



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 06:53 PM EDT

PDB ID : 6XA2 / pdb_00006xa2
Title : Structure of the tirandamycin C-bound P450 monooxygenase TamI
Authors : Newmister, S.A.; Srivastava, K.R.; Espinoza, R.V.; Haatveit, K.C.; Khatri, Y.; Martini, R.M.; Garcia-Borras, M.; Podust, L.M.; Houk, K.N.; Sherman, D.H.
Deposited on : 2020-06-03
Resolution : 2.64 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

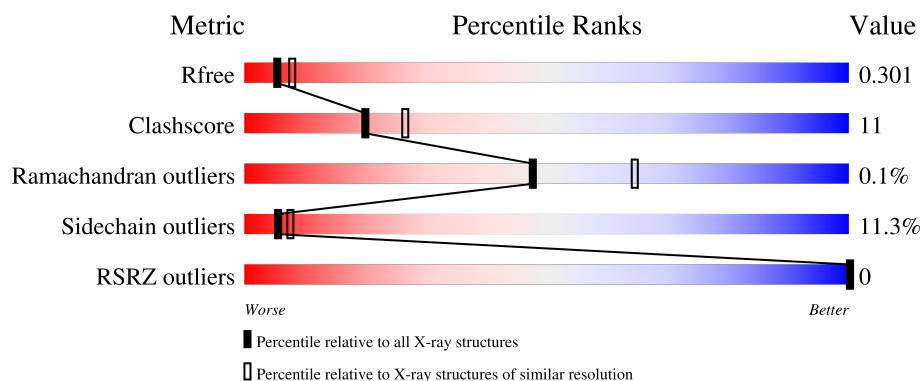
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.64 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	2053 (2.66-2.62)
Clashscore	190562	2097 (2.66-2.62)
Ramachandran outliers	187476	2066 (2.66-2.62)
Sidechain outliers	187428	2066 (2.66-2.62)
RSRZ outliers	180081	2052 (2.66-2.62)

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	414	
1	B	414	
1	C	414	
1	D	414	

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Mol	Chain	Length	Quality of chain
1	E	414	 70%22%5%•
1	F	414	 71%23%••
1	G	414	 66%26%5%•
1	H	414	 66%26%••

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 25091 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 TamI.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	399	Total	C	N	O	S	0	0	0
			3056	1930	542	570	14			
1	B	399	Total	C	N	O	S	0	0	0
			3060	1932	542	572	14			
1	C	393	Total	C	N	O	S	0	0	0
			2974	1874	531	555	14			
1	D	398	Total	C	N	O	S	0	0	0
			3042	1918	541	569	14			
1	E	399	Total	C	N	O	S	0	0	0
			3058	1931	545	568	14			
1	F	399	Total	C	N	O	S	0	0	0
			3059	1932	545	568	14			
1	G	399	Total	C	N	O	S	0	0	0
			3016	1904	534	564	14			
1	H	399	Total	C	N	O	S	0	0	0
			3037	1921	536	566	14			

There are 16 discrepancies between the modelled and reference sequences:

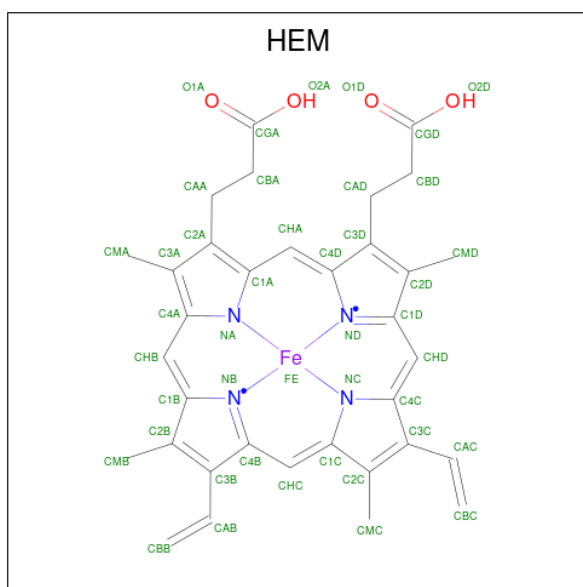
Chain	Residue	Modelled	Actual	Comment	Reference
A	0	ALA	-	expression tag	UNP D3Y1J3
A	1	VAL	-	expression tag	UNP D3Y1J3
B	0	ALA	-	expression tag	UNP D3Y1J3
B	1	VAL	-	expression tag	UNP D3Y1J3
C	0	ALA	-	expression tag	UNP D3Y1J3
C	1	VAL	-	expression tag	UNP D3Y1J3
D	0	ALA	-	expression tag	UNP D3Y1J3
D	1	VAL	-	expression tag	UNP D3Y1J3
E	0	ALA	-	expression tag	UNP D3Y1J3
E	1	VAL	-	expression tag	UNP D3Y1J3
F	0	ALA	-	expression tag	UNP D3Y1J3
F	1	VAL	-	expression tag	UNP D3Y1J3
G	0	ALA	-	expression tag	UNP D3Y1J3

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Chain	Residue	Modelled	Actual	Comment	Reference
G	1	VAL	-	expression tag	UNP D3Y1J3
H	0	ALA	-	expression tag	UNP D3Y1J3
H	1	VAL	-	expression tag	UNP D3Y1J3

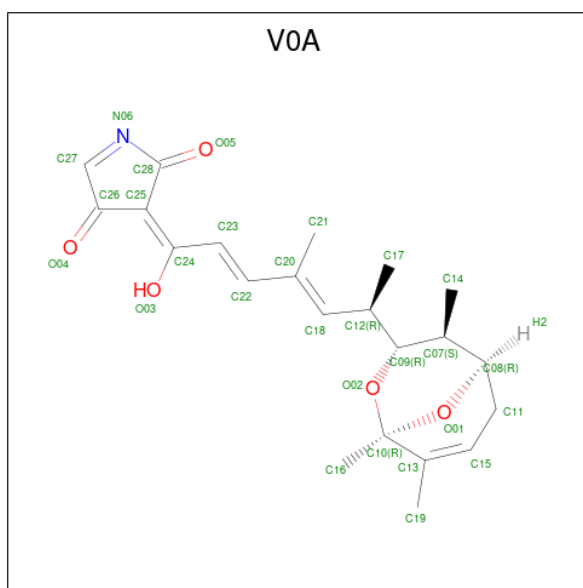
- Molecule 2 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$) (labeled as "Ligand of Interest" by depositor).



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
2	F	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	G	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	H	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

- Molecule 3 is (3E)-3-{(2E,4E,6R)-1-hydroxy-4-methyl-6-[(1R,3R,4S,5R)-1,4,8-trimethyl-2,9-dioxabicyclo[3.3.1]non-7-en-3-yl]hepta-2,4-dien-1-ylidene}-2H-pyrrole-2,4(3H)-dione (CCD

ID: V0A) (formula: $C_{22}H_{27}NO_5$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			28	22	1	5		
3	B	1	Total	C	N	O	0	0
			28	22	1	5		
3	C	1	Total	C	N	O	0	0
			28	22	1	5		
3	D	1	Total	C	N	O	0	0
			28	22	1	5		
3	E	1	Total	C	N	O	0	0
			28	22	1	5		
3	F	1	Total	C	N	O	0	0
			28	22	1	5		
3	G	1	Total	C	N	O	0	0
			28	22	1	5		
3	H	1	Total	C	N	O	0	0
			28	22	1	5		

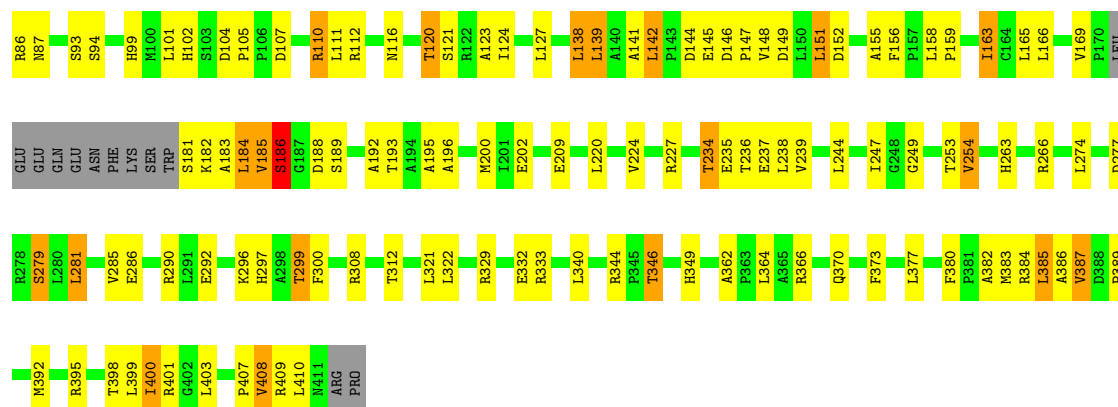
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	39	Total	O	0	0
			39	39		
4	B	30	Total	O	0	0
			30	30		
4	C	23	Total	O	0	0
			23	23		

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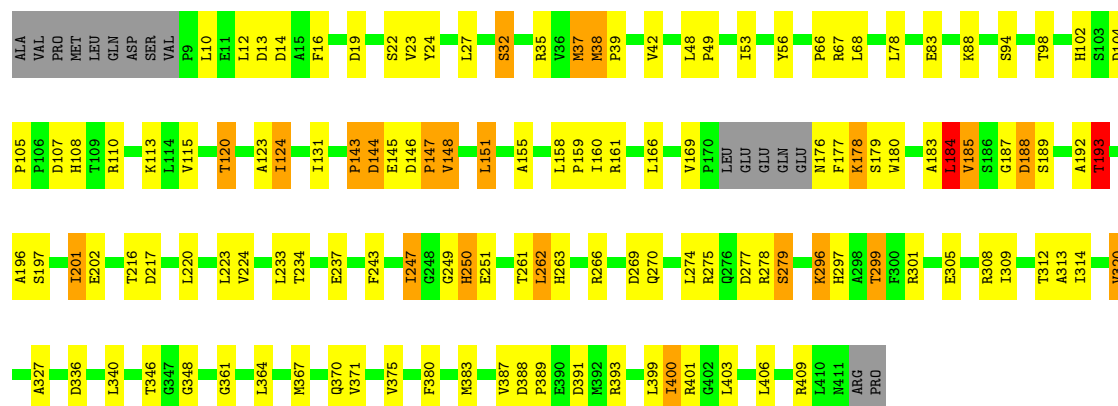
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	D	24	Total 24	O 24	0	0
4	E	24	Total 24	O 24	0	0
4	F	41	Total 41	O 41	0	0
4	G	19	Total 19	O 19	0	0
4	H	21	Total 21	O 21	0	0



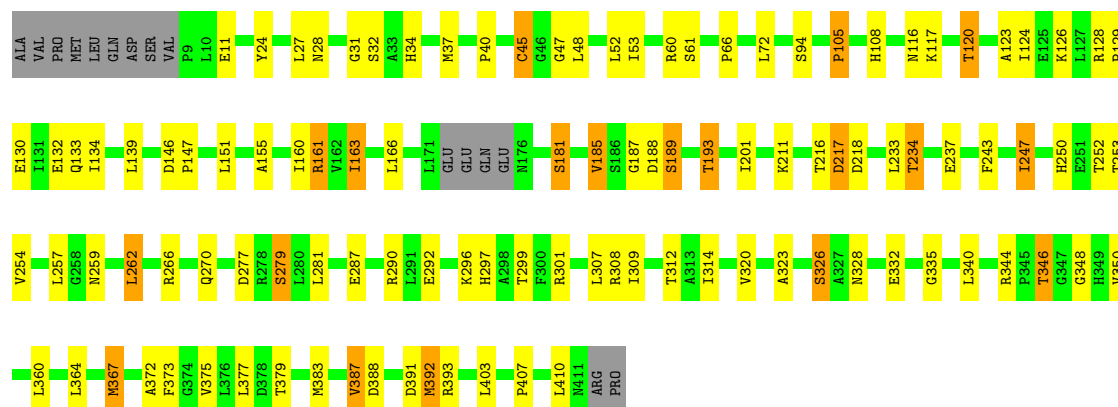
• Molecule 1: TamI

Chain D: 65% 26% 5% .



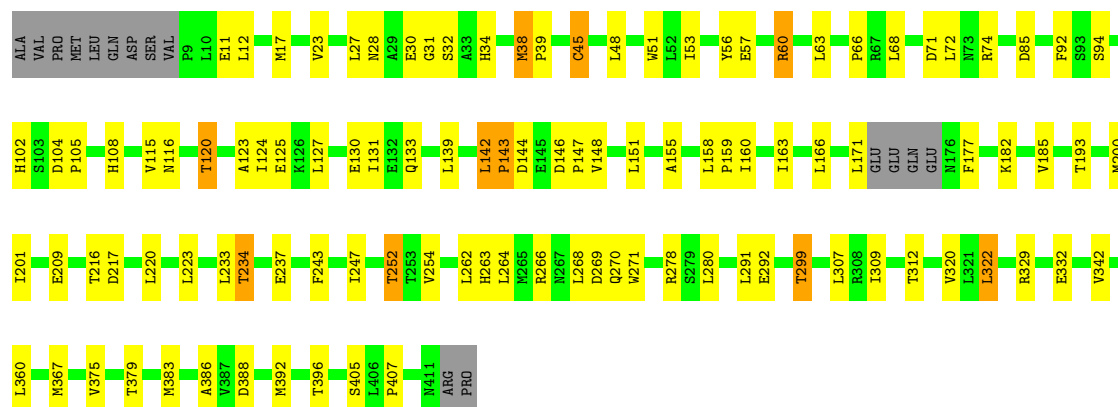
• Molecule 1: TamI

Chain E: 70% 22% 5% .



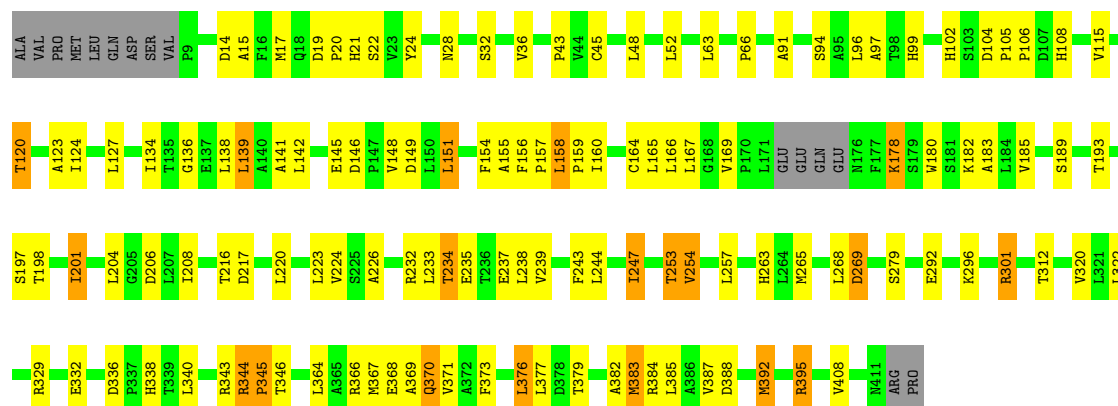
• Molecule 1: TamI

Chain F: 71% 23% . .



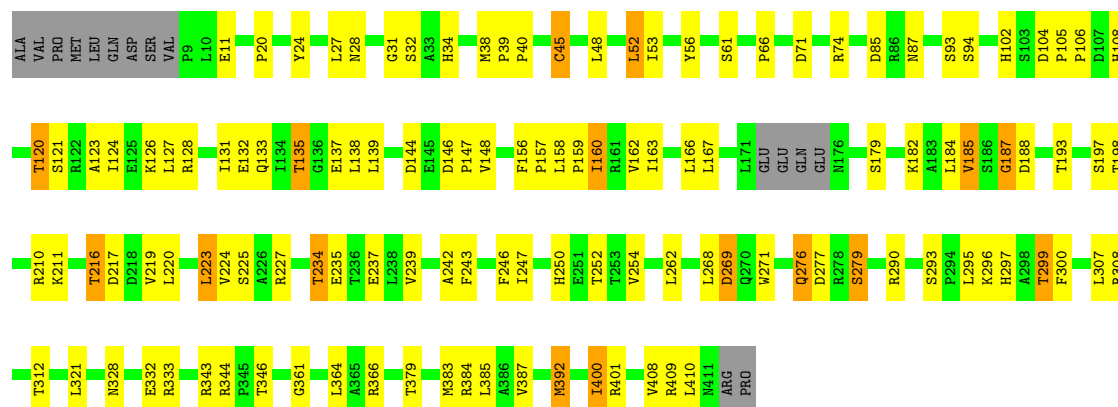
• Molecule 1: TamI

Chain G: 66% 26% 5% .



• Molecule 1: TamI

Chain H: 66% 26% . .



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	224.55Å 57.16Å 282.66Å 90.00° 90.89° 90.00°	Depositor
Resolution (Å)	48.55 – 2.64 48.55 – 2.64	Depositor EDS
% Data completeness (in resolution range)	99.6 (48.55-2.64) 95.6 (48.55-2.64)	Depositor EDS
R_{merge}	0.24	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.66 (at 2.65Å)	Xtriage
Refinement program	PHENIX 1.18_3845	Depositor
R, R_{free}	0.252 , 0.299 0.254 , 0.301	Depositor DCC
R_{free} test set	2001 reflections (1.87%)	wwPDB-VP
Wilson B-factor (Å ²)	48.9	Xtriage
Anisotropy	0.578	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 37.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	0.238 for -h,-k,l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	25091	wwPDB-VP
Average B, all atoms (Å ²)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 40.54 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.6931e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: HEM, V0A

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	0.63	1/3123 (0.0%)	0.73	9/4255 (0.2%)
1	B	0.40	0/3127	0.58	3/4260 (0.1%)
1	C	0.62	1/3037 (0.0%)	0.81	14/4141 (0.3%)
1	D	0.63	2/3108 (0.1%)	0.80	17/4235 (0.4%)
1	E	0.49	1/3125 (0.0%)	0.69	7/4257 (0.2%)
1	F	0.56	2/3126 (0.1%)	0.65	7/4258 (0.2%)
1	G	0.65	1/3080 (0.0%)	0.84	10/4199 (0.2%)
1	H	0.58	1/3104 (0.0%)	0.65	3/4232 (0.1%)
All	All	0.58	9/24830 (0.0%)	0.72	70/33837 (0.2%)

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	85	ASP	C-N	7.28	1.44	1.33
1	G	336	ASP	C-O	6.97	1.27	1.23
1	C	169	VAL	CA-C	6.81	1.57	1.52
1	D	336	ASP	C-O	6.44	1.26	1.23
1	A	189	SER	CA-C	-6.35	1.46	1.52
1	D	145	GLU	CA-C	-5.66	1.46	1.52
1	H	344	ARG	CA-C	-5.51	1.47	1.53
1	F	182	LYS	C-O	-5.18	1.18	1.24
1	E	388	ASP	CA-C	-5.13	1.47	1.53

All (70) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	105	PRO	N-CA-C	14.90	128.88	110.70
1	C	184	LEU	N-CA-C	-14.14	96.93	114.75
1	A	105	PRO	N-CA-C	13.23	126.84	110.70
1	D	184	LEU	N-CA-C	-13.13	97.88	114.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	346	THR	N-CA-C	12.80	125.31	111.36
1	E	346	THR	N-CA-C	10.77	123.10	111.36
1	C	188	ASP	N-CA-C	-10.69	98.97	113.18
1	C	279	SER	N-CA-C	-10.18	100.86	113.38
1	F	144	ASP	N-CA-C	-9.16	102.22	112.57
1	A	42	VAL	N-CA-C	-9.14	100.77	108.63
1	G	346	THR	N-CA-C	9.08	121.18	111.28
1	E	185	VAL	N-CA-C	7.98	118.78	110.72
1	C	346	THR	N-CA-C	7.97	119.97	111.28
1	G	180	TRP	N-CA-C	7.82	119.80	111.28
1	C	141	ALA	N-CA-C	-7.79	101.41	113.02
1	D	146	ASP	CA-C-N	-7.67	110.25	119.84
1	D	146	ASP	C-N-CA	-7.67	110.25	119.84
1	C	186	SER	N-CA-C	-7.57	97.89	109.85
1	D	185	VAL	N-CA-CB	-7.54	105.45	111.64
1	G	183	ALA	N-CA-C	-7.49	104.38	113.97
1	D	193	THR	N-CA-C	-7.39	102.18	112.45
1	C	138	LEU	N-CA-C	-7.34	102.98	112.23
1	E	391	ASP	N-CA-C	-7.31	103.96	113.17
1	H	269	ASP	N-CA-C	-7.26	103.30	111.07
1	D	16	PHE	N-CA-C	-7.24	103.47	111.36
1	A	185	VAL	N-CA-C	7.22	118.01	110.72
1	D	188	ASP	N-CA-C	-6.99	104.01	114.64
1	D	143	PRO	N-CA-C	6.54	121.51	111.11
1	F	143	PRO	N-CA-C	6.51	121.17	111.41
1	D	148	VAL	N-CA-C	6.46	117.22	108.17
1	F	146	ASP	CA-C-N	-6.39	111.85	119.84
1	F	146	ASP	C-N-CA	-6.39	111.85	119.84
1	C	139	LEU	N-CA-C	-6.38	101.94	110.55
1	G	134	ILE	N-CA-CB	-6.30	103.51	110.51
1	E	348	GLY	N-CA-C	6.27	123.42	114.64
1	D	187	GLY	N-CA-C	6.25	118.39	110.96
1	A	42	VAL	CB-CA-C	6.12	116.64	110.94
1	G	253	THR	N-CA-C	6.07	118.86	111.82
1	B	185	VAL	N-CA-C	6.07	116.85	110.72
1	C	169	VAL	N-CA-C	6.05	114.81	107.61
1	D	88	LYS	N-CA-C	-6.05	104.54	112.41
1	A	105	PRO	CA-C-N	-5.94	112.46	119.05
1	A	105	PRO	C-N-CA	-5.94	112.46	119.05
1	D	185	VAL	N-CA-C	-5.93	106.93	111.62
1	C	146	ASP	CA-C-N	-5.80	112.59	119.84
1	C	146	ASP	C-N-CA	-5.80	112.59	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	142	LEU	N-CA-C	5.80	117.27	110.31
1	C	142	LEU	CA-C-N	-5.79	112.60	119.84
1	C	142	LEU	C-N-CA	-5.79	112.60	119.84
1	B	92	PHE	N-CA-C	-5.79	104.89	112.41
1	A	168	GLY	N-CA-C	5.79	124.17	113.76
1	G	279	SER	N-CA-C	-5.78	105.89	113.17
1	H	276	GLN	CB-CG-CD	-5.74	102.84	112.60
1	A	43	PRO	N-CA-C	5.65	122.94	113.78
1	D	147	PRO	N-CA-C	-5.60	100.93	112.47
1	D	393	ARG	N-CA-C	5.55	118.31	110.14
1	H	187	GLY	N-CA-C	5.54	120.90	111.15
1	A	347	GLY	N-CA-C	-5.40	104.65	111.72
1	G	141	ALA	N-CA-C	5.38	118.94	112.38
1	G	269	ASP	CB-CA-C	-5.36	102.41	110.92
1	D	144	ASP	N-CA-C	-5.30	107.00	112.93
1	D	348	GLY	N-CA-C	-5.27	107.39	114.25
1	D	37	MET	N-CA-C	-5.19	101.18	109.23
1	E	105	PRO	CA-C-N	-5.18	113.58	118.97
1	E	105	PRO	C-N-CA	-5.18	113.58	118.97
1	F	56	TYR	N-CA-C	5.13	117.28	111.02
1	C	144	ASP	N-CA-C	-5.08	101.48	109.25
1	F	92	PHE	N-CA-C	-5.05	105.84	112.41
1	G	206	ASP	CB-CA-C	-5.03	102.77	110.81
1	G	345	PRO	N-CA-C	-5.02	103.30	111.03

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	3056	0	3026	59	0
1	B	3060	0	3030	72	0
1	C	2974	0	2933	97	0
1	D	3042	0	3008	76	0
1	E	3058	0	3033	60	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	3059	0	3035	56	0
1	G	3016	0	2972	82	0
1	H	3037	0	2998	78	0
2	A	43	0	30	5	0
2	B	43	0	30	3	0
2	C	43	0	30	3	0
2	D	43	0	30	5	0
2	E	43	0	30	4	0
2	F	43	0	30	3	0
2	G	43	0	30	4	0
2	H	43	0	30	4	0
3	A	28	0	0	0	0
3	B	28	0	0	0	0
3	C	28	0	0	8	0
3	D	28	0	0	1	0
3	E	28	0	0	0	0
3	F	28	0	0	0	0
3	G	28	0	0	2	0
3	H	28	0	0	2	0
4	A	39	0	0	1	0
4	B	30	0	0	0	0
4	C	23	0	0	1	0
4	D	24	0	0	0	0
4	E	24	0	0	0	0
4	F	41	0	0	1	0
4	G	19	0	0	1	0
4	H	21	0	0	1	0
All	All	25091	0	24275	562	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 11.

All (562) 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:H:120:THR:HG22	1:H:123:ALA:H	1.33	0.93
1:G:120:THR:HG22	1:G:123:ALA:H	1.33	0.93
1:C:185:VAL:HG22	3:C:502:V0A:C22	1.99	0.92
1:C:185:VAL:HG22	3:C:502:V0A:C23	1.98	0.92
1:C:120:THR:HG22	1:C:123:ALA:H	1.34	0.90
1:B:120:THR:HG22	1:B:123:ALA:H	1.41	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:129:PRO:O	1:E:133:GLN:HG3	1.78	0.83
1:F:234:THR:HG22	1:F:237:GLU:H	1.46	0.80
1:G:234:THR:HG22	1:G:237:GLU:H	1.47	0.80
1:C:263:HIS:HB3	1:C:340:LEU:HD22	1.64	0.79
1:H:185:VAL:HG22	3:H:502:V0A:C23	2.12	0.79
1:F:105:PRO:HG3	1:H:66:PRO:HG2	1.66	0.78
1:B:66:PRO:HG2	1:C:105:PRO:HG3	1.66	0.77
1:A:120:THR:HG22	1:A:123:ALA:H	1.49	0.77
1:F:120:THR:HG22	1:F:123:ALA:H	1.52	0.75
1:F:71:ASP:HB3	1:F:74:ARG:HG3	1.68	0.74
1:F:66:PRO:HG2	1:H:105:PRO:HG3	1.69	0.73
1:B:234:THR:HG22	1:B:237:GLU:H	1.56	0.71
1:H:71:ASP:HB3	1:H:74:ARG:HG3	1.72	0.70
1:D:262:LEU:HD12	1:D:403:LEU:HD11	1.71	0.70
1:G:265:MET:HE1	1:G:384:ARG:HA	1.74	0.70
1:B:275:ARG:O	1:B:278:ARG:NH2	2.25	0.69
1:B:156:PHE:HB3	1:B:178:LYS:HD3	1.74	0.69
1:E:66:PRO:HG2	1:G:105:PRO:HG3	1.75	0.69
1:C:385:LEU:HD21	1:C:392:MET:HE1	1.75	0.69
1:G:91:ALA:HB3	3:G:502:V0A:C21	2.24	0.68
1:E:234:THR:HG22	1:E:237:GLU:H	1.58	0.68
1:A:105:PRO:HG3	1:D:66:PRO:HG2	1.76	0.68
1:G:329:ARG:HH21	1:G:338:HIS:HA	1.59	0.67
1:D:48:LEU:HD13	1:D:78:LEU:HG	1.76	0.67
1:E:24:TYR:OH	1:E:297:HIS:NE2	2.28	0.67
1:D:296:LYS:HG2	1:D:401:ARG:HB2	1.75	0.67
1:A:66:PRO:HG2	1:D:105:PRO:HG3	1.77	0.66
1:B:105:PRO:HG3	1:C:66:PRO:HG2	1.79	0.65
1:G:96:LEU:HD11	1:G:201:ILE:HG12	1.79	0.65
1:E:262:LEU:HD12	1:E:403:LEU:HD11	1.79	0.64
1:B:65:ASP:HB3	1:B:68:LEU:HD23	1.79	0.64
1:H:124:ILE:HG21	1:H:364:LEU:HA	1.79	0.64
1:G:157:PRO:O	1:G:160:ILE:HG22	1.97	0.64
1:H:234:THR:HG22	1:H:237:GLU:H	1.62	0.64
1:C:32:SER:O	1:C:53:ILE:HA	1.98	0.64
1:G:96:LEU:CD1	1:G:201:ILE:HG12	2.27	0.64
1:E:130:GLU:O	1:E:133:GLN:HB2	1.99	0.63
1:G:197:SER:O	1:G:201:ILE:HG13	1.98	0.63
1:C:184:LEU:HG	1:C:196:ALA:HB1	1.81	0.63
1:A:63:LEU:HG	1:A:322:LEU:HD23	1.81	0.62
1:A:17:MET:HG2	1:A:396:THR:HA	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:501:HEM:HBB2	2:C:501:HEM:HMB2	1.81	0.62
1:A:234:THR:HG22	1:A:237:GLU:H	1.65	0.62
1:H:211:LYS:HE2	1:H:220:LEU:HD23	1.81	0.62
2:D:501:HEM:HBB2	2:D:501:HEM:HMB2	1.82	0.62
1:H:160:ILE:HA	1:H:163:ILE:HG22	1.80	0.62
1:C:24:TYR:OH	1:C:297:HIS:NE2	2.32	0.61
1:A:26:ARG:HH11	1:A:26:ARG:HB3	1.65	0.61
1:G:263:HIS:HB3	1:G:340:LEU:HD22	1.81	0.61
1:B:133:GLN:NE2	1:B:137:GLU:OE1	2.33	0.61
1:C:290:ARG:HH12	1:C:344:ARG:HE	1.49	0.61
1:D:67:ARG:HG2	1:D:305:GLU:HG2	1.82	0.61
1:H:128:ARG:O	1:H:132:GLU:HG3	1.99	0.61
1:G:243:PHE:O	1:G:247:ILE:HG22	2.00	0.61
2:A:501:HEM:HBB2	2:A:501:HEM:HMB2	1.83	0.61
1:D:309:ILE:HD12	1:D:314:ILE:HD12	1.83	0.61
1:A:124:ILE:HD12	1:A:364:LEU:HD13	1.83	0.60
1:D:23:VAL:O	1:D:27:LEU:HD12	2.01	0.60
2:E:501:HEM:HBB2	2:E:501:HEM:HMB2	1.83	0.60
1:B:386:ALA:HB3	1:B:407:PRO:HB2	1.84	0.60
1:B:278:ARG:NH1	1:B:378:ASP:OD1	2.29	0.60
1:C:186:SER:HB3	1:C:395:ARG:HH11	1.67	0.60
1:B:390:GLU:CD	1:B:390:GLU:H	2.10	0.59
1:F:51:TRP:HB2	1:F:320:VAL:HG22	1.84	0.59
1:C:55:GLY:O	1:C:59:VAL:HG23	2.01	0.59
1:E:105:PRO:HA	1:E:108:HIS:HB3	1.82	0.59
1:E:123:ALA:HA	1:E:126:LYS:HE2	1.83	0.59
1:B:270:GLN:NE2	1:B:340:LEU:O	2.35	0.59
1:D:39:PRO:HB2	1:D:42:VAL:HG23	1.83	0.59
1:F:263:HIS:NE2	1:F:292:GLU:HG3	2.17	0.59
2:G:501:HEM:HMC2	2:G:501:HEM:HBC2	1.83	0.59
1:H:156:PHE:HD1	1:H:250:HIS:HE2	1.50	0.59
1:C:20:PRO:HD2	1:C:21:HIS:CE1	2.37	0.59
1:C:185:VAL:CG2	3:C:502:V0A:C23	2.76	0.59
1:E:277:ASP:OD1	1:E:279:SER:OG	2.20	0.59
1:F:270:GLN:HG2	1:F:342:VAL:HG22	1.84	0.59
1:B:169:VAL:HG21	1:B:246:PHE:HZ	1.66	0.59
1:C:382:ALA:HB1	1:G:382:ALA:HB1	1.84	0.59
1:D:184:LEU:HG	1:D:196:ALA:CB	2.33	0.59
1:B:291:LEU:O	1:B:329:ARG:NH1	2.30	0.59
1:C:46:GLY:O	1:C:82:ASN:ND2	2.35	0.58
1:C:192:ALA:O	1:C:195:ALA:HB3	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:124:ILE:HG21	1:E:364:LEU:HA	1.85	0.58
1:G:124:ILE:HG21	1:G:364:LEU:HA	1.86	0.58
1:H:32:SER:O	1:H:53:ILE:HA	2.04	0.58
1:C:124:ILE:HA	1:C:127:LEU:HD23	1.85	0.58
1:G:301:ARG:NH1	2:G:501:HEM:O1A	2.32	0.58
2:F:501:HEM:HMB2	2:F:501:HEM:HBB2	1.85	0.57
1:G:14:ASP:O	1:G:17:MET:N	2.38	0.57
1:C:234:THR:HG22	1:C:237:GLU:H	1.69	0.57
1:E:335:GLY:O	1:E:344:ARG:NH1	2.35	0.57
1:C:71:ASP:OD1	1:C:73:ASN:N	2.35	0.57
1:C:184:LEU:HG	1:C:196:ALA:CB	2.35	0.57
1:E:116:ASN:HA	1:E:360:LEU:HD11	1.85	0.56
1:E:134:ILE:HD13	1:E:161:ARG:HB3	1.86	0.56
1:G:265:MET:CE	1:G:384:ARG:HA	2.34	0.56
1:B:387:VAL:HG22	1:B:407:PRO:HG2	1.88	0.56
1:D:10:LEU:HD22	1:D:12:LEU:HD23	1.87	0.56
1:E:151:LEU:HD12	1:E:155:ALA:HB3	1.88	0.56
1:C:56:TYR:CD2	1:C:333:ARG:HG3	2.40	0.56
1:E:181:SER:HB3	1:E:247:ILE:HD11	1.87	0.56
1:H:361:GLY:HA3	2:H:501:HEM:C3C	2.41	0.56
1:D:275:ARG:HA	1:D:278:ARG:HH12	1.71	0.56
1:H:24:TYR:OH	1:H:297:HIS:NE2	2.32	0.55
1:H:268:LEU:HA	1:H:271:TRP:HB3	1.88	0.55
1:H:87:ASN:HA	1:H:93:SER:HB3	1.88	0.55
1:G:124:ILE:HD12	1:G:364:LEU:HB2	1.87	0.55
1:C:76:ASP:OD2	1:C:86:ARG:NH1	2.38	0.55
1:F:278:ARG:HG2	1:F:278:ARG:HH11	1.71	0.55
1:D:115:VAL:HG13	1:D:223:LEU:HD11	1.89	0.55
1:H:45:CYS:HA	1:H:48:LEU:HD12	1.88	0.55
2:G:501:HEM:HMB1	2:G:501:HEM:HBB2	1.88	0.55
1:H:219:VAL:O	1:H:223:LEU:HD12	2.06	0.55
1:E:11:GLU:OE1	1:E:40:PRO:HD3	2.07	0.54
1:C:149:ASP:HB3	1:C:152:ASP:HB3	1.89	0.54
1:G:91:ALA:CB	3:G:502:V0A:C21	2.85	0.54
1:G:99:HIS:CD2	1:G:244:LEU:HD22	2.42	0.54
2:B:501:HEM:HMB1	2:B:501:HEM:HBB2	1.90	0.54
1:B:277:ASP:OD1	1:B:279:SER:OG	2.24	0.54
1:G:385:LEU:HD21	1:G:392:MET:HE1	1.90	0.54
1:B:148:VAL:HG23	1:B:408:VAL:O	2.07	0.54
1:G:366:ARG:O	1:G:370:GLN:HB2	2.07	0.54
1:H:163:ILE:HG13	1:H:167:LEU:HD22	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:115:VAL:CG1	1:G:223:LEU:HD11	2.38	0.54
1:A:124:ILE:HG21	1:A:364:LEU:HA	1.90	0.54
1:B:128:ARG:O	1:B:132:GLU:HG3	2.08	0.54
1:D:269:ASP:OD1	1:D:270:GLN:N	2.41	0.54
1:B:144:ASP:OD1	1:B:144:ASP:N	2.41	0.54
1:C:184:LEU:HD11	1:C:200:MET:HG3	1.89	0.54
1:A:133:GLN:O	1:A:137:GLU:HG3	2.07	0.53
1:C:383:MET:HA	1:C:409:ARG:O	2.09	0.53
1:F:177:PHE:HE1	1:F:200:MET:HE1	1.73	0.53
1:G:383:MET:SD	1:G:408:VAL:HG21	2.48	0.53
1:H:252:THR:HB	2:H:501:HEM:HAB	1.90	0.53
1:C:373:PHE:O	1:C:377:LEU:HD22	2.07	0.53
1:A:109:THR:O	1:A:113:LYS:HG3	2.07	0.53
1:C:249:GLY:HA2	2:C:501:HEM:C2C	2.43	0.53
1:D:158:LEU:HB3	1:D:159:PRO:HD3	1.91	0.53
1:F:139:LEU:O	1:F:142:LEU:HG	2.08	0.53
1:C:158:LEU:HB3	1:C:159:PRO:HD3	1.90	0.53
1:D:115:VAL:CG1	1:D:223:LEU:HD11	2.39	0.53
1:F:53:ILE:HD12	1:F:309:ILE:HG21	1.89	0.53
1:C:387:VAL:HG23	1:C:407:PRO:HG2	1.91	0.53
1:H:131:ILE:O	1:H:135:THR:OG1	2.27	0.53
1:G:158:LEU:HB3	1:G:159:PRO:HD3	1.91	0.52
1:H:102:HIS:NE2	1:H:299:THR:HG21	2.23	0.52
1:H:243:PHE:O	1:H:247:ILE:HG22	2.09	0.52
1:D:269:ASP:OD1	1:D:270:GLN:HG2	2.08	0.52
1:G:235:GLU:O	1:G:239:VAL:HG23	2.10	0.52
1:E:262:LEU:O	1:E:266:ARG:HG3	2.10	0.52
1:G:45:CYS:HA	1:G:48:LEU:HD12	1.91	0.52
1:B:27:LEU:HB3	1:B:34:HIS:CE1	2.45	0.52
1:A:371:VAL:O	1:A:375:VAL:HG23	2.09	0.51
1:E:105:PRO:HG3	1:G:66:PRO:HG2	1.90	0.51
1:E:146:ASP:HB3	1:E:147:PRO:HD3	1.91	0.51
1:H:235:GLU:O	1:H:239:VAL:HG23	2.10	0.51
1:C:185:VAL:CG2	3:C:502:V0A:C20	2.87	0.51
1:D:124:ILE:HG21	1:D:364:LEU:HA	1.91	0.51
1:A:158:LEU:HB3	1:A:159:PRO:HD3	1.92	0.51
1:C:185:VAL:HG22	3:C:502:V0A:C20	2.40	0.51
1:C:235:GLU:O	1:C:239:VAL:HG23	2.10	0.51
1:C:227:ARG:HG3	1:C:238:LEU:HD12	1.92	0.51
1:D:220:LEU:O	1:D:224:VAL:HG23	2.11	0.51
1:F:158:LEU:HB3	1:F:159:PRO:HD3	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:66:PRO:CG	1:D:105:PRO:HG3	2.40	0.51
1:G:154:PHE:HE1	1:G:158:LEU:HD13	1.76	0.51
1:A:26:ARG:HB3	1:A:26:ARG:NH1	2.25	0.51
1:B:158:LEU:HB3	1:B:159:PRO:HD3	1.92	0.50
1:C:382:ALA:CB	1:G:382:ALA:HB1	2.41	0.50
1:D:131:ILE:HG22	1:D:371:VAL:HG11	1.93	0.50
1:D:275:ARG:C	1:D:278:ARG:HH12	2.19	0.50
1:A:265:MET:HE2	1:A:265:MET:HA	1.92	0.50
1:B:169:VAL:HG22	1:B:207:LEU:HD11	1.93	0.50
1:F:105:PRO:HA	1:F:108:HIS:HB3	1.93	0.50
1:G:344:ARG:HG2	1:G:345:PRO:HD2	1.93	0.50
1:H:105:PRO:HG2	1:H:106:PRO:HD3	1.93	0.50
1:G:156:PHE:CE1	1:G:254:VAL:HG11	2.46	0.50
1:D:184:LEU:HG	1:D:196:ALA:HB3	1.94	0.50
1:A:160:ILE:HA	1:A:163:ILE:HG22	1.92	0.50
1:A:270:GLN:HG2	1:A:342:VAL:HG22	1.94	0.50
1:B:63:LEU:HG	1:B:322:LEU:HD23	1.93	0.50
1:F:386:ALA:HB3	1:F:407:PRO:HB2	1.93	0.50
1:A:148:VAL:HG23	1:A:408:VAL:O	2.11	0.50
1:D:184:LEU:HG	1:D:196:ALA:HB1	1.94	0.50
1:C:21:HIS:HE1	1:C:401:ARG:NH2	2.09	0.50
1:C:43:PRO:HB3	1:C:193:THR:HG21	1.94	0.50
1:E:139:LEU:HD21	1:E:375:VAL:HG12	1.93	0.50
1:B:160:ILE:HA	1:B:163:ILE:HG22	1.92	0.50
1:G:376:LEU:HD12	1:G:383:MET:HE3	1.92	0.50
1:H:252:THR:HB	2:H:501:HEM:C3B	2.47	0.50
1:B:145:GLU:HG2	1:B:147:PRO:HD2	1.93	0.50
1:F:104:ASP:HB3	1:F:105:PRO:HD2	1.93	0.50
1:F:105:PRO:HG3	1:H:66:PRO:CG	2.39	0.50
1:F:160:ILE:HA	1:F:163:ILE:HG22	1.92	0.50
1:B:43:PRO:HB3	1:B:193:THR:HG21	1.94	0.49
1:B:105:PRO:HG3	1:C:66:PRO:CG	2.41	0.49
1:F:127:LEU:HD11	1:F:166:LEU:HD13	1.94	0.49
1:H:242:ALA:O	1:H:246:PHE:HD1	1.95	0.49
1:A:259:ASN:HB3	1:A:292:GLU:HB3	1.94	0.49
1:E:250:HIS:O	1:E:254:VAL:HG12	2.12	0.49
1:F:243:PHE:CE1	1:F:247:ILE:HG13	2.46	0.49
1:C:56:TYR:CE2	1:C:333:ARG:HG3	2.47	0.49
1:D:399:LEU:HD12	3:D:502:V0A:C22	2.43	0.49
1:E:66:PRO:CG	1:G:105:PRO:HG3	2.42	0.49
1:E:139:LEU:HD21	1:E:375:VAL:CG1	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:120:THR:HG21	1:H:332:GLU:HG3	1.95	0.49
1:F:332:GLU:OE1	1:H:120:THR:HG21	2.12	0.49
1:B:66:PRO:CG	1:C:105:PRO:HG3	2.38	0.49
1:B:113:LYS:NZ	1:C:308:ARG:HH11	2.11	0.49
1:B:66:PRO:HB3	1:C:66:PRO:HB3	1.93	0.49
1:D:160:ILE:HD12	1:D:250:HIS:HB2	1.95	0.49
1:D:249:GLY:HA2	2:D:501:HEM:C2C	2.48	0.49
1:D:250:HIS:CE1	1:D:251:GLU:HG2	2.48	0.49
1:C:286:GLU:OE1	1:C:349:HIS:NE2	2.42	0.49
1:D:234:THR:HG22	1:D:237:GLU:HB2	1.95	0.49
1:C:87:ASN:HA	1:C:93:SER:HB3	1.95	0.49
1:C:104:ASP:HB3	1:C:105:PRO:HD2	1.93	0.49
1:E:301:ARG:HH22	2:E:501:HEM:CGA	2.26	0.49
1:H:277:ASP:OD1	1:H:279:SER:OG	2.31	0.49
1:C:13:ASP:OD1	1:C:15:ALA:N	2.46	0.49
1:D:197:SER:O	1:D:201:ILE:HG23	2.13	0.49
1:D:277:ASP:OD1	1:D:279:SER:OG	2.22	0.49
1:H:296:LYS:HG2	1:H:401:ARG:HB2	1.94	0.49
1:B:57:GLU:OE2	1:C:112:ARG:NE	2.40	0.48
1:F:234:THR:HG21	4:F:641:HOH:O	2.12	0.48
1:C:124:ILE:HG21	1:C:364:LEU:HA	1.95	0.48
1:G:151:LEU:HA	1:G:155:ALA:HB3	1.95	0.48
1:H:160:ILE:HD12	1:H:250:HIS:HB2	1.95	0.48
1:E:187:GLY:HA3	1:E:193:THR:HG22	1.96	0.48
1:A:262:LEU:HD12	1:A:403:LEU:HD11	1.96	0.48
1:D:56:TYR:HA	1:D:327:ALA:HB1	1.95	0.48
1:B:24:TYR:HE1	1:B:52:LEU:HD21	1.78	0.48
1:D:32:SER:O	1:D:53:ILE:HA	2.13	0.48
1:E:270:GLN:NE2	1:E:340:LEU:O	2.46	0.48
1:F:45:CYS:HA	1:F:48:LEU:HD12	1.95	0.48
1:G:63:LEU:HG	1:G:322:LEU:HD13	1.95	0.48
1:G:364:LEU:O	1:G:368:GLU:HG3	2.14	0.48
1:D:183:ALA:O	1:D:193:THR:HA	2.14	0.48
1:H:104:ASP:HB3	1:H:105:PRO:HD2	1.95	0.48
1:F:115:VAL:HG13	1:F:223:LEU:HD21	1.96	0.48
1:G:164:CYS:SG	1:G:169:VAL:HB	2.54	0.48
1:G:265:MET:HE2	1:G:385:LEU:H	1.78	0.48
1:C:386:ALA:HB3	1:C:407:PRO:HB2	1.95	0.48
1:D:104:ASP:HB3	1:D:105:PRO:HD2	1.95	0.48
1:D:278:ARG:HG2	1:D:278:ARG:HH11	1.79	0.48
1:G:19:ASP:OD2	1:G:22:SER:OG	2.26	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:301:ARG:HH12	2:G:501:HEM:CGA	2.24	0.48
1:B:45:CYS:HA	1:B:48:LEU:HD12	1.95	0.48
1:B:251:GLU:OE1	1:B:395:ARG:NH1	2.45	0.48
1:C:99:HIS:CD2	1:C:244:LEU:HD22	2.48	0.48
1:C:124:ILE:HD12	1:C:364:LEU:HD13	1.95	0.48
1:A:28:ASN:HA	1:A:31:GLY:O	2.13	0.47
1:E:28:ASN:HA	1:E:31:GLY:O	2.13	0.47
1:A:146:ASP:HB3	1:A:147:PRO:HD3	1.95	0.47
1:D:185:VAL:HG13	1:D:400:ILE:HG13	1.96	0.47
1:H:56:TYR:CD1	1:H:333:ARG:HG3	2.49	0.47
1:B:250:HIS:O	1:B:254:VAL:HG12	2.14	0.47
1:C:296:LYS:HE3	1:C:400:ILE:O	2.14	0.47
1:D:263:HIS:HB3	1:D:340:LEU:HD22	1.96	0.47
1:D:120:THR:CG2	1:D:123:ALA:H	2.27	0.47
1:G:226:ALA:O	1:G:232:ARG:HB2	2.14	0.47
1:B:17:MET:HG2	1:B:396:THR:HA	1.97	0.47
1:D:38:MET:H	1:D:38:MET:HG2	1.27	0.47
1:D:107:ASP:CG	1:D:110:ARG:HH21	2.23	0.47
1:E:45:CYS:HA	1:E:48:LEU:HD12	1.96	0.47
1:E:163:ILE:HD12	1:E:163:ILE:HA	1.73	0.47
1:F:125:GLU:HA	1:F:367:MET:HE1	1.96	0.47
1:G:154:PHE:CE1	1:G:158:LEU:HD13	2.50	0.47
1:H:252:THR:HB	2:H:501:HEM:CAB	2.44	0.47
1:H:296:LYS:HE2	1:H:400:ILE:O	2.15	0.47
1:B:124:ILE:HG21	1:B:364:LEU:HA	1.97	0.47
1:C:234:THR:CG2	1:C:237:GLU:H	2.27	0.47
1:D:266:ARG:HE	1:D:389:PRO:HB3	1.80	0.47
2:B:501:HEM:HMC1	2:B:501:HEM:HBC2	1.96	0.47
1:H:293:SER:OG	1:H:328:ASN:ND2	2.47	0.47
1:H:295:LEU:HD23	1:H:295:LEU:HA	1.79	0.47
1:G:105:PRO:HG2	1:G:106:PRO:HD3	1.97	0.46
1:C:59:VAL:HG13	1:C:322:LEU:HB3	1.97	0.46
1:C:274:LEU:HD23	1:C:274:LEU:HA	1.69	0.46
1:E:234:THR:CG2	1:E:237:GLU:H	2.27	0.46
1:A:116:ASN:HA	1:A:360:LEU:HD11	1.96	0.46
1:C:383:MET:SD	1:C:408:VAL:HG21	2.55	0.46
1:F:220:LEU:HA	1:F:223:LEU:HD12	1.96	0.46
1:F:262:LEU:HD13	1:F:392:MET:HE1	1.97	0.46
1:H:216:THR:OG1	1:H:217:ASP:N	2.47	0.46
1:F:262:LEU:O	1:F:266:ARG:HG2	2.16	0.46
1:G:189:SER:O	1:G:193:THR:HG23	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:21:HIS:CD2	1:C:329:ARG:HE	2.34	0.46
1:C:151:LEU:HA	1:C:155:ALA:HB3	1.97	0.46
1:C:281:LEU:O	1:C:285:VAL:HG23	2.15	0.46
1:C:300:PHE:CE1	1:C:321:LEU:HD13	2.50	0.46
1:C:383:MET:HE3	1:C:408:VAL:HG21	1.97	0.46
1:G:220:LEU:O	1:G:224:VAL:HG23	2.16	0.46
1:H:383:MET:SD	1:H:408:VAL:HG21	2.56	0.46
1:A:128:ARG:O	1:A:132:GLU:HG3	2.15	0.46
1:B:138:LEU:HD23	1:B:138:LEU:HA	1.78	0.46
1:D:38:MET:HE2	1:D:38:MET:HB3	1.79	0.46
1:D:233:LEU:HD11	1:D:237:GLU:HB3	1.98	0.46
1:E:259:ASN:HB3	1:E:292:GLU:HB3	1.97	0.46
1:E:297:HIS:HD2	1:E:323:ALA:HA	1.80	0.46
1:D:216:THR:OG1	1:D:217:ASP:N	2.49	0.46
1:D:308:ARG:HG2	1:D:313:ALA:HA	1.98	0.46
1:H:383:MET:HA	1:H:409:ARG:O	2.16	0.46
1:A:298:ALA:HB1	2:A:501:HEM:O1A	2.15	0.46
1:F:28:ASN:HA	1:F:31:GLY:O	2.16	0.46
1:B:220:LEU:HA	1:B:223:LEU:HD12	1.98	0.46
1:C:398:THR:HG22	1:C:399:LEU:HD23	1.96	0.46
1:D:234:THR:CG2	1:D:237:GLU:H	2.29	0.46
2:E:501:HEM:HMC1	2:E:501:HEM:HBC2	1.98	0.46
1:E:270:GLN:HE22	1:E:340:LEU:C	2.24	0.45
2:F:501:HEM:HBC2	2:F:501:HEM:HMC1	1.98	0.45
1:E:189:SER:O	1:E:193:THR:HG23	2.16	0.45
1:D:299:THR:OG1	2:D:501:HEM:O1A	2.35	0.45
1:G:373:PHE:O	1:G:377:LEU:HG	2.17	0.45
1:D:275:ARG:CA	1:D:278:ARG:HH12	2.29	0.45
1:E:299:THR:HG22	2:E:501:HEM:O1A	2.15	0.45
1:D:151:LEU:HA	1:D:155:ALA:HB3	1.98	0.45
1:A:99:HIS:CD2	1:A:244:LEU:HD22	2.51	0.45
1:A:117:LYS:HD3	1:A:117:LYS:HA	1.69	0.45
1:C:292:GLU:OE2	1:C:329:ARG:NH2	2.50	0.45
1:D:19:ASP:OD2	1:D:22:SER:OG	2.27	0.45
1:G:14:ASP:O	1:G:15:ALA:C	2.59	0.45
1:G:329:ARG:HH21	1:G:338:HIS:CA	2.29	0.45
1:F:233:LEU:HD11	1:F:237:GLU:HB3	1.98	0.45
1:G:263:HIS:NE2	1:G:292:GLU:HG2	2.32	0.45
1:H:184:LEU:HD23	1:H:184:LEU:HA	1.72	0.45
1:B:104:ASP:HB3	1:B:105:PRO:HD2	1.98	0.45
1:B:110:ARG:HD3	1:B:232:ARG:O	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:43:PRO:CB	1:C:193:THR:HG21	2.47	0.45
1:H:158:LEU:O	1:H:162:VAL:HG23	2.17	0.45
1:D:261:THR:HB	1:D:406:LEU:HD21	1.98	0.45
1:F:263:HIS:HE2	1:F:292:GLU:HG3	1.80	0.45
1:G:216:THR:OG1	1:G:217:ASP:N	2.49	0.45
1:G:233:LEU:HD23	1:G:238:LEU:HD23	1.99	0.45
1:G:265:MET:HE3	1:G:265:MET:HA	1.99	0.45
1:A:249:GLY:HA2	2:A:501:HEM:C2C	2.52	0.45
1:A:250:HIS:O	1:A:254:VAL:HG12	2.17	0.45
1:C:14:ASP:O	1:C:17:MET:N	2.50	0.45
1:C:399:LEU:HD12	3:C:502:V0A:C22	2.47	0.45
1:E:257:LEU:HD21	1:E:372:ALA:HB3	1.99	0.45
1:F:216:THR:OG1	1:F:217:ASP:N	2.49	0.45
1:G:387:VAL:HG22	1:G:388:ASP:N	2.32	0.45
1:B:105:PRO:HA	1:B:108:HIS:HB3	2.00	0.44
1:B:233:LEU:HD12	1:B:233:LEU:HA	1.79	0.44
1:C:112:ARG:O	1:C:116:ASN:HB3	2.17	0.44
1:E:24:TYR:HB3	1:E:326:SER:HB2	1.98	0.44
1:C:19:ASP:OD2	1:C:22:SER:OG	2.25	0.44
1:D:234:THR:HG23	1:D:237:GLU:H	1.82	0.44
1:D:361:GLY:HA3	2:D:501:HEM:C3C	2.52	0.44
1:E:211:LYS:NZ	1:E:218:ASP:OD2	2.47	0.44
1:H:133:GLN:O	1:H:137:GLU:HG3	2.17	0.44
1:H:366:ARG:HD3	4:H:613:HOH:O	2.17	0.44
1:A:387:VAL:HG22	1:A:407:PRO:HG2	1.99	0.44
1:B:264:LEU:HD13	1:B:271:TRP:HE3	1.82	0.44
1:F:155:ALA:C	1:F:254:VAL:HG23	2.42	0.44
1:G:367:MET:O	1:G:371:VAL:HG23	2.18	0.44
1:H:139:LEU:HD11	1:H:379:THR:OG1	2.18	0.44
2:A:501:HEM:HBC2	2:A:501:HEM:HMC1	2.00	0.44
1:E:296:LYS:HG3	1:E:297:HIS:CG	2.52	0.44
1:F:139:LEU:HD21	1:F:375:VAL:CG1	2.47	0.44
1:A:156:PHE:HD1	1:A:250:HIS:NE2	2.15	0.44
1:D:105:PRO:HA	1:D:108:HIS:HB3	1.99	0.44
1:D:166:LEU:HD23	1:D:166:LEU:HA	1.87	0.44
1:D:274:LEU:O	1:D:278:ARG:NH1	2.51	0.44
1:E:105:PRO:HG3	1:G:66:PRO:CG	2.47	0.44
1:E:128:ARG:HD2	1:E:367:MET:HE1	1.99	0.44
1:A:135:THR:HG23	1:A:154:PHE:HZ	1.83	0.44
1:H:20:PRO:HB2	1:H:24:TYR:CE2	2.53	0.44
1:A:287:GLU:HG3	1:A:340:LEU:HD12	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:388:ASP:HA	1:A:389:PRO:HD2	1.85	0.44
1:C:107:ASP:CG	1:C:110:ARG:HH21	2.24	0.44
1:C:183:ALA:HA	1:C:186:SER:O	2.18	0.44
1:C:185:VAL:CG2	3:C:502:V0A:C22	2.84	0.44
1:C:400:ILE:HD11	3:C:502:V0A:C18	2.48	0.44
1:D:178:LYS:H	1:D:178:LYS:HG3	1.47	0.44
1:F:102:HIS:NE2	1:F:299:THR:HG21	2.33	0.44
1:G:156:PHE:HE2	1:G:395:ARG:HH22	1.64	0.44
1:H:27:LEU:HB3	1:H:34:HIS:CD2	2.53	0.44
1:B:120:THR:HG23	1:C:332:GLU:O	2.18	0.44
1:B:252:THR:HB	2:B:501:HEM:C3B	2.52	0.44
1:C:151:LEU:HD11	1:C:403:LEU:HB2	2.00	0.44
1:D:180:TRP:O	1:D:196:ALA:HB2	2.17	0.44
1:H:243:PHE:CZ	1:H:247:ILE:HG21	2.53	0.44
1:A:144:ASP:OD1	1:A:144:ASP:N	2.51	0.43
1:B:291:LEU:O	1:B:329:ARG:HD2	2.18	0.43
2:C:501:HEM:HMC1	2:C:501:HEM:HBC2	1.98	0.43
1:G:20:PRO:HB2	1:G:24:TYR:CE2	2.53	0.43
1:G:165:LEU:HD23	1:G:165:LEU:HA	1.86	0.43
1:B:39:PRO:HD2	1:B:42:VAL:HG21	2.00	0.43
1:B:281:LEU:O	1:B:285:VAL:HG23	2.18	0.43
1:C:220:LEU:O	1:C:224:VAL:HG23	2.18	0.43
1:E:387:VAL:HG22	1:E:407:PRO:HG2	1.99	0.43
1:F:264:LEU:HD13	1:F:271:TRP:HE3	1.83	0.43
1:H:124:ILE:HA	1:H:127:LEU:HD13	1.99	0.43
1:B:269:ASP:OD1	1:B:269:ASP:N	2.51	0.43
1:D:266:ARG:HE	1:D:389:PRO:CB	2.31	0.43
1:H:105:PRO:HA	1:H:108:HIS:HB3	1.99	0.43
1:H:234:THR:CG2	1:H:237:GLU:H	2.28	0.43
1:H:384:ARG:O	1:H:408:VAL:HG23	2.18	0.43
1:A:66:PRO:HB3	1:D:66:PRO:HB3	2.01	0.43
1:A:308:ARG:HD3	1:D:113:LYS:NZ	2.34	0.43
1:B:270:GLN:OE1	1:B:340:LEU:HG	2.18	0.43
1:E:233:LEU:HD12	1:E:233:LEU:HA	1.66	0.43
1:E:290:ARG:HG2	1:E:328:ASN:HB3	2.00	0.43
1:G:243:PHE:CZ	1:G:247:ILE:HG21	2.53	0.43
1:B:52:LEU:HD11	1:B:323:ALA:HB2	2.00	0.43
1:A:105:PRO:HG3	1:D:66:PRO:CG	2.45	0.43
1:C:163:ILE:HD12	1:C:163:ILE:HA	1.73	0.43
1:C:380:PHE:CD1	1:C:410:LEU:HB3	2.53	0.43
1:F:12:LEU:O	1:F:39:PRO:HG3	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:130:GLU:O	1:F:133:GLN:HB2	2.17	0.43
1:H:27:LEU:HB3	1:H:34:HIS:NE2	2.33	0.43
1:B:332:GLU:CD	1:C:120:THR:HG21	2.44	0.43
1:C:124:ILE:HA	1:C:127:LEU:CD2	2.48	0.43
1:E:373:PHE:O	1:E:377:LEU:HG	2.19	0.43
1:H:250:HIS:O	1:H:254:VAL:HG12	2.19	0.43
1:E:392:MET:HE2	1:E:392:MET:HB3	1.82	0.43
1:F:291:LEU:O	1:F:329:ARG:NH1	2.39	0.43
1:G:392:MET:HE2	1:G:392:MET:HB2	1.53	0.43
1:H:163:ILE:HD12	1:H:163:ILE:HA	1.85	0.43
1:H:300:PHE:CD1	1:H:321:LEU:HD13	2.53	0.43
1:A:48:LEU:HA	1:A:49:PRO:HD3	1.83	0.43
1:C:48:LEU:HA	1:C:49:PRO:HD3	1.92	0.43
1:F:12:LEU:HD12	1:F:38:MET:SD	2.59	0.43
1:F:116:ASN:HA	1:F:360:LEU:HD11	2.00	0.43
1:G:97:ALA:HA	1:G:99:HIS:CE1	2.54	0.43
1:H:148:VAL:HG21	1:H:410:LEU:HD13	2.01	0.43
1:A:278:ARG:HH11	1:A:278:ARG:HD2	1.69	0.42
1:A:301:ARG:HH22	2:A:501:HEM:CGA	2.30	0.42
1:B:139:LEU:HD22	1:B:380:PHE:HE2	1.83	0.42
1:C:101:LEU:HD12	1:C:101:LEU:O	2.19	0.42
1:D:24:TYR:OH	1:D:297:HIS:NE2	2.49	0.42
1:D:102:HIS:NE2	1:D:299:THR:HG21	2.34	0.42
1:A:241:MET:O	1:A:245:LEU:HG	2.19	0.42
1:D:98:THR:HG22	1:D:237:GLU:HG3	2.00	0.42
1:F:142:LEU:HB2	1:F:143:PRO:CD	2.48	0.42
1:F:262:LEU:CD1	1:F:392:MET:HE1	2.49	0.42
1:F:278:ARG:HG2	1:F:278:ARG:NH1	2.35	0.42
1:A:111:LEU:O	1:A:241:MET:HE1	2.19	0.42
1:A:163:ILE:HD12	1:A:163:ILE:HA	1.83	0.42
1:B:135:THR:HG23	1:B:154:PHE:HZ	1.84	0.42
1:D:35:ARG:NH1	1:D:49:PRO:HB2	2.34	0.42
1:E:120:THR:OG1	1:G:332:GLU:HG3	2.19	0.42
1:G:43:PRO:CB	1:G:193:THR:HG21	2.49	0.42
1:G:233:LEU:HD12	1:G:234:THR:H	1.84	0.42
1:G:376:LEU:HD13	1:G:376:LEU:HA	1.79	0.42
1:H:138:LEU:HD23	1:H:138:LEU:HA	1.77	0.42
1:D:23:VAL:HG12	1:D:27:LEU:CD1	2.50	0.42
1:F:139:LEU:HD21	1:F:375:VAL:HG12	2.01	0.42
1:A:33:ALA:HB3	1:A:312:THR:HG21	2.01	0.42
1:A:344:ARG:O	1:A:345:PRO:C	2.63	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:272:GLU:OE1	1:B:272:GLU:HA	2.19	0.42
1:B:297:HIS:HD2	1:B:323:ALA:HA	1.84	0.42
1:B:335:GLY:O	1:B:344:ARG:NH1	2.47	0.42
1:D:278:ARG:HG2	1:D:278:ARG:NH1	2.35	0.42
1:E:37:MET:HG2	1:E:47:GLY:HA2	2.01	0.42
1:E:287:GLU:OE1	1:E:287:GLU:HA	2.20	0.42
1:G:28:ASN:ND2	4:G:602:HOH:O	2.49	0.42
1:G:104:ASP:HB3	1:G:105:PRO:HD2	2.00	0.42
1:H:227:ARG:HH21	1:H:235:GLU:HB2	1.85	0.42
1:B:120:THR:HG21	1:C:332:GLU:OE1	2.20	0.42
1:B:262:LEU:O	1:B:266:ARG:HG2	2.20	0.42
1:C:156:PHE:HD1	1:C:254:VAL:HG21	1.85	0.42
1:C:189:SER:O	1:C:193:THR:HG23	2.20	0.42
1:E:53:ILE:HD12	1:E:309:ILE:HG21	2.01	0.42
1:E:66:PRO:HB3	1:G:66:PRO:HB3	2.02	0.42
1:F:27:LEU:HB3	1:F:34:HIS:CE1	2.55	0.42
1:F:66:PRO:HB3	1:H:66:PRO:HB3	2.01	0.42
1:G:36:VAL:HG21	1:G:52:LEU:HB2	2.00	0.42
1:G:96:LEU:HD13	1:G:201:ILE:HG12	2.00	0.42
1:H:52:LEU:HD23	1:H:321:LEU:HB3	2.01	0.42
1:H:138:LEU:HD13	1:H:157:PRO:HG2	2.00	0.42
1:H:400:ILE:HD11	3:H:502:V0A:C17	2.50	0.42
1:B:139:LEU:HD23	1:B:139:LEU:HA	1.70	0.42
1:C:68:LEU:HD23	1:C:68:LEU:HA	1.88	0.42
1:C:362:ALA:O	1:C:366:ARG:HG3	2.18	0.42
1:D:189:SER:HB3	1:D:192:ALA:HB3	2.02	0.42
1:F:63:LEU:HG	1:F:322:LEU:HD23	2.00	0.42
1:F:291:LEU:O	1:F:329:ARG:HD2	2.19	0.42
1:G:97:ALA:HB1	1:G:102:HIS:HD1	1.84	0.42
1:G:257:LEU:HD21	1:G:369:ALA:HA	2.00	0.42
1:A:266:ARG:CD	1:A:389:PRO:HB3	2.50	0.42
1:B:234:THR:CG2	1:B:237:GLU:H	2.29	0.42
1:C:21:HIS:HA	1:C:24:TYR:CD2	2.55	0.42
1:C:185:VAL:HG11	1:C:400:ILE:HD12	2.02	0.42
1:D:243:PHE:CZ	1:D:247:ILE:HG21	2.55	0.42
1:G:265:MET:HE2	1:G:385:LEU:N	2.34	0.42
1:H:187:GLY:HA3	1:H:193:THR:CG2	2.49	0.42
1:A:86:ARG:HB3	1:A:94:SER:OG	2.19	0.42
1:C:181:SER:O	1:C:184:LEU:HB2	2.19	0.42
1:F:23:VAL:O	1:F:27:LEU:HG	2.20	0.42
1:G:178:LYS:HG2	1:G:182:LYS:HE3	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:252:THR:OG1	1:E:253:THR:N	2.53	0.42
1:F:60:ARG:HE	1:F:60:ARG:HB3	1.70	0.42
1:G:124:ILE:HA	1:G:127:LEU:HD12	2.01	0.42
1:H:166:LEU:HD23	1:H:166:LEU:HA	1.74	0.42
1:E:187:GLY:HA3	1:E:193:THR:CG2	2.50	0.41
1:E:243:PHE:CZ	1:E:247:ILE:HG21	2.55	0.41
1:H:28:ASN:HA	1:H:31:GLY:O	2.20	0.41
1:H:126:LYS:HB2	1:H:126:LYS:HE2	1.73	0.41
1:A:180:TRP:CZ2	1:A:199:ALA:HB1	2.55	0.41
1:C:266:ARG:HE	1:C:389:PRO:HG3	1.85	0.41
1:C:384:ARG:O	1:C:408:VAL:HG23	2.21	0.41
2:D:501:HEM:HMC1	2:D:501:HEM:HBC2	2.01	0.41
1:B:223:LEU:HD22	1:B:241:MET:HG2	2.03	0.41
1:D:23:VAL:HG12	1:D:27:LEU:HD11	2.03	0.41
1:H:290:ARG:HG2	1:H:328:ASN:HB3	2.03	0.41
1:H:385:LEU:HD21	1:H:392:MET:HE1	2.01	0.41
1:B:12:LEU:O	1:B:39:PRO:HG3	2.20	0.41
1:B:48:LEU:HA	1:B:49:PRO:HD3	1.93	0.41
1:D:383:MET:HA	1:D:409:ARG:O	2.20	0.41
1:G:105:PRO:HA	1:G:108:HIS:HB3	2.03	0.41
1:H:276:GLN:OE1	1:H:277:ASP:HB2	2.20	0.41
1:A:262:LEU:O	1:A:266:ARG:HG2	2.21	0.41
1:E:332:GLU:HG3	1:G:120:THR:HG21	2.01	0.41
1:G:204:LEU:O	1:G:208:ILE:HD12	2.21	0.41
1:A:269:ASP:OD1	1:A:269:ASP:N	2.53	0.41
1:A:371:VAL:HA	4:A:629:HOH:O	2.21	0.41
1:A:400:ILE:HD13	1:A:400:ILE:HA	1.87	0.41
1:F:17:MET:HG2	1:F:396:THR:HA	2.01	0.41
1:F:252:THR:HB	2:F:501:HEM:C3B	2.56	0.41
1:B:131:ILE:HG22	1:B:371:VAL:HG11	2.03	0.41
1:C:13:ASP:OD1	1:C:13:ASP:C	2.63	0.41
1:H:158:LEU:HB3	1:H:159:PRO:HD3	2.03	0.41
1:A:94:SER:O	1:A:98:THR:OG1	2.32	0.41
1:B:163:ILE:HD12	1:B:163:ILE:HA	1.90	0.41
1:E:328:ASN:OD1	1:E:350:VAL:HG12	2.21	0.41
1:F:332:GLU:HG3	1:H:120:THR:HG21	2.02	0.41
1:H:39:PRO:HA	1:H:40:PRO:HD3	1.99	0.41
1:B:220:LEU:O	1:B:224:VAL:HG23	2.20	0.41
1:C:35:ARG:NH2	4:C:601:HOH:O	2.33	0.41
1:C:151:LEU:O	1:C:156:PHE:HB2	2.21	0.41
1:C:366:ARG:O	1:C:370:GLN:HG3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:301:ARG:HB2	1:D:320:VAL:HG13	2.02	0.41
1:F:234:THR:CG2	1:F:237:GLU:H	2.24	0.41
1:G:21:HIS:NE2	1:G:292:GLU:OE1	2.53	0.41
1:G:383:MET:O	1:G:384:ARG:HD2	2.21	0.41
1:H:146:ASP:CB	1:H:147:PRO:HD3	2.50	0.41
1:H:220:LEU:O	1:H:224:VAL:HG23	2.21	0.41
1:B:219:VAL:O	1:B:223:LEU:HD12	2.21	0.41
1:G:136:GLY:HA2	1:G:139:LEU:HD23	2.03	0.40
1:H:296:LYS:CG	1:H:401:ARG:HB2	2.51	0.40
1:A:169:VAL:HG21	1:A:246:PHE:HZ	1.86	0.40
1:D:250:HIS:CG	1:D:251:GLU:N	2.86	0.40
1:B:243:PHE:CE1	1:B:247:ILE:HG13	2.57	0.40
1:E:27:LEU:HB3	1:E:34:HIS:NE2	2.36	0.40
1:E:128:ARG:O	1:E:132:GLU:HG3	2.21	0.40
1:E:166:LEU:HD12	1:E:166:LEU:HA	1.91	0.40
1:E:216:THR:OG1	1:E:217:ASP:N	2.52	0.40
1:A:233:LEU:HD12	1:A:233:LEU:HA	1.86	0.40
1:B:23:VAL:O	1:B:27:LEU:HD22	2.20	0.40
1:C:102:HIS:NE2	1:C:299:THR:HG21	2.35	0.40
1:D:184:LEU:HA	1:D:184:LEU:HD23	1.80	0.40
1:A:38:MET:HE3	1:A:398:THR:HG23	2.04	0.40
1:A:234:THR:CG2	1:A:237:GLU:H	2.33	0.40
1:B:53:ILE:HD12	1:B:309:ILE:HG21	2.03	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	395/414 (95%)	388 (98%)	7 (2%)	0	100	100
1	B	395/414 (95%)	389 (98%)	6 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	389/414 (94%)	373 (96%)	15 (4%)	1 (0%)	36	50
1	D	394/414 (95%)	383 (97%)	10 (2%)	1 (0%)	36	50
1	E	395/414 (95%)	386 (98%)	9 (2%)	0	100	100
1	F	395/414 (95%)	388 (98%)	6 (2%)	1 (0%)	36	50
1	G	395/414 (95%)	384 (97%)	10 (2%)	1 (0%)	36	50
1	H	395/414 (95%)	385 (98%)	10 (2%)	0	100	100
All	All	3153/3312 (95%)	3076 (98%)	73 (2%)	4 (0%)	48	64

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	147	PRO
1	G	145	GLU
1	F	147	PRO
1	D	147	PRO

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	324/345 (94%)	290 (90%)	34 (10%)	6	9
1	B	325/345 (94%)	294 (90%)	31 (10%)	8	12
1	C	311/345 (90%)	268 (86%)	43 (14%)	3	4
1	D	322/345 (93%)	280 (87%)	42 (13%)	4	5
1	E	324/345 (94%)	286 (88%)	38 (12%)	5	7
1	F	324/345 (94%)	291 (90%)	33 (10%)	7	10
1	G	316/345 (92%)	281 (89%)	35 (11%)	6	8
1	H	320/345 (93%)	285 (89%)	35 (11%)	6	8
All	All	2566/2760 (93%)	2275 (89%)	291 (11%)	5	7

All (291) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	ASP
1	A	17	MET
1	A	32	SER
1	A	42	VAL
1	A	45	CYS
1	A	60	ARG
1	A	87	ASN
1	A	94	SER
1	A	110	ARG
1	A	117	LYS
1	A	120	THR
1	A	144	ASP
1	A	151	LEU
1	A	171	LEU
1	A	179	SER
1	A	181	SER
1	A	185	VAL
1	A	188	ASP
1	A	193	THR
1	A	197	SER
1	A	201	ILE
1	A	214	THR
1	A	234	THR
1	A	240	SER
1	A	271	TRP
1	A	307	LEU
1	A	312	THR
1	A	320	VAL
1	A	345	PRO
1	A	346	THR
1	A	350	VAL
1	A	367	MET
1	A	383	MET
1	A	387	VAL
1	B	10	LEU
1	B	22	SER
1	B	32	SER
1	B	35	ARG
1	B	69	SER
1	B	109	THR
1	B	120	THR
1	B	122	ARG
1	B	144	ASP

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Mol	Chain	Res	Type
1	B	152	ASP
1	B	181	SER
1	B	185	VAL
1	B	189	SER
1	B	197	SER
1	B	201	ILE
1	B	225	SER
1	B	234	THR
1	B	269	ASP
1	B	271	TRP
1	B	274	LEU
1	B	276	GLN
1	B	299	THR
1	B	307	LEU
1	B	312	THR
1	B	322	LEU
1	B	346	THR
1	B	367	MET
1	B	379	THR
1	B	388	ASP
1	B	390	GLU
1	B	391	ASP
1	C	32	SER
1	C	35	ARG
1	C	38	MET
1	C	45	CYS
1	C	52	LEU
1	C	54	THR
1	C	60	ARG
1	C	72	LEU
1	C	85	ASP
1	C	94	SER
1	C	110	ARG
1	C	111	LEU
1	C	120	THR
1	C	121	SER
1	C	138	LEU
1	C	139	LEU
1	C	142	LEU
1	C	145	GLU
1	C	148	VAL
1	C	151	LEU

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Mol	Chain	Res	Type
1	C	163	ILE
1	C	165	LEU
1	C	166	LEU
1	C	182	LYS
1	C	185	VAL
1	C	186	SER
1	C	202	GLU
1	C	209	GLU
1	C	234	THR
1	C	236	THR
1	C	247	ILE
1	C	253	THR
1	C	254	VAL
1	C	277	ASP
1	C	279	SER
1	C	281	LEU
1	C	299	THR
1	C	312	THR
1	C	346	THR
1	C	385	LEU
1	C	387	VAL
1	C	400	ILE
1	C	408	VAL
1	D	13	ASP
1	D	14	ASP
1	D	32	SER
1	D	37	MET
1	D	38	MET
1	D	68	LEU
1	D	83	GLU
1	D	94	SER
1	D	120	THR
1	D	124	ILE
1	D	143	PRO
1	D	144	ASP
1	D	148	VAL
1	D	151	LEU
1	D	161	ARG
1	D	169	VAL
1	D	176	ASN
1	D	177	PHE
1	D	178	LYS

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Mol	Chain	Res	Type
1	D	179	SER
1	D	184	LEU
1	D	188	ASP
1	D	193	THR
1	D	201	ILE
1	D	202	GLU
1	D	247	ILE
1	D	250	HIS
1	D	262	LEU
1	D	279	SER
1	D	296	LYS
1	D	299	THR
1	D	312	THR
1	D	320	VAL
1	D	346	THR
1	D	367	MET
1	D	370	GLN
1	D	375	VAL
1	D	380	PHE
1	D	387	VAL
1	D	388	ASP
1	D	391	ASP
1	D	400	ILE
1	E	32	SER
1	E	45	CYS
1	E	52	LEU
1	E	60	ARG
1	E	61	SER
1	E	72	LEU
1	E	94	SER
1	E	117	LYS
1	E	120	THR
1	E	160	ILE
1	E	161	ARG
1	E	163	ILE
1	E	181	SER
1	E	185	VAL
1	E	188	ASP
1	E	189	SER
1	E	193	THR
1	E	201	ILE
1	E	217	ASP

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Mol	Chain	Res	Type
1	E	234	THR
1	E	247	ILE
1	E	262	LEU
1	E	279	SER
1	E	281	LEU
1	E	307	LEU
1	E	308	ARG
1	E	312	THR
1	E	314	ILE
1	E	320	VAL
1	E	326	SER
1	E	346	THR
1	E	367	MET
1	E	379	THR
1	E	383	MET
1	E	387	VAL
1	E	392	MET
1	E	393	ARG
1	E	410	LEU
1	F	11	GLU
1	F	30	GLU
1	F	32	SER
1	F	38	MET
1	F	45	CYS
1	F	57	GLU
1	F	60	ARG
1	F	68	LEU
1	F	72	LEU
1	F	94	SER
1	F	120	THR
1	F	124	ILE
1	F	131	ILE
1	F	148	VAL
1	F	151	LEU
1	F	171	LEU
1	F	185	VAL
1	F	193	THR
1	F	201	ILE
1	F	209	GLU
1	F	234	THR
1	F	252	THR
1	F	268	LEU

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Mol	Chain	Res	Type
1	F	269	ASP
1	F	280	LEU
1	F	299	THR
1	F	307	LEU
1	F	312	THR
1	F	322	LEU
1	F	379	THR
1	F	383	MET
1	F	388	ASP
1	F	405	SER
1	G	32	SER
1	G	94	SER
1	G	120	THR
1	G	138	LEU
1	G	139	LEU
1	G	142	LEU
1	G	146	ASP
1	G	148	VAL
1	G	149	ASP
1	G	151	LEU
1	G	158	LEU
1	G	166	LEU
1	G	167	LEU
1	G	178	LYS
1	G	185	VAL
1	G	198	THR
1	G	201	ILE
1	G	234	THR
1	G	247	ILE
1	G	253	THR
1	G	254	VAL
1	G	268	LEU
1	G	269	ASP
1	G	296	LYS
1	G	301	ARG
1	G	312	THR
1	G	320	VAL
1	G	343	ARG
1	G	344	ARG
1	G	370	GLN
1	G	376	LEU
1	G	379	THR

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Mol	Chain	Res	Type
1	G	383	MET
1	G	392	MET
1	G	395	ARG
1	H	11	GLU
1	H	38	MET
1	H	45	CYS
1	H	52	LEU
1	H	61	SER
1	H	85	ASP
1	H	94	SER
1	H	120	THR
1	H	121	SER
1	H	135	THR
1	H	144	ASP
1	H	160	ILE
1	H	179	SER
1	H	182	LYS
1	H	185	VAL
1	H	188	ASP
1	H	197	SER
1	H	198	THR
1	H	210	ARG
1	H	216	THR
1	H	223	LEU
1	H	225	SER
1	H	234	THR
1	H	262	LEU
1	H	269	ASP
1	H	279	SER
1	H	299	THR
1	H	307	LEU
1	H	308	ARG
1	H	312	THR
1	H	343	ARG
1	H	346	THR
1	H	387	VAL
1	H	392	MET
1	H	400	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	255	ASN
1	A	270	GLN
1	A	276	GLN
1	B	338	HIS
1	B	404	HIS
1	C	21	HIS
1	C	99	HIS
1	C	354	HIS
1	C	404	HIS
1	D	81	GLN
1	D	176	ASN
1	D	267	ASN
1	D	404	HIS
1	E	28	ASN
1	E	99	HIS
1	F	81	GLN
1	F	267	ASN
1	G	34	HIS
1	G	99	HIS
1	G	176	ASN
1	G	267	ASN
1	H	34	HIS
1	H	267	ASN

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 ⓘ

16 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	V0A	D	502	-	29,30,30	1.81	5 (17%)	27,45,45	3.14	10 (37%)
3	V0A	G	502	-	29,30,30	1.79	4 (13%)	27,45,45	3.76	14 (51%)
3	V0A	F	502	-	29,30,30	1.83	4 (13%)	27,45,45	3.35	10 (37%)
3	V0A	B	502	-	29,30,30	1.81	5 (17%)	27,45,45	3.42	9 (33%)
2	HEM	C	501	-	50,50,50	1.38	9 (18%)	67,82,82	1.10	6 (8%)
2	HEM	E	501	-	50,50,50	1.42	9 (18%)	67,82,82	1.13	5 (7%)
3	V0A	H	502	-	29,30,30	1.85	5 (17%)	27,45,45	2.91	8 (29%)
2	HEM	H	501	-	50,50,50	1.67	10 (20%)	67,82,82	1.64	11 (16%)
3	V0A	C	502	-	29,30,30	1.80	5 (17%)	27,45,45	3.19	11 (40%)
2	HEM	A	501	-	50,50,50	1.40	9 (18%)	67,82,82	1.13	6 (8%)
2	HEM	F	501	-	50,50,50	1.42	8 (16%)	67,82,82	1.07	5 (7%)
3	V0A	A	502	-	29,30,30	1.83	4 (13%)	27,45,45	3.40	10 (37%)
2	HEM	D	501	-	50,50,50	1.41	8 (16%)	67,82,82	1.16	6 (8%)
2	HEM	G	501	-	50,50,50	1.35	8 (16%)	67,82,82	1.11	4 (5%)
2	HEM	B	501	-	50,50,50	1.41	8 (16%)	67,82,82	1.11	5 (7%)
3	V0A	E	502	-	29,30,30	1.85	4 (13%)	27,45,45	3.34	11 (40%)

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	V0A	D	502	-	-	6/17/59/59	0/3/3/3
3	V0A	G	502	-	-	11/17/59/59	0/3/3/3
3	V0A	F	502	-	-	8/17/59/59	0/3/3/3
3	V0A	B	502	-	-	11/17/59/59	0/3/3/3
2	HEM	C	501	-	-	2/14/54/54	-
2	HEM	E	501	-	-	2/14/54/54	-
3	V0A	H	502	-	-	8/17/59/59	0/3/3/3
2	HEM	H	501	-	-	4/14/54/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	V0A	C	502	-	-	8/17/59/59	0/3/3/3
2	HEM	A	501	-	-	2/14/54/54	-
2	HEM	F	501	-	-	2/14/54/54	-
3	V0A	A	502	-	-	8/17/59/59	0/3/3/3
2	HEM	D	501	-	-	2/14/54/54	-
2	HEM	G	501	-	-	2/14/54/54	-
2	HEM	B	501	-	-	2/14/54/54	-
3	V0A	E	502	-	-	5/17/59/59	0/3/3/3

All (105) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	H	502	V0A	C27-C26	5.72	1.50	1.41
3	A	502	V0A	C27-C26	5.67	1.50	1.41
3	D	502	V0A	C27-N06	5.64	1.48	1.33
3	G	502	V0A	C27-N06	5.63	1.48	1.33
3	C	502	V0A	C27-N06	5.63	1.48	1.33
3	E	502	V0A	C27-N06	5.61	1.48	1.33
3	H	502	V0A	C27-N06	5.60	1.48	1.33
3	G	502	V0A	C27-C26	5.58	1.50	1.41
3	F	502	V0A	C27-N06	5.58	1.48	1.33
3	C	502	V0A	C27-C26	5.56	1.50	1.41
3	A	502	V0A	C27-N06	5.55	1.48	1.33
3	F	502	V0A	C27-C26	5.54	1.50	1.41
3	B	502	V0A	C27-N06	5.50	1.48	1.33
3	D	502	V0A	C27-C26	5.49	1.49	1.41
3	E	502	V0A	C27-C26	5.49	1.49	1.41
3	B	502	V0A	C27-C26	5.43	1.49	1.41
2	H	501	HEM	FE-NB	4.91	2.10	1.94
2	H	501	HEM	FE-NC	4.01	2.08	1.95
2	B	501	HEM	FE-NB	3.78	2.06	1.94
2	H	501	HEM	C1B-NB	-3.76	1.33	1.40
2	F	501	HEM	FE-NB	3.73	2.06	1.94
2	E	501	HEM	FE-NB	3.59	2.06	1.94
2	E	501	HEM	FE-NC	3.56	2.06	1.95
2	H	501	HEM	C4D-ND	-3.52	1.34	1.40
3	F	502	V0A	C25-C24	3.35	1.50	1.40
2	D	501	HEM	FE-NC	3.34	2.06	1.95
3	A	502	V0A	C25-C24	3.33	1.50	1.40
3	B	502	V0A	C25-C24	3.33	1.49	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	H	502	V0A	C25-C24	3.33	1.49	1.40
2	F	501	HEM	FE-NC	3.29	2.06	1.95
2	D	501	HEM	FE-NA	3.29	2.06	1.95
2	D	501	HEM	CAC-C3C	3.23	1.56	1.47
3	D	502	V0A	C25-C24	3.21	1.49	1.40
2	E	501	HEM	CAC-C3C	3.20	1.55	1.47
2	C	501	HEM	FE-NB	3.20	2.04	1.94
3	C	502	V0A	C25-C24	3.17	1.49	1.40
2	C	501	HEM	CAC-C3C	3.17	1.55	1.47
3	G	502	V0A	C25-C24	3.17	1.49	1.40
2	F	501	HEM	CAC-C3C	3.15	1.55	1.47
2	A	501	HEM	CAC-C3C	3.15	1.55	1.47
2	A	501	HEM	FE-ND	3.14	2.04	1.94
3	E	502	V0A	C25-C24	3.14	1.49	1.40
2	A	501	HEM	FE-NC	3.13	2.05	1.95
2	A	501	HEM	FE-NB	3.12	2.04	1.94
2	B	501	HEM	FE-NC	3.12	2.05	1.95
2	G	501	HEM	FE-NC	3.10	2.05	1.95
2	D	501	HEM	FE-NB	3.10	2.04	1.94
2	C	501	HEM	CAB-C3B	3.07	1.55	1.47
2	G	501	HEM	CAC-C3C	3.07	1.55	1.47
2	B	501	HEM	FE-ND	3.07	2.04	1.94
2	A	501	HEM	CAB-C3B	3.05	1.55	1.47
2	E	501	HEM	CAB-C3B	3.04	1.55	1.47
2	C	501	HEM	FE-NC	3.01	2.05	1.95
2	B	501	HEM	CAC-C3C	3.01	1.55	1.47
2	F	501	HEM	CAB-C3B	3.00	1.55	1.47
2	D	501	HEM	CAB-C3B	2.99	1.55	1.47
2	G	501	HEM	CAB-C3B	2.97	1.55	1.47
2	E	501	HEM	FE-ND	2.96	2.04	1.94
2	H	501	HEM	FE-ND	-2.96	1.85	1.94
2	F	501	HEM	FE-ND	2.95	2.04	1.94
3	E	502	V0A	O05-C28	2.94	1.29	1.23
3	F	502	V0A	O05-C28	2.93	1.29	1.23
2	B	501	HEM	CAB-C3B	2.92	1.55	1.47
3	G	502	V0A	O05-C28	2.92	1.29	1.23
3	D	502	V0A	O05-C28	2.91	1.29	1.23
3	C	502	V0A	O05-C28	2.90	1.29	1.23
3	H	502	V0A	O05-C28	2.89	1.29	1.23
2	G	501	HEM	FE-ND	2.89	2.03	1.94
2	A	501	HEM	FE-NA	2.89	2.04	1.95
3	A	502	V0A	O05-C28	2.86	1.28	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	501	HEM	FE-NA	2.80	2.04	1.95
2	G	501	HEM	FE-NB	2.80	2.03	1.94
2	H	501	HEM	C1C-C2C	-2.79	1.39	1.45
3	B	502	V0A	O05-C28	2.75	1.28	1.23
2	C	501	HEM	FE-ND	2.74	2.03	1.94
2	D	501	HEM	FE-ND	2.73	2.03	1.94
2	F	501	HEM	FE-NA	2.67	2.04	1.95
2	G	501	HEM	FE-NA	2.65	2.03	1.95
2	B	501	HEM	FE-NA	2.64	2.03	1.95
2	H	501	HEM	C1D-ND	-2.64	1.33	1.38
2	H	501	HEM	C4B-NB	-2.43	1.34	1.38
2	E	501	HEM	FE-NA	2.43	2.03	1.95
3	B	502	V0A	C23-C24	2.39	1.48	1.45
3	H	502	V0A	C23-C24	2.29	1.48	1.45
2	H	501	HEM	C1A-C2A	-2.29	1.40	1.44
2	D	501	HEM	CMC-C2C	2.26	1.55	1.50
2	G	501	HEM	CMC-C2C	2.26	1.55	1.50
2	B	501	HEM	CMC-C2C	2.23	1.55	1.50
2	C	501	HEM	CMC-C2C	2.23	1.55	1.50
2	A	501	HEM	CMC-C2C	2.20	1.55	1.50
3	D	502	V0A	C23-C24	2.19	1.48	1.45
2	B	501	HEM	CMB-C2B	2.18	1.55	1.50
2	A	501	HEM	CMB-C2B	2.18	1.55	1.50
2	E	501	HEM	CMC-C2C	2.17	1.55	1.50
2	E	501	HEM	CMB-C2B	2.16	1.55	1.50
2	F	501	HEM	CMB-C2B	2.16	1.55	1.50
2	F	501	HEM	CMC-C2C	2.15	1.55	1.50
2	C	501	HEM	CMB-C2B	2.08	1.55	1.50
2	H	501	HEM	C3C-C4C	-2.06	1.42	1.46
2	G	501	HEM	CMB-C2B	2.05	1.55	1.50
2	C	501	HEM	C2A-C3A	-2.03	1.33	1.38
2	D	501	HEM	CMB-C2B	2.03	1.54	1.50
2	E	501	HEM	CMD-C2D	2.01	1.54	1.50
2	A	501	HEM	CMD-C2D	2.00	1.54	1.50
3	C	502	V0A	C23-C24	2.00	1.48	1.45

All (131) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	502	V0A	C27-C26-C25	9.20	116.44	106.97
3	E	502	V0A	C27-C26-C25	9.11	116.34	106.97
3	B	502	V0A	C24-C25-C28	9.02	132.84	120.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	502	V0A	C27-C26-C25	9.02	116.25	106.97
3	E	502	V0A	C24-C25-C28	8.93	132.71	120.03
3	F	502	V0A	C27-C26-C25	8.93	116.15	106.97
3	C	502	V0A	C27-C26-C25	8.90	116.13	106.97
3	D	502	V0A	C27-C26-C25	8.89	116.11	106.97
3	G	502	V0A	C27-C26-C25	8.77	115.99	106.97
3	H	502	V0A	C27-C26-C25	8.70	115.91	106.97
3	C	502	V0A	C24-C25-C28	8.56	132.18	120.03
3	F	502	V0A	C24-C25-C28	8.42	131.99	120.03
3	D	502	V0A	C24-C25-C28	8.06	131.47	120.03
3	A	502	V0A	C24-C25-C28	7.70	130.96	120.03
3	G	502	V0A	C24-C25-C28	7.67	130.92	120.03
3	B	502	V0A	C23-C22-C20	-6.71	116.30	126.23
3	G	502	V0A	C23-C22-C20	-6.55	116.55	126.23
3	H	502	V0A	C24-C25-C28	6.31	128.99	120.03
3	G	502	V0A	C23-C24-C25	-6.04	117.93	124.39
3	G	502	V0A	O02-C09-C07	5.84	120.03	109.59
3	E	502	V0A	C23-C22-C20	-5.77	117.69	126.23
3	B	502	V0A	C26-C27-N06	-5.71	100.21	111.72
3	E	502	V0A	C26-C27-N06	-5.62	100.41	111.72
3	C	502	V0A	C26-C27-N06	-5.59	100.46	111.72
3	A	502	V0A	C26-C27-N06	-5.57	100.50	111.72
3	D	502	V0A	C26-C27-N06	-5.54	100.56	111.72
3	G	502	V0A	C26-C27-N06	-5.53	100.59	111.72
3	F	502	V0A	C26-C27-N06	-5.49	100.67	111.72
3	H	502	V0A	C26-C27-N06	-5.41	100.82	111.72
3	A	502	V0A	C23-C24-C25	-5.41	118.61	124.39
3	A	502	V0A	C23-C22-C20	-5.07	118.74	126.23
3	F	502	V0A	C23-C22-C20	-5.02	118.80	126.23
2	H	501	HEM	CHC-C4B-NB	4.79	129.58	124.42
2	H	501	HEM	CHD-C1D-ND	4.75	129.54	124.42
3	F	502	V0A	C09-C07-C08	4.46	117.52	108.21
3	G	502	V0A	C14-C07-C09	-4.43	103.66	112.22
3	B	502	V0A	C09-C07-C08	4.29	117.16	108.21
3	H	502	V0A	C09-C07-C08	4.28	117.14	108.21
3	D	502	V0A	C09-C07-C08	4.26	117.09	108.21
3	A	502	V0A	O02-C09-C07	4.25	117.19	109.59
3	G	502	V0A	O03-C24-C23	4.24	121.49	115.70
3	C	502	V0A	C09-C07-C08	4.19	116.94	108.21
3	A	502	V0A	C09-C07-C08	4.18	116.94	108.21
3	C	502	V0A	O02-C09-C07	4.06	116.84	109.59
3	H	502	V0A	O02-C09-C07	4.01	116.76	109.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	502	V0A	O02-C09-C07	3.87	116.50	109.59
3	H	502	V0A	C23-C22-C20	-3.87	120.52	126.23
3	F	502	V0A	C12-C09-C07	-3.84	109.36	115.56
3	F	502	V0A	C23-C24-C25	-3.81	120.31	124.39
3	E	502	V0A	C09-C07-C08	3.72	115.97	108.21
3	G	502	V0A	C17-C12-C18	-3.68	103.83	110.08
3	F	502	V0A	O02-C09-C07	3.63	116.08	109.59
3	B	502	V0A	O02-C09-C07	3.62	116.06	109.59
3	E	502	V0A	C09-C12-C18	-3.51	104.86	111.08
3	A	502	V0A	O03-C24-C23	3.46	120.42	115.70
3	D	502	V0A	C23-C24-C25	-3.42	120.73	124.39
3	C	502	V0A	C22-C23-C24	-3.41	117.03	122.49
2	H	501	HEM	CHA-C4D-ND	3.32	128.47	124.37
3	G	502	V0A	C09-C07-C08	3.27	115.04	108.21
2	H	501	HEM	C1B-NB-C4B	3.27	109.08	105.21
2	H	501	HEM	CHB-C1B-NB	3.26	128.40	124.37
3	D	502	V0A	O03-C24-C23	3.17	120.03	115.70
3	A	502	V0A	C12-C09-C07	-3.09	110.57	115.56
3	F	502	V0A	O03-C24-C23	3.09	119.92	115.70
3	G	502	V0A	C12-C18-C20	-3.06	117.21	126.72
2	H	501	HEM	CHD-C1D-C2D	-2.89	120.47	125.03
2	H	501	HEM	CAA-CBA-CGA	-2.83	106.15	113.67
3	E	502	V0A	C23-C24-C25	-2.82	121.38	124.39
2	A	501	HEM	C4D-ND-C1D	2.79	108.51	105.21
3	C	502	V0A	C12-C09-C07	-2.76	111.10	115.56
2	D	501	HEM	C4D-ND-C1D	2.75	108.46	105.21
2	B	501	HEM	C4D-ND-C1D	2.74	108.45	105.21
2	G	501	HEM	C4D-ND-C1D	2.72	108.42	105.21
2	E	501	HEM	C4D-ND-C1D	2.70	108.41	105.21
2	F	501	HEM	C4D-ND-C1D	2.68	108.38	105.21
3	G	502	V0A	C12-C09-C07	-2.65	111.28	115.56
3	E	502	V0A	O02-C09-C12	-2.61	101.15	106.26
2	C	501	HEM	C4D-ND-C1D	2.57	108.25	105.21
3	A	502	V0A	C14-C07-C08	-2.57	107.18	111.89
3	D	502	V0A	C14-C07-C08	-2.56	107.19	111.89
3	E	502	V0A	O03-C24-C23	2.54	119.16	115.70
3	C	502	V0A	O03-C24-C23	2.47	119.07	115.70
2	D	501	HEM	C3D-C4D-ND	-2.46	107.48	110.17
2	H	501	HEM	C1A-CHA-C4D	-2.37	120.67	126.25
2	E	501	HEM	C2A-C1A-NA	-2.34	107.55	110.15
2	C	501	HEM	CAA-CBA-CGA	-2.33	107.48	113.67
2	H	501	HEM	CHA-C4D-C3D	-2.33	120.93	125.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	501	HEM	C2A-C1A-NA	-2.33	107.57	110.15
3	C	502	V0A	C23-C24-C25	-2.32	121.91	124.39
3	B	502	V0A	C22-C23-C24	2.32	126.21	122.49
3	H	502	V0A	C14-C07-C08	-2.31	107.64	111.89
3	H	502	V0A	C12-C09-C07	-2.31	111.84	115.56
3	B	502	V0A	C12-C09-C07	-2.30	111.85	115.56
2	A	501	HEM	C1B-NB-C4B	2.30	107.93	105.21
2	B	501	HEM	C2A-C1A-NA	-2.28	107.62	110.15
2	D	501	HEM	CHD-C1D-ND	2.26	126.86	124.42
2	H	501	HEM	CHA-C1A-NA	2.26	127.95	123.86
2	D	501	HEM	C1B-NB-C4B	2.26	107.88	105.21
2	C	501	HEM	C2A-C1A-NA	-2.24	107.66	110.15
3	E	502	V0A	C21-C20-C22	-2.24	114.67	118.09
2	A	501	HEM	C2D-C1D-ND	-2.24	107.32	109.90
3	E	502	V0A	C11-C15-C13	-2.21	121.22	125.12
2	B	501	HEM	C3D-C4D-ND	-2.20	107.75	110.17
2	G	501	HEM	C2D-C1D-ND	-2.19	107.37	109.90
2	E	501	HEM	C1B-NB-C4B	2.18	107.79	105.21
3	F	502	V0A	C11-C15-C13	-2.18	121.27	125.12
2	A	501	HEM	C3D-C4D-ND	-2.18	107.78	110.17
2	D	501	HEM	C2A-C1A-NA	-2.18	107.74	110.15
2	F	501	HEM	C2A-C1A-NA	-2.17	107.74	110.15
2	G	501	HEM	C1B-NB-C4B	2.16	107.76	105.21
3	C	502	V0A	C14-C07-C08	-2.15	107.94	111.89
2	B	501	HEM	C2D-C1D-ND	-2.14	107.43	109.90
2	A	501	HEM	C3B-C2B-C1B	2.14	108.02	106.41
2	C	501	HEM	C1B-NB-C4B	2.13	107.73	105.21
2	A	501	HEM	C2A-C1A-NA	-2.13	107.79	110.15
2	E	501	HEM	C3D-C4D-ND	-2.12	107.85	110.17
3	G	502	V0A	O01-C08-C07	-2.11	107.37	109.97
2	E	501	HEM	C2D-C1D-ND	-2.11	107.47	109.90
3	D	502	V0A	C22-C23-C24	-2.10	119.12	122.49
2	C	501	HEM	C3D-C4D-ND	-2.10	107.87	110.17
3	G	502	V0A	C22-C20-C18	2.09	124.43	118.82
2	D	501	HEM	C2D-C1D-ND	-2.08	107.49	109.90
3	B	502	V0A	C11-C15-C13	-2.08	121.44	125.12
2	F	501	HEM	C1B-NB-C4B	2.08	107.67	105.21
2	F	501	HEM	C2D-C1D-ND	-2.08	107.50	109.90
2	F	501	HEM	C3D-C4D-ND	-2.07	107.90	110.17
2	H	501	HEM	O2D-CGD-O1D	-2.06	118.04	123.33
3	C	502	V0A	C11-C15-C13	-2.04	121.52	125.12
3	D	502	V0A	C23-C22-C20	-2.04	123.22	126.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	501	HEM	C1B-NB-C4B	2.02	107.60	105.21
2	C	501	HEM	C2D-C1D-ND	-2.01	107.58	109.90

There are no chirality outliers.

All (83) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	H	501	HEM	C2B-C3B-CAB-CBB
3	A	502	V0A	C07-C09-C12-C18
3	A	502	V0A	O02-C09-C12-C17
3	A	502	V0A	O02-C09-C12-C18
3	A	502	V0A	C17-C12-C18-C20
3	A	502	V0A	O03-C24-C25-C28
3	B	502	V0A	O02-C09-C12-C18
3	B	502	V0A	C18-C20-C22-C23
3	B	502	V0A	C22-C23-C24-C25
3	B	502	V0A	C22-C23-C24-O03
3	B	502	V0A	C23-C24-C25-C26
3	B	502	V0A	C23-C24-C25-C28
3	B	502	V0A	O03-C24-C25-C26
3	B	502	V0A	O03-C24-C25-C28
3	C	502	V0A	C18-C20-C22-C23
3	C	502	V0A	C23-C24-C25-C28
3	C	502	V0A	O03-C24-C25-C28
3	D	502	V0A	O02-C09-C12-C18
3	D	502	V0A	C18-C20-C22-C23
3	E	502	V0A	O02-C09-C12-C18
3	E	502	V0A	C17-C12-C18-C20
3	F	502	V0A	C07-C09-C12-C18
3	F	502	V0A	O02-C09-C12-C17
3	F	502	V0A	O02-C09-C12-C18
3	F	502	V0A	C17-C12-C18-C20
3	F	502	V0A	O03-C24-C25-C28
3	G	502	V0A	C07-C09-C12-C18
3	G	502	V0A	O02-C09-C12-C18
3	G	502	V0A	C18-C20-C22-C23
3	G	502	V0A	C21-C20-C22-C23
3	G	502	V0A	C22-C23-C24-C25
3	G	502	V0A	C22-C23-C24-O03
3	G	502	V0A	C23-C24-C25-C28
3	G	502	V0A	O03-C24-C25-C28
3	H	502	V0A	C18-C20-C22-C23

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Mol	Chain	Res	Type	Atoms
3	H	502	V0A	C21-C20-C22-C23
3	H	502	V0A	C22-C23-C24-C25
3	H	502	V0A	C22-C23-C24-O03
3	H	502	V0A	O03-C24-C25-C26
3	B	502	V0A	C21-C20-C22-C23
3	C	502	V0A	C21-C20-C22-C23
3	D	502	V0A	C21-C20-C22-C23
3	B	502	V0A	O02-C09-C12-C17
3	G	502	V0A	O02-C09-C12-C17
3	G	502	V0A	C07-C09-C12-C17
3	A	502	V0A	C09-C12-C18-C20
3	E	502	V0A	C09-C12-C18-C20
3	F	502	V0A	C09-C12-C18-C20
2	H	501	HEM	C2C-C3C-CAC-CBC
3	D	502	V0A	O02-C09-C12-C17
3	A	502	V0A	C07-C09-C12-C17
3	B	502	V0A	C07-C09-C12-C17
3	E	502	V0A	C07-C09-C12-C17
3	F	502	V0A	C07-C09-C12-C17
3	H	502	V0A	C23-C24-C25-C26
3	C	502	V0A	O02-C09-C12-C17
3	E	502	V0A	O02-C09-C12-C17
2	H	501	HEM	C4B-C3B-CAB-CBB
3	C	502	V0A	O03-C24-C25-C26
3	G	502	V0A	O03-C24-C25-C26
3	A	502	V0A	C23-C24-C25-C28
3	C	502	V0A	O02-C09-C12-C18
3	D	502	V0A	O03-C24-C25-C28
3	F	502	V0A	C23-C24-C25-C28
3	H	502	V0A	O02-C09-C12-C17
3	H	502	V0A	O02-C09-C12-C18
3	D	502	V0A	C07-C09-C12-C17
2	H	501	HEM	C4C-C3C-CAC-CBC
2	F	501	HEM	CAA-CBA-CGA-O2A
2	G	501	HEM	CAA-CBA-CGA-O2A
2	E	501	HEM	CAA-CBA-CGA-O2A
2	C	501	HEM	CAA-CBA-CGA-O2A
2	B	501	HEM	CAA-CBA-CGA-O2A
2	A	501	HEM	CAA-CBA-CGA-O2A
2	D	501	HEM	CAA-CBA-CGA-O2A
2	E	501	HEM	CAA-CBA-CGA-O1A
2	F	501	HEM	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
2	G	501	HEM	CAA-CBA-CGA-O1A
2	C	501	HEM	CAA-CBA-CGA-O1A
2	B	501	HEM	CAA-CBA-CGA-O1A
2	A	501	HEM	CAA-CBA-CGA-O1A
3	C	502	V0A	C07-C09-C12-C17
2	D	501	HEM	CAA-CBA-CGA-O1A

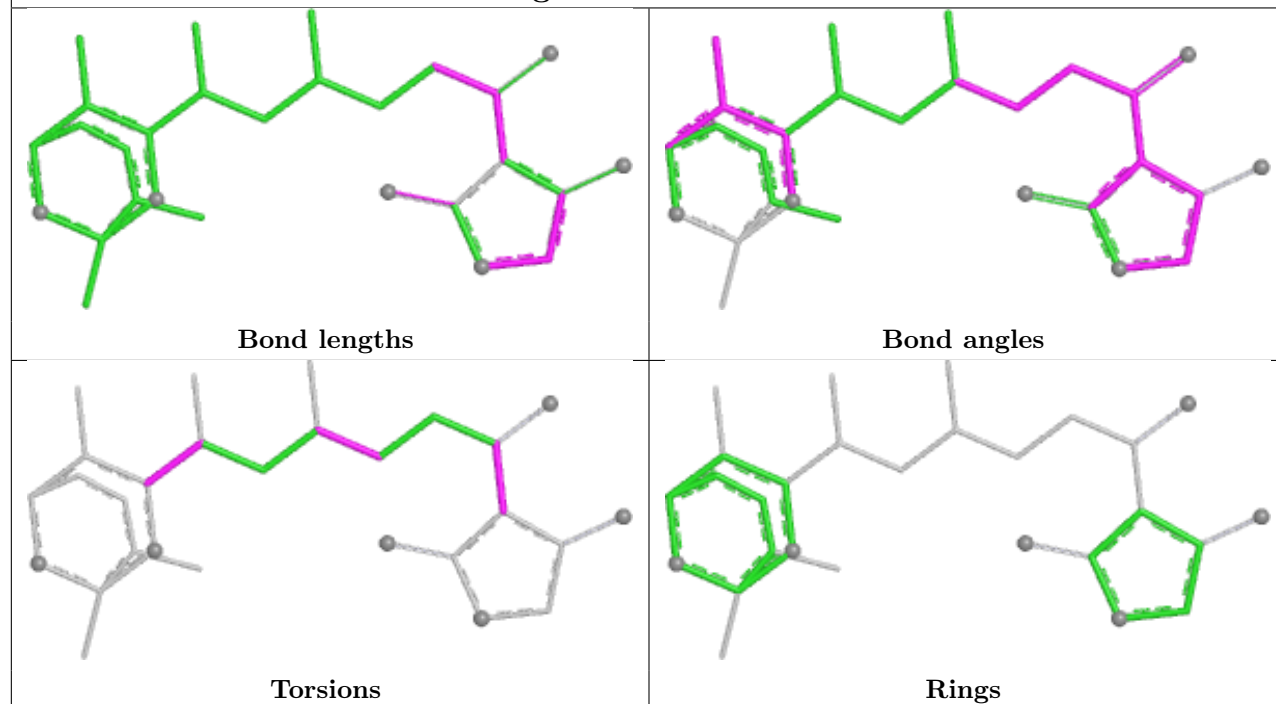
There are no ring outliers.

12 monomers are involved in 44 short contacts:

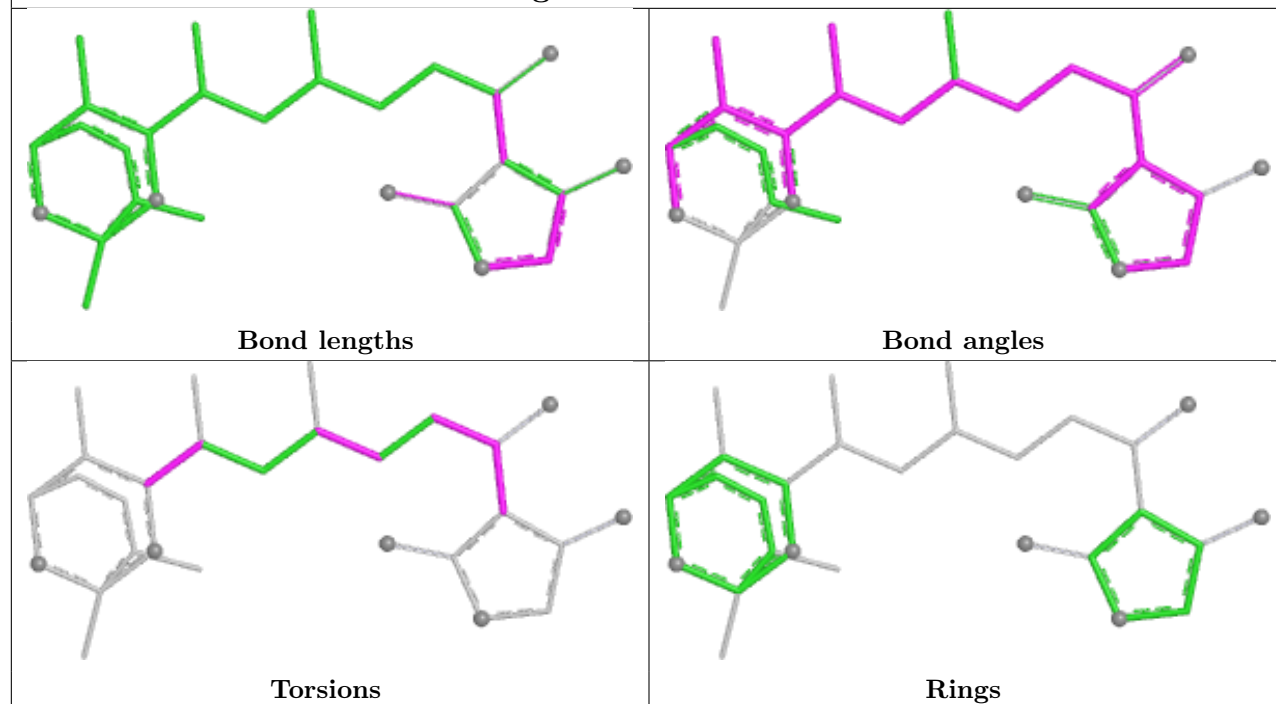
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	502	V0A	1	0
3	G	502	V0A	2	0
2	C	501	HEM	3	0
2	E	501	HEM	4	0
3	H	502	V0A	2	0
2	H	501	HEM	4	0
3	C	502	V0A	8	0
2	A	501	HEM	5	0
2	F	501	HEM	3	0
2	D	501	HEM	5	0
2	G	501	HEM	4	0
2	B	501	HEM	3	0

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.

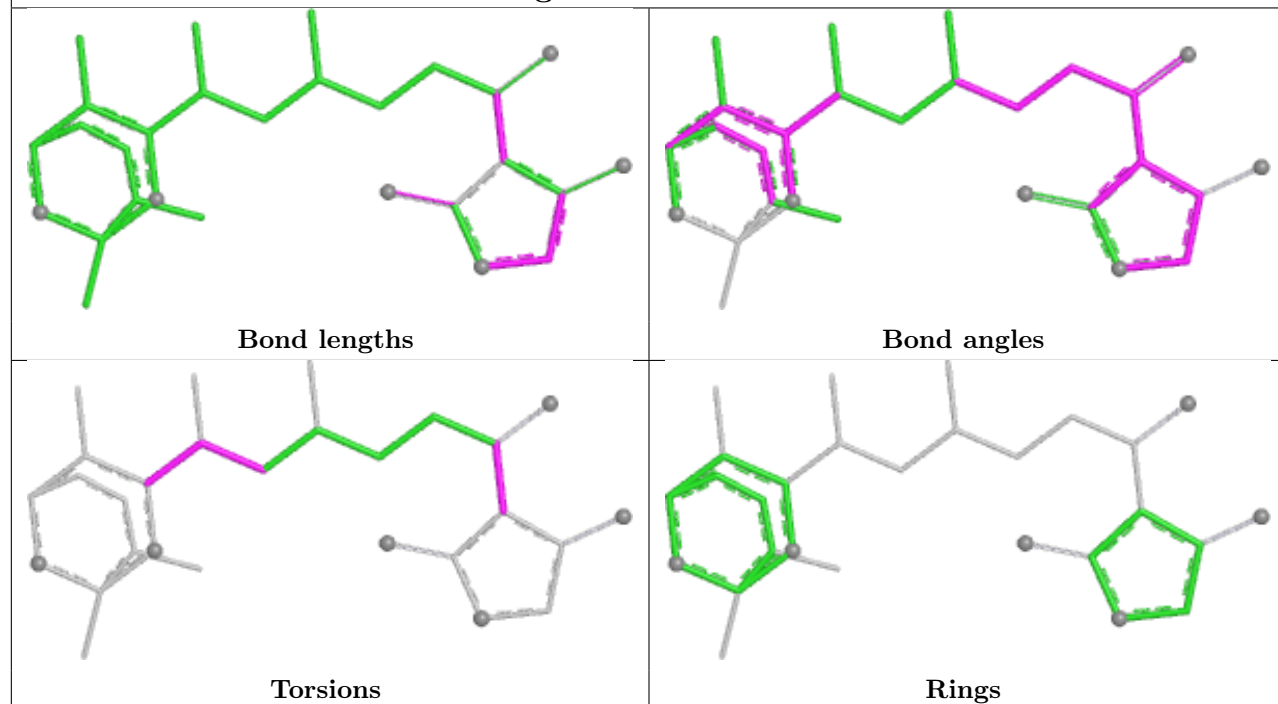
Ligand V0A D 502



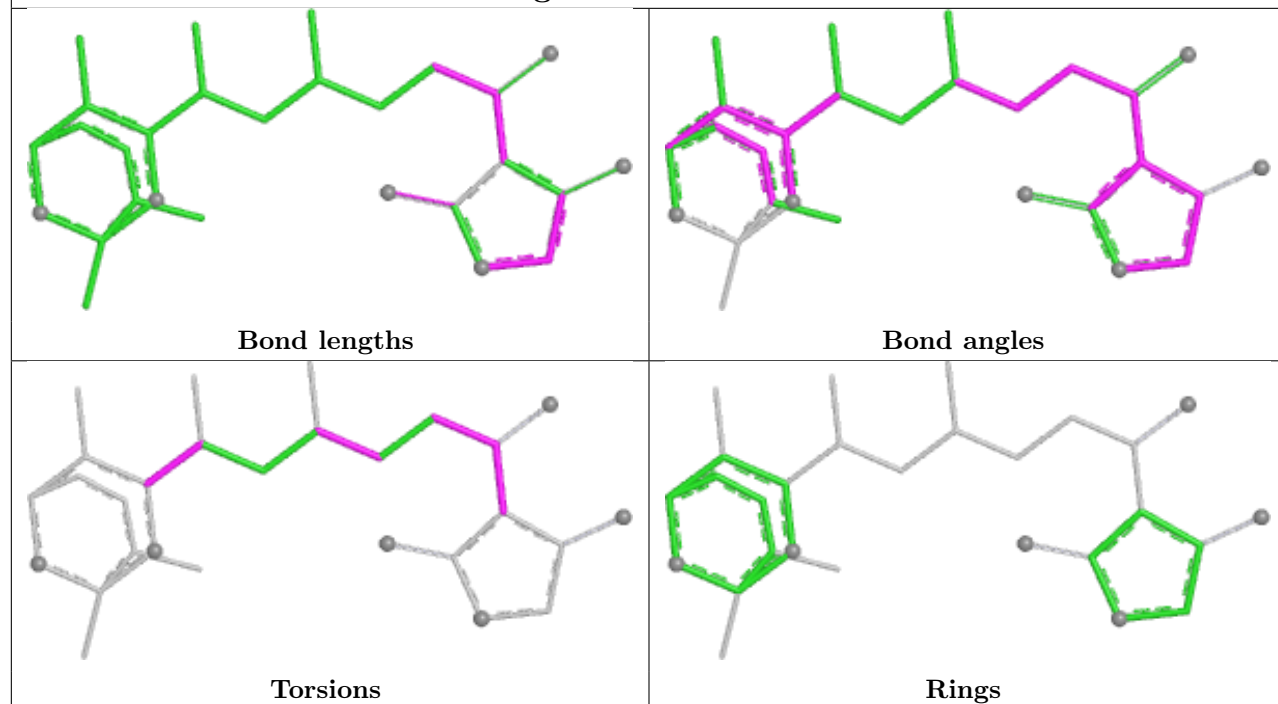
Ligand V0A G 502

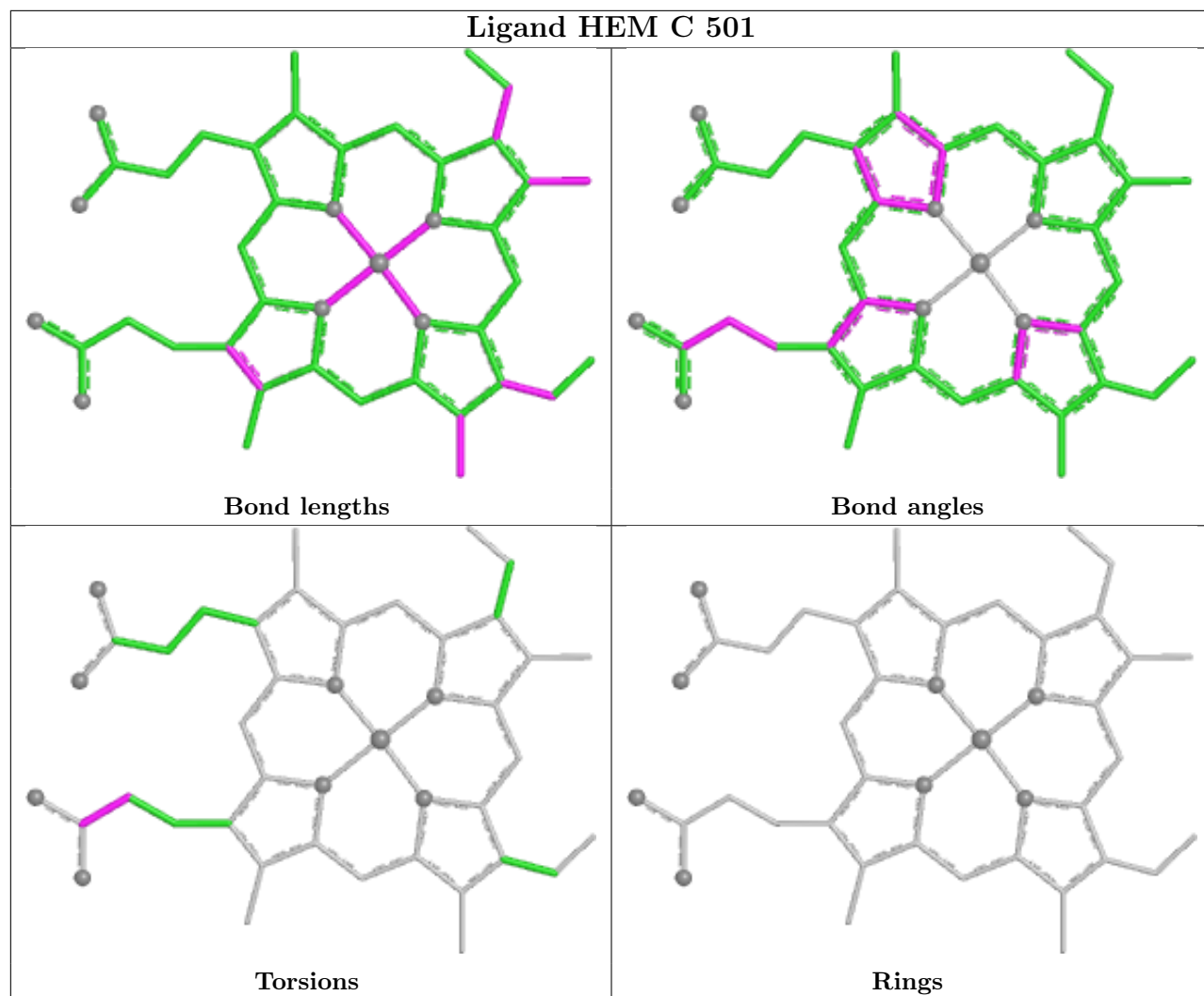


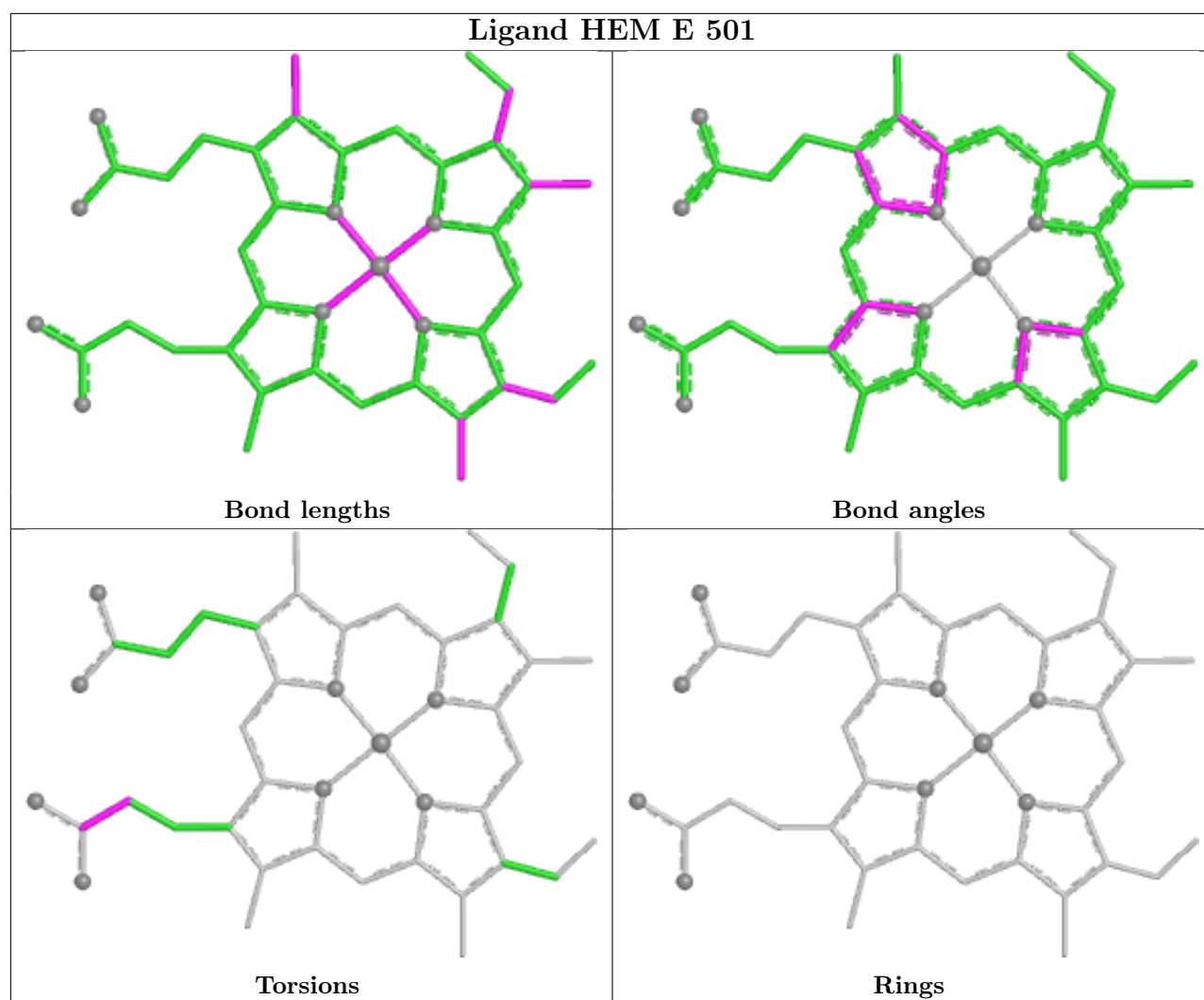
Ligand V0A F 502

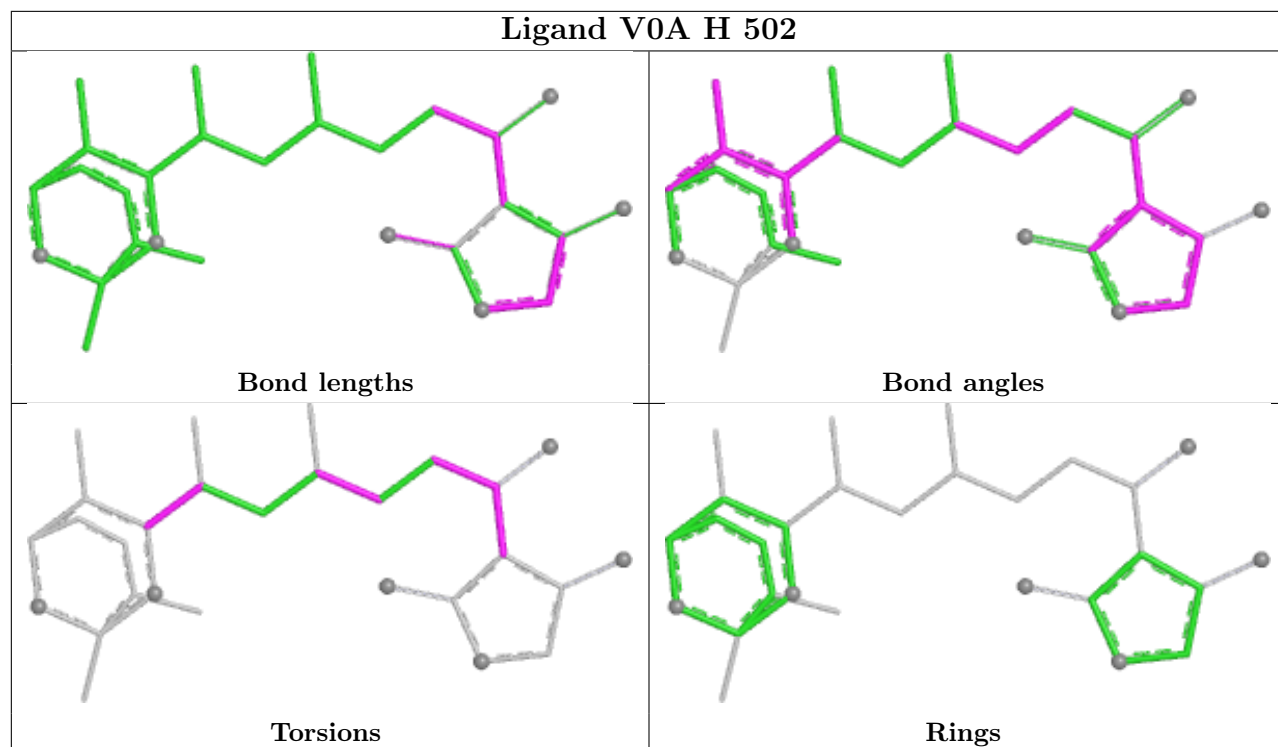


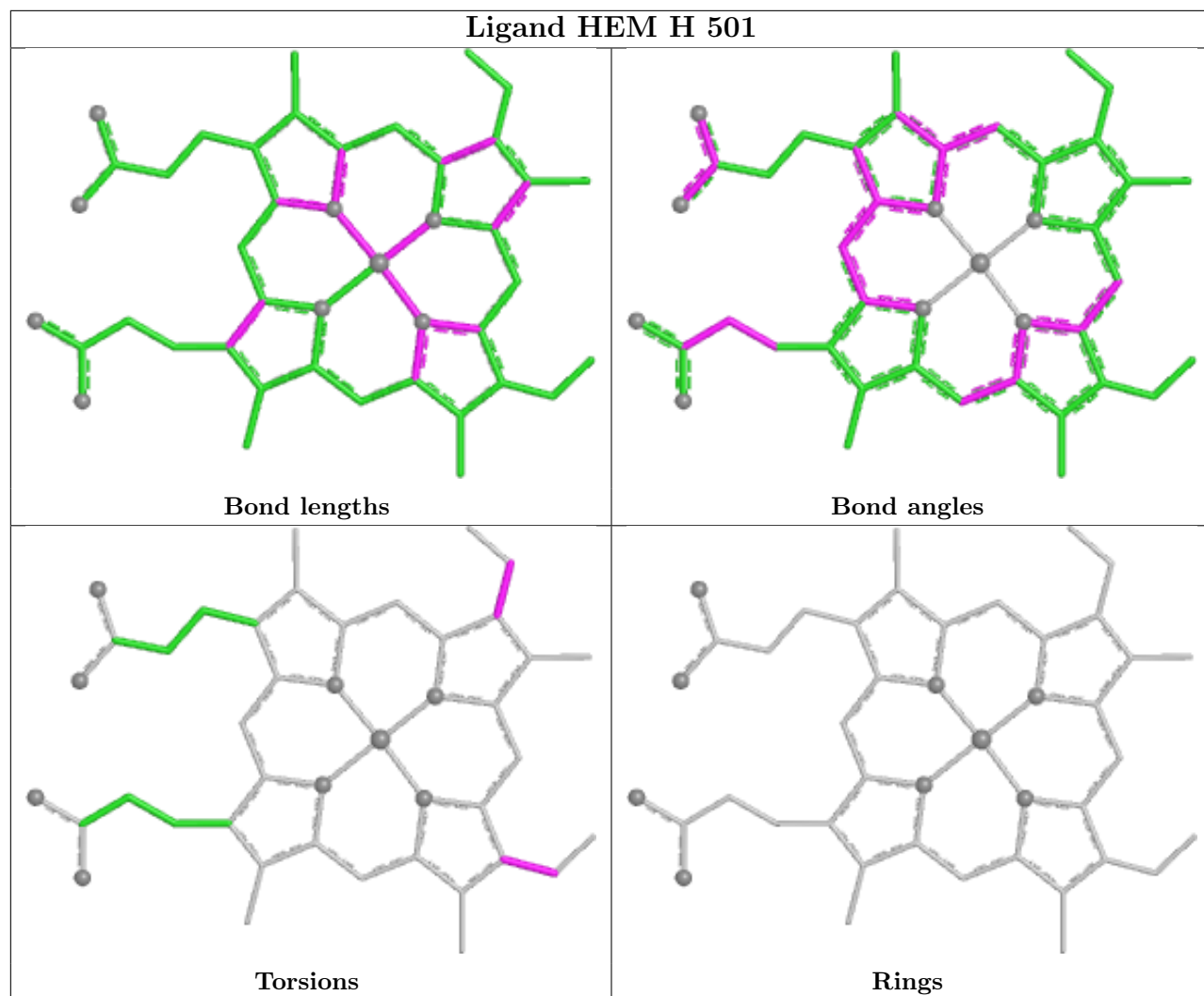
Ligand V0A B 502

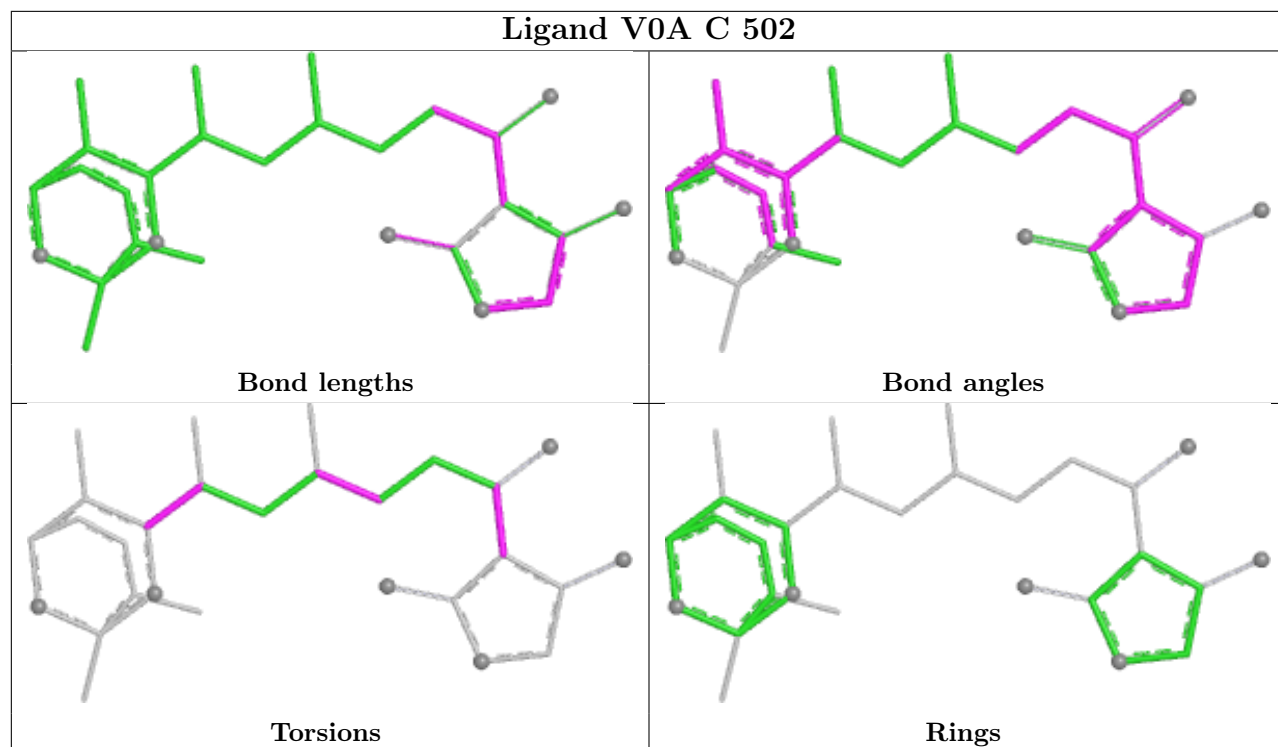


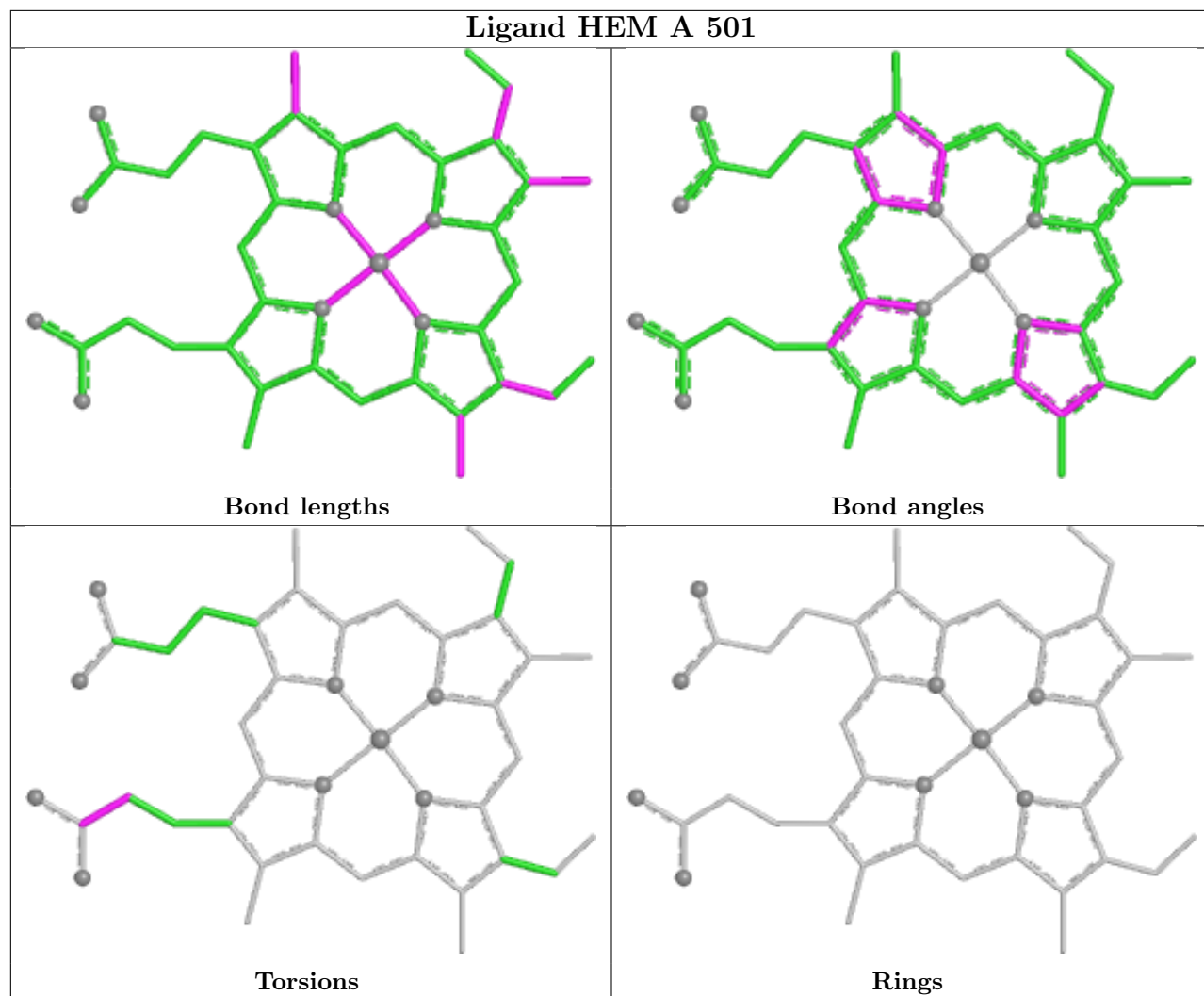


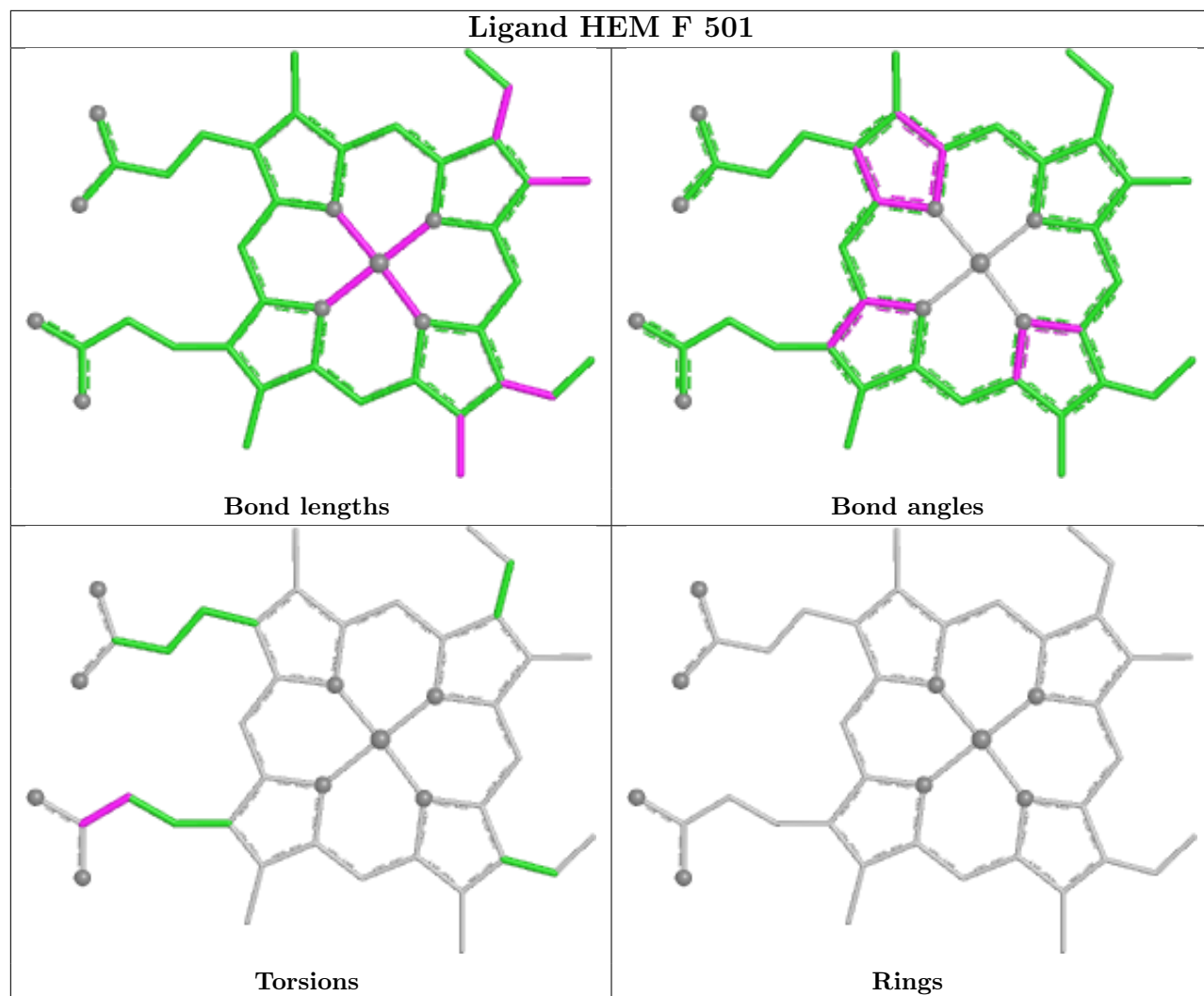


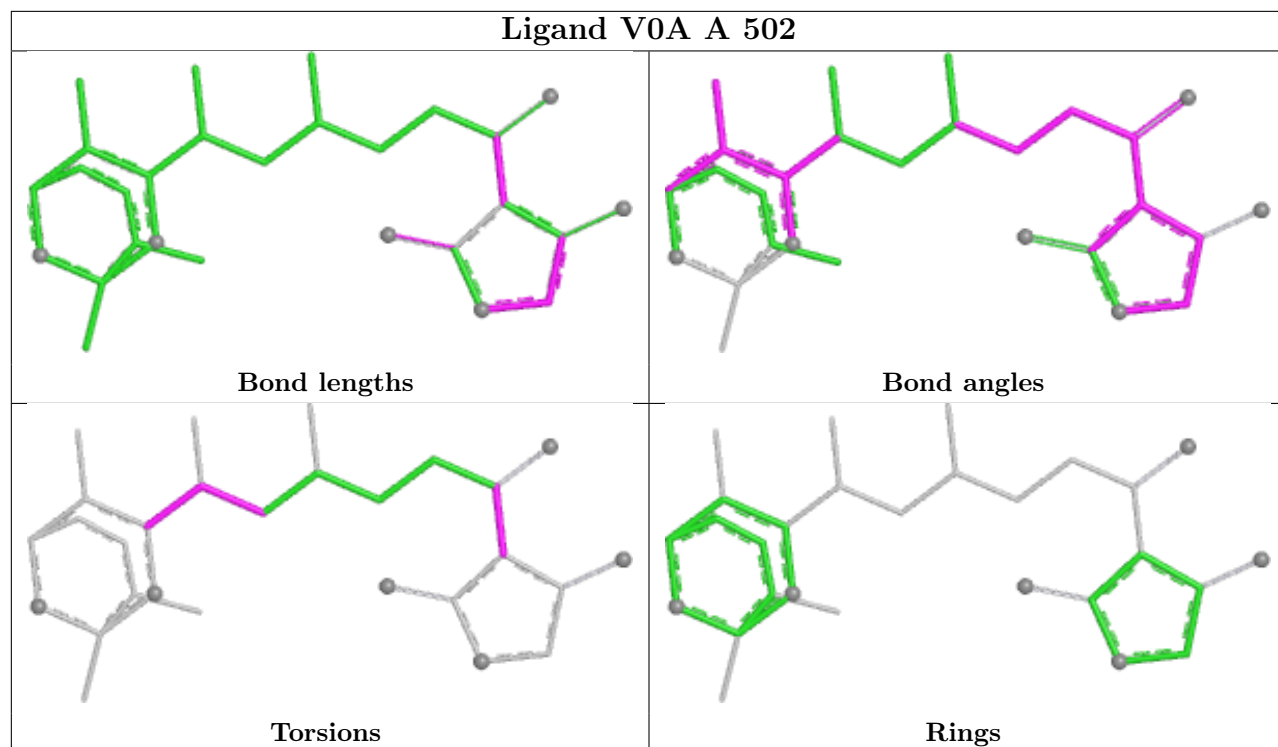


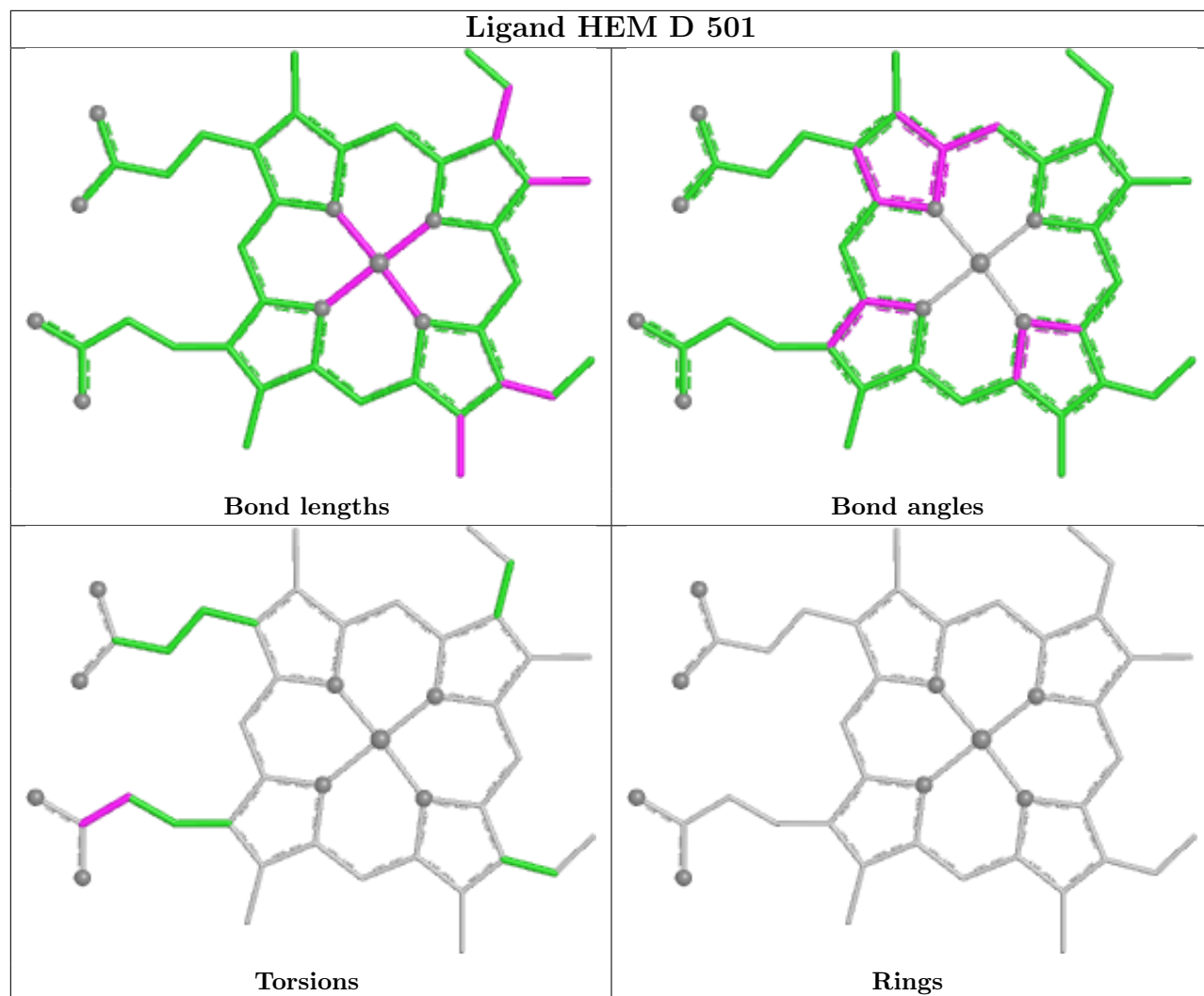


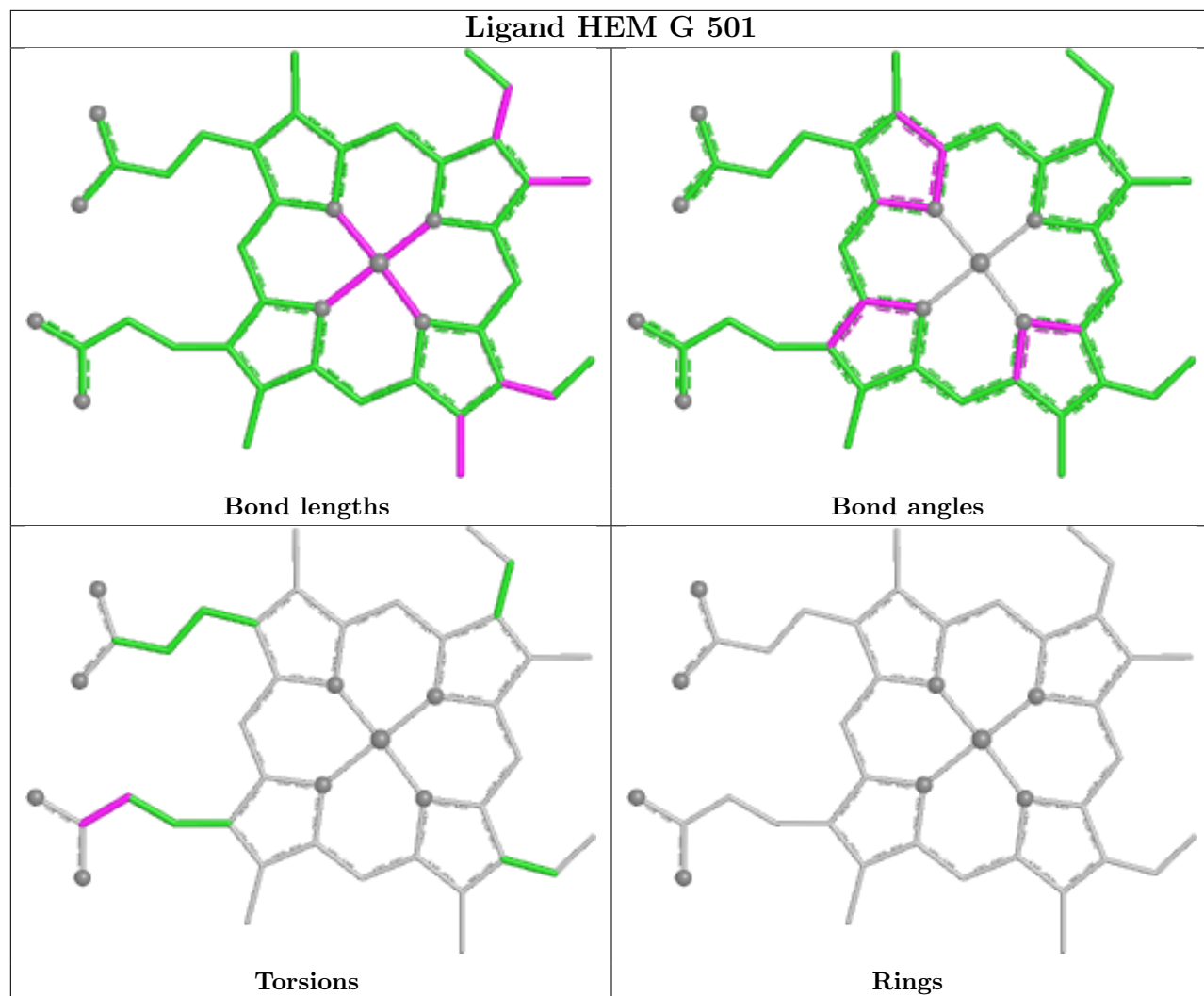


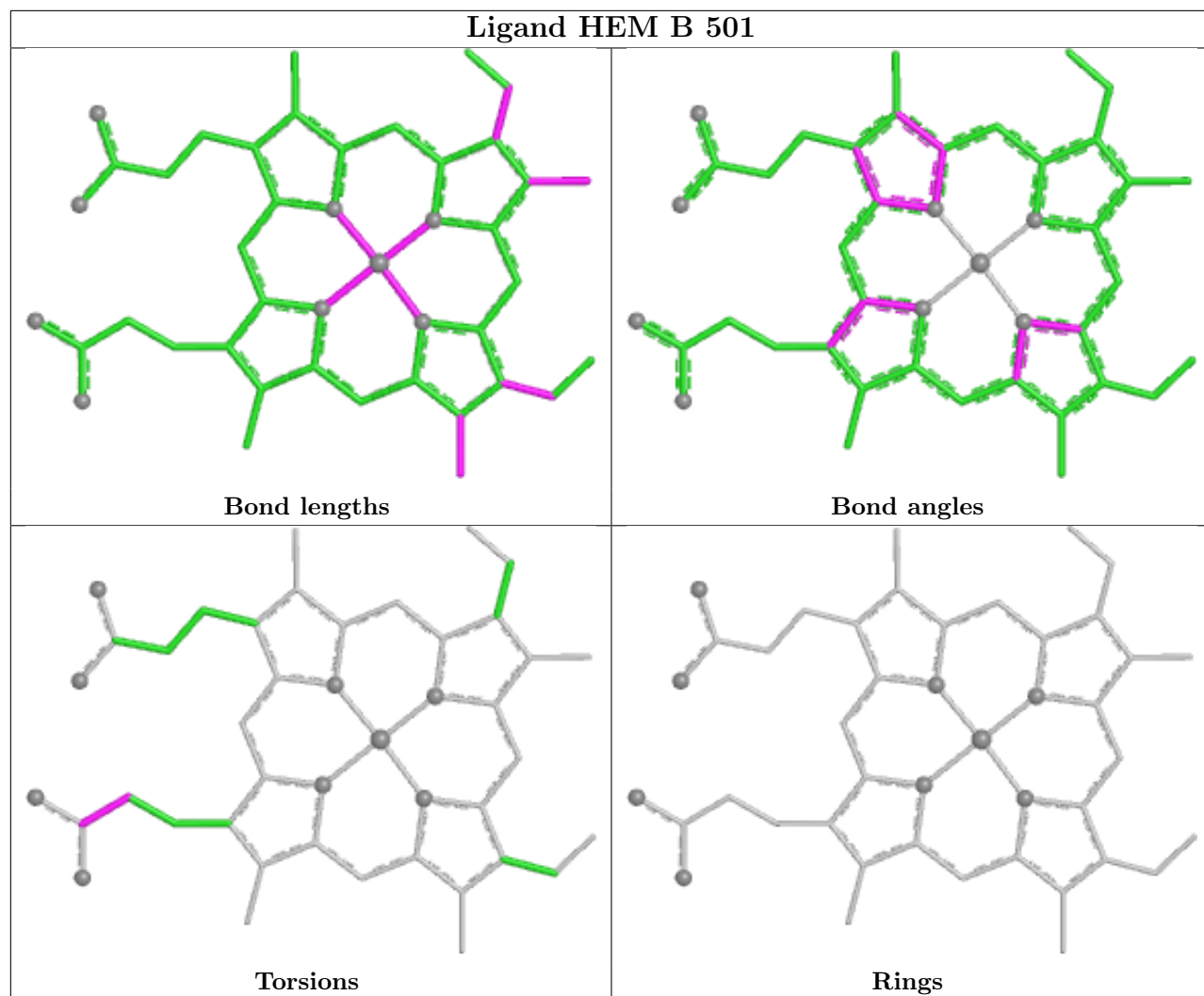


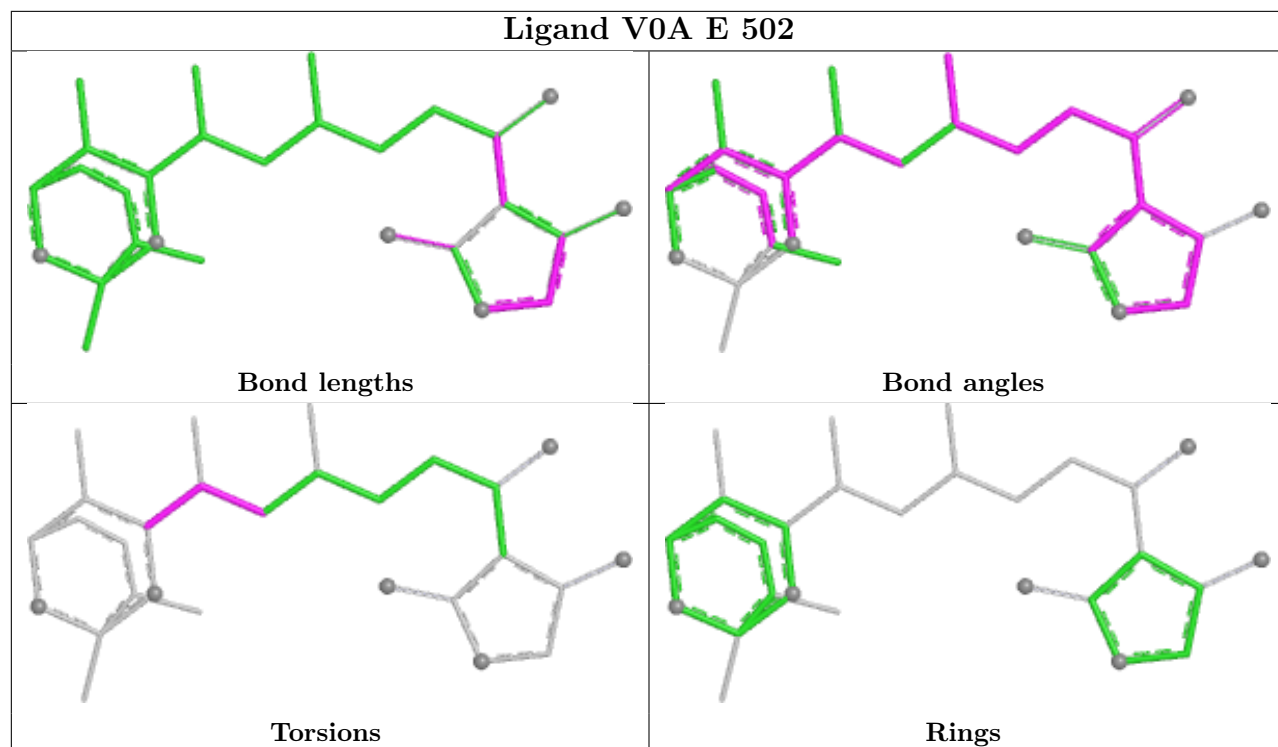












5.7 Other polymers [i](#)

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	399/414 (96%)	-1.36	0 100 100	28, 42, 67, 97	0
1	B	399/414 (96%)	-1.35	0 100 100	30, 44, 73, 99	0
1	C	393/414 (94%)	-1.24	0 100 100	33, 58, 83, 103	0
1	D	398/414 (96%)	-1.30	0 100 100	29, 51, 78, 90	0
1	E	399/414 (96%)	-1.32	0 100 100	32, 47, 69, 92	0
1	F	399/414 (96%)	-1.36	0 100 100	26, 42, 67, 95	0
1	G	399/414 (96%)	-1.26	0 100 100	37, 59, 85, 103	0
1	H	399/414 (96%)	-1.28	0 100 100	29, 56, 81, 98	0
All	All	3185/3312 (96%)	-1.31	0 100 100	26, 50, 78, 103	0

There are no RSRZ outliers to report.

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](#)

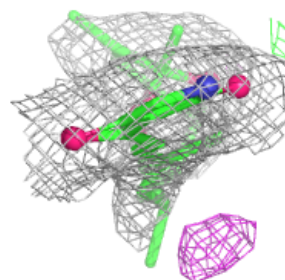
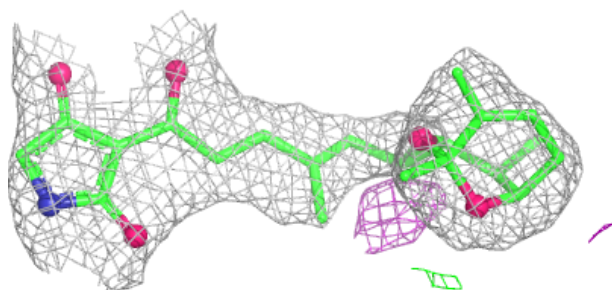
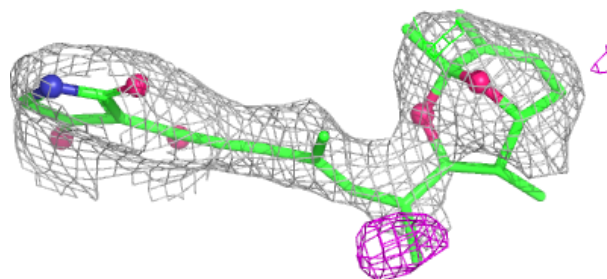
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists 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
3	V0A	C	502	28/28	0.98	0.06	42,54,61,66	0
2	HEM	B	501	43/43	0.99	0.04	24,32,37,40	0
2	HEM	C	501	43/43	0.99	0.04	28,39,45,47	0
2	HEM	D	501	43/43	0.99	0.04	27,35,45,50	0
2	HEM	E	501	43/43	0.99	0.04	28,41,50,52	0
2	HEM	F	501	43/43	0.99	0.04	27,35,39,47	0
2	HEM	G	501	43/43	0.99	0.04	28,42,50,60	0
2	HEM	H	501	43/43	0.99	0.04	20,20,20,20	0
3	V0A	A	502	28/28	0.99	0.06	36,47,56,70	0
3	V0A	B	502	28/28	0.99	0.06	39,49,59,59	0
2	HEM	A	501	43/43	0.99	0.04	24,33,37,41	0
3	V0A	D	502	28/28	0.99	0.04	38,48,55,55	0
3	V0A	E	502	28/28	0.99	0.05	45,55,66,70	0
3	V0A	F	502	28/28	0.99	0.05	36,46,52,57	0
3	V0A	G	502	28/28	0.99	0.05	53,60,67,71	0
3	V0A	H	502	28/28	0.99	0.05	42,49,57,61	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.

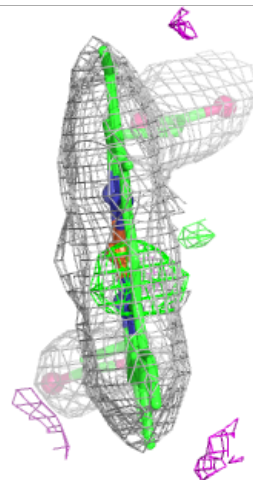
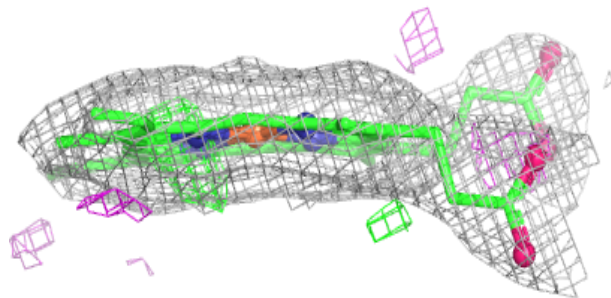
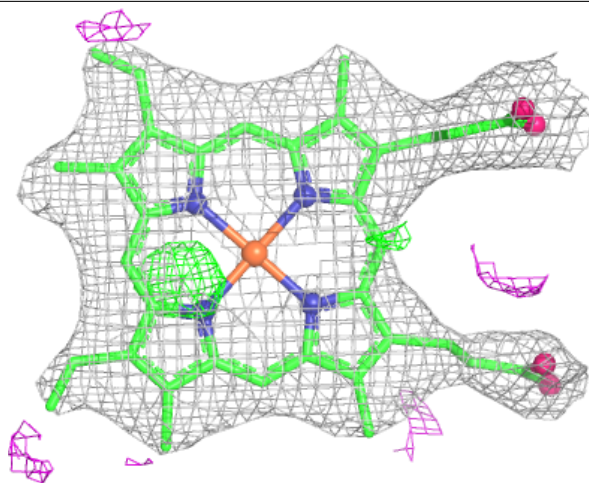
Electron density around V0A C 502:

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



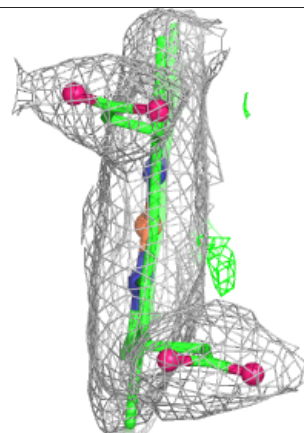
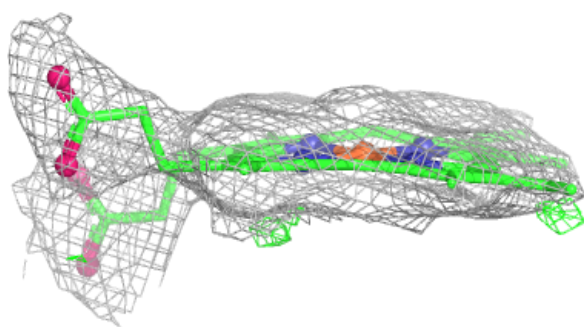
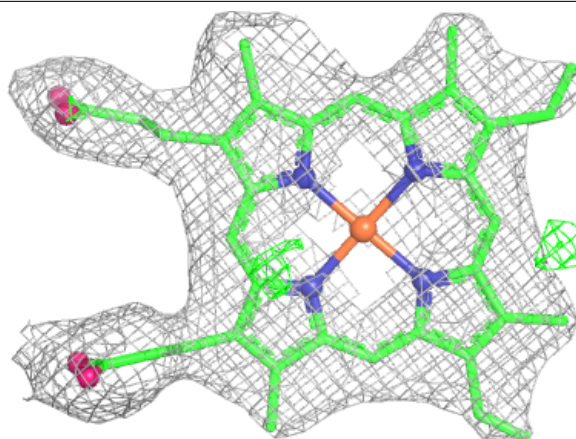
Electron density around HEM B 501:

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



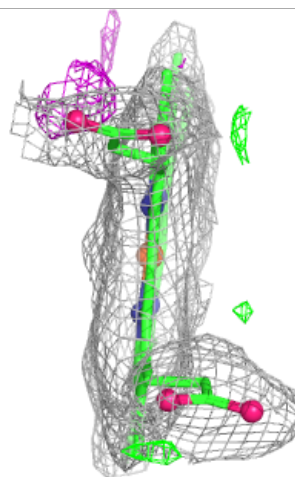
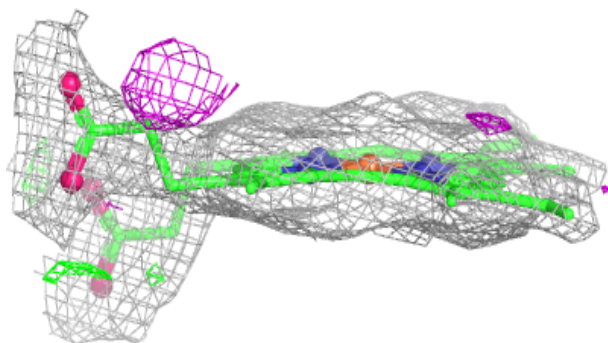
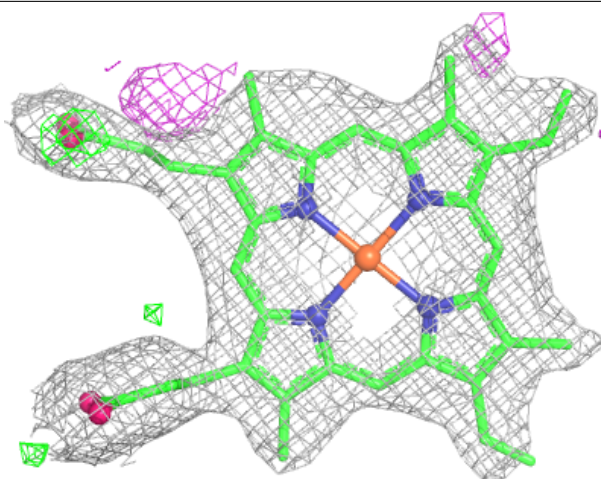
Electron density around HEM C 501:

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



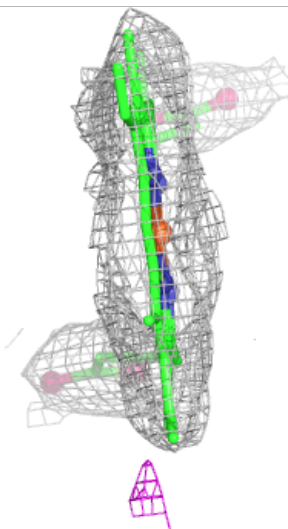
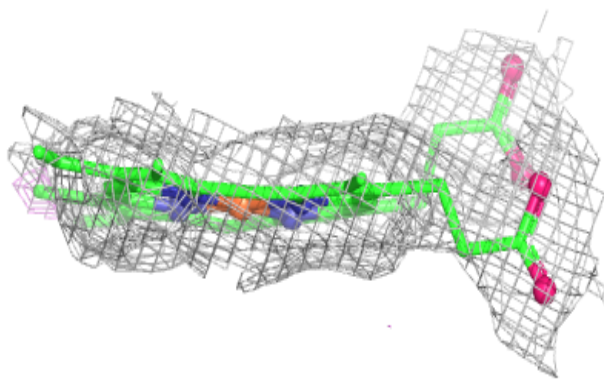
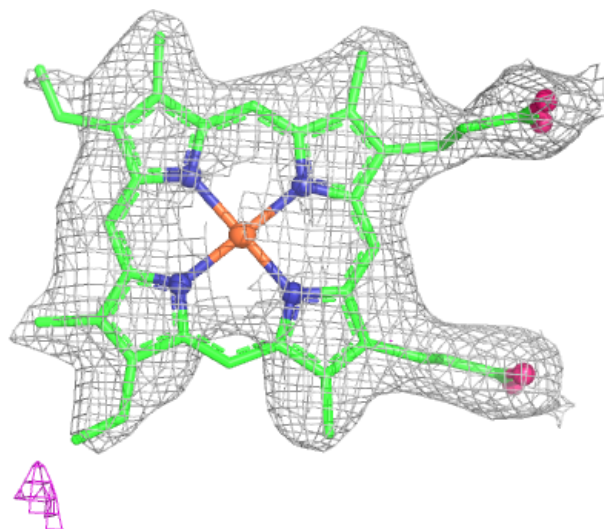
Electron density around HEM D 501:

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



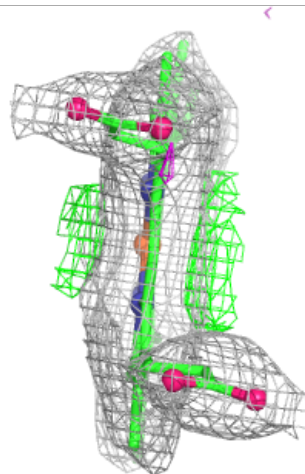
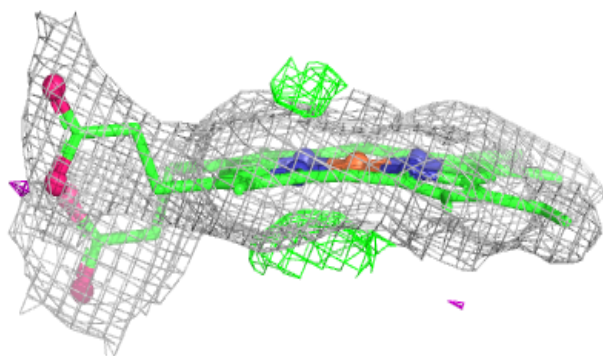
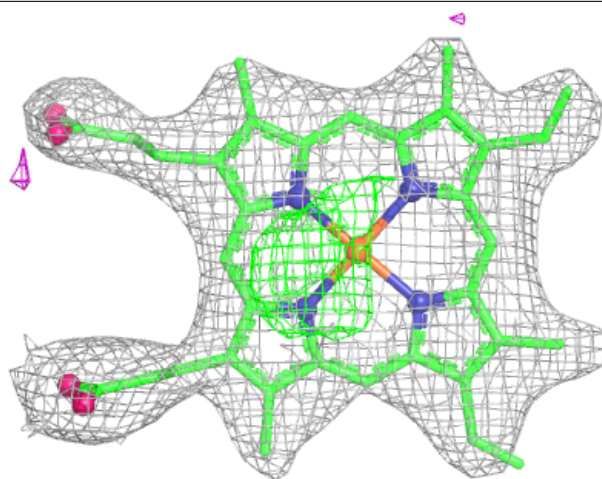
Electron density around HEM E 501:

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



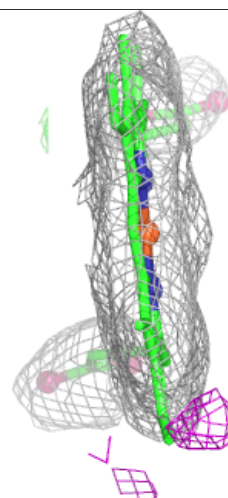
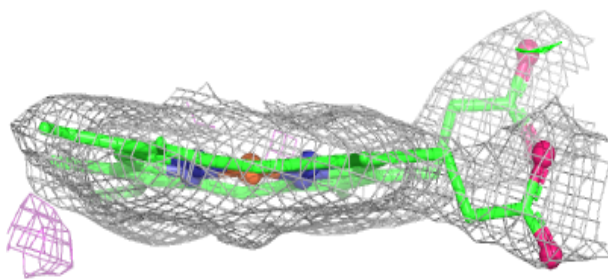
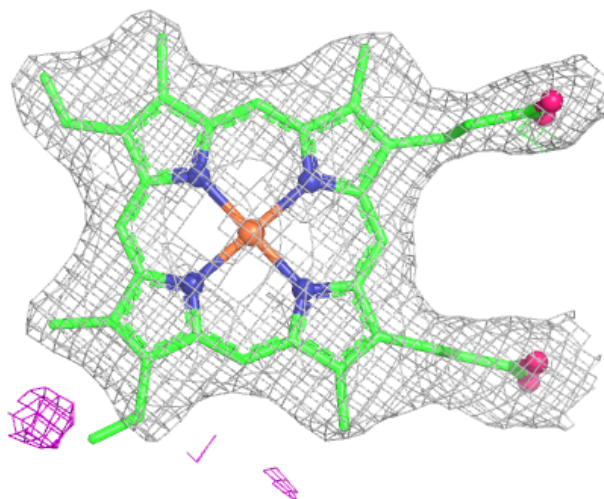
Electron density around HEM F 501:

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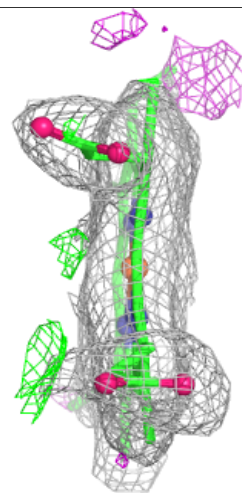
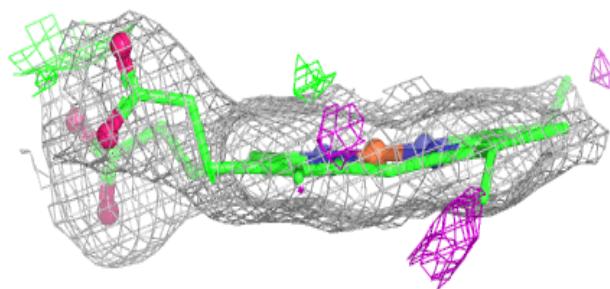
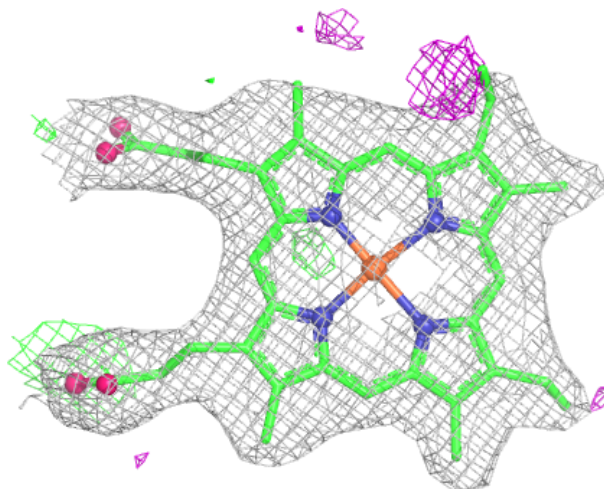
Electron density around HEM G 501:

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



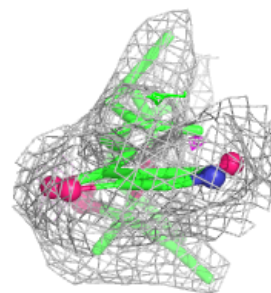
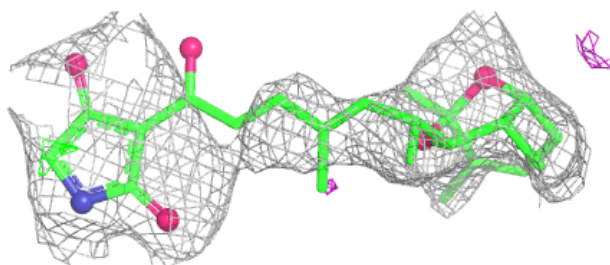
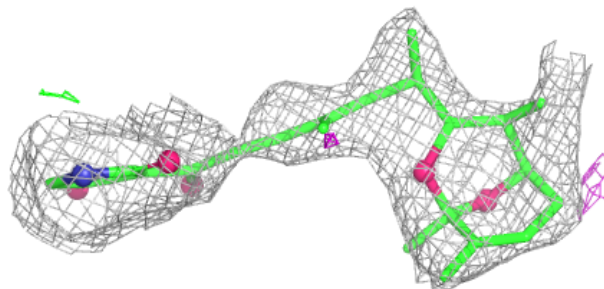
Electron density around HEM H 501:

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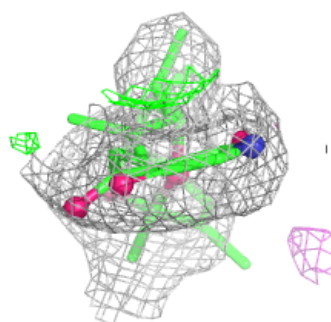
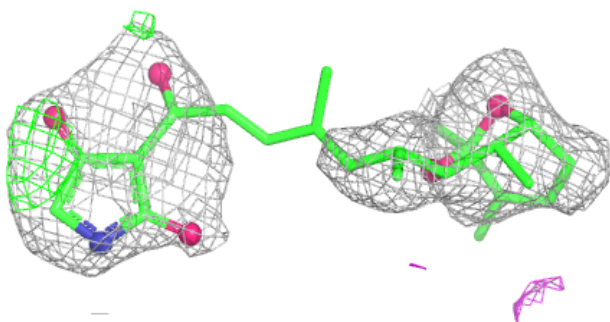
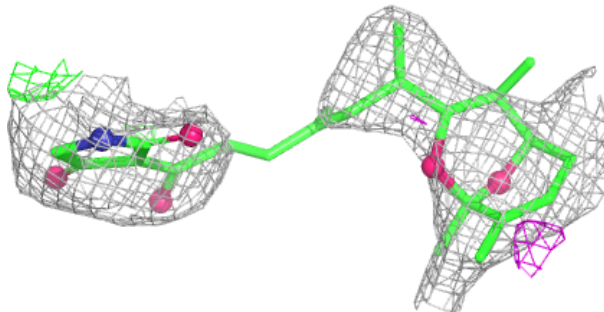


Electron density around V0A A 502:

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

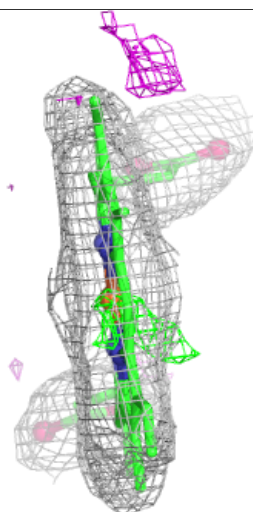
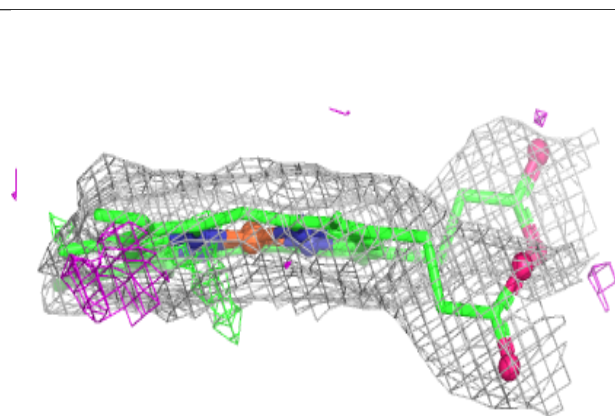
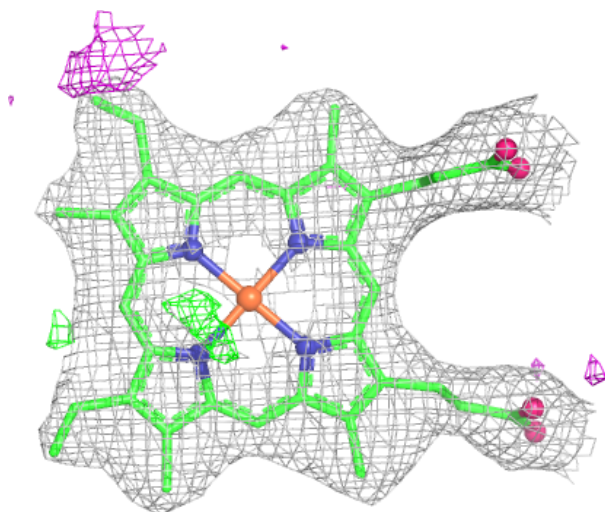
**Electron density around V0A B 502:**

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



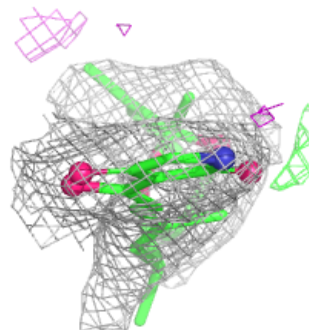
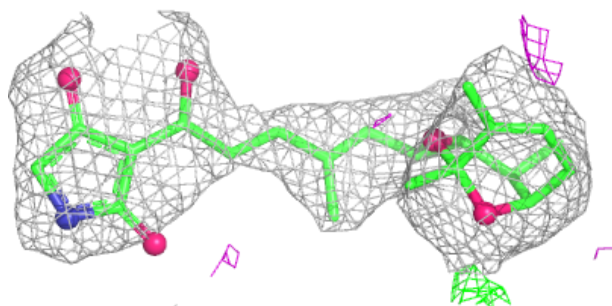
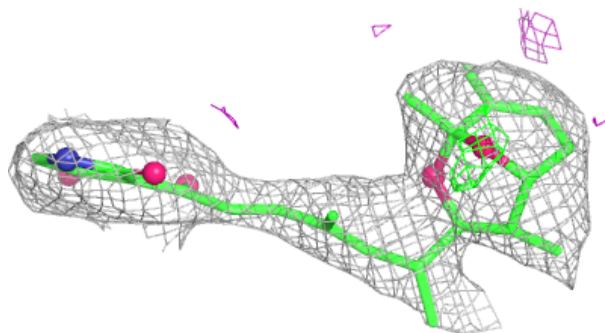
Electron density around HEM A 501:

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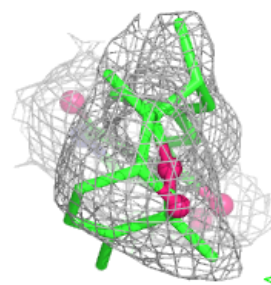
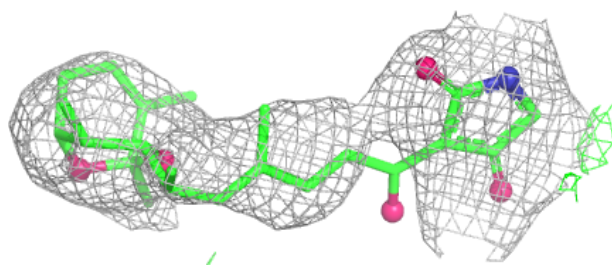
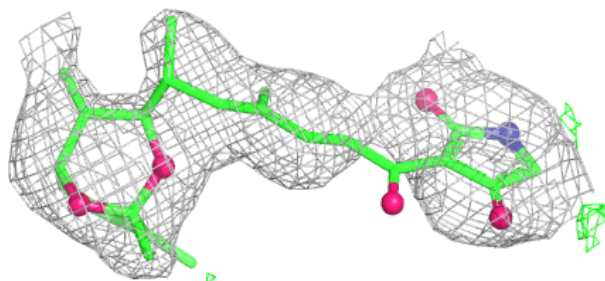


Electron density around V0A D 502:

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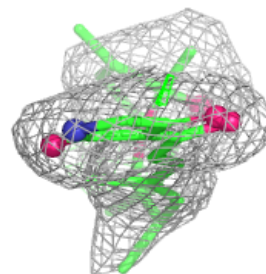
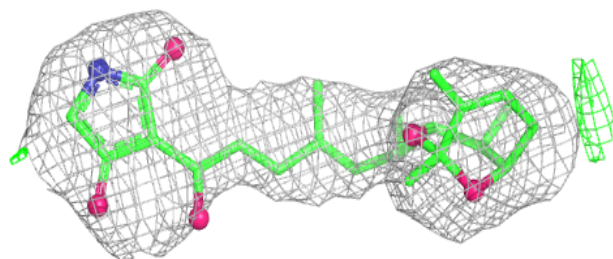
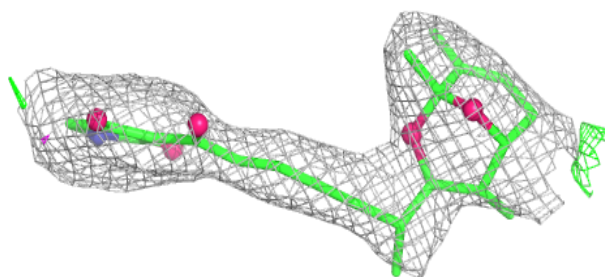
**Electron density around V0A E 502:**

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

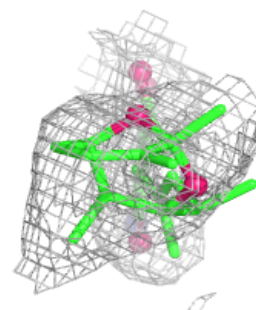
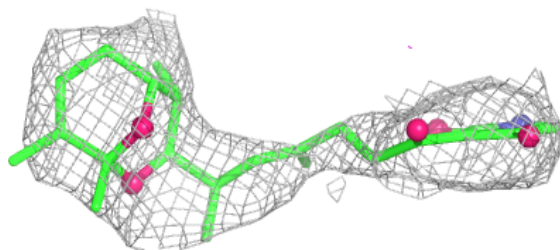
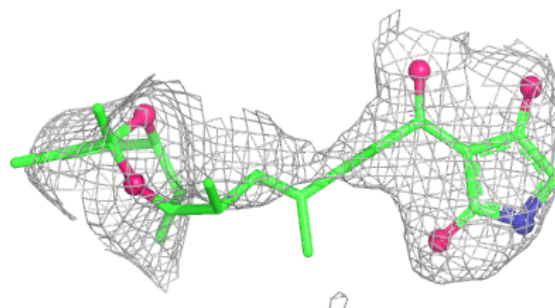


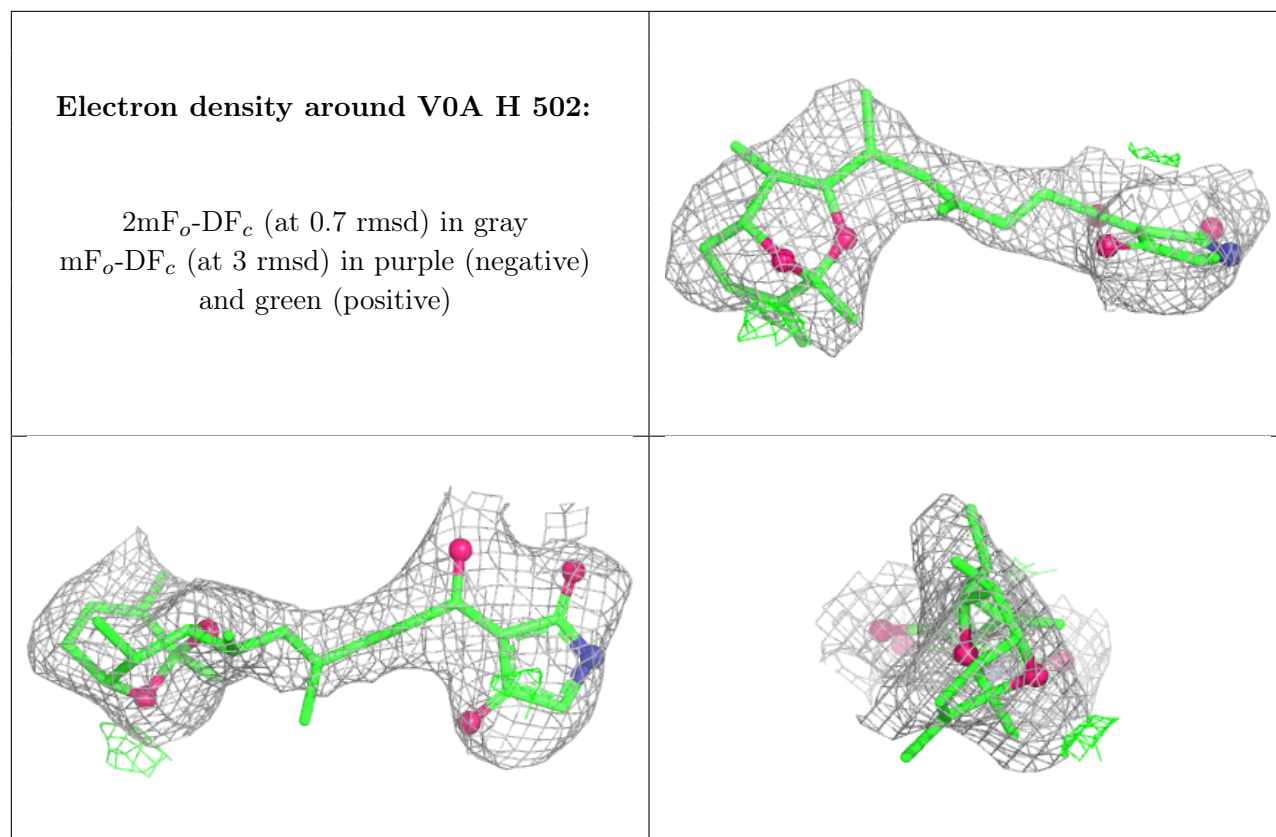
Electron density around V0A F 502:

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

**Electron density around V0A G 502:**

$2mF_o-DF_c$ (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.