



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 5, 2026 – 08:01 AM EDT

PDB ID : 3A50 / pdb_00003a50
Title : Structure of cytochrome P450 Vdh mutant (Vdh-K1) obtained by directed evolution with bound vitamin D3
Authors : Yasutake, Y.; Fujii, Y.; Cheon, W.K.; Arisawa, A.; Tamura, T.
Deposited on : 2009-07-24
Resolution : 2.05 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

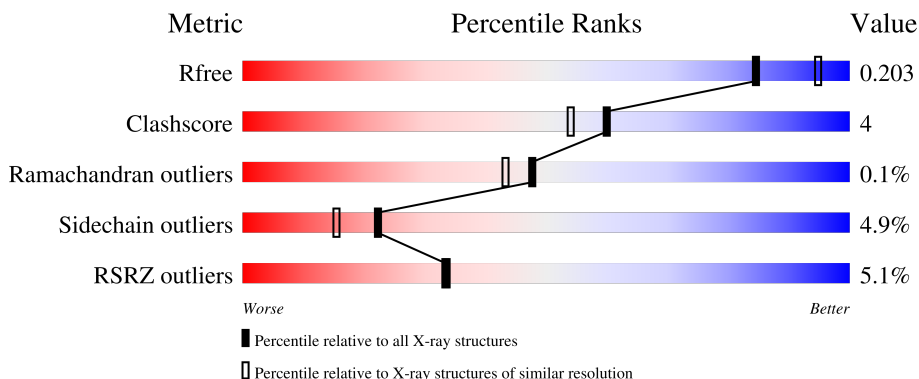
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.05 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	2260 (2.04-2.04)
Clashscore	190562	2333 (2.04-2.04)
Ramachandran outliers	187476	2318 (2.04-2.04)
Sidechain outliers	187428	2318 (2.04-2.04)
RSRZ outliers	180081	2260 (2.04-2.04)

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	411	2% 91% 5% ..
1	B	411	8% 87% 10% ..
1	C	411	9% 84% 12% ..
1	D	411	3% 85% 12% ..
1	E	411	4% 88% 8% ..

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 16977 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 hydroxylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	402	Total	C	N	O	S	0	0	0
			3113	1958	549	589	17			
1	B	402	Total	C	N	O	S	0	0	0
			3113	1958	549	589	17			
1	C	401	Total	C	N	O	S	0	0	0
			3108	1955	548	588	17			
1	D	401	Total	C	N	O	S	0	0	0
			3108	1955	548	588	17			
1	E	401	Total	C	N	O	S	0	0	0
			3108	1955	548	588	17			

There are 60 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	70	ARG	THR	engineered mutation	UNP C4B644
A	156	LEU	VAL	engineered mutation	UNP C4B644
A	216	MET	GLU	engineered mutation	UNP C4B644
A	384	ARG	GLU	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
B	70	ARG	THR	engineered mutation	UNP C4B644
B	156	LEU	VAL	engineered mutation	UNP C4B644
B	216	MET	GLU	engineered mutation	UNP C4B644
B	384	ARG	GLU	engineered mutation	UNP C4B644
B	404	LEU	-	expression tag	UNP C4B644
B	405	GLU	-	expression tag	UNP C4B644
B	406	HIS	-	expression tag	UNP C4B644

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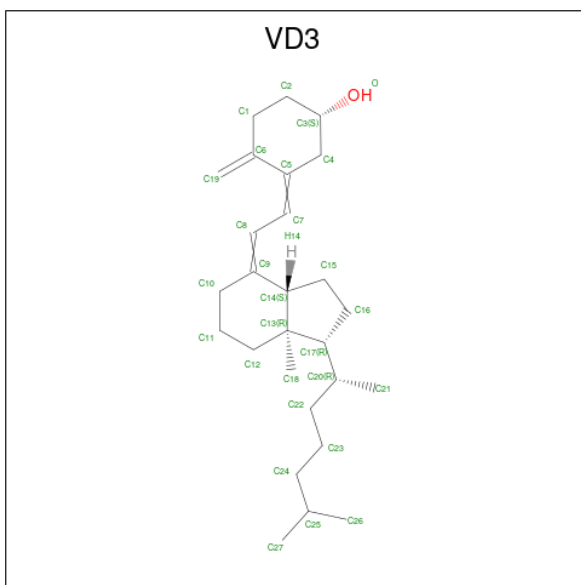
Chain	Residue	Modelled	Actual	Comment	Reference
B	407	HIS	-	expression tag	UNP C4B644
B	408	HIS	-	expression tag	UNP C4B644
B	409	HIS	-	expression tag	UNP C4B644
B	410	HIS	-	expression tag	UNP C4B644
B	411	HIS	-	expression tag	UNP C4B644
C	70	ARG	THR	engineered mutation	UNP C4B644
C	156	LEU	VAL	engineered mutation	UNP C4B644
C	216	MET	GLU	engineered mutation	UNP C4B644
C	384	ARG	GLU	engineered mutation	UNP C4B644
C	404	LEU	-	expression tag	UNP C4B644
C	405	GLU	-	expression tag	UNP C4B644
C	406	HIS	-	expression tag	UNP C4B644
C	407	HIS	-	expression tag	UNP C4B644
C	408	HIS	-	expression tag	UNP C4B644
C	409	HIS	-	expression tag	UNP C4B644
C	410	HIS	-	expression tag	UNP C4B644
C	411	HIS	-	expression tag	UNP C4B644
D	70	ARG	THR	engineered mutation	UNP C4B644
D	156	LEU	VAL	engineered mutation	UNP C4B644
D	216	MET	GLU	engineered mutation	UNP C4B644
D	384	ARG	GLU	engineered mutation	UNP C4B644
D	404	LEU	-	expression tag	UNP C4B644
D	405	GLU	-	expression tag	UNP C4B644
D	406	HIS	-	expression tag	UNP C4B644
D	407	HIS	-	expression tag	UNP C4B644
D	408	HIS	-	expression tag	UNP C4B644
D	409	HIS	-	expression tag	UNP C4B644
D	410	HIS	-	expression tag	UNP C4B644
D	411	HIS	-	expression tag	UNP C4B644
E	70	ARG	THR	engineered mutation	UNP C4B644
E	156	LEU	VAL	engineered mutation	UNP C4B644
E	216	MET	GLU	engineered mutation	UNP C4B644
E	384	ARG	GLU	engineered mutation	UNP C4B644
E	404	LEU	-	expression tag	UNP C4B644
E	405	GLU	-	expression tag	UNP C4B644
E	406	HIS	-	expression tag	UNP C4B644
E	407	HIS	-	expression tag	UNP C4B644
E	408	HIS	-	expression tag	UNP C4B644
E	409	HIS	-	expression tag	UNP C4B644
E	410	HIS	-	expression tag	UNP C4B644
E	411	HIS	-	expression tag	UNP C4B644

- Molecule 2 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula:

HEM

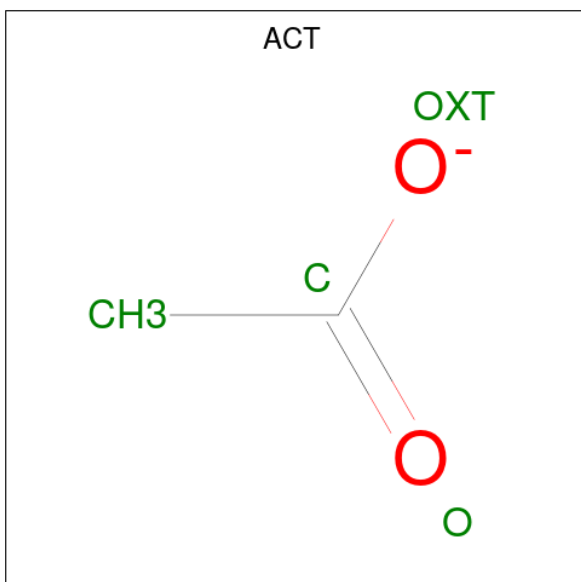
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	B	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	C	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	D	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	E	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

- 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]ETHYLIDENE]-4-METHY LIDENE-CYCLOHEXAN-1-OL (CCD ID: VD3) (formula: C₂₇H₄₄O).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			28	27	1		
3	B	1	Total	C	O	0	0
			28	27	1		
3	C	1	Total	C	O	0	0
			28	27	1		
3	D	1	Total	C	O	0	0
			28	27	1		
3	E	1	Total	C	O	0	0
			28	27	1		

- Molecule 4 is ACETATE ION (CCD ID: ACT) (formula: $C_2H_3O_2$).

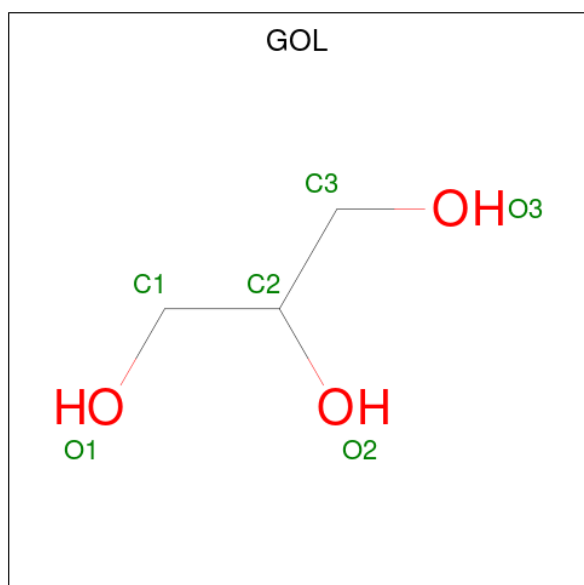


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 4 2 2	0	0
4	C	1	Total C O 4 2 2	0	0
4	C	1	Total C O 4 2 2	0	0
4	D	1	Total C O 4 2 2	0	0
4	E	1	Total C O 4 2 2	0	0
4	E	1	Total C O 4 2 2	0	0

- Molecule 5 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	3	Total Ca 3 3	0	0
5	C	1	Total Ca 1 1	0	0
5	D	1	Total Ca 1 1	0	0
5	E	1	Total Ca 1 1	0	0

- Molecule 6 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			6	3	3		
6	A	1	Total	C	O	0	0
			6	3	3		

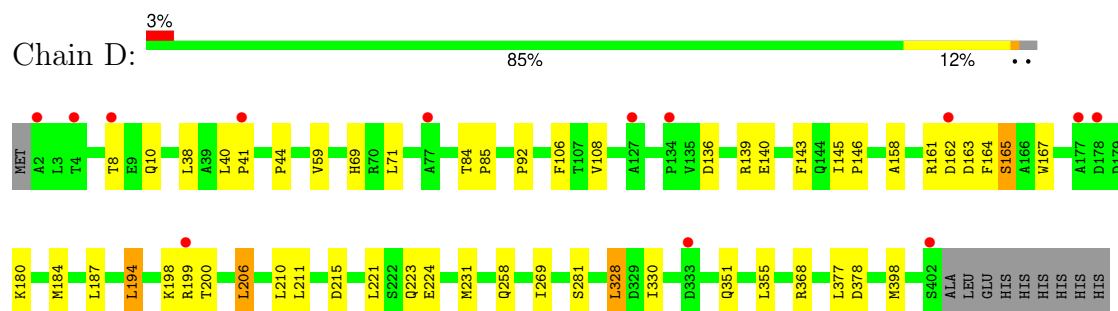
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	303	Total	O	0	0
			303	303		
7	B	174	Total	O	0	0
			174	174		
7	C	150	Total	O	0	0
			150	150		
7	D	198	Total	O	0	0
			198	198		
7	E	205	Total	O	0	0
			205	205		

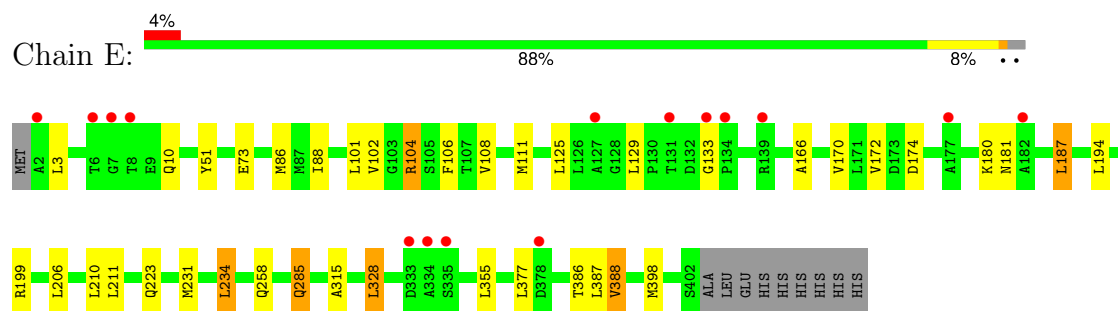
- Molecule 1: Vitamin D hydroxylase



● Molecule 1: Vitamin D hydroxylase



● Molecule 1: Vitamin D hydroxylase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	77.38Å 172.27Å 189.06Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.09 – 2.05 49.09 – 2.05	Depositor EDS
% Data completeness (in resolution range)	99.9 (49.09-2.05) 99.9 (49.09-2.05)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.02 (at 2.05Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.201 , 0.240 0.203 , 0.203	Depositor DCC
R_{free} test set	7920 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	26.7	Xtriage
Anisotropy	0.223	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 38.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	16977	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.74% 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: VD3, ACT, CA, GOL, HEM

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	0.84	0/3179	0.96	1/4325 (0.0%)
1	B	0.75	1/3179 (0.0%)	0.94	2/4325 (0.0%)
1	C	0.75	0/3174	0.96	2/4318 (0.0%)
1	D	0.76	1/3174 (0.0%)	0.94	3/4318 (0.1%)
1	E	0.75	0/3174	0.94	1/4318 (0.0%)
All	All	0.77	2/15880 (0.0%)	0.95	9/21604 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	92	PRO	CA-C	7.12	1.55	1.51
1	D	92	PRO	CA-C	6.37	1.55	1.51

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	281	SER	CA-C-N	5.97	125.68	119.05
1	D	281	SER	C-N-CA	5.97	125.68	119.05
1	B	156	LEU	CA-C-N	5.82	126.73	119.98
1	B	156	LEU	C-N-CA	5.82	126.73	119.98
1	C	281	SER	CA-C-N	5.65	125.33	119.05

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	3113	0	3095	19	0
1	B	3113	0	3095	29	0
1	C	3108	0	3090	34	0
1	D	3108	0	3090	26	0
1	E	3108	0	3090	22	0
2	A	43	0	30	1	0
2	B	43	0	30	0	0
2	C	43	0	30	7	0
2	D	43	0	30	1	0
2	E	43	0	30	0	0
3	A	28	0	44	1	0
3	B	28	0	44	6	0
3	C	28	0	44	2	0
3	D	28	0	44	4	0
3	E	28	0	43	6	0
4	A	4	0	3	0	0
4	C	8	0	6	0	0
4	D	4	0	3	0	0
4	E	8	0	6	0	0
5	A	3	0	0	0	0
5	C	1	0	0	0	0
5	D	1	0	0	0	0
5	E	1	0	0	0	0
6	A	12	0	14	0	0
7	A	303	0	0	3	0
7	B	174	0	0	1	0
7	C	150	0	0	2	0
7	D	198	0	0	1	0
7	E	205	0	0	1	0
All	All	16977	0	15861	137	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 4.

The worst 5 of 137 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:82:THR:HG21	1:A:85:PRO:HA	1.51	0.90
1:B:87:MET:CE	1:B:229:MET:HE1	2.03	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:187:LEU:HD13	1:E:231:MET:HG3	1.60	0.83
1:D:184:MET:HE1	3:D:2001:VD3:H102	1.61	0.81
1:C:258:GLN:HG3	1:C:328:LEU:HD13	1.63	0.80

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%)	388 (97%)	12 (3%)	0	100	100
1	B	400/411 (97%)	386 (96%)	14 (4%)	0	100	100
1	C	399/411 (97%)	386 (97%)	13 (3%)	0	100	100
1	D	399/411 (97%)	385 (96%)	13 (3%)	1 (0%)	36	30
1	E	399/411 (97%)	388 (97%)	11 (3%)	0	100	100
All	All	1997/2055 (97%)	1933 (97%)	63 (3%)	1 (0%)	48	43

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	8	THR

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	334/343 (97%)	323 (97%)	11 (3%)	33	28
1	B	334/343 (97%)	321 (96%)	13 (4%)	28	23
1	C	334/343 (97%)	312 (93%)	22 (7%)	15	9
1	D	334/343 (97%)	317 (95%)	17 (5%)	21	14
1	E	334/343 (97%)	316 (95%)	18 (5%)	20	12
All	All	1670/1715 (97%)	1589 (95%)	81 (5%)	22	15

5 of 81 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	221	LEU
1	E	187	LEU
1	D	328	LEU
1	E	73	GLU
1	E	234	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 15 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	69	HIS
1	E	69	HIS
1	C	238	HIS
1	E	223	GLN
1	D	69	HIS

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 oligosaccharides in this entry.

5.6 Ligand geometry

Of 24 ligands modelled in this entry, 6 are monoatomic - leaving 18 for Mogul analysis.

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	HEM	E	412	1	50,50,50	2.13	10 (20%)	67,82,82	1.58	10 (14%)
4	ACT	C	4004	5	3,3,3	0.70	0	3,3,3	1.52	1 (33%)
6	GOL	A	3002	5	5,5,5	0.30	0	5,5,5	1.90	1 (20%)
2	HEM	D	412	1	50,50,50	2.02	11 (22%)	67,82,82	1.36	5 (7%)
2	HEM	B	412	1	50,50,50	2.18	11 (22%)	67,82,82	1.43	8 (11%)
4	ACT	E	4008	-	3,3,3	0.78	0	3,3,3	1.34	0
3	VD3	B	2001	-	30,30,30	1.05	1 (3%)	43,43,43	2.12	11 (25%)
4	ACT	A	4006	-	3,3,3	0.86	0	3,3,3	1.29	0
4	ACT	C	4007	-	3,3,3	0.71	0	3,3,3	1.35	0
4	ACT	D	4001	-	3,3,3	0.98	0	3,3,3	1.23	0
3	VD3	C	2001	-	30,30,30	0.94	1 (3%)	43,43,43	2.07	10 (23%)
2	HEM	C	412	1	50,50,50	2.00	12 (24%)	67,82,82	1.51	8 (11%)
6	GOL	A	3001	-	5,5,5	0.52	0	5,5,5	0.33	0
3	VD3	E	2001	-	30,30,30	0.94	0	43,43,43	2.55	13 (30%)
4	ACT	E	4005	5	3,3,3	0.74	0	3,3,3	1.30	0
3	VD3	A	2001	-	30,30,30	0.68	0	43,43,43	2.26	13 (30%)
3	VD3	D	2001	-	30,30,30	1.21	3 (10%)	43,43,43	1.77	13 (30%)
2	HEM	A	412	1	50,50,50	2.25	11 (22%)	67,82,82	1.58	12 (17%)

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	HEM	E	412	1	-	1/14/54/54	-
6	GOL	A	3002	5	-	3/4/4/4	-
2	HEM	D	412	1	-	2/14/54/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	HEM	B	412	1	-	0/14/54/54	-
3	VD3	B	2001	-	-	5/15/56/56	0/3/3/3
3	VD3	C	2001	-	-	5/15/56/56	0/3/3/3
2	HEM	C	412	1	-	1/14/54/54	-
6	GOL	A	3001	-	-	0/4/4/4	-
3	VD3	E	2001	-	-	7/15/56/56	0/3/3/3
3	VD3	A	2001	-	-	9/15/56/56	0/3/3/3
3	VD3	D	2001	-	-	9/15/56/56	0/3/3/3
2	HEM	A	412	1	-	0/14/54/54	-

The worst 5 of 60 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	412	HEM	C3D-C2D	7.88	1.53	1.36
2	D	412	HEM	C3D-C2D	7.49	1.52	1.36
2	A	412	HEM	C3D-C2D	7.33	1.52	1.36
2	E	412	HEM	C3D-C2D	7.28	1.52	1.36
2	C	412	HEM	C3D-C2D	7.25	1.52	1.36

The worst 5 of 105 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	2001	VD3	C14-C13-C17	-8.93	90.39	99.72
3	A	2001	VD3	C7-C8-C9	-7.03	115.75	126.13
2	E	412	HEM	C4D-ND-C1D	6.49	112.90	105.21
2	C	412	HEM	C4D-ND-C1D	6.08	112.41	105.21
2	A	412	HEM	C4D-ND-C1D	5.96	112.27	105.21

There are no chirality outliers.

5 of 42 torsion outliers are listed below:

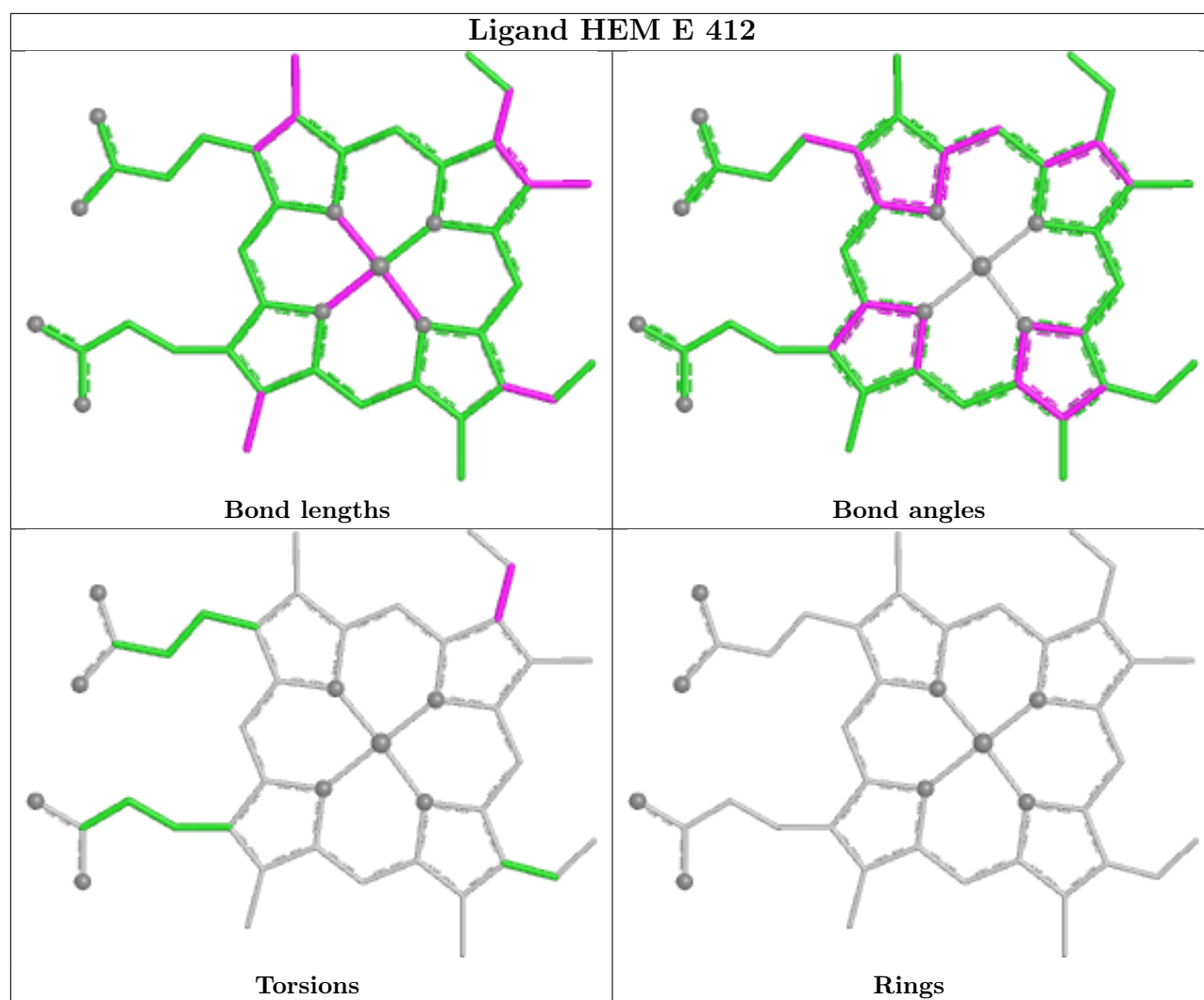
Mol	Chain	Res	Type	Atoms
2	D	412	HEM	C2C-C3C-CAC-CBC
3	A	2001	VD3	C5-C7-C8-C9
3	D	2001	VD3	C5-C7-C8-C9
3	E	2001	VD3	C5-C7-C8-C9
6	A	3002	GOL	O1-C1-C2-C3

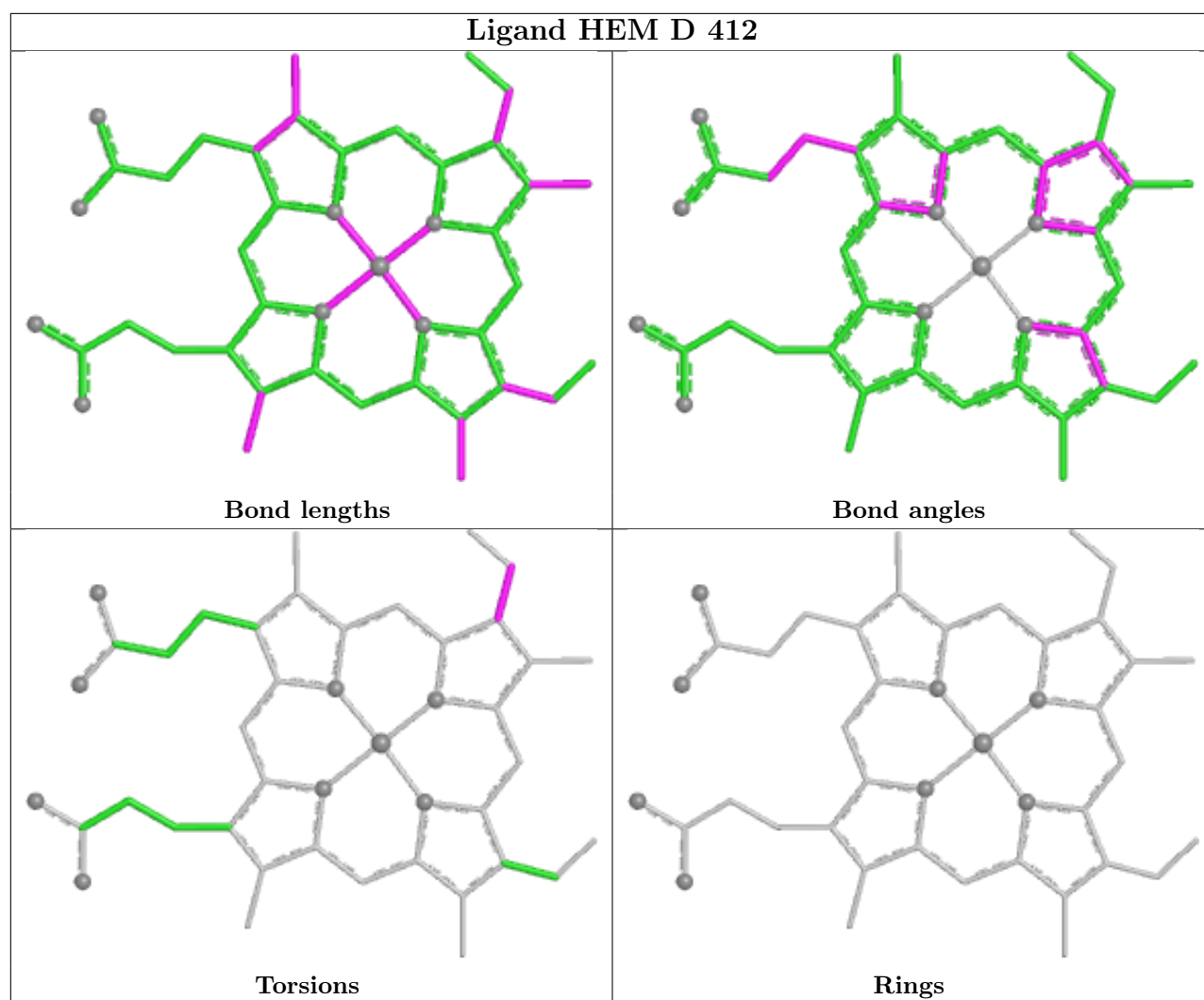
There are no ring outliers.

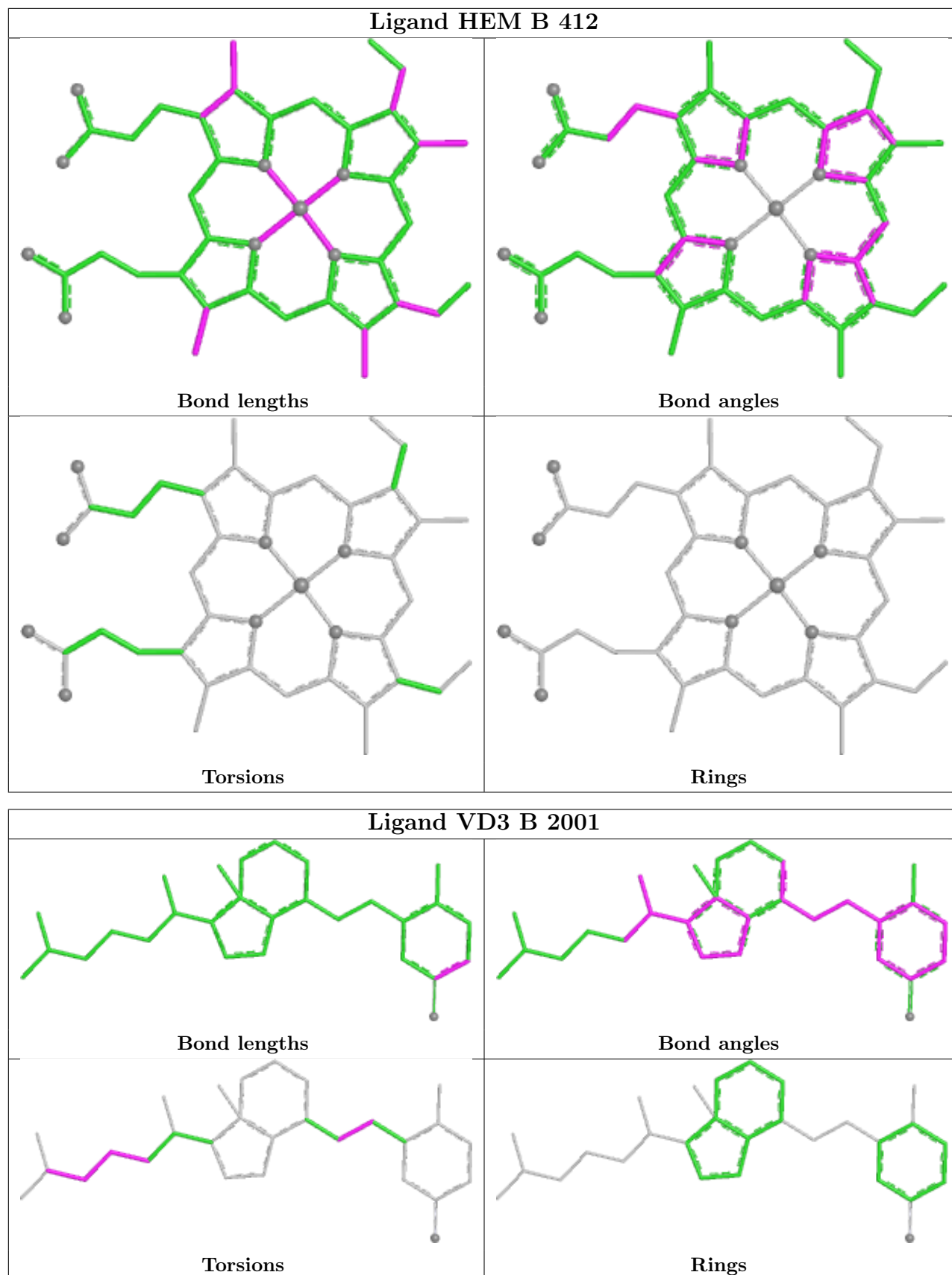
8 monomers are involved in 28 short contacts:

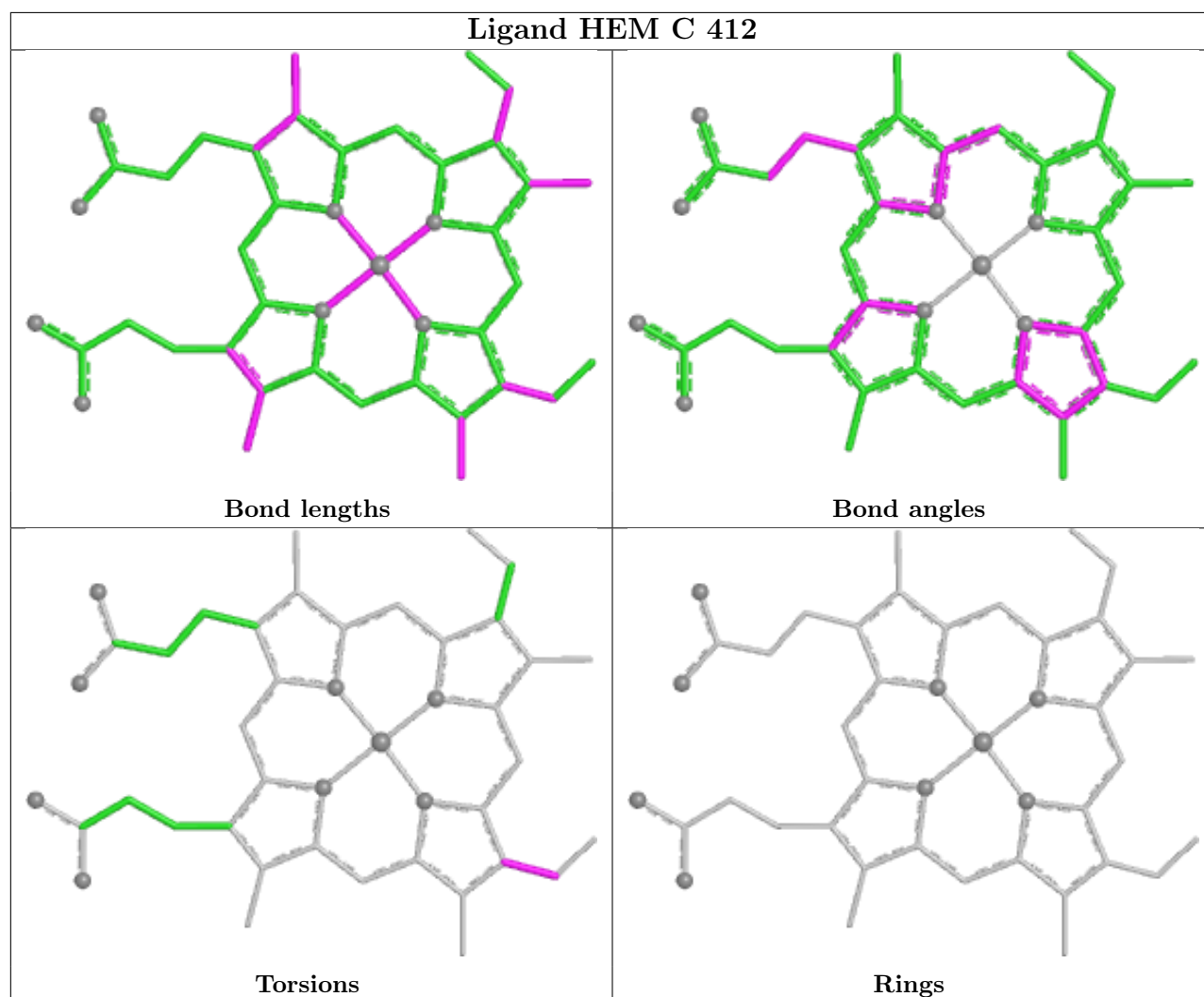
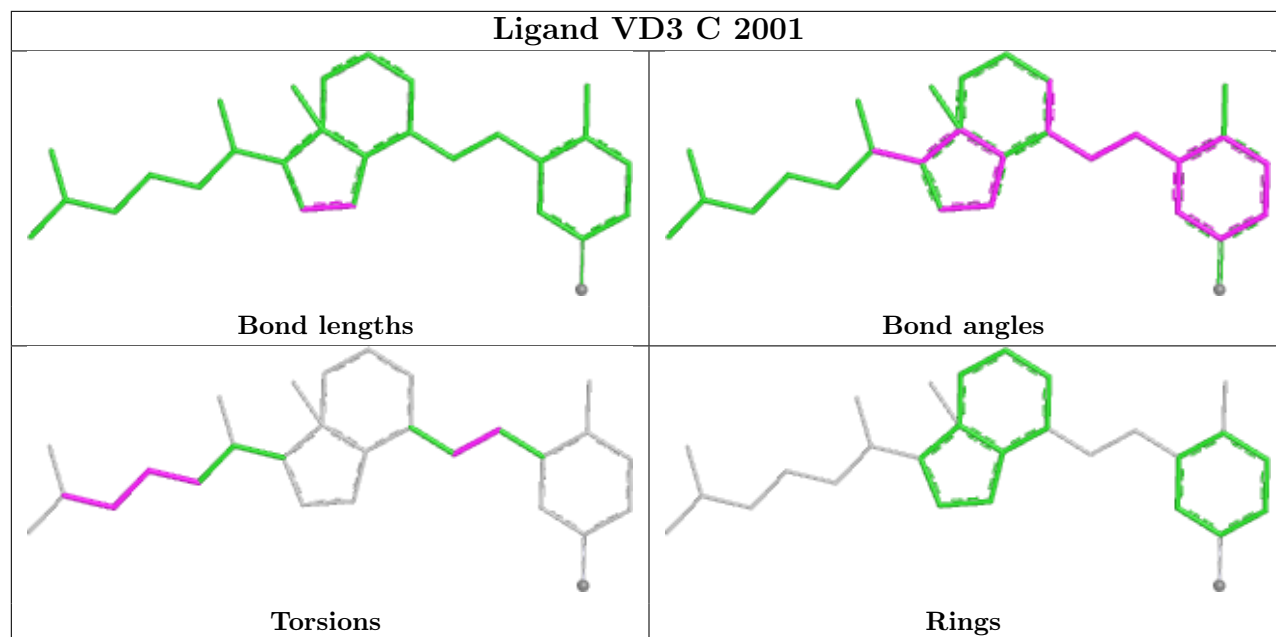
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	412	HEM	1	0
3	B	2001	VD3	6	0
3	C	2001	VD3	2	0
2	C	412	HEM	7	0
3	E	2001	VD3	6	0
3	A	2001	VD3	1	0
3	D	2001	VD3	4	0
2	A	412	HEM	1	0

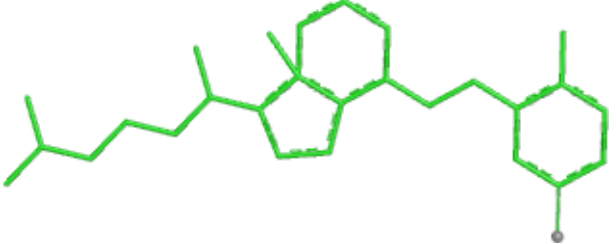
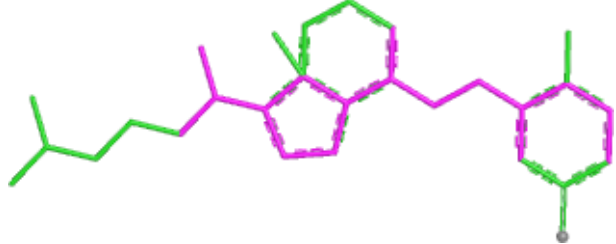
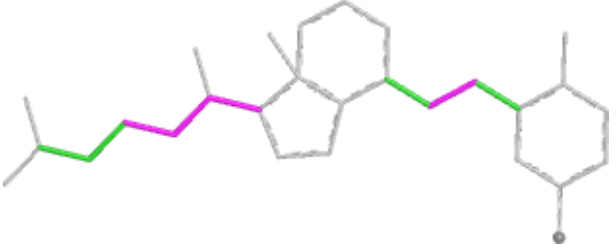
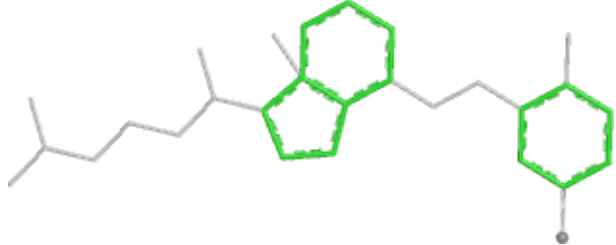
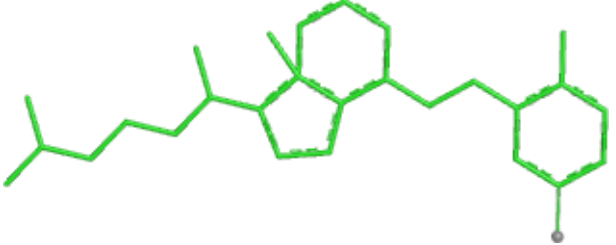
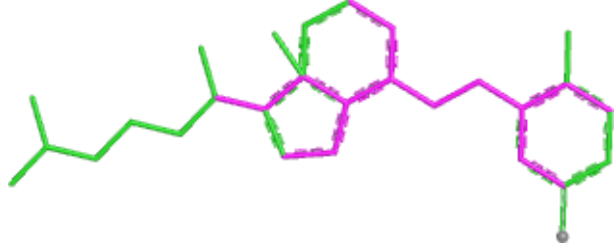
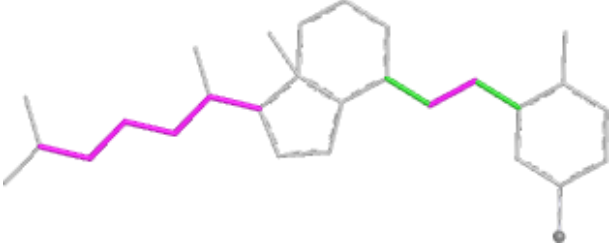
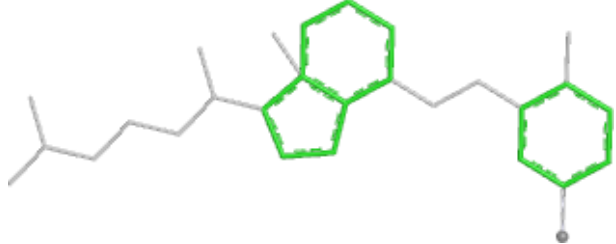
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 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.

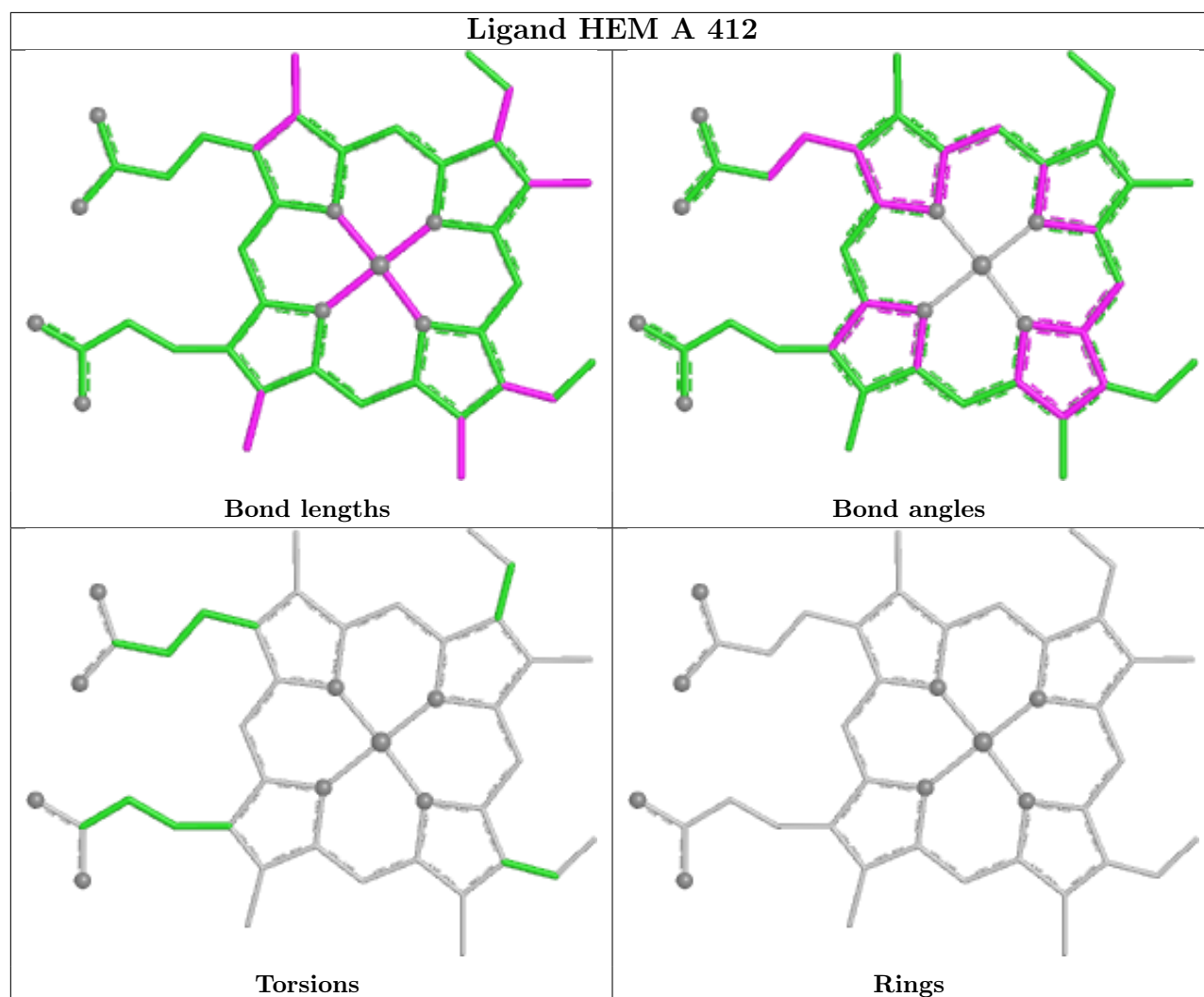
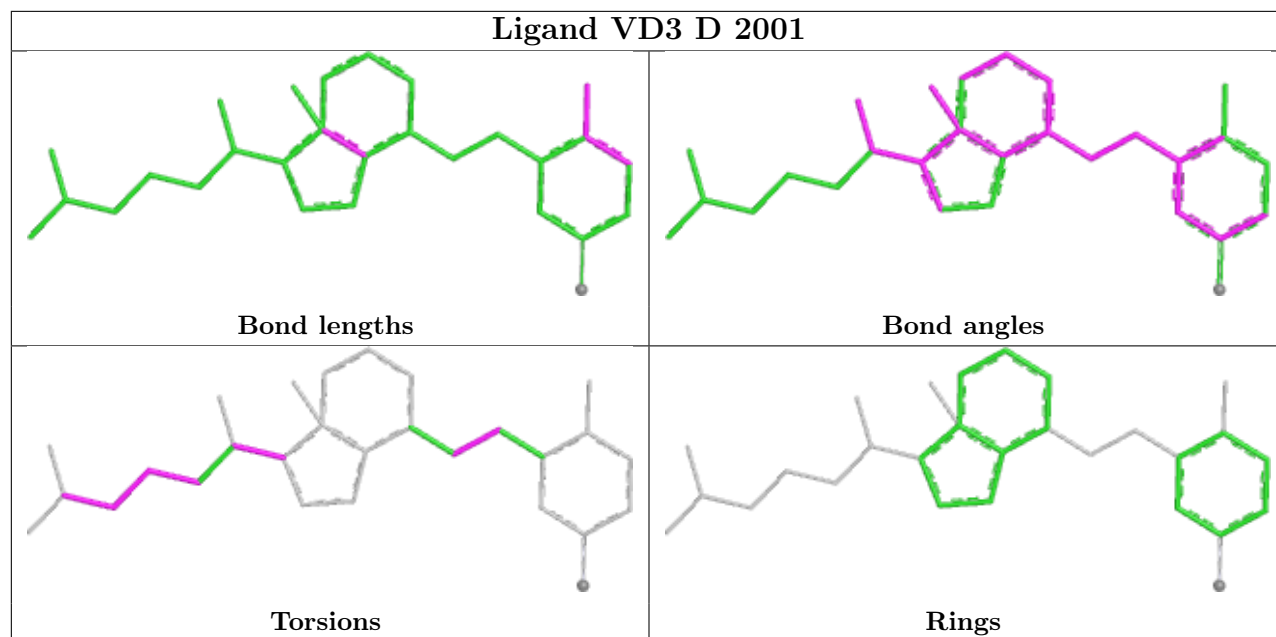








Ligand VD3 E 2001	
	
Bond lengths	Bond angles
	
Torsions	Rings
Ligand VD3 A 2001	
	
Bond lengths	Bond angles
	
Torsions	Rings



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%)	-0.27	7 (1%) 69 70	11, 20, 35, 45	0
1	B	402/411 (97%)	0.42	33 (8%) 17 18	16, 29, 52, 64	0
1	C	401/411 (97%)	0.48	35 (8%) 16 16	14, 29, 49, 61	0
1	D	401/411 (97%)	0.26	13 (3%) 50 50	14, 29, 48, 56	0
1	E	401/411 (97%)	0.17	15 (3%) 45 45	17, 27, 42, 52	0
All	All	2007/2055 (97%)	0.21	103 (5%) 33 33	11, 27, 47, 64	0

The worst 5 of 103 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	403	ALA	5.3
1	E	133	GLY	4.7
1	C	6	THR	4.1
1	C	135	VAL	4.1
1	D	134	PRO	3.9

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,

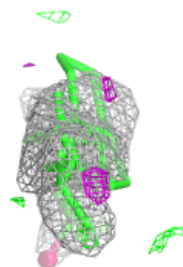
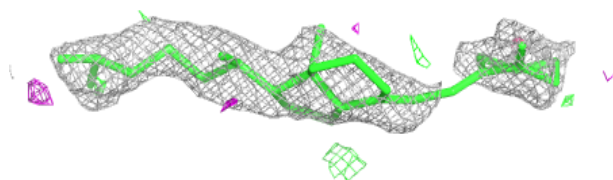
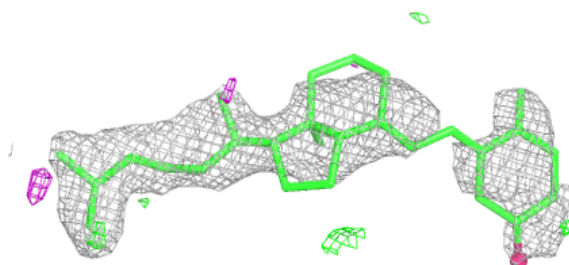
median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	ACT	E	4005	4/4	0.72	0.20	42,42,42,42	0
3	VD3	C	2001	28/28	0.80	0.23	45,64,71,71	0
3	VD3	E	2001	28/28	0.80	0.27	62,74,82,82	0
3	VD3	A	2001	28/28	0.80	0.23	45,60,68,68	0
3	VD3	B	2001	28/28	0.81	0.29	67,78,83,83	0
3	VD3	D	2001	28/28	0.81	0.24	56,69,77,77	0
4	ACT	C	4007	4/4	0.82	0.16	30,30,31,31	0
4	ACT	C	4004	4/4	0.83	0.15	43,43,43,43	0
4	ACT	E	4008	4/4	0.90	0.12	36,36,36,36	0
6	GOL	A	3002	6/6	0.90	0.10	29,32,33,38	0
4	ACT	A	4006	4/4	0.92	0.10	20,20,20,20	0
6	GOL	A	3001	6/6	0.93	0.09	23,23,24,25	0
4	ACT	D	4001	4/4	0.94	0.09	18,18,18,18	0
5	CA	A	2506	1/1	0.95	0.07	41,41,41,41	0
2	HEM	B	412	43/43	0.97	0.07	19,25,28,30	0
5	CA	E	2504	1/1	0.97	0.05	35,35,35,35	0
5	CA	C	2503	1/1	0.98	0.03	33,33,33,33	0
5	CA	D	2502	1/1	0.98	0.04	35,35,35,35	0
2	HEM	C	412	43/43	0.98	0.06	12,16,19,29	0
2	HEM	D	412	43/43	0.98	0.05	13,16,18,23	0
2	HEM	E	412	43/43	0.98	0.05	15,18,19,23	0
2	HEM	A	412	43/43	0.99	0.05	9,13,15,23	0
5	CA	A	2501	1/1	0.99	0.03	29,29,29,29	0
5	CA	A	2505	1/1	0.99	0.03	27,27,27,27	0

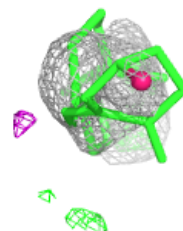
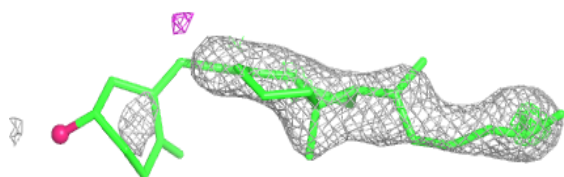
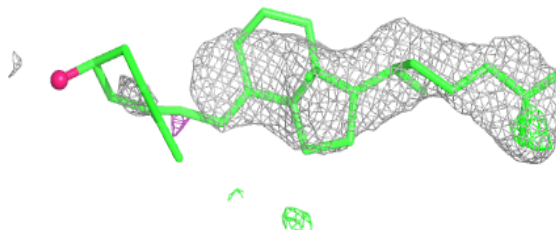
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around VD3 C 2001:

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

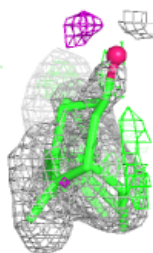
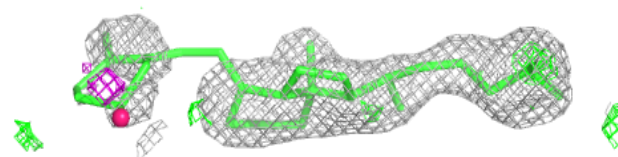
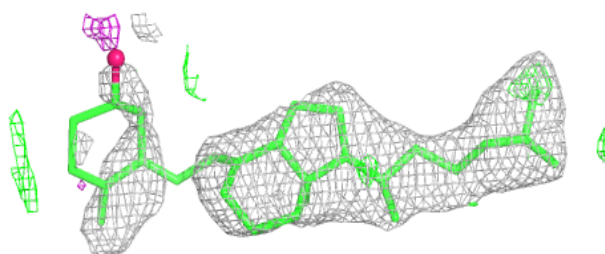
**Electron density around VD3 E 2001:**

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

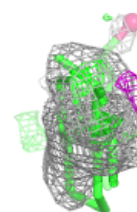
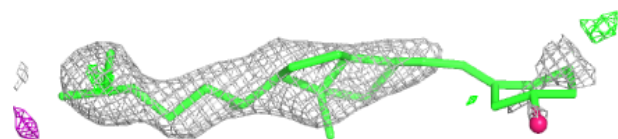
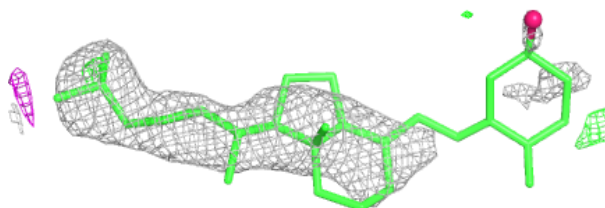


Electron density around VD3 A 2001:

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

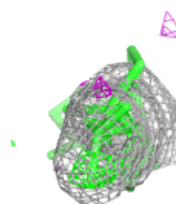
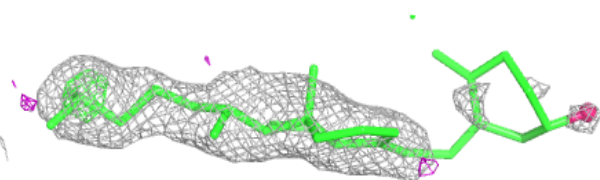
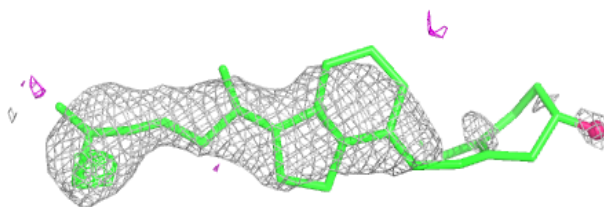
**Electron density around VD3 B 2001:**

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



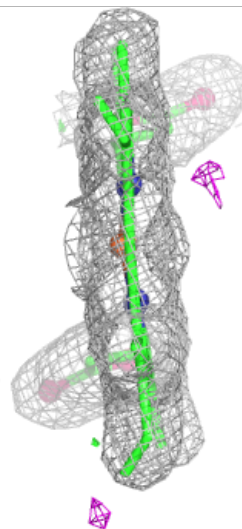
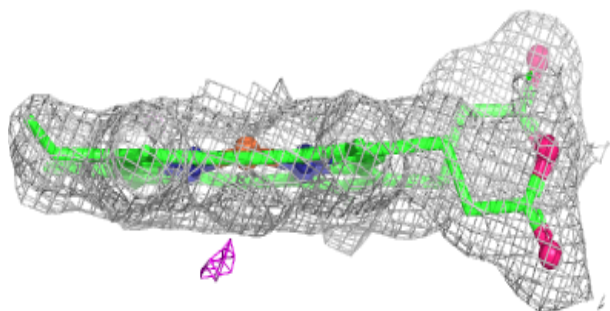
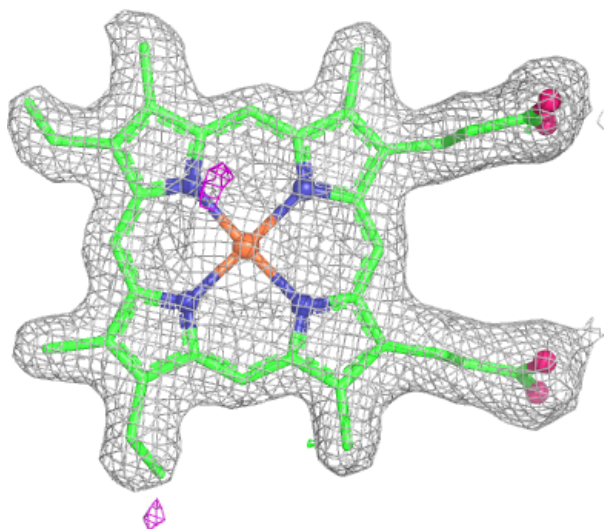
Electron density around VD3 D 2001:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



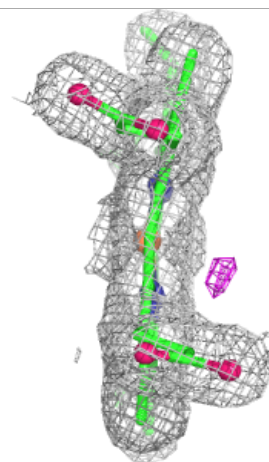
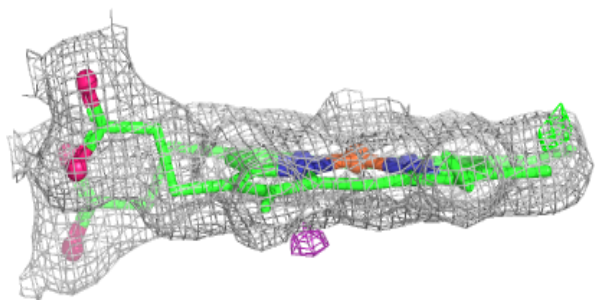
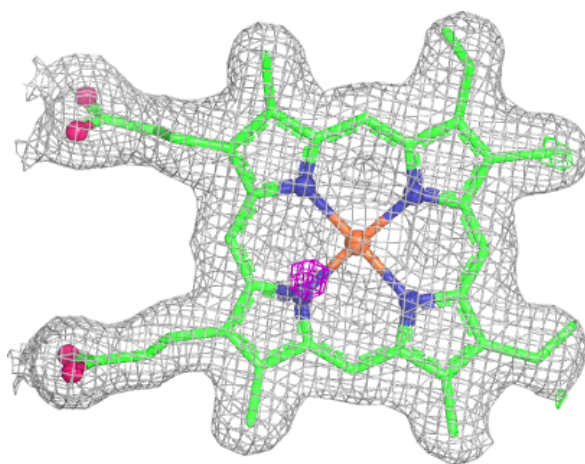
Electron density around HEM B 412:

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



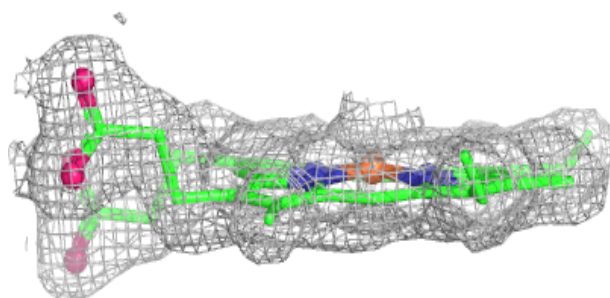
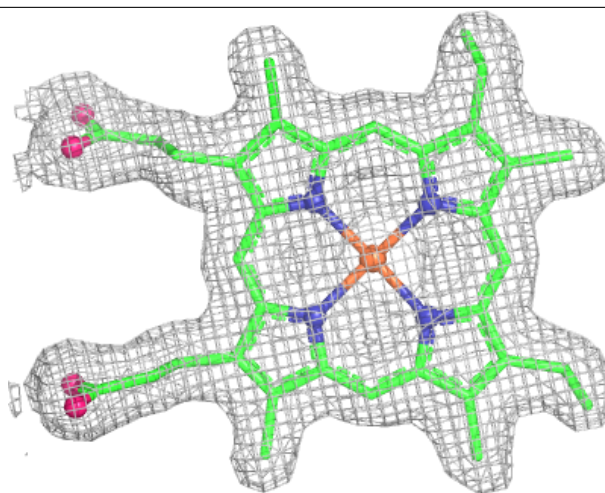
Electron density around HEM C 412:

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



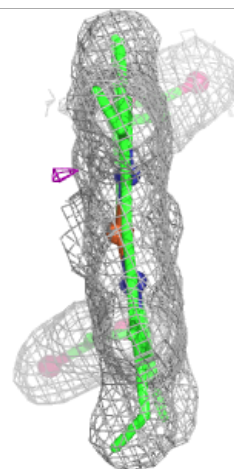
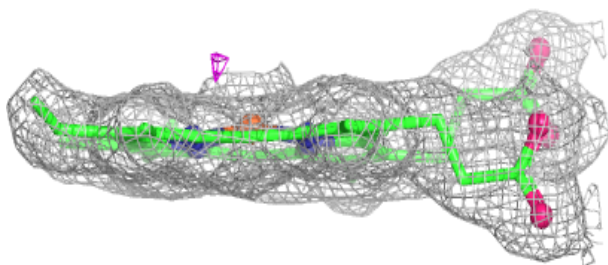
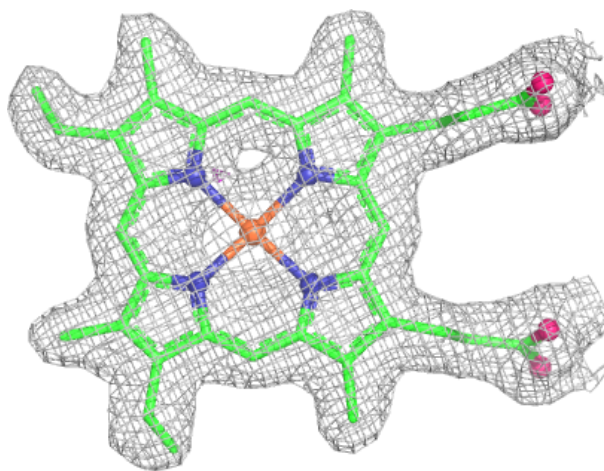
Electron density around HEM D 412:

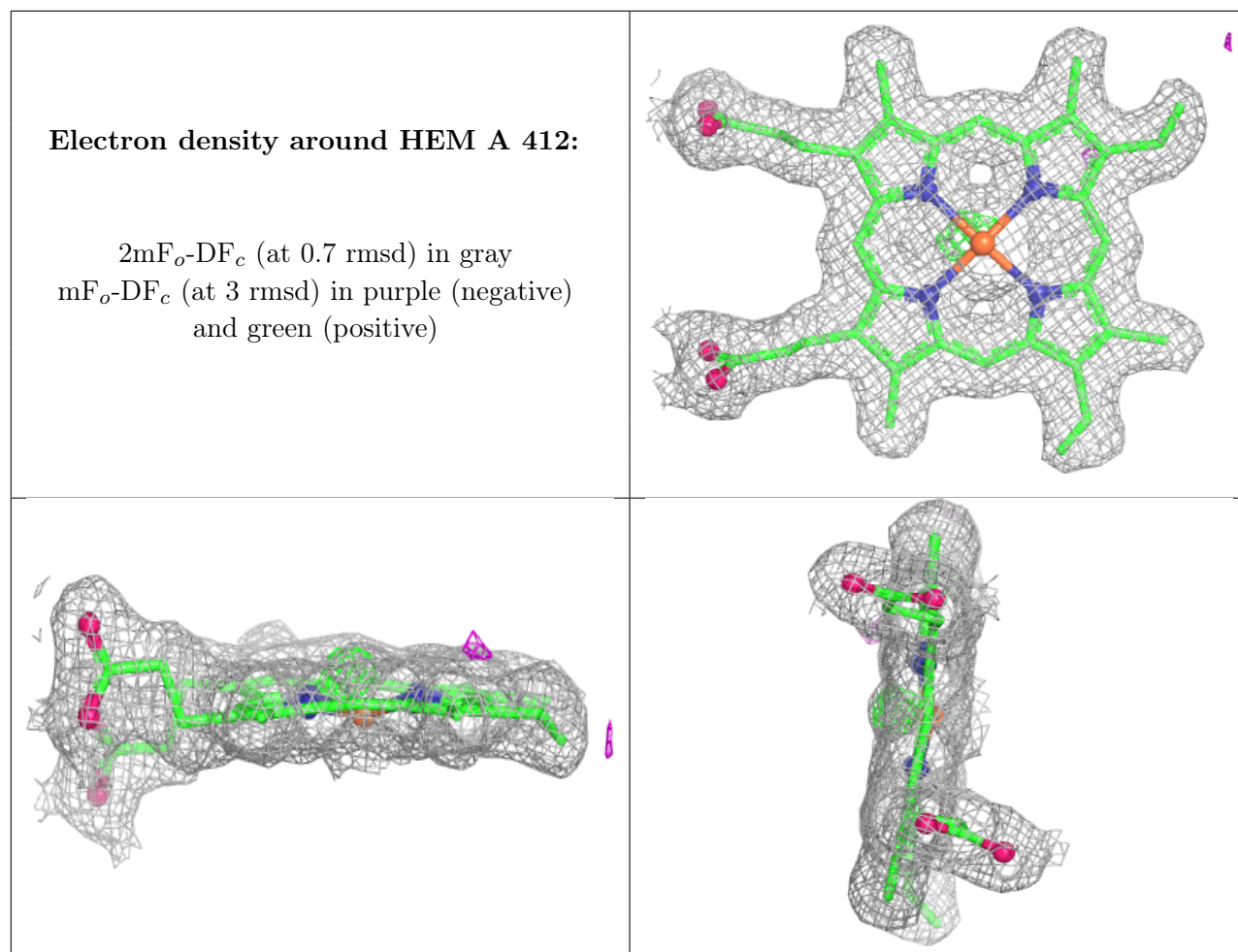
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around HEM E 412:

$2mF_o-DF_c$ (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.