



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 5, 2026 – 07:46 PM EDT

PDB ID : 3P9P / pdb_00003p9p
Title : Structure of I274V variant of E. coli KatE
Authors : Loewen, P.C.; Jha, V.; Louis, S.; Chelikani, P.; Carpena, X.; Fita, I.
Deposited on : 2010-10-18
Resolution : 1.50 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 : 9.0.015 (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

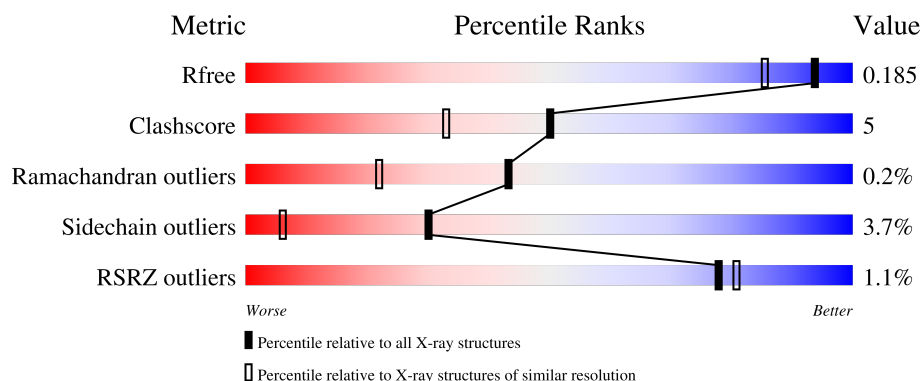
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.50 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	4037 (1.50-1.50)
Clashscore	190562	4235 (1.50-1.50)
Ramachandran outliers	187476	4153 (1.50-1.50)
Sidechain outliers	187428	4150 (1.50-1.50)
RSRZ outliers	180081	4039 (1.50-1.50)

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	753	% 86% 9% ...
1	B	753	2% 83% 12% ...
1	C	753	% 84% 11% ...
1	D	753	% 83% 12% ...

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	HDD	A	760[D]	X	-	-	-
4	HDD	B	760[D]	X	-	-	-
4	HDD	C	760[D]	X	-	-	-
4	HDD	D	760[D]	X	-	-	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 27001 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.

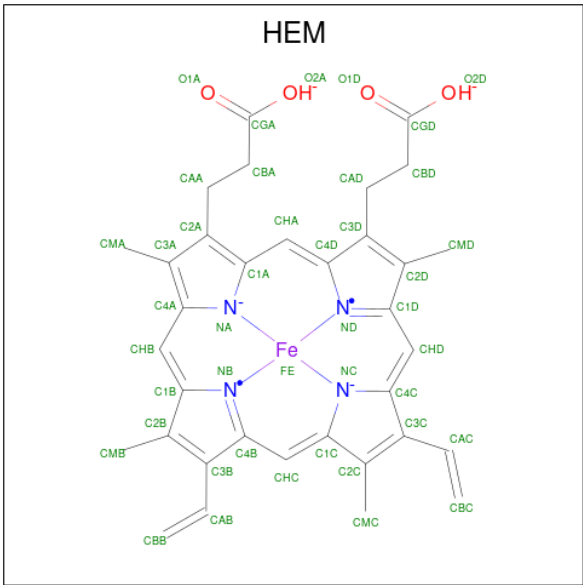
- Molecule 1 is a protein called Catalase HP11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	726	Total	C	N	O	S	0	5	0
			5764	3658	1011	1083	12			
1	B	726	Total	C	N	O	S	0	3	0
			5749	3649	1007	1081	12			
1	C	726	Total	C	N	O	S	0	5	0
			5766	3661	1008	1085	12			
1	D	726	Total	C	N	O	S	0	6	0
			5757	3652	1008	1085	12			

There are 4 discrepancies between the modelled and reference sequences:

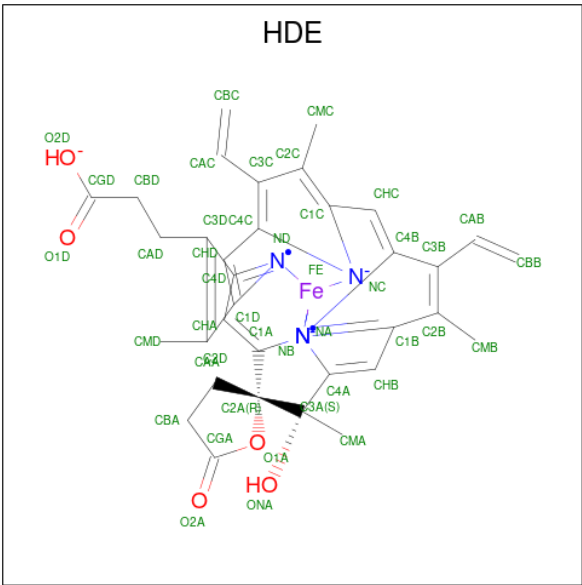
Chain	Residue	Modelled	Actual	Comment	Reference
A	274	VAL	ILE	engineered mutation	UNP P21179
B	274	VAL	ILE	engineered mutation	UNP P21179
C	274	VAL	ILE	engineered mutation	UNP P21179
D	274	VAL	ILE	engineered mutation	UNP P21179

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



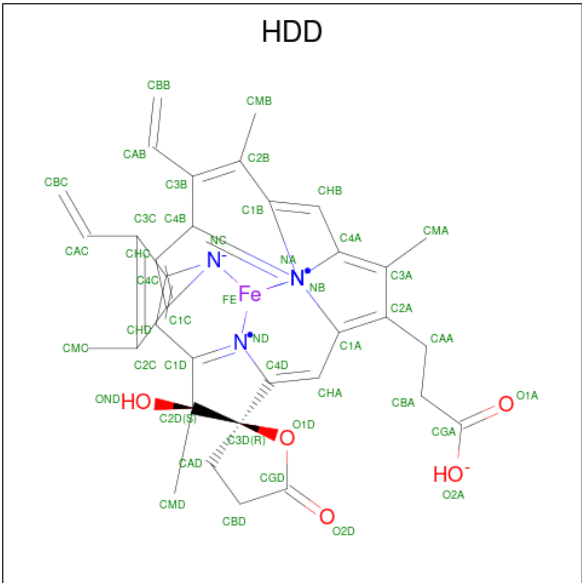
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	1
2	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	1
2	B	1	Total 43	C 34	Fe 1	N 4	O 4	0	1
2	B	1	Total 43	C 34	Fe 1	N 4	O 4	0	1
2	C	1	Total 43	C 34	Fe 1	N 4	O 4	0	1
2	C	1	Total 43	C 34	Fe 1	N 4	O 4	0	1
2	D	1	Total 43	C 34	Fe 1	N 4	O 4	0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

- Molecule 3 is CIS-HEME D HYDROXYCHLORIN GAMMA-SPIROLACTONE 17R, 18S (CCD ID: HDE) (formula: C₃₄H₃₂FeN₄O₅).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	Fe	N	O	0	1
			44	34	1	4	5		
3	B	1	Total	C	Fe	N	O	0	1
			44	34	1	4	5		
3	C	1	Total	C	Fe	N	O	0	1
			44	34	1	4	5		
3	D	1	Total	C	Fe	N	O	0	1
			44	34	1	4	5		

- Molecule 4 is CIS-HEME D HYDROXYCHLORIN GAMMA-SPIROLACTONE (CCD ID: HDD) (formula: C₃₄H₃₂FeN₄O₅).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total 44	C 34	Fe 1	N 4	O 5	0	1
4	B	1	Total 44	C 34	Fe 1	N 4	O 5	0	1
4	C	1	Total 44	C 34	Fe 1	N 4	O 5	0	1
4	D	1	Total 44	C 34	Fe 1	N 4	O 5	0	1

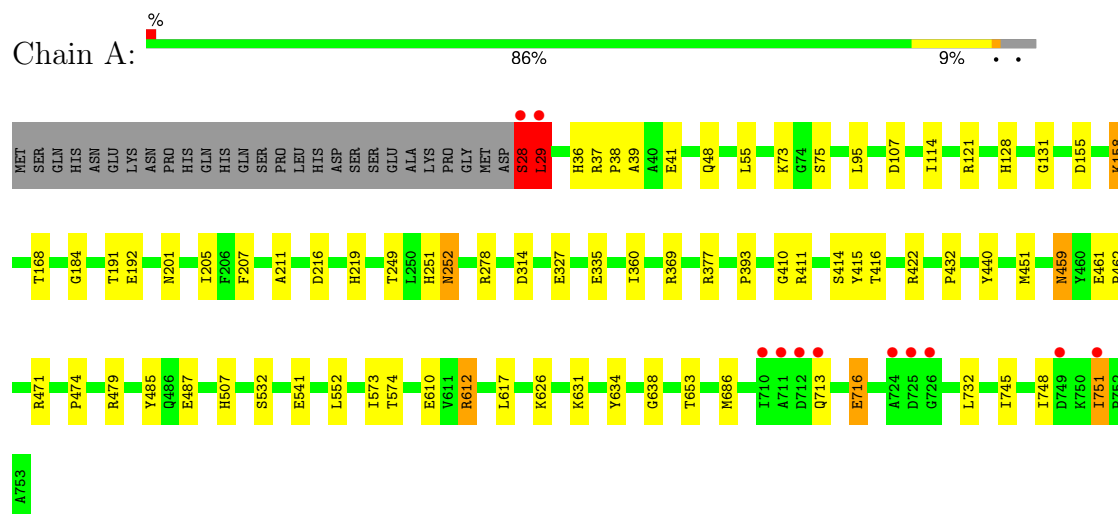
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	842	Total 842	O 842	0	0
5	B	754	Total 754	O 754	0	0
5	C	807	Total 807	O 807	0	0
5	D	866	Total 866	O 866	0	0

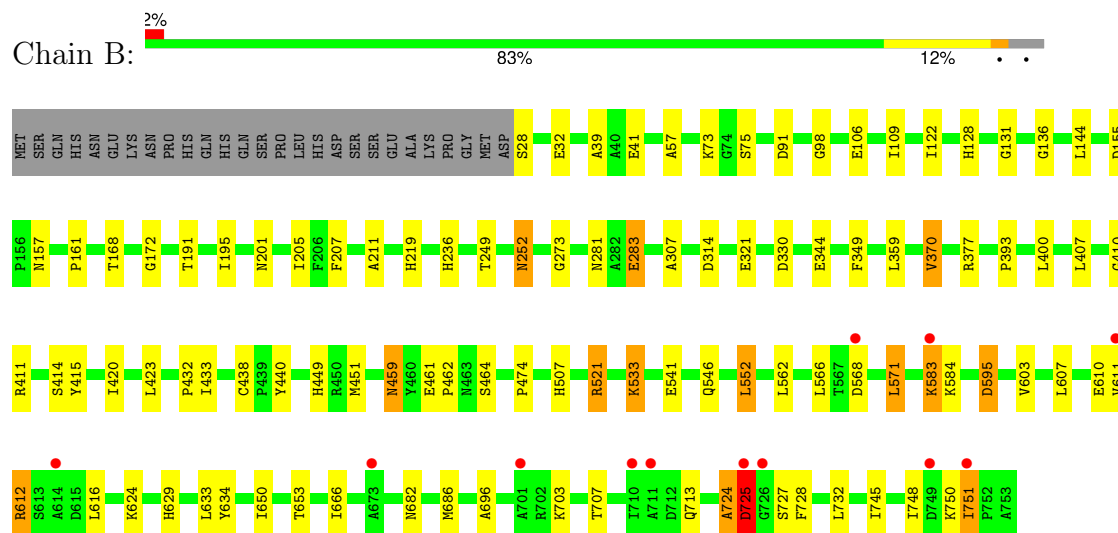
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

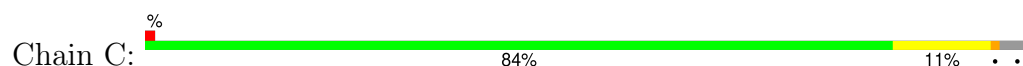
• Molecule 1: Catalase HP1I

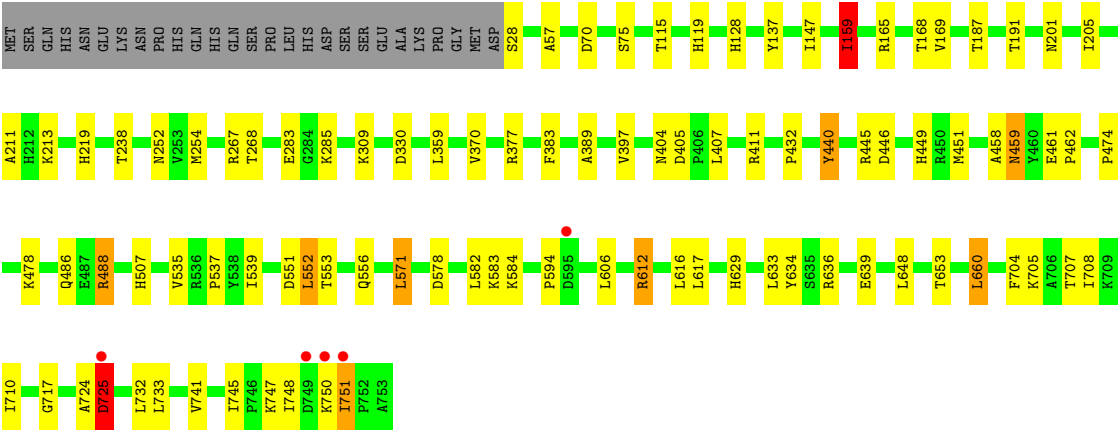


• Molecule 1: Catalase HP1I

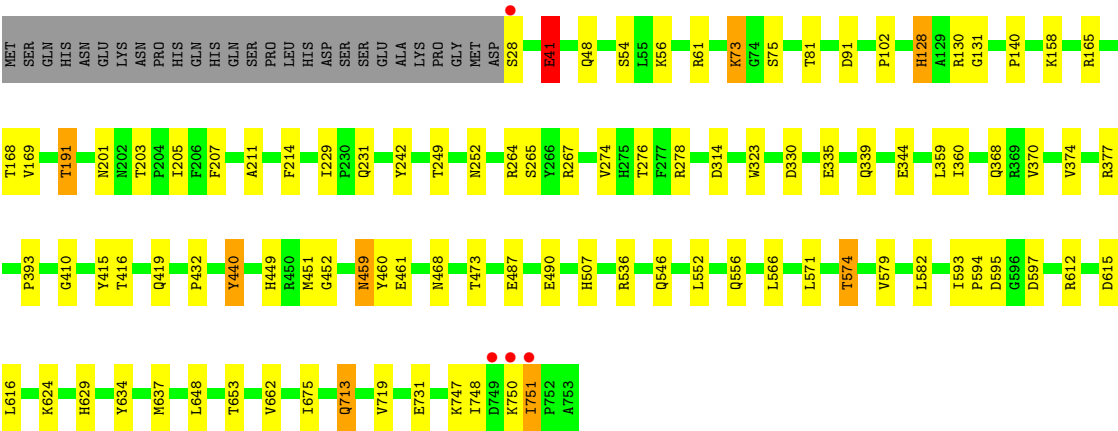
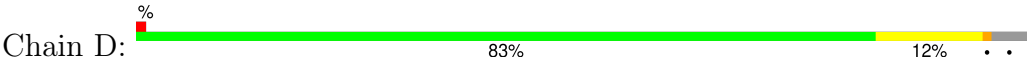


• Molecule 1: Catalase HP1I





● Molecule 1: Catalase HP1I



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	93.50Å 132.82Å 122.59Å 90.00° 109.47° 90.00°	Depositor
Resolution (Å)	29.16 – 1.50 29.16 – 1.50	Depositor EDS
% Data completeness (in resolution range)	94.8 (29.16-1.50) 94.8 (29.16-1.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.12	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.81 (at 1.50Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.149 , 0.185 0.148 , 0.185	Depositor DCC
R_{free} test set	21394 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	9.4	Xtriage
Anisotropy	0.048	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 34.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.024 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	27001	wwPDB-VP
Average B, all atoms (Å ²)	13.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.43% 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 i

5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: HDD, HDE, 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	1.53	14/5937 (0.2%)	1.30	12/8071 (0.1%)
1	B	1.50	23/5918 (0.4%)	1.31	11/8046 (0.1%)
1	C	1.49	18/5940 (0.3%)	1.30	7/8076 (0.1%)
1	D	1.56	34/5938 (0.6%)	1.33	21/8073 (0.3%)
All	All	1.52	89/23733 (0.4%)	1.31	51/32266 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	C	1	2
All	All	1	3

All (89) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	474	PRO	CA-C	10.78	1.57	1.51
1	C	57	ALA	CA-CB	8.56	1.62	1.53
1	D	203	THR	N-CA	7.70	1.52	1.45
1	C	159	ILE	CB-CG1	-7.50	1.38	1.53
1	A	29	LEU	N-CA	-7.35	1.36	1.45
1	A	360	ILE	N-CA	6.82	1.51	1.46
1	C	159	ILE	CA-CB	-6.79	1.46	1.54
1	C	389	ALA	N-CA	6.75	1.54	1.46
1	D	214	PHE	C-O	-6.71	1.18	1.24
1	D	314	ASP	N-CA	6.44	1.52	1.46
1	C	159	ILE	CG1-CD1	-6.38	1.26	1.51
1	B	136	GLY	N-CA	6.26	1.53	1.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	377	ARG	CZ-NH1	6.24	1.41	1.32
1	D	276	THR	C-O	6.21	1.31	1.24
1	C	187	THR	N-CA	6.07	1.53	1.46
1	B	98	GLY	N-CA	6.06	1.51	1.45
1	A	327	GLU	N-CA	6.05	1.53	1.46
1	D	191	THR	CA-CB	6.01	1.63	1.53
1	B	307	ALA	N-CA	5.95	1.53	1.46
1	D	229	ILE	CA-C	5.93	1.59	1.52
1	A	485	TYR	C-O	5.93	1.31	1.23
1	D	360	ILE	CA-C	5.93	1.58	1.53
1	B	400	LEU	N-CA	5.88	1.53	1.45
1	A	184	GLY	N-CA	5.86	1.54	1.45
1	D	323	TRP	C-O	-5.85	1.17	1.24
1	C	383	PHE	C-O	5.78	1.30	1.24
1	A	314	ASP	N-CA	5.75	1.52	1.46
1	D	452	GLY	N-CA	5.73	1.52	1.45
1	D	377	ARG	N-CA	5.73	1.53	1.46
1	D	140	PRO	C-O	-5.72	1.17	1.23
1	B	273	GLY	C-O	5.71	1.30	1.23
1	B	433	ILE	CA-CB	5.70	1.62	1.54
1	C	458	ALA	C-O	5.68	1.30	1.23
1	C	397	VAL	CA-CB	5.68	1.61	1.55
1	A	638	GLY	N-CA	5.68	1.51	1.45
1	B	109	ILE	C-O	5.62	1.30	1.24
1	D	536	ARG	N-CA	5.59	1.52	1.46
1	B	541	GLU	C-O	5.58	1.30	1.24
1	D	231	GLN	C-O	5.58	1.30	1.23
1	C	397	VAL	N-CA	5.58	1.51	1.46
1	D	91	ASP	C-O	5.57	1.31	1.24
1	D	131	GLY	N-CA	5.57	1.51	1.45
1	D	419	GLN	CA-C	-5.55	1.45	1.52
1	A	745	ILE	CA-CB	5.52	1.56	1.54
1	B	122	ILE	C-O	-5.51	1.18	1.24
1	B	725	ASP	CA-C	5.51	1.60	1.52
1	C	119	HIS	CA-C	-5.51	1.46	1.53
1	B	236	HIS	C-O	5.50	1.30	1.23
1	B	423	LEU	C-O	5.49	1.31	1.24
1	D	274	VAL	N-CA	5.48	1.53	1.46
1	A	131	GLY	N-CA	5.48	1.51	1.45
1	B	57	ALA	CA-CB	5.47	1.60	1.53
1	D	452	GLY	C-O	5.46	1.29	1.24
1	C	432	PRO	N-CA	-5.46	1.40	1.47

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	675	ILE	N-CA	5.45	1.51	1.46
1	A	573	ILE	CA-CB	5.44	1.60	1.54
1	C	446	ASP	N-CA	5.44	1.53	1.46
1	A	474	PRO	CA-C	-5.41	1.49	1.51
1	D	128	HIS	N-CA	5.38	1.54	1.46
1	B	195	ILE	CG1-CD1	-5.37	1.30	1.51
1	D	719	VAL	C-O	-5.36	1.17	1.24
1	D	579	VAL	CA-CB	5.35	1.60	1.53
1	B	420	ILE	N-CA	-5.30	1.40	1.46
1	C	445	ARG	CD-NE	5.30	1.53	1.46
1	D	130	ARG	N-CA	5.29	1.53	1.46
1	D	264	ARG	N-CA	5.29	1.52	1.46
1	D	370	VAL	CA-CB	5.27	1.63	1.54
1	A	216	ASP	C-O	5.26	1.30	1.24
1	D	41	GLU	CG-CD	5.25	1.65	1.52
1	D	56	LYS	CA-CB	5.20	1.61	1.53
1	B	521	ARG	CG-CD	5.19	1.68	1.52
1	B	106	GLU	CA-C	5.17	1.59	1.52
1	B	131	GLY	N-CA	5.13	1.50	1.45
1	D	662	VAL	CA-CB	5.12	1.62	1.54
1	D	440	TYR	CE1-CZ	5.10	1.50	1.38
1	B	172	GLY	N-CA	5.10	1.51	1.45
1	C	147	ILE	C-O	-5.09	1.18	1.24
1	D	81	THR	C-O	5.09	1.30	1.23
1	C	268	THR	CA-CB	5.08	1.60	1.53
1	D	339	GLN	N-CA	5.08	1.52	1.46
1	A	631	LYS	CA-CB	5.06	1.62	1.53
1	B	321	GLU	CB-CG	5.05	1.67	1.52
1	D	54	SER	CA-C	5.05	1.59	1.52
1	D	102	PRO	CA-CB	5.04	1.59	1.53
1	C	115	THR	N-CA	5.02	1.52	1.46
1	C	370	VAL	CA-CB	5.02	1.62	1.54
1	B	314	ASP	N-CA	5.01	1.51	1.46
1	D	165	ARG	CZ-NH2	5.00	1.40	1.33
1	B	438	CYS	C-O	5.00	1.29	1.23

All (51) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	159	ILE	CB-CG1-CD1	-10.16	92.46	113.80
1	C	725	ASP	N-CA-C	7.62	127.04	110.80
1	D	615	ASP	N-CA-C	-6.61	104.00	111.14

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	55	LEU	N-CA-C	-6.30	105.72	113.41
1	D	377	ARG	CG-CD-NE	-6.29	98.17	112.00
1	A	360	ILE	N-CA-C	-6.28	100.88	107.60
1	B	349	PHE	CA-C-N	-5.98	112.73	122.65
1	B	349	PHE	C-N-CA	-5.98	112.73	122.65
1	D	368	GLN	CA-CB-CG	-5.85	102.39	114.10
1	A	114	ILE	CA-C-O	-5.85	114.15	120.47
1	B	377	ARG	CA-CB-CG	-5.81	102.47	114.10
1	B	161	PRO	CB-CA-C	-5.68	103.95	111.23
1	A	574	THR	CA-C-N	5.67	123.80	119.66
1	A	574	THR	C-N-CA	5.67	123.80	119.66
1	D	377	ARG	NE-CZ-NH1	-5.56	115.94	121.50
1	A	745	ILE	CA-C-N	-5.55	113.90	119.56
1	A	745	ILE	C-N-CA	-5.55	113.90	119.56
1	C	539	ILE	N-CA-C	-5.54	105.13	110.72
1	D	377	ARG	NH1-CZ-NH2	5.48	126.42	119.30
1	A	28	SER	CA-C-N	-5.45	113.63	122.36
1	A	28	SER	C-N-CA	-5.45	113.63	122.36
1	A	612	ARG	NE-CZ-NH2	5.44	124.10	119.20
1	B	595	ASP	CB-CA-C	5.44	121.24	110.42
1	B	533	LYS	CA-CB-CG	-5.43	103.24	114.10
1	D	242	TYR	O-C-N	5.41	127.64	122.07
1	D	595	ASP	N-CA-C	-5.39	104.97	112.03
1	D	360	ILE	N-CA-C	-5.34	101.89	107.60
1	A	471	ARG	N-CA-C	5.29	118.69	110.17
1	B	377	ARG	NE-CZ-NH1	-5.24	116.26	121.50
1	D	91	ASP	N-CA-C	-5.23	106.76	112.72
1	D	374	VAL	CA-C-N	-5.15	115.92	122.77
1	D	374	VAL	C-N-CA	-5.15	115.92	122.77
1	D	675	ILE	CA-C-O	5.15	123.62	118.98
1	C	159	ILE	CG1-CB-CG2	5.15	126.15	110.70
1	D	574	THR	CB-CA-C	5.14	116.82	109.26
1	B	724	ALA	N-CA-C	5.12	119.09	113.21
1	D	265	SER	N-CA-CB	-5.11	103.64	111.56
1	D	468	ASN	N-CA-C	5.10	120.65	113.56
1	D	335	GLU	CB-CG-CD	-5.10	103.94	112.60
1	B	370	VAL	CA-CB-CG2	-5.09	101.74	110.40
1	C	751	ILE	CB-CA-C	5.09	116.64	110.78
1	C	474	PRO	CB-CA-C	-5.08	106.61	111.39
1	D	637	MET	CA-C-N	5.06	126.16	121.86
1	D	637	MET	C-N-CA	5.06	126.16	121.86
1	A	686	MET	CG-SD-CE	5.06	112.03	100.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	727	SER	N-CA-C	5.04	116.47	111.07
1	C	745	ILE	O-C-N	5.04	123.65	120.42
1	B	464	SER	N-CA-C	-5.03	107.31	113.50
1	D	473	THR	CA-C-N	-5.01	115.22	120.38
1	D	473	THR	C-N-CA	-5.01	115.22	120.38
1	D	377	ARG	CA-CB-CG	-5.01	104.08	114.10

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	C	159	ILE	CB

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	121	ARG	Sidechain
1	C	724	ALA	Peptide
1	C	725	ASP	Peptide

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	5764	0	5599	44	0
1	B	5749	0	5577	63	0
1	C	5766	0	5595	55	0
1	D	5757	0	5585	49	0
2	A	86	0	60	8	0
2	B	86	0	60	10	0
2	C	86	0	60	9	0
2	D	86	0	60	4	0
3	A	44	0	37	7	0
3	B	44	0	37	5	0
3	C	44	0	37	8	0
3	D	44	0	37	5	0
4	A	44	0	31	4	0
4	B	44	0	31	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	C	44	0	31	3	0
4	D	44	0	31	3	0
5	A	842	0	0	12	0
5	B	754	0	0	14	0
5	C	807	0	0	18	0
5	D	866	0	0	16	1
All	All	27001	0	22868	248	1

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 5.

All (248) 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:C:449[B]:HIS:CE1	5:C:3363:HOH:O	1.74	1.36
1:B:451:MET:HE2	1:D:451:MET:HE2	1.23	1.19
5:A:2649:HOH:O	1:C:28:SER:HA	1.44	1.16
1:D:451:MET:SD	5:D:3617:HOH:O	1.99	1.15
1:A:369[B]:ARG:HH21	1:A:369[B]:ARG:HG3	1.12	1.15
1:A:451:MET:HE2	1:C:451:MET:HE2	1.23	1.13
1:B:157:ASN:HB2	5:B:3138:HOH:O	1.48	1.11
5:B:2705:HOH:O	1:D:73:LYS:HD3	1.49	1.10
1:D:41:GLU:HG2	5:D:3312:HOH:O	1.52	1.06
1:D:267:ARG:HG3	5:D:1920:HOH:O	1.57	1.04
1:B:546:GLN:HG3	5:B:3324:HOH:O	1.58	1.03
1:A:369[B]:ARG:HH21	1:A:369[B]:ARG:CG	1.73	1.00
1:C:267:ARG:HG3	5:C:2916:HOH:O	1.62	0.99
1:A:713:GLN:HG2	5:A:3248:HOH:O	1.65	0.94
1:A:28:SER:O	1:A:28:SER:OG	1.84	0.93
1:A:748:ILE:O	1:A:751:ILE:HG22	1.69	0.93
1:B:521:ARG:HH21	1:B:745:ILE:HG21	1.33	0.91
1:D:28:SER:HB3	5:D:2467:HOH:O	1.76	0.85
1:A:541:GLU:OE2	5:A:2550:HOH:O	1.94	0.85
2:B:754[A]:HEM:CMB	2:B:754[A]:HEM:HBB2	2.05	0.83
1:B:521:ARG:NH2	1:B:745:ILE:HG21	1.94	0.82
1:A:416[B]:THR:HG22	5:A:901:HOH:O	1.79	0.81
1:C:751:ILE:HB	5:C:2367:HOH:O	1.81	0.80
2:B:755[C]:HEM:HMC2	2:B:755[C]:HEM:HBC2	1.63	0.79
1:B:155:ASP:OD1	5:B:3138:HOH:O	1.98	0.79
1:D:416[B]:THR:CG2	5:D:1415:HOH:O	2.30	0.78
3:C:761[B]:HDE:HMB	3:C:761[B]:HDE:HBBB	1.66	0.78

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:416[B]:THR:HG22	5:D:1415:HOH:O	1.83	0.77
3:D:761[B]:HDE:HMB	3:D:761[B]:HDE:HBBB	1.65	0.77
1:D:552:LEU:CD1	1:D:556:GLN:NE2	2.49	0.75
1:C:636:ARG:HD3	5:C:2717:HOH:O	1.87	0.75
2:A:755[C]:HEM:HMC2	2:A:755[C]:HEM:HBC2	1.68	0.75
2:B:754[A]:HEM:HBB2	2:B:754[A]:HEM:HMB1	1.70	0.74
1:C:748:ILE:O	1:C:751:ILE:HG22	1.86	0.74
1:B:546:GLN:CG	5:B:3324:HOH:O	2.27	0.74
1:B:533:LYS:HE2	5:B:3100:HOH:O	1.88	0.73
1:D:552:LEU:HD13	1:D:556:GLN:NE2	2.04	0.72
1:B:144:LEU:HD11	1:B:370:VAL:HG13	1.71	0.71
1:B:330:ASP:OD1	1:B:629:HIS:HE1	1.73	0.71
2:A:755[C]:HEM:CMB	2:A:755[C]:HEM:HBB2	2.22	0.69
1:C:70:ASP:OD1	5:C:2554:HOH:O	2.09	0.69
2:A:755[C]:HEM:HBB2	2:A:755[C]:HEM:HMB2	1.75	0.68
1:C:578[A]:ASP:OD1	5:C:3157:HOH:O	2.11	0.68
1:D:748:ILE:O	1:D:751:ILE:HG22	1.93	0.68
1:B:607:LEU:HD12	1:B:650[B]:ILE:CD1	2.23	0.68
1:B:546:GLN:CD	5:B:3324:HOH:O	2.36	0.68
1:A:612:ARG:NH1	5:A:3360:HOH:O	2.26	0.67
1:A:369[B]:ARG:HG3	1:A:369[B]:ARG:NH2	1.96	0.66
3:D:761[B]:HDE:HMB	3:D:761[B]:HDE:CBB	2.25	0.66
1:D:597:ASP:OD1	5:D:3292:HOH:O	2.14	0.66
1:C:486:GLN:OE1	5:C:2892:HOH:O	2.13	0.65
1:C:612:ARG:HB2	1:C:612:ARG:CZ	2.27	0.65
1:C:583:LYS:O	1:C:584:LYS:HB3	1.97	0.64
5:B:2705:HOH:O	1:D:73:LYS:CD	2.23	0.64
3:A:761[B]:HDE:HMB	3:A:761[B]:HDE:HBBB	1.80	0.64
2:B:754[A]:HEM:HMB1	2:B:754[A]:HEM:CBB	2.26	0.64
1:A:411:ARG:HG3	3:A:761[B]:HDE:HBBA	1.78	0.64
1:B:407:LEU:HD12	2:B:755[C]:HEM:HBB1	1.79	0.63
1:C:556:GLN:NE2	5:C:2533:HOH:O	2.31	0.63
2:C:755[C]:HEM:HMB2	2:C:755[C]:HEM:HBB2	1.80	0.63
1:A:416[B]:THR:CG2	5:A:901:HOH:O	2.43	0.62
1:C:634:TYR:O	1:C:653:THR:HA	1.99	0.62
1:C:330:ASP:OD1	1:C:629:HIS:HE1	1.83	0.62
1:D:629:HIS:HD2	5:D:1554:HOH:O	1.83	0.62
1:B:583:LYS:NZ	1:B:583:LYS:H	1.98	0.61
1:D:552:LEU:HD11	1:D:556:GLN:NE2	2.14	0.61
1:C:211:ALA:CB	2:C:755[C]:HEM:HBB1	2.30	0.61
1:A:29:LEU:HB2	5:C:2405:HOH:O	2.01	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:532[A]:SER:OG	5:A:3443:HOH:O	2.12	0.60
1:D:556:GLN:NE2	5:D:2773:HOH:O	2.33	0.60
2:B:755[C]:HEM:HBC2	2:B:755[C]:HEM:CMC	2.30	0.60
1:B:748:ILE:O	1:B:751:ILE:HG22	2.02	0.60
1:D:330:ASP:OD1	1:D:629:HIS:HE1	1.84	0.59
1:A:369[B]:ARG:CG	1:A:369[B]:ARG:NH2	2.44	0.59
1:D:552:LEU:HD13	1:D:556:GLN:HE21	1.68	0.58
1:A:479:ARG:NH2	5:A:2607:HOH:O	2.18	0.57
1:C:449[B]:HIS:NE2	5:C:3363:HOH:O	2.04	0.57
1:B:411:ARG:HG3	3:B:761[B]:HDE:HBBA	1.85	0.57
1:B:201:ASN:CG	4:B:760[D]:HDD:HMB1	2.29	0.57
1:C:578[A]:ASP:HB2	1:C:582:LEU:O	2.04	0.57
1:A:713:GLN:HA	1:A:713:GLN:HE21	1.68	0.57
1:C:411:ARG:HG3	3:C:761[B]:HDE:HBBA	1.86	0.57
1:D:211:ALA:HB2	2:D:755[C]:HEM:HBB1	1.86	0.56
3:C:761[B]:HDE:HMC	3:C:761[B]:HDE:HBCB	1.87	0.56
1:C:359:LEU:H	1:C:507:HIS:HD2	1.52	0.56
1:B:634:TYR:O	1:B:653:THR:HA	2.05	0.56
1:B:521:ARG:NH2	1:B:745:ILE:HD13	2.21	0.56
3:D:761[B]:HDE:CBB	3:D:761[B]:HDE:CMB	2.82	0.56
3:B:761[B]:HDE:HMBB	3:B:761[B]:HDE:CBB	2.36	0.55
1:B:359:LEU:H	1:B:507:HIS:HD2	1.53	0.55
1:C:636:ARG:NH2	1:C:639:GLU:O	2.39	0.55
2:C:754[A]:HEM:HBB2	2:C:754[A]:HEM:CMB	2.37	0.55
3:C:761[B]:HDE:HBBB	3:C:761[B]:HDE:CMB	2.37	0.55
4:A:760[D]:HDD:HBC1	4:A:760[D]:HDD:HMC1	1.88	0.54
1:A:201:ASN:CG	4:A:760[D]:HDD:HMB1	2.32	0.54
1:B:629:HIS:HD2	5:B:1052:HOH:O	1.92	0.53
1:B:724:ALA:O	1:B:725:ASP:O	2.27	0.53
1:A:278:ARG:HH12	1:A:487:GLU:CD	2.17	0.53
1:D:158:LYS:HB3	5:D:3367:HOH:O	2.08	0.53
4:A:760[D]:HDD:HBC1	4:A:760[D]:HDD:CMC	2.39	0.52
3:B:761[B]:HDE:HMBB	3:B:761[B]:HDE:HBBB	1.91	0.52
1:D:211:ALA:CB	2:D:755[C]:HEM:HBB1	2.40	0.52
1:C:440[B]:TYR:CZ	5:C:1792:HOH:O	2.54	0.52
3:A:761[B]:HDE:HBBB	3:A:761[B]:HDE:CMB	2.39	0.52
3:C:761[B]:HDE:HBAA	5:C:964:HOH:O	2.09	0.52
1:D:201:ASN:CG	4:D:760[D]:HDD:HMB1	2.35	0.51
1:B:533:LYS:HE3	5:C:2623:HOH:O	2.12	0.50
1:B:552:LEU:HD21	1:B:571:LEU:HD12	1.93	0.50
1:C:535:VAL:O	1:C:537:PRO:HD3	2.11	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:36:HIS:CD2	1:A:36:HIS:H	2.30	0.49
2:A:755[C]:HEM:HBC2	2:A:755[C]:HEM:CMC	2.41	0.49
1:A:192:GLU:OE1	1:A:479:ARG:NH2	2.45	0.49
1:B:603:VAL:HG11	1:B:666:ILE:HD12	1.95	0.49
4:C:760[D]:HDD:HBD2	5:C:964:HOH:O	2.12	0.49
4:C:760[D]:HDD:HBC1	4:C:760[D]:HDD:CMC	2.43	0.49
1:B:583:LYS:O	1:B:584:LYS:HB3	2.13	0.49
1:C:201:ASN:CG	4:C:760[D]:HDD:HMB1	2.38	0.49
1:D:61:ARG:NH2	5:D:3239:HOH:O	2.36	0.49
1:B:449[B]:HIS:HE1	5:B:1789:HOH:O	1.96	0.48
1:D:278:ARG:HH12	1:D:487:GLU:CD	2.21	0.48
1:D:359:LEU:H	1:D:507:HIS:HD2	1.61	0.48
1:A:414:SER:OG	2:A:754[A]:HEM:HHD	2.13	0.48
1:D:713:GLN:O	1:D:713:GLN:HG2	2.14	0.48
1:B:612:ARG:HB2	1:B:612:ARG:CZ	2.43	0.48
1:C:128:HIS:HA	1:C:168:THR:O	2.13	0.47
1:C:748:ILE:O	1:C:751:ILE:CG2	2.58	0.47
3:C:761[B]:HDE:HAAA	3:C:761[B]:HDE:HMA	1.49	0.47
1:A:459:ASN:HD22	1:A:459:ASN:H	1.63	0.47
1:B:281:ASN:OD1	1:B:283:GLU:HG3	2.15	0.47
4:B:760[D]:HDD:HBC1	4:B:760[D]:HDD:CMC	2.44	0.47
1:C:488:ARG:HE	1:C:488:ARG:HB2	1.39	0.47
1:B:73:LYS:NZ	5:B:1110:HOH:O	2.47	0.47
1:B:407:LEU:CD1	2:B:755[C]:HEM:HBB1	2.45	0.47
1:B:359:LEU:H	1:B:507:HIS:CD2	2.31	0.47
1:D:207:PHE:O	1:D:249:THR:HA	2.14	0.47
4:D:760[D]:HDD:HMC1	4:D:760[D]:HDD:CBC	2.44	0.47
1:A:612:ARG:CZ	5:A:3400:HOH:O	2.62	0.47
1:C:583:LYS:O	1:C:584:LYS:CB	2.63	0.47
1:C:629:HIS:HD2	5:C:1129:HOH:O	1.98	0.47
1:D:731:GLU:OE2	5:D:3028:HOH:O	2.20	0.47
2:D:755[C]:HEM:HBC2	2:D:755[C]:HEM:CMC	2.46	0.47
1:B:583:LYS:H	1:B:583:LYS:HZ2	1.62	0.46
1:A:155:ASP:HB3	1:A:158:LYS:HB2	1.97	0.46
1:B:603:VAL:HG11	1:B:666:ILE:CD1	2.46	0.46
1:B:634:TYR:HB2	1:B:650[B]:ILE:HD12	1.96	0.46
1:D:128:HIS:HA	1:D:168:THR:O	2.15	0.46
1:B:546:GLN:NE2	5:B:3324:HOH:O	2.47	0.46
1:C:411:ARG:HG2	2:C:755[C]:HEM:C3B	2.50	0.46
4:A:760[D]:HDD:HMC1	4:A:760[D]:HDD:CBC	2.45	0.46
1:B:521:ARG:NH2	1:B:745:ILE:CG2	2.74	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:612:ARG:HG3	5:C:3087:HOH:O	2.15	0.45
1:A:211:ALA:CB	1:A:410:GLY:HA3	2.46	0.45
1:D:552:LEU:HD21	1:D:571:LEU:HD23	1.97	0.45
1:B:696:ALA:HB1	1:B:728:PHE:CZ	2.51	0.45
2:A:754[A]:HEM:CMB	2:A:754[A]:HEM:HBB2	2.47	0.45
1:C:137:TYR:HB2	1:C:159:ILE:HD11	1.97	0.45
1:D:359:LEU:HD21	5:D:2971:HOH:O	2.17	0.45
3:D:761[B]:HDE:HMA	3:D:761[B]:HDE:HAAA	1.44	0.45
1:B:211:ALA:HA	2:B:755[C]:HEM:HBB1	1.98	0.45
1:B:414:SER:OG	2:B:754[A]:HEM:HHD	2.16	0.45
1:B:533:LYS:CE	5:C:2623:HOH:O	2.65	0.45
5:A:1788:HOH:O	1:C:449[A]:HIS:HE1	1.99	0.45
1:B:39:ALA:HB1	1:B:41:GLU:HG2	1.98	0.45
1:C:165:ARG:HD3	2:C:755[C]:HEM:O1D	2.16	0.45
1:C:254:MET:HB3	1:C:254:MET:HE3	1.80	0.45
1:C:704:PHE:O	1:C:707:THR:HG22	2.17	0.45
2:C:755[C]:HEM:HBB2	2:C:755[C]:HEM:CMB	2.46	0.45
1:A:128:HIS:HA	1:A:168:THR:O	2.17	0.45
1:A:411:ARG:CG	3:A:761[B]:HDE:HBBA	2.46	0.45
1:A:634:TYR:O	1:A:653:THR:HA	2.16	0.45
1:C:201:ASN:CG	2:C:755[C]:HEM:HAC	2.41	0.45
1:D:393:PRO:HD2	1:D:415:TYR:CG	2.52	0.45
1:B:459:ASN:HD22	1:B:459:ASN:H	1.65	0.44
1:B:211:ALA:CB	1:B:410:GLY:HA3	2.47	0.44
1:B:686:MET:HB3	1:B:751:ILE:HD11	1.98	0.44
1:C:488:ARG:NH1	5:C:2379:HOH:O	2.25	0.44
1:C:717:GLY:HA3	1:C:741:VAL:HG11	1.99	0.44
1:B:157:ASN:CB	5:B:3138:HOH:O	2.28	0.44
1:D:556:GLN:HG2	1:D:566:LEU:HD12	1.98	0.44
1:B:461:GLU:HA	1:B:462:PRO:C	2.42	0.44
1:C:552:LEU:HD22	1:C:556:GLN:HG3	2.00	0.44
1:C:705:LYS:HG2	1:C:710:ILE:HB	2.00	0.44
1:B:128:HIS:HA	1:B:168:THR:O	2.18	0.44
2:B:754[A]:HEM:HBB2	2:B:754[A]:HEM:HMB3	1.93	0.44
1:C:309:LYS:HB3	1:C:660:LEU:HD21	1.98	0.44
1:C:128:HIS:CE1	1:C:169:VAL:HG22	2.53	0.44
1:C:551:ASP:OD1	1:C:553:THR:HB	2.18	0.44
1:C:461:GLU:HA	1:C:462:PRO:C	2.42	0.44
1:A:393:PRO:HD2	1:A:415:TYR:CG	2.53	0.43
1:C:359:LEU:H	1:C:507:HIS:CD2	2.32	0.43
1:B:393:PRO:HD2	1:B:415:TYR:CG	2.54	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:755[C]:HEM:HMB2	2:A:755[C]:HEM:CBB	2.46	0.43
1:B:521:ARG:NH2	1:B:745:ILE:CD1	2.81	0.43
2:D:755[C]:HEM:HBC2	2:D:755[C]:HEM:HMC2	2.00	0.43
1:A:252:ASN:HD22	1:A:252:ASN:HA	1.69	0.43
4:D:760[D]:HDD:HMC1	4:D:760[D]:HDD:HBC1	2.00	0.43
1:A:461:GLU:HA	1:A:462:PRO:C	2.43	0.43
5:B:1789:HOH:O	1:D:449[A]:HIS:HE1	2.02	0.43
1:D:128:HIS:CE1	1:D:169:VAL:HG22	2.54	0.43
1:C:404:ASN:O	1:C:405:ASP:C	2.60	0.43
1:B:583:LYS:H	1:B:583:LYS:HZ3	1.65	0.43
2:C:754[A]:HEM:HBB2	2:C:754[A]:HEM:HMB1	2.00	0.43
1:C:552:LEU:HD21	1:C:571:LEU:HD12	2.00	0.42
1:D:48:GLN:HE21	1:D:48:GLN:HB3	1.69	0.42
1:D:393:PRO:HD2	1:D:415:TYR:CD2	2.54	0.42
1:A:335:GLU:OE1	1:A:369[B]:ARG:HD3	2.20	0.42
1:B:252:ASN:HD22	1:B:252:ASN:HA	1.75	0.42
1:C:578[B]:ASP:CG	1:C:583:LYS:HG3	2.44	0.42
1:D:416[B]:THR:HG21	5:D:1415:HOH:O	2.07	0.42
3:A:761[B]:HDE:HABA	3:A:761[B]:HDE:HHCA	1.86	0.42
3:A:761[B]:HDE:HMAB	3:A:761[B]:HDE:HAAA	1.65	0.42
1:D:597:ASP:OD2	5:D:2709:HOH:O	2.21	0.42
1:A:414:SER:OG	3:A:761[B]:HDE:HHB	2.20	0.42
3:C:761[B]:HDE:CMB	3:C:761[B]:HDE:CBB	2.98	0.42
1:A:610:GLU:HG2	5:A:2551:HOH:O	2.19	0.42
1:C:211:ALA:HB2	2:C:755[C]:HEM:HBB1	2.02	0.42
1:A:422:ARG:NE	2:A:754[A]:HEM:O1D	2.53	0.41
1:B:682:ASN:HB3	1:B:707:THR:HG21	2.02	0.41
1:A:38:PRO:HA	1:A:48:GLN:OE1	2.19	0.41
1:D:593:ILE:HA	1:D:594:PRO:HD3	1.94	0.41
1:C:219:HIS:HB3	1:D:459:ASN:ND2	2.36	0.41
1:C:459:ASN:H	1:C:459:ASN:HD22	1.68	0.41
1:D:211:ALA:CB	1:D:410:GLY:HA3	2.51	0.41
1:D:459:ASN:HD22	1:D:459:ASN:H	1.68	0.41
1:A:459:ASN:ND2	1:B:219:HIS:HB3	2.36	0.41
1:A:219:HIS:HB3	1:B:459:ASN:ND2	2.36	0.41
1:A:716:GLU:HG2	5:A:1656:HOH:O	2.21	0.41
1:B:207:PHE:O	1:B:249:THR:HA	2.21	0.41
1:B:91:ASP:OD1	1:D:461:GLU:OE1	2.39	0.41
1:B:359:LEU:HD12	1:B:359:LEU:C	2.46	0.41
3:B:761[B]:HDE:HAAA	3:B:761[B]:HDE:HMA	1.41	0.41
1:C:583:LYS:HE3	1:C:583:LYS:HB2	1.90	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:556:GLN:CG	1:D:566:LEU:HD12	2.51	0.41
1:D:634:TYR:O	1:D:653:THR:HA	2.20	0.41
3:D:761[B]:HDE:CMB	3:D:761[B]:HDE:HBBA	2.50	0.41
1:B:521:ARG:HH22	1:B:745:ILE:CD1	2.34	0.40
1:B:607:LEU:HD22	1:B:611:VAL:HG21	2.02	0.40
1:B:732:LEU:C	1:B:732:LEU:HD13	2.45	0.40
1:A:39:ALA:HB1	1:A:41:GLU:HG2	2.04	0.40
1:A:207:PHE:O	1:A:249:THR:HA	2.21	0.40
1:C:238:THR:HB	1:D:460:TYR:CE2	2.56	0.40
1:D:61:ARG:NH1	5:D:3245:HOH:O	2.53	0.40
1:A:95:LEU:HB3	1:A:107:ASP:HB2	2.03	0.40
1:A:251:HIS:CE1	1:A:507:HIS:HB3	2.56	0.40
1:B:411:ARG:HG2	3:B:761[B]:HDE:C3B	2.51	0.40
1:C:407:LEU:HD12	3:C:761[B]:HDE:HBB	2.04	0.40
1:B:144:LEU:HD11	1:B:370:VAL:CG1	2.48	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:D:2178:HOH:O	5:D:2976:HOH:O[1_655]	2.13	0.07

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	729/753 (97%)	713 (98%)	15 (2%)	1 (0%)	48 24
1	B	727/753 (96%)	706 (97%)	19 (3%)	2 (0%)	36 17
1	C	729/753 (97%)	717 (98%)	11 (2%)	1 (0%)	48 24
1	D	730/753 (97%)	716 (98%)	13 (2%)	1 (0%)	48 24

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	2915/3012 (97%)	2852 (98%)	58 (2%)	5 (0%)	43 22

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	725	ASP
1	A	75	SER
1	B	75	SER
1	C	75	SER
1	D	75	SER

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	616/636 (97%)	599 (97%)	17 (3%)	38 11
1	B	614/636 (96%)	588 (96%)	26 (4%)	26 4
1	C	616/636 (97%)	587 (95%)	29 (5%)	23 3
1	D	617/636 (97%)	597 (97%)	20 (3%)	34 8
All	All	2463/2544 (97%)	2371 (96%)	92 (4%)	30 6

All (92) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	28	SER
1	A	29	LEU
1	A	37	ARG
1	A	73	LYS
1	A	158	LYS
1	A	191	THR
1	A	205	ILE
1	A	252	ASN
1	A	432	PRO
1	A	440	TYR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	459	ASN
1	A	552	LEU
1	A	617	LEU
1	A	626	LYS
1	A	716	GLU
1	A	732	LEU
1	A	751	ILE
1	B	28	SER
1	B	32	GLU
1	B	191	THR
1	B	205	ILE
1	B	252	ASN
1	B	283	GLU
1	B	344	GLU
1	B	432	PRO
1	B	440	TYR
1	B	459	ASN
1	B	552	LEU
1	B	562	LEU
1	B	566	LEU
1	B	568	ASP
1	B	571	LEU
1	B	583	LYS
1	B	595	ASP
1	B	610	GLU
1	B	612	ARG
1	B	616	LEU
1	B	624	LYS
1	B	633	LEU
1	B	703	LYS
1	B	713	GLN
1	B	750	LYS
1	B	751	ILE
1	C	159	ILE
1	C	191	THR
1	C	205	ILE
1	C	213	LYS
1	C	252	ASN
1	C	283	GLU
1	C	285	LYS
1	C	377	ARG
1	C	440[A]	TYR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	440[B]	TYR
1	C	459	ASN
1	C	478	LYS
1	C	488	ARG
1	C	552	LEU
1	C	571	LEU
1	C	594	PRO
1	C	606	LEU
1	C	612	ARG
1	C	616	LEU
1	C	617	LEU
1	C	633	LEU
1	C	648	LEU
1	C	660	LEU
1	C	708	ILE
1	C	725	ASP
1	C	732	LEU
1	C	733	LEU
1	C	747	LYS
1	C	750	LYS
1	D	41	GLU
1	D	73	LYS
1	D	191	THR
1	D	205	ILE
1	D	252	ASN
1	D	344	GLU
1	D	432	PRO
1	D	440	TYR
1	D	459	ASN
1	D	490	GLU
1	D	574	THR
1	D	582	LEU
1	D	612	ARG
1	D	616	LEU
1	D	624	LYS
1	D	648	LEU
1	D	713	GLN
1	D	747	LYS
1	D	750	LYS
1	D	751	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	36	HIS
1	A	66	ASN
1	A	84	GLN
1	A	212	HIS
1	A	246	GLN
1	A	252	ASN
1	A	459	ASN
1	A	671	ASN
1	A	713	GLN
1	B	157	ASN
1	B	252	ASN
1	B	459	ASN
1	B	507	HIS
1	B	546	GLN
1	B	629	HIS
1	C	252	ASN
1	C	459	ASN
1	C	486	GLN
1	C	507	HIS
1	C	556	GLN
1	C	629	HIS
1	C	671	ASN
1	D	48	GLN
1	D	252	ASN
1	D	459	ASN
1	D	486	GLN
1	D	507	HIS
1	D	549	HIS
1	D	556	GLN
1	D	629	HIS
1	D	682	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	HDE	A	761[B]	5,1	50,52,52	2.44	21 (42%)	60,89,89	2.26	20 (33%)
2	HEM	C	755[C]	5,1	50,50,50	1.64	7 (14%)	67,82,82	1.65	16 (23%)
2	HEM	B	754[A]	5,1	50,50,50	1.87	10 (20%)	67,82,82	1.76	16 (23%)
2	HEM	A	754[A]	5,1	50,50,50	1.89	9 (18%)	67,82,82	1.84	15 (22%)
4	HDD	C	760[D]	5,1	49,52,52	2.15	10 (20%)	62,89,89	1.96	20 (32%)
4	HDD	D	760[D]	1	49,52,52	2.34	12 (24%)	62,89,89	1.67	14 (22%)
3	HDE	C	761[B]	5,1	50,52,52	2.50	21 (42%)	60,89,89	2.19	22 (36%)
2	HEM	C	754[A]	5,1	50,50,50	1.87	6 (12%)	67,82,82	1.75	19 (28%)
2	HEM	D	754[A]	1	50,50,50	1.98	9 (18%)	67,82,82	1.72	11 (16%)
3	HDE	B	761[B]	5,1	50,52,52	2.53	23 (46%)	60,89,89	2.17	22 (36%)
3	HDE	D	761[B]	1	50,52,52	2.44	20 (40%)	60,89,89	2.08	21 (35%)
4	HDD	A	760[D]	5,1	49,52,52	2.35	11 (22%)	62,89,89	2.12	21 (33%)
2	HEM	D	755[C]	1	50,50,50	1.70	9 (18%)	67,82,82	1.44	11 (16%)
2	HEM	B	755[C]	5,1	50,50,50	1.77	9 (18%)	67,82,82	1.45	12 (17%)
4	HDD	B	760[D]	5,1	49,52,52	2.25	12 (24%)	62,89,89	2.01	21 (33%)
2	HEM	A	755[C]	5,1	50,50,50	1.81	10 (20%)	67,82,82	1.66	15 (22%)

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	HDE	A	761[B]	5,1	-	2/9/89/89	0/1/9/9
2	HEM	C	755[C]	5,1	-	3/14/54/54	-
2	HEM	A	754[A]	5,1	-	4/14/54/54	-
4	HDD	D	760[D]	1	1/1/8/14	4/9/89/89	0/1/9/9
4	HDD	C	760[D]	5,1	1/1/8/14	4/9/89/89	0/1/9/9
2	HEM	B	754[A]	5,1	-	4/14/54/54	-
3	HDE	C	761[B]	5,1	-	3/9/89/89	0/1/9/9
4	HDD	A	760[D]	5,1	1/1/8/14	3/9/89/89	0/1/9/9
2	HEM	C	754[A]	5,1	-	2/14/54/54	-
2	HEM	D	754[A]	1	-	3/14/54/54	-
3	HDE	B	761[B]	5,1	-	2/9/89/89	0/1/9/9
3	HDE	D	761[B]	1	-	2/9/89/89	0/1/9/9
2	HEM	D	755[C]	1	-	5/14/54/54	-
2	HEM	B	755[C]	5,1	-	2/14/54/54	-
4	HDD	B	760[D]	5,1	1/1/8/14	4/9/89/89	0/1/9/9
2	HEM	A	755[C]	5,1	-	2/14/54/54	-

All (199) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	760[D]	HDD	FE-ND	9.08	2.22	1.94
4	C	760[D]	HDD	FE-ND	8.86	2.22	1.94
4	A	760[D]	HDD	FE-ND	8.86	2.22	1.94
4	A	760[D]	HDD	C1D-ND	7.85	1.40	1.35
4	B	760[D]	HDD	FE-ND	7.75	2.18	1.94
4	D	760[D]	HDD	C1D-ND	7.62	1.40	1.35
2	D	754[A]	HEM	C3D-C2D	7.53	1.53	1.36
2	D	754[A]	HEM	FE-NB	7.33	2.17	1.94
2	A	754[A]	HEM	C3D-C2D	7.29	1.52	1.36
4	B	760[D]	HDD	C1D-ND	7.21	1.40	1.35
2	C	754[A]	HEM	C3D-C2D	7.13	1.52	1.36
2	D	755[C]	HEM	C3D-C2D	7.10	1.52	1.36
2	B	754[A]	HEM	C3D-C2D	7.01	1.51	1.36
2	C	755[C]	HEM	C3D-C2D	6.93	1.51	1.36
2	A	755[C]	HEM	C3D-C2D	6.85	1.51	1.36
2	B	755[C]	HEM	C3D-C2D	6.81	1.51	1.36
4	A	760[D]	HDD	O1D-C3D	-6.79	1.35	1.46
2	C	754[A]	HEM	FE-NB	6.48	2.14	1.94
2	B	754[A]	HEM	FE-NC	5.74	2.14	1.95
3	C	761[B]	HDE	C3B-C2B	5.69	1.48	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	761[B]	HDE	C3B-C2B	5.49	1.48	1.37
4	C	760[D]	HDD	O1D-C3D	-5.41	1.38	1.46
2	A	755[C]	HEM	FE-NC	5.36	2.12	1.95
3	D	761[B]	HDE	C3B-C2B	5.27	1.47	1.37
2	A	754[A]	HEM	FE-NB	5.24	2.11	1.94
3	C	761[B]	HDE	C3D-C2D	5.23	1.48	1.36
4	B	760[D]	HDD	FE-NB	5.12	2.10	1.94
4	C	760[D]	HDD	FE-NB	5.11	2.10	1.94
3	A	761[B]	HDE	C3D-C2D	5.11	1.47	1.36
4	C	760[D]	HDD	C1D-ND	5.07	1.38	1.35
3	A	761[B]	HDE	C3B-C2B	5.04	1.47	1.37
4	D	760[D]	HDD	FE-NB	5.00	2.10	1.94
4	B	760[D]	HDD	O1D-C3D	-4.84	1.38	1.46
3	C	761[B]	HDE	O1A-CGA	4.80	1.43	1.35
3	B	761[B]	HDE	C4A-NA	4.74	1.45	1.37
3	B	761[B]	HDE	O1A-CGA	4.72	1.43	1.35
2	B	755[C]	HEM	FE-NB	4.68	2.09	1.94
3	B	761[B]	HDE	FE-ND	4.61	2.09	1.94
4	D	760[D]	HDD	O1D-C3D	-4.58	1.39	1.46
3	D	761[B]	HDE	FE-ND	4.57	2.09	1.94
2	C	754[A]	HEM	FE-NC	4.53	2.10	1.95
3	A	761[B]	HDE	FE-ND	4.43	2.08	1.94
2	A	755[C]	HEM	FE-NA	4.43	2.09	1.95
3	B	761[B]	HDE	C1A-NA	4.42	1.45	1.37
3	D	761[B]	HDE	C3B-C4B	-4.41	1.36	1.44
3	D	761[B]	HDE	CHA-C4D	4.34	1.49	1.39
3	C	761[B]	HDE	CHC-C4B	4.34	1.47	1.38
3	A	761[B]	HDE	O1A-CGA	4.30	1.42	1.35
3	D	761[B]	HDE	C4A-NA	4.29	1.45	1.37
2	A	754[A]	HEM	FE-NC	4.23	2.09	1.95
3	B	761[B]	HDE	CHD-C1D	4.16	1.46	1.38
3	C	761[B]	HDE	FE-ND	4.15	2.07	1.94
3	B	761[B]	HDE	CBB-CAB	4.08	1.50	1.30
2	B	755[C]	HEM	FE-NC	4.07	2.08	1.95
2	B	754[A]	HEM	FE-NB	4.05	2.07	1.94
3	D	761[B]	HDE	O1A-CGA	4.04	1.42	1.35
3	D	761[B]	HDE	C3D-C2D	3.99	1.45	1.36
3	C	761[B]	HDE	CBC-CAC	3.98	1.49	1.30
3	A	761[B]	HDE	C1A-NA	3.97	1.44	1.37
3	D	761[B]	HDE	CBC-CAC	3.89	1.49	1.30
3	A	761[B]	HDE	CHA-C4D	3.89	1.48	1.39
3	A	761[B]	HDE	C3B-C4B	-3.88	1.37	1.44

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	761[B]	HDE	CBB-CAB	3.86	1.48	1.30
3	B	761[B]	HDE	CHA-C4D	3.80	1.47	1.39
3	A	761[B]	HDE	CHB-C1B	3.79	1.47	1.39
3	C	761[B]	HDE	CHB-C1B	3.77	1.47	1.39
3	B	761[B]	HDE	CBC-CAC	3.76	1.48	1.30
2	D	755[C]	HEM	FE-NB	3.76	2.06	1.94
3	C	761[B]	HDE	C1A-NA	3.71	1.44	1.37
3	C	761[B]	HDE	CHD-C1D	3.70	1.45	1.38
3	A	761[B]	HDE	CBB-CAB	3.69	1.48	1.30
2	C	755[C]	HEM	FE-NB	3.67	2.06	1.94
3	D	761[B]	HDE	CBB-CAB	3.67	1.48	1.30
3	D	761[B]	HDE	C1A-NA	3.66	1.43	1.37
3	B	761[B]	HDE	CHC-C1C	3.62	1.47	1.39
3	C	761[B]	HDE	C4A-NA	3.61	1.43	1.37
3	A	761[B]	HDE	CHC-C4B	3.58	1.45	1.38
3	B	761[B]	HDE	CHB-C1B	3.57	1.47	1.39
3	A	761[B]	HDE	CBC-CAC	3.53	1.47	1.30
3	B	761[B]	HDE	C3D-C2D	3.52	1.44	1.36
3	D	761[B]	HDE	CHD-C1D	3.52	1.45	1.38
3	A	761[B]	HDE	C4A-NA	3.51	1.43	1.37
3	C	761[B]	HDE	C3B-C4B	-3.48	1.38	1.44
3	C	761[B]	HDE	CHA-C4D	3.47	1.47	1.39
3	A	761[B]	HDE	CHC-C1C	3.42	1.47	1.39
2	B	755[C]	HEM	CAB-C3B	3.41	1.56	1.47
4	A	760[D]	HDD	FE-NB	3.32	2.05	1.94
3	D	761[B]	HDE	CHB-C1B	3.30	1.46	1.39
4	B	760[D]	HDD	FE-NC	3.28	2.06	1.95
4	D	760[D]	HDD	CMD-C2D	3.26	1.57	1.53
3	B	761[B]	HDE	C3B-C4B	-3.26	1.38	1.44
3	B	761[B]	HDE	CHC-C4B	3.26	1.45	1.38
2	D	754[A]	HEM	FE-NC	3.23	2.05	1.95
2	A	754[A]	HEM	FE-ND	3.23	2.04	1.94
3	A	761[B]	HDE	CHD-C4C	3.18	1.46	1.39
3	B	761[B]	HDE	CHD-C4C	3.16	1.46	1.39
3	D	761[B]	HDE	CHC-C4B	3.13	1.44	1.38
3	A	761[B]	HDE	CHD-C1D	3.11	1.44	1.38
3	C	761[B]	HDE	CHD-C4C	3.04	1.46	1.39
2	D	754[A]	HEM	FE-ND	2.97	2.04	1.94
2	C	755[C]	HEM	C2A-C3A	-2.96	1.31	1.38
4	C	760[D]	HDD	FE-NC	2.94	2.04	1.95
2	C	755[C]	HEM	FE-NC	2.94	2.04	1.95
4	A	760[D]	HDD	FE-NC	2.92	2.04	1.95

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	761[B]	HDE	C1D-ND	-2.87	1.35	1.40
4	B	760[D]	HDD	C2A-C3A	-2.87	1.31	1.38
2	A	754[A]	HEM	FE-NA	2.85	2.04	1.95
4	D	760[D]	HDD	CAC-C3C	2.83	1.54	1.47
3	A	761[B]	HDE	C1D-C2D	-2.83	1.38	1.44
3	D	761[B]	HDE	C1D-C2D	-2.81	1.38	1.44
2	A	754[A]	HEM	CAC-C3C	2.80	1.54	1.47
4	B	760[D]	HDD	CMD-C2D	2.78	1.57	1.53
2	D	754[A]	HEM	CMC-C2C	2.78	1.56	1.50
2	B	755[C]	HEM	C2A-C3A	-2.77	1.31	1.38
4	D	760[D]	HDD	CAB-C3B	2.75	1.54	1.47
4	B	760[D]	HDD	CAB-C3B	2.71	1.54	1.47
3	A	761[B]	HDE	C1C-NC	2.71	1.44	1.39
3	C	761[B]	HDE	C4D-ND	-2.70	1.33	1.38
3	D	761[B]	HDE	C1D-ND	-2.63	1.35	1.40
2	D	755[C]	HEM	FE-ND	2.62	2.03	1.94
4	D	760[D]	HDD	OND-C2D	2.61	1.47	1.42
3	D	761[B]	HDE	CHD-C4C	2.60	1.45	1.39
2	A	755[C]	HEM	CAC-C3C	2.60	1.54	1.47
2	B	754[A]	HEM	C2A-C3A	-2.60	1.32	1.38
2	D	754[A]	HEM	CAC-C3C	2.58	1.54	1.47
2	B	754[A]	HEM	CMA-C3A	2.57	1.56	1.50
2	A	755[C]	HEM	C2A-C3A	-2.55	1.32	1.38
2	D	755[C]	HEM	CAB-C3B	2.54	1.54	1.47
2	D	755[C]	HEM	C3B-C2B	-2.54	1.32	1.37
2	A	755[C]	HEM	CAB-C3B	2.51	1.54	1.47
3	C	761[B]	HDE	C1D-C2D	-2.50	1.39	1.44
2	C	754[A]	HEM	CAB-C3B	2.49	1.54	1.47
2	C	754[A]	HEM	CAC-C3C	2.48	1.54	1.47
3	D	761[B]	HDE	CHC-C1C	2.47	1.45	1.39
2	B	754[A]	HEM	CMC-C2C	2.46	1.55	1.50
2	D	755[C]	HEM	FE-NC	2.46	2.03	1.95
2	B	754[A]	HEM	FE-NA	2.44	2.03	1.95
2	A	754[A]	HEM	CAB-C3B	2.44	1.53	1.47
2	B	755[C]	HEM	C1B-NB	-2.44	1.36	1.40
4	C	760[D]	HDD	CAC-C3C	2.44	1.53	1.47
4	B	760[D]	HDD	CMC-C2C	2.43	1.55	1.50
3	C	761[B]	HDE	C1D-ND	-2.42	1.36	1.40
4	B	760[D]	HDD	CMA-C3A	2.40	1.55	1.50
3	C	761[B]	HDE	FE-NC	2.40	2.03	1.95
2	B	755[C]	HEM	CAC-C3C	2.40	1.53	1.47
4	C	760[D]	HDD	CAB-C3B	2.39	1.53	1.47

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	760[D]	HDD	CAC-C3C	2.38	1.53	1.47
4	C	760[D]	HDD	CMD-C2D	2.37	1.56	1.53
3	B	761[B]	HDE	FE-NA	2.37	2.03	1.95
4	D	760[D]	HDD	C2A-C3A	-2.33	1.32	1.38
4	B	760[D]	HDD	C3B-C2B	-2.32	1.32	1.37
2	B	755[C]	HEM	CMD-C2D	2.30	1.55	1.50
3	C	761[B]	HDE	CHC-C1C	2.30	1.44	1.39
3	D	761[B]	HDE	FE-NC	2.30	2.02	1.95
3	B	761[B]	HDE	C3C-C4C	2.29	1.49	1.42
3	B	761[B]	HDE	C3C-C2C	2.28	1.48	1.41
2	C	755[C]	HEM	CAB-C3B	2.27	1.53	1.47
2	A	754[A]	HEM	CMC-C2C	2.27	1.55	1.50
3	D	761[B]	HDE	C4D-C3D	2.27	1.48	1.45
2	B	754[A]	HEM	CAB-C3B	2.26	1.53	1.47
3	B	761[B]	HDE	FE-NC	2.25	2.02	1.95
2	D	755[C]	HEM	C2A-C3A	-2.25	1.33	1.38
4	A	760[D]	HDD	CMC-C2C	2.24	1.55	1.50
2	C	755[C]	HEM	CMC-C2C	2.22	1.55	1.50
2	D	755[C]	HEM	CAC-C3C	2.21	1.53	1.47
4	D	760[D]	HDD	C3C-C2C	-2.20	1.32	1.37
2	D	754[A]	HEM	CAB-C3B	2.20	1.53	1.47
3	D	761[B]	HDE	C3C-C2C	2.20	1.48	1.41
3	A	761[B]	HDE	C1D-ND	-2.19	1.36	1.40
3	A	761[B]	HDE	FE-NC	2.18	2.02	1.95
2	A	755[C]	HEM	FE-NB	2.18	2.01	1.94
2	A	755[C]	HEM	CMB-C2B	2.18	1.55	1.50
2	A	755[C]	HEM	CMC-C2C	2.17	1.55	1.50
4	B	760[D]	HDD	CAC-C3C	2.17	1.53	1.47
3	B	761[B]	HDE	CAC-C3C	2.16	1.53	1.47
3	B	761[B]	HDE	C1D-C2D	-2.16	1.40	1.44
4	D	760[D]	HDD	FE-NC	2.16	2.02	1.95
3	C	761[B]	HDE	FE-NB	2.14	2.01	1.94
4	A	760[D]	HDD	C3C-C2C	-2.13	1.32	1.37
4	D	760[D]	HDD	CMA-C3A	2.13	1.55	1.50
2	C	755[C]	HEM	CAC-C3C	2.11	1.53	1.47
4	A	760[D]	HDD	CAB-C3B	2.10	1.53	1.47
2	D	754[A]	HEM	C2A-C3A	-2.09	1.33	1.38
4	C	760[D]	HDD	C2A-C3A	-2.09	1.33	1.38
2	A	754[A]	HEM	C2A-C3A	-2.08	1.33	1.38
2	C	754[A]	HEM	FE-ND	2.08	2.01	1.94
2	D	754[A]	HEM	CMA-C3A	2.07	1.55	1.50
3	A	761[B]	HDE	O1A-C2A	-2.07	1.43	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	754[A]	HEM	CAC-C3C	2.06	1.52	1.47
3	A	761[B]	HDE	C4D-ND	-2.06	1.34	1.38
3	C	761[B]	HDE	C3C-C4C	2.06	1.48	1.42
2	A	755[C]	HEM	CMA-C3A	2.05	1.55	1.50
2	B	754[A]	HEM	C3B-C2B	-2.05	1.33	1.37
4	A	760[D]	HDD	CMD-C2D	2.04	1.55	1.53
3	B	761[B]	HDE	FE-NB	2.03	2.01	1.94
2	D	755[C]	HEM	CMD-C2D	2.01	1.54	1.50
4	C	760[D]	HDD	OND-C2D	2.01	1.46	1.42
4	A	760[D]	HDD	C2A-C3A	-2.00	1.33	1.38
2	B	755[C]	HEM	CMC-C2C	2.00	1.54	1.50

All (276) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	761[B]	HDE	C2D-C1D-ND	6.92	117.79	109.84
3	C	761[B]	HDE	C2D-C1D-ND	6.55	117.37	109.84
3	A	761[B]	HDE	C2D-C1D-ND	6.49	117.30	109.84
3	B	761[B]	HDE	C2D-C1D-ND	6.24	117.01	109.84
2	D	754[A]	HEM	C3B-C4B-NB	-5.93	105.21	109.47
4	A	760[D]	HDD	C4D-ND-C1D	5.78	112.06	105.27
2	A	754[A]	HEM	C4D-ND-C1D	5.72	111.98	105.21
4	A	760[D]	HDD	CAD-CBD-CGD	-5.49	96.32	104.48
4	C	760[D]	HDD	C3B-C4B-NB	-5.48	105.53	109.47
2	A	754[A]	HEM	C3B-C4B-NB	-5.38	105.61	109.47
2	D	754[A]	HEM	C4D-ND-C1D	4.92	111.04	105.21
2	C	754[A]	HEM	C3B-C4B-NB	-4.91	105.94	109.47
3	A	761[B]	HDE	C3C-C2C-C1C	-4.77	101.55	107.17
4	A	760[D]	HDD	O1D-CGD-CBD	-4.76	105.83	110.17
3	A	761[B]	HDE	CBA-CAA-C2A	4.76	110.77	103.98
2	B	754[A]	HEM	C3B-C4B-NB	-4.73	106.07	109.47
4	B	760[D]	HDD	C4D-ND-C1D	4.71	110.80	105.27
4	D	760[D]	HDD	C4D-ND-C1D	4.65	110.72	105.27
4	C	760[D]	HDD	O1D-CGD-O2D	4.64	124.72	120.81
2	C	754[A]	HEM	CBD-CAD-C3D	-4.63	99.73	112.53
3	A	761[B]	HDE	CMC-C2C-C1C	4.59	132.40	125.42
2	B	754[A]	HEM	C4D-ND-C1D	4.52	110.56	105.21
2	D	754[A]	HEM	CBD-CAD-C3D	-4.48	100.15	112.53
2	B	755[C]	HEM	CAD-CBD-CGD	-4.47	101.80	113.67
3	C	761[B]	HDE	CBA-CAA-C2A	4.42	110.28	103.98
3	B	761[B]	HDE	C4B-C3B-C2B	-4.38	103.25	107.28
2	C	755[C]	HEM	CHC-C4B-NB	4.37	129.13	124.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	754[A]	HEM	CHA-C4D-ND	4.36	129.76	124.37
4	B	760[D]	HDD	O1D-CGD-O2D	4.36	124.48	120.81
2	B	754[A]	HEM	CBD-CAD-C3D	-4.36	100.49	112.53
3	C	761[B]	HDE	C2C-C1C-NC	4.28	117.00	110.14
3	A	761[B]	HDE	CAD-CBD-CGD	-4.26	102.36	113.67
2	A	754[A]	HEM	CBD-CAD-C3D	-4.20	100.92	112.53
3	B	761[B]	HDE	C2C-C1C-NC	4.18	116.85	110.14
4	A	760[D]	HDD	C3B-C2B-C1B	4.17	109.54	106.41
3	C	761[B]	HDE	C1D-C2D-C3D	-4.13	102.64	106.98
4	B	760[D]	HDD	CHD-C4C-NC	4.12	128.94	124.45
3	D	761[B]	HDE	CBB-CAB-C3B	-4.10	107.02	127.53
2	A	755[C]	HEM	CHA-C4D-ND	4.10	129.44	124.37
2	A	755[C]	HEM	CHD-C1D-ND	4.09	128.82	124.42
2	A	754[A]	HEM	CHA-C4D-ND	4.08	129.41	124.37
4	A	760[D]	HDD	C3B-C4B-NB	-4.08	106.54	109.47
2	D	754[A]	HEM	C1B-NB-C4B	4.07	110.02	105.21
3	C	761[B]	HDE	C3D-C4D-ND	4.06	114.27	110.35
2	D	755[C]	HEM	CAD-CBD-CGD	-4.00	103.05	113.67
4	A	760[D]	HDD	C3D-O1D-CGD	4.00	114.87	111.14
3	D	761[B]	HDE	CAD-CBD-CGD	-3.99	103.08	113.67
4	C	760[D]	HDD	C4D-ND-C1D	3.97	109.93	105.27
3	A	761[B]	HDE	CBB-CAB-C3B	-3.90	108.02	127.53
4	B	760[D]	HDD	CHC-C1C-NC	3.90	128.70	124.45
3	B	761[B]	HDE	C3C-C2C-C1C	-3.90	102.57	107.17
4	B	760[D]	HDD	C3B-C2B-C1B	3.89	109.33	106.41
4	B	760[D]	HDD	O1D-CGD-CBD	-3.88	106.64	110.17
4	B	760[D]	HDD	C3D-O1D-CGD	3.87	114.75	111.14
2	A	755[C]	HEM	C3B-C4B-NB	-3.86	106.69	109.47
4	C	760[D]	HDD	C3D-O1D-CGD	3.85	114.74	111.14
2	A	754[A]	HEM	C1B-NB-C4B	3.80	109.71	105.21
3	A	761[B]	HDE	C1D-C2D-C3D	-3.80	102.98	106.98
3	A	761[B]	HDE	C2A-O1A-CGA	3.79	114.68	111.14
3	C	761[B]	HDE	CHC-C1C-NC	-3.77	117.03	123.86
2	C	755[C]	HEM	C1B-NB-C4B	3.74	109.63	105.21
3	C	761[B]	HDE	C3C-C2C-C1C	-3.73	102.77	107.17
3	D	761[B]	HDE	CAD-C3D-C4D	3.72	131.19	124.70
3	B	761[B]	HDE	C3D-C4D-ND	3.70	113.92	110.35
3	B	761[B]	HDE	CAD-CBD-CGD	-3.68	103.92	113.67
2	C	754[A]	HEM	C4D-ND-C1D	3.66	109.54	105.21
2	B	755[C]	HEM	C4D-ND-C1D	3.64	109.52	105.21
4	D	760[D]	HDD	O1D-CGD-O2D	3.63	123.87	120.81
4	B	760[D]	HDD	CAA-CBA-CGA	-3.58	104.18	113.67

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	760[D]	HDD	C1B-NB-C4B	3.57	109.44	105.21
3	D	761[B]	HDE	C2C-C1C-NC	3.57	115.87	110.14
4	D	760[D]	HDD	C3B-C4B-NB	-3.55	106.92	109.47
3	C	761[B]	HDE	CAD-CBD-CGD	-3.49	104.42	113.67
2	C	755[C]	HEM	C3B-C4B-NB	-3.48	106.97	109.47
2	A	755[C]	HEM	C4D-ND-C1D	3.45	109.29	105.21
3	D	761[B]	HDE	C3C-C2C-C1C	-3.43	103.12	107.17
2	A	755[C]	HEM	CAD-CBD-CGD	-3.41	104.62	113.67
3	D	761[B]	HDE	CBA-CAA-C2A	3.38	108.80	103.98
2	C	754[A]	HEM	C1B-NB-C4B	3.36	109.19	105.21
2	B	754[A]	HEM	CAA-CBA-CGA	-3.32	104.87	113.67
3	A	761[B]	HDE	C2C-C1C-NC	3.31	115.45	110.14
2	A	755[C]	HEM	CHB-C1B-NB	3.30	128.45	124.37
3	A	761[B]	HDE	C3D-C4D-ND	3.28	113.52	110.35
4	B	760[D]	HDD	C4C-NC-C1C	3.22	111.07	105.82
2	A	754[A]	HEM	CHC-C4B-NB	3.20	127.86	124.42
4	B	760[D]	HDD	C3B-C4B-NB	-3.18	107.18	109.47
3	D	761[B]	HDE	C3B-C2B-C1B	-3.18	104.02	106.41
4	A	760[D]	HDD	C2A-C1A-NA	-3.16	106.65	110.15
3	D	761[B]	HDE	C1D-C2D-C3D	-3.14	103.68	106.98
3	B	761[B]	HDE	O1A-CGA-O2A	3.12	123.44	120.81
3	B	761[B]	HDE	CBA-CAA-C2A	3.11	108.42	103.98
3	B	761[B]	HDE	CHB-C4A-NA	-3.11	119.99	124.28
4	A	760[D]	HDD	C4C-C3C-C2C	3.09	109.50	106.81
3	A	761[B]	HDE	C1C-CHC-C4B	-3.07	119.04	126.25
4	D	760[D]	HDD	C3B-C2B-C1B	3.06	108.71	106.41
2	D	755[C]	HEM	C3B-C4B-NB	-3.05	107.28	109.47
2	C	755[C]	HEM	CHA-C4D-ND	3.05	128.13	124.37
4	C	760[D]	HDD	C4B-C3B-C2B	3.03	110.07	107.28
3	B	761[B]	HDE	C4B-NB-C1B	-3.03	101.62	105.21
2	C	755[C]	HEM	C4D-ND-C1D	3.02	108.78	105.21
3	B	761[B]	HDE	C4D-C3D-C2D	-3.01	102.51	106.89
3	C	761[B]	HDE	CMB-C2B-C1B	3.01	129.74	125.03
4	A	760[D]	HDD	C1B-NB-C4B	3.00	108.77	105.21
2	B	754[A]	HEM	C1B-NB-C4B	3.00	108.76	105.21
4	A	760[D]	HDD	CHC-C4B-NB	3.00	127.65	124.42
3	C	761[B]	HDE	C4B-C3B-C2B	-3.00	104.53	107.28
4	C	760[D]	HDD	C4C-C3C-C2C	2.96	109.38	106.81
2	C	755[C]	HEM	C2B-C1B-NB	-2.94	106.46	109.84
2	B	754[A]	HEM	CHD-C1D-ND	2.94	127.59	124.42
4	C	760[D]	HDD	CHD-C4C-NC	2.94	127.66	124.45
4	A	760[D]	HDD	CHB-C4A-NA	2.94	129.18	123.86

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	760[D]	HDD	CHD-C4C-NC	2.93	127.65	124.45
2	C	755[C]	HEM	CBA-CAA-C2A	-2.93	104.42	112.53
2	D	755[C]	HEM	CBA-CAA-C2A	-2.93	104.44	112.53
4	A	760[D]	HDD	CAA-CBA-CGA	-2.93	105.91	113.67
2	D	755[C]	HEM	C1D-C2D-C3D	-2.92	103.91	106.98
3	A	761[B]	HDE	CAD-C3D-C2D	2.92	133.34	127.87
2	C	754[A]	HEM	C4C-C3C-C2C	2.92	109.35	106.81
2	D	754[A]	HEM	CAC-C3C-C4C	-2.91	117.87	124.82
2	C	755[C]	HEM	CAD-CBD-CGD	-2.90	105.97	113.67
3	C	761[B]	HDE	CHC-C4B-NB	-2.88	120.80	124.37
3	C	761[B]	HDE	C4D-C3D-C2D	-2.88	102.70	106.89
2	C	755[C]	HEM	CMB-C2B-C1B	-2.88	120.54	125.03
3	D	761[B]	HDE	CMA-C3A-C4A	-2.86	107.83	112.68
2	D	755[C]	HEM	C4D-ND-C1D	2.86	108.59	105.21
4	C	760[D]	HDD	CHC-C1C-NC	2.85	127.55	124.45
3	C	761[B]	HDE	CBB-CAB-C3B	-2.84	113.35	127.53
3	D	761[B]	HDE	C3D-C4D-ND	2.84	113.09	110.35
4	D	760[D]	HDD	C1B-NB-C4B	2.82	108.55	105.21
3	D	761[B]	HDE	C4D-C3D-C2D	-2.79	102.82	106.89
4	C	760[D]	HDD	C4C-CHD-C1D	2.78	130.48	125.99
3	B	761[B]	HDE	C1C-CHC-C4B	-2.78	119.71	126.25
2	B	755[C]	HEM	CHA-C4D-ND	2.78	127.80	124.37
3	D	761[B]	HDE	CHD-C1D-C2D	-2.77	119.07	126.95
2	A	754[A]	HEM	C3D-C4D-ND	-2.77	107.13	110.17
3	B	761[B]	HDE	CBB-CAB-C3B	-2.76	113.72	127.53
4	B	760[D]	HDD	C1B-NB-C4B	2.76	108.47	105.21
4	D	760[D]	HDD	O1D-CGD-CBD	-2.75	107.66	110.17
4	B	760[D]	HDD	C4A-C3A-C2A	2.73	109.95	106.82
4	C	760[D]	HDD	CAA-CBA-CGA	-2.73	106.42	113.67
3	C	761[B]	HDE	CBC-CAC-C3C	-2.72	113.92	127.53
2	C	754[A]	HEM	CHB-C4A-NA	2.72	128.78	123.86
3	C	761[B]	HDE	CAA-CBA-CGA	-2.70	100.46	104.48
2	D	754[A]	HEM	C4B-C3B-C2B	2.68	109.75	107.28
4	A	760[D]	HDD	CBC-CAC-C3C	-2.67	114.17	127.53
4	C	760[D]	HDD	C2B-C1B-NB	-2.67	106.77	109.84
2	B	755[C]	HEM	C1B-NB-C4B	2.66	108.36	105.21
2	C	754[A]	HEM	CHA-C4D-ND	2.66	127.66	124.37
3	B	761[B]	HDE	C1D-C2D-C3D	-2.64	104.20	106.98
3	B	761[B]	HDE	CMA-C3A-C4A	-2.64	108.21	112.68
2	B	755[C]	HEM	CHC-C4B-NB	2.62	127.25	124.42
4	A	760[D]	HDD	C4A-C3A-C2A	2.61	109.81	106.82
3	A	761[B]	HDE	C4D-C3D-C2D	-2.61	103.09	106.89

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	754[A]	HEM	CHC-C1C-NC	2.61	127.30	124.45
3	C	761[B]	HDE	CHB-C4A-NA	-2.58	120.72	124.28
2	D	755[C]	HEM	CHD-C4C-NC	2.58	127.26	124.45
2	C	755[C]	HEM	CHB-C1B-NB	2.57	127.55	124.37
4	D	760[D]	HDD	CAA-CBA-CGA	-2.55	106.89	113.67
2	A	754[A]	HEM	CHB-C4A-NA	2.54	128.47	123.86
2	C	754[A]	HEM	CBA-CAA-C2A	-2.54	105.52	112.53
4	D	760[D]	HDD	C2A-C1A-NA	-2.53	107.34	110.15
2	A	754[A]	HEM	C3B-C2B-C1B	2.53	108.31	106.41
2	A	754[A]	HEM	CMD-C2D-C1D	2.53	128.98	125.03
3	A	761[B]	HDE	CHD-C4C-NC	2.52	128.42	123.86
4	C	760[D]	HDD	CHA-C1A-NA	2.52	128.42	123.86
2	C	754[A]	HEM	C4B-C3B-C2B	2.51	109.59	107.28
4	A	760[D]	HDD	CMC-C2C-C1C	-2.51	120.32	124.73
2	B	755[C]	HEM	CMB-C2B-C1B	-2.50	121.12	125.03
2	A	755[C]	HEM	CHA-C4D-C3D	-2.50	120.62	125.23
2	B	754[A]	HEM	C3D-C4D-ND	-2.49	107.44	110.17
4	C	760[D]	HDD	CHB-C4A-NA	2.49	128.38	123.86
2	C	754[A]	HEM	CHC-C4B-NB	2.47	127.08	124.42
4	A	760[D]	HDD	C2B-C1B-NB	-2.47	107.00	109.84
3	C	761[B]	HDE	CAD-C3D-C2D	2.47	132.49	127.87
2	C	754[A]	HEM	C4A-C3A-C2A	2.46	109.63	106.82
2	C	755[C]	HEM	C4C-C3C-C2C	2.46	108.95	106.81
4	A	760[D]	HDD	CMA-C3A-C4A	-2.46	121.68	125.42
4	C	760[D]	HDD	O1D-CGD-CBD	-2.45	107.94	110.17
4	C	760[D]	HDD	C2A-C1A-NA	-2.45	107.44	110.15
2	C	754[A]	HEM	CMD-C2D-C1D	2.44	128.85	125.03
2	B	755[C]	HEM	CHD-C1D-ND	2.44	127.05	124.42
2	C	754[A]	HEM	C3A-C4A-NA	-2.44	106.24	110.14
2	A	755[C]	HEM	CMB-C2B-C1B	-2.42	121.25	125.03
3	B	761[B]	HDE	C1D-ND-C4D	-2.42	102.34	105.21
2	A	755[C]	HEM	C1B-NB-C4B	2.40	108.05	105.21
2	C	754[A]	HEM	C2B-C1B-NB	-2.40	107.08	109.84
3	D	761[B]	HDE	C1C-CHC-C4B	-2.39	120.62	126.25
2	A	754[A]	HEM	O1A-CGA-CBA	-2.39	115.50	123.09
2	A	755[C]	HEM	C3B-C2B-C1B	2.39	108.20	106.41
2	D	755[C]	HEM	C4B-C3B-C2B	2.39	109.47	107.28
2	A	755[C]	HEM	CBB-CAB-C3B	-2.38	115.63	127.53
2	C	754[A]	HEM	O2D-CGD-CBD	2.38	121.52	114.00
4	D	760[D]	HDD	CHB-C4A-NA	2.37	128.16	123.86
3	A	761[B]	HDE	CHD-C1D-C2D	-2.36	120.23	126.95
4	B	760[D]	HDD	C4C-C3C-C2C	2.36	108.86	106.81

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	755[C]	HEM	CHC-C4B-NB	2.36	126.96	124.42
3	A	761[B]	HDE	C4B-C3B-C2B	-2.35	105.12	107.28
4	B	760[D]	HDD	CHB-C4A-NA	2.34	128.11	123.86
3	C	761[B]	HDE	CHA-C4D-C3D	-2.33	121.38	124.77
3	D	761[B]	HDE	CHB-C1B-NB	-2.33	121.92	124.42
3	D	761[B]	HDE	C1D-ND-C4D	-2.32	102.46	105.21
2	C	755[C]	HEM	CHA-C4D-C3D	-2.32	120.95	125.23
3	C	761[B]	HDE	CHD-C1D-ND	-2.32	121.50	124.37
2	C	755[C]	HEM	CHD-C4C-NC	2.31	126.97	124.45
3	B	761[B]	HDE	C2B-C1B-NB	2.31	112.57	109.90
4	B	760[D]	HDD	C2B-C1B-NB	-2.30	107.19	109.84
2	B	754[A]	HEM	CBA-CAA-C2A	-2.30	106.18	112.53
2	D	754[A]	HEM	CBB-CAB-C3B	-2.29	116.06	127.53
3	A	761[B]	HDE	CMD-C2D-C3D	2.29	132.35	126.15
4	B	760[D]	HDD	C2D-C1D-CHD	2.28	126.88	123.28
2	B	754[A]	HEM	C4C-NC-C1C	2.28	109.54	105.82
2	D	755[C]	HEM	CHA-C4D-ND	2.28	127.19	124.37
4	A	760[D]	HDD	C2D-C1D-CHD	2.28	126.87	123.28
3	B	761[B]	HDE	CHD-C1D-C2D	-2.28	120.48	126.95
2	B	754[A]	HEM	CBB-CAB-C3B	-2.28	116.15	127.53
2	A	754[A]	HEM	C2B-C1B-NB	-2.26	107.24	109.84
2	D	754[A]	HEM	CHC-C4B-C3B	2.26	129.58	125.07
2	D	754[A]	HEM	CHA-C4D-ND	2.26	127.16	124.37
3	B	761[B]	HDE	CHC-C4B-NB	-2.25	121.58	124.37
2	D	754[A]	HEM	CMD-C2D-C1D	2.24	128.54	125.03
4	C	760[D]	HDD	CBC-CAC-C3C	-2.22	116.41	127.53
3	D	761[B]	HDE	C2B-C1B-NB	2.22	112.47	109.90
4	C	760[D]	HDD	C4C-NC-C1C	2.21	109.43	105.82
2	C	755[C]	HEM	CMD-C2D-C1D	2.20	128.48	125.03
2	A	754[A]	HEM	CAA-CBA-CGA	-2.20	107.82	113.67
2	A	754[A]	HEM	O2A-CGA-CBA	2.20	120.96	114.00
2	D	755[C]	HEM	CHB-C4A-NA	2.19	127.84	123.86
2	B	755[C]	HEM	CBA-CAA-C2A	-2.19	106.47	112.53
4	B	760[D]	HDD	C2A-C1A-NA	-2.19	107.72	110.15
2	B	754[A]	HEM	C4B-C3B-C2B	2.19	109.29	107.28
3	C	761[B]	HDE	C4C-NC-C1C	-2.18	102.26	105.82
4	D	760[D]	HDD	CBD-CAD-C3D	-2.18	100.88	103.98
4	C	760[D]	HDD	C4A-C3A-C2A	2.18	109.31	106.82
2	C	754[A]	HEM	CBB-CAB-C3B	-2.17	116.67	127.53
2	A	755[C]	HEM	CAA-CBA-CGA	-2.17	107.91	113.67
4	A	760[D]	HDD	CBD-CAD-C3D	-2.17	100.89	103.98
2	A	754[A]	HEM	C4C-C3C-C2C	2.16	108.69	106.81

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	755[C]	HEM	CAA-CBA-CGA	-2.16	107.93	113.67
3	D	761[B]	HDE	C4B-NB-C1B	-2.16	102.65	105.21
2	D	754[A]	HEM	O2D-CGD-CBD	2.16	120.82	114.00
3	A	761[B]	HDE	CMA-C3A-C4A	-2.15	109.04	112.68
2	C	755[C]	HEM	C3B-C2B-C1B	2.15	108.03	106.41
2	D	755[C]	HEM	O2A-CGA-CBA	2.14	120.75	114.00
3	D	761[B]	HDE	CHA-C4D-ND	-2.14	122.12	124.42
3	B	761[B]	HDE	CHC-C1C-NC	-2.14	119.99	123.86
4	B	760[D]	HDD	CBC-CAC-C3C	-2.13	116.89	127.53
3	D	761[B]	HDE	C3A-C4A-CHB	-2.12	120.97	124.27
4	D	760[D]	HDD	C3C-C2C-C1C	2.12	109.05	107.05
3	B	761[B]	HDE	CMC-C2C-C3C	2.12	131.53	126.55
3	D	761[B]	HDE	CMC-C2C-C3C	2.11	131.52	126.55
3	A	761[B]	HDE	CHC-C1C-NC	-2.11	120.03	123.86
2	C	755[C]	HEM	CAD-C3D-C4D	2.11	128.38	124.70
2	A	755[C]	HEM	C2A-C1A-NA	-2.11	107.81	110.15
4	B	760[D]	HDD	CBA-CAA-C2A	-2.10	106.71	112.53
4	A	760[D]	HDD	C3A-C4A-NA	-2.09	106.80	110.14
4	C	760[D]	HDD	C3A-C4A-NA	-2.09	106.80	110.14
3	B	761[B]	HDE	O2D-CGD-CBD	2.07	120.55	114.00
2	C	754[A]	HEM	C4C-NC-C1C	2.06	109.19	105.82
3	C	761[B]	HDE	CHD-C1D-C2D	-2.06	121.09	126.95
2	B	755[C]	HEM	O2D-CGD-CBD	2.06	120.51	114.00
4	D	760[D]	HDD	C3D-O1D-CGD	2.06	113.06	111.14
2	B	754[A]	HEM	CHC-C1C-NC	2.06	126.69	124.45
2	C	754[A]	HEM	CAA-CBA-CGA	-2.06	108.21	113.67
3	C	761[B]	HDE	CMD-C2D-C3D	2.05	131.70	126.15
3	A	761[B]	HDE	C4C-CHD-C1D	-2.05	121.42	126.25
2	B	755[C]	HEM	CHA-C1A-NA	2.05	127.57	123.86
2	B	754[A]	HEM	CBC-CAC-C3C	-2.04	117.31	127.53
4	D	760[D]	HDD	C2D-C1D-CHD	2.04	126.49	123.28
4	B	760[D]	HDD	C2C-C1C-NC	-2.03	105.88	109.64
2	B	755[C]	HEM	C2A-C1A-NA	-2.03	107.90	110.15
2	D	755[C]	HEM	CHA-C4D-C3D	-2.02	121.49	125.23
4	B	760[D]	HDD	O1D-C3D-CAD	2.02	106.80	103.06
4	D	760[D]	HDD	CMC-C2C-C3C	-2.02	123.53	128.43
2	B	754[A]	HEM	CAD-C3D-C4D	2.02	128.21	124.70
2	A	755[C]	HEM	CBA-CAA-C2A	-2.00	107.00	112.53
2	B	754[A]	HEM	CHC-C4B-NB	2.00	126.58	124.42

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	A	760[D]	HDD	NC
4	B	760[D]	HDD	NC
4	C	760[D]	HDD	NC
4	D	760[D]	HDD	NC

All (49) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	754[A]	HEM	C2C-C3C-CAC-CBC
4	B	760[D]	HDD	C2B-C3B-CAB-CBB
2	B	754[A]	HEM	C4C-C3C-CAC-CBC
4	B	760[D]	HDD	C4B-C3B-CAB-CBB
2	A	754[A]	HEM	C2C-C3C-CAC-CBC
4	C	760[D]	HDD	C2B-C3B-CAB-CBB
4	D	760[D]	HDD	C2B-C3B-CAB-CBB
2	D	755[C]	HEM	C4B-C3B-CAB-CBB
4	D	760[D]	HDD	C4B-C3B-CAB-CBB
4	A	760[D]	HDD	CAA-CBA-CGA-O1A
2	D	755[C]	HEM	CAD-CBD-CGD-O1D
4	D	760[D]	HDD	CAA-CBA-CGA-O1A
2	B	754[A]	HEM	CAA-CBA-CGA-O1A
4	A	760[D]	HDD	CAA-CBA-CGA-O2A
2	A	754[A]	HEM	CAA-CBA-CGA-O1A
2	A	755[C]	HEM	CAD-CBD-CGD-O1D
2	A	754[A]	HEM	CAA-CBA-CGA-O2A
2	A	755[C]	HEM	CAD-CBD-CGD-O2D
3	C	761[B]	HDE	CAD-CBD-CGD-O2D
4	D	760[D]	HDD	CAA-CBA-CGA-O2A
4	C	760[D]	HDD	CAA-CBA-CGA-O1A
4	C	760[D]	HDD	CAA-CBA-CGA-O2A
2	B	754[A]	HEM	CAA-CBA-CGA-O2A
3	A	761[B]	HDE	CAD-CBD-CGD-O1D
3	B	761[B]	HDE	CAD-CBD-CGD-O2D
3	D	761[B]	HDE	CAD-CBD-CGD-O2D
4	B	760[D]	HDD	CAA-CBA-CGA-O1A
3	B	761[B]	HDE	CAD-CBD-CGD-O1D
2	D	755[C]	HEM	CAD-CBD-CGD-O2D
3	A	761[B]	HDE	CAD-CBD-CGD-O2D
3	C	761[B]	HDE	CAD-CBD-CGD-O1D
2	D	754[A]	HEM	CAA-CBA-CGA-O2A
2	B	755[C]	HEM	CAD-CBD-CGD-O2D
4	B	760[D]	HDD	CAA-CBA-CGA-O2A
3	D	761[B]	HDE	CAD-CBD-CGD-O1D

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	C	755[C]	HEM	CAD-CBD-CGD-O1D
2	C	755[C]	HEM	CAD-CBD-CGD-O2D
2	D	755[C]	HEM	C2B-C3B-CAB-CBB
2	C	754[A]	HEM	CAA-CBA-CGA-O2A
2	D	754[A]	HEM	CAA-CBA-CGA-O1A
2	B	755[C]	HEM	CAD-CBD-CGD-O1D
2	A	754[A]	HEM	C4C-C3C-CAC-CBC
4	C	760[D]	HDD	C4B-C3B-CAB-CBB
2	C	754[A]	HEM	CAA-CBA-CGA-O1A
2	D	755[C]	HEM	CAA-CBA-CGA-O2A
3	C	761[B]	HDE	C2D-C3D-CAD-CBD
2	C	755[C]	HEM	C2B-C3B-CAB-CBB
2	D	754[A]	HEM	C2C-C3C-CAC-CBC
4	A	760[D]	HDD	C2B-C3B-CAB-CBB

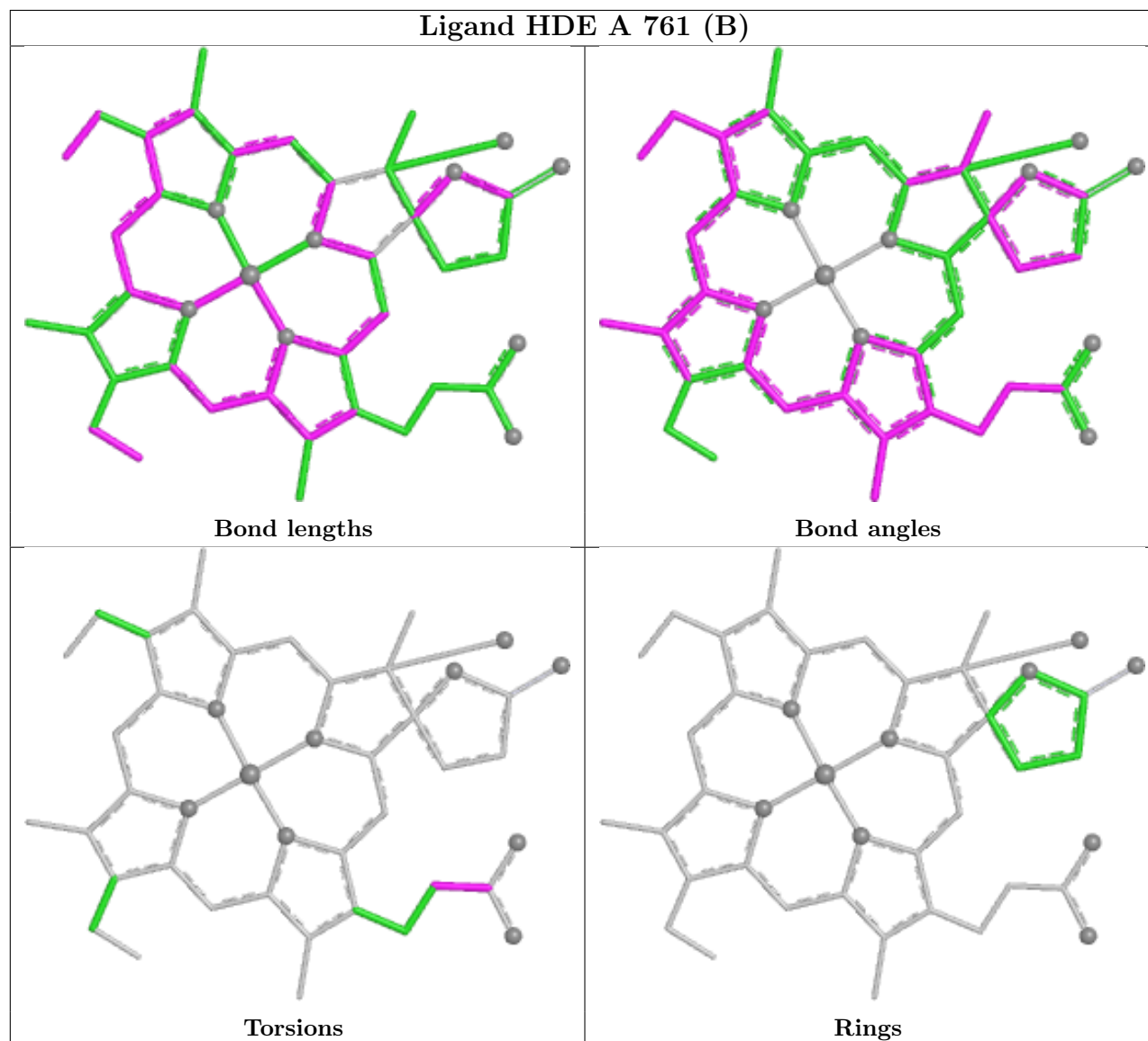
There are no ring outliers.

15 monomers are involved in 68 short contacts:

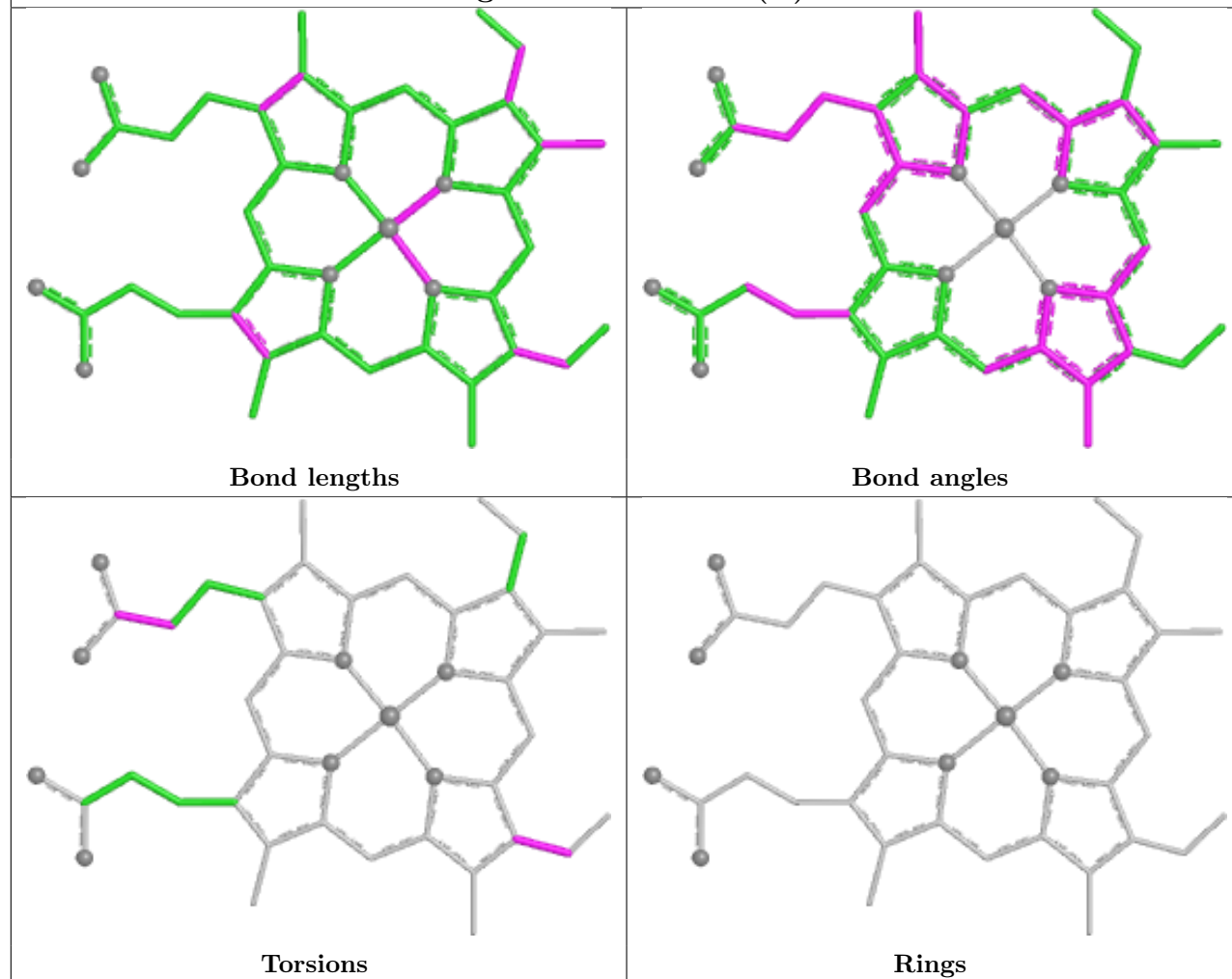
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	761[B]	HDE	7	0
2	C	755[C]	HEM	7	0
2	B	754[A]	HEM	5	0
2	A	754[A]	HEM	3	0
4	C	760[D]	HDD	3	0
4	D	760[D]	HDD	3	0
3	C	761[B]	HDE	8	0
2	C	754[A]	HEM	2	0
3	B	761[B]	HDE	5	0
3	D	761[B]	HDE	5	0
4	A	760[D]	HDD	4	0
2	D	755[C]	HEM	4	0
2	B	755[C]	HEM	5	0
4	B	760[D]	HDD	2	0
2	A	755[C]	HEM	5	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

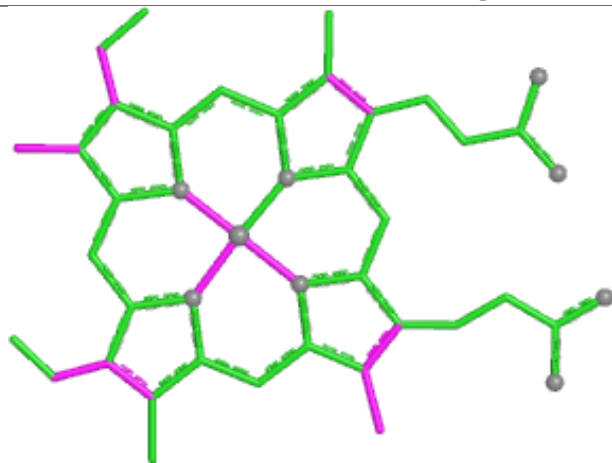
in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



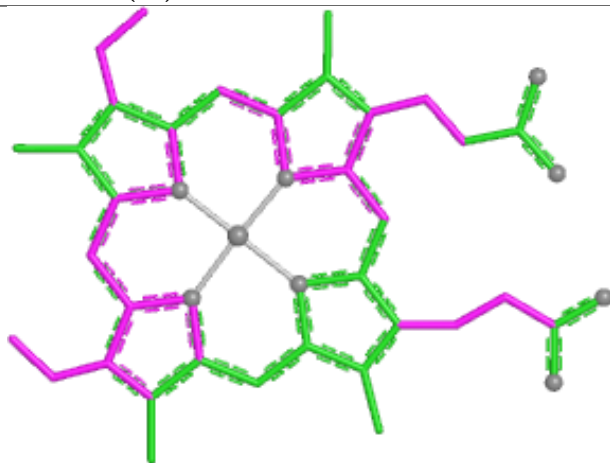
Ligand HEM C 755 (C)



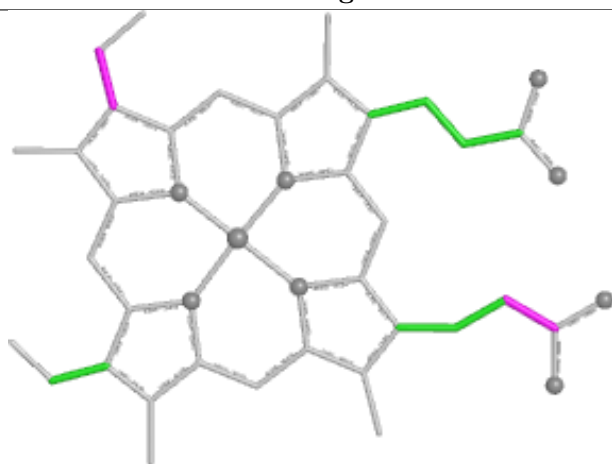
Ligand HEM B 754 (A)



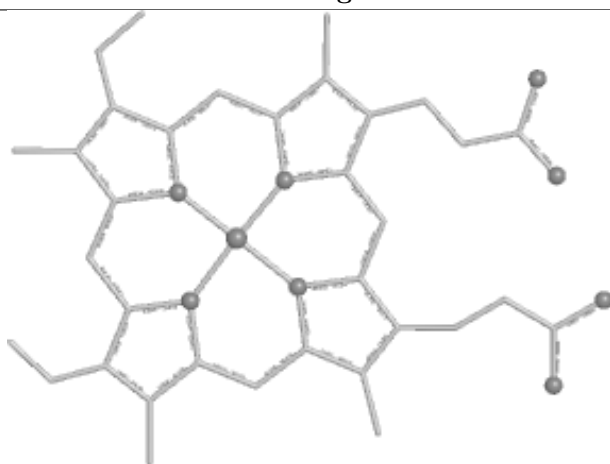
Bond lengths



Bond angles

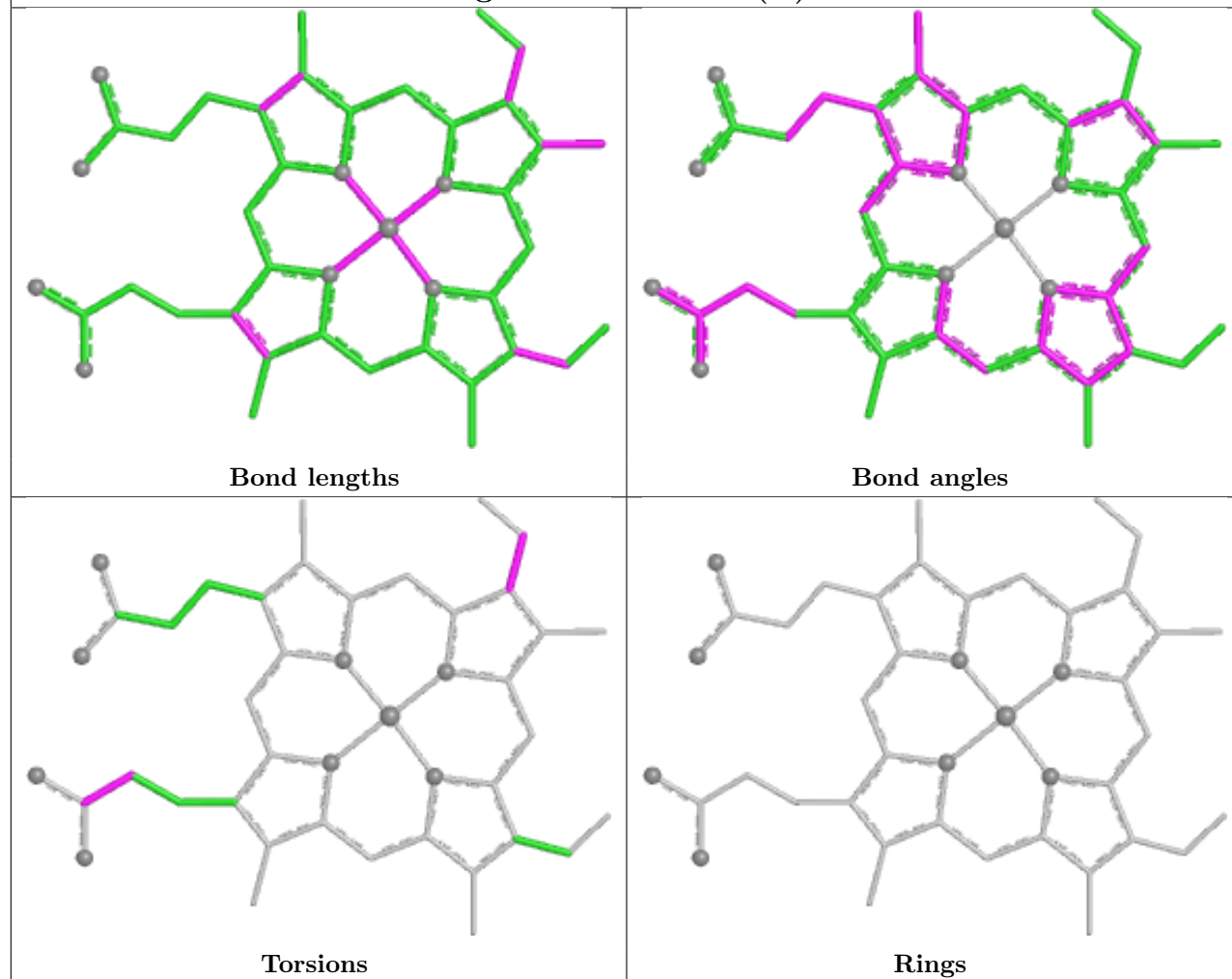


Torsions

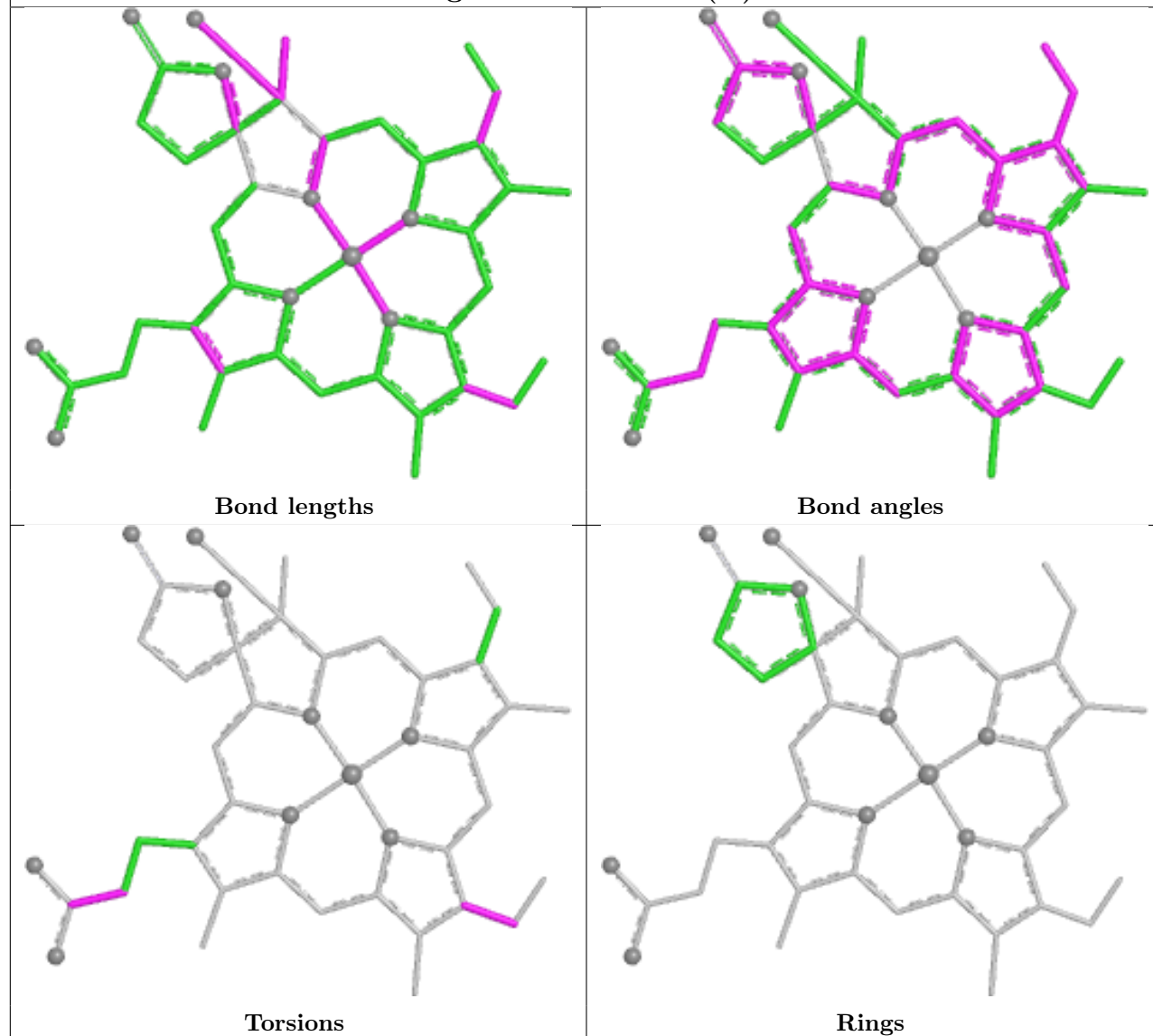


Rings

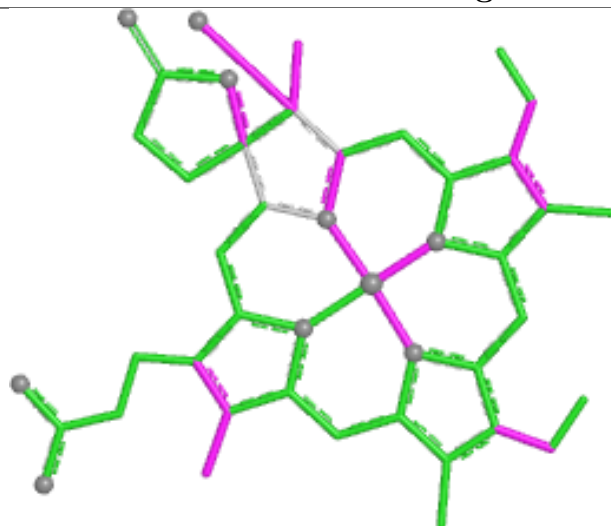
Ligand HEM A 754 (A)



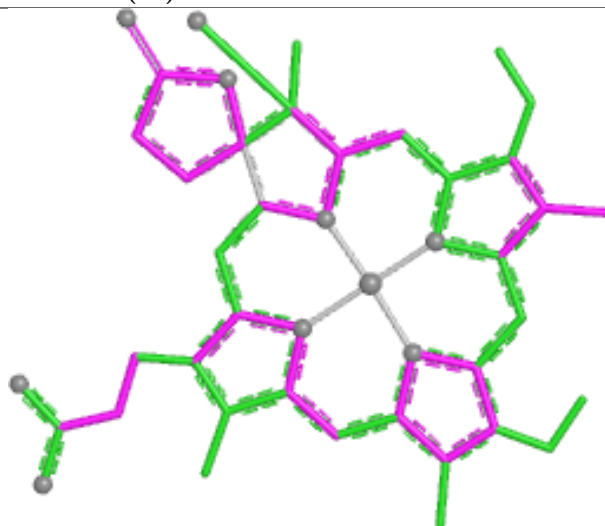
Ligand HDD C 760 (D)



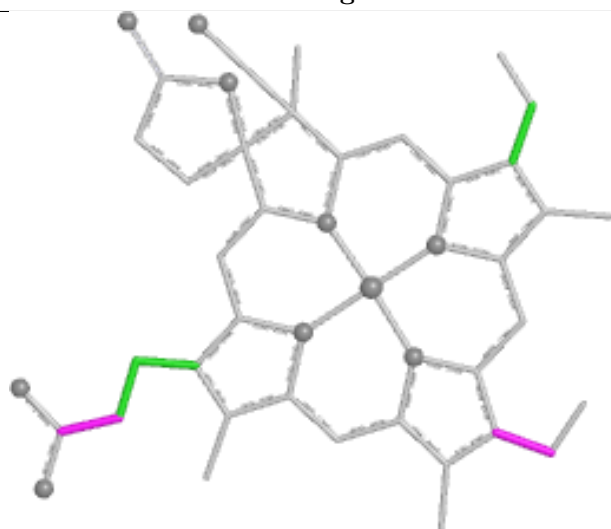
Ligand HDD D 760 (D)



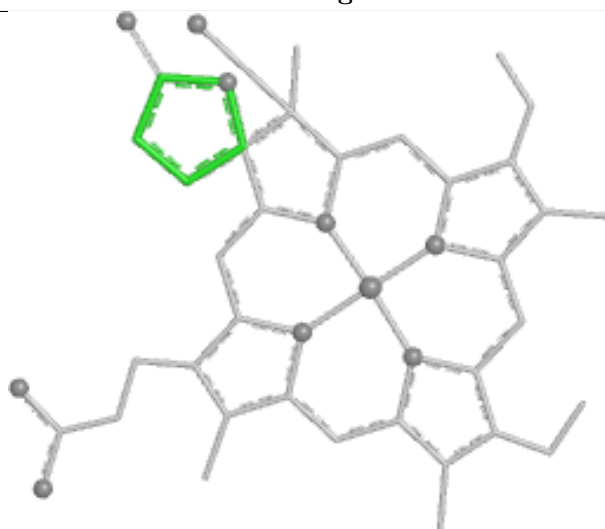
Bond lengths



Bond angles

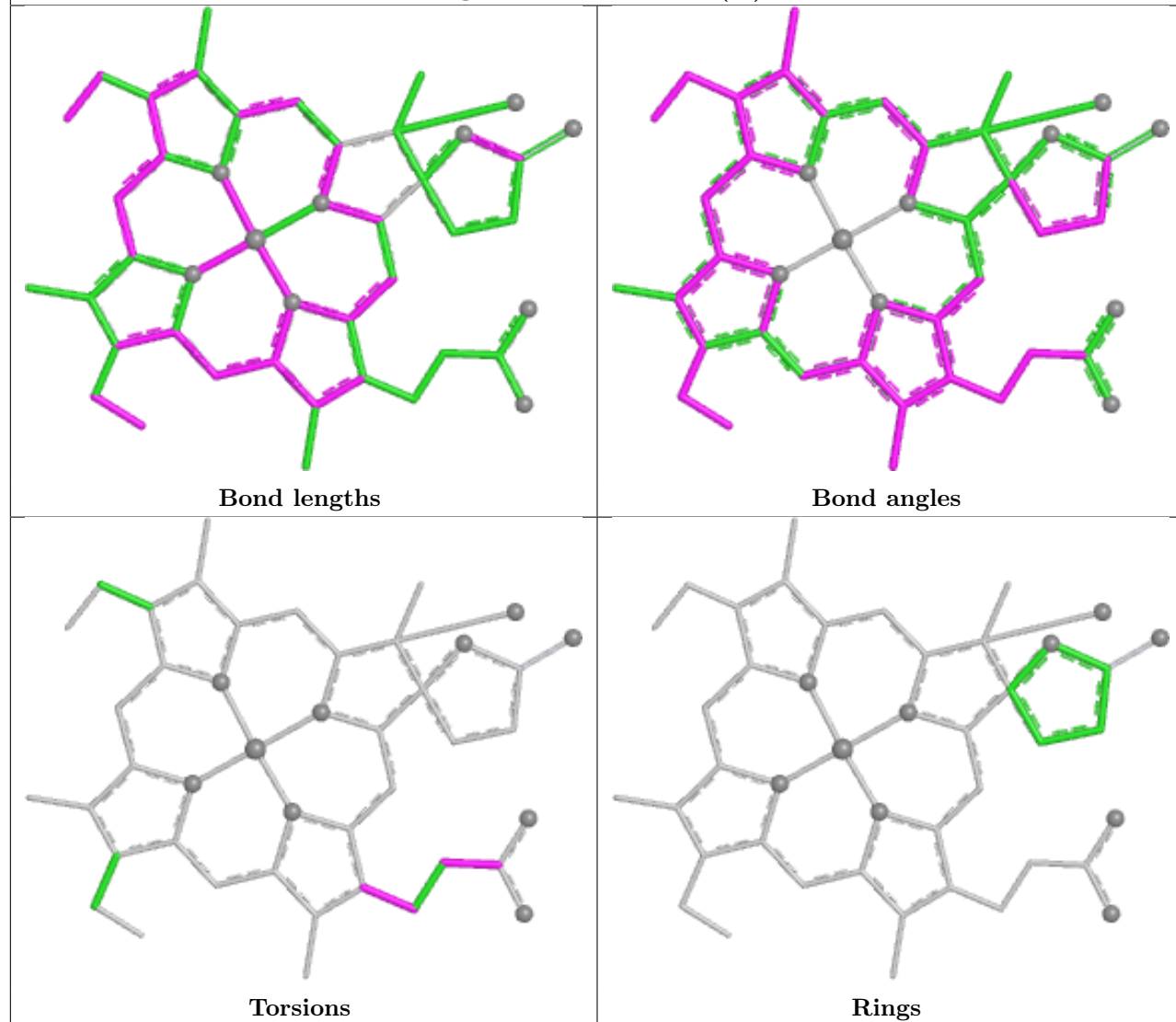


Torsions

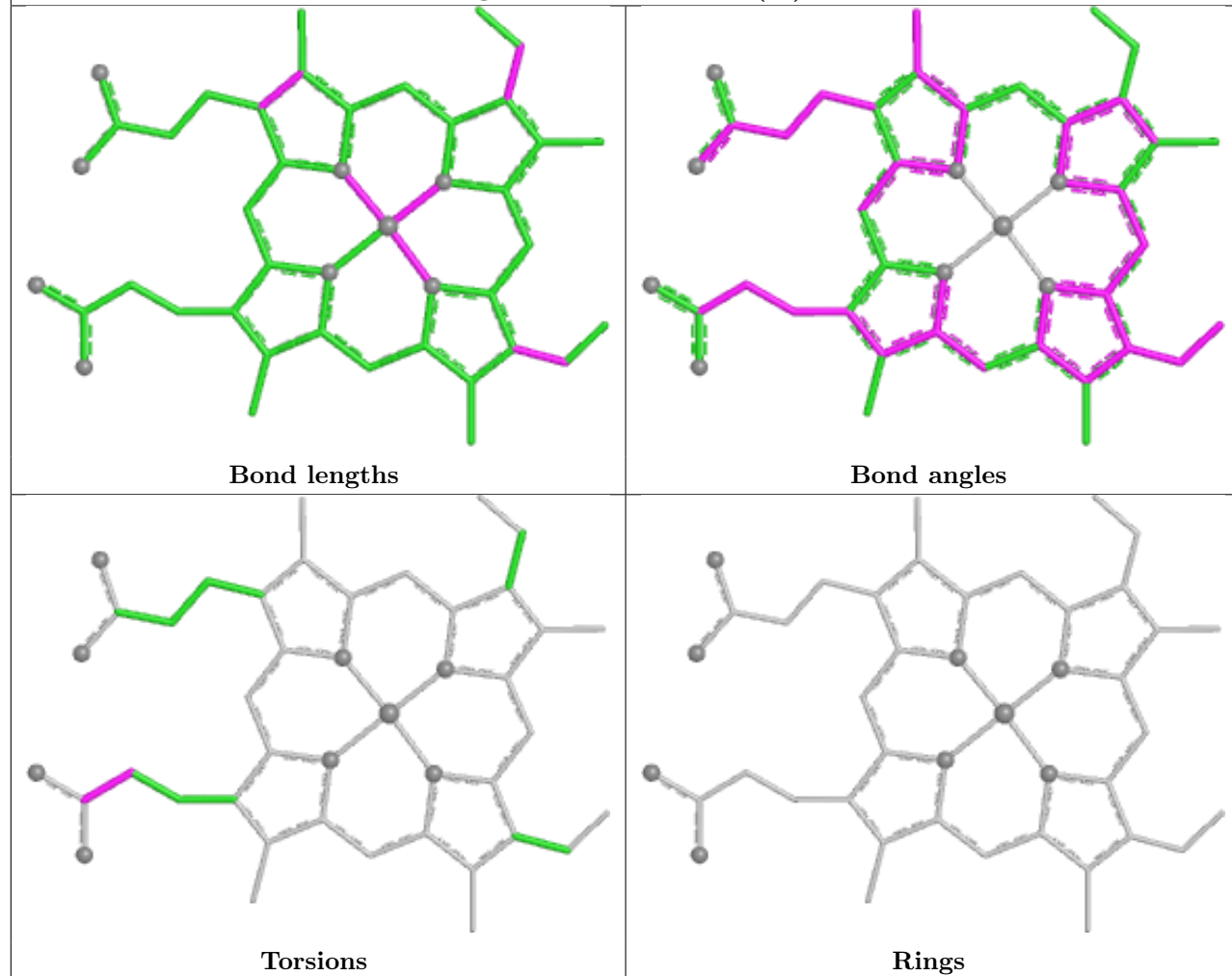


Rings

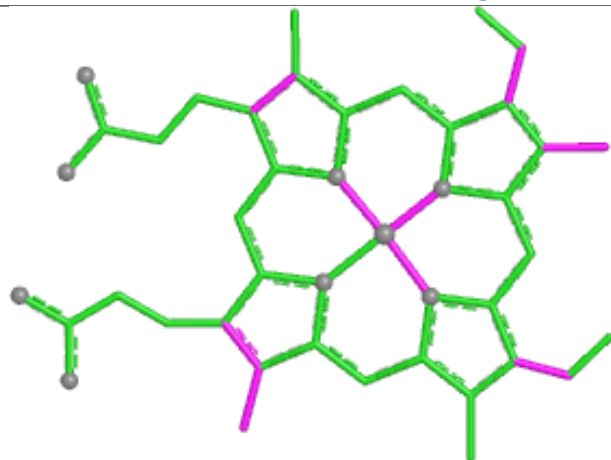
Ligand HDE C 761 (B)



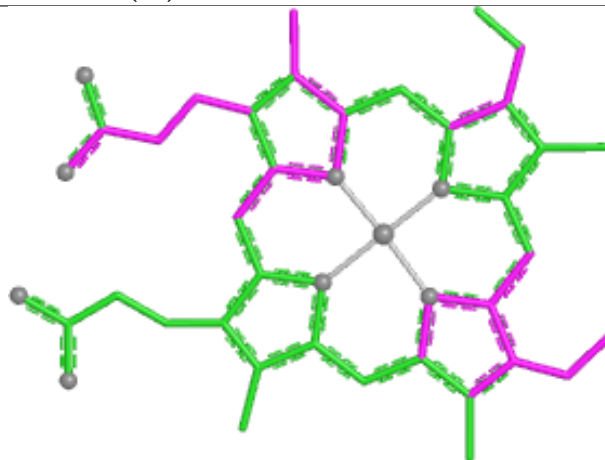
Ligand HEM C 754 (A)



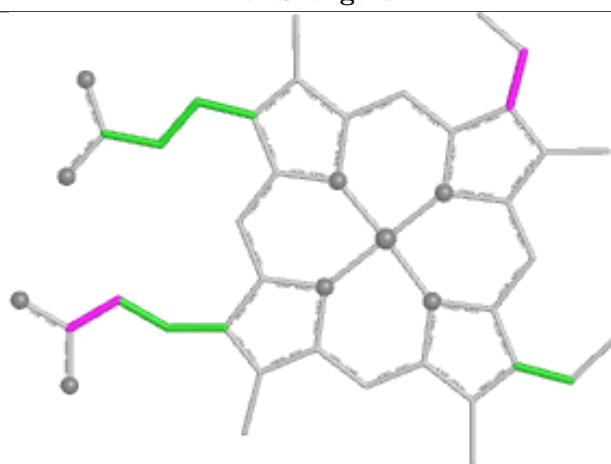
Ligand HEM D 754 (A)



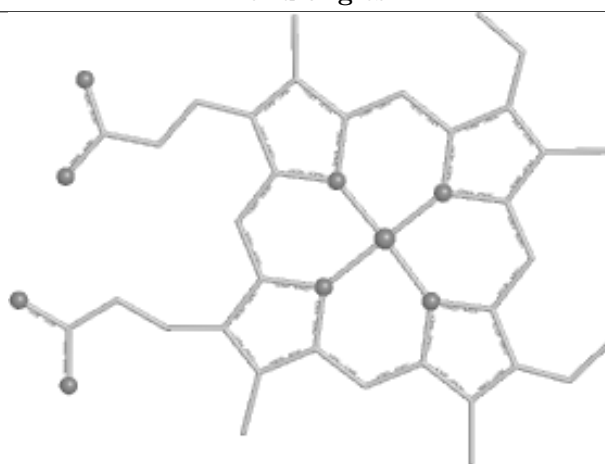
Bond lengths



Bond angles

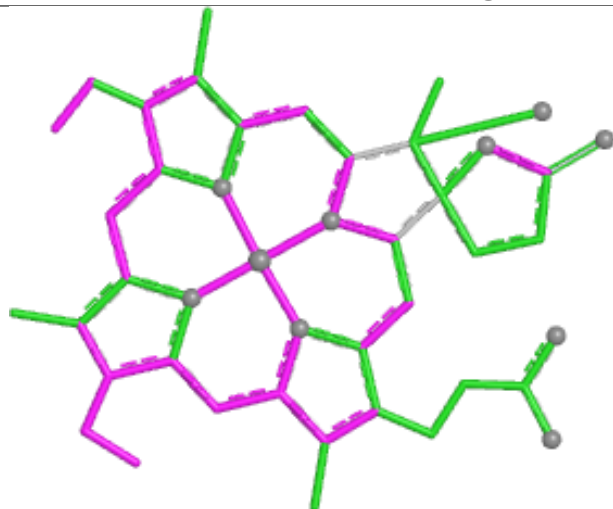


Torsions

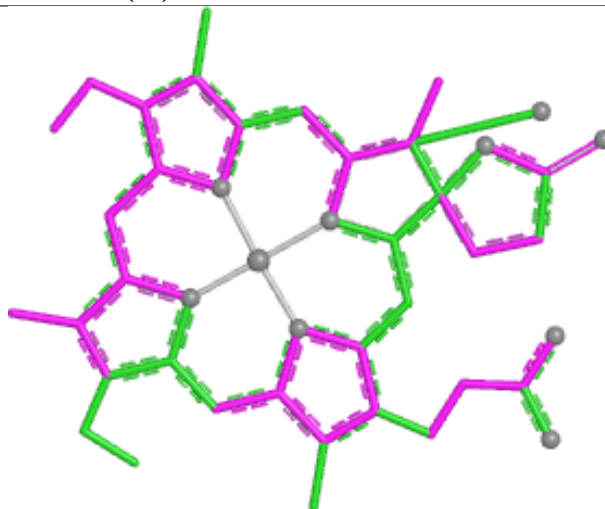


Rings

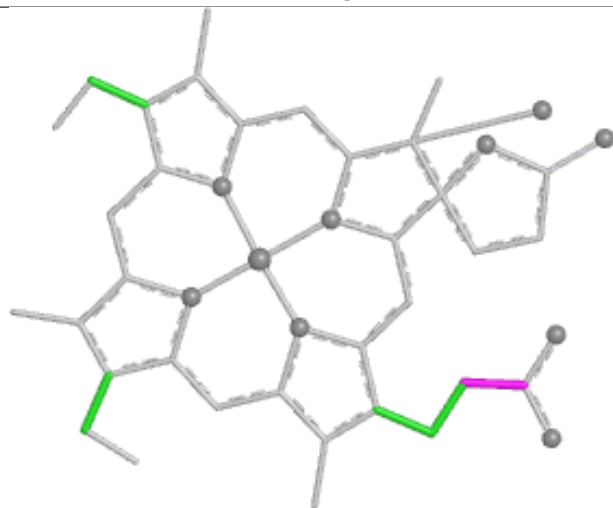
Ligand HDE B 761 (B)



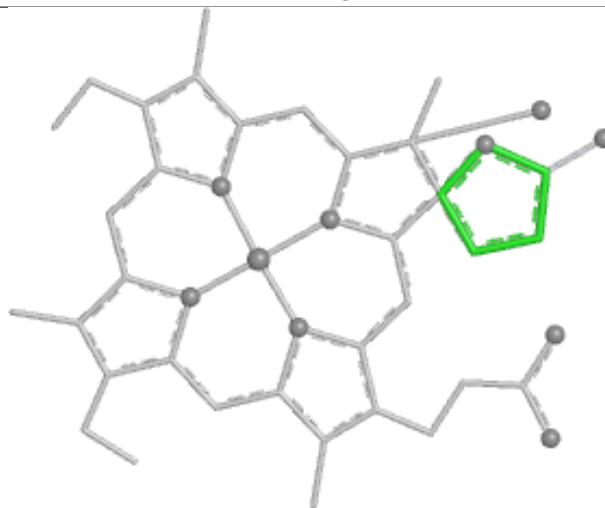
Bond lengths



Bond angles

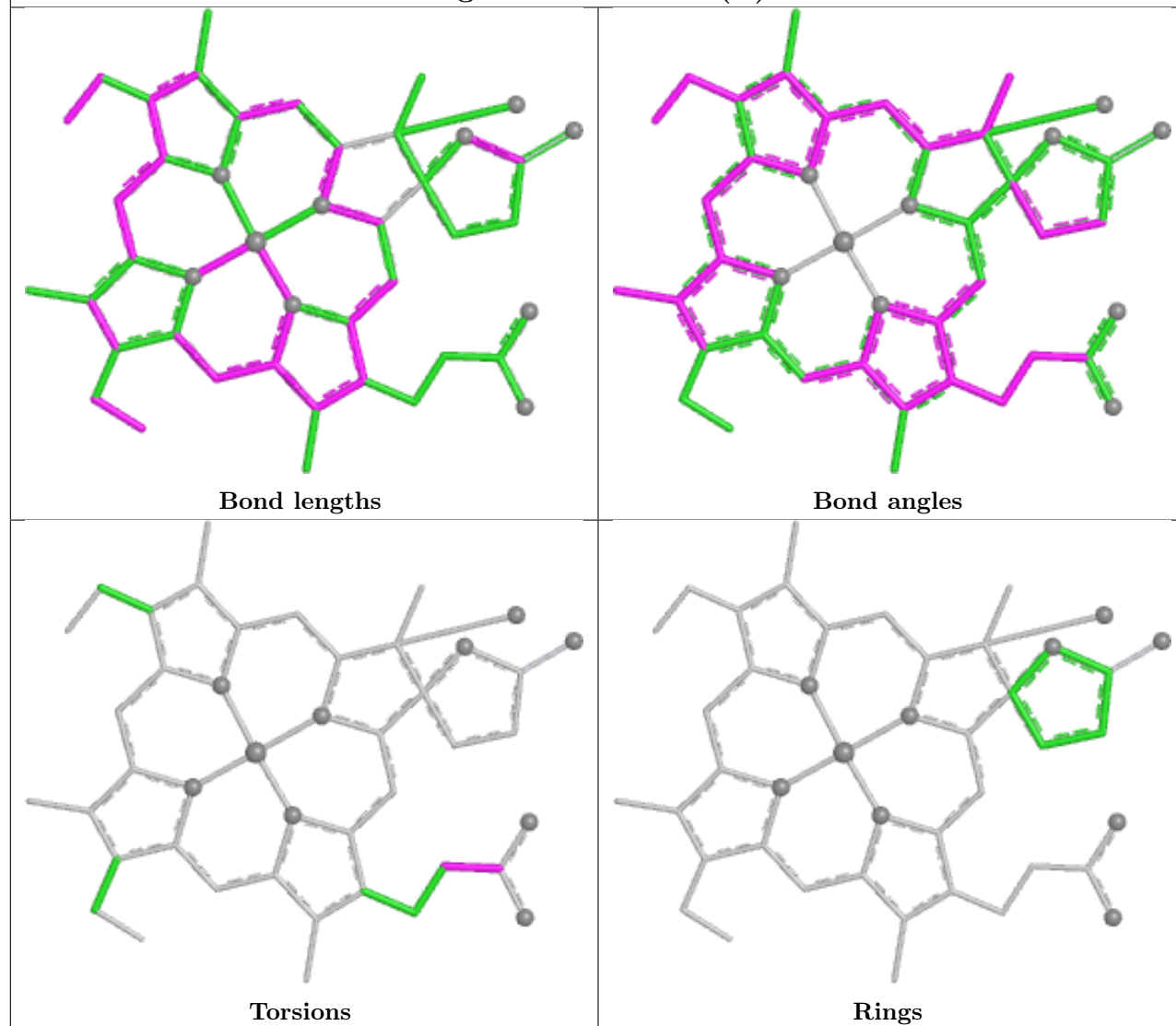


Torsions

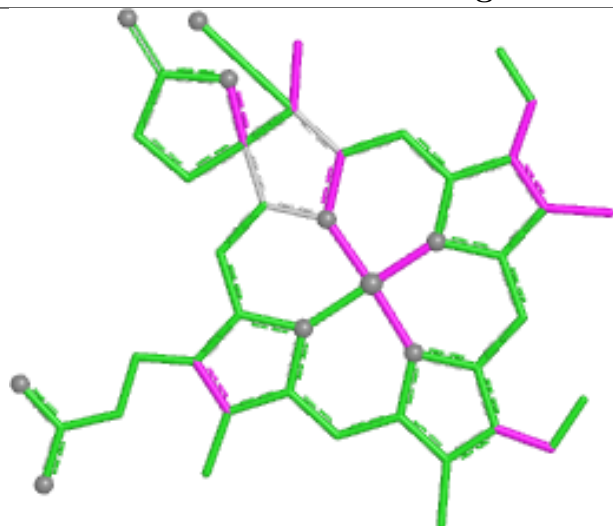


Rings

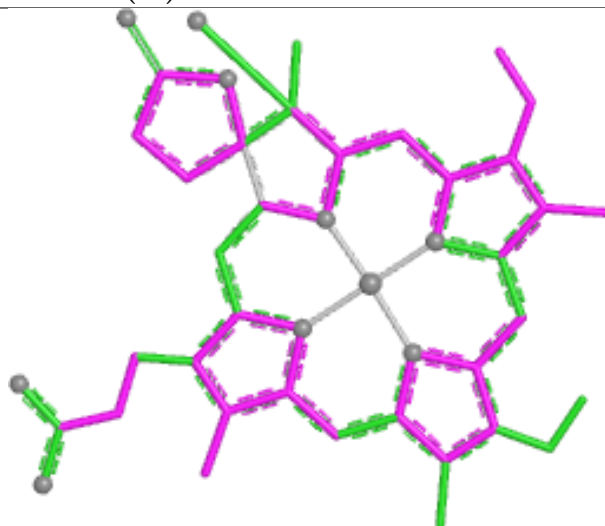
Ligand HDE D 761 (B)



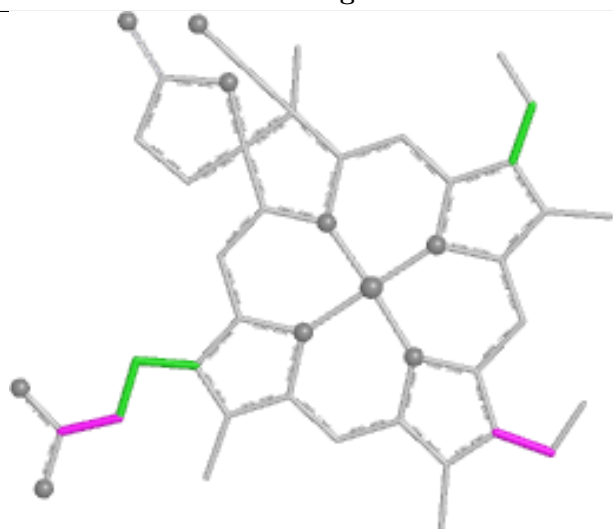
Ligand HDD A 760 (D)



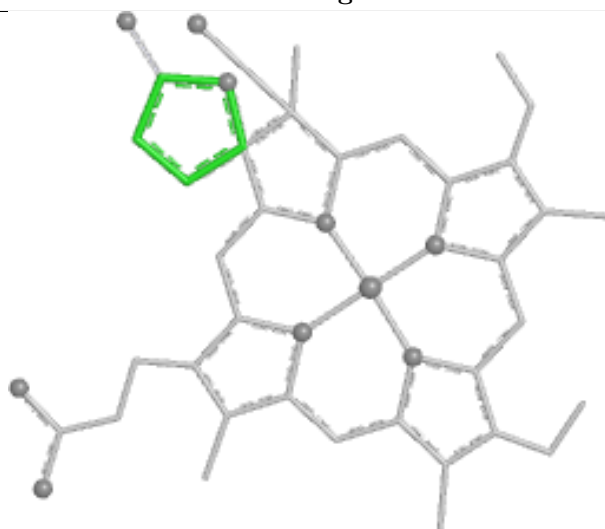
Bond lengths



Bond angles

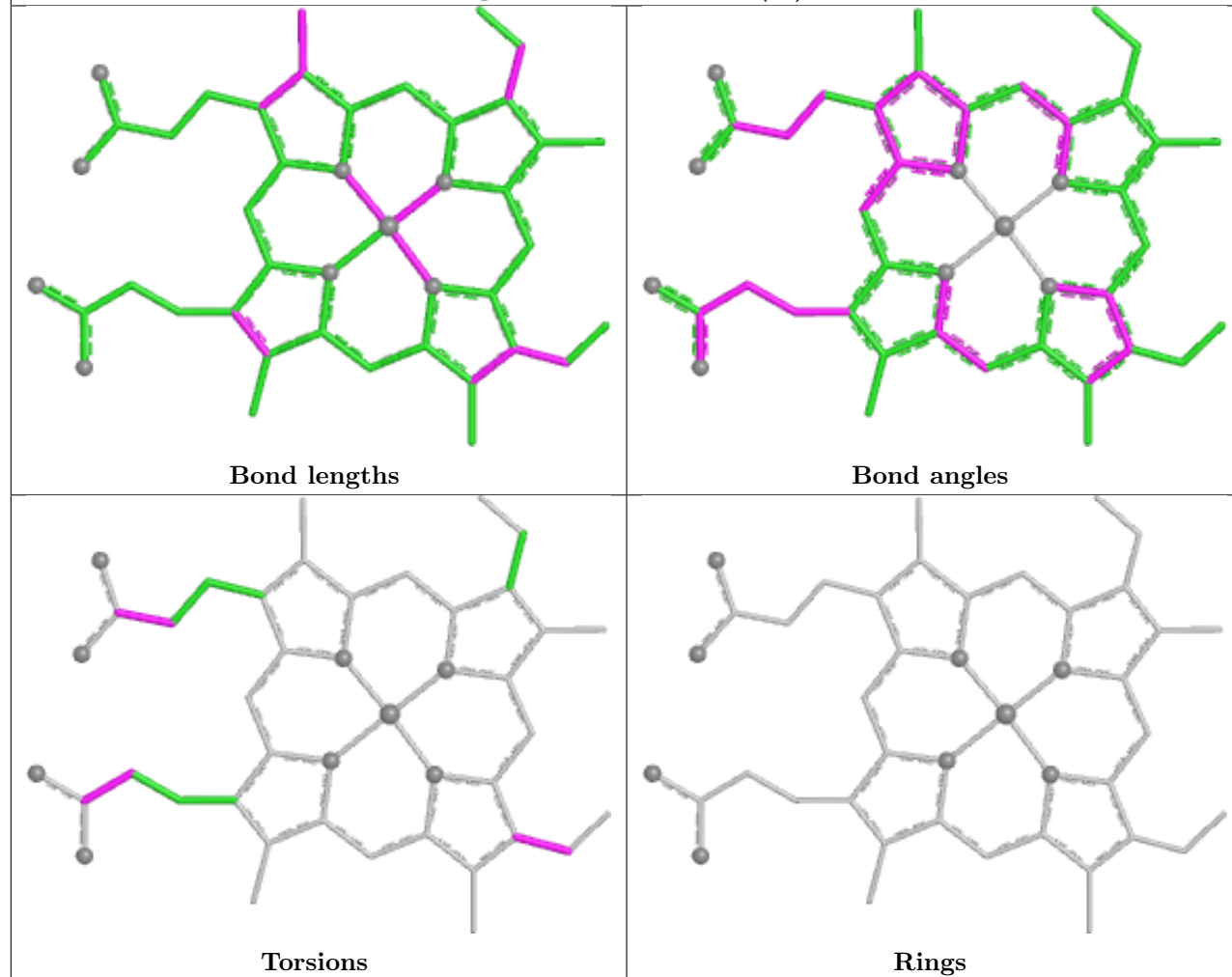


Torsions

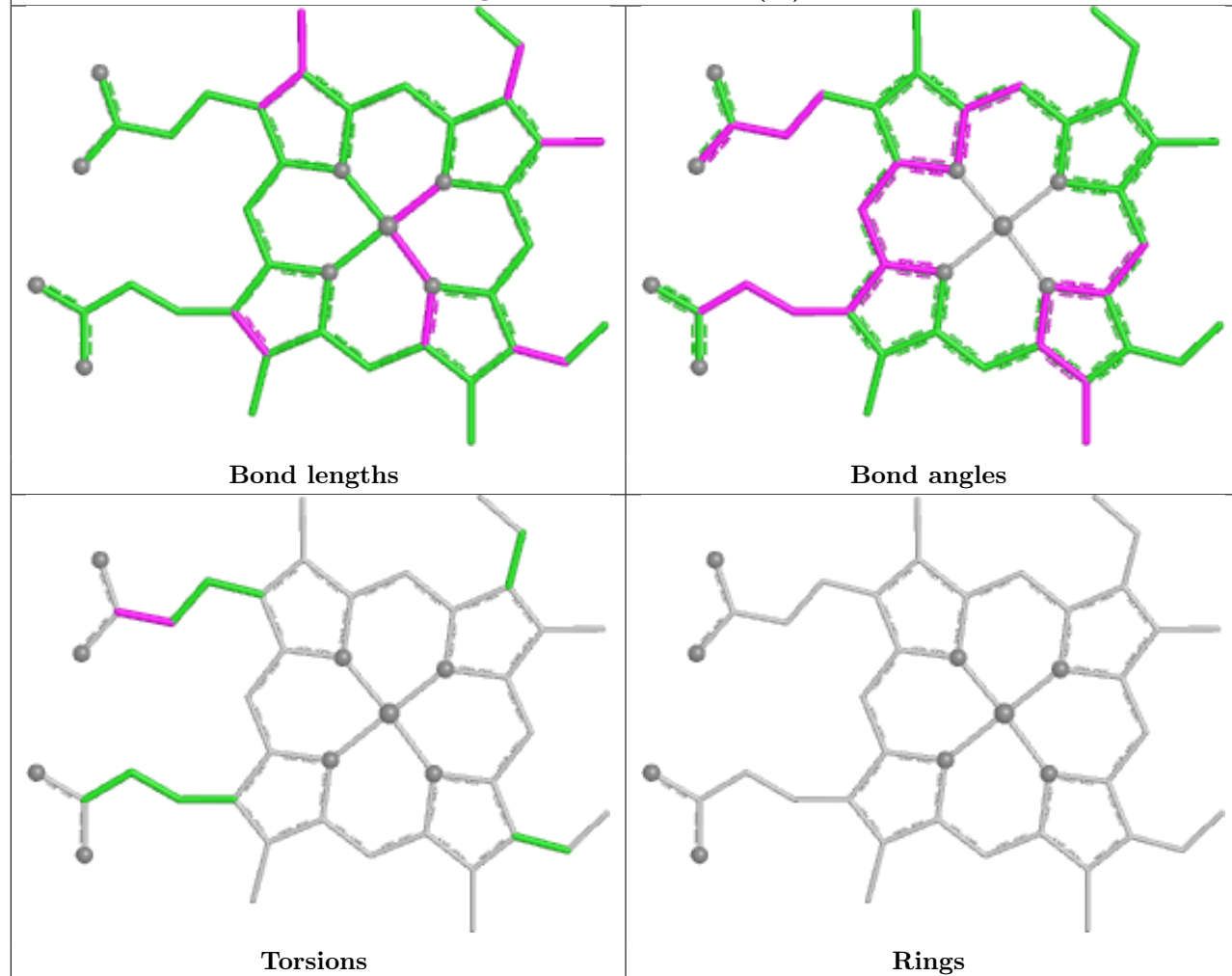


Rings

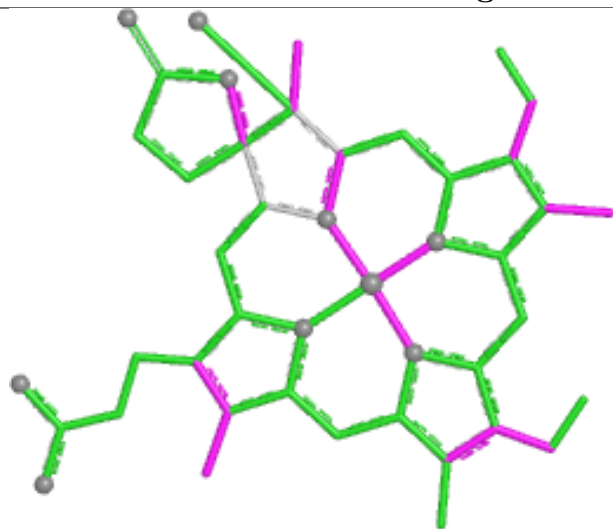
Ligand HEM D 755 (C)



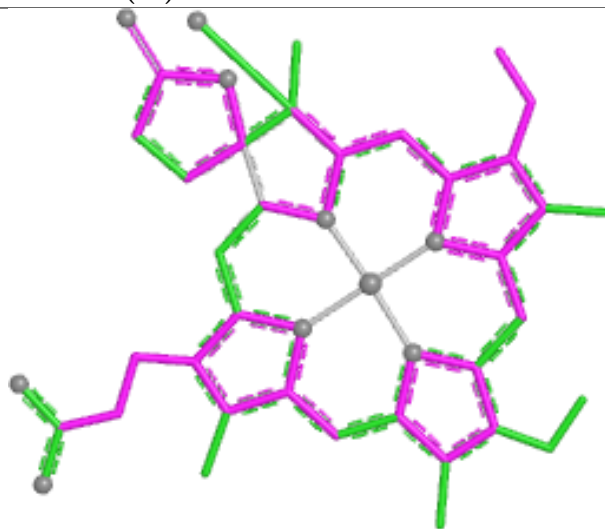
Ligand HEM B 755 (C)



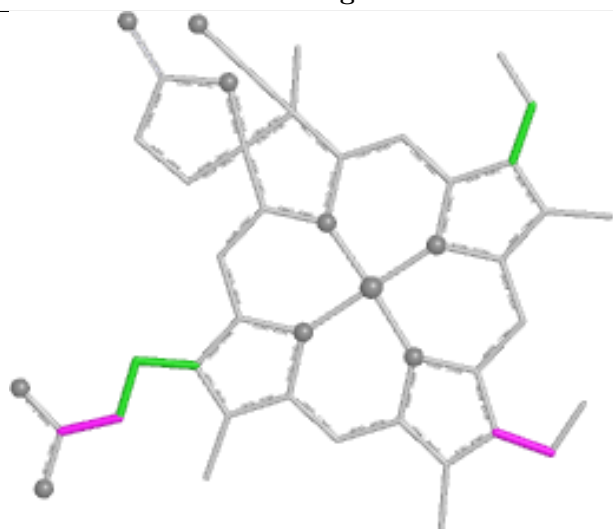
Ligand HDD B 760 (D)



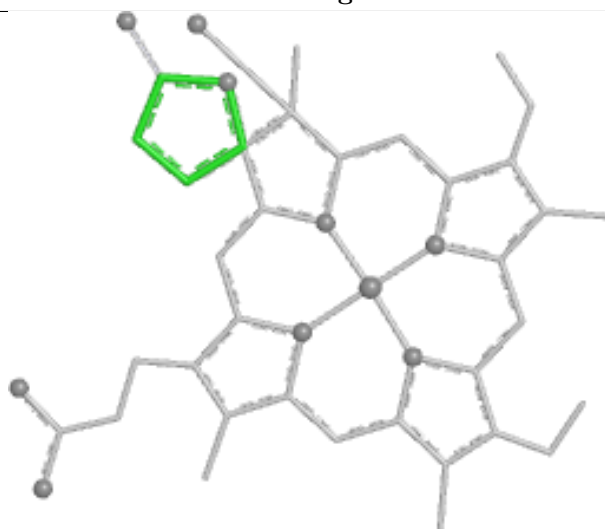
Bond lengths



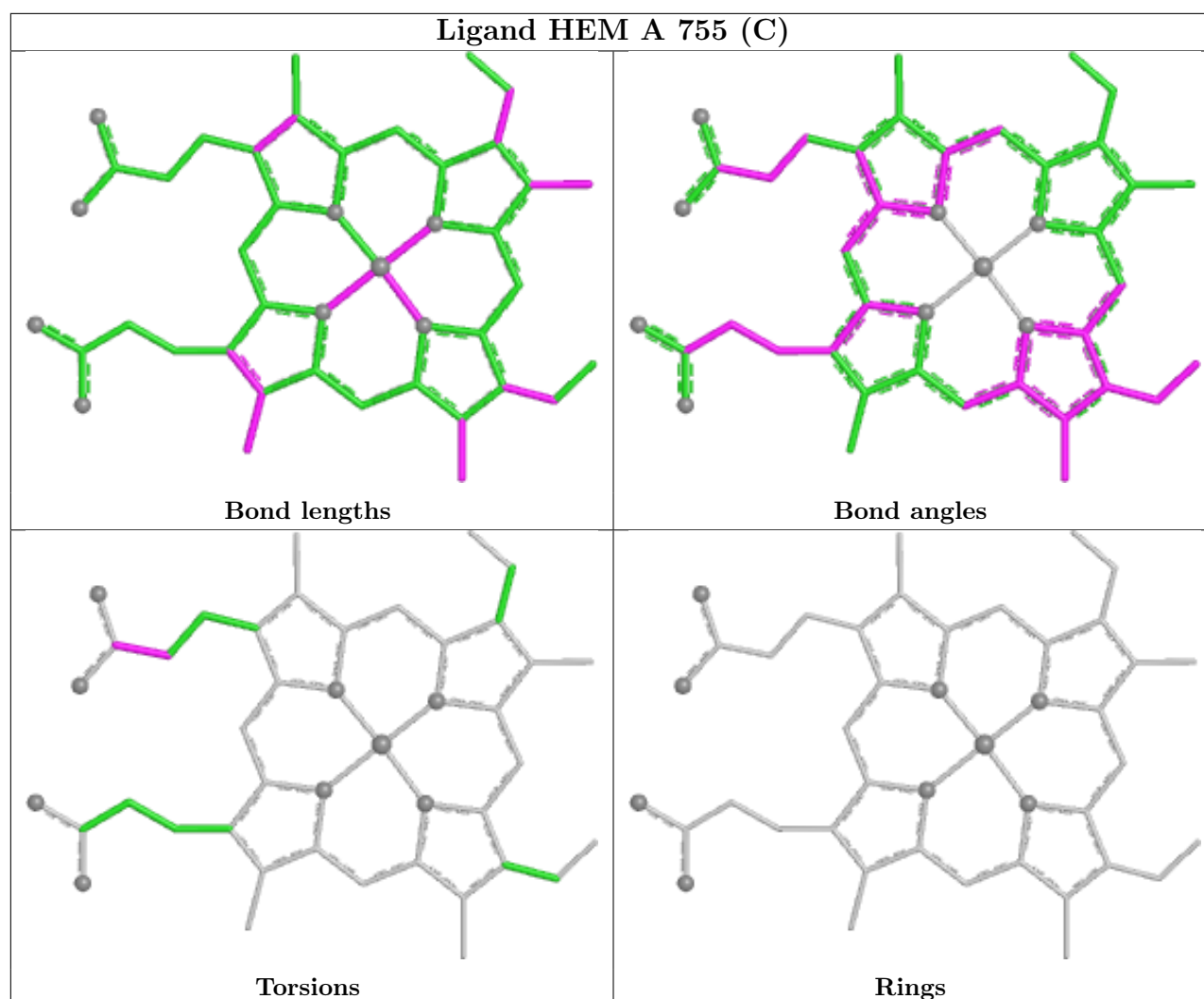
Bond angles



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 ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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	726/753 (96%)	-0.60	11 (1%) 72 75	3, 10, 28, 48	6 (0%)
1	B	726/753 (96%)	-0.44	12 (1%) 69 72	2, 11, 34, 50	4 (0%)
1	C	726/753 (96%)	-0.51	5 (0%) 84 87	3, 11, 33, 50	6 (0%)
1	D	726/753 (96%)	-0.61	4 (0%) 85 88	2, 9, 28, 48	6 (0%)
All	All	2904/3012 (96%)	-0.54	32 (1%) 78 81	2, 10, 31, 50	22 (0%)

All (32) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	28	SER	3.6
1	D	28	SER	3.5
1	B	726	GLY	3.4
1	B	673	ALA	3.3
1	D	751	ILE	3.1
1	A	711	ALA	3.1
1	A	726	GLY	3.0
1	D	749	ASP	2.9
1	B	583	LYS	2.9
1	C	751	ILE	2.7
1	A	725	ASP	2.6
1	A	29	LEU	2.6
1	B	611	VAL	2.5
1	A	712	ASP	2.5
1	B	725	ASP	2.5
1	D	750	LYS	2.4
1	C	750	LYS	2.4
1	A	751	ILE	2.4
1	A	713	GLN	2.2
1	C	595	ASP	2.2
1	B	751	ILE	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	749	ASP	2.2
1	B	614	ALA	2.1
1	B	701	ALA	2.1
1	B	710	ILE	2.1
1	B	568	ASP	2.1
1	A	710	ILE	2.1
1	C	725	ASP	2.1
1	A	749	ASP	2.1
1	B	711	ALA	2.0
1	A	724	ALA	2.0
1	C	749	ASP	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no 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(Å ²)	Q<0.9
2	HEM	A	755[C]	43/43	0.98	0.04	2,4,7,10	43
2	HEM	B	754[A]	43/43	0.98	0.05	2,4,7,9	43
2	HEM	B	755[C]	43/43	0.98	0.05	2,4,9,12	43
2	HEM	D	755[C]	43/43	0.98	0.05	2,2,7,8	43
3	HDE	B	761[B]	44/44	0.98	0.05	2,3,6,11	44
3	HDE	C	761[B]	44/44	0.98	0.05	2,2,4,12	44
3	HDE	D	761[B]	44/44	0.98	0.05	2,2,6,10	44
2	HEM	A	754[A]	43/43	0.99	0.03	2,3,4,5	43
3	HDE	A	761[B]	44/44	0.99	0.04	2,2,4,7	44
2	HEM	C	754[A]	43/43	0.99	0.04	2,4,6,8	43
2	HEM	C	755[C]	43/43	0.99	0.04	2,5,8,11	43
2	HEM	D	754[A]	43/43	0.99	0.04	2,2,6,8	43

Continued on next page...

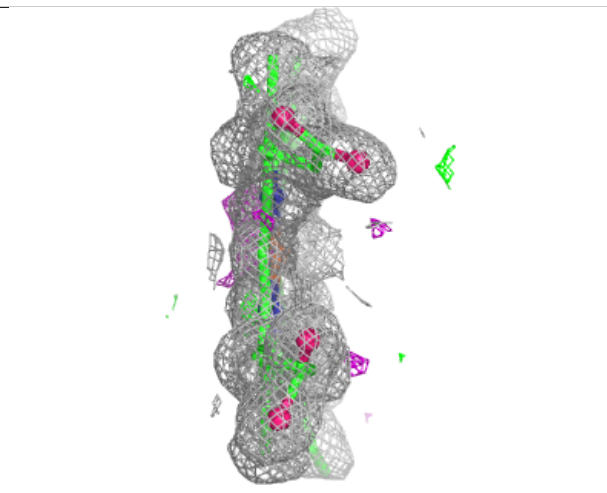
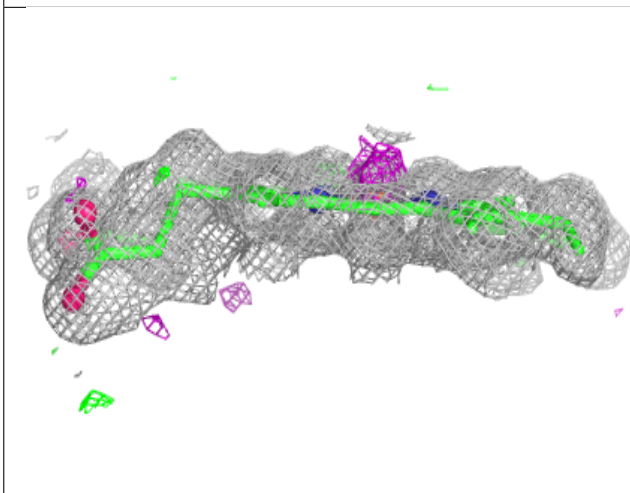
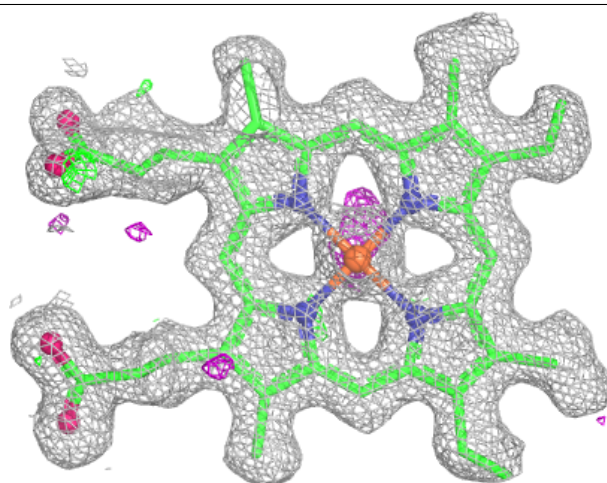
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	HDD	A	760[D]	44/44	0.99	0.04	2,2,3,6	44
4	HDD	B	760[D]	44/44	0.99	0.05	2,3,5,7	44
4	HDD	C	760[D]	44/44	0.99	0.04	2,3,7,9	44
4	HDD	D	760[D]	44/44	0.99	0.04	2,2,4,7	44

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.

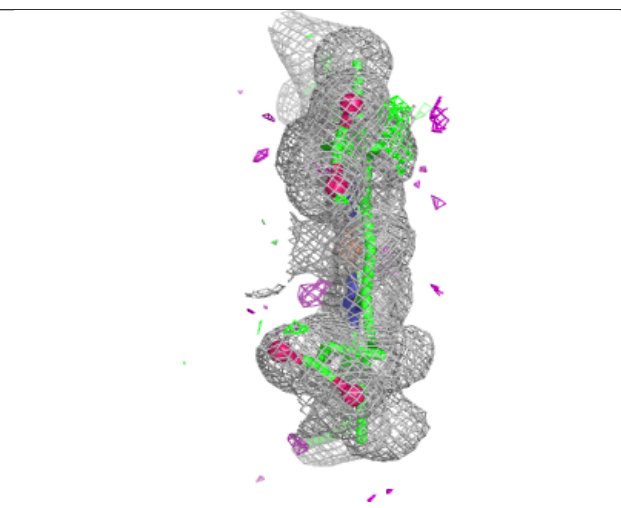
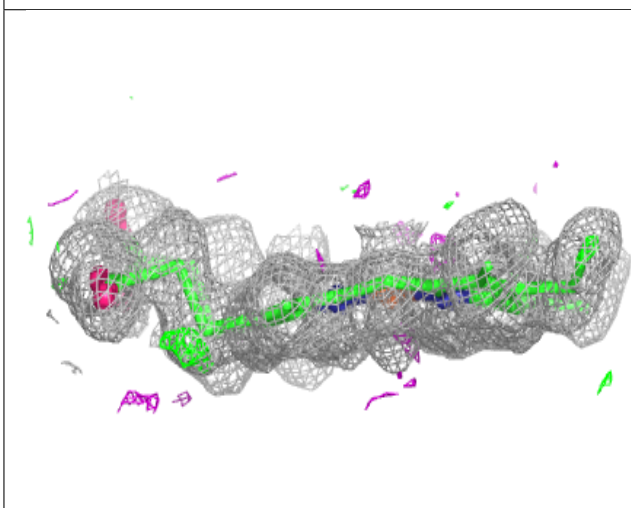
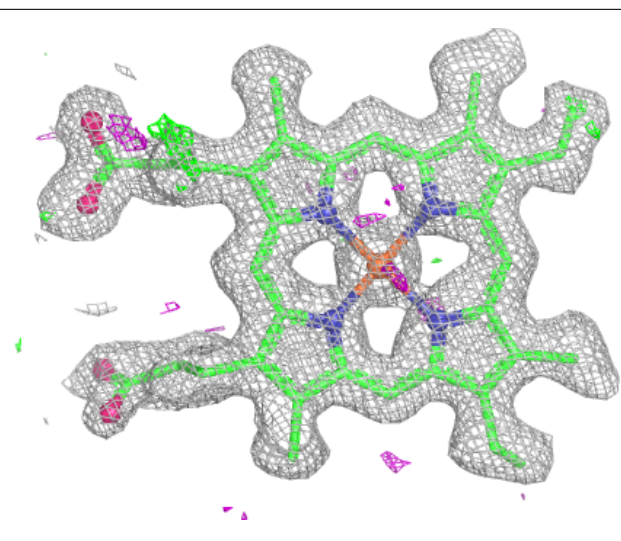
Electron density around HEM A 755 (C):

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



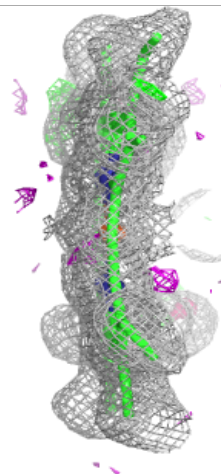
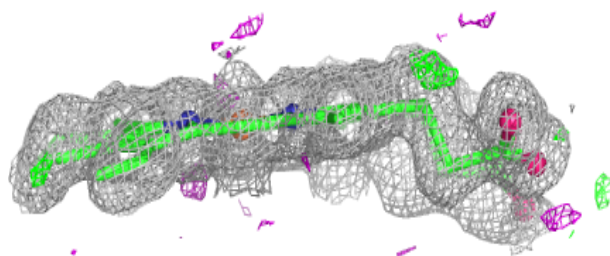
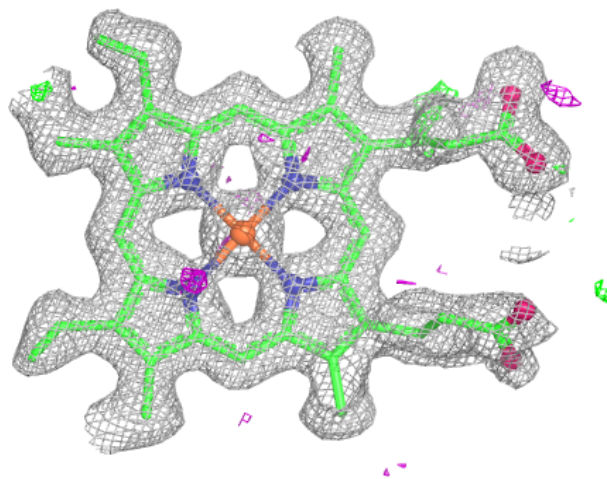
Electron density around HEM B 754 (A):

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



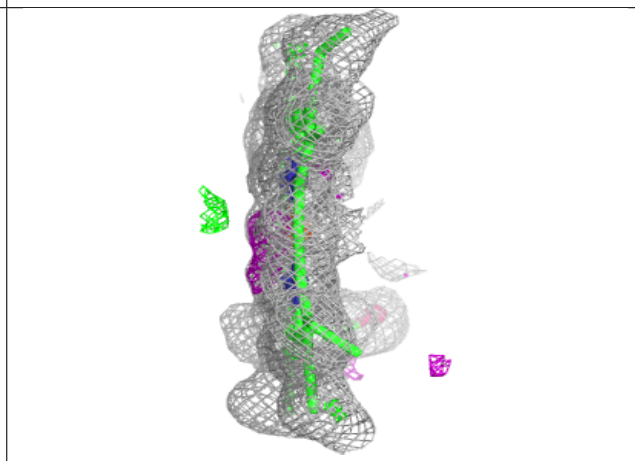
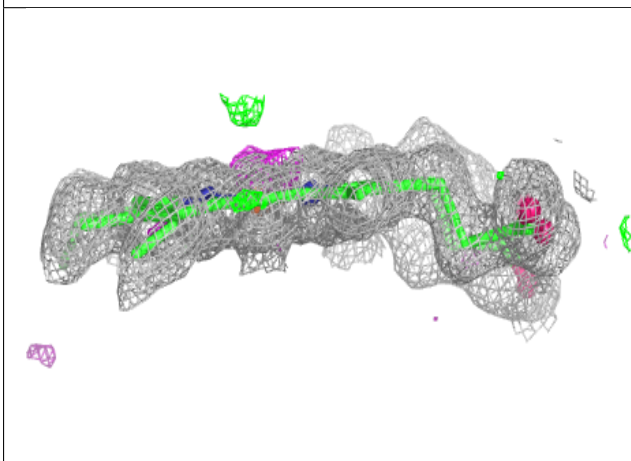
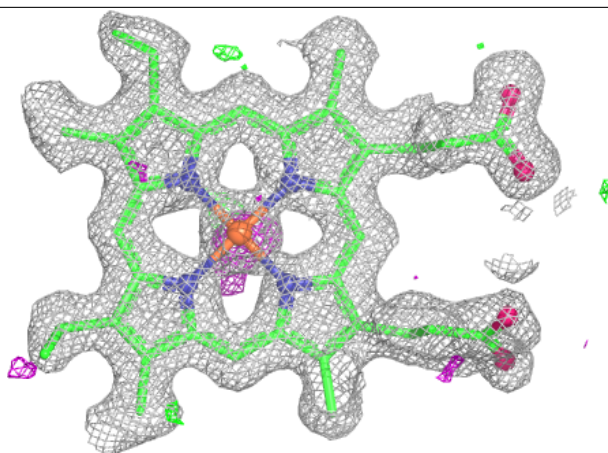
Electron density around HEM B 755 (C):

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



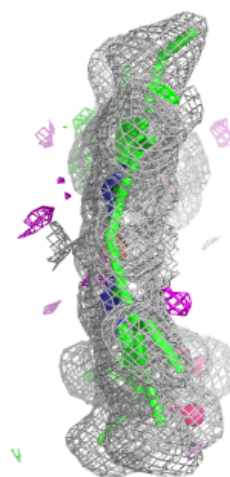
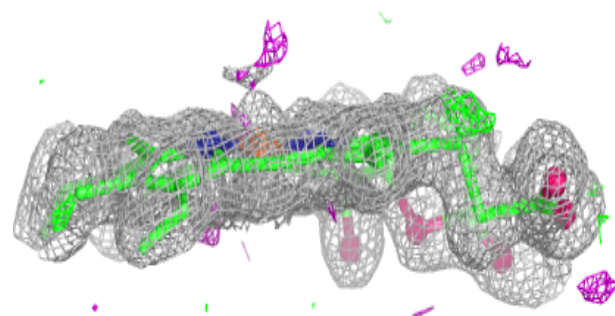
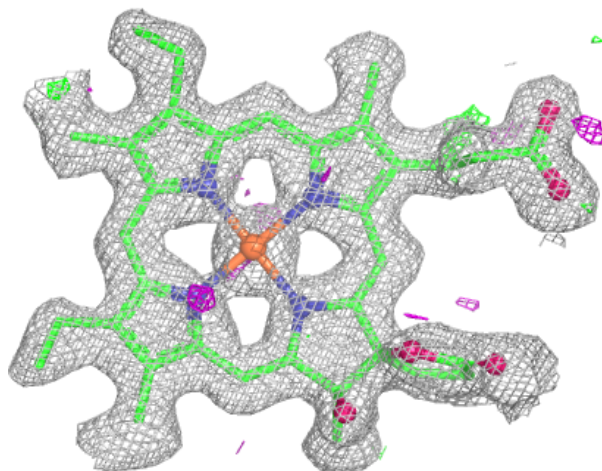
Electron density around HEM D 755 (C):

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



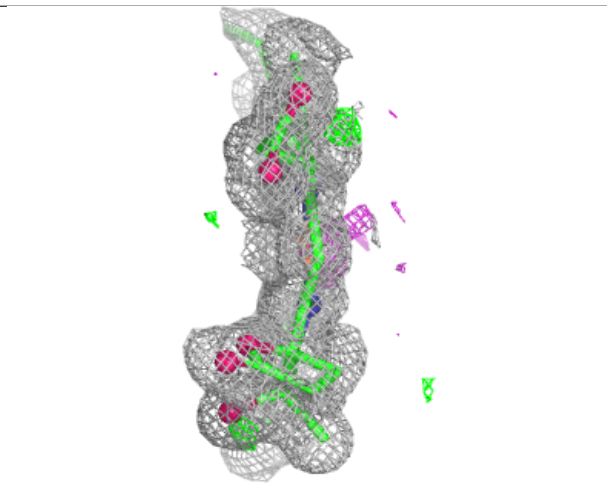
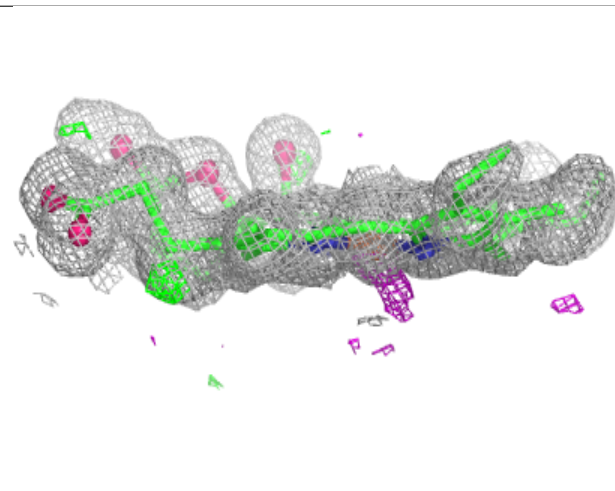
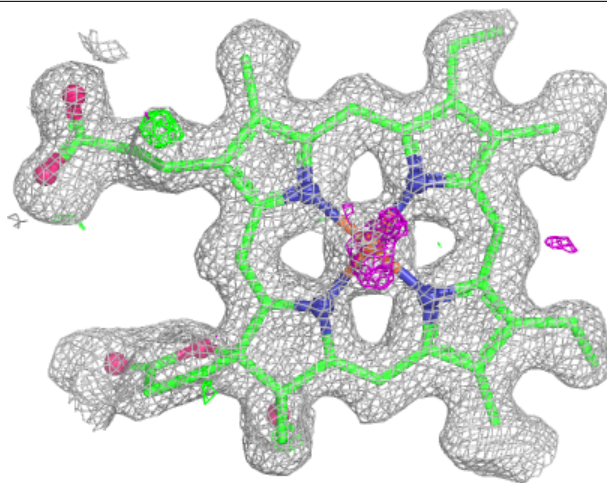
Electron density around HDE B 761 (B):

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



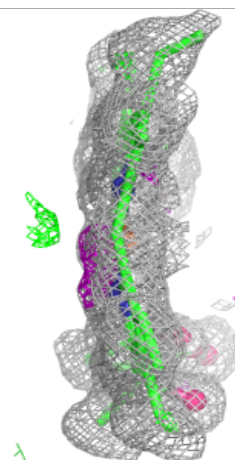
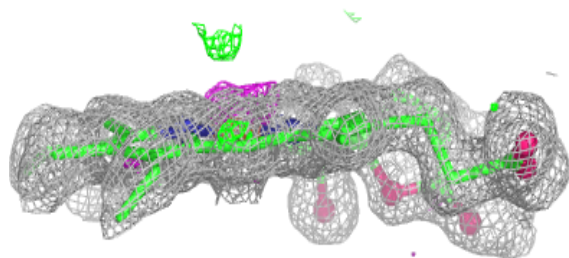
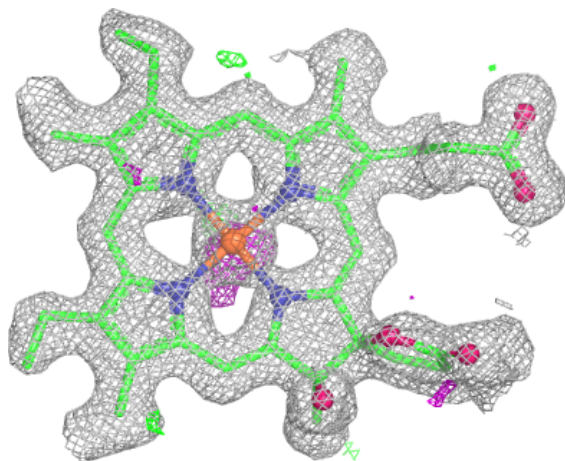
Electron density around HDE C 761 (B):

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



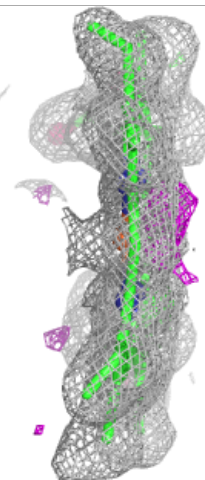
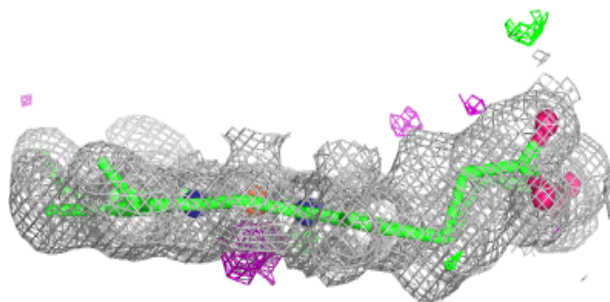
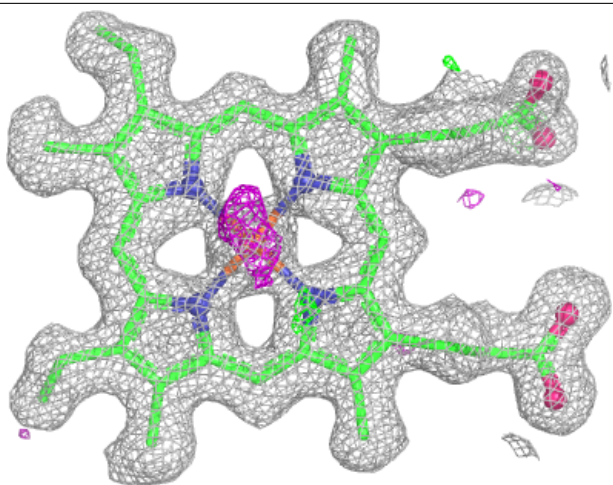
Electron density around HDE D 761 (B):

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



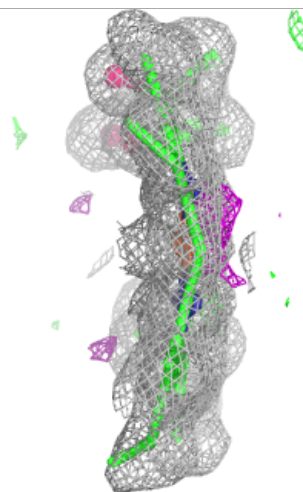
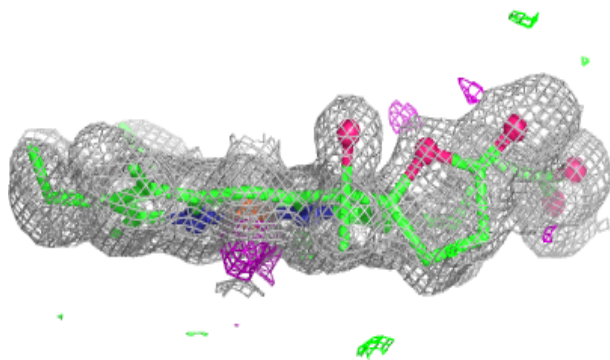
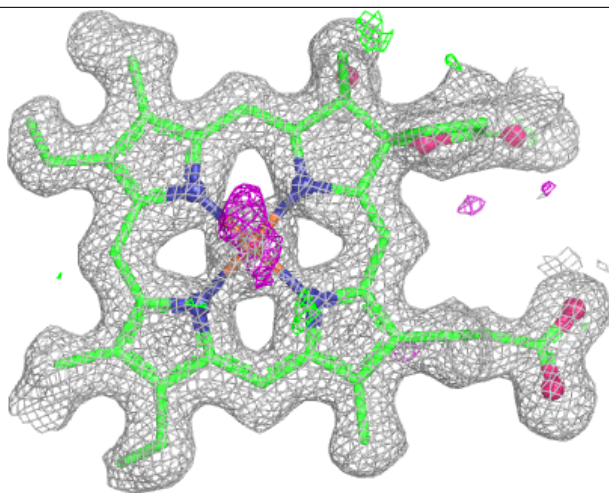
Electron density around HEM A 754 (A):

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



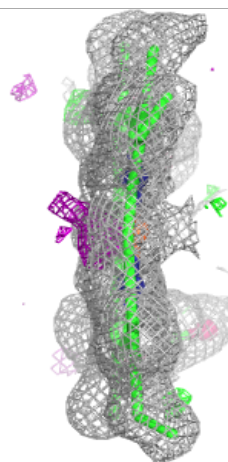
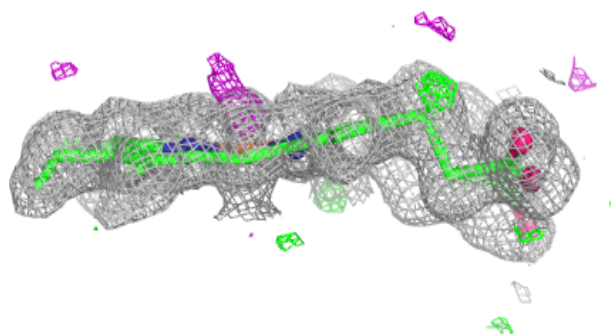
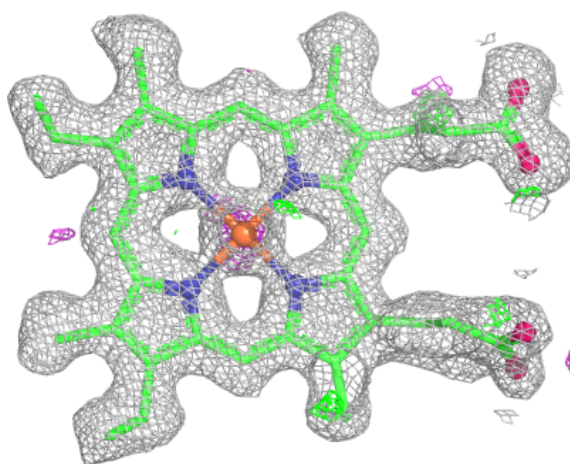
Electron density around HDE A 761 (B):

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



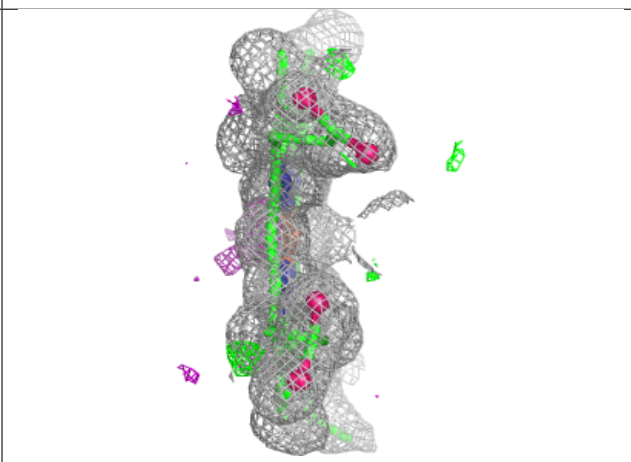
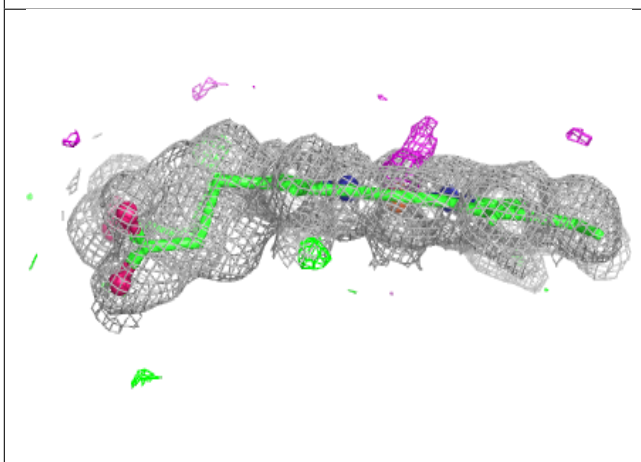
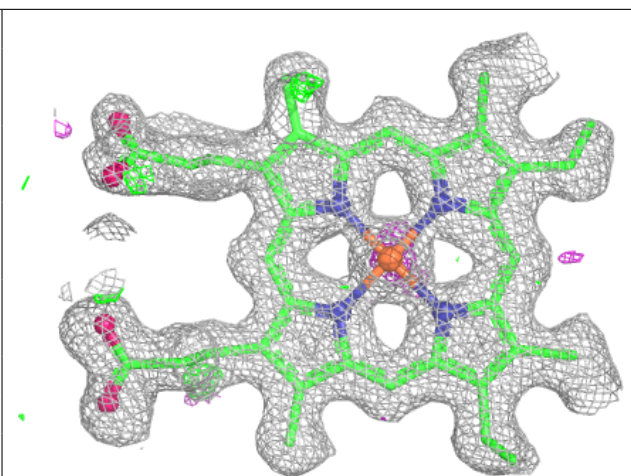
Electron density around HEM C 754 (A):

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



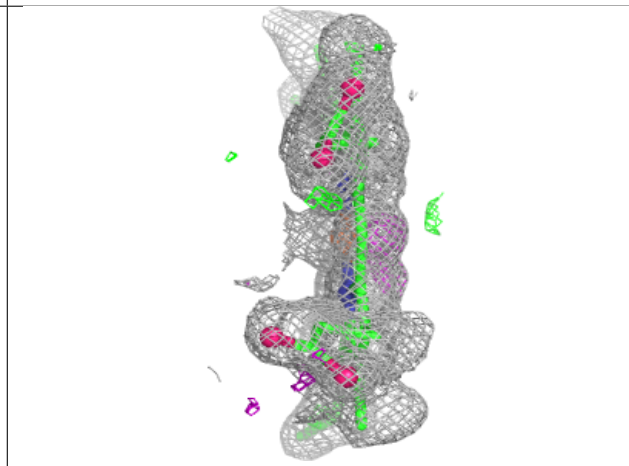
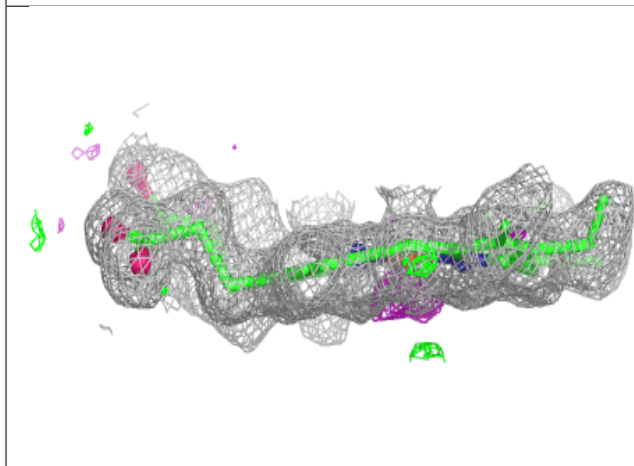
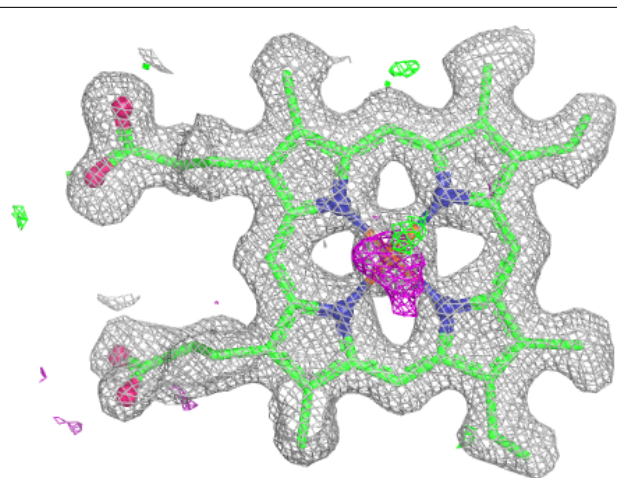
Electron density around HEM C 755 (C):

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



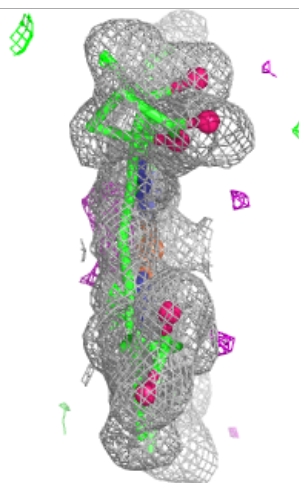
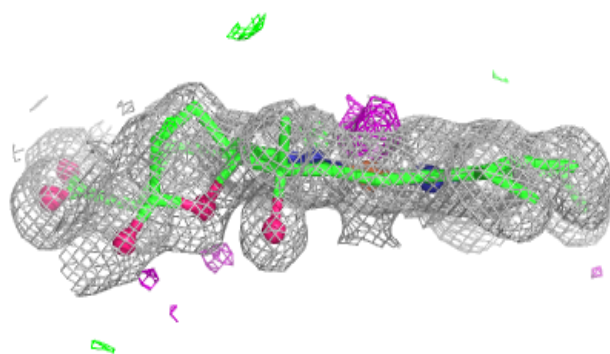
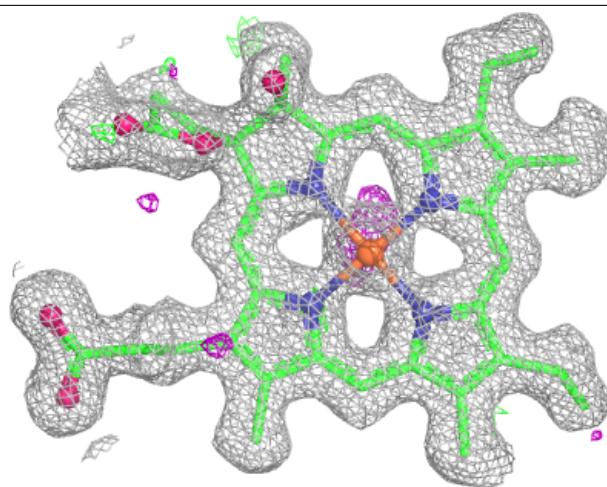
Electron density around HEM D 754 (A):

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



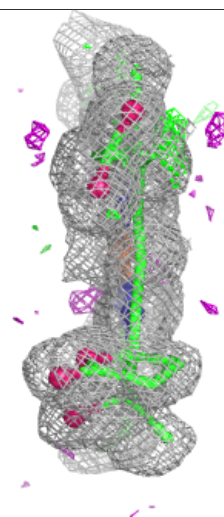
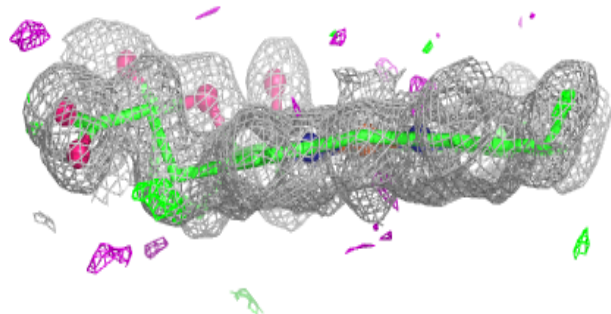
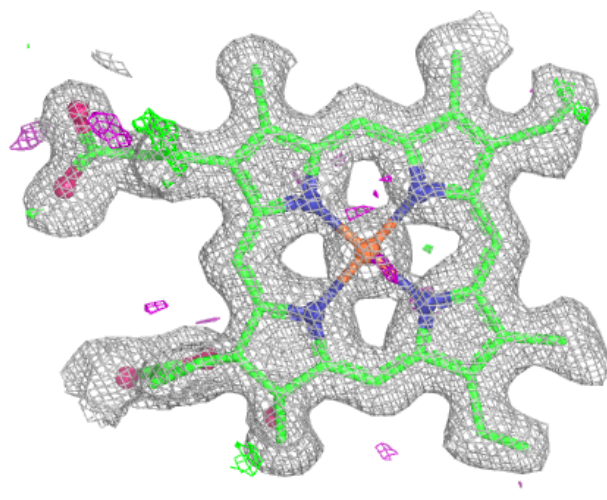
Electron density around HDD A 760 (D):

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



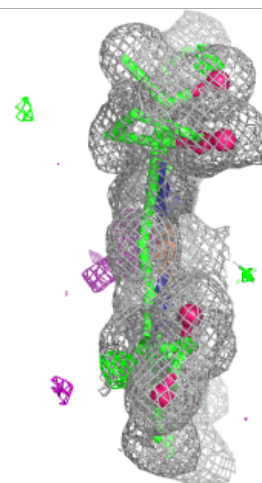
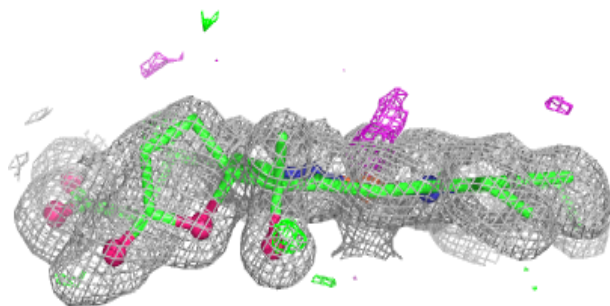
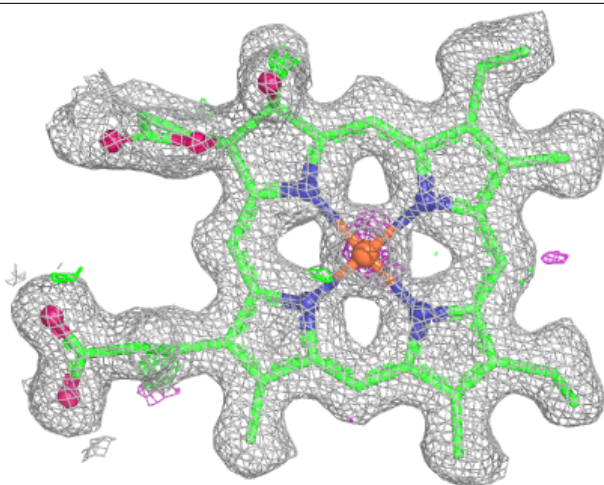
Electron density around HDD B 760 (D):

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



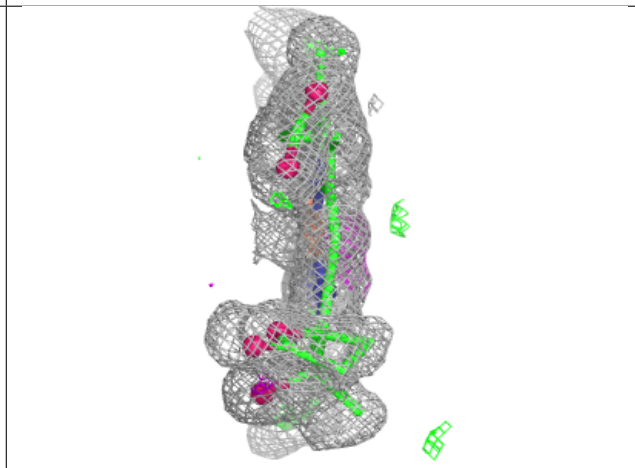
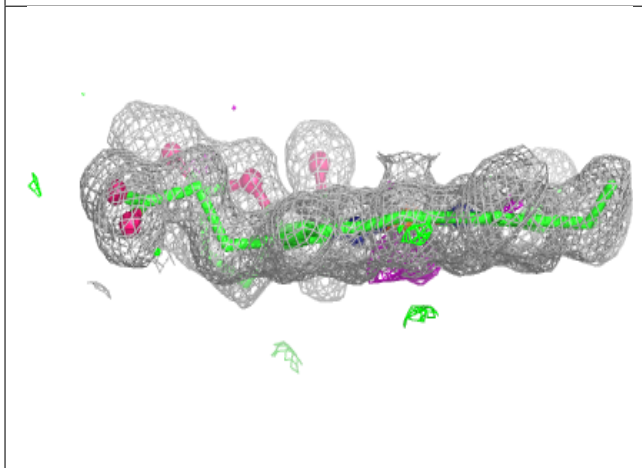
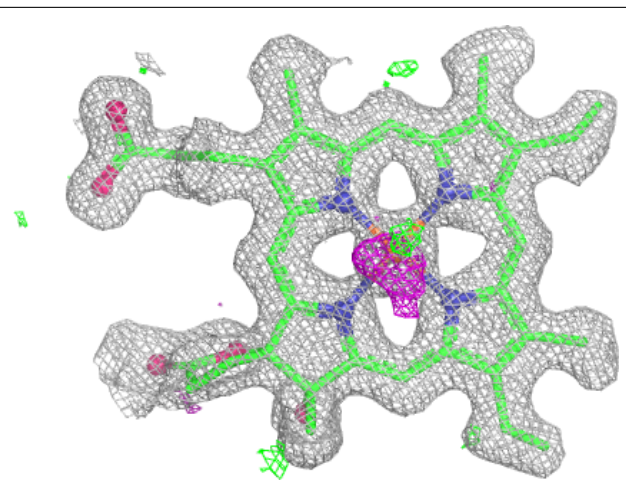
Electron density around HDD C 760 (D):

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



Electron density around HDD D 760 (D):

$2mF_o-DF_c$ (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.