Full wwPDB X-ray Structure Validation Report (i)

Jun 12, 2024 – 09:23 PM EDT

PDB ID	:	3VRM
Title	:	Structure of cytochrome P450 Vdh mutant T107A with bound vitamin D3
Authors	:	Nishioka, T.; Yasutake, Y.; Tamura, T.
Deposited on	:	2012-04-12
Resolution	:	2.57 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:

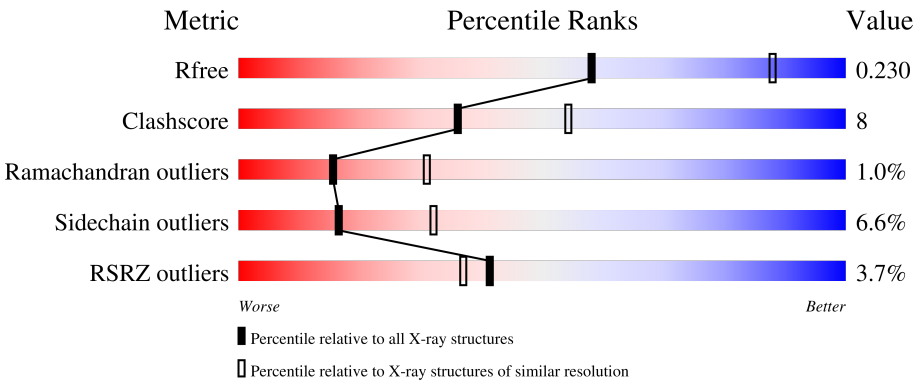
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.36.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

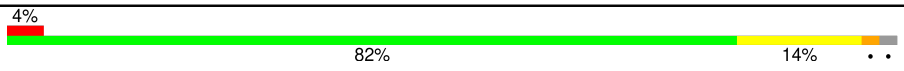
The reported resolution of this entry is 2.57 Å.

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	3676 (2.60-2.56)
Clashscore	141614	4049 (2.60-2.56)
Ramachandran outliers	138981	3979 (2.60-2.56)
Sidechain outliers	138945	3979 (2.60-2.56)
RSRZ outliers	127900	3614 (2.60-2.56)

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	411	

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 3240 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.

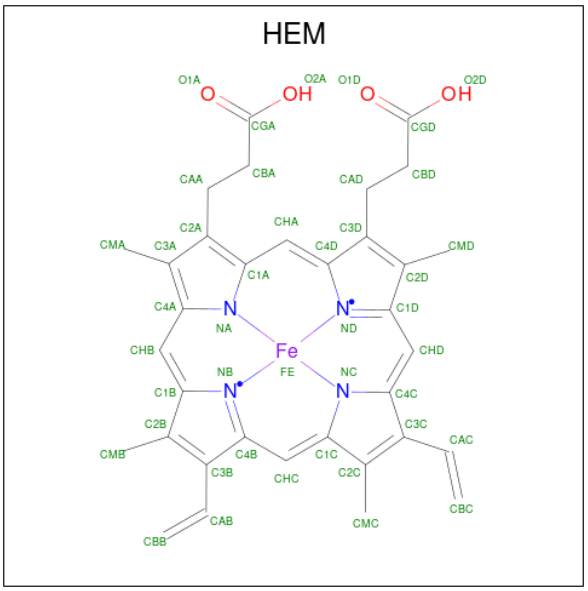
- Molecule 1 is a protein called Vitamin D(3) 25-hydroxylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	402	3105	1953	543	593	16	0	0	0

There are 9 discrepancies between the modelled and reference sequences:

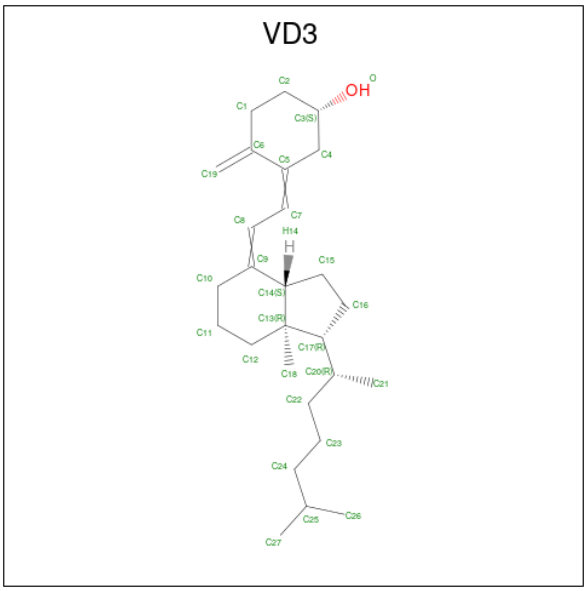
Chain	Residue	Modelled	Actual	Comment	Reference
A	107	ALA	THR	engineered mutation	UNP C4B644
A	404	LEU	-	expression tag	UNP C4B644
A	405	GLU	-	expression tag	UNP C4B644
A	406	HIS	-	expression tag	UNP C4B644
A	407	HIS	-	expression tag	UNP C4B644
A	408	HIS	-	expression tag	UNP C4B644
A	409	HIS	-	expression tag	UNP C4B644
A	410	HIS	-	expression tag	UNP C4B644
A	411	HIS	-	expression tag	UNP C4B644

- Molecule 2 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Fe	N	O		
2	A	1	43	34	1	4	4	0	0

- Molecule 3 is (1S,3Z)-3-[(2E)-2-[(1R,3AR,7AS)-7A-METHYL-1-[(2R)-6-METHYLHEPTA N-2-YL]-2,3,3A,5,6,7-HEXAHYDRO-1H-INDEN-4-YLIDENE]ETHYLI DENE]-4-METHY LIDENE-CYCLOHEXAN-1-OL (three-letter code: VD3) (formula: $C_{27}H_{44}O$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
3	A	1	56	54	2	0	1

- Molecule 4 is water.

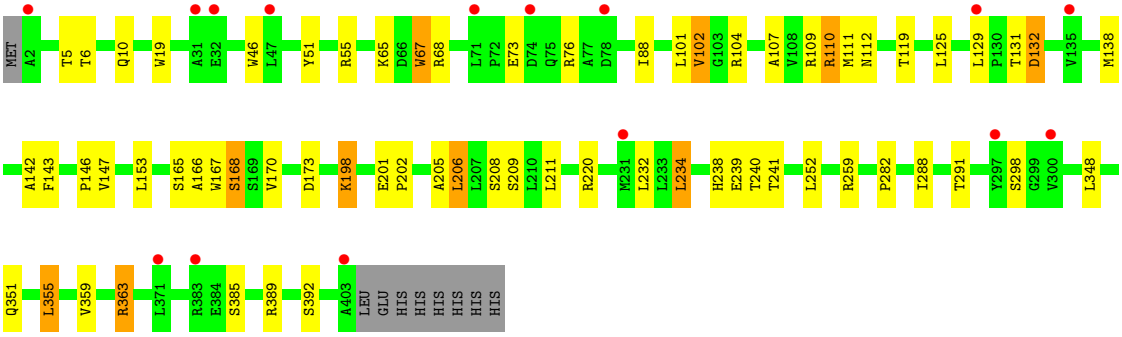
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	36	36	36	0	0

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: Vitamin D(3) 25-hydroxylase

Chain A:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	61.42Å 105.52Å 141.99Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.57 42.51 – 2.57	Depositor EDS
% Data completeness (in resolution range)	98.6 (50.00-2.57) 98.7 (42.51-2.57)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.85 (at 2.58Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.187 , 0.231 0.186 , 0.230	Depositor DCC
R_{free} test set	741 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å^2)	62.3	Xtriage
Anisotropy	0.642	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 42.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.022 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l 0.038 for 1/2*h+1/2*k,3/2*h-1/2*k,-l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	3240	wwPDB-VP
Average B, all atoms (Å^2)	76.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.79% 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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: HEM, VD3

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	0.52	4/3171 (0.1%)	0.64	0/4317

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	167	TRP	CD2-CE2	5.24	1.47	1.41
1	A	46	TRP	CD2-CE2	5.12	1.47	1.41
1	A	67	TRP	CD2-CE2	5.02	1.47	1.41
1	A	19	TRP	CD2-CE2	5.01	1.47	1.41

There are no bond angle outliers.

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	3105	0	3075	37	0
2	A	43	0	30	6	0
3	A	56	0	88	13	0
4	A	36	0	0	1	0
All	All	3240	0	3193	51	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 8.

All (51) 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)
3:A:502[A]:VD3:H192	3:A:502[A]:VD3:C8	1.49	1.23
3:A:502[A]:VD3:H192	3:A:502[A]:VD3:H8	1.30	1.11
1:A:288:ILE:HD12	1:A:288:ILE:H	1.28	0.99
3:A:502[A]:VD3:C8	3:A:502[A]:VD3:C19	2.27	0.98
1:A:143:PHE:O	1:A:147:VAL:HG23	1.78	0.84
3:A:502[A]:VD3:H8	3:A:502[A]:VD3:C19	2.02	0.82
3:A:502[A]:VD3:H212	3:A:502[A]:VD3:H121	1.67	0.77
1:A:282:PRO:HG2	2:A:501:HEM:HMB2	1.68	0.74
3:A:502[B]:VD3:H101	3:A:502[B]:VD3:C6	2.18	0.74
1:A:288:ILE:H	1:A:288:ILE:CD1	2.00	0.74
3:A:502[A]:VD3:H192	3:A:502[A]:VD3:C9	2.17	0.70
3:A:502[B]:VD3:H101	3:A:502[B]:VD3:C5	2.24	0.67
1:A:288:ILE:HD12	1:A:288:ILE:N	2.08	0.65
2:A:501:HEM:HHD	2:A:501:HEM:HBC2	1.77	0.65
1:A:68:ARG:HB3	1:A:76:ARG:HG2	1.80	0.63
1:A:359:VAL:O	1:A:363:ARG:HB2	2.03	0.58
1:A:101:LEU:HD21	1:A:220:ARG:HG2	1.90	0.54
1:A:102:VAL:CG1	1:A:348:LEU:HD21	2.39	0.52
1:A:252:LEU:HD22	1:A:259:ARG:HA	1.92	0.52
3:A:502[B]:VD3:C6	3:A:502[B]:VD3:O	2.58	0.51
1:A:102:VAL:HG13	1:A:348:LEU:HD21	1.93	0.50
1:A:110:ARG:HE	1:A:110:ARG:HB3	1.40	0.49
1:A:119:THR:HG23	1:A:363:ARG:HE	1.79	0.48
3:A:502[B]:VD3:H192	3:A:502[B]:VD3:C8	2.44	0.48
3:A:502[B]:VD3:C8	3:A:502[B]:VD3:C19	2.92	0.48
1:A:132:ASP:OD1	1:A:132:ASP:N	2.46	0.47
1:A:240:THR:HB	2:A:501:HEM:C3B	2.50	0.47
1:A:125:LEU:O	1:A:129:LEU:HG	2.15	0.46
1:A:198:LYS:HB3	1:A:211:LEU:HD22	1.97	0.46
1:A:107:ALA:HB3	1:A:110:ARG:HG3	1.97	0.46
1:A:168:SER:OG	1:A:238:HIS:HE1	1.98	0.45
1:A:173:ASP:HA	1:A:385:SER:HB2	1.98	0.45
1:A:234:LEU:HD23	1:A:234:LEU:HA	1.81	0.44
1:A:147:VAL:HG13	1:A:238:HIS:HD2	1.82	0.44
1:A:143:PHE:HZ	1:A:165:SER:CB	2.31	0.44
1:A:112:ASN:HA	1:A:355:LEU:HD21	1.99	0.43
1:A:351:GLN:HE21	1:A:351:GLN:HA	1.83	0.43
3:A:502[B]:VD3:H183	3:A:502[B]:VD3:H20	1.86	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:502[A]:VD3:H212	3:A:502[A]:VD3:C12	2.43	0.43
1:A:111:MET:HA	1:A:111:MET:CE	2.49	0.42
1:A:153:LEU:O	1:A:205:ALA:HB1	2.19	0.41
1:A:232:LEU:HD21	2:A:501:HEM:HMD2	2.02	0.41
1:A:146:PRO:HB3	1:A:241:THR:HB	2.01	0.41
1:A:88:ILE:HG13	2:A:501:HEM:HAD2	2.02	0.41
1:A:138:MET:HA	1:A:142:ALA:HB3	2.02	0.41
1:A:201:GLU:HA	1:A:202:PRO:HD3	1.81	0.41
1:A:282:PRO:HG2	2:A:501:HEM:CMB	2.44	0.41
1:A:206:LEU:HD23	1:A:206:LEU:HA	1.83	0.41
1:A:198:LYS:NZ	4:A:617:HOH:O	2.54	0.40
1:A:65:LYS:HD2	1:A:88:ILE:O	2.21	0.40
1:A:166:ALA:O	1:A:170:VAL:HG23	2.20	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	400/411 (97%)	367 (92%)	29 (7%)	4 (1%)	15 31

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	239	GLU
1	A	73	GLU
1	A	298	SER
1	A	51	TYR

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.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	333/342 (97%)	311 (93%)	22 (7%)	16 32

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	THR
1	A	6	THR
1	A	10	GLN
1	A	55	ARG
1	A	67	TRP
1	A	102	VAL
1	A	104	ARG
1	A	109	ARG
1	A	110	ARG
1	A	131	THR
1	A	132	ASP
1	A	168	SER
1	A	198	LYS
1	A	206	LEU
1	A	208	SER
1	A	209	SER
1	A	234	LEU
1	A	291	THR
1	A	355	LEU
1	A	363	ARG
1	A	389	ARG
1	A	392	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	238	HIS
1	A	285	GLN
1	A	351	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

3 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	$\#\|Z\| > 2$
3	VD3	A	502[B]	-	30,30,30	0.79	1 (3%)	43,43,43	2.06	11 (25%)
2	HEM	A	501	1	42,50,50	2.49	16 (38%)	46,82,82	3.27	22 (47%)
3	VD3	A	502[A]	-	30,30,30	0.83	1 (3%)	43,43,43	2.58	14 (32%)

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
3	VD3	A	502[B]	-	-	10/15/56/56	0/3/3/3
2	HEM	A	501	1	-	3/12/54/54	-
3	VD3	A	502[A]	-	-	4/15/56/56	0/3/3/3

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	HEM	C4A-NA	5.42	1.47	1.36
2	A	501	HEM	C3C-C2C	4.98	1.47	1.40
2	A	501	HEM	C1A-NA	4.98	1.46	1.36
2	A	501	HEM	C3C-C4C	4.96	1.48	1.41
2	A	501	HEM	C3B-C2B	4.57	1.46	1.37
2	A	501	HEM	CHA-C4D	4.16	1.44	1.34
2	A	501	HEM	C3D-C2D	3.80	1.45	1.36
2	A	501	HEM	CHB-C1B	3.73	1.43	1.34
2	A	501	HEM	C2A-C3A	3.60	1.48	1.37
2	A	501	HEM	C2C-C1C	3.13	1.49	1.42
3	A	502[A]	VD3	C13-C14	-2.88	1.51	1.56
3	A	502[B]	VD3	C13-C14	-2.61	1.51	1.56
2	A	501	HEM	C1B-NB	-2.60	1.35	1.40
2	A	501	HEM	FE-ND	2.56	2.12	1.98
2	A	501	HEM	C4D-ND	-2.56	1.35	1.40
2	A	501	HEM	FE-NB	2.45	2.11	1.98
2	A	501	HEM	CHD-C1D	2.37	1.47	1.40
2	A	501	HEM	C1D-C2D	2.29	1.49	1.44

All (47) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	501	HEM	C3B-C4B-NB	9.41	116.22	109.47
2	A	501	HEM	C3D-C4D-ND	7.65	118.56	110.17
3	A	502[A]	VD3	C4-C5-C6	7.47	122.36	113.86
2	A	501	HEM	C3B-C2B-C1B	-7.40	100.85	106.41
3	A	502[A]	VD3	C7-C5-C6	-6.96	118.00	125.15
2	A	501	HEM	C2B-C1B-NB	6.53	117.35	109.84
3	A	502[A]	VD3	C8-C7-C5	-6.40	116.55	126.54
2	A	501	HEM	C2D-C1D-ND	6.14	117.00	109.90
3	A	502[B]	VD3	C10-C9-C8	-5.46	119.38	125.27
3	A	502[B]	VD3	C11-C12-C13	-4.91	107.43	113.19
3	A	502[B]	VD3	C7-C8-C9	-4.86	118.95	126.13
3	A	502[B]	VD3	C3-C4-C5	-4.58	105.82	112.51
2	A	501	HEM	C4D-ND-C1D	-4.53	99.84	105.21
3	A	502[A]	VD3	C7-C8-C9	-4.46	119.54	126.13
3	A	502[A]	VD3	C11-C12-C13	-4.18	108.28	113.19
2	A	501	HEM	C1D-C2D-C3D	-4.17	102.60	106.98
3	A	502[A]	VD3	C1-C6-C5	4.10	120.36	114.51
2	A	501	HEM	C4A-C3A-C2A	-3.99	104.22	107.00
3	A	502[A]	VD3	C10-C9-C8	-3.95	121.00	125.27
2	A	501	HEM	CHA-C4D-C3D	-3.90	118.03	125.23
3	A	502[B]	VD3	C13-C17-C20	-3.76	113.69	119.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	501	HEM	CBD-CAD-C3D	-3.70	102.30	112.53
2	A	501	HEM	CMD-C2D-C1D	3.58	130.63	125.03
2	A	501	HEM	C4D-C3D-C2D	-3.52	101.76	106.89
2	A	501	HEM	C4B-C3B-C2B	-3.48	104.08	107.28
2	A	501	HEM	CHD-C1D-C2D	-3.35	119.74	125.03
2	A	501	HEM	C1B-NB-C4B	-3.15	101.48	105.21
3	A	502[A]	VD3	C15-C14-C9	-3.14	117.04	120.68
3	A	502[B]	VD3	C4-C5-C6	3.09	117.37	113.86
2	A	501	HEM	CMB-C2B-C1B	2.96	129.65	125.03
3	A	502[A]	VD3	C19-C6-C5	-2.87	119.86	123.05
3	A	502[A]	VD3	C14-C9-C8	-2.86	119.04	123.56
3	A	502[A]	VD3	C10-C9-C14	2.80	119.90	113.33
2	A	501	HEM	CHC-C4B-C3B	-2.74	120.38	124.57
2	A	501	HEM	CHB-C1B-NB	-2.63	121.11	124.37
2	A	501	HEM	CAD-C3D-C4D	2.60	129.22	124.70
3	A	502[B]	VD3	C1-C6-C5	2.56	118.16	114.51
3	A	502[B]	VD3	C10-C9-C14	2.44	119.04	113.33
2	A	501	HEM	O2A-CGA-CBA	2.43	121.66	114.00
3	A	502[A]	VD3	C13-C17-C20	-2.38	115.83	119.50
2	A	501	HEM	CMA-C3A-C2A	2.31	129.30	124.94
3	A	502[A]	VD3	C16-C15-C14	-2.31	101.49	105.25
3	A	502[B]	VD3	C16-C15-C14	-2.22	101.63	105.25
3	A	502[A]	VD3	C21-C20-C17	-2.04	109.82	112.88
2	A	501	HEM	O1A-CGA-CBA	-2.04	116.64	123.09
3	A	502[B]	VD3	C18-C13-C17	-2.03	107.99	111.68
3	A	502[B]	VD3	C21-C20-C17	-2.03	109.84	112.88

There are no chirality outliers.

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	502[A]	VD3	C5-C7-C8-C9
3	A	502[B]	VD3	C5-C7-C8-C9
3	A	502[B]	VD3	C21-C20-C22-C23
3	A	502[B]	VD3	C13-C17-C20-C22
3	A	502[B]	VD3	C13-C17-C20-C21
3	A	502[A]	VD3	C21-C20-C22-C23
3	A	502[A]	VD3	C17-C20-C22-C23
3	A	502[B]	VD3	C17-C20-C22-C23
3	A	502[A]	VD3	C20-C22-C23-C24
3	A	502[B]	VD3	C22-C23-C24-C25
3	A	502[B]	VD3	C23-C24-C25-C27

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Mol	Chain	Res	Type	Atoms
3	A	502[B]	VD3	C16-C17-C20-C21
3	A	502[B]	VD3	C23-C24-C25-C26
3	A	502[B]	VD3	C16-C17-C20-C22
2	A	501	HEM	CAA-CBA-CGA-O2A
2	A	501	HEM	CAA-CBA-CGA-O1A
2	A	501	HEM	C2B-C3B-CAB-CBB

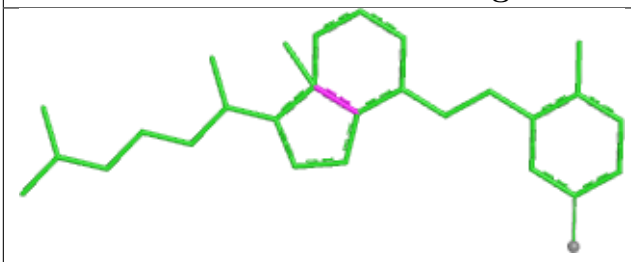
There are no ring outliers.

3 monomers are involved in 19 short contacts:

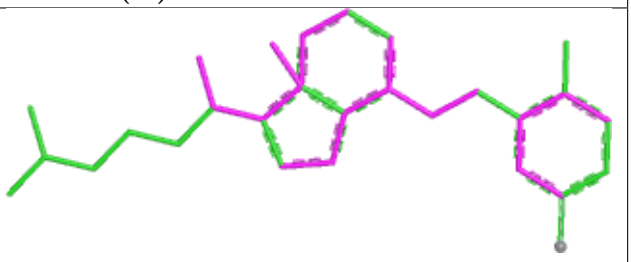
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	502[B]	VD3	6	0
2	A	501	HEM	6	0
3	A	502[A]	VD3	7	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

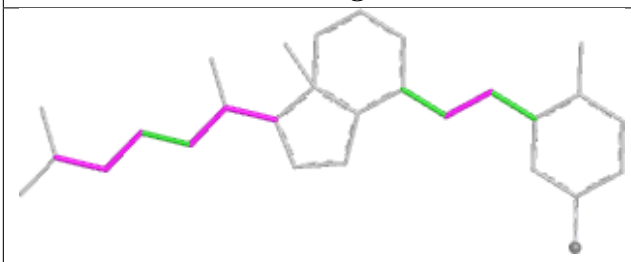
Ligand VD3 A 502 (B)



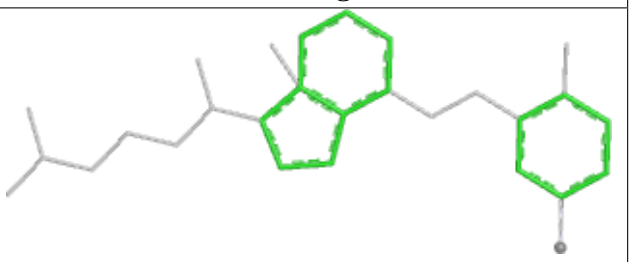
Bond lengths



Bond angles

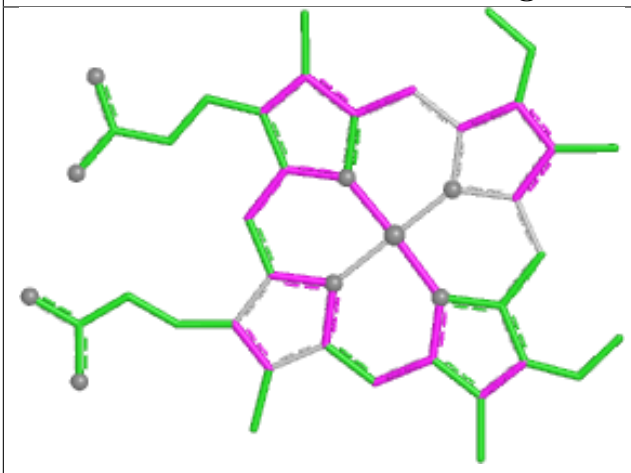


Torsions

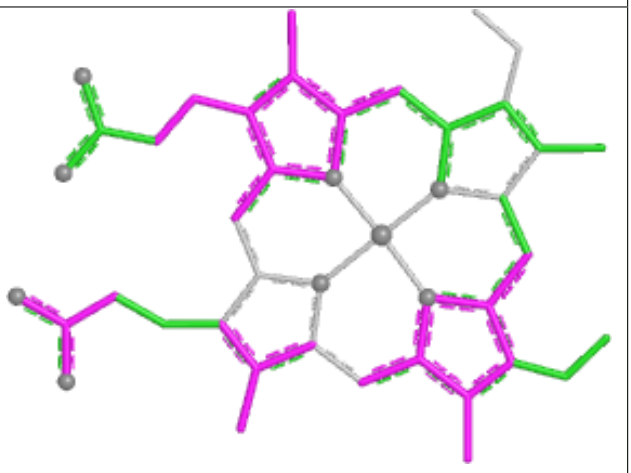


Rings

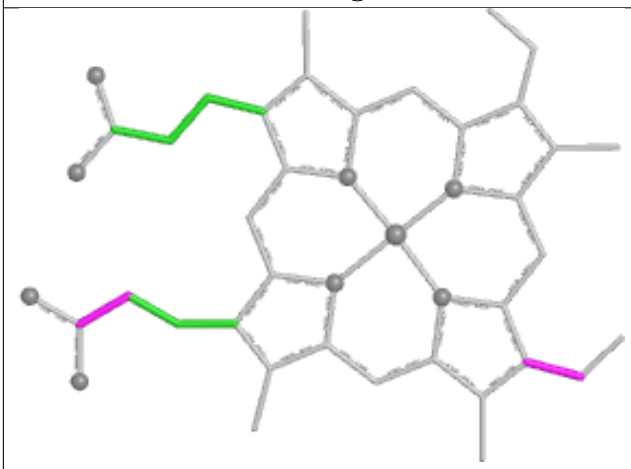
Ligand HEM A 501



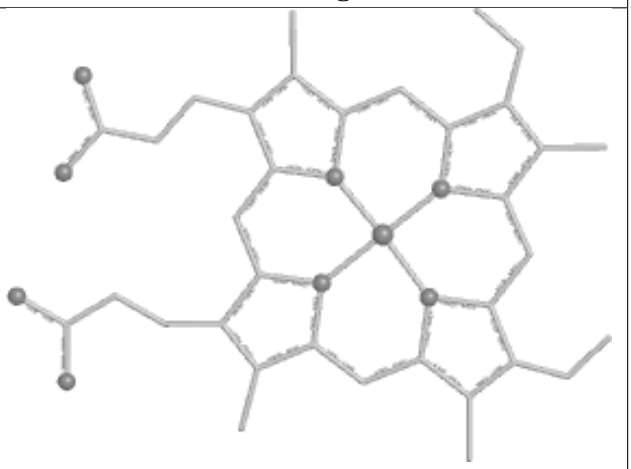
Bond lengths



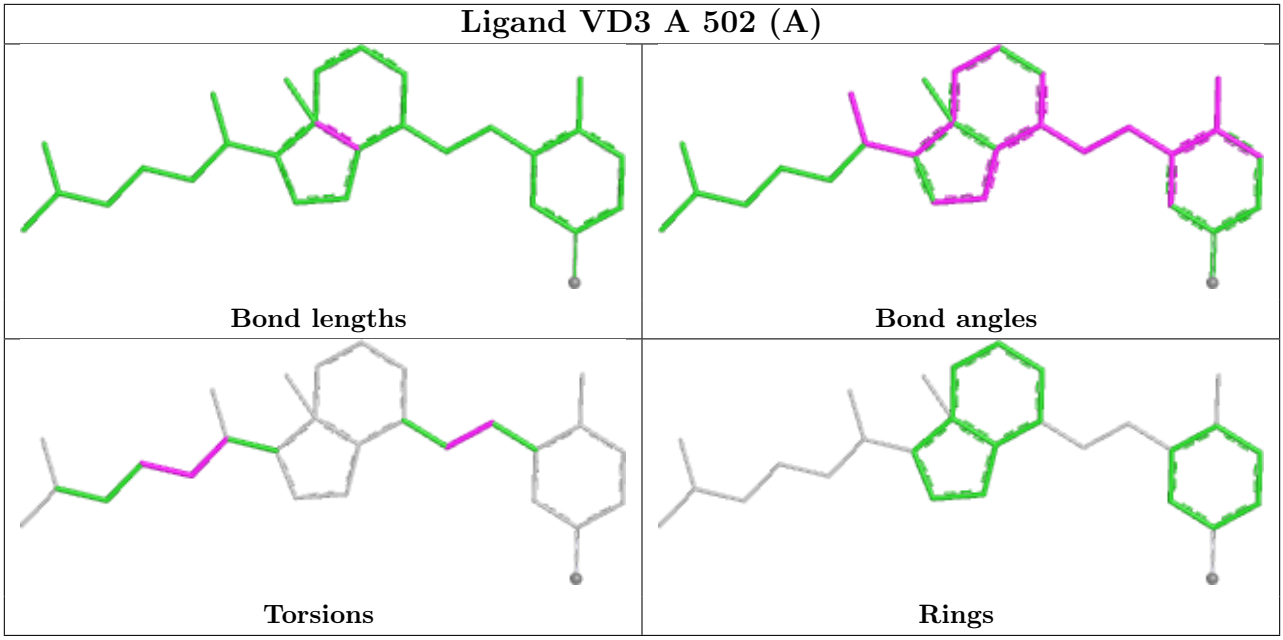
Bond angles



Torsions



Rings



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 (i)

6.1 Protein, DNA and RNA chains (i)

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	402/411 (97%)	0.26	15 (3%) 41 37	42, 75, 115, 141	2 (0%)

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	78	ASP	4.3
1	A	403	ALA	4.2
1	A	31	ALA	2.9
1	A	47	LEU	2.8
1	A	129	LEU	2.8
1	A	300	VAL	2.8
1	A	135	VAL	2.7
1	A	231	MET	2.5
1	A	2	ALA	2.5
1	A	32	GLU	2.4
1	A	297	TYR	2.3
1	A	383	ARG	2.2
1	A	71	LEU	2.1
1	A	74	ASP	2.0
1	A	371	LEU	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)

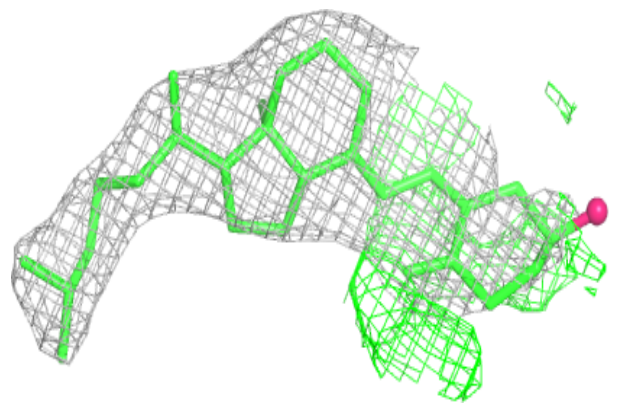
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

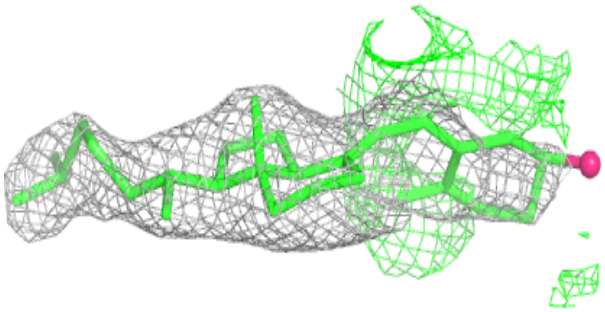
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	VD3	A	502[A]	28/28	0.90	0.26	59,65,68,69	28
3	VD3	A	502[B]	28/28	0.90	0.26	60,67,70,71	28
2	HEM	A	501	43/43	0.99	0.20	33,41,49,55	0

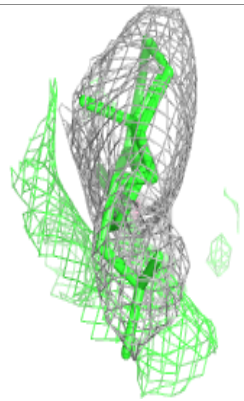
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around VD3 A 502 (A):

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

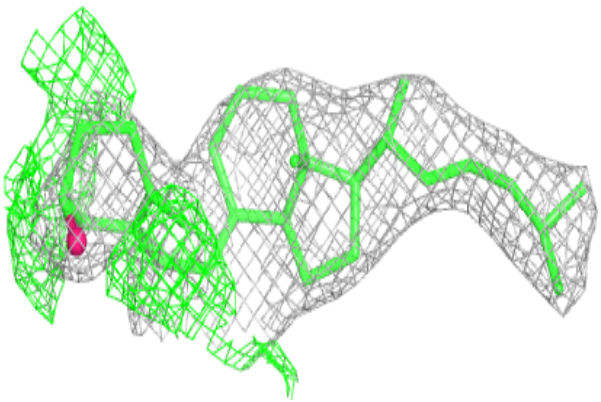


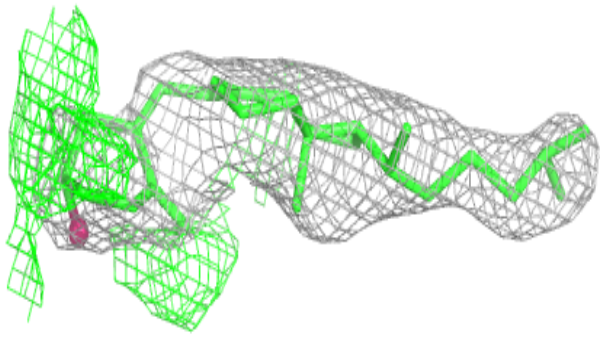


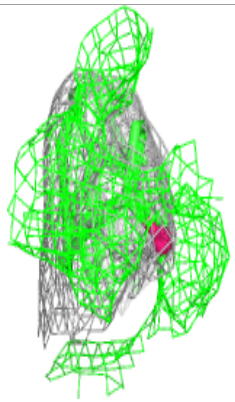


Electron density around VD3 A 502 (B):

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

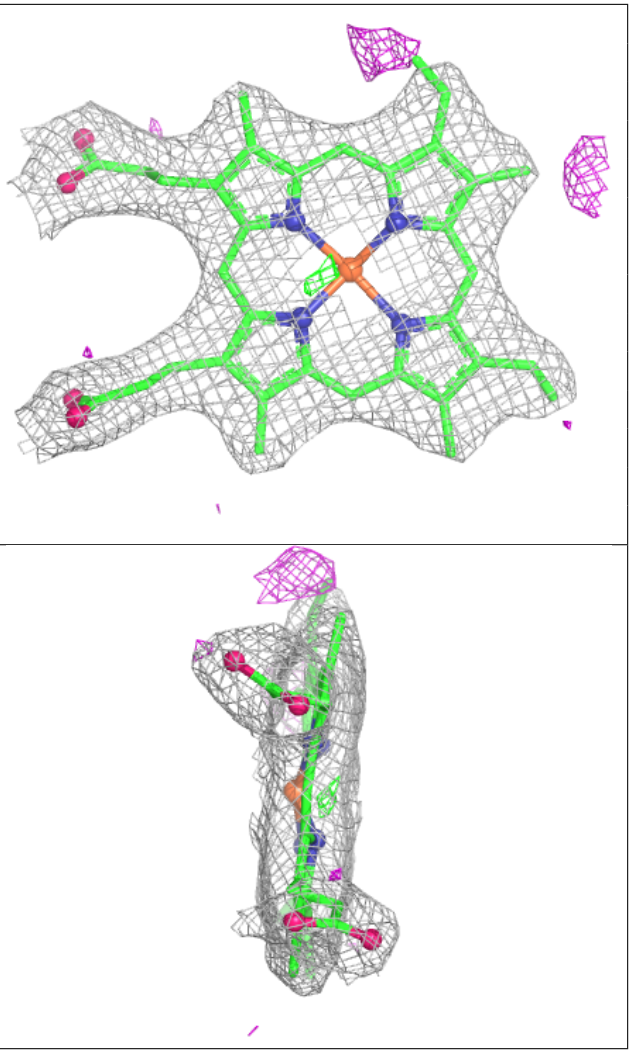






Electron density around HEM A 501:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers (i)

There are no such residues in this entry.