



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 1, 2017 – 07:12 AM EDT

PDB ID : 1KPM  
Title : First Structural Evidence of a Specific Inhibition of Phospholipase A2 by Vitamin E and its Implications in Inflammation: Crystal Structure of the Complex Formed between Phospholipase A2 and Vitamin E at 1.8 Å Resolution.  
Authors : Chandra, V.; Jasti, J.; Kaur, P.; Betzel, C.; Srinivasan, A.; Singh, T.P.  
Deposited on : unknown  
Resolution : 1.80 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) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20030345

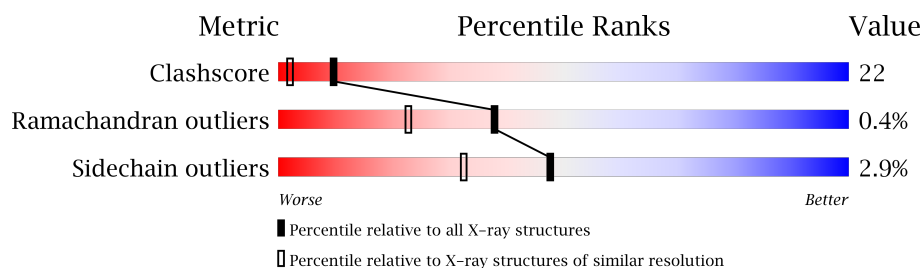
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.80 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	112137	5742 (1.80-1.80)
Ramachandran outliers	110173	5676 (1.80-1.80)
Sidechain outliers	110143	5675 (1.80-1.80)

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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	121	
1	B	121	

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	VIT	A	401	X	-	X	-
3	ACY	A	504	-	-	X	-

## 2 Entry composition [i](#)

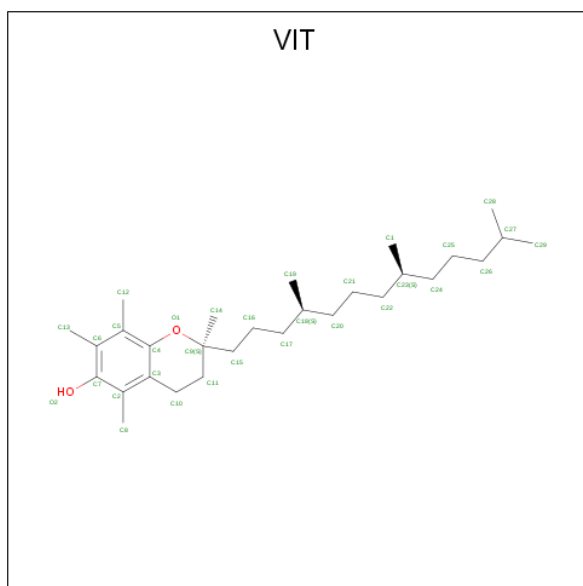
There are 4 unique types of molecules in this entry. The entry contains 2241 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Phospholipase A2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	121	Total	C	N	O	S	0	0	0
			944	591	159	178	16			
1	B	121	Total	C	N	O	S	0	0	0
			944	591	159	178	16			

- Molecule 2 is VITAMIN E (three-letter code: VIT) (formula:  $C_{29}H_{50}O_2$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			31	29	2		

- Molecule 3 is ACETIC ACID (three-letter code: ACY) (formula:  $C_2H_4O_2$ ).



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

- Molecule 4 is water.

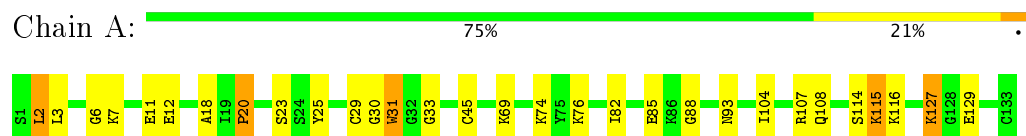
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	143	Total	O	0	0
			143	143		
4	B	163	Total	O	0	0
			163	163		

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

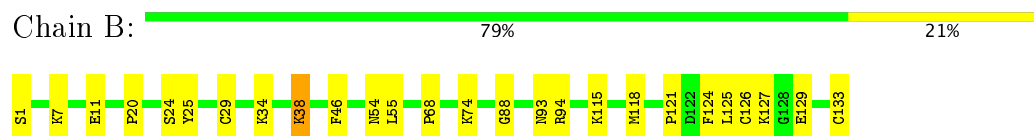
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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.

Note EDS was not executed.

- Molecule 1: Phospholipase A2



- Molecule 1: Phospholipase A2



## 4 Data and refinement statistics

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

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	75.79 Å 88.51 Å 78.04 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 1.80	Depositor
% Data completeness (in resolution range)	95.8 (20.00-1.80)	Depositor
$R_{merge}$	0.04	Depositor
$R_{sym}$	0.04	Depositor
Refinement program	CNS 0.9	Depositor
R, $R_{free}$	0.197 , 0.228	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2241	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	29.0	wwPDB-VP

## 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: ACY, VIT

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	0.75	5/964 (0.5%)	1.08	5/1292 (0.4%)
1	B	0.31	0/964	0.57	0/1292
All	All	0.58	5/1928 (0.3%)	0.86	5/2584 (0.2%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	31	TRP	CA-CB	-15.00	1.21	1.53
1	A	127	LYS	CD-CE	-9.77	1.26	1.51
1	A	30	GLY	C-N	-7.58	1.16	1.34
1	A	127	LYS	CG-CD	-6.73	1.29	1.52
1	A	31	TRP	C-N	6.37	1.44	1.33

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	31	TRP	CA-CB-CG	21.64	154.82	113.70
1	A	127	LYS	CG-CD-CE	16.36	160.96	111.90
1	A	31	TRP	CB-CA-C	11.27	132.94	110.40
1	A	31	TRP	N-CA-CB	-10.16	92.31	110.60
1	A	127	LYS	CB-CG-CD	-8.84	88.61	111.60

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	944	0	906	40	0
1	B	944	0	907	23	0
2	A	31	0	50	40	0
3	A	4	0	3	2	0
3	B	12	0	9	0	0
4	A	143	0	0	9	0
4	B	163	0	0	2	0
All	All	2241	0	1875	82	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 22.

All (82) 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:401:VIT:C18	2:A:401:VIT:C17	1.80	1.56
2:A:401:VIT:C9	2:A:401:VIT:C15	1.83	1.55
2:A:401:VIT:C16	2:A:401:VIT:C17	1.89	1.49
2:A:401:VIT:C16	2:A:401:VIT:C15	2.02	1.38
2:A:401:VIT:C11	2:A:401:VIT:C15	2.20	1.20
1:A:7:LYS:HA	2:A:401:VIT:HC13	1.32	1.10
2:A:401:VIT:H151	2:A:401:VIT:C11	1.78	1.10
2:A:401:VIT:H151	2:A:401:VIT:H111	1.09	1.08
2:A:401:VIT:C15	2:A:401:VIT:H111	1.88	0.98
1:A:2:LEU:O	2:A:401:VIT:H171	1.67	0.93
2:A:401:VIT:C20	2:A:401:VIT:C17	2.46	0.93
1:A:7:LYS:CA	2:A:401:VIT:HC13	2.03	0.87
2:A:401:VIT:H143	4:A:517:HOH:O	1.78	0.83
2:A:401:VIT:H201	2:A:401:VIT:H171	1.60	0.83
2:A:401:VIT:C14	4:A:517:HOH:O	2.26	0.82
2:A:401:VIT:H191	1:B:54:ASN:HD21	1.43	0.82
2:A:401:VIT:H201	2:A:401:VIT:C17	2.10	0.81
1:A:88:GLY:H	1:A:93:ASN:HD21	1.28	0.81
1:B:88:GLY:H	1:B:93:ASN:HD21	1.26	0.80
1:A:7:LYS:HA	2:A:401:VIT:C1	2.12	0.80
1:B:74:LYS:HE2	4:B:519:HOH:O	1.83	0.79
3:A:504:ACY:H1	4:A:537:HOH:O	1.82	0.78
1:B:55:LEU:HD22	1:B:94:ARG:HD3	1.66	0.78
1:A:6:GLY:HA3	2:A:401:VIT:H212	1.67	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:23:SER:HB3	2:A:401:VIT:H141	1.67	0.74
2:A:401:VIT:H152	2:A:401:VIT:C9	2.14	0.74
2:A:401:VIT:O1	2:A:401:VIT:C15	2.38	0.70
1:B:88:GLY:H	1:B:93:ASN:ND2	1.90	0.69
1:A:2:LEU:HD11	2:A:401:VIT:H123	1.77	0.67
1:A:115:LYS:N	1:A:115:LYS:HD3	2.10	0.66
1:A:115:LYS:H	1:A:115:LYS:HD3	1.61	0.66
1:A:129:GLU:H	1:A:129:GLU:CD	2.01	0.63
1:A:7:LYS:O	1:A:11:GLU:HG3	1.99	0.63
1:B:55:LEU:CD2	1:B:94:ARG:HD3	2.30	0.61
1:A:114:SER:OG	1:A:116:LYS:HG2	2.01	0.60
1:B:115:LYS:HG2	1:B:118:MET:HE2	1.82	0.60
1:A:23:SER:CB	2:A:401:VIT:H141	2.32	0.58
2:A:401:VIT:H152	2:A:401:VIT:O1	2.04	0.57
2:A:401:VIT:C19	1:B:54:ASN:HD21	2.15	0.57
2:A:401:VIT:H142	4:A:517:HOH:O	1.98	0.56
2:A:401:VIT:H191	1:B:54:ASN:ND2	2.18	0.56
1:B:38:LYS:HA	1:B:38:LYS:HE3	1.89	0.55
1:A:7:LYS:HD2	2:A:401:VIT:H261	1.89	0.55
1:A:6:GLY:CA	2:A:401:VIT:H212	2.36	0.54
1:A:69:LYS:HE3	2:A:401:VIT:H121	1.89	0.54
1:B:7:LYS:O	1:B:11:GLU:HG3	2.08	0.53
1:B:129:GLU:O	1:B:129:GLU:HG3	2.09	0.53
1:B:24:SER:O	1:B:118:MET:HA	2.10	0.52
1:B:1:SER:HA	1:B:68:PRO:O	2.10	0.51
1:A:104:ILE:O	1:A:108:GLN:HG3	2.11	0.50
1:A:7:LYS:CB	2:A:401:VIT:HC13	2.42	0.50
1:B:121:PRO:HG2	1:B:125:LEU:CD1	2.41	0.50
1:A:115:LYS:H	1:A:115:LYS:HZ2	1.59	0.49
2:A:401:VIT:H122	4:A:508:HOH:O	2.12	0.48
1:B:34:LYS:O	1:B:126:CYS:HB3	2.13	0.48
1:B:124:PHE:HA	1:B:127:LYS:NZ	2.29	0.48
1:A:115:LYS:H	1:A:115:LYS:CD	2.26	0.48
1:A:88:GLY:H	1:A:93:ASN:ND2	2.05	0.47
2:A:401:VIT:H202	1:B:133:CYS:O	2.14	0.47
1:A:76:LYS:HE3	1:A:85:GLU:HG2	1.97	0.47
1:A:31:TRP:HZ2	1:B:46:PHE:HD2	1.63	0.46
1:B:121:PRO:HG2	1:B:125:LEU:HG	1.96	0.46
3:A:504:ACY:CH3	4:A:537:HOH:O	2.54	0.45
1:B:25:TYR:HB3	1:B:29:CYS:HB2	2.00	0.44
1:A:20:PRO:HB3	4:B:576:HOH:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:45:CYS:SG	2:A:401:VIT:C8	3.06	0.44
1:A:76:LYS:HD3	1:A:85:GLU:OE2	2.17	0.44
1:A:3:LEU:O	2:A:401:VIT:H221	2.18	0.44
1:B:88:GLY:N	1:B:93:ASN:HD21	2.04	0.43
1:A:115:LYS:NZ	4:A:599:HOH:O	2.51	0.43
1:A:74:LYS:HD3	4:A:622:HOH:O	2.17	0.43
1:A:31:TRP:HZ2	1:B:46:PHE:CD2	2.36	0.43
1:A:25:TYR:O	1:A:29:CYS:HB2	2.19	0.42
1:A:7:LYS:HB2	2:A:401:VIT:H241	2.01	0.42
1:A:18:ALA:HB3	2:A:401:VIT:H193	2.01	0.42
2:A:401:VIT:HC11	2:A:401:VIT:H252	1.63	0.42
1:A:25:TYR:HB3	1:A:29:CYS:HB2	2.01	0.41
1:A:82:ILE:HG13	4:A:530:HOH:O	2.20	0.41
1:A:12:GLU:O	1:A:107:ARG:HD3	2.20	0.41
1:A:107:ARG:HH21	1:A:107:ARG:HG2	1.86	0.41
1:A:115:LYS:N	1:A:115:LYS:CD	2.83	0.40
1:A:6:GLY:HA3	2:A:401:VIT:C20	2.51	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	119/121 (98%)	115 (97%)	3 (2%)	1 (1%)	22	8
1	B	119/121 (98%)	118 (99%)	1 (1%)	0	100	100
All	All	238/242 (98%)	233 (98%)	4 (2%)	1 (0%)	38	23

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	33	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	104/104 (100%)	100 (96%)	4 (4%)	38	21
1	B	104/104 (100%)	102 (98%)	2 (2%)	62	50
All	All	208/208 (100%)	202 (97%)	6 (3%)	48	32

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	LEU
1	A	20	PRO
1	A	115	LYS
1	A	127	LYS
1	B	20	PRO
1	B	38	LYS

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

Mol	Chain	Res	Type
1	A	93	ASN
1	B	54	ASN
1	B	93	ASN
1	B	108	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules 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

5 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	VIT	A	401	-	32,32,32	4.92	16 (50%)	40,45,45	4.50	20 (50%)
3	ACY	A	504	-	1,3,3	2.02	1 (100%)	0,3,3	0.00	-
3	ACY	B	501	-	1,3,3	2.13	1 (100%)	0,3,3	0.00	-
3	ACY	B	502	-	1,3,3	2.04	1 (100%)	0,3,3	0.00	-
3	ACY	B	503	-	1,3,3	2.13	1 (100%)	0,3,3	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
2	VIT	A	401	-	2/2/4/4	0/19/30/30	0/2/2/2
3	ACY	A	504	-	-	0/0/0/0	0/0/0/0
3	ACY	B	501	-	-	0/0/0/0	0/0/0/0
3	ACY	B	502	-	-	0/0/0/0	0/0/0/0
3	ACY	B	503	-	-	0/0/0/0	0/0/0/0

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	401	VIT	C13-C6	-4.21	1.43	1.51
2	A	401	VIT	C21-C22	-2.97	1.39	1.52
2	A	401	VIT	C21-C20	-2.51	1.41	1.52
3	A	504	ACY	CH3-C	2.02	1.51	1.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	401	VIT	C3-C2	2.04	1.44	1.40
3	B	502	ACY	CH3-C	2.04	1.51	1.48
3	B	501	ACY	CH3-C	2.13	1.51	1.48
3	B	503	ACY	CH3-C	2.13	1.51	1.48
2	A	401	VIT	O2-C7	2.39	1.42	1.37
2	A	401	VIT	C6-C5	2.47	1.45	1.40
2	A	401	VIT	C4-C5	2.58	1.44	1.39
2	A	401	VIT	C11-C10	2.77	1.59	1.52
2	A	401	VIT	C11-C9	3.20	1.62	1.53
2	A	401	VIT	O1-C9	3.30	1.51	1.46
2	A	401	VIT	O1-C4	3.42	1.43	1.37
2	A	401	VIT	C10-C3	4.33	1.58	1.51
2	A	401	VIT	C17-C18	5.06	1.80	1.52
2	A	401	VIT	C16-C17	8.31	1.89	1.52
2	A	401	VIT	C15-C16	13.31	2.02	1.52
2	A	401	VIT	C15-C9	19.22	1.83	1.53

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	401	VIT	C13-C6-C5	-5.87	109.23	119.87
2	A	401	VIT	C14-C9-C11	-4.49	101.91	112.11
2	A	401	VIT	O1-C4-C3	-4.21	118.12	122.43
2	A	401	VIT	C20-C18-C17	-3.95	93.13	112.10
2	A	401	VIT	C1-C23-C24	-3.59	98.27	111.36
2	A	401	VIT	C10-C3-C4	-3.11	116.66	120.31
2	A	401	VIT	C12-C5-C4	-2.68	117.23	121.30
2	A	401	VIT	O2-C7-C6	2.77	125.67	118.14
2	A	401	VIT	C1-C23-C22	3.00	122.30	111.36
2	A	401	VIT	C11-C10-C3	3.88	118.16	111.75
2	A	401	VIT	C21-C22-C23	4.17	129.43	115.73
2	A	401	VIT	C9-O1-C4	4.27	125.02	118.10
2	A	401	VIT	C22-C21-C20	4.57	135.33	113.25
2	A	401	VIT	O1-C4-C5	5.54	121.37	115.29
2	A	401	VIT	C19-C18-C17	5.60	131.78	111.36
2	A	401	VIT	C13-C6-C7	6.06	131.00	120.54
2	A	401	VIT	C21-C20-C18	6.14	135.88	115.73
2	A	401	VIT	C16-C15-C9	10.19	164.25	114.56
2	A	401	VIT	C15-C16-C17	10.78	135.80	112.80
2	A	401	VIT	O1-C9-C14	14.80	140.68	105.16

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	401	VIT	C23
2	A	401	VIT	C18

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 42 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	401	VIT	40	0
3	A	504	ACY	2	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	30:GLY	C	31:TRP	N	1.16

## 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.