:232:ARG:H	1:A:576:GLN:NE2	1.98	0.42
1:A:49:LEU:HD11	1:A:179:ALA:HB2	2.02	0.41
1:A:349:SER:O	1:A:353:LYS:HG3	2.20	0.41
1:A:82:THR:CG2	1:A:88:ARG:HA	2.50	0.41
1:A:430:GLU:HB3	1:A:431:PRO:HD2	2.02	0.41
1:A:400:TYR:HA	1:A:401:PRO:HA	1.90	0.41
1:A:405:ALA:HB1	1:A:553:VAL:HG23	2.03	0.41
1:A:569:LYS:HA	1:A:570:PRO:HD3	1.96	0.41
1:A:345:ALA:HB1	1:A:406:THR:HG22	2.01	0.40
1:A:181:GLN:HG3	1:A:221:TYR:HB2	2.02	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	574/609 (94%)	544 (95%)	24 (4%)	6 (1%)	12 9

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	120	GLN
1	A	124	ASN
1	A	128	ASN
1	A	290	ALA
1	A	122	ASN
1	A	126	GLY

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	466/506 (92%)	453 (97%)	13 (3%)	38 43

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

Mol	Chain	Res	Type
1	A	59	LEU
1	A	108	LYS
1	A	164	ASP
1	A	187	THR
1	A	196	GLU

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Mol	Chain	Res	Type
1	A	219	ARG
1	A	301	PRO
1	A	401	PRO
1	A	449	ARG
1	A	461	ILE
1	A	519	VAL
1	A	574	GLU
1	A	576	GLN

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

Mol	Chain	Res	Type
1	A	27	ASN
1	A	132	ASN
1	A	174	ASN
1	A	305	ASN
1	A	486	ASN
1	A	576	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 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	610	1,3	0,3,4	-	-	-		
3	AZI	A	611	2	2,2,2	3.29	2 (100%)	0,1,1	-	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	611	AZI	N1-N2	-3.29	1.16	1.23
3	A	611	AZI	N3-N2	-3.29	1.16	1.23

There are no bond angle outliers.

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	610	VO4	2	0
3	A	611	AZI	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

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.