



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 9, 2026 – 05:04 am BST

PDB ID : 8RXU / pdb_00008rxu
Title : Crystal structure of octaheme nitrite reductase from Trichlorobacter ammonif-
icans in space group P21
Authors : Polyakov, K.M.; Safonova, T.N.; Osipov, E.; Popov, A.N.; Tikhonova, T.V.;
Popov, V.O.
Deposited on : 2024-02-08
Resolution : 1.74 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	:	1.8.4, CSD as541be (2020)
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

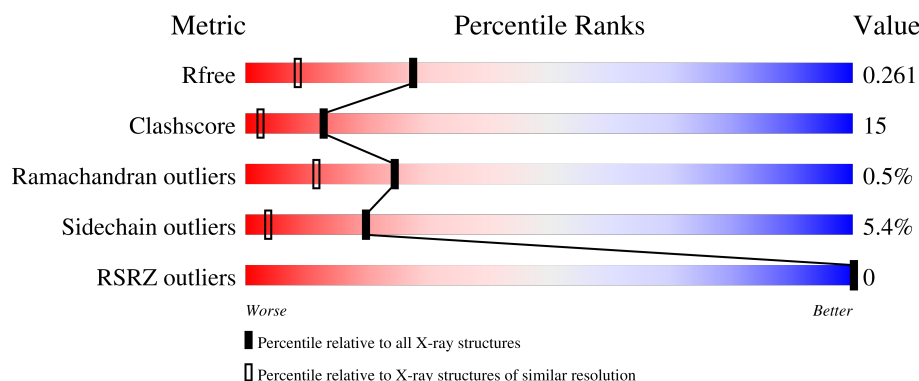
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.74 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	1187 (1.74-1.74)
Clashscore	190562	1207 (1.74-1.74)
Ramachandran outliers	187476	1200 (1.74-1.74)
Sidechain outliers	187428	1200 (1.74-1.74)
RSRZ outliers	180081	1188 (1.74-1.74)

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	AAA	495	 64% 31% 5%
1	MMM	495	 66% 29% 5%
1	YYY	495	 64% 31% 5%

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

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	HEC	AAA	601	X	-	-	-
2	HEC	AAA	602	X	-	-	-
2	HEC	AAA	603	X	-	-	-
2	HEC	AAA	604	X	-	-	-
2	HEC	AAA	605	X	-	-	-
2	HEC	AAA	606	X	-	-	-
2	HEC	AAA	607[A]	X	-	-	-
2	HEC	AAA	607[B]	X	-	-	-
2	HEC	AAA	608	X	-	-	-
2	HEC	MMM	601	X	-	-	-
2	HEC	MMM	602	X	-	-	-
2	HEC	MMM	603	X	-	-	-
2	HEC	MMM	604	X	-	-	-
2	HEC	MMM	605	X	-	-	-
2	HEC	MMM	606	X	-	-	-
2	HEC	MMM	607	X	-	-	-
2	HEC	MMM	608	X	-	-	-
2	HEC	YYY	601	X	-	-	-
2	HEC	YYY	602	X	-	-	-
2	HEC	YYY	603	X	-	-	-
2	HEC	YYY	604	X	-	-	-
2	HEC	YYY	605	X	-	-	-
2	HEC	YYY	606	X	-	-	-
2	HEC	YYY	607	X	-	-	-
2	HEC	YYY	608	X	-	-	-
4	PO4	YYY	610	-	-	X	-

2 Entry composition [i](#)

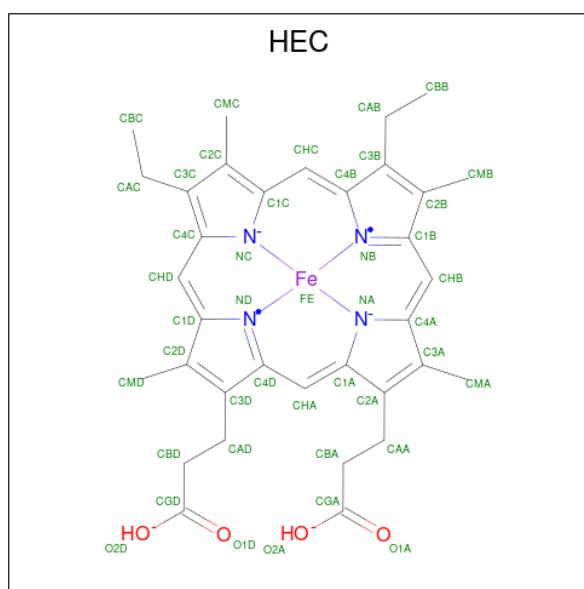
There are 5 unique types of molecules in this entry. The entry contains 13690 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Octaheme nitrite reductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AAA	495	Total	C	N	O	S	0	2	0
			3895	2437	714	717	27			
1	MMM	495	Total	C	N	O	S	0	3	0
			3894	2438	714	715	27			
1	YYY	495	Total	C	N	O	S	0	2	0
			3898	2440	712	717	29			

- Molecule 2 is HEME C (CCD ID: HEC) (formula: $C_{34}H_{36}FeN_4O_4$) (labeled as "Ligand of Interest" by depositor).



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

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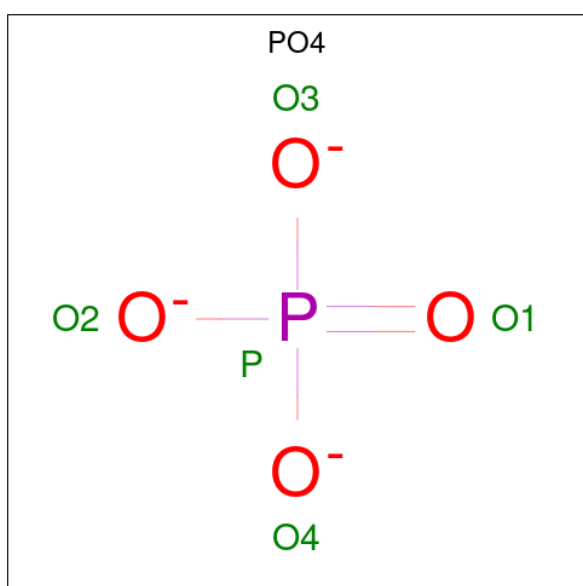
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	AAA	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	AAA	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	AAA	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	AAA	1	Total 46	C 35	Fe 1	N 4	O 6	0	1
2	AAA	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	MMM	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	MMM	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	MMM	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	MMM	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	MMM	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	MMM	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	MMM	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	MMM	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	YYY	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	YYY	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	YYY	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	YYY	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	YYY	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	YYY	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	YYY	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	YYY	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

- Molecule 3 is CALCIUM ION (CCD ID: CA) (formula: Ca) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	AAA	1	Total Ca 1 1	0	0
3	MMM	1	Total Ca 1 1	0	0
3	YYY	1	Total Ca 1 1	0	0

- Molecule 4 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	AAA	1	Total O P 5 4 1	0	0
4	MMM	1	Total O P 5 4 1	0	0
4	YYY	1	Total O P 5 4 1	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	AAA	323	Total O 323 323	0	0
5	MMM	308	Total O 308 308	0	0

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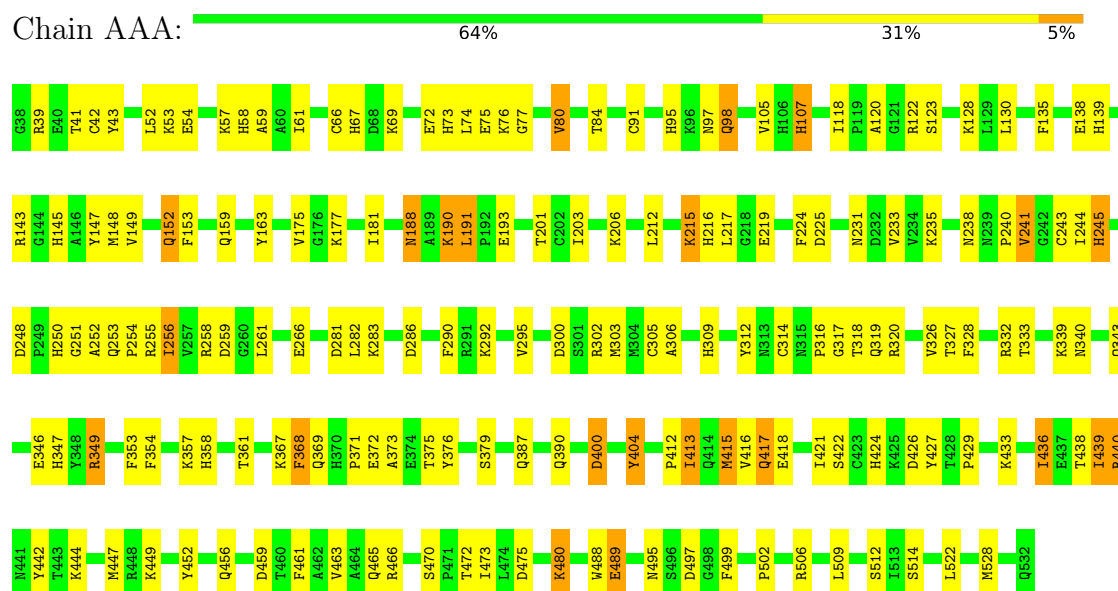
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	YYY	319	Total 319	O 319	0	0

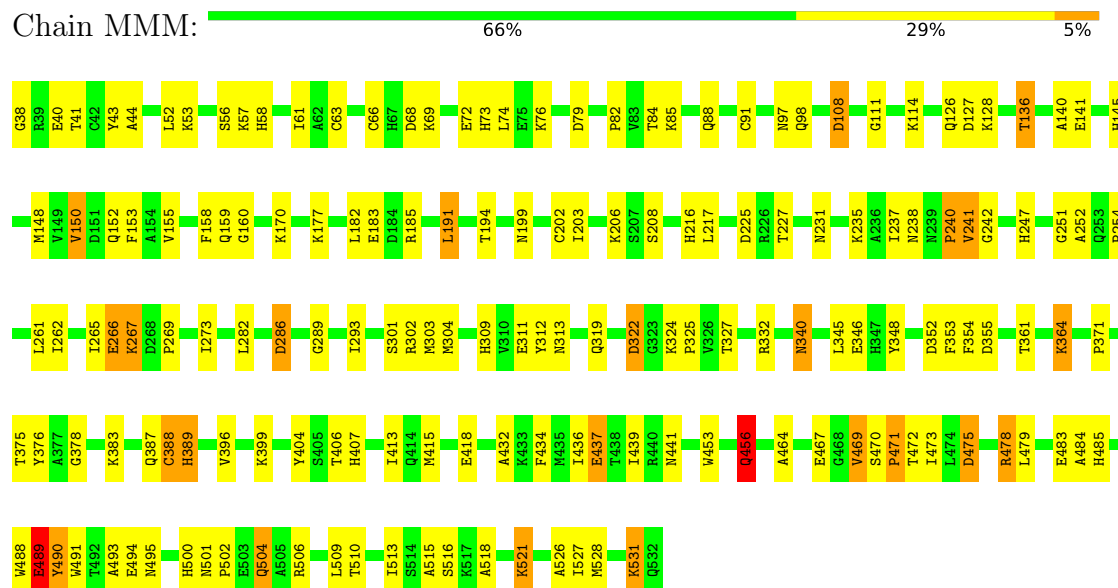
3 Residue-property plots

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: Octaheme nitrite reductase

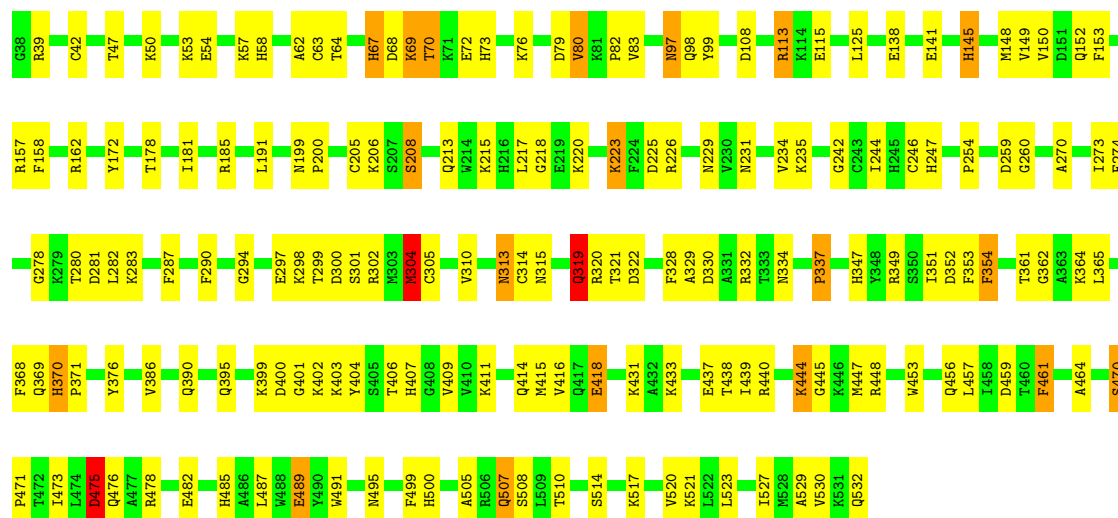


• Molecule 1: Octaheme nitrite reductase



● Molecule 1: Octaheme nitrite reductase

Chain YYY:  64% 31% . .



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	114.20Å 64.80Å 114.20Å 90.00° 119.90° 90.00°	Depositor
Resolution (Å)	42.88 – 1.74 42.88 – 1.74	Depositor EDS
% Data completeness (in resolution range)	97.8 (42.88-1.74) 97.8 (42.88-1.74)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.53 (at 1.74Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.191 , 0.254 0.196 , 0.261	Depositor DCC
R_{free} test set	7348 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å ²)	22.0	Xtriage
Anisotropy	0.333	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 14.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	0.457 for -h-l,k,h 0.457 for l,k,-h-l 0.023 for h,-k,-h-l 0.029 for -h-l,-k,l 0.024 for l,-k,h	Xtriage
Reported twinning fraction	0.400 for H, K, L 0.290 for L, K, -H-L 0.310 for -H-L, K, H	Depositor
Outliers	0 of 145920 reflections	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	13690	wwPDB-VP
Average B, all atoms (Å ²)	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.16% 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: HEC, PO4, CA

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	AAA	1.23	13/4002 (0.3%)	1.70	30/5390 (0.6%)
1	MMM	1.24	8/4003 (0.2%)	1.66	39/5391 (0.7%)
1	YYY	1.24	12/4000 (0.3%)	1.66	36/5388 (0.7%)
All	All	1.24	33/12005 (0.3%)	1.67	105/16169 (0.6%)

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	YYY	0	1

All (33) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	MMM	432	ALA	C-O	8.07	1.33	1.24
1	YYY	507	GLN	C-O	7.76	1.33	1.24
1	YYY	453	TRP	C-O	6.55	1.31	1.24
1	AAA	357	LYS	C-O	6.26	1.31	1.24
1	AAA	120	ALA	C-O	6.15	1.32	1.24
1	MMM	199	ASN	N-CA	6.06	1.50	1.46
1	AAA	440	ARG	C-O	6.04	1.31	1.24
1	AAA	305	CYS	C-O	6.02	1.31	1.24
1	MMM	202	CYS	C-O	5.96	1.31	1.24
1	YYY	97	ASN	C-O	5.73	1.30	1.24
1	YYY	444	LYS	C-O	5.73	1.30	1.24
1	YYY	500	HIS	CE1-NE2	5.68	1.38	1.32
1	YYY	67	HIS	C-O	5.61	1.30	1.24
1	AAA	376	TYR	C-O	5.56	1.31	1.24
1	YYY	371	PRO	C-O	-5.54	1.14	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	MMM	340	ASN	C-O	5.52	1.31	1.23
1	YYY	145	HIS	CE1-NE2	5.46	1.38	1.32
1	MMM	388	CYS	C-O	5.37	1.30	1.24
1	AAA	438	THR	C-O	5.34	1.30	1.24
1	YYY	370	HIS	CE1-NE2	5.33	1.37	1.32
1	AAA	379	SER	C-O	5.28	1.30	1.23
1	AAA	206	LYS	C-O	5.28	1.30	1.24
1	YYY	440	ARG	C-O	5.27	1.30	1.24
1	YYY	514	SER	C-O	5.25	1.30	1.24
1	MMM	500	HIS	C-O	-5.21	1.17	1.24
1	MMM	309	HIS	C-O	5.15	1.30	1.24
1	AAA	95	HIS	CE1-NE2	5.14	1.37	1.32
1	YYY	337	PRO	C-O	-5.13	1.17	1.24
1	MMM	128	LYS	C-O	5.11	1.30	1.24
1	AAA	145	HIS	CE1-NE2	5.10	1.37	1.32
1	AAA	456	GLN	C-O	5.09	1.29	1.24
1	AAA	300	ASP	C-O	5.06	1.29	1.23
1	AAA	358	HIS	CE1-NE2	5.04	1.37	1.32

All (105) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	YYY	406	THR	CA-CB-OG1	-9.73	95.00	109.60
1	MMM	325	PRO	N-CA-C	7.68	123.25	111.19
1	MMM	153	PHE	CA-C-O	-7.65	112.79	120.82
1	AAA	120	ALA	CA-C-N	7.32	131.83	121.30
1	AAA	120	ALA	C-N-CA	7.32	131.83	121.30
1	MMM	108	ASP	CB-CA-C	7.14	119.66	109.38
1	AAA	440	ARG	CA-C-N	7.14	130.07	120.65
1	AAA	440	ARG	C-N-CA	7.14	130.07	120.65
1	MMM	262	ILE	CA-C-O	-7.03	113.96	121.27
1	MMM	456	GLN	CB-CG-CD	6.84	124.23	112.60
1	YYY	259	ASP	CA-CB-CG	6.75	119.36	112.60
1	YYY	199	ASN	CB-CA-C	6.71	119.08	110.22
1	MMM	247	HIS	CA-CB-CG	6.70	120.50	113.80
1	YYY	254	PRO	N-CA-C	-6.69	100.74	111.38
1	AAA	371	PRO	CB-CA-C	-6.48	104.40	112.89
1	YYY	313	ASN	CA-CB-CG	-6.40	106.20	112.60
1	MMM	489	GLU	N-CA-C	-6.27	104.55	111.82
1	MMM	150	VAL	CA-C-O	-6.25	114.44	120.95
1	YYY	70	THR	CA-C-N	6.24	128.88	120.65
1	YYY	70	THR	C-N-CA	6.24	128.88	120.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AAA	98	GLN	N-CA-C	-6.23	104.11	111.03
1	YYY	299	THR	CA-CB-OG1	-6.12	100.42	109.60
1	MMM	91	CYS	CA-C-N	6.07	127.73	120.14
1	MMM	91	CYS	C-N-CA	6.07	127.73	120.14
1	MMM	441	ASN	CA-C-O	-6.07	114.45	120.82
1	YYY	115	GLU	CB-CA-C	6.06	119.35	109.90
1	YYY	440	ARG	N-CA-C	-6.03	104.62	111.07
1	YYY	499	PHE	CA-C-O	-5.96	114.20	120.63
1	MMM	325	PRO	CB-CA-C	-5.91	103.35	111.21
1	YYY	459	ASP	CA-CB-CG	5.86	118.46	112.60
1	AAA	426	ASP	CA-CB-CG	5.85	118.45	112.60
1	AAA	436	ILE	N-CA-C	-5.81	104.84	110.42
1	MMM	266	GLU	CA-C-N	5.81	128.87	120.79
1	MMM	266	GLU	C-N-CA	5.81	128.87	120.79
1	MMM	490	TYR	N-CA-C	-5.77	104.19	111.11
1	YYY	439	ILE	CA-C-N	5.74	127.90	120.44
1	YYY	439	ILE	C-N-CA	5.74	127.90	120.44
1	YYY	69	LYS	CB-CA-C	-5.71	101.72	111.26
1	MMM	432	ALA	CA-C-N	5.69	128.22	120.54
1	MMM	432	ALA	C-N-CA	5.69	128.22	120.54
1	AAA	91	CYS	N-CA-C	-5.69	105.08	111.28
1	YYY	489	GLU	CB-CG-CD	5.67	122.24	112.60
1	MMM	485	HIS	CA-C-O	-5.64	114.89	120.70
1	AAA	123	SER	O-C-N	5.61	125.28	121.19
1	MMM	439	ILE	N-CA-C	-5.61	105.06	110.72
1	YYY	510	THR	O-C-N	5.57	128.50	122.15
1	YYY	319	GLN	CB-CA-C	5.56	118.71	109.53
1	YYY	254	PRO	CA-C-O	-5.55	114.90	121.67
1	YYY	50	LYS	CA-C-N	5.55	128.03	120.54
1	YYY	50	LYS	C-N-CA	5.55	128.03	120.54
1	AAA	163	TYR	CB-CA-C	5.52	118.86	109.75
1	AAA	188	ASN	CB-CA-C	5.52	120.76	109.67
1	AAA	286	ASP	CA-CB-CG	5.52	118.12	112.60
1	MMM	313	ASN	CB-CA-C	5.51	118.95	110.14
1	MMM	506	ARG	CA-C-O	-5.50	115.04	120.82
1	YYY	400	ASP	N-CA-C	-5.47	107.61	114.56
1	YYY	349	ARG	CB-CA-C	5.47	120.44	110.11
1	YYY	304	MET	N-CA-C	-5.44	105.35	111.28
1	AAA	368	PHE	CA-CB-CG	-5.42	108.38	113.80
1	AAA	438	THR	CA-C-N	5.36	127.42	120.56
1	AAA	438	THR	C-N-CA	5.36	127.42	120.56
1	MMM	231	ASN	CB-CA-C	5.35	120.94	110.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AAA	480	LYS	N-CA-C	-5.34	105.54	111.36
1	MMM	108	ASP	CA-C-O	5.34	123.27	119.32
1	MMM	262	ILE	O-C-N	5.33	127.27	121.94
1	YYY	80	VAL	CA-C-N	5.32	128.04	120.49
1	YYY	80	VAL	C-N-CA	5.32	128.04	120.49
1	AAA	375	THR	N-CA-C	-5.30	105.41	111.14
1	AAA	281	ASP	CA-CB-CG	-5.30	107.30	112.60
1	AAA	188	ASN	CA-CB-CG	-5.29	107.31	112.60
1	YYY	337	PRO	CA-C-N	5.28	129.86	122.36
1	YYY	337	PRO	C-N-CA	5.28	129.86	122.36
1	MMM	52	LEU	CA-C-O	-5.26	114.84	120.42
1	YYY	461	PHE	CA-C-N	5.26	127.33	120.28
1	YYY	461	PHE	C-N-CA	5.26	127.33	120.28
1	AAA	439	ILE	N-CA-C	-5.26	105.59	110.53
1	AAA	152	GLN	CA-C-O	-5.24	115.32	120.82
1	YYY	438	THR	N-CA-C	-5.24	105.47	111.07
1	YYY	354	PHE	CA-CB-CG	5.22	119.03	113.80
1	AAA	245	HIS	CA-CB-CG	-5.22	108.58	113.80
1	MMM	153	PHE	CB-CA-C	5.21	119.06	110.88
1	MMM	389	HIS	CA-CB-CG	5.19	118.99	113.80
1	YYY	141	GLU	CB-CG-CD	5.18	121.41	112.60
1	MMM	327	THR	CA-C-O	-5.18	116.03	121.88
1	YYY	259	ASP	CA-C-N	5.17	126.60	120.14
1	YYY	259	ASP	C-N-CA	5.17	126.60	120.14
1	MMM	136	THR	CB-CA-C	5.15	121.19	110.32
1	MMM	97	ASN	CB-CA-C	5.15	120.56	110.67
1	AAA	512	SER	CA-C-N	5.15	127.24	120.60
1	AAA	512	SER	C-N-CA	5.15	127.24	120.60
1	MMM	145	HIS	CA-C-O	-5.14	114.05	119.97
1	AAA	404	TYR	CA-C-N	5.14	128.64	121.24
1	AAA	404	TYR	C-N-CA	5.14	128.64	121.24
1	MMM	510	THR	CA-C-N	5.12	125.77	119.99
1	MMM	510	THR	C-N-CA	5.12	125.77	119.99
1	AAA	375	THR	O-C-N	5.11	127.61	122.09
1	AAA	254	PRO	N-CA-C	-5.11	103.09	110.80
1	MMM	262	ILE	CA-C-N	5.11	127.08	120.44
1	MMM	262	ILE	C-N-CA	5.11	127.08	120.44
1	MMM	84	THR	CB-CA-C	5.09	119.96	111.51
1	AAA	107	HIS	CA-CB-CG	-5.07	108.73	113.80
1	YYY	368	PHE	CA-C-O	-5.07	115.17	120.80
1	MMM	126	GLN	CA-C-N	5.04	127.04	120.28
1	MMM	126	GLN	C-N-CA	5.04	127.04	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	MMM	437	GLU	CA-C-O	-5.03	114.65	120.24

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	YYY	310	VAL	Peptide

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	AAA	3895	0	3804	125	0
1	MMM	3894	0	3811	112	0
1	YYY	3898	0	3812	127	0
2	AAA	347	0	214	34	0
2	MMM	344	0	240	25	0
2	YYY	344	0	240	26	0
3	AAA	1	0	0	0	0
3	MMM	1	0	0	0	0
3	YYY	1	0	0	0	0
4	AAA	5	0	0	1	0
4	MMM	5	0	0	0	0
4	YYY	5	0	0	2	0
5	AAA	323	0	0	13	1
5	MMM	308	0	0	9	0
5	YYY	319	0	0	13	1
All	All	13690	0	12121	374	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 15.

All (374) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:AAA:603:HEC:HBC3	5:AAA:1015:HOH:O	1.56	1.05

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:YYY:319:GLN:NE2	1:YYY:322:ASP:OD2	1.98	0.97
1:MMM:456:GLN:HE21	1:MMM:456:GLN:HA	1.30	0.95
1:MMM:415:MET:SD	1:MMM:418:GLU:HG3	2.14	0.88
1:YYY:495:ASN:HB3	2:YYY:607:HEC:HAA1	1.59	0.84
1:AAA:327:THR:HB	5:AAA:907:HOH:O	1.78	0.84
1:YYY:319:GLN:O	5:YYY:701:HOH:O	1.97	0.81
1:YYY:260:GLY:O	5:YYY:702:HOH:O	2.00	0.80
1:MMM:495:ASN:HB3	2:MMM:607:HEC:HAA1	1.62	0.80
1:AAA:400:ASP:OD1	5:AAA:702:HOH:O	1.99	0.79
1:AAA:480:LYS:HE2	5:AAA:949:HOH:O	1.85	0.76
1:YYY:415:MET:HG2	1:YYY:418:GLU:HG2	1.66	0.76
1:MMM:319:GLN:NE2	1:MMM:332:ARG:HH22	1.83	0.75
1:MMM:38:GLY:N	5:MMM:704:HOH:O	2.19	0.75
1:YYY:320:ARG:N	1:YYY:352:ASP:OD1	2.20	0.75
1:AAA:98:GLN:HE21	2:AAA:605:HEC:HBA2	1.51	0.75
2:AAA:605:HEC:HBC2	2:AAA:605:HEC:HHD	1.68	0.74
1:MMM:267:LYS:O	1:MMM:269:PRO:HD3	1.88	0.74
1:MMM:177[A]:LYS:HD3	1:MMM:238:ASN:HB3	1.70	0.74
1:YYY:235:LYS:HD3	5:YYY:773:HOH:O	1.88	0.74
1:AAA:72:GLU:HG2	1:AAA:76:LYS:HE3	1.71	0.73
1:MMM:148:MET:HB2	2:MMM:606:HEC:HMD2	1.71	0.71
1:MMM:312:TYR:CE2	2:MMM:604:HEC:HMC1	2.26	0.70
1:MMM:527:ILE:O	1:MMM:531:LYS:NZ	2.23	0.70
1:MMM:415:MET:SD	1:MMM:418:GLU:CG	2.79	0.70
1:MMM:72:GLU:O	1:MMM:76:LYS:HB2	1.92	0.70
1:MMM:473:ILE:HG21	1:MMM:526:ALA:CB	2.23	0.69
1:MMM:413:ILE:HD12	1:MMM:436:ILE:HD12	1.74	0.69
1:AAA:367:LYS:NZ	1:AAA:489:GLU:OE2	2.18	0.68
1:YYY:53:LYS:NZ	1:YYY:58:HIS:O	2.27	0.68
1:AAA:314:CYS:HA	1:AAA:333:THR:O	1.94	0.67
1:AAA:216:HIS:CE1	1:AAA:292:LYS:HD2	2.29	0.67
2:MMM:606:HEC:HBB3	2:MMM:606:HEC:CMB	2.24	0.67
2:AAA:603:HEC:HBC2	2:AAA:603:HEC:HHD	1.77	0.66
1:AAA:415:MET:CG	1:AAA:415:MET:O	2.42	0.66
1:AAA:61:ILE:HG22	2:AAA:602:HEC:CMC	2.25	0.66
1:MMM:319:GLN:HE22	1:MMM:332:ARG:HH22	1.42	0.66
1:AAA:497:ASP:OD2	5:AAA:703:HOH:O	2.13	0.66
1:AAA:461:PHE:HE1	1:AAA:465:GLN:HE21	1.44	0.65
1:MMM:456:GLN:HE21	1:MMM:456:GLN:CA	2.07	0.65
1:YYY:495:ASN:HB3	2:YYY:607:HEC:CAA	2.27	0.65
1:YYY:456:GLN:HE21	1:YYY:520:VAL:HG11	1.62	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:YYY:376:TYR:CE1	2:YYY:607:HEC:HMC1	2.31	0.65
2:MMM:606:HEC:HBB3	2:MMM:606:HEC:HMB1	1.79	0.64
1:AAA:256:ILE:HD12	1:AAA:261:LEU:HD23	1.79	0.64
1:AAA:417:GLN:HB2	5:AAA:811:HOH:O	1.96	0.64
1:AAA:67:HIS:HD1	1:AAA:84:THR:HB	1.61	0.64
1:MMM:378:GLY:O	1:MMM:383:LYS:HE2	1.98	0.64
1:YYY:471:PRO:O	1:YYY:475:ASP:OD1	2.16	0.64
1:MMM:266:GLU:O	5:MMM:703:HOH:O	2.16	0.64
1:MMM:40:GLU:HA	1:MMM:43:TYR:HB2	1.79	0.63
1:AAA:39:ARG:HG3	1:AAA:43:TYR:CE2	2.34	0.63
1:YYY:246:CYS:HB3	1:YYY:304:MET:HE2	1.82	0.62
1:AAA:98:GLN:NE2	2:AAA:605:HEC:HBA2	2.14	0.62
1:YYY:149:VAL:HG11	1:YYY:178:THR:OG1	1.99	0.62
2:AAA:605:HEC:HBC3	2:AAA:606:HEC:CBB	2.30	0.61
1:YYY:491:TRP:CZ3	1:YYY:505:ALA:HB2	2.35	0.61
1:YYY:215:LYS:HB2	1:YYY:290:PHE:CE2	2.35	0.61
1:AAA:42:CYS:HA	2:AAA:601:HEC:CHC	2.31	0.60
1:YYY:70:THR:O	1:YYY:73:HIS:HB3	2.00	0.60
1:YYY:162:ARG:O	1:YYY:185:ARG:HG2	2.02	0.60
1:MMM:286:ASP:OD1	1:MMM:286:ASP:C	2.44	0.60
1:MMM:518:ALA:O	1:MMM:521:LYS:HB3	2.02	0.60
1:AAA:506:ARG:NH1	1:MMM:191:LEU:CD2	2.65	0.59
1:YYY:376:TYR:CZ	2:YYY:607:HEC:HMC1	2.37	0.59
1:YYY:321:THR:OG1	1:YYY:322:ASP:N	2.34	0.59
1:YYY:470:SER:HB3	1:YYY:473:ILE:HD12	1.84	0.59
1:AAA:72:GLU:HG2	1:AAA:76:LYS:CE	2.33	0.59
1:YYY:125:LEU:HD23	5:YYY:977:HOH:O	2.03	0.59
1:MMM:73:HIS:CG	1:MMM:82:PRO:HD3	2.38	0.59
1:YYY:444:LYS:HA	1:YYY:447[B]:MET:HE3	1.85	0.58
1:AAA:302:ARG:O	1:AAA:306:ALA:HB2	2.04	0.58
1:YYY:79:ASP:HB2	5:YYY:705:HOH:O	2.03	0.58
1:AAA:367:LYS:NZ	1:AAA:368:PHE:O	2.37	0.57
1:YYY:365:LEU:HD22	1:YYY:485:HIS:CD2	2.39	0.57
2:YYY:608:HEC:HBC3	2:YYY:608:HEC:HMC1	1.86	0.57
1:MMM:502:PRO:HG2	5:MMM:786:HOH:O	2.05	0.57
1:MMM:155:VAL:HG12	1:MMM:158:PHE:HB2	1.86	0.57
1:AAA:215:LYS:HB3	1:AAA:219:GLU:O	2.05	0.57
1:AAA:215:LYS:HD3	1:AAA:290:PHE:CE1	2.40	0.56
1:AAA:243:CYS:CB	2:AAA:603:HEC:HMB1	2.35	0.56
1:MMM:437:GLU:HA	1:MMM:437:GLU:OE1	2.05	0.56
1:YYY:300:ASP:OD1	1:YYY:302:ARG:HB2	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:YYY:218:GLY:O	1:YYY:225:ASP:HB2	2.05	0.56
1:MMM:183:GLU:OE2	1:MMM:185:ARG:NE	2.39	0.56
1:MMM:216:HIS:CE1	1:MMM:217:LEU:HG	2.42	0.55
1:YYY:76:LYS:O	5:YYY:705:HOH:O	2.17	0.55
1:AAA:67:HIS:ND1	1:AAA:84:THR:HB	2.21	0.55
1:YYY:415:MET:HG2	1:YYY:418:GLU:CG	2.37	0.55
1:MMM:66:CYS:HB2	2:MMM:602:HEC:C4C	2.36	0.55
1:YYY:280:THR:HA	5:YYY:748:HOH:O	2.07	0.55
1:YYY:395:GLN:OE1	1:YYY:403:LYS:HE3	2.07	0.55
1:AAA:74:LEU:HD21	2:AAA:601:HEC:CBB	2.37	0.55
1:MMM:265:ILE:HG21	1:MMM:282:LEU:HD22	1.88	0.55
1:YYY:351:ILE:O	1:YYY:352:ASP:C	2.50	0.55
1:MMM:225:ASP:OD2	1:MMM:227:THR:OG1	2.15	0.55
1:AAA:480:LYS:CE	5:AAA:949:HOH:O	2.49	0.54
1:AAA:52:LEU:O	1:AAA:251:GLY:HA3	2.07	0.54
1:MMM:114:LYS:O	1:MMM:140:ALA:HA	2.07	0.54
1:AAA:135:PHE:HD2	1:AAA:139:HIS:CD2	2.25	0.54
1:YYY:320:ARG:NH1	1:YYY:482:GLU:OE1	2.35	0.54
1:MMM:58:HIS:HE1	2:MMM:603:HEC:NB	1.98	0.54
1:YYY:313:ASN:ND2	1:YYY:353:PHE:CZ	2.76	0.54
1:YYY:529:ALA:HA	1:YYY:532:GLN:CD	2.31	0.54
1:AAA:415:MET:O	1:AAA:415:MET:HG3	2.07	0.54
2:AAA:603:HEC:HHD	2:AAA:603:HEC:CBC	2.36	0.54
1:YYY:244:ILE:HG21	2:YYY:602:HEC:HMD2	1.90	0.54
1:YYY:523:LEU:O	1:YYY:527:ILE:HG13	2.08	0.54
1:MMM:456:GLN:HA	1:MMM:456:GLN:NE2	2.08	0.54
1:AAA:442:TYR:HA	5:MMM:717:HOH:O	2.08	0.53
1:MMM:495:ASN:HB3	2:MMM:607:HEC:CAA	2.36	0.53
1:MMM:488:TRP:CZ3	1:MMM:489:GLU:HG3	2.43	0.53
1:YYY:113:ARG:HD2	1:YYY:172:TYR:OH	2.08	0.53
1:YYY:273:ILE:HD11	1:YYY:274:PHE:CZ	2.44	0.53
1:AAA:312:TYR:CD2	2:AAA:604:HEC:HMC2	2.43	0.53
1:MMM:53:LYS:HD3	2:MMM:602:HEC:HBB2	1.89	0.53
1:YYY:365:LEU:HD22	1:YYY:485:HIS:CG	2.44	0.52
1:YYY:461:PHE:O	1:YYY:464:ALA:HB3	2.09	0.52
1:AAA:250:HIS:HA	5:AAA:807:HOH:O	2.09	0.52
1:AAA:320:ARG:NH1	1:AAA:349:ARG:HD3	2.25	0.52
1:MMM:241:VAL:HB	2:MMM:606:HEC:HBC2	1.91	0.52
1:MMM:177[B]:LYS:HD3	1:MMM:238:ASN:HB3	1.92	0.52
1:MMM:304:MET:SD	2:MMM:605:HEC:HMD2	2.50	0.52
1:AAA:440:ARG:NH2	5:AAA:728:HOH:O	2.41	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:YYY:330:ASP:OD2	1:YYY:332:ARG:NH2	2.43	0.51
1:AAA:243:CYS:HB3	2:AAA:603:HEC:HMB1	1.91	0.51
1:YYY:217:LEU:O	1:YYY:226:ARG:NH1	2.35	0.51
2:AAA:604:HEC:O1D	2:AAA:604:HEC:HHA	2.11	0.51
1:YYY:354:PHE:CE1	1:YYY:364:LYS:HD3	2.45	0.51
1:MMM:203:ILE:HG21	1:MMM:237:ILE:CD1	2.41	0.51
1:AAA:152:GLN:NE2	1:AAA:203:ILE:HD12	2.26	0.51
1:YYY:456:GLN:NE2	1:YYY:520:VAL:HG11	2.26	0.51
1:YYY:475:ASP:O	1:YYY:478:ARG:N	2.44	0.51
1:MMM:38:GLY:HA2	5:MMM:950:HOH:O	2.10	0.50
1:AAA:387:GLN:N	1:AAA:390:GLN:OE1	2.40	0.50
1:AAA:84:THR:HG21	1:AAA:212:LEU:CD1	2.40	0.50
1:YYY:67:HIS:ND1	2:YYY:601:HEC:HMA3	2.27	0.50
1:YYY:205:CYS:O	1:YYY:206:LYS:HD3	2.11	0.50
1:YYY:445:GLY:HA3	5:YYY:802:HOH:O	2.10	0.50
1:AAA:340:ASN:C	1:AAA:340:ASN:OD1	2.54	0.50
1:YYY:390:GLN:HG2	5:YYY:718:HOH:O	2.11	0.50
1:AAA:240:PRO:O	1:AAA:241:VAL:C	2.54	0.50
1:AAA:152:GLN:HE22	1:AAA:203:ILE:HD12	1.76	0.50
1:MMM:58:HIS:CG	1:MMM:61:ILE:HD11	2.47	0.50
1:YYY:148:MET:SD	1:YYY:206:LYS:HA	2.52	0.50
1:AAA:61:ILE:CG2	2:AAA:602:HEC:CMC	2.89	0.50
1:MMM:484:ALA:HB2	1:MMM:515:ALA:HB3	1.94	0.50
1:AAA:303:MET:O	1:AAA:306:ALA:HB3	2.12	0.49
1:AAA:212:LEU:HD11	2:AAA:602:HEC:HAD2	1.93	0.49
1:AAA:412:PRO:HB3	2:AAA:608:HEC:HBB1	1.95	0.49
1:AAA:472:THR:HA	1:AAA:475:ASP:OD2	2.11	0.49
1:YYY:329:ALA:HA	5:YYY:965:HOH:O	2.11	0.49
1:AAA:53:LYS:HD3	2:AAA:602:HEC:HBB2	1.94	0.49
1:AAA:266:GLU:OE2	1:AAA:292:LYS:NZ	2.42	0.49
1:MMM:58:HIS:HE1	2:MMM:603:HEC:C4B	2.25	0.49
1:AAA:57:LYS:HD2	2:AAA:603:HEC:O2A	2.12	0.49
1:YYY:67:HIS:CE1	2:YYY:601:HEC:CMA	2.96	0.49
1:AAA:361:THR:HA	1:AAA:461:PHE:CE1	2.48	0.49
1:YYY:150:VAL:HG11	1:YYY:181:ILE:HG21	1.94	0.49
1:YYY:456:GLN:O	1:YYY:457:LEU:C	2.56	0.49
1:MMM:354:PHE:CG	1:MMM:364:LYS:HB3	2.47	0.49
1:YYY:314:CYS:SG	2:YYY:604:HEC:HMC1	2.52	0.49
1:AAA:177:LYS:HA	1:AAA:238:ASN:O	2.13	0.49
1:MMM:88:GLN:NE2	1:MMM:240:PRO:O	2.43	0.49
1:AAA:74:LEU:HD21	2:AAA:601:HEC:HBB2	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AAA:148:MET:HB2	2:AAA:606:HEC:HMD2	1.95	0.49
2:AAA:608:HEC:CAA	1:MMM:170:LYS:HB3	2.43	0.48
1:MMM:453:TRP:HB3	1:MMM:516:SER:HB2	1.95	0.48
1:MMM:471:PRO:O	1:MMM:475:ASP:HB2	2.13	0.48
1:AAA:135:PHE:CD2	1:AAA:139:HIS:CD2	3.00	0.48
1:YYY:152:GLN:HA	2:YYY:604:HEC:HMA1	1.96	0.48
1:AAA:463:VAL:HG22	1:AAA:466:ARG:HH21	1.79	0.48
1:YYY:319:GLN:HE21	1:YYY:322:ASP:CG	2.21	0.48
1:YYY:409:VAL:HG23	2:YYY:606:HEC:HBA2	1.96	0.48
1:AAA:243:CYS:HB2	2:AAA:603:HEC:HMB1	1.96	0.48
1:MMM:311:GLU:OE2	1:MMM:348:TYR:OH	2.31	0.48
1:YYY:97:ASN:HD21	1:YYY:399:LYS:CG	2.27	0.48
1:YYY:399:LYS:HG3	1:YYY:402:LYS:HB3	1.96	0.47
1:YYY:67:HIS:ND1	2:YYY:601:HEC:CMA	2.77	0.47
1:AAA:69:LYS:NZ	1:AAA:72:GLU:OE2	2.47	0.47
1:MMM:56:SER:OG	1:MMM:251:GLY:HA2	2.14	0.47
1:AAA:400:ASP:OD1	1:AAA:400:ASP:N	2.47	0.47
1:YYY:62:ALA:C	1:YYY:64:THR:H	2.22	0.47
1:AAA:76:LYS:HB2	1:AAA:80:VAL:HG21	1.96	0.47
1:MMM:111:GLY:O	1:MMM:114:LYS:HE2	2.13	0.47
1:MMM:251:GLY:O	1:MMM:252:ALA:HB3	2.15	0.47
1:MMM:261:LEU:O	1:MMM:265:ILE:HD12	2.14	0.47
1:MMM:319:GLN:HA	1:MMM:352:ASP:O	2.15	0.47
1:MMM:361:THR:O	1:MMM:478:ARG:NH2	2.47	0.47
1:YYY:67:HIS:CE1	2:YYY:601:HEC:HMA2	2.50	0.47
1:YYY:229:ASN:OD1	1:YYY:231:ASN:HB2	2.15	0.47
1:MMM:340:ASN:HD22	1:MMM:504:GLN:HE22	1.61	0.47
1:YYY:53:LYS:HD3	2:YYY:602:HEC:HBB2	1.97	0.47
1:YYY:475:ASP:O	1:YYY:478:ARG:HB2	2.14	0.47
1:AAA:413:ILE:HD12	1:AAA:433:LYS:HG2	1.96	0.46
1:MMM:319:GLN:NE2	1:MMM:332:ARG:NH2	2.60	0.46
1:YYY:97:ASN:ND2	1:YYY:399:LYS:HG2	2.30	0.46
1:YYY:153:PHE:CE1	1:YYY:234:VAL:HG12	2.51	0.46
1:AAA:465:GLN:NE2	5:AAA:736:HOH:O	2.49	0.46
1:YYY:145:HIS:CD2	2:YYY:606:HEC:ND	2.84	0.46
1:AAA:224:PHE:CD1	1:AAA:233:VAL:HG22	2.51	0.46
1:MMM:273:ILE:CG2	5:MMM:906:HOH:O	2.63	0.46
2:MMM:608:HEC:HMC3	2:MMM:608:HEC:HBC3	1.97	0.46
1:YYY:246:CYS:HB3	1:YYY:304:MET:HG2	1.97	0.46
1:AAA:84:THR:CG2	1:AAA:212:LEU:HD12	2.44	0.46
1:AAA:470:SER:HB3	1:AAA:473:ILE:HD12	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:MMM:491:TRP:CZ2	1:MMM:504:GLN:HG2	2.50	0.46
1:YYY:361:THR:HA	1:YYY:461:PHE:CE1	2.50	0.46
1:MMM:68:ASP:O	1:MMM:69:LYS:CB	2.63	0.46
1:YYY:63:CYS:HB3	2:YYY:601:HEC:HMB1	1.96	0.46
1:YYY:72:GLU:O	1:YYY:76:LYS:HG2	2.15	0.46
1:YYY:157:ARG:NH2	4:YYY:610:PO4:O1	2.49	0.46
1:YYY:282:LEU:HD11	1:YYY:294:GLY:C	2.40	0.46
1:YYY:217:LEU:HA	1:YYY:334:ASN:HD22	1.80	0.46
1:AAA:424:HIS:O	1:AAA:427:TYR:HB2	2.15	0.46
1:AAA:440:ARG:O	1:AAA:444:LYS:HG3	2.15	0.46
1:MMM:473:ILE:HG21	1:MMM:526:ALA:HB1	1.94	0.46
1:YYY:370:HIS:NE2	2:YYY:604:HEC:C1D	2.79	0.46
1:YYY:487:LEU:HB3	1:YYY:508:SER:O	2.16	0.46
1:YYY:362:GLY:HA2	5:YYY:887:HOH:O	2.15	0.46
1:YYY:97:ASN:ND2	1:YYY:399:LYS:CG	2.79	0.45
1:AAA:105:VAL:CG1	1:AAA:107:HIS:CE1	2.99	0.45
1:MMM:301:SER:HA	1:MMM:304:MET:HB2	1.98	0.45
1:MMM:322:ASP:HB2	1:MMM:324:LYS:HG2	1.98	0.45
1:YYY:247:HIS:CG	2:YYY:603:HEC:HMA1	2.51	0.45
1:AAA:39:ARG:NH1	1:AAA:59:ALA:O	2.50	0.45
1:AAA:326:VAL:HG22	1:AAA:332:ARG:NH2	2.31	0.45
1:MMM:254:PRO:HB3	1:MMM:304:MET:HE3	1.99	0.45
1:YYY:281:ASP:OD1	1:YYY:297:GLU:N	2.42	0.45
1:AAA:118:ILE:HB	1:YYY:448:ARG:HG3	1.98	0.45
1:AAA:318:THR:HB	1:AAA:354:PHE:CE1	2.52	0.45
1:AAA:436:ILE:HG13	2:AAA:608:HEC:HMB2	1.99	0.45
1:YYY:213:GLN:HB3	1:YYY:223:LYS:HB3	1.98	0.45
1:AAA:190:LYS:O	1:AAA:191:LEU:CD2	2.64	0.45
1:MMM:41:THR:O	1:MMM:44:ALA:HB3	2.16	0.45
1:MMM:152:GLN:CD	1:MMM:206:LYS:HG3	2.42	0.45
1:AAA:175:VAL:C	1:AAA:181:ILE:HD11	2.42	0.44
1:MMM:38:GLY:O	1:MMM:41:THR:HB	2.16	0.44
1:MMM:208:SER:OG	1:MMM:242:GLY:N	2.50	0.44
1:YYY:369:GLN:HG2	4:YYY:610:PO4:O3	2.16	0.44
1:AAA:193:GLU:OE1	1:YYY:517:LYS:NZ	2.49	0.44
1:YYY:337:PRO:HB3	1:YYY:347:HIS:CD2	2.52	0.44
1:AAA:73:HIS:O	1:AAA:77:GLY:O	2.35	0.44
1:MMM:456:GLN:CD	5:MMM:741:HOH:O	2.60	0.44
1:YYY:437:GLU:OE1	1:YYY:437:GLU:HA	2.16	0.44
1:MMM:82:PRO:HG2	2:MMM:601:HEC:C3A	2.48	0.44
1:YYY:491:TRP:CZ2	1:YYY:505:ALA:HA	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:YYY:527:ILE:HG22	1:YYY:527:ILE:O	2.17	0.44
1:MMM:467:GLU:HB3	1:MMM:531:LYS:NZ	2.33	0.44
2:MMM:607:HEC:HBD1	2:MMM:607:HEC:O2A	2.18	0.44
1:AAA:317:GLY:HA3	1:AAA:353:PHE:CE2	2.52	0.44
1:MMM:53:LYS:O	1:MMM:56:SER:OG	2.32	0.44
1:AAA:97:ASN:HB3	1:AAA:404:TYR:CE2	2.53	0.44
1:AAA:248:ASP:O	1:AAA:252:ALA:HA	2.18	0.44
1:AAA:312:TYR:OH	4:AAA:610:PO4:O4	2.14	0.44
2:AAA:605:HEC:HBC3	2:AAA:606:HEC:HBB2	1.99	0.44
1:MMM:312:TYR:CD2	2:MMM:604:HEC:CMC	3.00	0.44
1:AAA:488:TRP:CE3	1:AAA:489:GLU:HB2	2.53	0.44
1:YYY:407:HIS:HD2	2:YYY:605:HEC:CHC	2.31	0.44
1:AAA:107:HIS:CE1	1:YYY:431:LYS:HD2	2.53	0.43
1:AAA:159:GLN:HG2	1:AAA:231:ASN:OD1	2.18	0.43
1:MMM:57:LYS:HD2	2:MMM:603:HEC:CGA	2.48	0.43
1:MMM:63:CYS:HA	2:MMM:602:HEC:CHC	2.48	0.43
1:AAA:190:LYS:O	1:AAA:191:LEU:HD22	2.18	0.43
1:MMM:407:HIS:HD2	2:MMM:605:HEC:CHC	2.30	0.43
1:AAA:316:PRO:HD3	1:AAA:328:PHE:CE1	2.54	0.43
1:YYY:376:TYR:OH	1:YYY:386:VAL:O	2.34	0.43
1:AAA:421:ILE:HD11	1:AAA:429:PRO:HA	2.01	0.43
1:MMM:286:ASP:OD2	1:MMM:289:GLY:HA2	2.19	0.43
1:AAA:130:LEU:N	1:AAA:130:LEU:HD23	2.33	0.43
2:AAA:606:HEC:HMA2	2:AAA:607[A]:HEC:HBA1	2.00	0.43
1:MMM:434:PHE:CD1	1:MMM:434:PHE:C	2.96	0.43
1:YYY:42:CYS:HA	2:YYY:601:HEC:CHC	2.48	0.43
1:YYY:444:LYS:HB2	1:YYY:444:LYS:HE3	1.81	0.43
1:AAA:73:HIS:CE1	2:AAA:601:HEC:ND	2.86	0.43
1:YYY:205:CYS:C	1:YYY:206:LYS:HG2	2.43	0.43
1:YYY:304:MET:HE2	2:YYY:605:HEC:CHD	2.48	0.43
1:YYY:376:TYR:CE1	2:YYY:607:HEC:CMC	3.01	0.43
1:YYY:411:LYS:O	1:YYY:414:GLN:HB2	2.18	0.43
1:AAA:415:MET:HE3	1:AAA:415:MET:HB2	1.77	0.43
1:AAA:449:LYS:NZ	1:MMM:136:THR:O	2.52	0.43
1:YYY:97:ASN:HD21	1:YYY:399:LYS:HG2	1.84	0.43
1:YYY:200:PRO:HD2	5:YYY:789:HOH:O	2.18	0.43
1:MMM:150:VAL:HA	1:MMM:182:LEU:HD11	2.01	0.43
1:AAA:75:GLU:OE2	1:AAA:75:GLU:N	2.52	0.42
1:MMM:160:GLY:HA2	1:MMM:194:THR:OG1	2.18	0.42
1:MMM:267:LYS:C	1:MMM:269:PRO:HD3	2.44	0.42
1:MMM:265:ILE:CD1	1:MMM:303:MET:HE2	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:MMM:376:TYR:CE1	2:MMM:607:HEC:HMC2	2.54	0.42
1:YYY:395:GLN:HA	1:YYY:404:TYR:O	2.18	0.42
1:AAA:216:HIS:O	1:AAA:217:LEU:HB2	2.19	0.42
1:MMM:345:LEU:HD22	1:MMM:483:GLU:HA	2.01	0.42
1:YYY:72:GLU:HB3	1:YYY:80:VAL:HG11	2.01	0.42
1:MMM:312:TYR:CD2	2:MMM:604:HEC:HMC1	2.54	0.42
1:MMM:396:VAL:HG21	1:MMM:406:THR:HB	2.01	0.42
1:AAA:416:VAL:O	1:AAA:417:GLN:C	2.62	0.42
1:AAA:418:GLU:HA	1:AAA:422:SER:HB3	2.01	0.42
1:AAA:439:ILE:HG21	1:AAA:499:PHE:HA	2.00	0.42
1:AAA:309:HIS:HB3	1:AAA:372:GLU:HB2	2.02	0.42
1:MMM:301:SER:OG	1:MMM:387:GLN:HB3	2.19	0.42
1:MMM:387:GLN:OE1	1:MMM:389:HIS:HE1	2.02	0.42
2:MMM:604:HEC:HBC3	2:MMM:604:HEC:HMC3	2.01	0.42
1:YYY:98:GLN:H	1:YYY:98:GLN:CD	2.27	0.42
1:YYY:475:ASP:O	1:YYY:476:GLN:C	2.63	0.42
1:AAA:128:LYS:NZ	1:AAA:459:ASP:OD1	2.46	0.42
1:AAA:143:ARG:HD2	1:AAA:147:TYR:CD2	2.55	0.42
1:MMM:41:THR:CG2	1:MMM:74:LEU:HD21	2.50	0.42
1:YYY:82:PRO:HG2	2:YYY:601:HEC:CHB	2.50	0.42
1:YYY:215:LYS:HD3	1:YYY:220:LYS:O	2.20	0.42
1:YYY:152:GLN:O	1:YYY:158:PHE:HB2	2.20	0.42
1:YYY:287:PHE:O	1:YYY:290:PHE:N	2.39	0.42
1:AAA:98:GLN:HG2	2:AAA:605:HEC:C4A	2.50	0.41
1:MMM:225:ASP:HB2	5:MMM:718:HOH:O	2.20	0.41
1:MMM:353:PHE:CD1	1:MMM:353:PHE:C	2.98	0.41
1:YYY:68:ASP:O	1:YYY:69:LYS:HB2	2.20	0.41
1:AAA:43:TYR:OH	1:AAA:54:GLU:OE1	2.29	0.41
1:MMM:509:LEU:O	1:MMM:513:ILE:HG13	2.20	0.41
1:AAA:347:HIS:CD2	1:AAA:347:HIS:C	2.98	0.41
1:MMM:340:ASN:ND2	1:MMM:504:GLN:HE22	2.18	0.41
1:YYY:138:GLU:O	1:YYY:157:ARG:HD3	2.20	0.41
1:YYY:301:SER:O	1:YYY:305:CYS:SG	2.78	0.41
1:MMM:312:TYR:CE2	2:MMM:604:HEC:CMC	3.00	0.41
1:YYY:337:PRO:HB3	1:YYY:347:HIS:NE2	2.36	0.41
1:AAA:188:ASN:ND2	5:AAA:724:HOH:O	2.40	0.41
1:MMM:43:TYR:O	1:MMM:44:ALA:C	2.64	0.41
1:YYY:270:ALA:HA	1:YYY:278:GLY:C	2.46	0.41
1:YYY:407:HIS:HD2	2:YYY:605:HEC:C1C	2.33	0.41
1:YYY:416:VAL:HG11	1:YYY:433:LYS:HG3	2.01	0.41
1:AAA:319:GLN:OE1	1:AAA:332:ARG:NH2	2.47	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:MMM:464:ALA:O	1:MMM:469:VAL:HG13	2.21	0.41
1:MMM:490:TYR:O	1:MMM:493:ALA:HB3	2.20	0.41
1:YYY:208:SER:OG	1:YYY:242:GLY:N	2.50	0.41
1:AAA:201:THR:HG22	1:AAA:314:CYS:HB2	2.01	0.41
1:MMM:82:PRO:HG2	2:MMM:601:HEC:CMA	2.51	0.41
1:AAA:61:ILE:CG2	2:AAA:602:HEC:HMC1	2.51	0.41
1:AAA:312:TYR:CE2	2:AAA:604:HEC:HMC2	2.55	0.41
2:AAA:605:HEC:HBC3	2:AAA:606:HEC:HBB1	2.00	0.41
1:MMM:114:LYS:HB2	1:MMM:141:GLU:HG3	2.03	0.41
1:MMM:302:ARG:HA	1:MMM:388:CYS:SG	2.61	0.41
1:YYY:153:PHE:CZ	1:YYY:234:VAL:HG12	2.55	0.41
1:YYY:282:LEU:HD11	1:YYY:294:GLY:CA	2.51	0.41
1:AAA:244:ILE:HB	1:AAA:255:ARG:HH21	1.86	0.41
1:AAA:339:LYS:HB3	1:AAA:343:GLN:HB2	2.02	0.41
1:AAA:447:MET:HG3	1:AAA:509:LEU:CD1	2.50	0.41
1:MMM:98:GLN:HG2	2:MMM:605:HEC:C4A	2.50	0.41
1:MMM:387:GLN:OE1	1:MMM:389:HIS:CE1	2.74	0.41
1:AAA:149:VAL:HG12	1:AAA:153:PHE:CE2	2.56	0.40
1:AAA:253:GLN:CB	1:AAA:295:VAL:HG13	2.51	0.40
1:AAA:439:ILE:HG21	1:AAA:502:PRO:HG3	2.02	0.40
1:AAA:452:TYR:CE2	1:MMM:127:ASP:HB3	2.56	0.40
1:MMM:79:ASP:CA	5:MMM:907:HOH:O	2.68	0.40
1:YYY:246:CYS:HB3	1:YYY:304:MET:CE	2.50	0.40
1:AAA:66:CYS:HB2	2:AAA:602:HEC:C4C	2.51	0.40
1:AAA:369:GLN:HA	5:AAA:921:HOH:O	2.21	0.40
1:YYY:226:ARG:NE	1:YYY:328:PHE:O	2.49	0.40
1:YYY:321:THR:OG1	1:YYY:352:ASP:OD2	2.34	0.40
1:AAA:302:ARG:O	1:AAA:306:ALA:CB	2.69	0.40
1:YYY:82:PRO:HG2	2:YYY:601:HEC:C4A	2.51	0.40
1:YYY:99:TYR:OH	5:YYY:704:HOH:O	2.12	0.40
1:YYY:108:ASP:OD1	1:YYY:108:ASP:C	2.64	0.40
1:AAA:42:CYS:HB3	2:AAA:602:HEC:CMB	2.52	0.40
1:MMM:371:PRO:HD2	1:MMM:494:GLU:CA	2.51	0.40
1:MMM:396:VAL:HG23	1:MMM:404:TYR:CZ	2.55	0.40
1:YYY:98:GLN:NE2	2:YYY:605:HEC:O2A	2.41	0.40
1:AAA:58:HIS:CE1	2:AAA:603:HEC:NB	2.88	0.40
1:AAA:258:ARG:HD2	1:AAA:259:ASP:OD1	2.21	0.40
1:MMM:375:THR:O	1:MMM:501:ASN:HB2	2.21	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:AAA:1019:HOH:O	5:YYY:1013:HOH:O[2_546]	2.12	0.08

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	AAA	495/495 (100%)	459 (93%)	33 (7%)	3 (1%)	21	8
1	MMM	496/495 (100%)	453 (91%)	41 (8%)	2 (0%)	30	16
1	YYY	495/495 (100%)	448 (90%)	45 (9%)	2 (0%)	30	16
All	All	1486/1485 (100%)	1360 (92%)	119 (8%)	7 (0%)	24	12

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	AAA	138	GLU
1	AAA	241	VAL
1	AAA	282	LEU
1	YYY	475	ASP
1	MMM	241	VAL
1	YYY	401	GLY
1	MMM	471	PRO

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	AAA	416/414 (100%)	393 (94%)	23 (6%)	19 3
1	MMM	415/414 (100%)	390 (94%)	25 (6%)	17 3
1	YYY	416/414 (100%)	395 (95%)	21 (5%)	22 4
All	All	1247/1242 (100%)	1178 (94%)	69 (6%)	20 3

All (69) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AAA	41	THR
1	AAA	80	VAL
1	AAA	122	ARG
1	AAA	190	LYS
1	AAA	191	LEU
1	AAA	215	LYS
1	AAA	225	ASP
1	AAA	235[A]	LYS
1	AAA	235[B]	LYS
1	AAA	245	HIS
1	AAA	256	ILE
1	AAA	283[A]	LYS
1	AAA	283[B]	LYS
1	AAA	346	GLU
1	AAA	349	ARG
1	AAA	400	ASP
1	AAA	413	ILE
1	AAA	415	MET
1	AAA	417	GLN
1	AAA	489	GLU
1	AAA	514	SER
1	AAA	522	LEU
1	AAA	528	MET
1	MMM	85	LYS
1	MMM	108	ASP
1	MMM	159	GLN
1	MMM	191	LEU
1	MMM	240	PRO
1	MMM	267	LYS
1	MMM	286	ASP
1	MMM	293	ILE

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Mol	Chain	Res	Type
1	MMM	322	ASP
1	MMM	346	GLU
1	MMM	355	ASP
1	MMM	364	LYS
1	MMM	399	LYS
1	MMM	456	GLN
1	MMM	469	VAL
1	MMM	470	SER
1	MMM	472	THR
1	MMM	475	ASP
1	MMM	478	ARG
1	MMM	479	LEU
1	MMM	489	GLU
1	MMM	504	GLN
1	MMM	521	LYS
1	MMM	528	MET
1	MMM	531	LYS
1	YYY	39	ARG
1	YYY	47	THR
1	YYY	54	GLU
1	YYY	57	LYS
1	YYY	83	VAL
1	YYY	113	ARG
1	YYY	191	LEU
1	YYY	208	SER
1	YYY	223	LYS
1	YYY	283	LYS
1	YYY	298	LYS
1	YYY	304	MET
1	YYY	315	ASN
1	YYY	319	GLN
1	YYY	418	GLU
1	YYY	470	SER
1	YYY	475	ASP
1	YYY	489	GLU
1	YYY	507	GLN
1	YYY	521	LYS
1	YYY	530	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 31 ligands modelled in this entry, 3 are monoatomic - leaving 28 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	HEC	MMM	602	1	50,50,50	2.45	22 (44%)	68,82,82	3.04	33 (48%)
2	HEC	AAA	608	1	50,50,50	2.66	25 (50%)	68,82,82	2.29	23 (33%)
2	HEC	MMM	604	1,4	50,50,50	2.42	24 (48%)	68,82,82	2.96	27 (39%)
2	HEC	YYY	608	1	50,50,50	2.59	26 (52%)	68,82,82	2.14	21 (30%)
2	HEC	MMM	605	1	50,50,50	2.71	25 (50%)	68,82,82	2.72	27 (39%)
2	HEC	YYY	606	1	50,50,50	2.66	26 (52%)	68,82,82	2.69	31 (45%)
2	HEC	AAA	601	1	50,50,50	2.60	24 (48%)	68,82,82	3.14	38 (55%)
2	HEC	AAA	603	1	50,50,50	2.71	27 (54%)	68,82,82	2.58	28 (41%)
2	HEC	MMM	606	1	50,50,50	2.60	29 (58%)	68,82,82	2.90	33 (48%)
2	HEC	YYY	603	1	50,50,50	2.70	26 (52%)	68,82,82	2.51	26 (38%)
2	HEC	YYY	607	1	50,50,50	2.69	25 (50%)	68,82,82	2.78	29 (42%)
2	HEC	AAA	602	1	50,50,50	2.53	26 (52%)	68,82,82	2.65	36 (52%)
2	HEC	AAA	607[A]	-	50,50,50	2.51	21 (42%)	68,82,82	3.61	36 (52%)
2	HEC	YYY	602	1	50,50,50	2.43	23 (46%)	68,82,82	2.62	33 (48%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	HEC	YYY	604	1,4	50,50,50	2.48	22 (44%)	68,82,82	2.62	28 (41%)
4	PO4	MMM	610	2	4,4,4	1.76	2 (50%)	6,6,6	1.27	0
4	PO4	YYY	610	2	4,4,4	0.45	0	6,6,6	0.91	0
2	HEC	YYY	605	1	50,50,50	2.69	25 (50%)	68,82,82	2.57	28 (41%)
2	HEC	AAA	606	1	50,50,50	2.70	22 (44%)	68,82,82	2.82	36 (52%)
2	HEC	AAA	605	1	50,50,50	2.61	26 (52%)	68,82,82	2.43	28 (41%)
2	HEC	AAA	607[B]	-	50,50,50	2.50	21 (42%)	68,82,82	3.55	34 (50%)
2	HEC	MMM	603	1	50,50,50	2.59	21 (42%)	68,82,82	2.86	33 (48%)
2	HEC	AAA	604	1,4	50,50,50	2.48	27 (54%)	68,82,82	2.57	24 (35%)
2	HEC	MMM	607	1	50,50,50	2.67	22 (44%)	68,82,82	2.97	31 (45%)
2	HEC	YYY	601	1	50,50,50	2.54	25 (50%)	68,82,82	2.78	32 (47%)
2	HEC	MMM	608	1	50,50,50	2.53	21 (42%)	68,82,82	2.45	24 (35%)
2	HEC	MMM	601	1	50,50,50	2.55	27 (54%)	68,82,82	2.86	35 (51%)
4	PO4	AAA	610	2	4,4,4	1.94	2 (50%)	6,6,6	0.93	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	HEC	MMM	602	1	1/1/3/7	7/14/54/54	-
2	HEC	AAA	608	1	1/1/3/7	4/14/54/54	-
2	HEC	MMM	604	1,4	1/1/3/7	6/14/54/54	-
2	HEC	YYY	608	1	1/1/3/7	4/14/54/54	-
2	HEC	MMM	605	1	1/1/3/7	6/14/54/54	-
2	HEC	YYY	606	1	1/1/3/7	3/14/54/54	-
2	HEC	AAA	601	1	1/1/3/7	6/14/54/54	-
2	HEC	AAA	603	1	1/1/3/7	7/14/54/54	-
2	HEC	MMM	606	1	1/1/3/7	4/14/54/54	-
2	HEC	YYY	603	1	1/1/3/7	8/14/54/54	-
2	HEC	YYY	607	1	1/1/3/7	7/14/54/54	-
2	HEC	AAA	602	1	1/1/3/7	7/14/54/54	-
2	HEC	AAA	607[A]	-	1/1/3/7	8/14/54/54	-
2	HEC	YYY	602	1	1/1/3/7	8/14/54/54	-
2	HEC	YYY	604	1,4	1/1/3/7	5/14/54/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	HEC	YYY	605	1	1/1/3/7	4/14/54/54	-
2	HEC	AAA	606	1	1/1/3/7	3/14/54/54	-
2	HEC	AAA	605	1	1/1/3/7	4/14/54/54	-
2	HEC	AAA	607[B]	-	1/1/3/7	9/14/54/54	-
2	HEC	MMM	603	1	1/1/3/7	5/14/54/54	-
2	HEC	AAA	604	1,4	1/1/3/7	6/14/54/54	-
2	HEC	MMM	607	1	1/1/3/7	8/14/54/54	-
2	HEC	YYY	601	1	1/1/3/7	11/14/54/54	-
2	HEC	MMM	608	1	1/1/3/7	5/14/54/54	-
2	HEC	MMM	601	1	1/1/3/7	5/14/54/54	-

All (612) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	MMM	607	HEC	C4B-NB	-6.92	1.28	1.40
2	MMM	604	HEC	C4B-NB	-6.85	1.28	1.40
2	YYY	607	HEC	CHA-C1A	6.56	1.51	1.38
2	AAA	604	HEC	C4B-NB	-6.10	1.29	1.40
2	AAA	606	HEC	C1D-ND	-6.02	1.29	1.40
2	AAA	607[A]	HEC	C3D-C2D	5.96	1.49	1.36
2	AAA	607[B]	HEC	C3D-C2D	5.96	1.49	1.36
2	YYY	603	HEC	C3D-C2D	5.84	1.49	1.36
2	MMM	608	HEC	C3D-C2D	5.82	1.49	1.36
2	MMM	602	HEC	C1D-ND	-5.81	1.30	1.40
2	MMM	606	HEC	C1A-NA	-5.80	1.28	1.39
2	AAA	608	HEC	CHA-C1A	5.78	1.49	1.38
2	YYY	607	HEC	C4B-NB	-5.69	1.30	1.40
2	AAA	607[A]	HEC	C1C-NC	-5.65	1.28	1.39
2	AAA	607[B]	HEC	C1C-NC	-5.65	1.28	1.39
2	MMM	605	HEC	FE-ND	5.55	2.12	1.94
2	AAA	601	HEC	C4B-NB	-5.51	1.30	1.40
2	AAA	608	HEC	CHC-C4B	5.49	1.49	1.38
2	AAA	603	HEC	CHA-C1A	5.41	1.48	1.38
2	YYY	604	HEC	C3B-C2B	5.38	1.48	1.36
2	MMM	608	HEC	CHC-C4B	5.37	1.49	1.38
2	AAA	606	HEC	C1B-NB	-5.33	1.27	1.38
2	AAA	608	HEC	C3D-C2D	5.28	1.47	1.36
2	AAA	604	HEC	C1A-NA	-5.26	1.29	1.39
2	MMM	607	HEC	C1C-NC	-5.24	1.29	1.39
2	MMM	603	HEC	C3D-C2D	5.22	1.47	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	YYY	608	HEC	CHA-C1A	5.17	1.48	1.38
2	AAA	605	HEC	C4A-NA	-5.14	1.29	1.39
2	AAA	603	HEC	FE-ND	5.10	2.10	1.94
2	MMM	607	HEC	CHB-C4A	5.10	1.48	1.38
2	MMM	608	HEC	CHA-C4D	5.10	1.50	1.39
2	AAA	602	HEC	C1D-ND	-5.09	1.31	1.40
2	MMM	605	HEC	CHA-C1A	5.07	1.48	1.38
2	YYY	605	HEC	CHA-C1A	5.06	1.48	1.38
2	MMM	605	HEC	C4B-NB	-5.05	1.31	1.40
2	MMM	608	HEC	C4A-NA	-5.01	1.30	1.39
2	YYY	603	HEC	FE-NB	4.99	2.10	1.94
2	YYY	605	HEC	C2A-C3A	4.99	1.47	1.36
2	YYY	601	HEC	C3B-C2B	4.98	1.47	1.36
2	MMM	607	HEC	C4D-ND	-4.97	1.28	1.38
2	AAA	601	HEC	CHB-C4A	4.97	1.48	1.38
2	MMM	603	HEC	FE-NB	4.96	2.10	1.94
2	MMM	606	HEC	FE-ND	4.95	2.10	1.94
2	AAA	601	HEC	FE-NC	4.91	2.11	1.95
2	AAA	605	HEC	C1D-ND	-4.91	1.31	1.40
2	YYY	601	HEC	CHB-C4A	4.89	1.47	1.38
2	MMM	605	HEC	C3B-C2B	4.88	1.47	1.36
2	AAA	603	HEC	C3B-C2B	4.87	1.47	1.36
2	MMM	602	HEC	C4B-NB	-4.86	1.31	1.40
2	YYY	604	HEC	CHD-C1D	4.86	1.48	1.38
2	YYY	606	HEC	C1D-ND	-4.85	1.31	1.40
2	MMM	601	HEC	C3B-C2B	4.84	1.47	1.36
2	YYY	605	HEC	C4C-NC	-4.82	1.30	1.39
2	AAA	608	HEC	C1D-ND	-4.80	1.32	1.40
2	AAA	605	HEC	C2A-C3A	4.79	1.46	1.36
2	YYY	606	HEC	C1B-NB	-4.78	1.28	1.38
2	AAA	601	HEC	C2A-C3A	4.77	1.46	1.36
2	AAA	605	HEC	CHA-C1A	4.77	1.47	1.38
2	MMM	605	HEC	C4D-ND	-4.75	1.29	1.38
2	YYY	608	HEC	CHB-C1B	4.74	1.50	1.39
2	YYY	606	HEC	C3D-C2D	4.73	1.46	1.36
2	AAA	602	HEC	FE-NB	4.72	2.09	1.94
2	YYY	601	HEC	C3D-C2D	4.70	1.46	1.36
2	YYY	607	HEC	C1D-ND	-4.69	1.32	1.40
2	YYY	601	HEC	C2A-C3A	4.68	1.46	1.36
2	MMM	607	HEC	C3D-C2D	4.68	1.46	1.36
2	YYY	605	HEC	C3B-C2B	4.66	1.46	1.36
2	AAA	607[A]	HEC	C4B-NB	-4.65	1.32	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	AAA	607[B]	HEC	C4B-NB	-4.65	1.32	1.40
2	YYY	606	HEC	FE-NB	4.64	2.09	1.94
2	YYY	608	HEC	C2A-C3A	4.62	1.46	1.36
2	YYY	605	HEC	C3D-C2D	4.59	1.46	1.36
2	YYY	603	HEC	FE-ND	4.57	2.09	1.94
2	AAA	608	HEC	C4B-NB	-4.57	1.32	1.40
2	YYY	603	HEC	CHA-C1A	4.55	1.47	1.38
2	MMM	605	HEC	CHC-C4B	4.55	1.47	1.38
2	AAA	605	HEC	C3B-C2B	4.54	1.46	1.36
2	YYY	602	HEC	CHB-C4A	4.54	1.47	1.38
2	YYY	608	HEC	C3D-C2D	4.52	1.46	1.36
2	AAA	607[A]	HEC	C4A-NA	-4.50	1.31	1.39
2	AAA	607[B]	HEC	C4A-NA	-4.50	1.31	1.39
2	MMM	602	HEC	C1A-NA	-4.47	1.31	1.39
2	MMM	601	HEC	C2A-C3A	4.47	1.46	1.36
2	AAA	606	HEC	CHA-C1A	4.47	1.47	1.38
2	AAA	606	HEC	C2A-C3A	4.46	1.46	1.36
2	AAA	606	HEC	CHB-C4A	4.43	1.47	1.38
2	YYY	604	HEC	C4C-NC	-4.41	1.31	1.39
2	AAA	606	HEC	C1A-NA	-4.41	1.31	1.39
2	YYY	607	HEC	C4D-ND	-4.41	1.29	1.38
2	MMM	603	HEC	CHA-C1A	4.39	1.46	1.38
2	AAA	602	HEC	FE-ND	4.38	2.08	1.94
2	YYY	608	HEC	C4B-NB	-4.37	1.32	1.40
2	MMM	608	HEC	C4C-NC	-4.37	1.31	1.39
2	MMM	603	HEC	C1D-ND	-4.36	1.32	1.40
2	AAA	606	HEC	FE-ND	4.36	2.08	1.94
2	YYY	601	HEC	CHC-C4B	4.35	1.47	1.38
2	YYY	604	HEC	C3D-C2D	4.35	1.46	1.36
2	MMM	607	HEC	C1A-NA	-4.34	1.31	1.39
2	MMM	606	HEC	C4B-NB	-4.33	1.32	1.40
2	AAA	606	HEC	FE-NB	4.33	2.08	1.94
2	YYY	604	HEC	C4B-NB	-4.33	1.32	1.40
2	YYY	604	HEC	C2A-C3A	4.33	1.45	1.36
2	MMM	605	HEC	C2A-C3A	4.33	1.45	1.36
2	AAA	601	HEC	C3B-C2B	4.31	1.45	1.36
2	YYY	602	HEC	C1C-NC	-4.31	1.31	1.39
2	YYY	608	HEC	CHB-C4A	4.30	1.46	1.38
2	YYY	605	HEC	FE-ND	4.30	2.08	1.94
2	MMM	601	HEC	FE-NA	4.29	2.09	1.95
2	AAA	601	HEC	CHD-C1D	4.28	1.47	1.38
2	AAA	602	HEC	CHD-C4C	4.25	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	YYY	604	HEC	FE-ND	4.24	2.08	1.94
2	YYY	603	HEC	C3B-C2B	4.24	1.45	1.36
2	YYY	601	HEC	CHA-C1A	4.23	1.46	1.38
2	MMM	606	HEC	C1D-ND	-4.22	1.33	1.40
2	AAA	601	HEC	FE-NA	4.21	2.09	1.95
2	YYY	602	HEC	C4B-NB	-4.21	1.33	1.40
2	MMM	606	HEC	CHD-C1D	4.21	1.47	1.38
2	AAA	607[A]	HEC	CHD-C1D	4.21	1.47	1.38
2	AAA	607[B]	HEC	CHD-C1D	4.21	1.47	1.38
2	AAA	603	HEC	C4A-NA	-4.20	1.31	1.39
2	MMM	602	HEC	CHC-C4B	4.19	1.47	1.38
2	MMM	601	HEC	CHD-C1D	4.19	1.47	1.38
2	MMM	603	HEC	C4C-NC	-4.17	1.31	1.39
2	AAA	608	HEC	CHA-C4D	4.17	1.48	1.39
2	AAA	603	HEC	C3D-C2D	4.16	1.45	1.36
2	MMM	606	HEC	C1C-NC	-4.16	1.31	1.39
2	YYY	603	HEC	CHD-C1D	4.16	1.47	1.38
2	AAA	604	HEC	CHD-C1D	4.15	1.47	1.38
2	MMM	604	HEC	C2A-C3A	4.15	1.45	1.36
2	AAA	607[A]	HEC	C4C-NC	-4.15	1.31	1.39
2	AAA	607[B]	HEC	C4C-NC	-4.15	1.31	1.39
2	YYY	607	HEC	C2A-C3A	4.15	1.45	1.36
2	AAA	601	HEC	CHC-C4B	4.15	1.46	1.38
2	YYY	605	HEC	C4B-NB	-4.13	1.33	1.40
2	AAA	605	HEC	C1B-NB	-4.13	1.30	1.38
2	YYY	605	HEC	FE-NB	4.12	2.07	1.94
2	AAA	605	HEC	CHC-C1C	4.11	1.48	1.39
2	AAA	606	HEC	CHD-C4C	4.11	1.48	1.39
2	MMM	603	HEC	C3B-C2B	4.11	1.45	1.36
2	AAA	604	HEC	FE-NC	4.11	2.09	1.95
2	MMM	603	HEC	FE-ND	4.10	2.07	1.94
2	YYY	601	HEC	CHB-C1B	4.10	1.48	1.39
2	AAA	603	HEC	FE-NC	4.10	2.09	1.95
2	MMM	608	HEC	FE-NB	4.09	2.07	1.94
2	YYY	605	HEC	C1D-ND	-4.09	1.33	1.40
2	YYY	605	HEC	C4D-ND	-4.08	1.30	1.38
2	MMM	601	HEC	CHB-C4A	4.08	1.46	1.38
2	YYY	606	HEC	CHD-C1D	4.07	1.46	1.38
2	MMM	603	HEC	C4B-NB	-4.06	1.33	1.40
2	YYY	603	HEC	CHD-C4C	4.06	1.48	1.39
2	YYY	602	HEC	FE-NB	4.06	2.07	1.94
2	AAA	603	HEC	C4B-NB	-4.06	1.33	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	MMM	601	HEC	CHD-C4C	4.04	1.48	1.39
2	MMM	607	HEC	C2A-C3A	4.03	1.45	1.36
2	AAA	606	HEC	CHD-C1D	4.03	1.46	1.38
2	YYY	606	HEC	CHA-C4D	4.03	1.48	1.39
2	AAA	606	HEC	C4B-NB	-4.02	1.33	1.40
2	MMM	604	HEC	CHA-C1A	4.02	1.46	1.38
2	MMM	608	HEC	C3B-C2B	4.01	1.45	1.36
2	MMM	601	HEC	C3D-C2D	4.01	1.45	1.36
2	MMM	601	HEC	CHA-C1A	4.01	1.46	1.38
2	MMM	603	HEC	C1C-NC	-3.97	1.32	1.39
2	MMM	605	HEC	C3D-C2D	3.96	1.45	1.36
2	AAA	602	HEC	CHB-C4A	3.96	1.46	1.38
2	YYY	603	HEC	C4B-NB	-3.96	1.33	1.40
2	AAA	607[A]	HEC	C1A-NA	-3.95	1.32	1.39
2	AAA	607[B]	HEC	C1A-NA	-3.95	1.32	1.39
2	MMM	603	HEC	FE-NA	3.95	2.08	1.95
2	YYY	607	HEC	C4C-NC	-3.94	1.32	1.39
2	MMM	603	HEC	CHD-C1D	3.94	1.46	1.38
2	MMM	606	HEC	C4A-NA	-3.93	1.32	1.39
2	MMM	602	HEC	C3B-C2B	3.93	1.45	1.36
2	YYY	606	HEC	C4A-NA	-3.92	1.32	1.39
2	YYY	601	HEC	FE-NC	3.92	2.08	1.95
2	AAA	605	HEC	C3D-C2D	3.92	1.45	1.36
2	YYY	605	HEC	CHB-C4A	3.90	1.46	1.38
2	MMM	604	HEC	C3B-C2B	3.90	1.45	1.36
2	YYY	606	HEC	C1A-NA	-3.90	1.32	1.39
2	YYY	608	HEC	CHD-C4C	3.89	1.48	1.39
2	MMM	602	HEC	C3D-C2D	3.89	1.45	1.36
2	YYY	603	HEC	FE-NA	3.89	2.08	1.95
2	YYY	602	HEC	C3B-C2B	3.89	1.45	1.36
2	MMM	601	HEC	FE-NB	3.88	2.06	1.94
2	MMM	607	HEC	CHB-C1B	3.87	1.48	1.39
2	AAA	608	HEC	C1B-NB	-3.87	1.30	1.38
2	YYY	605	HEC	CHA-C4D	3.85	1.48	1.39
2	YYY	606	HEC	CHC-C4B	3.85	1.46	1.38
2	YYY	606	HEC	C3B-C2B	3.84	1.44	1.36
2	YYY	601	HEC	FE-NA	3.84	2.08	1.95
2	AAA	605	HEC	C4B-NB	-3.84	1.33	1.40
2	YYY	607	HEC	FE-NB	3.83	2.06	1.94
2	AAA	608	HEC	C4C-NC	-3.83	1.32	1.39
2	MMM	604	HEC	FE-ND	3.83	2.06	1.94
2	AAA	608	HEC	C4A-NA	-3.83	1.32	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	YYY	608	HEC	CHD-C1D	3.82	1.46	1.38
2	MMM	607	HEC	C1D-ND	-3.82	1.33	1.40
2	YYY	602	HEC	C3D-C2D	3.82	1.44	1.36
2	AAA	605	HEC	FE-NB	3.80	2.06	1.94
2	MMM	602	HEC	FE-NC	3.79	2.08	1.95
2	MMM	607	HEC	CHD-C1D	3.79	1.46	1.38
2	AAA	604	HEC	FE-NA	3.79	2.08	1.95
2	YYY	602	HEC	CHA-C1A	3.78	1.45	1.38
2	AAA	602	HEC	CHD-C1D	3.76	1.46	1.38
2	AAA	603	HEC	C3C-C2C	3.76	1.48	1.38
2	MMM	603	HEC	CHB-C4A	3.76	1.45	1.38
2	MMM	605	HEC	FE-NB	3.75	2.06	1.94
2	AAA	601	HEC	CHB-C1B	3.74	1.47	1.39
2	AAA	605	HEC	FE-NA	3.74	2.07	1.95
2	AAA	608	HEC	C3C-C2C	3.74	1.48	1.38
2	YYY	602	HEC	C1D-ND	-3.73	1.33	1.40
2	AAA	602	HEC	C1A-NA	-3.73	1.32	1.39
2	YYY	604	HEC	CHB-C4A	3.73	1.45	1.38
2	YYY	605	HEC	CHB-C1B	3.73	1.47	1.39
2	MMM	607	HEC	C3B-C2B	3.72	1.44	1.36
2	YYY	603	HEC	CHB-C4A	3.72	1.45	1.38
2	YYY	602	HEC	C2A-C3A	3.72	1.44	1.36
2	MMM	605	HEC	C1D-ND	-3.71	1.33	1.40
2	YYY	603	HEC	CHA-C4D	3.71	1.47	1.39
2	YYY	603	HEC	C2A-C3A	3.70	1.44	1.36
2	YYY	604	HEC	C4A-NA	-3.68	1.32	1.39
2	AAA	603	HEC	C2A-C3A	3.68	1.44	1.36
2	YYY	606	HEC	CHB-C1B	3.67	1.47	1.39
2	MMM	608	HEC	CHD-C4C	3.66	1.47	1.39
2	MMM	605	HEC	C1A-NA	-3.66	1.32	1.39
2	MMM	601	HEC	C1A-NA	-3.66	1.32	1.39
2	MMM	608	HEC	FE-ND	3.65	2.06	1.94
2	AAA	606	HEC	FE-NC	3.63	2.07	1.95
2	MMM	605	HEC	CHD-C1D	3.63	1.45	1.38
2	MMM	602	HEC	C4C-NC	-3.62	1.32	1.39
2	AAA	606	HEC	C3D-C2D	3.61	1.44	1.36
2	YYY	608	HEC	CHA-C4D	3.60	1.47	1.39
2	YYY	602	HEC	CHA-C4D	3.60	1.47	1.39
2	MMM	605	HEC	CHB-C4A	3.60	1.45	1.38
2	MMM	608	HEC	CHA-C1A	3.59	1.45	1.38
2	AAA	602	HEC	CHC-C4B	3.59	1.45	1.38
2	AAA	601	HEC	CHA-C1A	3.58	1.45	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	AAA	603	HEC	FE-NB	3.58	2.05	1.94
2	YYY	601	HEC	CHD-C1D	3.57	1.45	1.38
2	YYY	603	HEC	C1A-NA	-3.56	1.32	1.39
2	AAA	603	HEC	C1D-ND	-3.56	1.34	1.40
2	YYY	606	HEC	FE-NA	3.56	2.07	1.95
2	MMM	602	HEC	CHA-C1A	3.55	1.45	1.38
2	YYY	601	HEC	C4B-NB	-3.55	1.34	1.40
2	AAA	602	HEC	CHA-C1A	3.55	1.45	1.38
2	YYY	604	HEC	C1A-NA	-3.54	1.32	1.39
2	AAA	608	HEC	FE-NB	3.54	2.05	1.94
2	YYY	608	HEC	FE-NA	3.53	2.07	1.95
2	YYY	601	HEC	CHA-C4D	3.53	1.47	1.39
2	YYY	607	HEC	C1B-NB	-3.53	1.31	1.38
2	AAA	603	HEC	CHC-C1C	3.51	1.47	1.39
2	AAA	605	HEC	FE-ND	3.51	2.05	1.94
2	YYY	604	HEC	FE-NA	3.50	2.07	1.95
2	YYY	603	HEC	C1D-ND	-3.50	1.34	1.40
2	YYY	607	HEC	FE-NC	3.49	2.06	1.95
2	YYY	602	HEC	CHD-C4C	3.49	1.47	1.39
2	MMM	605	HEC	FE-NC	3.48	2.06	1.95
2	YYY	607	HEC	C3D-C2D	3.48	1.44	1.36
2	MMM	603	HEC	C2A-C3A	3.47	1.44	1.36
2	AAA	603	HEC	CHB-C4A	3.47	1.45	1.38
2	YYY	603	HEC	CHC-C4B	3.47	1.45	1.38
2	MMM	601	HEC	C3C-C2C	3.46	1.48	1.38
2	AAA	602	HEC	C4B-C3B	3.46	1.51	1.45
2	YYY	602	HEC	FE-NA	3.46	2.06	1.95
2	AAA	601	HEC	CHA-C4D	3.46	1.47	1.39
2	MMM	601	HEC	CHC-C4B	3.46	1.45	1.38
2	MMM	607	HEC	FE-NC	3.45	2.06	1.95
2	MMM	606	HEC	FE-NC	3.45	2.06	1.95
2	MMM	608	HEC	CHB-C1B	3.44	1.47	1.39
2	MMM	603	HEC	CHD-C4C	3.44	1.47	1.39
2	YYY	607	HEC	C1D-C2D	3.44	1.51	1.44
2	MMM	603	HEC	CHA-C4D	3.44	1.47	1.39
2	YYY	602	HEC	FE-ND	3.43	2.05	1.94
2	AAA	607[A]	HEC	C3B-C2B	3.43	1.44	1.36
2	AAA	607[B]	HEC	C3B-C2B	3.43	1.44	1.36
2	YYY	606	HEC	C4C-NC	-3.42	1.33	1.39
2	YYY	605	HEC	C1C-NC	-3.42	1.33	1.39
2	YYY	602	HEC	CHC-C4B	3.40	1.45	1.38
2	YYY	608	HEC	FE-NC	3.40	2.06	1.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	AAA	605	HEC	C4D-ND	-3.39	1.31	1.38
2	AAA	603	HEC	CHD-C1D	3.39	1.45	1.38
2	AAA	603	HEC	CHD-C4C	3.39	1.47	1.39
2	YYY	608	HEC	FE-ND	3.38	2.05	1.94
2	MMM	606	HEC	CHA-C1A	3.37	1.44	1.38
2	MMM	601	HEC	CHB-C1B	3.37	1.46	1.39
2	MMM	601	HEC	C4C-NC	-3.37	1.33	1.39
2	MMM	604	HEC	C4A-NA	-3.37	1.33	1.39
2	YYY	605	HEC	CHC-C4B	3.36	1.45	1.38
2	MMM	604	HEC	C1B-NB	-3.35	1.31	1.38
2	YYY	607	HEC	C3B-C2B	3.35	1.43	1.36
2	MMM	604	HEC	C1D-ND	-3.34	1.34	1.40
2	AAA	602	HEC	C2A-C3A	3.34	1.43	1.36
2	AAA	607[A]	HEC	FE-ND	3.34	2.05	1.94
2	AAA	607[B]	HEC	FE-ND	3.34	2.05	1.94
2	YYY	602	HEC	CHB-C1B	3.33	1.46	1.39
2	YYY	607	HEC	C1C-NC	-3.33	1.33	1.39
2	YYY	604	HEC	FE-NC	3.33	2.06	1.95
2	YYY	607	HEC	O2D-CGD	-3.33	1.19	1.30
2	AAA	601	HEC	C1C-NC	-3.33	1.33	1.39
2	MMM	606	HEC	C3D-C2D	3.31	1.43	1.36
2	MMM	601	HEC	FE-NC	3.31	2.06	1.95
2	YYY	603	HEC	C3C-C2C	3.31	1.47	1.38
2	YYY	606	HEC	C4B-NB	-3.31	1.34	1.40
2	AAA	604	HEC	C1B-C2B	3.30	1.51	1.44
2	AAA	606	HEC	C1B-C2B	3.30	1.50	1.44
2	AAA	603	HEC	FE-NA	3.30	2.06	1.95
2	YYY	604	HEC	CHD-C4C	3.30	1.46	1.39
2	MMM	606	HEC	CAD-C3D	-3.29	1.42	1.51
2	MMM	606	HEC	CAA-C2A	-3.29	1.42	1.51
2	AAA	604	HEC	C1D-ND	-3.29	1.34	1.40
2	YYY	606	HEC	C2A-C3A	3.29	1.43	1.36
2	MMM	603	HEC	C1A-NA	-3.28	1.33	1.39
2	MMM	602	HEC	CHB-C4A	3.27	1.44	1.38
2	MMM	606	HEC	C2A-C3A	3.26	1.43	1.36
2	AAA	601	HEC	C1B-NB	-3.25	1.32	1.38
2	MMM	604	HEC	FE-NC	3.25	2.06	1.95
2	MMM	604	HEC	C4C-NC	-3.25	1.33	1.39
2	MMM	605	HEC	CHB-C1B	3.24	1.46	1.39
2	AAA	602	HEC	CHC-C1C	3.24	1.46	1.39
2	AAA	607[A]	HEC	C1B-NB	-3.23	1.32	1.38
2	AAA	607[B]	HEC	C1B-NB	-3.23	1.32	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	MMM	604	HEC	CHD-C4C	3.23	1.46	1.39
2	YYY	606	HEC	O1A-CGA	3.23	1.32	1.22
2	MMM	606	HEC	CHD-C4C	3.23	1.46	1.39
2	YYY	608	HEC	C3C-C2C	3.22	1.47	1.38
2	AAA	603	HEC	CHA-C4D	3.22	1.46	1.39
2	AAA	601	HEC	C3D-C2D	3.22	1.43	1.36
2	MMM	606	HEC	CHB-C4A	3.21	1.44	1.38
2	MMM	602	HEC	C4B-C3B	3.21	1.50	1.45
2	AAA	607[A]	HEC	C3C-C2C	3.21	1.47	1.38
2	AAA	607[B]	HEC	C3C-C2C	3.21	1.47	1.38
2	AAA	606	HEC	C4D-ND	-3.20	1.32	1.38
2	AAA	604	HEC	CHB-C4A	3.19	1.44	1.38
2	YYY	608	HEC	C1D-ND	-3.19	1.34	1.40
2	MMM	604	HEC	FE-NA	3.19	2.05	1.95
2	YYY	608	HEC	C4C-NC	-3.19	1.33	1.39
2	YYY	607	HEC	CHD-C1D	3.18	1.45	1.38
2	YYY	607	HEC	C1A-NA	-3.18	1.33	1.39
2	MMM	602	HEC	CHD-C4C	3.18	1.46	1.39
2	AAA	608	HEC	CHB-C4A	3.18	1.44	1.38
2	AAA	604	HEC	C4D-C3D	3.16	1.50	1.45
2	AAA	602	HEC	C3C-C2C	3.15	1.47	1.38
2	AAA	601	HEC	C4A-C3A	3.15	1.51	1.45
2	AAA	602	HEC	C3D-C2D	3.14	1.43	1.36
2	AAA	607[A]	HEC	CHC-C1C	3.13	1.46	1.39
2	AAA	607[B]	HEC	CHC-C1C	3.13	1.46	1.39
2	AAA	606	HEC	C4A-NA	-3.13	1.33	1.39
2	YYY	607	HEC	FE-ND	3.13	2.04	1.94
2	MMM	607	HEC	FE-NA	3.13	2.05	1.95
2	MMM	602	HEC	FE-ND	3.12	2.04	1.94
2	YYY	603	HEC	FE-NC	3.12	2.05	1.95
2	AAA	602	HEC	C4C-NC	-3.10	1.33	1.39
2	AAA	605	HEC	C4C-NC	-3.10	1.33	1.39
2	AAA	602	HEC	C3B-C2B	3.10	1.43	1.36
2	AAA	607[A]	HEC	CHB-C1B	3.09	1.46	1.39
2	AAA	607[B]	HEC	CHB-C1B	3.09	1.46	1.39
2	YYY	601	HEC	C1C-NC	-3.08	1.33	1.39
2	MMM	602	HEC	FE-NB	3.08	2.04	1.94
2	YYY	603	HEC	C1D-C2D	3.08	1.50	1.44
2	YYY	605	HEC	C1A-C2A	3.07	1.50	1.45
2	AAA	604	HEC	C2A-C3A	3.07	1.43	1.36
2	AAA	608	HEC	CHD-C4C	3.04	1.46	1.39
2	AAA	603	HEC	CHC-C4B	3.03	1.44	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	MMM	602	HEC	C1C-NC	-3.02	1.33	1.39
2	YYY	607	HEC	C4A-NA	-3.02	1.33	1.39
2	AAA	602	HEC	C4B-NB	-3.02	1.35	1.40
2	AAA	602	HEC	C1C-NC	-3.02	1.33	1.39
2	AAA	604	HEC	C4D-ND	-3.00	1.32	1.38
2	MMM	604	HEC	CHC-C1C	3.00	1.46	1.39
2	AAA	608	HEC	FE-ND	3.00	2.04	1.94
2	AAA	603	HEC	C1A-NA	-2.99	1.34	1.39
2	AAA	608	HEC	FE-NA	2.99	2.05	1.95
2	MMM	608	HEC	CHC-C1C	2.98	1.46	1.39
2	MMM	601	HEC	FE-ND	2.98	2.04	1.94
2	AAA	604	HEC	CHD-C4C	2.98	1.46	1.39
2	MMM	606	HEC	C4D-C3D	2.98	1.50	1.45
2	YYY	601	HEC	CHC-C1C	2.98	1.46	1.39
2	YYY	604	HEC	CHC-C4B	2.98	1.44	1.38
2	AAA	603	HEC	C4D-C3D	2.97	1.50	1.45
2	AAA	604	HEC	C4A-NA	-2.97	1.34	1.39
2	MMM	605	HEC	C4C-NC	-2.97	1.34	1.39
2	AAA	601	HEC	C3C-C2C	2.96	1.46	1.38
2	YYY	606	HEC	FE-ND	2.95	2.04	1.94
2	MMM	603	HEC	C3C-C2C	2.95	1.46	1.38
2	AAA	604	HEC	FE-NB	2.95	2.04	1.94
2	YYY	602	HEC	CHD-C1D	2.94	1.44	1.38
2	YYY	605	HEC	CHD-C1D	2.94	1.44	1.38
2	YYY	608	HEC	C1C-NC	-2.93	1.34	1.39
2	YYY	604	HEC	CHA-C1A	2.92	1.44	1.38
2	AAA	603	HEC	CHB-C1B	2.92	1.45	1.39
2	YYY	603	HEC	C4A-NA	-2.91	1.34	1.39
4	AAA	610	PO4	P-O1	2.91	1.57	1.50
2	MMM	605	HEC	C1C-NC	-2.91	1.34	1.39
2	MMM	601	HEC	CHA-C4D	2.91	1.45	1.39
2	MMM	603	HEC	C4A-NA	-2.90	1.34	1.39
2	AAA	602	HEC	FE-NC	2.90	2.04	1.95
2	YYY	606	HEC	C4B-C3B	2.90	1.50	1.45
2	YYY	603	HEC	CHB-C1B	2.90	1.45	1.39
2	YYY	604	HEC	FE-NB	2.90	2.03	1.94
2	YYY	606	HEC	CHA-C1A	2.89	1.44	1.38
2	AAA	604	HEC	C1B-NB	-2.87	1.32	1.38
2	AAA	601	HEC	C1D-ND	-2.86	1.35	1.40
2	MMM	601	HEC	C1D-ND	-2.86	1.35	1.40
2	MMM	602	HEC	CHD-C1D	2.85	1.44	1.38
2	AAA	608	HEC	CHC-C1C	2.85	1.45	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	YYY	607	HEC	C1B-C2B	2.85	1.50	1.44
2	MMM	605	HEC	CHC-C1C	2.84	1.45	1.39
2	AAA	608	HEC	C2A-C3A	2.84	1.42	1.36
2	YYY	601	HEC	C4A-NA	-2.83	1.34	1.39
2	AAA	606	HEC	C4B-C3B	2.83	1.49	1.45
2	YYY	601	HEC	C4C-NC	-2.83	1.34	1.39
2	MMM	601	HEC	CHC-C1C	2.83	1.45	1.39
2	MMM	606	HEC	C3B-C2B	2.82	1.42	1.36
2	MMM	608	HEC	FE-NA	2.81	2.04	1.95
2	YYY	605	HEC	C4A-NA	-2.81	1.34	1.39
2	YYY	605	HEC	FE-NC	2.80	2.04	1.95
2	MMM	607	HEC	CHA-C1A	2.80	1.43	1.38
2	AAA	604	HEC	C1C-C2C	2.79	1.49	1.43
2	MMM	608	HEC	C1A-NA	-2.79	1.34	1.39
2	MMM	606	HEC	FE-NB	2.78	2.03	1.94
2	MMM	604	HEC	C1A-NA	-2.77	1.34	1.39
2	YYY	608	HEC	C4D-ND	-2.76	1.33	1.38
2	AAA	601	HEC	C4A-NA	-2.76	1.34	1.39
2	YYY	607	HEC	C1C-C2C	2.76	1.49	1.43
2	MMM	601	HEC	C1C-NC	-2.76	1.34	1.39
2	YYY	608	HEC	C4A-NA	-2.75	1.34	1.39
2	YYY	605	HEC	FE-NA	2.75	2.04	1.95
2	AAA	608	HEC	C3B-C2B	2.75	1.42	1.36
2	MMM	605	HEC	FE-NA	2.74	2.04	1.95
2	YYY	608	HEC	C1C-C2C	2.74	1.49	1.43
2	AAA	605	HEC	CHA-C4D	2.74	1.45	1.39
2	YYY	605	HEC	C1A-NA	-2.73	1.34	1.39
2	MMM	608	HEC	C2A-C3A	2.73	1.42	1.36
2	YYY	603	HEC	CHC-C1C	2.73	1.45	1.39
2	MMM	604	HEC	CHA-C4D	2.72	1.45	1.39
2	MMM	605	HEC	CHD-C4C	2.72	1.45	1.39
2	YYY	608	HEC	C1B-NB	-2.72	1.33	1.38
2	AAA	608	HEC	C1A-NA	-2.72	1.34	1.39
2	MMM	604	HEC	O1D-CGD	2.71	1.31	1.22
2	AAA	605	HEC	CHD-C4C	2.71	1.45	1.39
2	AAA	605	HEC	CHD-C1D	2.71	1.44	1.38
2	YYY	607	HEC	CHA-C4D	2.71	1.45	1.39
2	YYY	606	HEC	CBA-CGA	2.71	1.56	1.50
2	YYY	601	HEC	FE-NB	2.71	2.03	1.94
2	AAA	606	HEC	C3B-C2B	2.71	1.42	1.36
2	MMM	604	HEC	C4D-ND	-2.70	1.33	1.38
2	AAA	607[A]	HEC	FE-NB	2.69	2.03	1.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	AAA	607[B]	HEC	FE-NB	2.69	2.03	1.94
2	YYY	604	HEC	CHC-C1C	2.69	1.45	1.39
2	MMM	607	HEC	C4C-NC	-2.69	1.34	1.39
2	MMM	601	HEC	C4A-NA	-2.68	1.34	1.39
2	YYY	607	HEC	CHC-C1C	2.68	1.45	1.39
2	AAA	602	HEC	C4D-ND	-2.67	1.33	1.38
2	MMM	607	HEC	C1B-C2B	2.66	1.49	1.44
2	MMM	606	HEC	FE-NA	2.66	2.04	1.95
2	YYY	601	HEC	C3C-C2C	2.66	1.45	1.38
2	YYY	606	HEC	C4C-C3C	2.66	1.49	1.44
2	AAA	601	HEC	CHC-C1C	2.65	1.45	1.39
2	MMM	606	HEC	CHB-C1B	2.65	1.45	1.39
2	AAA	605	HEC	CHB-C1B	2.64	1.45	1.39
2	MMM	606	HEC	C1B-NB	-2.63	1.33	1.38
2	AAA	606	HEC	C3C-C2C	2.63	1.45	1.38
2	MMM	604	HEC	CHB-C4A	2.63	1.43	1.38
2	MMM	604	HEC	FE-NB	2.62	2.03	1.94
2	AAA	605	HEC	CHB-C4A	2.62	1.43	1.38
2	YYY	607	HEC	C3C-C2C	2.61	1.45	1.38
2	AAA	608	HEC	FE-NC	2.60	2.03	1.95
2	AAA	603	HEC	C1C-NC	-2.60	1.34	1.39
2	AAA	603	HEC	O2A-CGA	-2.59	1.22	1.30
2	YYY	602	HEC	C3C-C2C	2.59	1.45	1.38
2	YYY	606	HEC	CHD-C4C	2.59	1.45	1.39
2	MMM	607	HEC	C1B-NB	-2.58	1.33	1.38
2	MMM	606	HEC	C1C-C2C	2.57	1.49	1.43
2	AAA	606	HEC	CHA-C4D	2.57	1.45	1.39
2	MMM	606	HEC	CHA-C4D	2.57	1.45	1.39
2	YYY	602	HEC	C1B-NB	-2.57	1.33	1.38
2	AAA	604	HEC	C1D-C2D	2.56	1.49	1.44
2	AAA	607[A]	HEC	CHA-C1A	2.56	1.43	1.38
2	AAA	607[B]	HEC	CHA-C1A	2.56	1.43	1.38
2	MMM	605	HEC	C3C-C2C	2.55	1.45	1.38
2	MMM	604	HEC	CHD-C1D	2.55	1.43	1.38
2	YYY	601	HEC	C4D-ND	-2.54	1.33	1.38
2	MMM	602	HEC	C2A-C3A	2.54	1.42	1.36
2	AAA	604	HEC	FE-ND	2.54	2.02	1.94
2	MMM	603	HEC	FE-NC	2.54	2.03	1.95
4	AAA	610	PO4	P-O4	-2.54	1.47	1.54
2	AAA	607[A]	HEC	FE-NC	2.53	2.03	1.95
2	AAA	607[B]	HEC	FE-NC	2.53	2.03	1.95
2	AAA	605	HEC	FE-NC	2.53	2.03	1.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	YYY	606	HEC	C1C-NC	-2.52	1.34	1.39
2	AAA	608	HEC	CHD-C1D	2.52	1.43	1.38
2	AAA	605	HEC	C3C-C2C	2.52	1.45	1.38
2	MMM	606	HEC	C4C-NC	-2.51	1.34	1.39
2	YYY	608	HEC	CHC-C1C	2.51	1.45	1.39
2	AAA	603	HEC	C1D-C2D	2.50	1.49	1.44
2	AAA	607[A]	HEC	CHA-C4D	2.50	1.44	1.39
2	AAA	607[B]	HEC	CHA-C4D	2.50	1.44	1.39
2	YYY	604	HEC	C3C-C2C	2.49	1.45	1.38
2	YYY	608	HEC	C4D-C3D	2.49	1.49	1.45
2	YYY	601	HEC	C1D-ND	-2.48	1.36	1.40
2	YYY	603	HEC	C1B-C2B	2.48	1.49	1.44
2	AAA	607[A]	HEC	C2A-C3A	2.48	1.42	1.36
2	AAA	607[B]	HEC	C2A-C3A	2.48	1.42	1.36
2	MMM	606	HEC	C4D-ND	-2.48	1.33	1.38
2	YYY	607	HEC	CHD-C4C	2.47	1.44	1.39
2	MMM	601	HEC	C1D-C2D	2.46	1.49	1.44
2	AAA	601	HEC	FE-NB	2.45	2.02	1.94
2	AAA	606	HEC	C1C-C2C	2.45	1.49	1.43
2	MMM	602	HEC	CHC-C1C	2.45	1.44	1.39
2	MMM	608	HEC	C4B-NB	-2.45	1.36	1.40
2	AAA	605	HEC	C1C-NC	-2.44	1.35	1.39
2	MMM	603	HEC	C4D-ND	-2.44	1.33	1.38
2	MMM	606	HEC	CBA-CAA	2.44	1.59	1.52
2	AAA	604	HEC	C3C-C2C	2.44	1.45	1.38
2	YYY	602	HEC	C1A-C2A	2.43	1.49	1.45
2	MMM	604	HEC	C3D-C2D	2.41	1.41	1.36
2	YYY	603	HEC	C1C-NC	-2.41	1.35	1.39
2	MMM	602	HEC	FE-NA	2.40	2.03	1.95
2	YYY	601	HEC	FE-ND	2.40	2.02	1.94
2	MMM	607	HEC	C4D-C3D	2.40	1.49	1.45
4	MMM	610	PO4	P-O3	2.40	1.61	1.54
2	AAA	604	HEC	CHC-C1C	2.40	1.44	1.39
2	YYY	605	HEC	C1B-NB	-2.39	1.33	1.38
2	AAA	601	HEC	C4D-ND	-2.38	1.33	1.38
2	MMM	602	HEC	C4D-ND	-2.38	1.33	1.38
2	AAA	602	HEC	C1B-NB	-2.37	1.33	1.38
2	MMM	604	HEC	C1B-C2B	2.37	1.49	1.44
2	AAA	604	HEC	CAA-C2A	-2.37	1.45	1.51
2	AAA	604	HEC	C3D-C2D	2.36	1.41	1.36
2	AAA	605	HEC	O2D-CGD	-2.36	1.22	1.30
2	AAA	602	HEC	CMC-C2C	-2.35	1.45	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	MMM	607	HEC	CMB-C2B	-2.34	1.45	1.50
2	YYY	601	HEC	C1C-C2C	2.34	1.48	1.43
2	YYY	603	HEC	C4D-ND	-2.33	1.34	1.38
2	YYY	605	HEC	O2A-CGA	-2.33	1.22	1.30
2	YYY	602	HEC	FE-NC	2.33	2.03	1.95
2	YYY	603	HEC	C4D-C3D	2.32	1.49	1.45
2	YYY	608	HEC	C3B-C2B	2.31	1.41	1.36
2	MMM	608	HEC	CHD-C1D	2.31	1.43	1.38
2	AAA	606	HEC	CAA-C2A	-2.31	1.45	1.51
2	AAA	608	HEC	C4D-ND	-2.31	1.34	1.38
2	AAA	603	HEC	C1B-NB	-2.29	1.34	1.38
2	YYY	608	HEC	FE-NB	2.28	2.01	1.94
2	AAA	607[A]	HEC	C1D-ND	-2.28	1.36	1.40
2	AAA	607[B]	HEC	C1D-ND	-2.28	1.36	1.40
2	YYY	601	HEC	C1A-NA	-2.28	1.35	1.39
2	AAA	601	HEC	C4B-C3B	-2.28	1.41	1.45
2	YYY	604	HEC	CBD-CGD	2.27	1.55	1.50
2	AAA	602	HEC	O1D-CGD	2.27	1.29	1.22
2	YYY	602	HEC	CHC-C1C	2.27	1.44	1.39
2	YYY	604	HEC	CHA-C4D	2.26	1.44	1.39
2	YYY	602	HEC	C1B-C2B	2.26	1.48	1.44
4	MMM	610	PO4	P-O2	-2.25	1.47	1.54
2	MMM	603	HEC	CHB-C1B	2.24	1.44	1.39
2	MMM	607	HEC	FE-ND	2.24	2.01	1.94
2	AAA	602	HEC	C1A-C2A	-2.24	1.41	1.45
2	YYY	606	HEC	CBA-CAA	2.23	1.59	1.52
2	MMM	605	HEC	CHA-C4D	2.23	1.44	1.39
2	MMM	608	HEC	CHB-C4A	2.23	1.42	1.38
2	AAA	604	HEC	O2D-CGD	-2.23	1.23	1.30
2	AAA	607[A]	HEC	CHB-C4A	2.22	1.42	1.38
2	AAA	607[B]	HEC	CHB-C4A	2.22	1.42	1.38
2	AAA	601	HEC	C1A-C2A	2.22	1.49	1.45
2	MMM	608	HEC	C1D-ND	-2.22	1.36	1.40
2	YYY	601	HEC	C4A-C3A	2.22	1.49	1.45
2	AAA	604	HEC	CHA-C1A	2.21	1.42	1.38
2	YYY	604	HEC	O1D-CGD	2.21	1.29	1.22
2	YYY	604	HEC	C1B-C2B	2.21	1.48	1.44
2	AAA	608	HEC	C1D-C2D	2.21	1.48	1.44
2	MMM	601	HEC	C4D-ND	-2.20	1.34	1.38
2	YYY	606	HEC	O2D-CGD	-2.20	1.23	1.30
2	AAA	602	HEC	CHA-C4D	2.20	1.44	1.39
2	AAA	603	HEC	C4D-ND	-2.20	1.34	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	YYY	607	HEC	CAA-C2A	-2.19	1.45	1.51
2	MMM	605	HEC	C4D-C3D	2.19	1.48	1.45
2	AAA	604	HEC	CBA-CGA	2.18	1.55	1.50
2	YYY	608	HEC	C1A-NA	-2.18	1.35	1.39
2	AAA	605	HEC	CHC-C4B	2.18	1.42	1.38
2	MMM	604	HEC	C1C-C2C	2.17	1.48	1.43
2	MMM	607	HEC	C4A-NA	-2.16	1.35	1.39
2	MMM	604	HEC	C3C-C2C	2.16	1.44	1.38
2	MMM	606	HEC	C3C-C2C	2.16	1.44	1.38
2	AAA	605	HEC	C1A-C2A	2.16	1.49	1.45
2	YYY	608	HEC	CHC-C4B	2.16	1.42	1.38
2	AAA	601	HEC	C1C-C2C	2.16	1.48	1.43
2	AAA	602	HEC	C1B-C2B	2.15	1.48	1.44
2	MMM	601	HEC	C4C-C3C	2.15	1.48	1.44
2	MMM	606	HEC	O2D-CGD	-2.14	1.23	1.30
2	MMM	601	HEC	C1B-C2B	2.14	1.48	1.44
2	MMM	606	HEC	CMB-C2B	-2.14	1.46	1.50
2	MMM	608	HEC	C1B-NB	-2.13	1.34	1.38
2	MMM	601	HEC	C4A-C3A	2.12	1.49	1.45
2	AAA	608	HEC	CMB-C2B	-2.12	1.46	1.50
2	AAA	607[A]	HEC	CMA-C3A	2.11	1.55	1.50
2	AAA	607[B]	HEC	CMA-C3A	2.11	1.55	1.50
2	YYY	605	HEC	C1B-C2B	2.11	1.48	1.44
2	MMM	607	HEC	O1D-CGD	2.10	1.29	1.22
2	MMM	608	HEC	C3C-C2C	2.09	1.44	1.38
2	YYY	605	HEC	CHD-C4C	2.09	1.44	1.39
2	MMM	602	HEC	CHA-C4D	2.09	1.44	1.39
2	MMM	605	HEC	C1B-C2B	2.09	1.48	1.44
2	MMM	605	HEC	C1B-NB	-2.09	1.34	1.38
2	YYY	603	HEC	C4C-NC	-2.09	1.35	1.39
2	MMM	602	HEC	C3C-C2C	2.08	1.44	1.38
2	YYY	606	HEC	C1B-C2B	2.08	1.48	1.44
2	AAA	603	HEC	O2D-CGD	-2.07	1.23	1.30
2	YYY	601	HEC	C1A-C2A	2.07	1.48	1.45
2	AAA	605	HEC	CBD-CGD	2.06	1.55	1.50
2	YYY	602	HEC	C4B-C3B	2.05	1.48	1.45
2	AAA	604	HEC	CHA-C4D	2.05	1.43	1.39
2	AAA	604	HEC	CHB-C1B	2.04	1.43	1.39
2	AAA	608	HEC	C1C-C2C	2.00	1.48	1.43
2	MMM	601	HEC	C4B-NB	-2.00	1.36	1.40

All (754) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	AAA	607[A]	HEC	C3D-C4D-ND	11.53	121.52	110.36
2	AAA	607[B]	HEC	C3D-C4D-ND	11.53	121.52	110.36
2	MMM	601	HEC	CAA-CBA-CGA	-8.53	95.26	113.60
2	MMM	603	HEC	C1B-C2B-C3B	-8.32	98.21	106.96
2	MMM	603	HEC	C1C-C2C-C3C	-8.22	97.22	106.83
2	MMM	602	HEC	C2A-C1A-NA	8.11	118.22	110.32
2	AAA	607[A]	HEC	CHB-C1B-NB	-7.99	115.74	124.42
2	AAA	607[B]	HEC	CHB-C1B-NB	-7.99	115.74	124.42
2	MMM	606	HEC	CAB-C3B-C4B	7.94	135.11	124.81
2	AAA	601	HEC	C2A-C1A-NA	7.88	117.99	110.32
2	MMM	607	HEC	C3D-C4D-ND	7.86	117.97	110.36
2	MMM	605	HEC	C3D-C4D-ND	7.73	117.84	110.36
2	YYY	602	HEC	C2A-C1A-NA	7.70	117.82	110.32
2	YYY	606	HEC	CAB-C3B-C4B	7.52	134.57	124.81
2	AAA	607[A]	HEC	C3B-C4B-NB	7.48	118.49	110.17
2	AAA	607[B]	HEC	C3B-C4B-NB	7.48	118.49	110.17
2	MMM	603	HEC	C2B-C1B-NB	7.43	118.78	109.88
2	MMM	607	HEC	C2A-C1A-NA	7.38	117.51	110.32
2	MMM	604	HEC	C1C-C2C-C3C	-7.38	98.20	106.83
2	MMM	604	HEC	C1B-C2B-C3B	-7.32	99.26	106.96
2	MMM	604	HEC	C2A-C1A-NA	7.23	117.36	110.32
2	AAA	601	HEC	C3C-C4C-NC	7.16	118.16	110.15
2	MMM	606	HEC	C2D-C1D-ND	7.14	118.30	109.84
2	YYY	604	HEC	C1B-C2B-C3B	-7.09	99.51	106.96
2	MMM	602	HEC	C4A-NA-C1A	-7.04	98.46	105.35
2	YYY	601	HEC	C2A-C1A-NA	7.03	117.16	110.32
2	AAA	602	HEC	C2B-C1B-NB	6.98	118.24	109.88
2	AAA	608	HEC	CBA-CAA-C2A	-6.96	93.29	112.63
2	YYY	601	HEC	C2D-C1D-ND	6.96	118.09	109.84
2	YYY	607	HEC	C3C-C4C-NC	6.94	117.90	110.15
2	AAA	607[A]	HEC	C2B-C1B-NB	6.89	118.14	109.88
2	AAA	607[B]	HEC	C2B-C1B-NB	6.89	118.14	109.88
2	MMM	605	HEC	C2D-C1D-ND	6.85	117.95	109.84
2	AAA	601	HEC	CAD-CBD-CGD	-6.83	98.90	113.60
2	MMM	606	HEC	C1C-C2C-C3C	-6.80	98.88	106.83
2	YYY	607	HEC	C1B-C2B-C3B	-6.78	99.83	106.96
2	YYY	608	HEC	C1C-C2C-C3C	-6.76	98.93	106.83
2	MMM	608	HEC	C1B-C2B-C3B	-6.64	99.98	106.96
2	MMM	605	HEC	C1B-C2B-C3B	-6.56	100.06	106.96
2	AAA	607[A]	HEC	C1B-C2B-C3B	-6.56	100.06	106.96
2	AAA	607[B]	HEC	C1B-C2B-C3B	-6.56	100.06	106.96
2	YYY	607	HEC	C3D-C4D-ND	6.52	116.67	110.36
2	YYY	605	HEC	C1B-C2B-C3B	-6.44	100.18	106.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	MMM	608	HEC	C2B-C1B-NB	6.44	117.59	109.88
2	MMM	606	HEC	C2B-C1B-NB	6.35	117.49	109.88
2	YYY	601	HEC	C3D-C4D-ND	6.33	116.49	110.36
2	YYY	605	HEC	C3D-C4D-ND	6.31	116.47	110.36
2	AAA	606	HEC	C1C-C2C-C3C	-6.31	99.45	106.83
2	MMM	605	HEC	C1D-C2D-C3D	-6.28	100.36	106.96
2	MMM	602	HEC	CHA-C4D-C3D	-6.24	115.67	124.84
2	YYY	606	HEC	C2B-C1B-NB	6.24	117.36	109.88
2	AAA	607[A]	HEC	C2D-C1D-ND	6.22	117.21	109.84
2	AAA	607[B]	HEC	C2D-C1D-ND	6.22	117.21	109.84
2	YYY	605	HEC	C1D-C2D-C3D	-6.20	100.44	106.96
2	YYY	608	HEC	CBA-CAA-C2A	-6.19	95.43	112.63
2	AAA	603	HEC	CAD-C3D-C4D	6.16	135.43	124.66
2	YYY	603	HEC	C1B-C2B-C3B	-6.14	100.50	106.96
2	YYY	606	HEC	C2A-C1A-NA	6.12	116.28	110.32
2	AAA	606	HEC	C2C-C1C-NC	6.12	119.39	110.08
2	MMM	608	HEC	CBA-CAA-C2A	-6.11	95.64	112.63
2	AAA	601	HEC	C1B-C2B-C3B	-6.10	100.54	106.96
2	AAA	604	HEC	C1C-C2C-C3C	-6.06	99.74	106.83
2	YYY	601	HEC	C1D-C2D-C3D	-6.05	100.60	106.96
2	AAA	604	HEC	CMC-C2C-C1C	6.03	134.55	125.37
2	AAA	607[A]	HEC	C1D-ND-C4D	-6.00	98.87	105.07
2	AAA	607[B]	HEC	C1D-ND-C4D	-6.00	98.87	105.07
2	MMM	602	HEC	C1B-C2B-C3B	-6.00	100.64	106.96
2	YYY	604	HEC	C2B-C1B-NB	5.99	117.06	109.88
2	MMM	604	HEC	C2C-C1C-NC	5.93	119.11	110.08
2	MMM	602	HEC	CMA-C3A-C4A	5.90	135.12	124.71
2	AAA	607[A]	HEC	CHD-C1D-ND	-5.89	117.11	124.37
2	AAA	607[B]	HEC	CHD-C1D-ND	-5.89	117.11	124.37
2	MMM	605	HEC	CMC-C2C-C1C	5.86	134.30	125.37
2	MMM	607	HEC	C1C-C2C-C3C	-5.86	99.98	106.83
2	AAA	607[A]	HEC	C4D-C3D-C2D	-5.84	98.38	106.90
2	AAA	607[B]	HEC	C4D-C3D-C2D	-5.84	98.38	106.90
2	YYY	604	HEC	C3D-C4D-ND	5.83	116.00	110.36
2	AAA	603	HEC	C3D-C4D-ND	5.82	115.99	110.36
2	AAA	603	HEC	C1B-C2B-C3B	-5.79	100.87	106.96
2	YYY	601	HEC	C1A-C2A-C3A	-5.77	99.60	107.13
2	YYY	604	HEC	C1C-C2C-C3C	-5.77	100.08	106.83
2	AAA	606	HEC	CAA-C2A-C1A	5.76	135.75	124.89
2	MMM	606	HEC	CMC-C2C-C3C	5.72	137.98	125.61
2	YYY	603	HEC	C2A-C1A-NA	5.72	115.89	110.32
2	MMM	604	HEC	CHB-C4A-NA	-5.67	118.30	124.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	YYY	605	HEC	C2D-C1D-ND	5.65	116.53	109.84
2	MMM	604	HEC	C4A-NA-C1A	-5.61	99.85	105.35
2	MMM	602	HEC	CHA-C1A-NA	-5.60	118.38	124.44
2	AAA	603	HEC	C2D-C1D-ND	5.59	116.46	109.84
2	AAA	601	HEC	C1A-C2A-C3A	-5.58	99.86	107.13
2	AAA	606	HEC	C4C-NC-C1C	-5.51	99.95	105.35
2	MMM	608	HEC	CMD-C2D-C1D	5.48	133.39	125.04
2	MMM	605	HEC	C1C-C2C-C3C	-5.47	100.43	106.83
2	MMM	604	HEC	CMC-C2C-C1C	5.46	133.68	125.37
2	MMM	607	HEC	CHB-C4A-NA	-5.45	118.55	124.44
2	MMM	602	HEC	C2B-C1B-NB	5.45	116.41	109.88
2	YYY	602	HEC	C4A-NA-C1A	-5.44	100.03	105.35
2	MMM	607	HEC	C2C-C1C-NC	5.44	118.36	110.08
2	MMM	601	HEC	C3D-C4D-ND	5.41	115.59	110.36
2	YYY	607	HEC	C4A-C3A-C2A	-5.40	99.05	106.94
2	YYY	602	HEC	C1C-C2C-C3C	-5.38	100.54	106.83
2	MMM	601	HEC	C2A-C1A-NA	5.35	115.53	110.32
2	AAA	602	HEC	C1B-C2B-C3B	-5.34	101.34	106.96
2	YYY	606	HEC	C2D-C1D-ND	5.34	116.17	109.84
2	YYY	601	HEC	C1C-C2C-C3C	-5.32	100.60	106.83
2	AAA	608	HEC	C1C-C2C-C3C	-5.31	100.62	106.83
2	YYY	603	HEC	C2B-C1B-NB	5.30	116.23	109.88
2	YYY	606	HEC	C1B-C2B-C3B	-5.29	101.39	106.96
2	MMM	601	HEC	C1C-C2C-C3C	-5.29	100.64	106.83
2	AAA	606	HEC	C2A-C1A-NA	5.27	115.45	110.32
2	MMM	601	HEC	C3B-C4B-NB	5.26	116.02	110.17
2	AAA	607[A]	HEC	CHA-C4D-ND	-5.24	118.72	124.42
2	AAA	607[B]	HEC	CHA-C4D-ND	-5.24	118.72	124.42
2	YYY	603	HEC	C1C-C2C-C3C	-5.21	100.74	106.83
2	MMM	601	HEC	CMD-C2D-C1D	5.21	132.97	125.04
2	MMM	602	HEC	C3D-C4D-ND	5.19	115.38	110.36
2	YYY	604	HEC	C3B-C4B-NB	5.17	115.92	110.17
2	YYY	605	HEC	C2B-C1B-NB	5.14	116.04	109.88
2	AAA	601	HEC	CBC-CAC-C3C	5.14	126.60	112.43
2	AAA	604	HEC	C4A-C3A-C2A	-5.13	99.45	106.94
2	MMM	608	HEC	C1D-C2D-C3D	-5.12	101.58	106.96
2	YYY	606	HEC	C1D-C2D-C3D	-5.10	101.60	106.96
2	AAA	604	HEC	CMD-C2D-C1D	5.06	132.75	125.04
2	AAA	602	HEC	C2D-C1D-ND	5.06	115.83	109.84
2	AAA	605	HEC	CAC-C3C-C4C	5.06	131.93	124.92
2	MMM	601	HEC	C2B-C1B-NB	5.05	115.93	109.88
2	MMM	607	HEC	C1B-C2B-C3B	-5.04	101.65	106.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	AAA	601	HEC	CAC-C3C-C4C	5.02	131.88	124.92
2	YYY	602	HEC	CAA-C2A-C1A	4.97	134.26	124.89
2	AAA	607[A]	HEC	CHC-C4B-NB	-4.92	118.30	124.37
2	AAA	607[B]	HEC	CHC-C4B-NB	-4.92	118.30	124.37
2	AAA	604	HEC	C2C-C1C-NC	4.92	117.56	110.08
2	MMM	604	HEC	C3A-C4A-NA	4.90	118.73	109.69
2	MMM	602	HEC	C4A-C3A-C2A	-4.90	99.78	106.94
2	MMM	607	HEC	C4D-C3D-C2D	-4.87	99.80	106.90
2	AAA	607[A]	HEC	C4B-NB-C1B	-4.85	100.07	105.07
2	AAA	607[B]	HEC	C4B-NB-C1B	-4.85	100.07	105.07
2	AAA	603	HEC	CAA-CBA-CGA	-4.84	103.19	113.60
2	MMM	604	HEC	C4C-NC-C1C	-4.83	100.62	105.35
2	YYY	602	HEC	C2C-C1C-NC	4.81	117.40	110.08
2	MMM	606	HEC	C1B-C2B-C3B	-4.80	101.91	106.96
2	YYY	603	HEC	C3D-C4D-ND	4.80	115.01	110.36
2	AAA	604	HEC	C1B-C2B-C3B	-4.76	101.95	106.96
2	MMM	607	HEC	CHA-C4D-C3D	-4.74	117.87	124.84
2	AAA	604	HEC	C3C-C4C-NC	4.74	115.44	110.15
2	AAA	605	HEC	C3A-C4A-NA	4.73	118.42	109.69
2	AAA	601	HEC	C2D-C1D-ND	4.73	115.45	109.84
2	MMM	607	HEC	CBD-CAD-C3D	4.71	125.73	112.63
2	AAA	608	HEC	CAB-C3B-C4B	4.71	130.92	124.81
2	AAA	606	HEC	C3C-C4C-NC	4.71	115.41	110.15
2	AAA	601	HEC	CHD-C1D-ND	4.70	130.17	124.37
2	YYY	607	HEC	C2B-C1B-NB	4.70	115.51	109.88
2	AAA	605	HEC	C3D-C4D-ND	4.69	114.90	110.36
2	YYY	604	HEC	CMD-C2D-C1D	4.69	132.18	125.04
2	AAA	607[A]	HEC	CAD-CBD-CGD	-4.69	103.52	113.60
2	AAA	607[B]	HEC	CAD-CBD-CGD	-4.69	103.52	113.60
2	AAA	601	HEC	C4C-NC-C1C	-4.68	100.76	105.35
2	YYY	603	HEC	CAB-C3B-C4B	4.68	130.88	124.81
2	MMM	602	HEC	C3A-C4A-NA	4.67	118.31	109.69
2	AAA	608	HEC	C3C-C4C-NC	4.67	115.37	110.15
2	YYY	607	HEC	C1D-C2D-C3D	-4.67	102.05	106.96
2	AAA	605	HEC	C1D-C2D-C3D	-4.67	102.05	106.96
2	AAA	602	HEC	C3D-C4D-ND	4.66	114.87	110.36
2	MMM	604	HEC	C3C-C4C-NC	4.66	115.36	110.15
2	AAA	605	HEC	CAA-C2A-C1A	4.65	133.66	124.89
2	YYY	601	HEC	CBA-CAA-C2A	4.62	125.46	112.63
2	AAA	606	HEC	CMB-C2B-C1B	4.59	132.03	125.04
2	AAA	606	HEC	CBC-CAC-C3C	4.59	125.08	112.43
2	AAA	601	HEC	C1D-C2D-C3D	-4.59	102.13	106.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	MMM	606	HEC	C1D-C2D-C3D	-4.59	102.13	106.96
2	MMM	601	HEC	CMC-C2C-C3C	4.58	135.51	125.61
2	YYY	604	HEC	C4A-C3A-C2A	-4.56	100.27	106.94
2	AAA	601	HEC	C4B-NB-C1B	4.55	109.77	105.07
2	MMM	603	HEC	C2A-C1A-NA	4.54	114.74	110.32
2	MMM	601	HEC	C1B-C2B-C3B	-4.52	102.21	106.96
2	YYY	607	HEC	CMA-C3A-C4A	4.51	132.67	124.71
2	AAA	602	HEC	C2A-C1A-NA	4.50	114.70	110.32
2	AAA	604	HEC	CMA-C3A-C4A	4.49	132.63	124.71
2	YYY	607	HEC	C3B-C4B-NB	4.48	115.16	110.17
2	AAA	601	HEC	C2C-C1C-NC	4.48	116.90	110.08
2	YYY	601	HEC	C1B-C2B-C3B	-4.47	102.26	106.96
2	MMM	603	HEC	C2C-C1C-NC	4.46	116.88	110.08
2	MMM	603	HEC	C1D-C2D-C3D	-4.46	102.26	106.96
2	MMM	603	HEC	C3B-C4B-NB	4.46	115.13	110.17
2	AAA	607[A]	HEC	C4A-C3A-C2A	-4.45	100.44	106.94
2	AAA	607[B]	HEC	C4A-C3A-C2A	-4.45	100.44	106.94
2	YYY	604	HEC	C2D-C1D-ND	4.45	115.11	109.84
2	AAA	601	HEC	CHD-C1D-C2D	-4.45	114.37	126.73
2	AAA	608	HEC	C1B-C2B-C3B	-4.45	102.28	106.96
2	YYY	605	HEC	C1C-C2C-C3C	-4.44	101.63	106.83
2	AAA	604	HEC	CAB-C3B-C4B	4.44	130.56	124.81
2	AAA	604	HEC	CMB-C2B-C1B	4.43	131.79	125.04
2	MMM	608	HEC	C1C-C2C-C3C	-4.41	101.67	106.83
2	MMM	604	HEC	CMA-C3A-C4A	4.41	132.48	124.71
2	MMM	608	HEC	C2D-C1D-ND	4.41	115.06	109.84
2	AAA	603	HEC	C1D-C2D-C3D	-4.40	102.33	106.96
2	MMM	603	HEC	CMC-C2C-C3C	4.40	135.12	125.61
2	MMM	606	HEC	CHC-C4B-NB	-4.39	118.96	124.37
2	YYY	605	HEC	C3B-C4B-NB	4.39	115.05	110.17
2	MMM	604	HEC	C4B-NB-C1B	4.37	109.59	105.07
2	AAA	608	HEC	C1D-C2D-C3D	-4.37	102.36	106.96
2	AAA	607[A]	HEC	CMA-C3A-C4A	4.36	132.40	124.71
2	AAA	607[B]	HEC	CMA-C3A-C4A	4.36	132.40	124.71
2	AAA	607[A]	HEC	C4C-NC-C1C	4.33	109.59	105.35
2	AAA	607[B]	HEC	C4C-NC-C1C	4.33	109.59	105.35
2	AAA	603	HEC	C3C-C4C-NC	4.33	114.98	110.15
2	YYY	601	HEC	CMC-C2C-C1C	4.32	131.95	125.37
2	MMM	607	HEC	C3B-C4B-NB	4.32	114.97	110.17
2	AAA	605	HEC	CAB-C3B-C4B	4.30	130.39	124.81
2	YYY	602	HEC	C1A-C2A-C3A	-4.29	101.54	107.13
2	MMM	606	HEC	C2C-C1C-NC	4.28	116.60	110.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	AAA	602	HEC	C3B-C4B-NB	4.28	114.93	110.17
2	MMM	604	HEC	CHA-C1A-NA	-4.28	119.81	124.44
2	YYY	603	HEC	C1D-C2D-C3D	-4.26	102.48	106.96
2	AAA	606	HEC	CAB-C3B-C4B	4.25	130.33	124.81
2	AAA	602	HEC	CAD-C3D-C4D	4.25	132.09	124.66
2	AAA	601	HEC	C4C-C3C-C2C	-4.25	100.21	106.89
2	MMM	602	HEC	C1C-C2C-C3C	-4.24	101.86	106.83
2	MMM	603	HEC	CHB-C1B-C2B	-4.24	118.36	124.98
2	AAA	604	HEC	C3D-C4D-ND	4.24	114.46	110.36
2	YYY	607	HEC	CAD-CBD-CGD	-4.23	104.50	113.60
2	MMM	606	HEC	CMA-C3A-C4A	4.23	132.17	124.71
2	MMM	607	HEC	C3C-C4C-NC	4.23	114.87	110.15
2	AAA	602	HEC	C4A-C3A-C2A	-4.21	100.79	106.94
2	MMM	607	HEC	CHC-C4B-C3B	-4.20	117.44	125.33
2	AAA	603	HEC	CMA-C3A-C4A	4.20	132.11	124.71
2	YYY	603	HEC	C2C-C1C-NC	4.19	116.46	110.08
2	AAA	606	HEC	CAD-C3D-C4D	4.18	131.96	124.66
2	AAA	601	HEC	CAA-C2A-C1A	4.17	132.76	124.89
2	MMM	602	HEC	CHA-C4D-ND	4.17	128.95	124.42
2	YYY	608	HEC	C1D-C2D-C3D	-4.17	102.57	106.96
2	MMM	601	HEC	CAD-CBD-CGD	-4.16	104.64	113.60
2	AAA	607[A]	HEC	CAD-C3D-C4D	4.15	131.91	124.66
2	AAA	607[B]	HEC	CAD-C3D-C4D	4.15	131.91	124.66
2	MMM	601	HEC	C4A-C3A-C2A	-4.15	100.88	106.94
2	AAA	607[A]	HEC	CHA-C4D-C3D	-4.15	118.75	124.84
2	AAA	607[B]	HEC	CHA-C4D-C3D	-4.15	118.75	124.84
2	YYY	606	HEC	C1C-C2C-C3C	-4.14	101.98	106.83
2	MMM	606	HEC	C3D-C4D-ND	4.14	114.37	110.36
2	YYY	605	HEC	CHD-C1D-ND	-4.14	119.27	124.37
2	AAA	604	HEC	C4C-NC-C1C	-4.14	101.30	105.35
2	AAA	607[A]	HEC	CMD-C2D-C1D	4.11	131.29	125.04
2	AAA	607[B]	HEC	CMD-C2D-C1D	4.11	131.29	125.04
2	MMM	606	HEC	CHA-C4D-ND	-4.10	119.96	124.42
2	MMM	607	HEC	C1A-C2A-C3A	-4.10	101.78	107.13
2	YYY	603	HEC	C3B-C4B-NB	4.10	114.73	110.17
2	MMM	604	HEC	C4A-C3A-C2A	-4.09	100.97	106.94
2	MMM	602	HEC	C4D-C3D-C2D	-4.08	100.95	106.90
2	YYY	601	HEC	CAA-C2A-C1A	4.06	132.55	124.89
2	MMM	601	HEC	CBC-CAC-C3C	4.05	123.61	112.43
2	AAA	607[A]	HEC	CMB-C2B-C1B	4.04	131.19	125.04
2	AAA	607[B]	HEC	CMB-C2B-C1B	4.04	131.19	125.04
2	AAA	602	HEC	CAB-C3B-C4B	4.02	130.02	124.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	MMM	607	HEC	CHA-C1A-NA	-4.01	120.10	124.44
2	YYY	606	HEC	O2A-CGA-O1A	-4.01	113.30	123.30
2	YYY	601	HEC	CHA-C1A-C2A	-4.01	118.44	124.94
2	AAA	605	HEC	C1B-C2B-C3B	-4.00	102.75	106.96
2	AAA	601	HEC	CHC-C4B-NB	3.99	129.30	124.37
2	YYY	601	HEC	CAD-C3D-C2D	3.99	135.31	127.88
2	YYY	602	HEC	CMA-C3A-C4A	3.98	131.73	124.71
2	AAA	601	HEC	CAD-C3D-C4D	3.98	131.62	124.66
2	MMM	602	HEC	CMC-C2C-C1C	3.98	131.43	125.37
2	YYY	604	HEC	CMB-C2B-C1B	3.97	131.09	125.04
2	MMM	607	HEC	CMC-C2C-C1C	3.95	131.39	125.37
2	YYY	607	HEC	O2D-CGD-CBD	3.95	126.71	114.03
2	AAA	604	HEC	C3A-C4A-NA	3.94	116.97	109.69
2	AAA	605	HEC	C3B-C4B-NB	3.94	114.56	110.17
2	AAA	607[A]	HEC	C1C-C2C-C3C	-3.93	102.24	106.83
2	AAA	607[B]	HEC	C1C-C2C-C3C	-3.93	102.24	106.83
2	AAA	603	HEC	CMD-C2D-C1D	3.92	131.01	125.04
2	YYY	608	HEC	C2D-C1D-ND	3.91	114.47	109.84
2	MMM	607	HEC	CAD-CBD-CGD	-3.90	105.20	113.60
2	MMM	608	HEC	CMC-C2C-C3C	3.90	134.05	125.61
2	AAA	601	HEC	CBA-CAA-C2A	3.90	123.47	112.63
2	AAA	607[A]	HEC	O2A-CGA-CBA	3.90	126.56	114.03
2	MMM	606	HEC	CAB-C3B-C2B	-3.90	120.86	127.53
2	AAA	608	HEC	C2D-C1D-ND	3.89	114.45	109.84
2	MMM	605	HEC	CMB-C2B-C1B	3.88	130.95	125.04
2	YYY	603	HEC	CMB-C2B-C1B	3.87	130.93	125.04
2	AAA	605	HEC	C2B-C1B-NB	3.87	114.52	109.88
2	MMM	607	HEC	C4C-NC-C1C	-3.87	101.56	105.35
2	AAA	606	HEC	CHB-C4A-NA	-3.87	120.26	124.44
2	YYY	605	HEC	C3C-C4C-NC	3.86	114.46	110.15
2	YYY	603	HEC	CAA-CBA-CGA	-3.85	105.31	113.60
2	AAA	604	HEC	CHC-C1C-NC	-3.85	116.76	123.85
2	YYY	604	HEC	CMC-C2C-C1C	3.84	131.22	125.37
2	MMM	604	HEC	CMB-C2B-C1B	3.84	130.88	125.04
2	YYY	607	HEC	CHA-C4D-ND	-3.83	120.25	124.42
2	AAA	604	HEC	C3B-C4B-NB	3.82	114.42	110.17
2	MMM	604	HEC	C1D-C2D-C3D	-3.81	102.95	106.96
2	YYY	601	HEC	CHA-C4D-C3D	-3.80	119.25	124.84
2	YYY	606	HEC	C4A-C3A-C2A	-3.80	101.39	106.94
2	MMM	606	HEC	C3B-C4B-NB	3.79	114.39	110.17
2	MMM	603	HEC	CHC-C1C-C2C	-3.79	116.52	127.24
2	MMM	605	HEC	CMD-C2D-C1D	3.79	130.81	125.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	YYY	601	HEC	C1D-ND-C4D	-3.77	101.17	105.07
2	YYY	602	HEC	C1B-C2B-C3B	-3.77	102.99	106.96
2	YYY	607	HEC	C2D-C1D-ND	3.77	114.31	109.84
2	MMM	603	HEC	CAD-CBD-CGD	-3.77	105.50	113.60
2	YYY	607	HEC	C1C-C2C-C3C	-3.76	102.44	106.83
2	MMM	603	HEC	C4B-NB-C1B	-3.75	101.20	105.07
2	AAA	606	HEC	C2D-C1D-ND	3.75	114.28	109.84
2	YYY	602	HEC	C3A-C4A-NA	3.74	116.59	109.69
2	AAA	607[A]	HEC	CAC-C3C-C4C	3.74	130.10	124.92
2	AAA	607[B]	HEC	CAC-C3C-C4C	3.74	130.10	124.92
2	MMM	602	HEC	O1A-CGA-CBA	-3.73	111.09	123.08
2	AAA	604	HEC	CHB-C4A-NA	-3.73	120.41	124.44
2	AAA	607[A]	HEC	O1A-CGA-CBA	-3.72	111.12	123.08
2	AAA	603	HEC	C4A-C3A-C2A	-3.72	101.50	106.94
2	YYY	604	HEC	C3A-C4A-NA	3.72	116.55	109.69
2	MMM	603	HEC	C3D-C4D-ND	3.72	113.96	110.36
2	AAA	606	HEC	CHA-C4D-ND	-3.71	120.38	124.42
2	YYY	607	HEC	CHB-C4A-NA	-3.71	120.42	124.44
2	AAA	602	HEC	CHB-C4A-C3A	-3.71	117.71	125.48
2	AAA	607[A]	HEC	CMC-C2C-C3C	3.70	133.61	125.61
2	AAA	607[B]	HEC	CMC-C2C-C3C	3.70	133.61	125.61
2	MMM	608	HEC	CHB-C1B-NB	-3.70	120.40	124.42
2	MMM	605	HEC	CHA-C4D-C3D	-3.69	119.42	124.84
2	MMM	603	HEC	C2D-C1D-ND	3.69	114.21	109.84
2	AAA	606	HEC	C1A-C2A-C3A	-3.68	102.33	107.13
2	MMM	601	HEC	CAC-C3C-C4C	3.67	130.01	124.92
2	AAA	602	HEC	CAA-CBA-CGA	-3.67	105.71	113.60
2	AAA	607[A]	HEC	CBA-CAA-C2A	-3.67	102.44	112.63
2	AAA	607[B]	HEC	CBA-CAA-C2A	-3.67	102.44	112.63
2	MMM	602	HEC	CMB-C2B-C1B	3.66	130.62	125.04
2	YYY	607	HEC	O2D-CGD-O1D	-3.66	114.19	123.30
2	MMM	605	HEC	CAD-CBD-CGD	-3.65	105.75	113.60
2	MMM	604	HEC	C1A-C2A-C3A	-3.65	102.37	107.13
2	MMM	601	HEC	CHA-C4D-C3D	-3.64	119.49	124.84
2	YYY	608	HEC	C3D-C4D-ND	3.64	113.88	110.36
2	YYY	603	HEC	C2D-C1D-ND	3.63	114.14	109.84
2	YYY	602	HEC	CHA-C1A-NA	-3.62	120.52	124.44
2	AAA	603	HEC	C2C-C1C-NC	3.62	115.59	110.08
2	AAA	602	HEC	CMA-C3A-C4A	3.59	131.05	124.71
2	AAA	602	HEC	CAD-CBD-CGD	3.59	121.32	113.60
2	AAA	603	HEC	CHA-C4D-ND	-3.58	120.52	124.42
2	YYY	602	HEC	CHA-C4D-C3D	-3.58	119.58	124.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	AAA	608	HEC	CAA-CBA-CGA	3.57	121.28	113.60
2	YYY	604	HEC	CHD-C1D-ND	-3.56	119.98	124.37
2	YYY	606	HEC	CHC-C4B-NB	-3.56	119.98	124.37
2	MMM	601	HEC	C1D-C2D-C3D	-3.55	103.22	106.96
2	AAA	608	HEC	C3D-C4D-ND	3.54	113.79	110.36
2	YYY	604	HEC	CHB-C1B-C2B	-3.53	119.47	124.98
2	AAA	604	HEC	C4D-C3D-C2D	-3.52	101.76	106.90
2	AAA	603	HEC	C2B-C1B-NB	3.52	114.10	109.88
2	AAA	602	HEC	C4D-C3D-C2D	-3.51	101.78	106.90
2	AAA	606	HEC	C1B-C2B-C3B	-3.51	103.27	106.96
2	AAA	605	HEC	C2D-C1D-ND	3.51	114.00	109.84
2	AAA	602	HEC	CHB-C1B-C2B	-3.50	119.50	124.98
2	YYY	601	HEC	C2C-C1C-NC	3.50	115.41	110.08
2	MMM	603	HEC	C3A-C4A-NA	3.50	116.15	109.69
2	YYY	608	HEC	C2A-C1A-NA	3.50	113.73	110.32
2	YYY	605	HEC	C4A-C3A-C2A	-3.49	101.84	106.94
2	YYY	605	HEC	C3A-C4A-NA	3.49	116.12	109.69
2	AAA	605	HEC	C1A-C2A-C3A	-3.48	102.59	107.13
2	MMM	603	HEC	CMA-C3A-C4A	3.47	130.83	124.71
2	MMM	605	HEC	C1D-ND-C4D	-3.46	101.50	105.07
2	YYY	603	HEC	C4A-C3A-C2A	-3.45	101.90	106.94
2	MMM	605	HEC	C2C-C1C-NC	3.45	115.34	110.08
2	MMM	608	HEC	C4C-NC-C1C	3.45	108.73	105.35
2	YYY	608	HEC	C1A-C2A-C3A	-3.45	102.63	107.13
2	MMM	607	HEC	CAC-C3C-C4C	3.43	129.67	124.92
2	YYY	602	HEC	CAD-C3D-C2D	3.42	134.25	127.88
2	MMM	606	HEC	CAD-C3D-C4D	3.42	130.63	124.66
2	MMM	601	HEC	CHC-C1C-C2C	-3.42	117.58	127.24
2	AAA	603	HEC	CAC-C3C-C4C	3.42	129.66	124.92
2	YYY	607	HEC	CMD-C2D-C1D	3.41	130.24	125.04
2	AAA	605	HEC	C4A-C3A-C2A	-3.40	101.97	106.94
2	MMM	603	HEC	C4A-C3A-C2A	-3.39	101.98	106.94
2	YYY	605	HEC	CMA-C3A-C4A	3.39	130.69	124.71
2	AAA	605	HEC	C1C-C2C-C3C	-3.39	102.87	106.83
2	AAA	606	HEC	C1D-C2D-C3D	-3.38	103.40	106.96
2	YYY	603	HEC	C3A-C4A-NA	3.37	115.90	109.69
2	YYY	605	HEC	CMD-C2D-C1D	3.37	130.17	125.04
2	YYY	607	HEC	C4C-C3C-C2C	-3.37	101.60	106.89
2	YYY	602	HEC	CHB-C4A-C3A	-3.36	118.43	125.48
2	MMM	603	HEC	CHB-C4A-C3A	-3.36	118.44	125.48
2	AAA	604	HEC	CBC-CAC-C3C	3.35	121.65	112.43
2	AAA	606	HEC	CAA-C2A-C3A	-3.34	121.66	127.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	MMM	607	HEC	C2D-C1D-ND	3.34	113.79	109.84
2	MMM	605	HEC	C2B-C1B-NB	3.33	113.87	109.88
2	MMM	608	HEC	CHC-C4B-NB	-3.32	120.28	124.37
2	YYY	601	HEC	C4B-NB-C1B	3.32	108.50	105.07
2	MMM	606	HEC	CHC-C1C-C2C	-3.32	117.86	127.24
2	MMM	607	HEC	CMD-C2D-C3D	3.30	135.07	126.12
2	AAA	607[A]	HEC	CBD-CAD-C3D	3.29	121.78	112.63
2	AAA	607[B]	HEC	CBD-CAD-C3D	3.29	121.78	112.63
2	MMM	602	HEC	O2A-CGA-CBA	3.29	124.61	114.03
2	MMM	608	HEC	CHD-C1D-ND	-3.29	120.32	124.37
2	AAA	602	HEC	C4B-NB-C1B	-3.29	101.67	105.07
2	YYY	608	HEC	C2C-C1C-NC	3.29	115.09	110.08
2	MMM	602	HEC	C3C-C4C-NC	3.29	113.82	110.15
2	YYY	607	HEC	C2C-C1C-NC	3.28	115.08	110.08
2	MMM	606	HEC	CHB-C1B-C2B	-3.28	119.85	124.98
2	YYY	607	HEC	CAB-C3B-C4B	3.28	129.06	124.81
2	YYY	606	HEC	CAA-C2A-C1A	3.27	131.07	124.89
2	YYY	606	HEC	CHB-C4A-C3A	-3.27	118.62	125.48
2	AAA	605	HEC	CAD-CBD-CGD	-3.27	106.56	113.60
2	AAA	605	HEC	CHA-C4D-C3D	-3.27	120.03	124.84
2	AAA	608	HEC	C3B-C4B-NB	3.27	113.80	110.17
2	AAA	603	HEC	CHB-C1B-C2B	-3.26	119.89	124.98
2	YYY	607	HEC	CHC-C4B-C3B	-3.26	119.21	125.33
2	AAA	606	HEC	CHD-C4C-NC	-3.25	117.86	123.85
2	AAA	602	HEC	C1C-C2C-C3C	-3.25	103.02	106.83
2	AAA	605	HEC	C2A-C1A-NA	3.25	113.49	110.32
2	MMM	604	HEC	CBC-CAC-C3C	3.25	121.39	112.43
2	AAA	606	HEC	C4B-NB-C1B	3.25	108.43	105.07
2	YYY	606	HEC	CHB-C1B-NB	-3.24	120.89	124.42
2	YYY	602	HEC	C3C-C4C-NC	3.24	113.77	110.15
2	AAA	605	HEC	CHB-C1B-C2B	-3.23	119.93	124.98
2	YYY	602	HEC	O2A-CGA-O1A	-3.22	115.28	123.30
2	MMM	608	HEC	C4A-NA-C1A	3.21	108.49	105.35
2	AAA	605	HEC	CHB-C4A-C3A	-3.21	118.75	125.48
2	YYY	606	HEC	CHA-C1A-C2A	-3.21	119.74	124.94
2	MMM	605	HEC	C2A-C1A-NA	3.21	113.44	110.32
2	AAA	603	HEC	C3A-C4A-NA	3.20	115.60	109.69
2	MMM	602	HEC	CAA-C2A-C1A	3.20	130.93	124.89
2	YYY	602	HEC	CHA-C4D-ND	3.19	127.88	124.42
2	MMM	601	HEC	CAB-C3B-C4B	3.19	128.95	124.81
2	YYY	604	HEC	CMA-C3A-C4A	3.18	130.32	124.71
2	MMM	601	HEC	C3A-C4A-NA	3.18	115.56	109.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	MMM	607	HEC	C4A-NA-C1A	-3.18	102.24	105.35
2	YYY	604	HEC	CAD-C3D-C4D	3.18	130.21	124.66
2	YYY	604	HEC	C1D-C2D-C3D	-3.17	103.62	106.96
2	AAA	603	HEC	CBC-CAC-C3C	3.17	121.17	112.43
2	YYY	608	HEC	CAD-CBD-CGD	-3.16	106.80	113.60
2	YYY	605	HEC	CAA-CBA-CGA	-3.16	106.81	113.60
2	MMM	601	HEC	C2C-C1C-NC	3.15	114.88	110.08
2	YYY	607	HEC	C4D-C3D-C2D	-3.15	102.31	106.90
2	AAA	602	HEC	CMC-C2C-C3C	3.15	132.41	125.61
2	MMM	601	HEC	CHA-C1A-C2A	-3.15	119.84	124.94
2	YYY	606	HEC	CAB-C3B-C2B	-3.14	122.15	127.53
2	AAA	601	HEC	CBD-CAD-C3D	3.14	121.35	112.63
2	AAA	605	HEC	C4B-C3B-C2B	-3.14	102.32	106.90
2	AAA	602	HEC	C3A-C4A-NA	3.14	115.48	109.69
2	AAA	603	HEC	C4C-C3C-C2C	-3.13	101.97	106.89
2	YYY	606	HEC	C2C-C1C-NC	3.13	114.85	110.08
2	MMM	601	HEC	C2D-C1D-ND	3.13	113.54	109.84
2	MMM	605	HEC	C4D-C3D-C2D	-3.12	102.34	106.90
2	MMM	604	HEC	CHC-C1C-NC	-3.12	118.10	123.85
2	MMM	604	HEC	C2D-C1D-ND	3.12	113.53	109.84
2	AAA	601	HEC	CHA-C1A-C2A	-3.12	119.89	124.94
2	AAA	608	HEC	C2C-C1C-NC	3.10	114.80	110.08
2	MMM	607	HEC	C3A-C4A-NA	3.10	115.41	109.69
2	AAA	603	HEC	C4D-C3D-C2D	-3.09	102.39	106.90
2	YYY	601	HEC	C3C-C4C-NC	3.09	113.60	110.15
2	YYY	608	HEC	CMD-C2D-C1D	3.09	129.74	125.04
2	YYY	604	HEC	CHC-C4B-C3B	-3.08	119.54	125.33
2	MMM	606	HEC	CHA-C1A-C2A	-3.08	119.94	124.94
2	MMM	605	HEC	CMA-C3A-C4A	3.08	130.14	124.71
2	AAA	608	HEC	C2B-C1B-NB	3.08	113.57	109.88
2	AAA	602	HEC	C1D-C2D-C3D	-3.07	103.73	106.96
2	AAA	606	HEC	CBD-CAD-C3D	-3.07	104.10	112.63
2	AAA	603	HEC	CAD-C3D-C2D	-3.07	122.17	127.88
2	YYY	604	HEC	C4D-C3D-C2D	-3.07	102.43	106.90
2	YYY	601	HEC	CHD-C1D-C2D	-3.06	118.22	126.73
2	AAA	605	HEC	C3C-C4C-NC	3.06	113.57	110.15
2	MMM	607	HEC	C1D-C2D-C3D	-3.05	103.75	106.96
2	MMM	607	HEC	CMA-C3A-C4A	3.05	130.09	124.71
2	MMM	601	HEC	CBD-CAD-C3D	3.04	121.08	112.63
2	MMM	605	HEC	CBC-CAC-C3C	3.04	120.81	112.43
2	YYY	608	HEC	C4B-NB-C1B	3.04	108.21	105.07
2	MMM	602	HEC	CAD-CBD-CGD	3.04	120.14	113.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	YYY	603	HEC	CHB-C1B-C2B	-3.04	120.23	124.98
2	YYY	604	HEC	C2C-C1C-NC	3.02	114.69	110.08
2	YYY	603	HEC	C4D-C3D-C2D	-3.02	102.49	106.90
2	YYY	606	HEC	C3D-C4D-ND	3.02	113.28	110.36
2	MMM	605	HEC	C4A-C3A-C2A	-3.00	102.56	106.94
2	YYY	602	HEC	C2D-C1D-ND	3.00	113.39	109.84
2	AAA	606	HEC	CMC-C2C-C3C	3.00	132.09	125.61
2	YYY	607	HEC	CAC-C3C-C4C	2.99	129.07	124.92
2	YYY	605	HEC	CBC-CAC-C3C	2.98	120.66	112.43
2	AAA	607[A]	HEC	C1D-C2D-C3D	-2.98	103.82	106.96
2	AAA	607[B]	HEC	C1D-C2D-C3D	-2.98	103.82	106.96
2	YYY	607	HEC	CMB-C2B-C1B	2.98	129.58	125.04
2	YYY	603	HEC	C1A-C2A-C3A	-2.98	103.24	107.13
2	MMM	603	HEC	CBD-CAD-C3D	-2.98	104.36	112.63
2	MMM	605	HEC	C3C-C4C-NC	2.97	113.47	110.15
2	AAA	606	HEC	CAD-CBD-CGD	-2.97	107.20	113.60
2	MMM	602	HEC	C2C-C1C-NC	2.97	114.60	110.08
2	AAA	604	HEC	CHA-C4D-C3D	-2.96	120.48	124.84
2	AAA	603	HEC	C1C-C2C-C3C	-2.96	103.37	106.83
2	MMM	608	HEC	CAB-C3B-C4B	2.96	128.65	124.81
2	MMM	602	HEC	CHB-C4A-C3A	-2.96	119.28	125.48
2	MMM	601	HEC	CMA-C3A-C4A	2.94	129.89	124.71
2	AAA	606	HEC	C4D-C3D-C2D	-2.93	102.62	106.90
2	AAA	607[A]	HEC	C3A-C4A-NA	2.93	115.09	109.69
2	AAA	607[B]	HEC	C3A-C4A-NA	2.93	115.09	109.69
2	MMM	604	HEC	CBD-CAD-C3D	-2.92	104.52	112.63
2	YYY	606	HEC	C3B-C4B-NB	2.91	113.41	110.17
2	AAA	603	HEC	C2A-C1A-NA	2.90	113.15	110.32
2	AAA	601	HEC	CMC-C2C-C3C	2.89	131.86	125.61
2	YYY	608	HEC	CMC-C2C-C1C	2.89	129.77	125.37
2	YYY	607	HEC	C3A-C4A-NA	2.89	115.02	109.69
2	MMM	606	HEC	C4A-C3A-C2A	-2.88	102.74	106.94
2	MMM	605	HEC	CHD-C4C-C3C	-2.87	119.09	125.36
2	YYY	605	HEC	CMC-C2C-C1C	2.86	129.73	125.37
2	YYY	606	HEC	C3A-C4A-NA	2.85	114.94	109.69
2	MMM	603	HEC	CMB-C2B-C1B	2.84	129.37	125.04
2	AAA	605	HEC	CHA-C1A-NA	-2.84	121.36	124.44
2	MMM	606	HEC	C4D-C3D-C2D	-2.84	102.76	106.90
2	MMM	601	HEC	C4B-NB-C1B	-2.83	102.15	105.07
2	MMM	607	HEC	CAD-C3D-C2D	2.83	133.14	127.88
2	MMM	601	HEC	C4C-NC-C1C	2.83	108.11	105.35
2	YYY	608	HEC	CAA-CBA-CGA	2.82	119.68	113.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	AAA	606	HEC	CBA-CAA-C2A	-2.82	104.80	112.63
2	MMM	603	HEC	CMD-C2D-C1D	2.82	129.33	125.04
2	YYY	606	HEC	CMC-C2C-C3C	2.81	131.69	125.61
2	MMM	604	HEC	CHB-C1B-C2B	-2.81	120.59	124.98
2	AAA	602	HEC	O2D-CGD-CBD	2.81	123.05	114.03
2	AAA	602	HEC	CHA-C1A-C2A	-2.80	120.40	124.94
2	AAA	601	HEC	CBB-CAB-C3B	-2.79	104.73	112.43
2	YYY	603	HEC	CMC-C2C-C3C	2.79	131.64	125.61
2	AAA	606	HEC	C4A-C3A-C2A	-2.78	102.88	106.94
2	YYY	602	HEC	C1D-C2D-C3D	-2.78	104.03	106.96
2	YYY	606	HEC	CAD-C3D-C4D	2.78	129.51	124.66
2	MMM	602	HEC	CBD-CAD-C3D	2.78	120.34	112.63
2	AAA	608	HEC	CMA-C3A-C4A	2.77	129.59	124.71
2	MMM	605	HEC	CHD-C1D-ND	-2.76	120.98	124.37
2	YYY	605	HEC	CHD-C4C-C3C	-2.75	119.34	125.36
2	MMM	606	HEC	C1D-ND-C4D	-2.75	102.23	105.07
2	YYY	605	HEC	CHA-C4D-C3D	-2.74	120.81	124.84
2	MMM	605	HEC	C3B-C4B-NB	2.74	113.22	110.17
2	AAA	603	HEC	CMB-C2B-C3B	2.74	133.55	126.12
2	AAA	606	HEC	CHC-C1C-NC	-2.74	118.81	123.85
2	YYY	602	HEC	CHC-C4B-C3B	-2.73	120.21	125.33
2	MMM	605	HEC	CAD-C3D-C4D	2.72	129.40	124.66
2	MMM	606	HEC	C4B-NB-C1B	-2.71	102.27	105.07
2	YYY	601	HEC	CMD-C2D-C3D	2.70	133.46	126.12
2	AAA	608	HEC	CMC-C2C-C1C	2.70	129.49	125.37
2	AAA	608	HEC	CHA-C4D-ND	-2.70	121.48	124.42
2	AAA	608	HEC	C4D-C3D-C2D	-2.70	102.96	106.90
2	MMM	603	HEC	CAA-C2A-C1A	2.70	129.98	124.89
2	YYY	606	HEC	CBA-CAA-C2A	-2.70	105.14	112.63
2	AAA	601	HEC	C3D-C4D-ND	2.70	112.97	110.36
2	AAA	608	HEC	C2A-C1A-NA	2.69	112.94	110.32
2	YYY	605	HEC	C2C-C1C-NC	2.69	114.17	110.08
2	AAA	602	HEC	CBA-CAA-C2A	-2.68	105.17	112.63
2	YYY	604	HEC	CHB-C4A-C3A	-2.68	119.86	125.48
2	MMM	607	HEC	C4A-C3A-C2A	-2.68	103.03	106.94
2	YYY	606	HEC	C1A-C2A-C3A	-2.68	103.64	107.13
2	YYY	601	HEC	CHB-C1B-C2B	-2.66	120.83	124.98
2	MMM	608	HEC	CAD-C3D-C4D	2.66	129.30	124.66
2	MMM	605	HEC	CAA-CBA-CGA	-2.66	107.88	113.60
2	MMM	605	HEC	C3A-C4A-NA	2.65	114.59	109.69
2	YYY	605	HEC	C2A-C1A-NA	2.65	112.90	110.32
2	MMM	604	HEC	C2B-C1B-NB	2.65	113.06	109.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	AAA	601	HEC	CHA-C4D-C3D	-2.64	120.96	124.84
2	MMM	608	HEC	C1A-C2A-C3A	-2.64	103.69	107.13
2	MMM	602	HEC	C4A-CHB-C1B	2.64	131.74	126.06
2	AAA	606	HEC	C2B-C1B-NB	2.63	113.03	109.88
2	MMM	603	HEC	C1A-C2A-C3A	-2.63	103.70	107.13
2	YYY	603	HEC	CMA-C3A-C4A	2.63	129.34	124.71
2	MMM	608	HEC	C3D-C4D-ND	2.63	112.90	110.36
2	MMM	606	HEC	C2A-C1A-NA	2.62	112.88	110.32
2	YYY	604	HEC	CHA-C4D-ND	-2.62	121.57	124.42
2	YYY	602	HEC	CHC-C4B-NB	2.62	127.60	124.37
2	MMM	601	HEC	CBA-CAA-C2A	2.62	119.90	112.63
2	MMM	608	HEC	CAA-C2A-C1A	2.62	129.83	124.89
2	YYY	608	HEC	CMC-C2C-C3C	2.61	131.26	125.61
2	YYY	602	HEC	C4B-NB-C1B	2.61	107.77	105.07
2	AAA	602	HEC	CHC-C4B-NB	-2.60	121.16	124.37
2	YYY	603	HEC	CHB-C4A-C3A	-2.59	120.04	125.48
2	YYY	604	HEC	CHC-C1C-C2C	-2.59	119.92	127.24
2	MMM	606	HEC	C4A-NA-C1A	2.59	107.88	105.35
2	MMM	601	HEC	CAC-C3C-C2C	-2.59	122.72	126.86
2	MMM	602	HEC	CAC-C3C-C4C	2.58	128.50	124.92
2	MMM	602	HEC	CAA-CBA-CGA	-2.58	108.05	113.60
2	AAA	602	HEC	CAC-C3C-C4C	2.58	128.50	124.92
2	YYY	607	HEC	O1A-CGA-CBA	-2.58	114.79	123.08
2	MMM	602	HEC	CHB-C1B-C2B	-2.57	120.96	124.98
2	YYY	603	HEC	CHC-C1C-C2C	-2.57	119.98	127.24
2	AAA	607[A]	HEC	C4B-C3B-C2B	-2.57	103.16	106.90
2	AAA	607[B]	HEC	C4B-C3B-C2B	-2.57	103.16	106.90
2	MMM	606	HEC	CHB-C4A-NA	-2.56	121.67	124.44
2	YYY	602	HEC	CMC-C2C-C3C	2.56	131.15	125.61
2	AAA	601	HEC	CHB-C4A-NA	-2.56	121.67	124.44
2	YYY	602	HEC	CHB-C1B-C2B	-2.56	120.98	124.98
2	YYY	603	HEC	CHA-C1A-C2A	-2.56	120.79	124.94
2	YYY	601	HEC	CAC-C3C-C4C	2.56	128.47	124.92
2	MMM	602	HEC	CAB-C3B-C4B	2.55	128.12	124.81
2	AAA	607[A]	HEC	CAB-C3B-C4B	2.54	128.11	124.81
2	AAA	607[B]	HEC	CAB-C3B-C4B	2.54	128.11	124.81
2	YYY	605	HEC	C1A-C2A-C3A	-2.54	103.81	107.13
2	MMM	607	HEC	CMD-C2D-C1D	-2.54	121.17	125.04
2	AAA	601	HEC	CAD-C3D-C2D	-2.54	123.15	127.88
2	YYY	602	HEC	O2A-CGA-CBA	2.53	122.17	114.03
2	MMM	606	HEC	C1A-C2A-C3A	-2.53	103.83	107.13
2	YYY	606	HEC	C4B-C3B-C2B	-2.53	103.21	106.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	AAA	601	HEC	C1C-C2C-C3C	-2.53	103.87	106.83
2	AAA	602	HEC	CHC-C1C-C2C	-2.53	120.09	127.24
2	YYY	608	HEC	CBB-CAB-C3B	-2.53	105.47	112.43
2	YYY	605	HEC	C4D-C3D-C2D	-2.52	103.22	106.90
2	AAA	604	HEC	C2B-C1B-NB	2.52	112.90	109.88
2	AAA	608	HEC	C4A-C3A-C2A	-2.52	103.26	106.94
2	AAA	605	HEC	CBB-CAB-C3B	-2.52	105.48	112.43
2	AAA	606	HEC	C3A-C4A-NA	2.52	114.33	109.69
2	MMM	601	HEC	CHB-C1B-C2B	-2.51	121.05	124.98
2	YYY	606	HEC	C1C-CHC-C4B	2.51	132.29	126.34
2	AAA	606	HEC	C3D-C4D-ND	2.50	112.77	110.36
2	MMM	601	HEC	C4D-C3D-C2D	-2.49	103.26	106.90
2	AAA	601	HEC	CHC-C4B-C3B	-2.49	120.65	125.33
2	MMM	604	HEC	C3D-C4D-ND	2.49	112.77	110.36
2	YYY	604	HEC	C4B-NB-C1B	-2.49	102.50	105.07
2	MMM	607	HEC	O1A-CGA-CBA	-2.48	115.10	123.08
2	AAA	602	HEC	C4C-NC-C1C	2.48	107.78	105.35
2	AAA	602	HEC	C4A-NA-C1A	-2.48	102.92	105.35
2	YYY	603	HEC	CAD-CBD-CGD	-2.47	108.28	113.60
2	AAA	602	HEC	CBC-CAC-C3C	2.47	119.25	112.43
2	AAA	603	HEC	CAB-C3B-C4B	2.47	128.01	124.81
2	MMM	603	HEC	C4D-C3D-C2D	-2.47	103.30	106.90
2	AAA	606	HEC	C4B-C3B-C2B	-2.47	103.30	106.90
2	MMM	606	HEC	CHA-C1A-NA	2.47	127.11	124.44
2	MMM	603	HEC	CAD-C3D-C4D	2.47	128.97	124.66
2	YYY	605	HEC	CAC-C3C-C4C	2.46	128.33	124.92
2	YYY	607	HEC	C4C-NC-C1C	-2.46	102.94	105.35
2	AAA	606	HEC	CHC-C4B-NB	2.45	127.40	124.37
2	MMM	606	HEC	CHD-C1D-C2D	-2.45	119.92	126.73
2	YYY	604	HEC	C1D-ND-C4D	-2.45	102.55	105.07
2	AAA	602	HEC	CHD-C1D-C2D	-2.45	119.93	126.73
2	MMM	605	HEC	C1A-C2A-C3A	-2.44	103.95	107.13
2	AAA	601	HEC	CMB-C2B-C3B	2.44	132.73	126.12
2	MMM	603	HEC	CBA-CAA-C2A	2.43	119.39	112.63
2	AAA	606	HEC	CHC-C4B-C3B	-2.42	120.78	125.33
2	YYY	608	HEC	C4D-C3D-C2D	-2.42	103.37	106.90
2	AAA	602	HEC	CMB-C2B-C1B	2.41	128.70	125.04
2	MMM	606	HEC	O2A-CGA-O1A	-2.40	117.31	123.30
2	YYY	603	HEC	C4A-NA-C1A	-2.40	103.00	105.35
2	AAA	605	HEC	CMC-C2C-C1C	2.40	129.02	125.37
2	MMM	601	HEC	CAD-C3D-C4D	2.38	128.82	124.66
2	YYY	605	HEC	CAB-C3B-C4B	2.38	127.90	124.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	YYY	602	HEC	C2B-C1B-NB	2.37	112.73	109.88
2	YYY	601	HEC	CHC-C4B-NB	2.37	127.29	124.37
2	YYY	608	HEC	CAB-C3B-C4B	2.37	127.88	124.81
2	AAA	605	HEC	CAC-C3C-C2C	-2.37	123.07	126.86
2	AAA	605	HEC	C2C-C1C-NC	2.37	113.68	110.08
2	YYY	608	HEC	O1D-CGD-CBD	-2.36	115.49	123.08
2	MMM	602	HEC	CAD-C3D-C2D	2.36	132.28	127.88
2	MMM	603	HEC	CHD-C1D-ND	-2.36	121.47	124.37
2	YYY	601	HEC	C1A-CHA-C4D	-2.36	120.97	126.06
2	YYY	606	HEC	CAC-C3C-C4C	2.35	128.18	124.92
2	YYY	601	HEC	O2D-CGD-CBD	2.34	121.55	114.03
2	AAA	608	HEC	CMD-C2D-C1D	2.34	128.60	125.04
2	MMM	604	HEC	CAA-C2A-C1A	2.34	129.30	124.89
2	MMM	602	HEC	CBC-CAC-C3C	2.33	118.85	112.43
2	YYY	607	HEC	O2A-CGA-CBA	2.32	121.49	114.03
2	YYY	602	HEC	CHC-C1C-C2C	-2.32	120.69	127.24
2	MMM	603	HEC	CMB-C2B-C3B	2.32	132.41	126.12
2	MMM	601	HEC	C1A-C2A-C3A	-2.31	104.11	107.13
2	YYY	606	HEC	CMA-C3A-C2A	2.30	132.37	126.12
2	AAA	605	HEC	C4D-C3D-C2D	-2.30	103.54	106.90
2	YYY	605	HEC	CHB-C4A-C3A	-2.29	120.68	125.48
2	AAA	604	HEC	CHC-C4B-C3B	-2.29	121.03	125.33
2	AAA	601	HEC	CAB-C3B-C4B	-2.29	121.84	124.81
2	YYY	601	HEC	C4D-C3D-C2D	-2.28	103.57	106.90
2	MMM	608	HEC	CAC-C3C-C4C	-2.28	121.75	124.92
2	AAA	602	HEC	CHA-C4D-ND	-2.28	121.94	124.42
2	MMM	607	HEC	CHC-C1C-NC	-2.28	119.65	123.85
2	AAA	605	HEC	CMB-C2B-C3B	2.27	132.28	126.12
2	YYY	604	HEC	CAD-CBD-CGD	2.27	118.48	113.60
2	AAA	606	HEC	O2D-CGD-CBD	2.26	121.30	114.03
2	YYY	605	HEC	CHB-C1B-NB	-2.26	121.96	124.42
2	AAA	601	HEC	C4A-NA-C1A	-2.26	103.14	105.35
2	YYY	601	HEC	CMB-C2B-C3B	2.25	132.22	126.12
2	YYY	602	HEC	C3D-C4D-ND	2.25	112.53	110.36
2	AAA	607[A]	HEC	C4C-C3C-C2C	-2.24	103.36	106.89
2	AAA	607[B]	HEC	C4C-C3C-C2C	-2.24	103.36	106.89
2	YYY	601	HEC	CHD-C4C-C3C	-2.24	120.46	125.36
2	AAA	604	HEC	CHB-C4A-C3A	-2.24	120.78	125.48
2	AAA	606	HEC	CMA-C3A-C4A	2.24	128.66	124.71
2	MMM	608	HEC	C3B-C4B-NB	2.24	112.66	110.17
2	AAA	604	HEC	C2A-C1A-NA	2.24	112.50	110.32
2	MMM	608	HEC	CHA-C1A-C2A	-2.23	121.32	124.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	AAA	605	HEC	CAA-C2A-C3A	-2.23	123.73	127.88
2	YYY	605	HEC	CMB-C2B-C1B	2.22	128.43	125.04
2	YYY	606	HEC	CHA-C4D-C3D	-2.22	121.58	124.84
2	AAA	601	HEC	CHD-C4C-NC	-2.22	119.77	123.85
2	AAA	603	HEC	C1D-ND-C4D	-2.21	102.79	105.07
2	AAA	601	HEC	C3A-C4A-NA	2.21	113.76	109.69
2	MMM	602	HEC	C3B-C4B-NB	2.21	112.62	110.17
2	MMM	606	HEC	CMD-C2D-C1D	2.20	128.39	125.04
2	MMM	601	HEC	C4B-C3B-C2B	-2.20	103.69	106.90
2	AAA	607[A]	HEC	CHB-C4A-C3A	-2.20	120.87	125.48
2	AAA	607[B]	HEC	CHB-C4A-C3A	-2.20	120.87	125.48
2	AAA	607[A]	HEC	C4A-CHB-C1B	2.20	130.79	126.06
2	AAA	607[B]	HEC	C4A-CHB-C1B	2.20	130.79	126.06
2	MMM	601	HEC	CHC-C4B-NB	-2.19	121.67	124.37
2	MMM	603	HEC	CHC-C4B-C3B	-2.19	121.21	125.33
2	AAA	608	HEC	CHD-C1D-C2D	-2.19	120.65	126.73
2	YYY	602	HEC	C4D-C3D-C2D	-2.19	103.70	106.90
2	AAA	602	HEC	CHB-C4A-NA	2.19	126.81	124.44
2	YYY	607	HEC	CHD-C1D-ND	-2.19	121.68	124.37
2	YYY	604	HEC	CBA-CAA-C2A	-2.19	106.56	112.63
2	YYY	607	HEC	CHB-C1B-C2B	-2.18	121.57	124.98
2	YYY	603	HEC	CHA-C4D-C3D	-2.17	121.64	124.84
2	MMM	607	HEC	CMB-C2B-C1B	2.17	128.34	125.04
2	MMM	606	HEC	O2A-CGA-CBA	2.16	120.98	114.03
2	AAA	601	HEC	CHA-C1A-NA	-2.16	122.10	124.44
2	AAA	601	HEC	CHB-C1B-C2B	-2.16	121.61	124.98
2	MMM	603	HEC	C4C-NC-C1C	2.16	107.46	105.35
2	AAA	607[A]	HEC	CHC-C1C-C2C	-2.15	121.15	127.24
2	AAA	607[B]	HEC	CHC-C1C-C2C	-2.15	121.15	127.24
2	YYY	601	HEC	C2B-C1B-NB	2.15	112.45	109.88
2	AAA	602	HEC	C4B-C3B-C2B	-2.15	103.77	106.90
2	YYY	602	HEC	CHD-C4C-C3C	-2.14	120.68	125.36
2	MMM	607	HEC	O2D-CGD-O1D	2.14	128.63	123.30
2	YYY	602	HEC	C4C-NC-C1C	-2.13	103.26	105.35
2	MMM	608	HEC	CMB-C2B-C3B	2.11	131.85	126.12
2	AAA	608	HEC	CBB-CAB-C3B	-2.11	106.61	112.43
2	YYY	608	HEC	CHD-C1D-ND	-2.11	121.77	124.37
2	MMM	606	HEC	CHD-C1D-ND	-2.11	121.78	124.37
2	AAA	608	HEC	CAB-C3B-C2B	-2.10	123.93	127.53
2	YYY	601	HEC	O1D-CGD-CBD	-2.10	116.33	123.08
2	YYY	605	HEC	O1A-CGA-CBA	-2.10	116.34	123.08
2	MMM	603	HEC	CAA-CBA-CGA	-2.10	109.09	113.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	AAA	607[A]	HEC	C2C-C1C-NC	2.09	113.27	110.08
2	AAA	607[B]	HEC	C2C-C1C-NC	2.09	113.27	110.08
2	MMM	602	HEC	C1A-CHA-C4D	-2.09	121.55	126.06
2	YYY	606	HEC	CHD-C1D-C2D	-2.09	120.92	126.73
2	AAA	601	HEC	O2A-CGA-CBA	2.09	120.73	114.03
2	AAA	603	HEC	CHA-C1A-C2A	-2.07	121.58	124.94
2	YYY	604	HEC	CBC-CAC-C3C	2.07	118.14	112.43
2	YYY	606	HEC	CHB-C1B-C2B	-2.07	121.75	124.98
2	MMM	601	HEC	CHB-C4A-C3A	-2.06	121.16	125.48
2	AAA	608	HEC	CBC-CAC-C3C	2.05	118.10	112.43
2	AAA	603	HEC	CHB-C4A-NA	-2.05	122.22	124.44
2	MMM	603	HEC	CHA-C1A-C2A	-2.05	121.61	124.94
2	YYY	602	HEC	CMB-C2B-C1B	2.05	128.16	125.04
2	AAA	601	HEC	CMA-C3A-C4A	2.05	128.33	124.71
2	AAA	602	HEC	CHB-C1B-NB	-2.05	122.19	124.42
2	MMM	604	HEC	CHB-C4A-C3A	-2.05	121.19	125.48
2	MMM	605	HEC	CHD-C1D-C2D	-2.04	121.06	126.73
2	YYY	601	HEC	CAD-C3D-C4D	-2.04	121.09	124.66
2	MMM	604	HEC	CHD-C1D-C2D	-2.04	121.07	126.73
2	AAA	603	HEC	CHD-C1D-C2D	-2.04	121.07	126.73
2	AAA	602	HEC	C2C-C1C-NC	2.04	113.18	110.08
2	YYY	601	HEC	O2A-CGA-CBA	2.04	120.57	114.03
2	MMM	602	HEC	CAA-C2A-C3A	-2.04	124.09	127.88
2	YYY	608	HEC	C4C-NC-C1C	2.04	107.34	105.35
2	YYY	602	HEC	CHA-C1A-C2A	-2.03	121.64	124.94
2	MMM	608	HEC	CMB-C2B-C1B	2.03	128.13	125.04
2	MMM	606	HEC	C4B-C3B-C2B	-2.03	103.94	106.90
2	YYY	601	HEC	CAD-CBD-CGD	-2.03	109.24	113.60
2	AAA	606	HEC	CHD-C1D-C2D	-2.03	121.10	126.73
2	MMM	603	HEC	C4A-NA-C1A	-2.02	103.37	105.35
2	AAA	604	HEC	CAD-C3D-C2D	2.02	131.64	127.88
2	MMM	608	HEC	CAC-C3C-C2C	2.02	130.10	126.86
2	YYY	606	HEC	CMB-C2B-C3B	2.02	131.60	126.12
2	MMM	601	HEC	O2D-CGD-CBD	2.02	120.52	114.03
2	YYY	604	HEC	CBD-CAD-C3D	-2.02	107.02	112.63
2	YYY	602	HEC	C4A-C3A-C2A	-2.01	104.00	106.94
2	YYY	608	HEC	CHC-C4B-NB	2.01	126.85	124.37
2	AAA	606	HEC	CMC-C2C-C1C	2.01	128.43	125.37
2	YYY	603	HEC	CAB-C3B-C2B	-2.00	124.11	127.53

All (25) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	AAA	601	HEC	NA
2	AAA	602	HEC	NA
2	AAA	603	HEC	NA
2	AAA	604	HEC	NA
2	AAA	605	HEC	NA
2	AAA	606	HEC	NA
2	AAA	607[A]	HEC	NA
2	AAA	607[B]	HEC	NA
2	AAA	608	HEC	NA
2	MMM	601	HEC	NA
2	MMM	602	HEC	NA
2	MMM	603	HEC	NA
2	MMM	604	HEC	NA
2	MMM	605	HEC	NA
2	MMM	606	HEC	NA
2	MMM	607	HEC	NA
2	MMM	608	HEC	NA
2	YYY	601	HEC	NA
2	YYY	602	HEC	NA
2	YYY	603	HEC	NA
2	YYY	604	HEC	NA
2	YYY	605	HEC	NA
2	YYY	606	HEC	NA
2	YYY	607	HEC	NA
2	YYY	608	HEC	NA

All (150) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	AAA	608	HEC	C2C-C3C-CAC-CBC
2	MMM	608	HEC	C2C-C3C-CAC-CBC
2	YYY	601	HEC	C4D-C3D-CAD-CBD
2	YYY	608	HEC	C2C-C3C-CAC-CBC
2	MMM	601	HEC	C4C-C3C-CAC-CBC
2	AAA	601	HEC	C2C-C3C-CAC-CBC
2	AAA	603	HEC	C2C-C3C-CAC-CBC
2	AAA	605	HEC	C2C-C3C-CAC-CBC
2	MMM	601	HEC	C2C-C3C-CAC-CBC
2	AAA	606	HEC	C4C-C3C-CAC-CBC
2	MMM	602	HEC	C4C-C3C-CAC-CBC
2	MMM	608	HEC	C4C-C3C-CAC-CBC
2	MMM	606	HEC	C2B-C3B-CAB-CBB
2	MMM	606	HEC	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
2	AAA	608	HEC	C4C-C3C-CAC-CBC
2	YYY	608	HEC	C4C-C3C-CAC-CBC
2	MMM	602	HEC	C2C-C3C-CAC-CBC
2	AAA	603	HEC	C4C-C3C-CAC-CBC
2	YYY	601	HEC	C2D-C3D-CAD-CBD
2	YYY	605	HEC	C4C-C3C-CAC-CBC
2	AAA	601	HEC	C4C-C3C-CAC-CBC
2	AAA	605	HEC	C4C-C3C-CAC-CBC
2	AAA	606	HEC	C2C-C3C-CAC-CBC
2	MMM	602	HEC	C2B-C3B-CAB-CBB
2	MMM	604	HEC	C4C-C3C-CAC-CBC
2	YYY	601	HEC	C4C-C3C-CAC-CBC
2	AAA	607[A]	HEC	C2C-C3C-CAC-CBC
2	AAA	607[B]	HEC	C2C-C3C-CAC-CBC
2	MMM	603	HEC	C4C-C3C-CAC-CBC
2	YYY	601	HEC	C2C-C3C-CAC-CBC
2	YYY	602	HEC	C4C-C3C-CAC-CBC
2	AAA	602	HEC	C4C-C3C-CAC-CBC
2	MMM	605	HEC	C4C-C3C-CAC-CBC
2	MMM	607	HEC	C4C-C3C-CAC-CBC
2	YYY	603	HEC	C4C-C3C-CAC-CBC
2	AAA	607[A]	HEC	C2B-C3B-CAB-CBB
2	AAA	607[B]	HEC	C2B-C3B-CAB-CBB
2	MMM	607	HEC	C2C-C3C-CAC-CBC
2	YYY	605	HEC	C2C-C3C-CAC-CBC
2	AAA	604	HEC	C4C-C3C-CAC-CBC
2	MMM	604	HEC	C2B-C3B-CAB-CBB
2	YYY	603	HEC	C2C-C3C-CAC-CBC
2	MMM	607	HEC	C2B-C3B-CAB-CBB
2	YYY	602	HEC	C2C-C3C-CAC-CBC
2	AAA	607[A]	HEC	C4C-C3C-CAC-CBC
2	AAA	607[B]	HEC	C4C-C3C-CAC-CBC
2	YYY	607	HEC	C4C-C3C-CAC-CBC
2	MMM	606	HEC	C2C-C3C-CAC-CBC
2	AAA	602	HEC	C2C-C3C-CAC-CBC
2	AAA	601	HEC	C2B-C3B-CAB-CBB
2	MMM	604	HEC	C2C-C3C-CAC-CBC
2	MMM	602	HEC	C4B-C3B-CAB-CBB
2	YYY	601	HEC	C3D-CAD-CBD-CGD
2	MMM	606	HEC	C4C-C3C-CAC-CBC
2	AAA	604	HEC	C2C-C3C-CAC-CBC
2	AAA	608	HEC	C3D-CAD-CBD-CGD

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Mol	Chain	Res	Type	Atoms
2	YYY	603	HEC	C2B-C3B-CAB-CBB
2	YYY	604	HEC	C2B-C3B-CAB-CBB
2	AAA	604	HEC	C2B-C3B-CAB-CBB
2	AAA	604	HEC	C4B-C3B-CAB-CBB
2	MMM	603	HEC	C2C-C3C-CAC-CBC
2	AAA	602	HEC	C4B-C3B-CAB-CBB
2	YYY	607	HEC	C2B-C3B-CAB-CBB
2	MMM	607	HEC	C2A-CAA-CBA-CGA
2	YYY	606	HEC	C2B-C3B-CAB-CBB
2	YYY	607	HEC	C2C-C3C-CAC-CBC
2	MMM	605	HEC	C2C-C3C-CAC-CBC
2	YYY	601	HEC	C2B-C3B-CAB-CBB
2	AAA	608	HEC	C2B-C3B-CAB-CBB
2	MMM	604	HEC	C4B-C3B-CAB-CBB
2	MMM	601	HEC	C2B-C3B-CAB-CBB
2	YYY	606	HEC	C4C-C3C-CAC-CBC
2	MMM	608	HEC	C2B-C3B-CAB-CBB
2	YYY	606	HEC	C2C-C3C-CAC-CBC
2	AAA	602	HEC	C2B-C3B-CAB-CBB
2	AAA	607[B]	HEC	C2A-CAA-CBA-CGA
2	YYY	602	HEC	C4B-C3B-CAB-CBB
2	AAA	607[A]	HEC	C4B-C3B-CAB-CBB
2	AAA	607[B]	HEC	C4B-C3B-CAB-CBB
2	AAA	606	HEC	C2B-C3B-CAB-CBB
2	YYY	603	HEC	CAD-CBD-CGD-O2D
2	YYY	601	HEC	C4B-C3B-CAB-CBB
2	AAA	603	HEC	CAD-CBD-CGD-O1D
2	AAA	602	HEC	CAA-CBA-CGA-O1A
2	YYY	602	HEC	C2B-C3B-CAB-CBB
2	YYY	608	HEC	CAD-CBD-CGD-O2D
2	YYY	601	HEC	CAA-CBA-CGA-O1A
2	YYY	603	HEC	CAD-CBD-CGD-O1D
2	YYY	603	HEC	C4B-C3B-CAB-CBB
2	MMM	601	HEC	CAA-CBA-CGA-O2A
2	MMM	607	HEC	CAA-CBA-CGA-O2A
2	MMM	608	HEC	CAD-CBD-CGD-O2D
2	YYY	608	HEC	CAD-CBD-CGD-O1D
2	AAA	603	HEC	C2D-C3D-CAD-CBD
2	AAA	604	HEC	CAA-CBA-CGA-O2A
2	AAA	607[A]	HEC	CAA-CBA-CGA-O2A
2	MMM	603	HEC	CAD-CBD-CGD-O1D
2	MMM	607	HEC	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
2	AAA	602	HEC	CAA-CBA-CGA-O2A
2	MMM	605	HEC	CAA-CBA-CGA-O1A
2	YYY	605	HEC	CAA-CBA-CGA-O1A
2	MMM	608	HEC	CAD-CBD-CGD-O1D
2	AAA	604	HEC	CAA-CBA-CGA-O1A
2	YYY	601	HEC	CAA-CBA-CGA-O2A
2	YYY	602	HEC	CAA-CBA-CGA-O1A
2	AAA	607[A]	HEC	CAA-CBA-CGA-O1A
2	MMM	603	HEC	CAD-CBD-CGD-O2D
2	MMM	604	HEC	CAA-CBA-CGA-O1A
2	AAA	603	HEC	CAD-CBD-CGD-O2D
2	YYY	604	HEC	CAA-CBA-CGA-O2A
2	YYY	605	HEC	CAA-CBA-CGA-O2A
2	MMM	602	HEC	CAA-CBA-CGA-O2A
2	MMM	605	HEC	CAA-CBA-CGA-O2A
2	AAA	607[A]	HEC	CAD-CBD-CGD-O1D
2	AAA	607[B]	HEC	CAD-CBD-CGD-O1D
2	YYY	602	HEC	CAA-CBA-CGA-O2A
2	YYY	603	HEC	CAA-CBA-CGA-O2A
2	MMM	604	HEC	CAA-CBA-CGA-O2A
2	YYY	602	HEC	CAD-CBD-CGD-O1D
2	YYY	604	HEC	CAA-CBA-CGA-O1A
2	MMM	601	HEC	CAA-CBA-CGA-O1A
2	YYY	603	HEC	CAA-CBA-CGA-O1A
2	AAA	603	HEC	CAA-CBA-CGA-O2A
2	AAA	607[B]	HEC	CAA-CBA-CGA-O1A
2	YYY	604	HEC	C4C-C3C-CAC-CBC
2	YYY	602	HEC	CAD-CBD-CGD-O2D
2	MMM	602	HEC	CAA-CBA-CGA-O1A
2	AAA	605	HEC	CAA-CBA-CGA-O2A
2	MMM	607	HEC	CAD-CBD-CGD-O1D
2	MMM	607	HEC	CAD-CBD-CGD-O2D
2	YYY	607	HEC	CAA-CBA-CGA-O2A
2	AAA	605	HEC	CAA-CBA-CGA-O1A
2	AAA	607[A]	HEC	CAD-CBD-CGD-O2D
2	AAA	607[B]	HEC	CAA-CBA-CGA-O2A
2	AAA	607[B]	HEC	CAD-CBD-CGD-O2D
2	YYY	607	HEC	CAA-CBA-CGA-O1A
2	AAA	603	HEC	CAA-CBA-CGA-O1A
2	MMM	603	HEC	C4B-C3B-CAB-CBB
2	AAA	602	HEC	C4D-C3D-CAD-CBD
2	MMM	605	HEC	CAD-CBD-CGD-O2D

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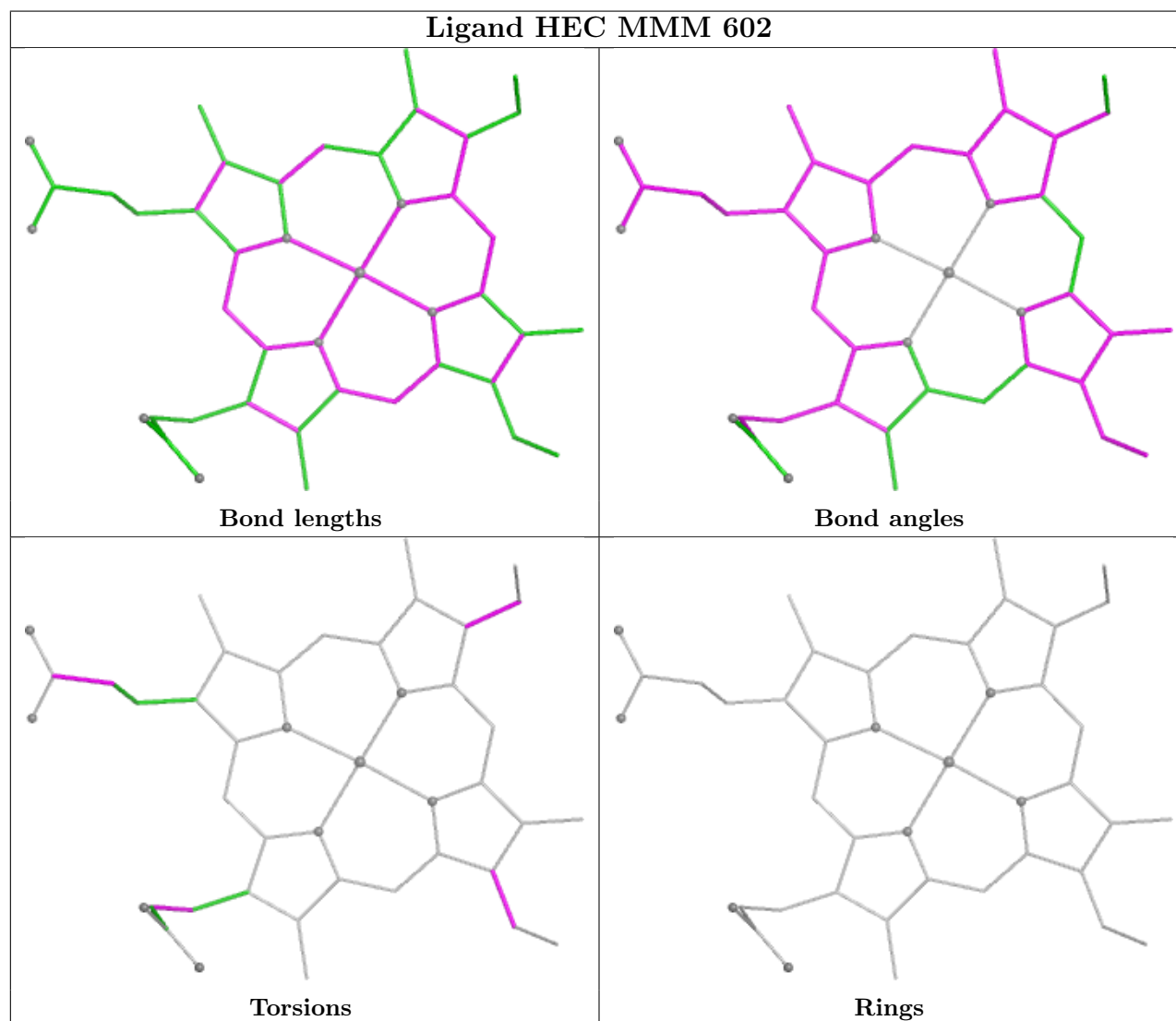
Mol	Chain	Res	Type	Atoms
2	YYY	601	HEC	CAD-CBD-CGD-O1D
2	MMM	602	HEC	C3D-CAD-CBD-CGD
2	AAA	601	HEC	CAA-CBA-CGA-O1A
2	YYY	604	HEC	C4B-C3B-CAB-CBB
2	YYY	607	HEC	C4D-C3D-CAD-CBD
2	MMM	605	HEC	CAD-CBD-CGD-O1D
2	AAA	601	HEC	CAD-CBD-CGD-O2D
2	YYY	601	HEC	CAD-CBD-CGD-O2D
2	AAA	601	HEC	CAA-CBA-CGA-O2A
2	YYY	607	HEC	CAD-CBD-CGD-O1D

There are no ring outliers.

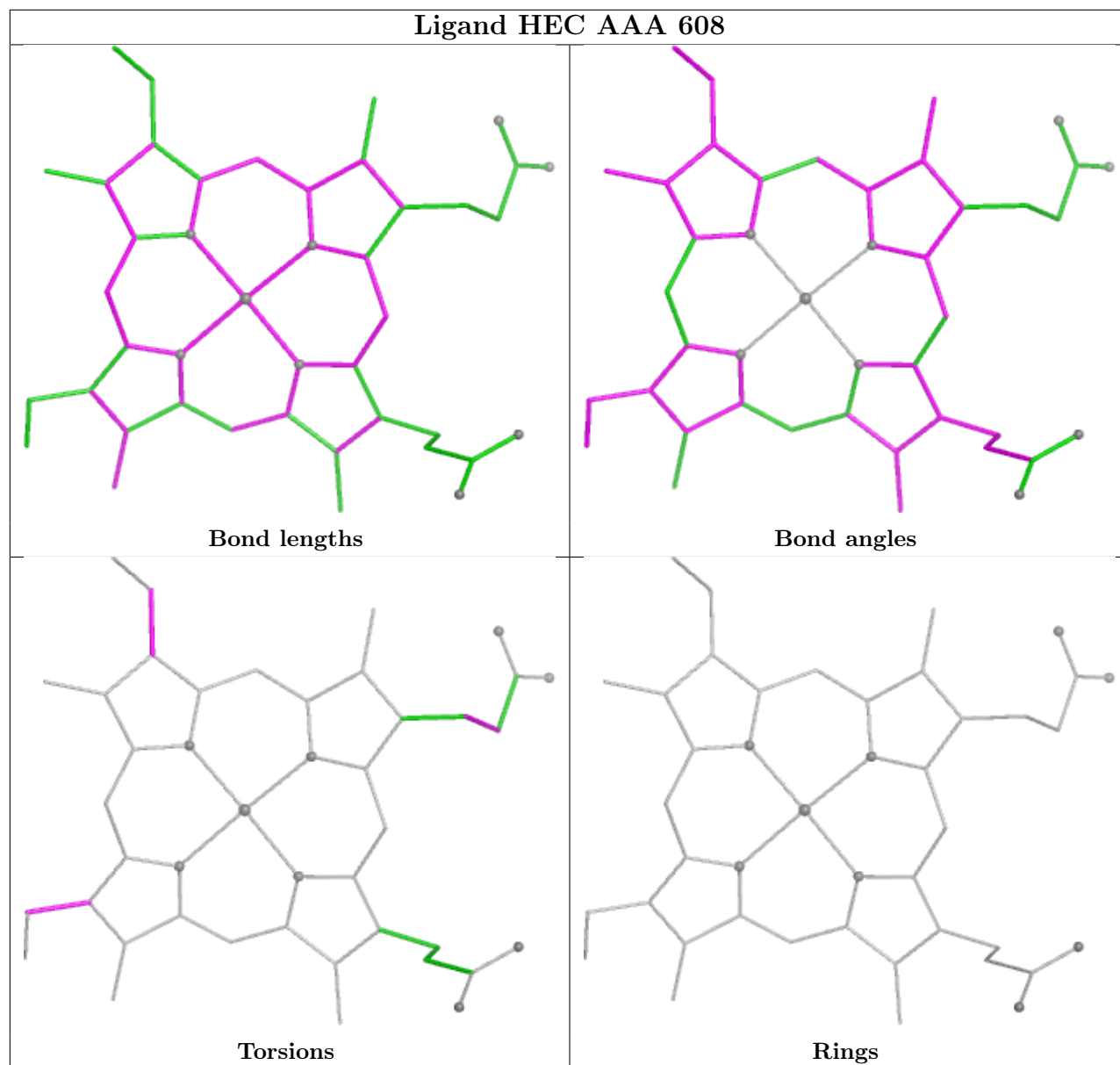
26 monomers are involved in 88 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	MMM	602	HEC	3	0
2	AAA	608	HEC	3	0
2	MMM	604	HEC	5	0
2	YYY	608	HEC	1	0
2	MMM	605	HEC	3	0
2	YYY	606	HEC	2	0
2	AAA	601	HEC	4	0
2	AAA	603	HEC	8	0
2	MMM	606	HEC	4	0
2	YYY	603	HEC	1	0
2	YYY	607	HEC	5	0
2	AAA	602	HEC	7	0
2	AAA	607[A]	HEC	1	0
2	YYY	602	HEC	2	0
2	YYY	604	HEC	3	0
4	YYY	610	PO4	2	0
2	YYY	605	HEC	4	0
2	AAA	606	HEC	5	0
2	AAA	605	HEC	7	0
2	MMM	603	HEC	3	0
2	AAA	604	HEC	3	0
2	MMM	607	HEC	4	0
2	YYY	601	HEC	8	0
2	MMM	608	HEC	1	0
2	MMM	601	HEC	2	0
4	AAA	610	PO4	1	0

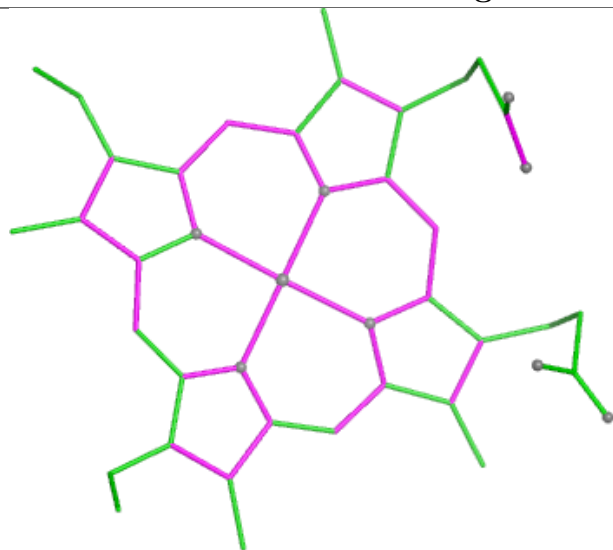
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



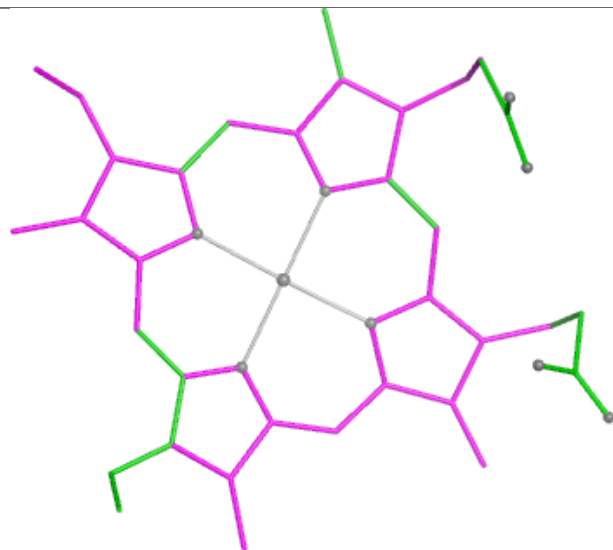
Ligand HEC AAA 608



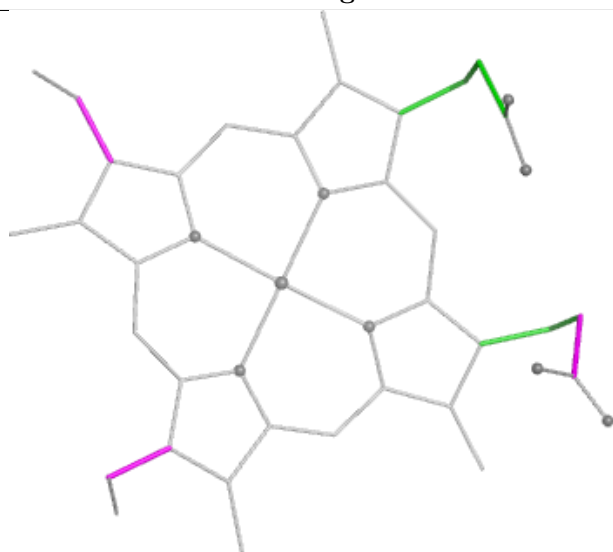
Ligand HEC MMM 604



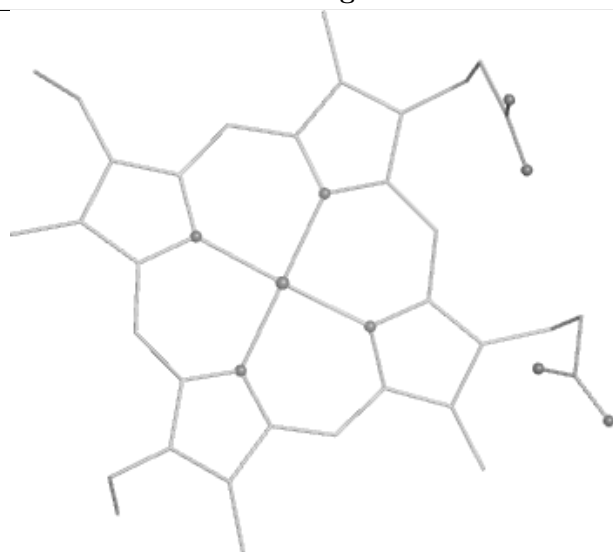
Bond lengths



Bond angles

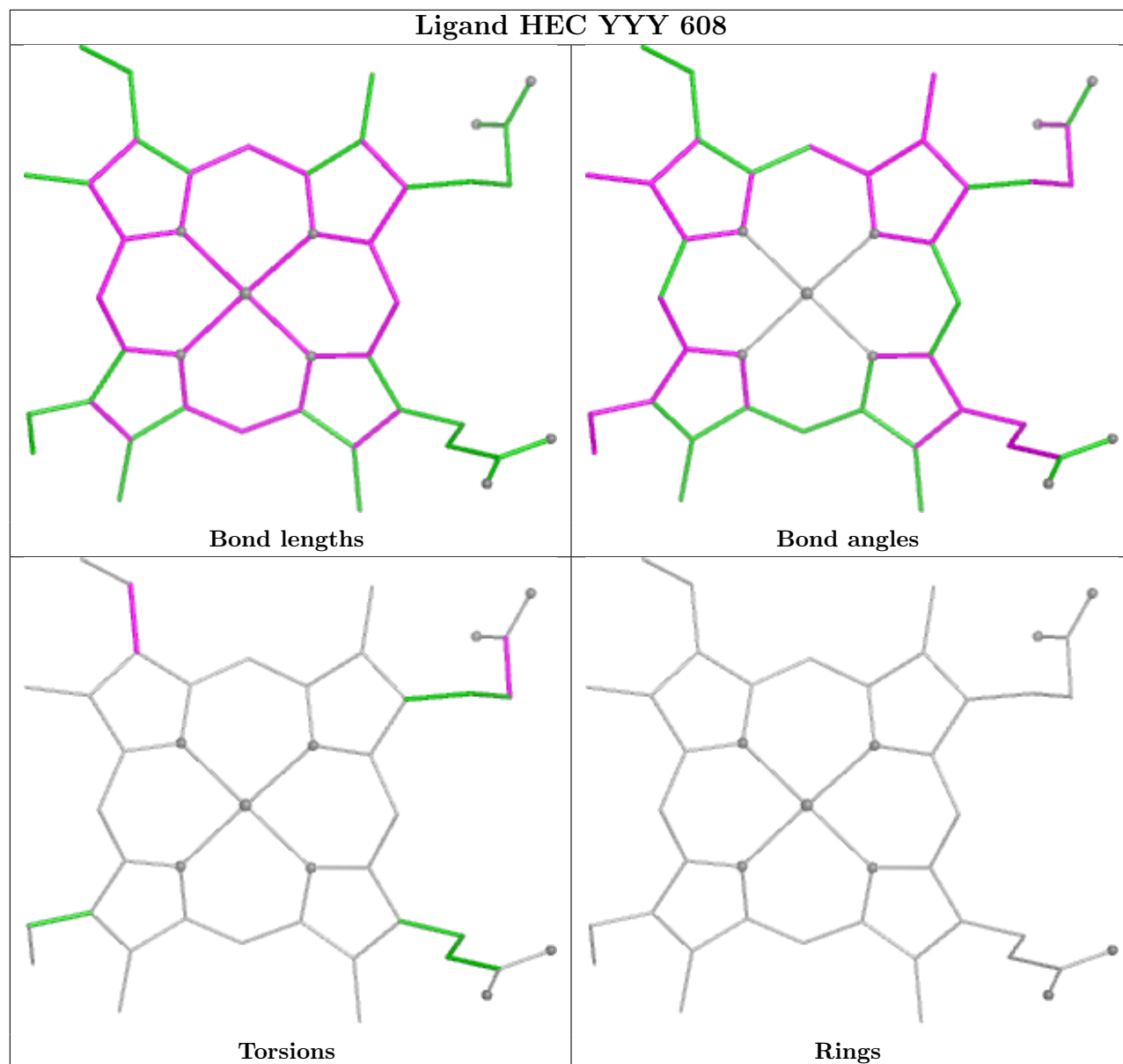


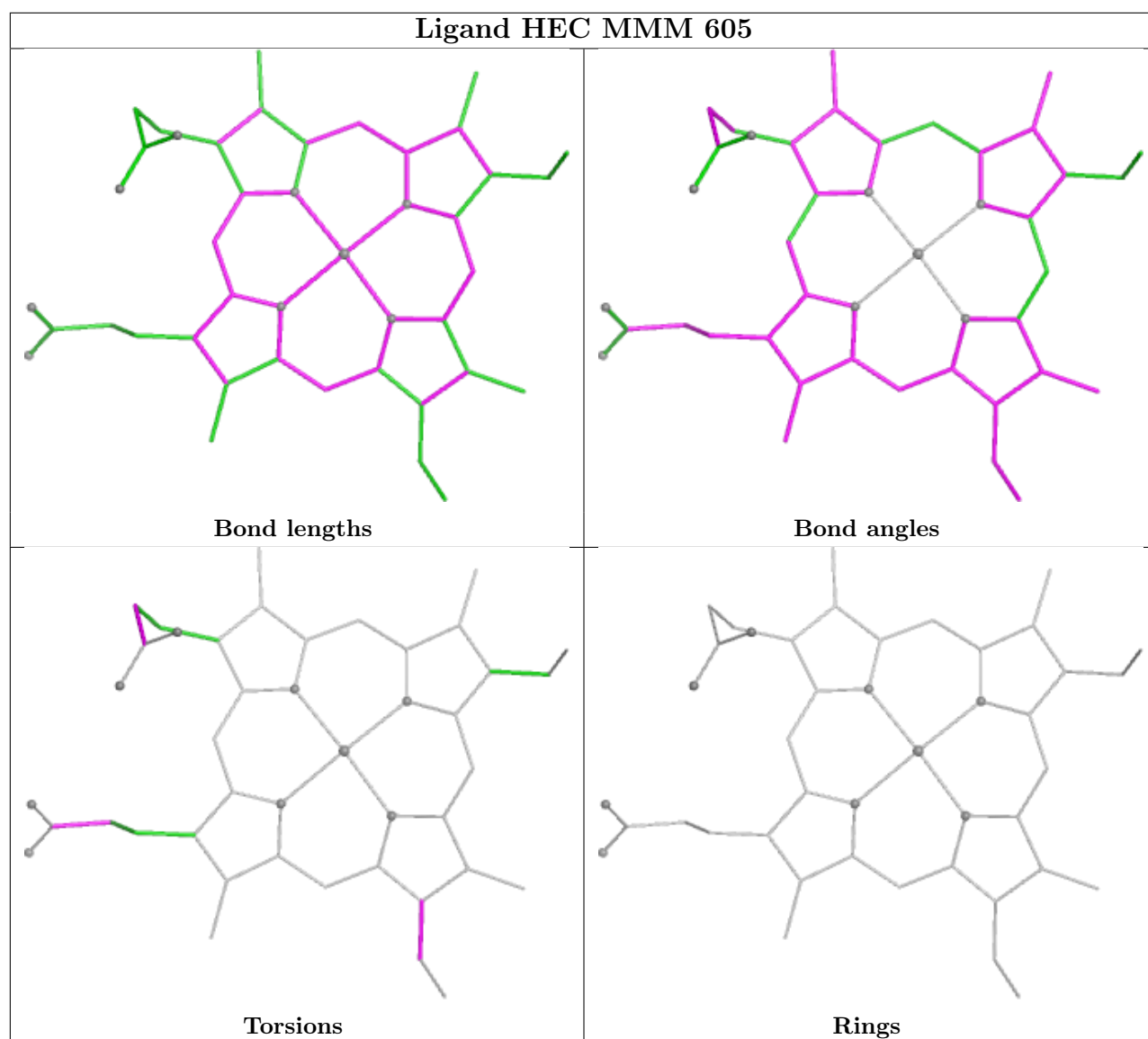
Torsions



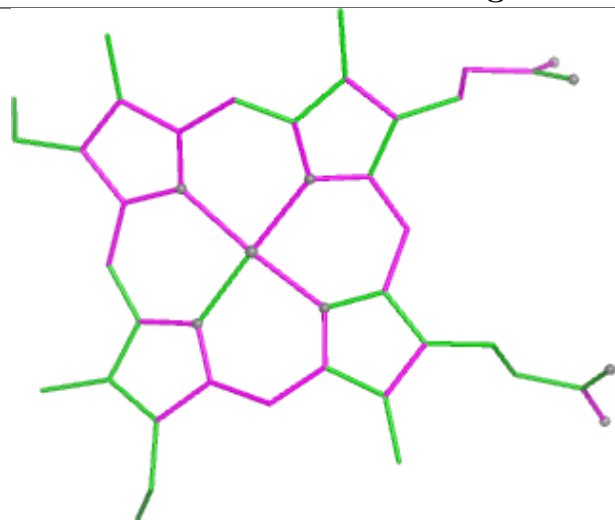
Rings

Ligand HEC YYY 608

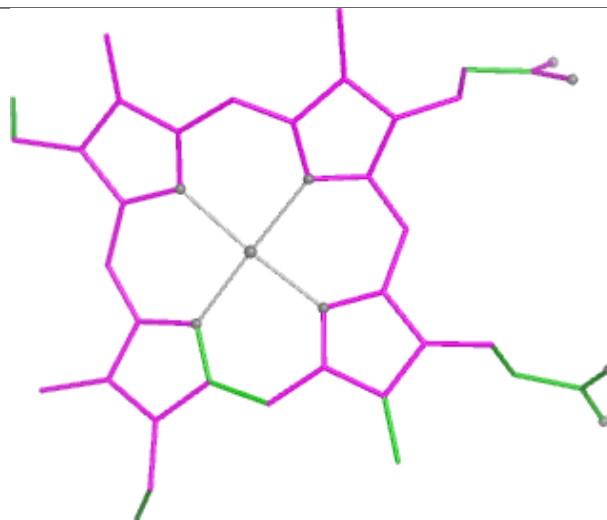




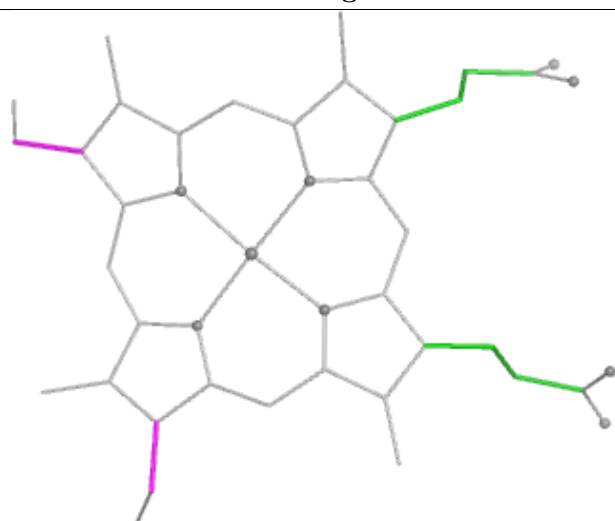
Ligand HEC YYY 606



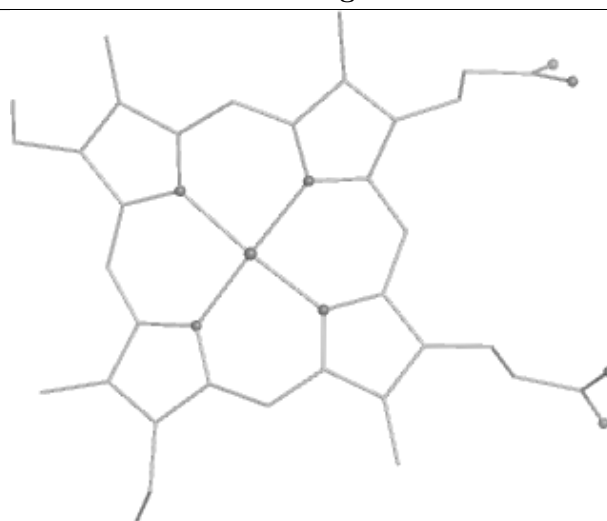
Bond lengths



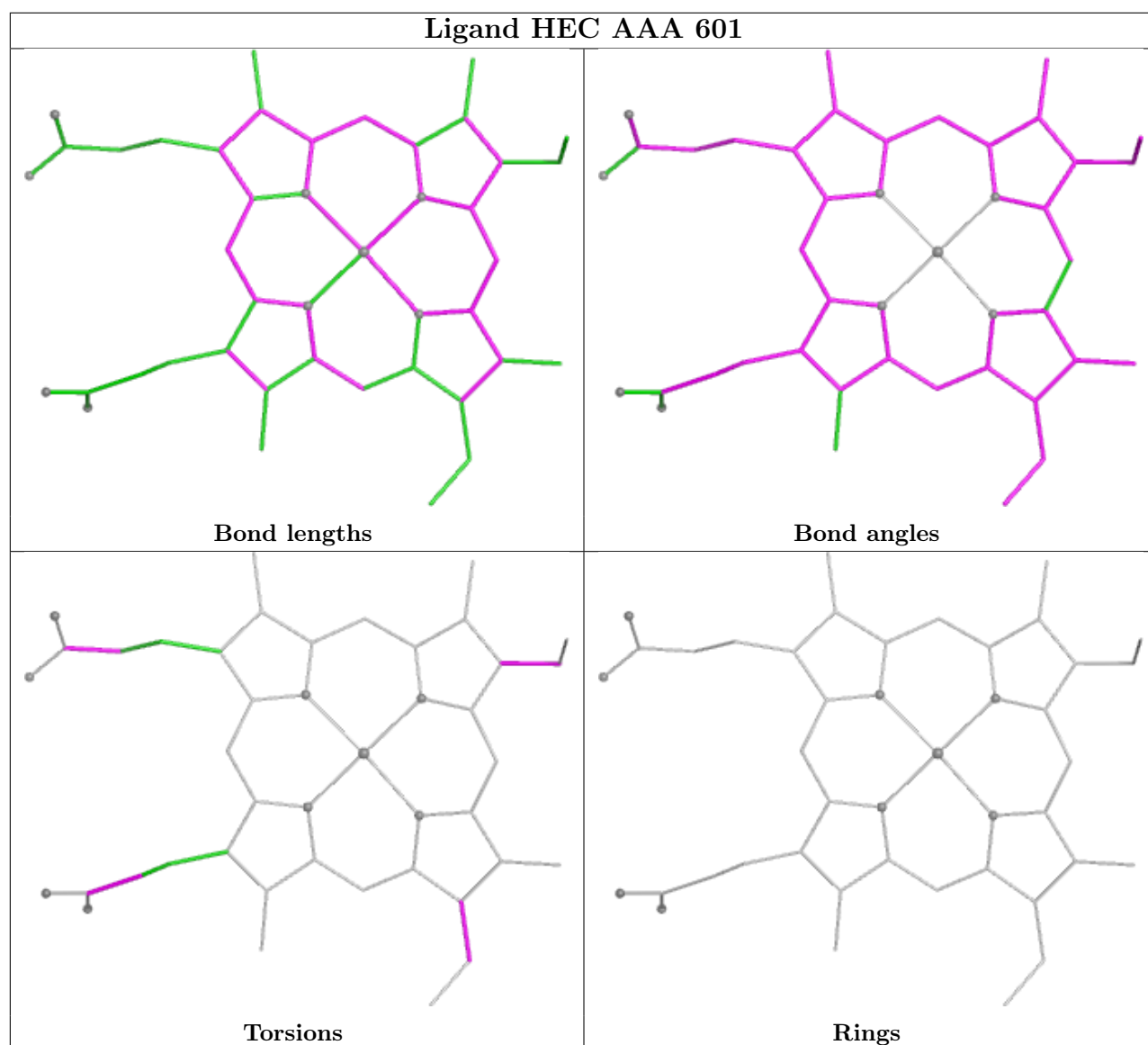
Bond angles



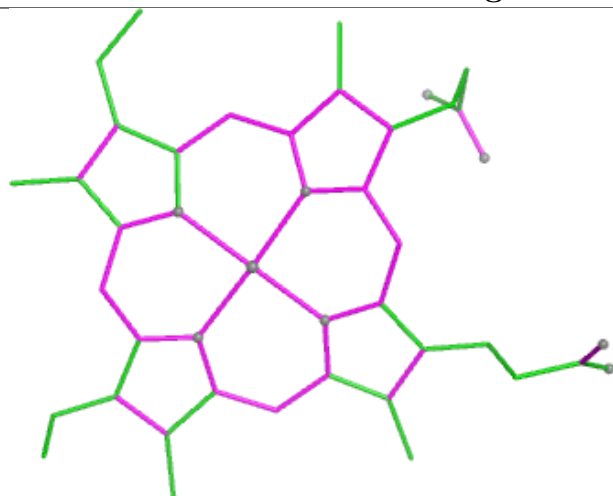
Torsions



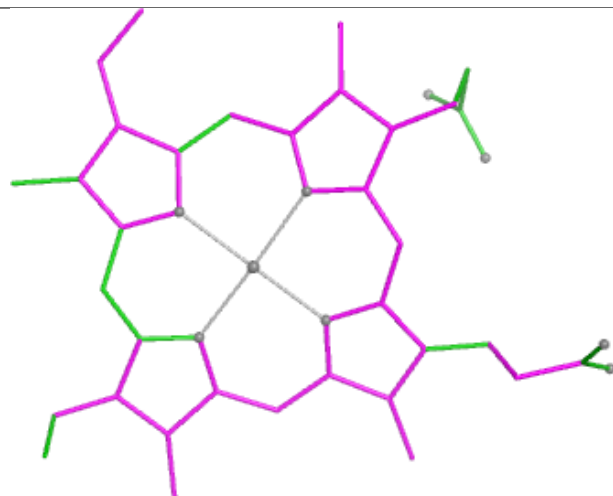
Rings



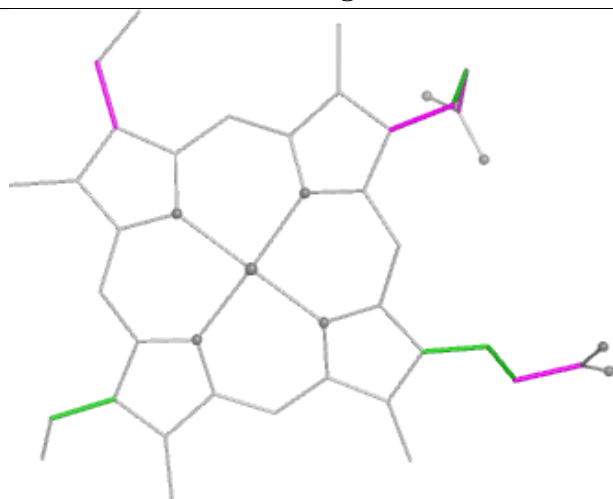
Ligand HEC AAA 603



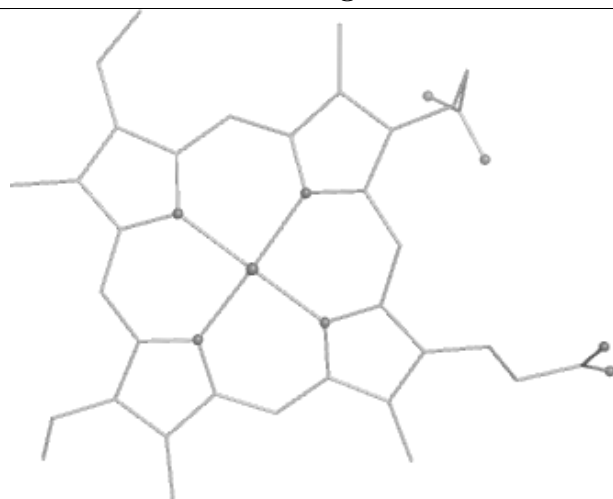
Bond lengths



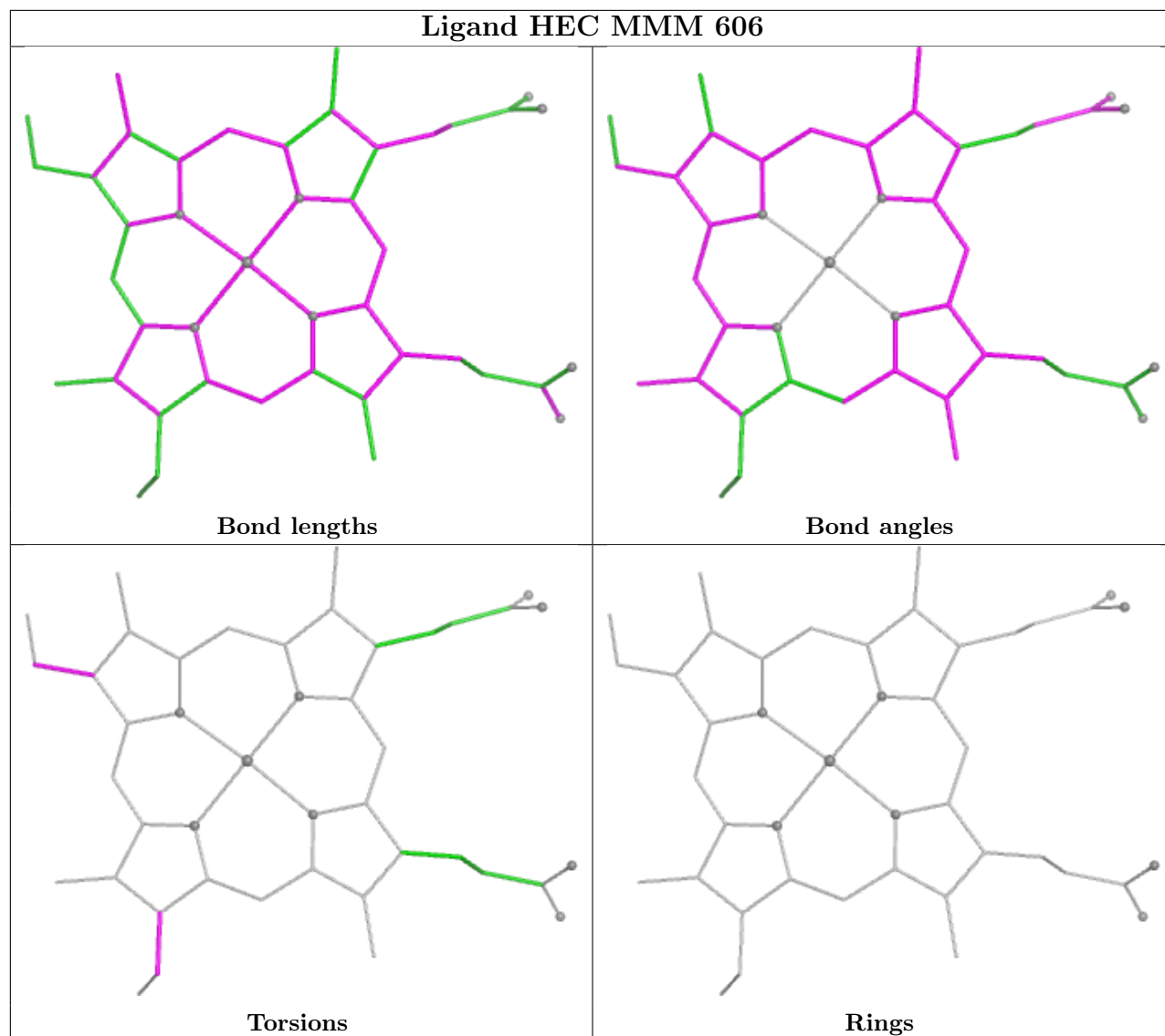
Bond angles



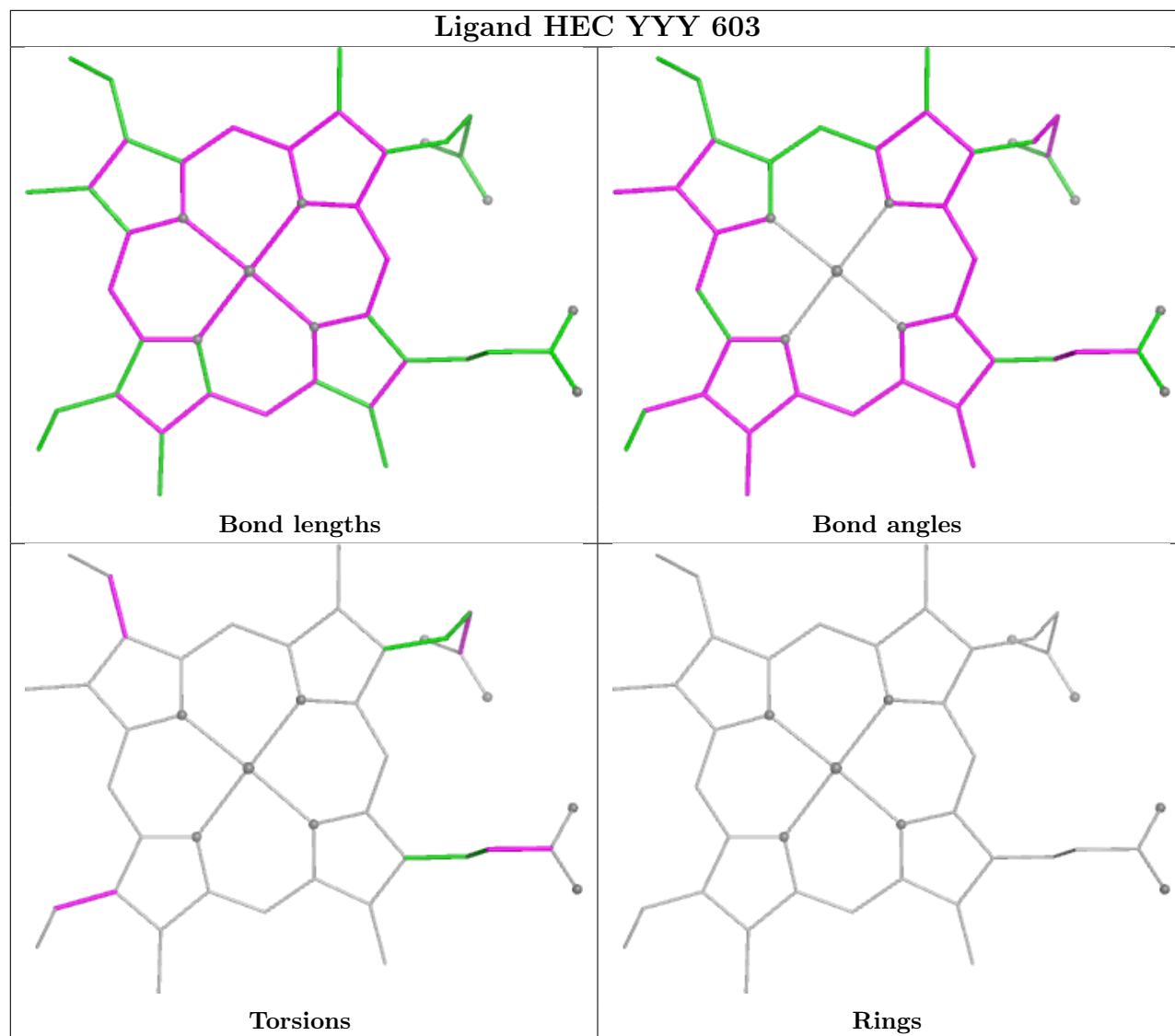
Torsions



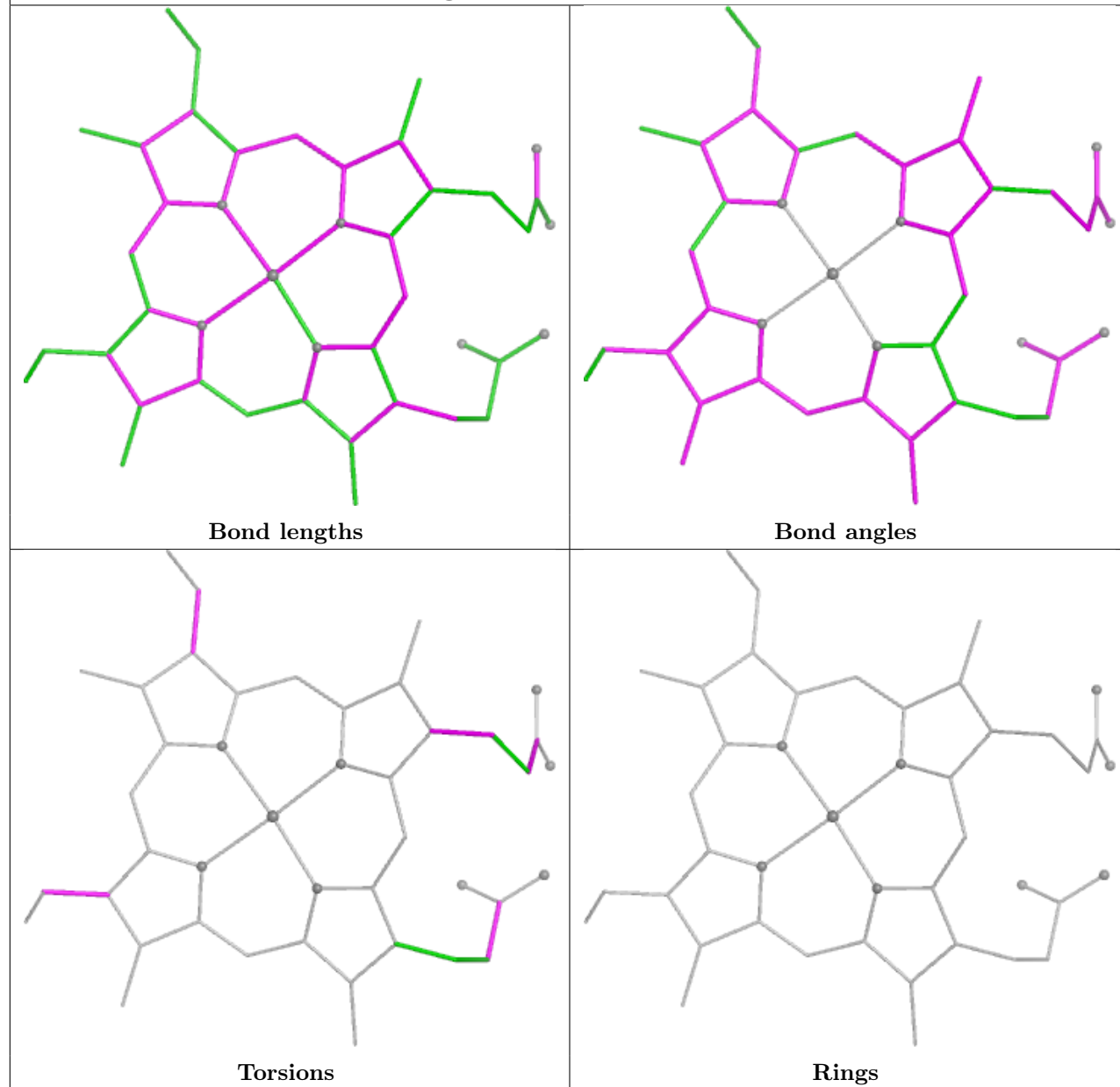
Rings



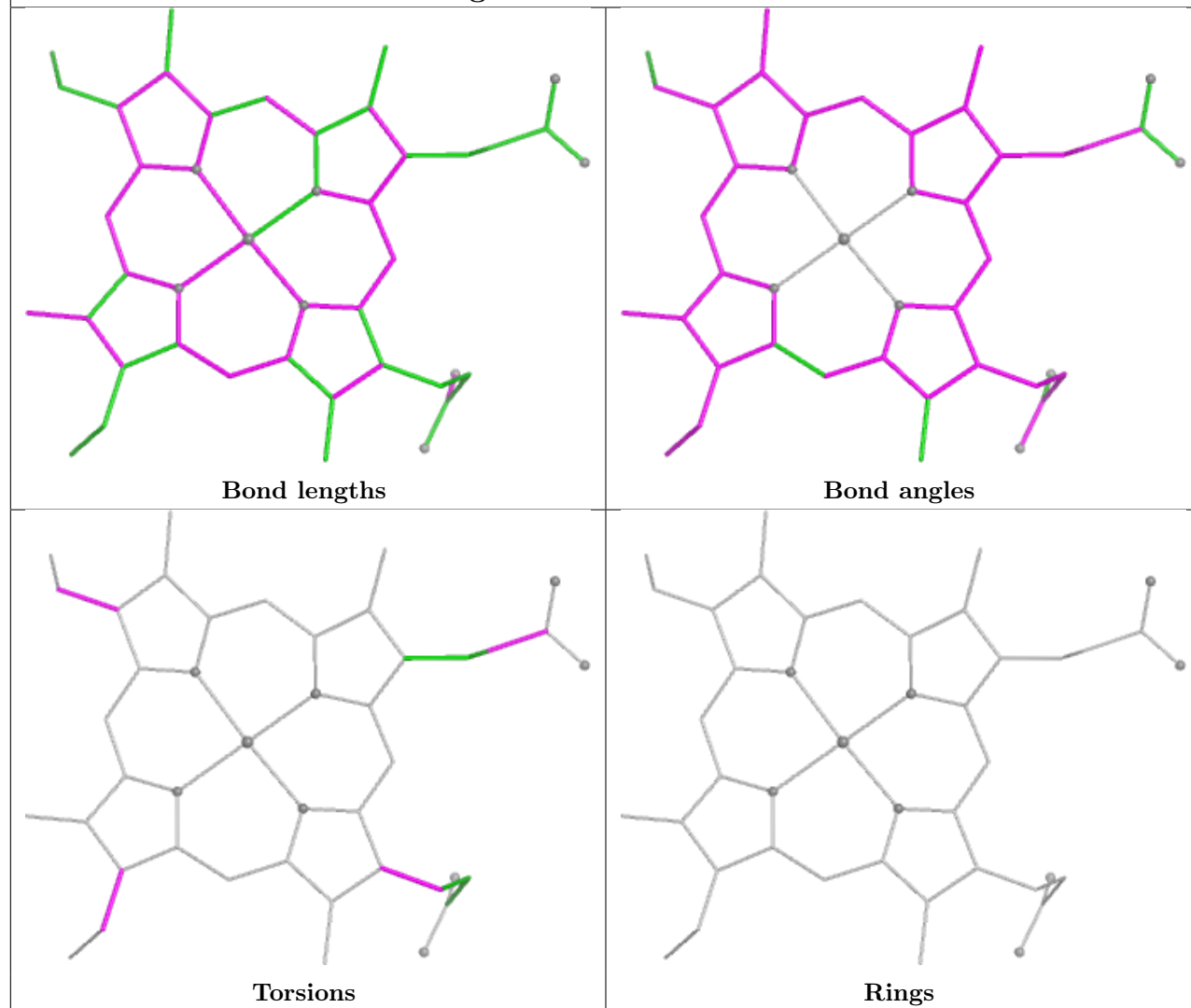
Ligand HEC YYY 603



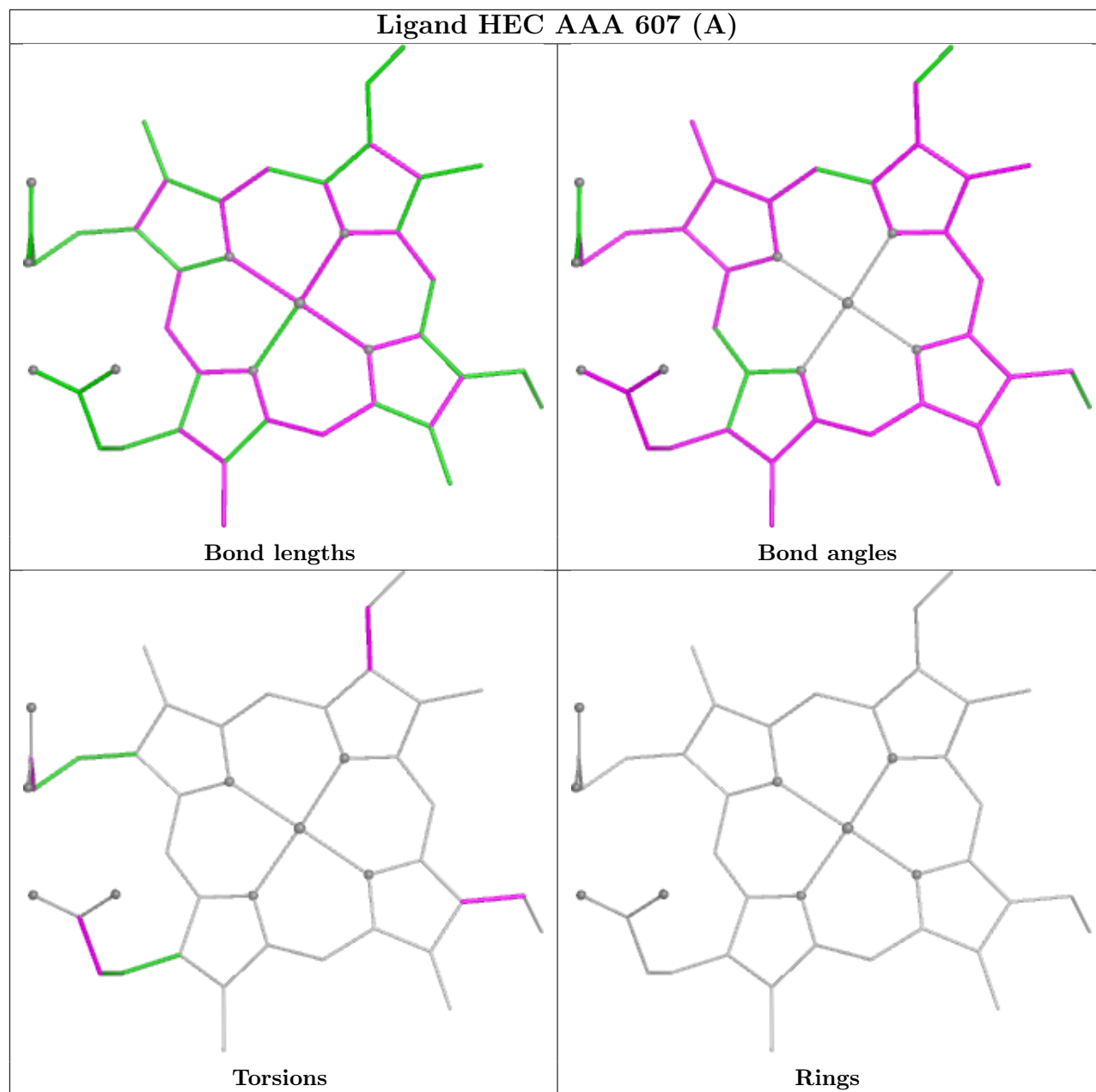
Ligand HEC YYY 607



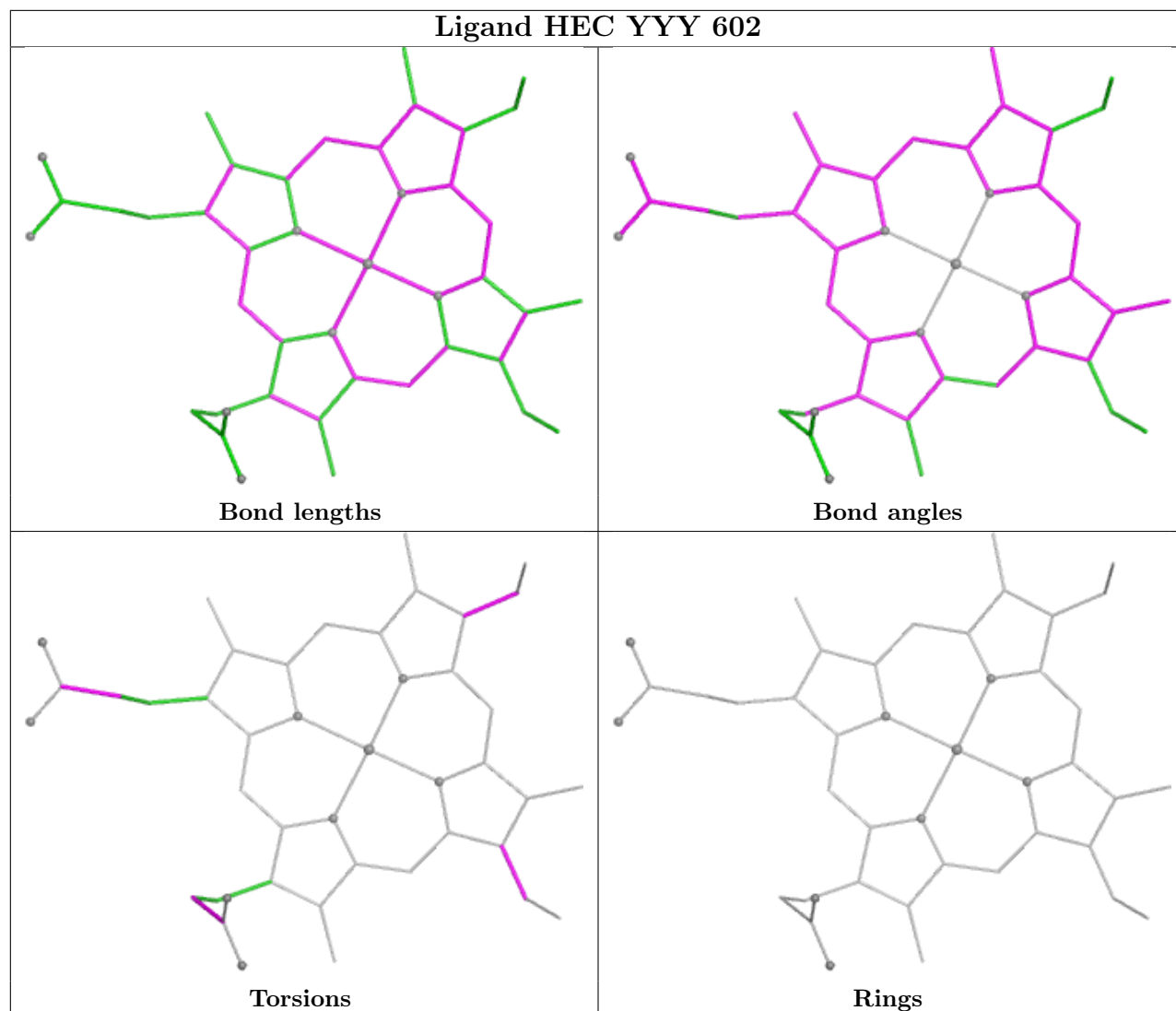
Ligand HEC AAA 602



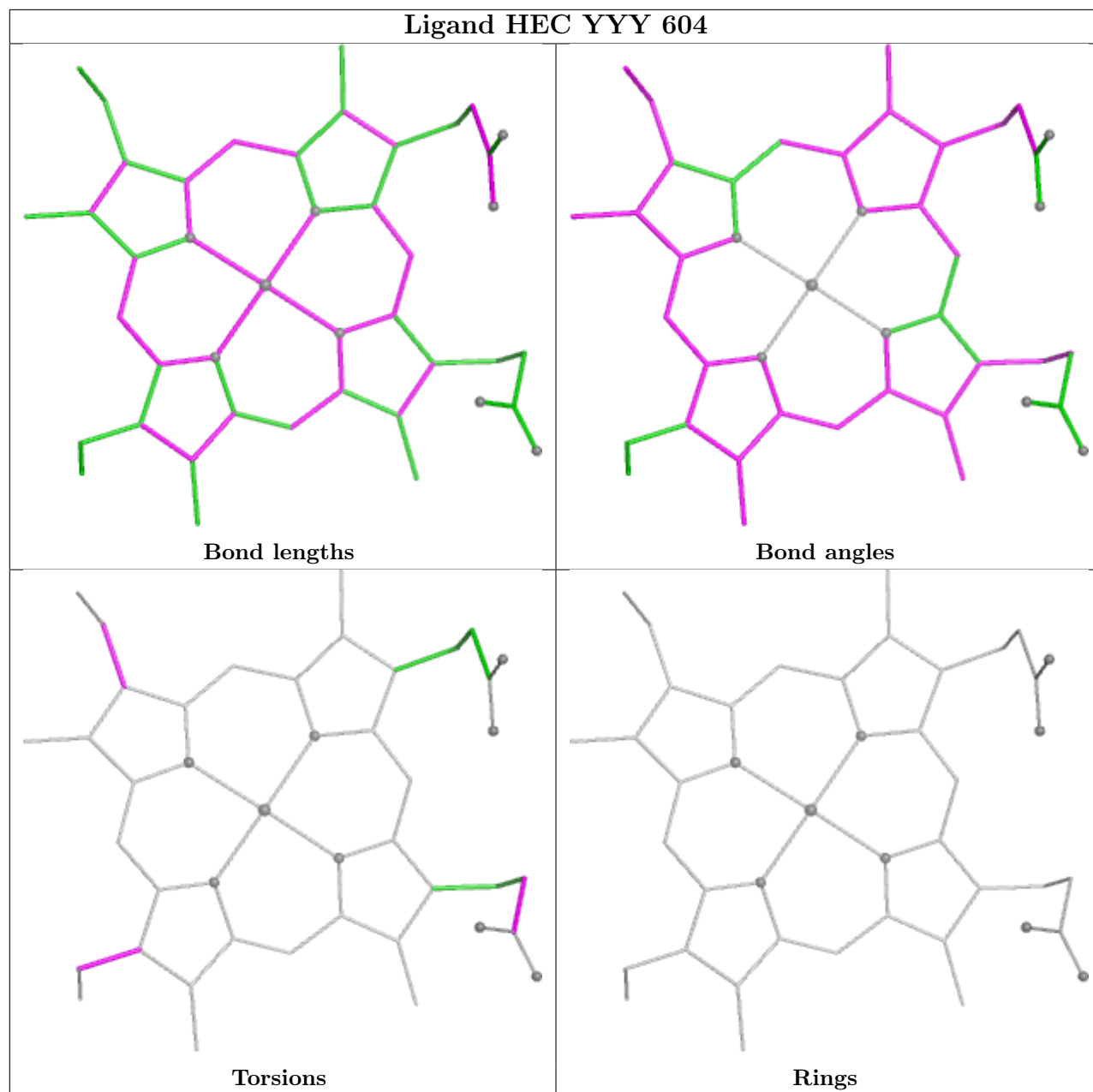
Ligand HEC AAA 607 (A)

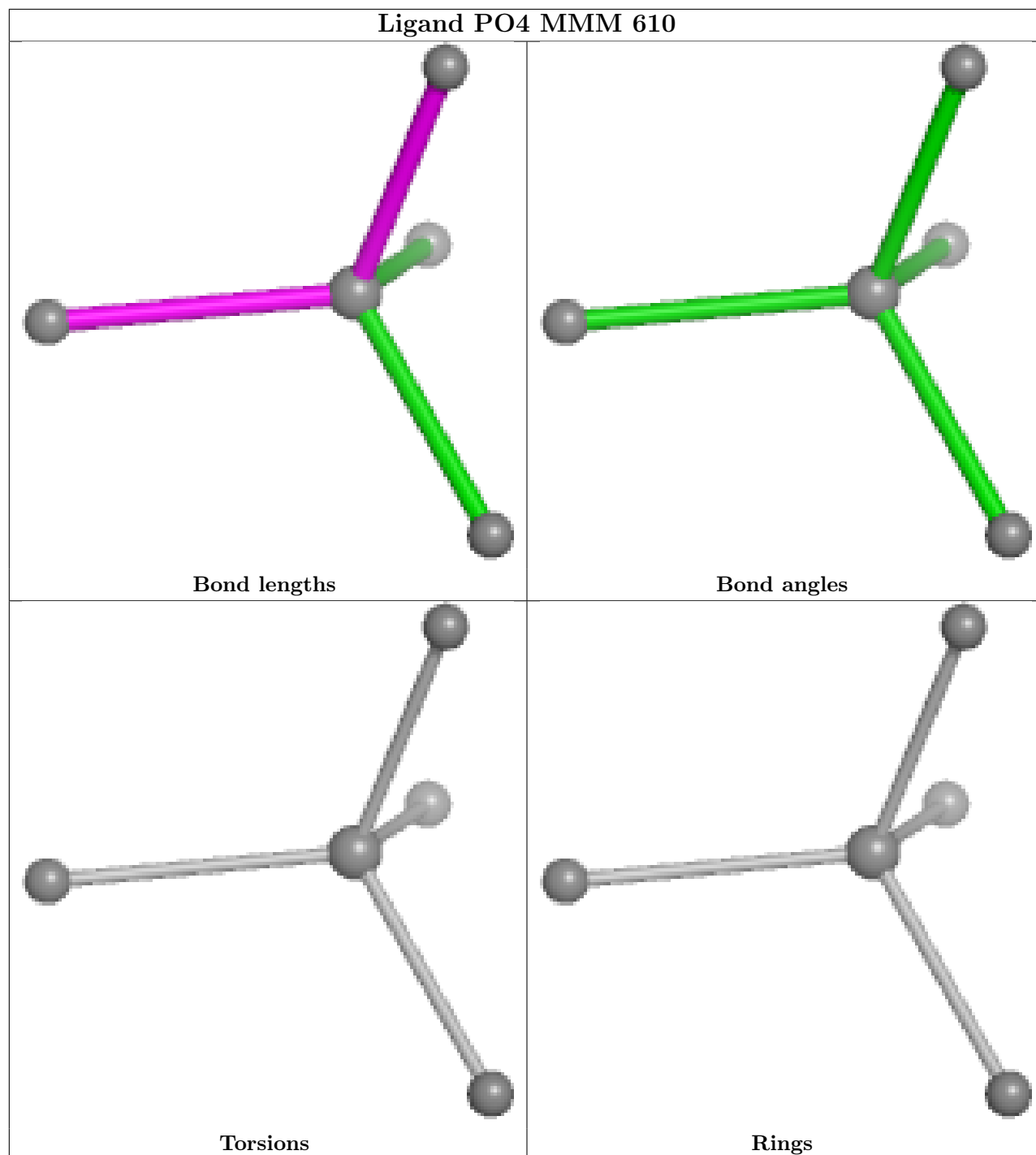


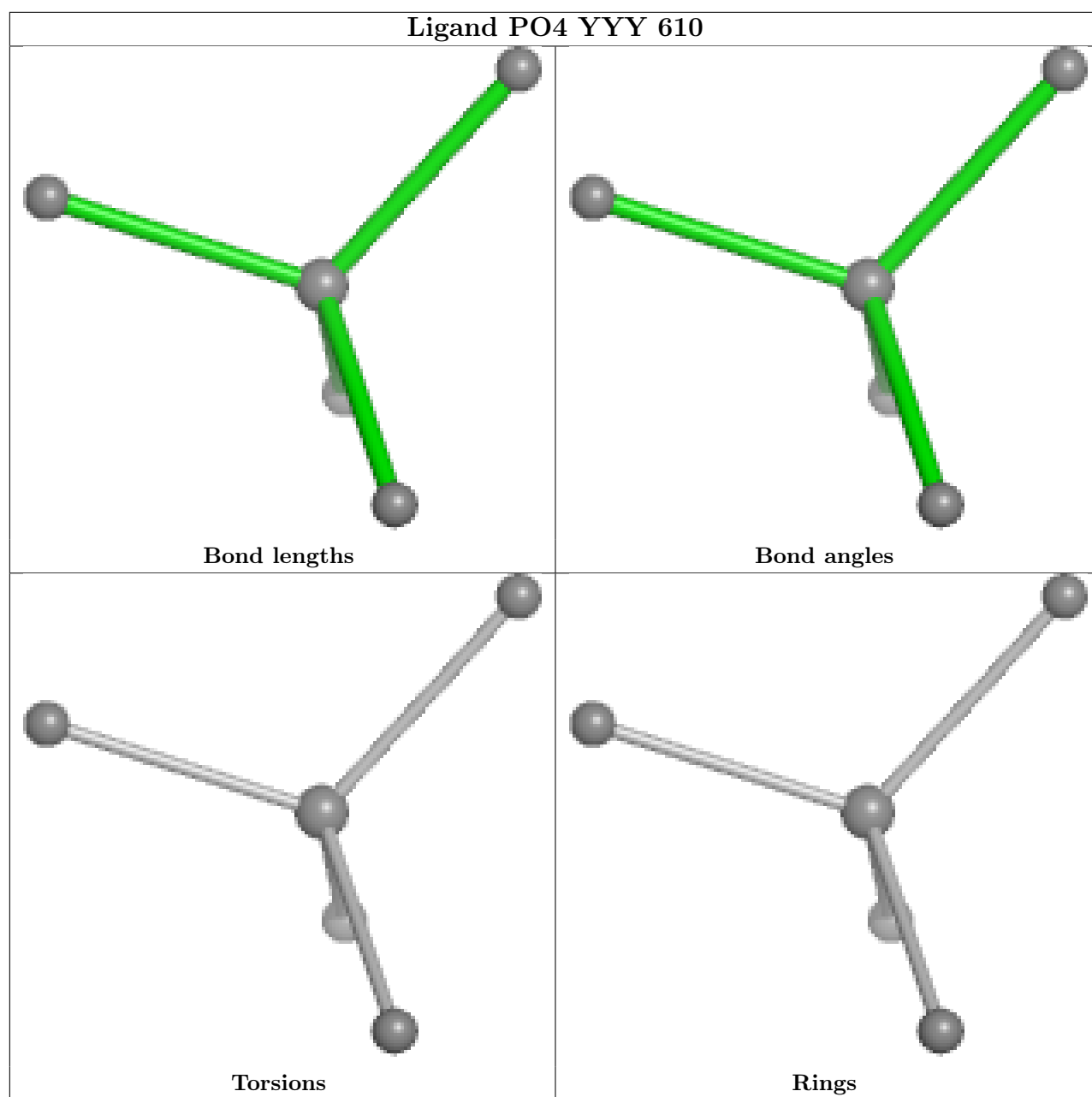
Ligand HEC YYY 602



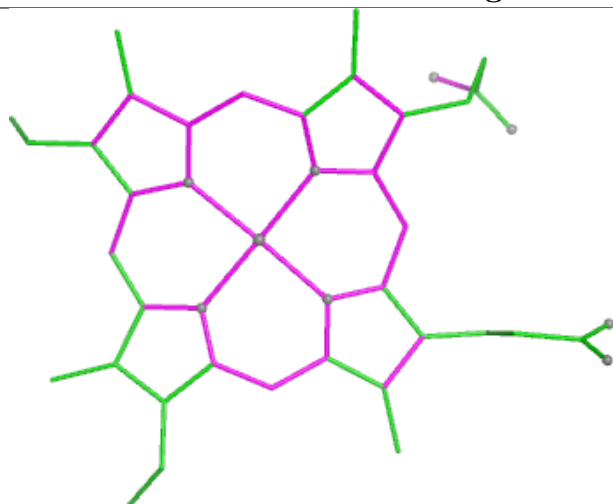
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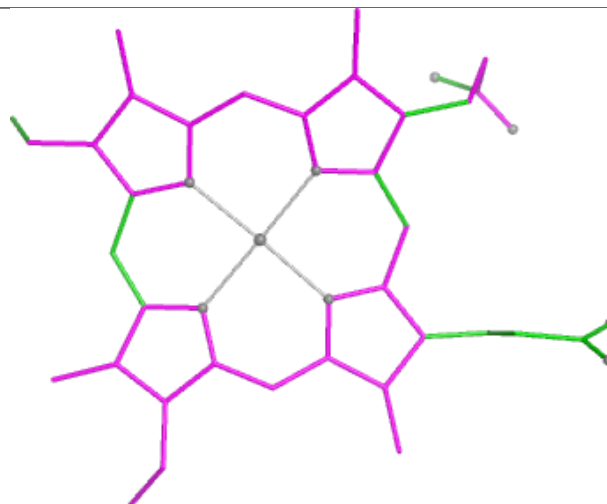




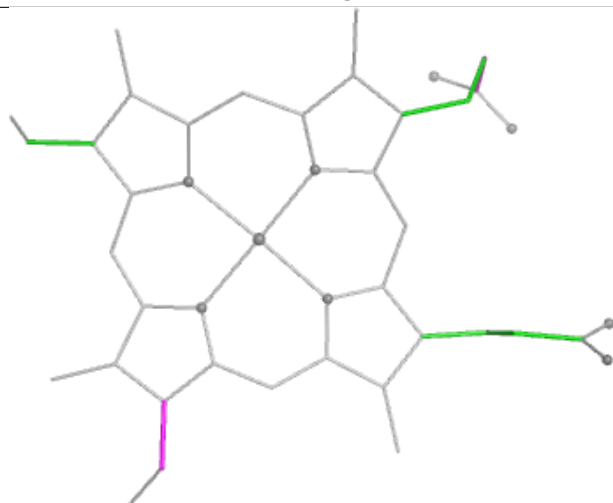
Ligand HEC YYY 605



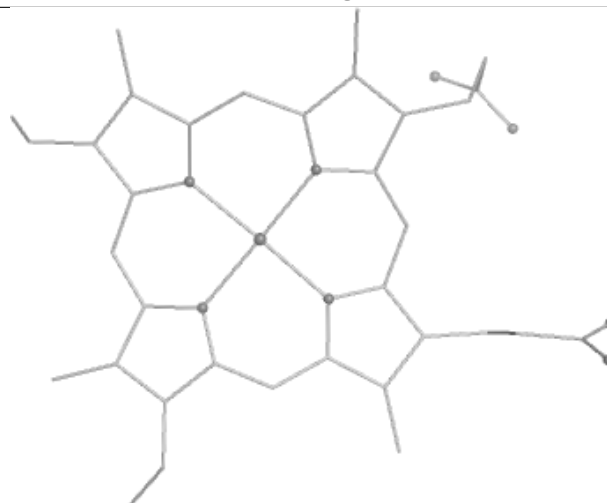
Bond lengths



Bond angles

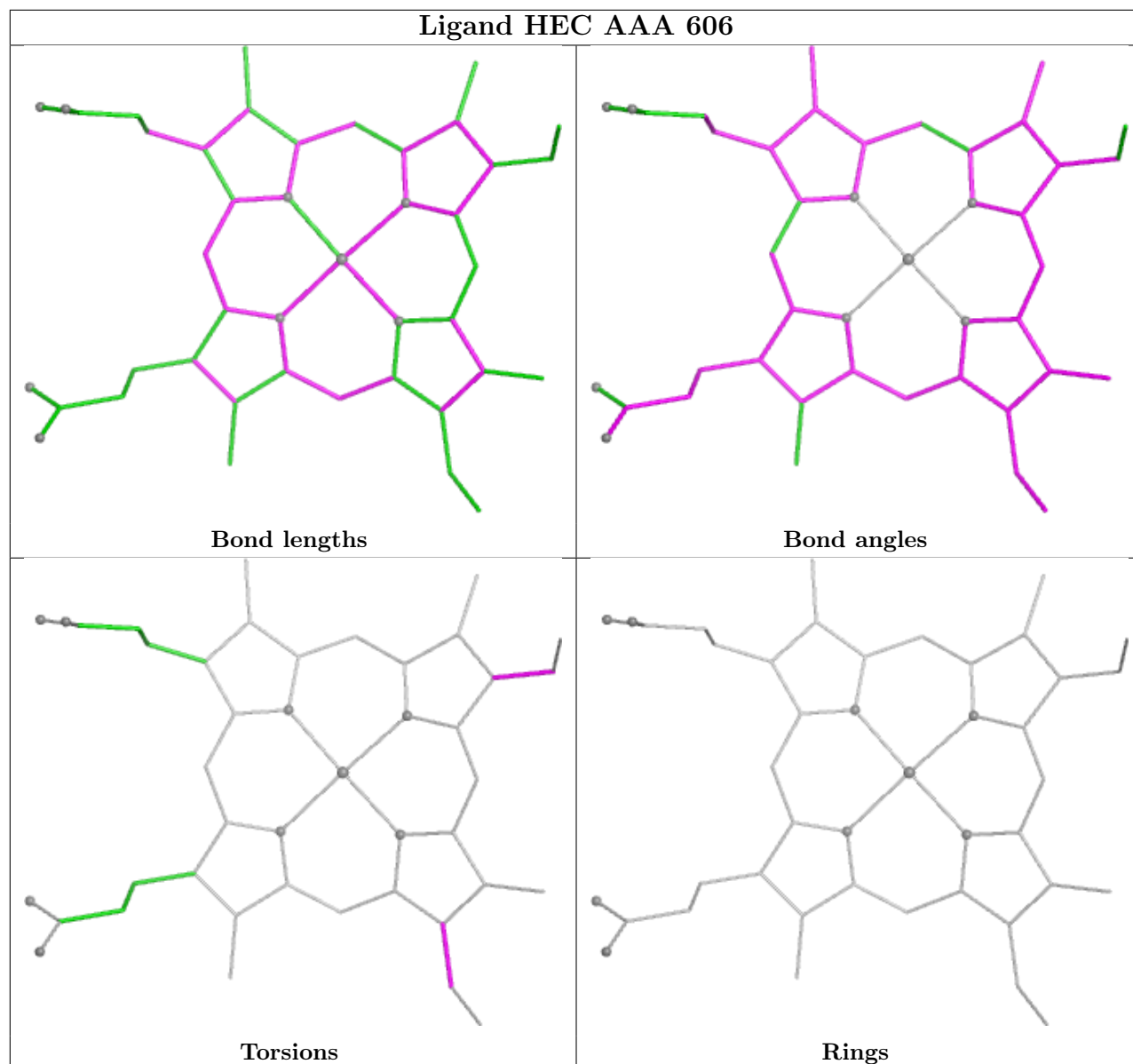


Torsions

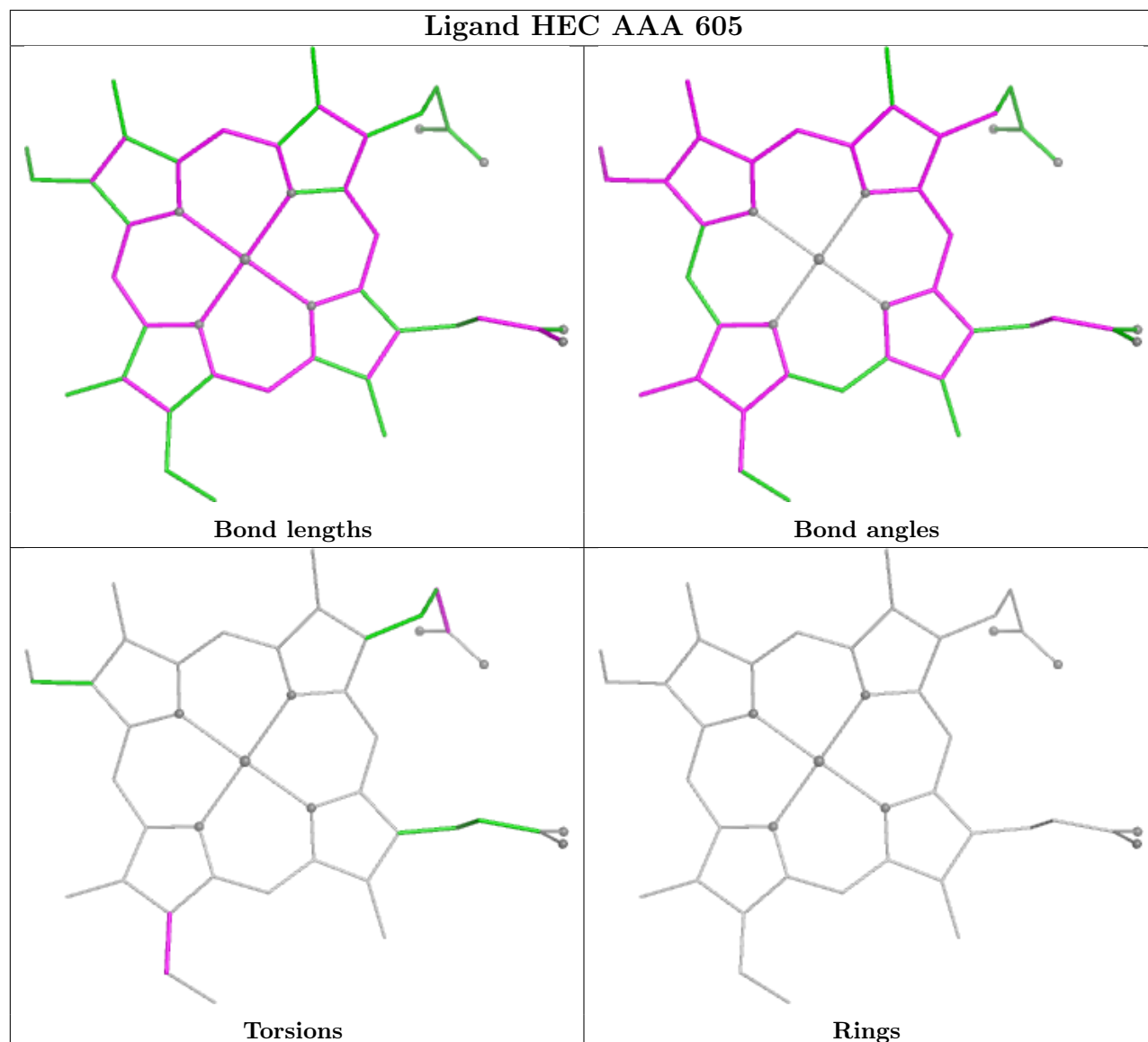


Rings

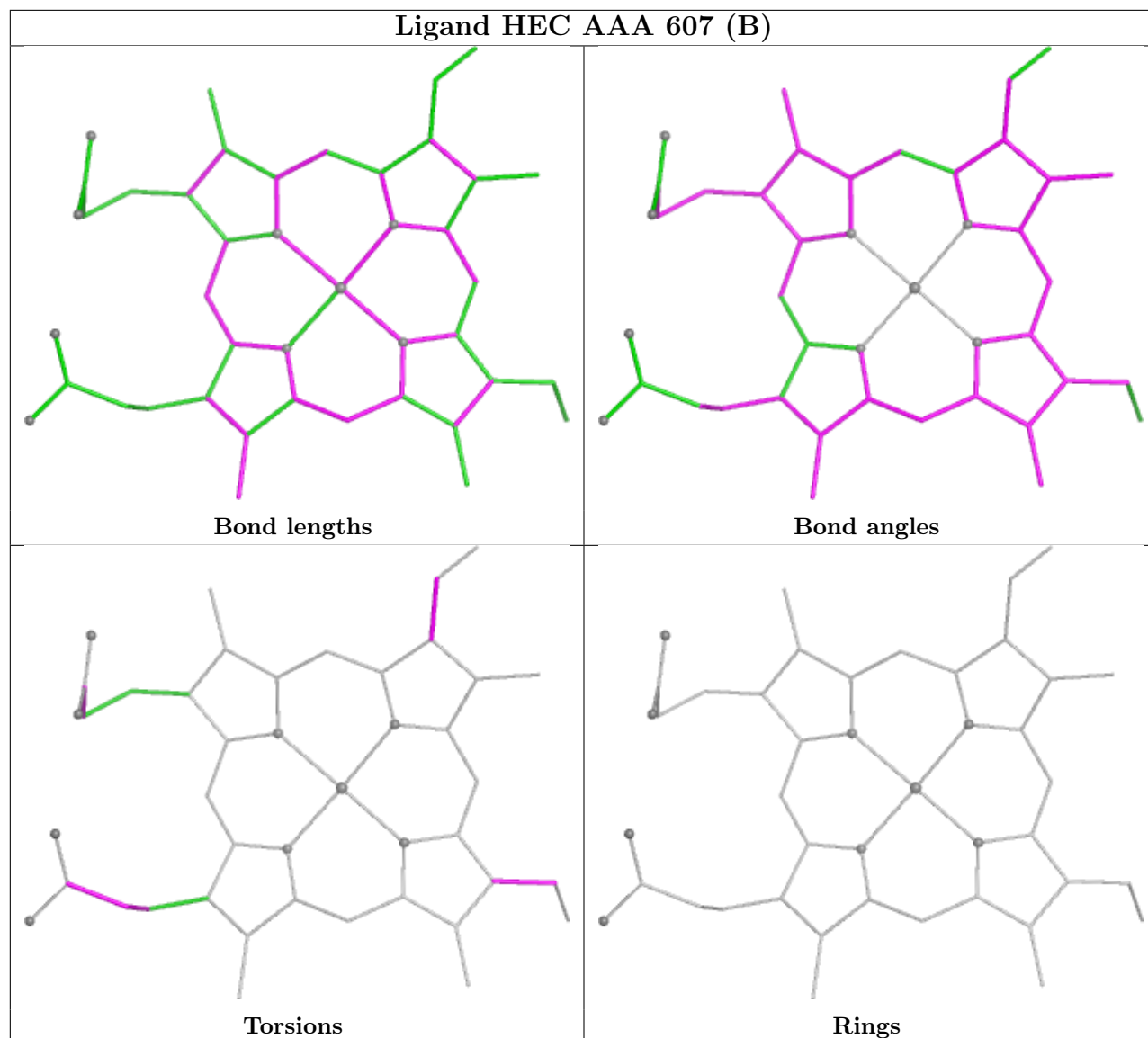
Ligand HEC AAA 606



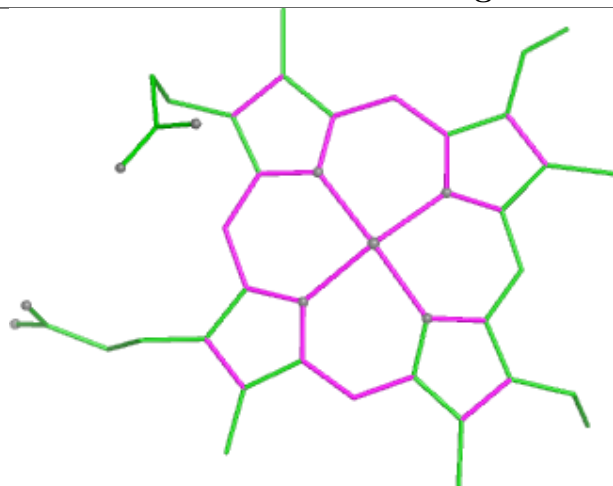
Ligand HEC AAA 605



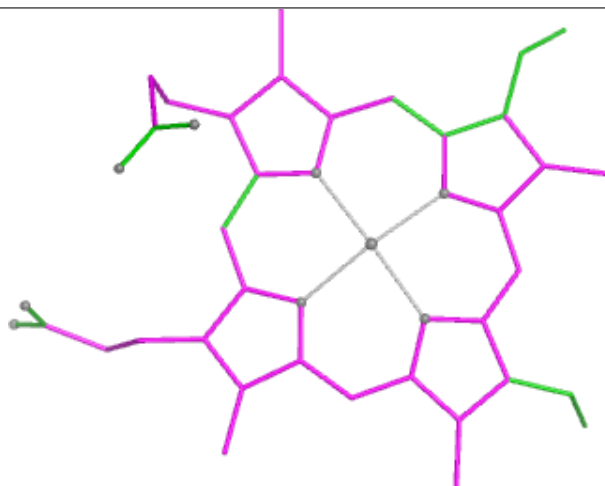
Ligand HEC AAA 607 (B)



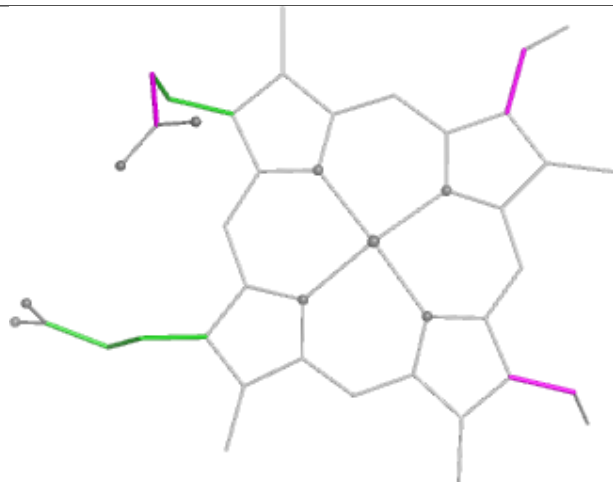
Ligand HEC MMM 603



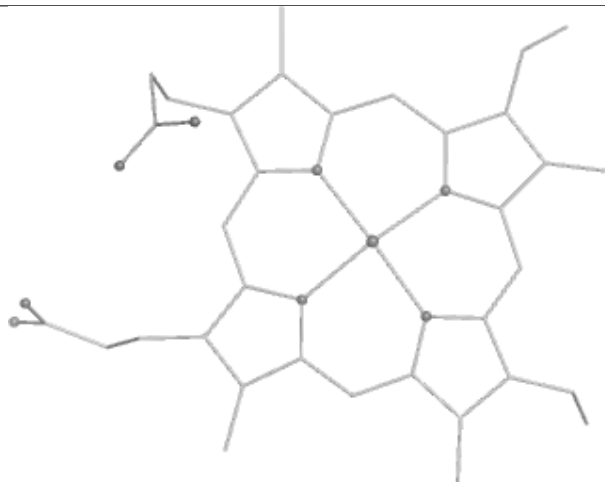
Bond lengths



Bond angles

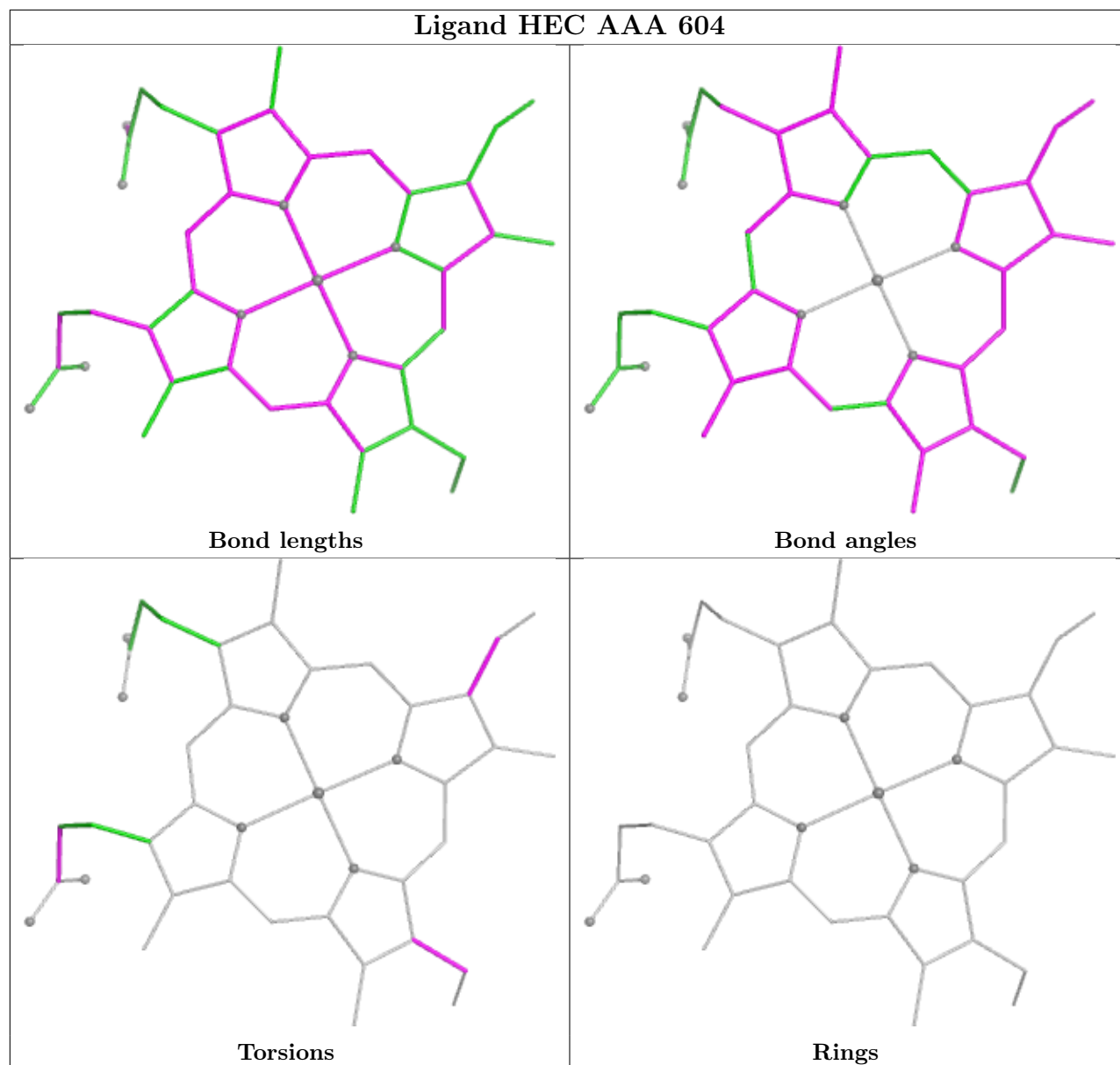


Torsions

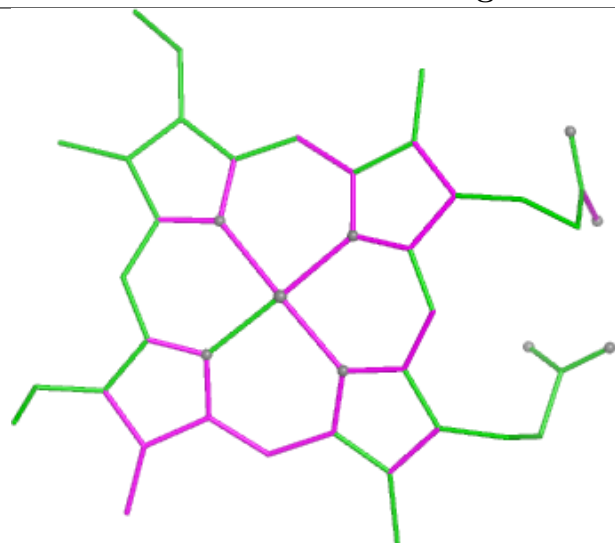


Rings

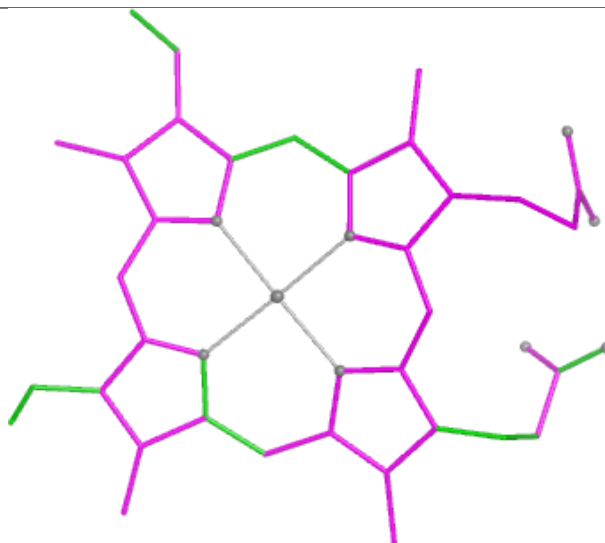
Ligand HEC AAA 604



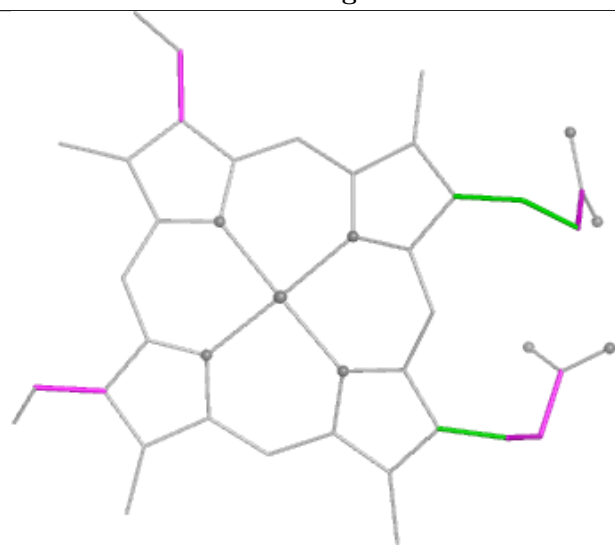
Ligand HEC MMM 607



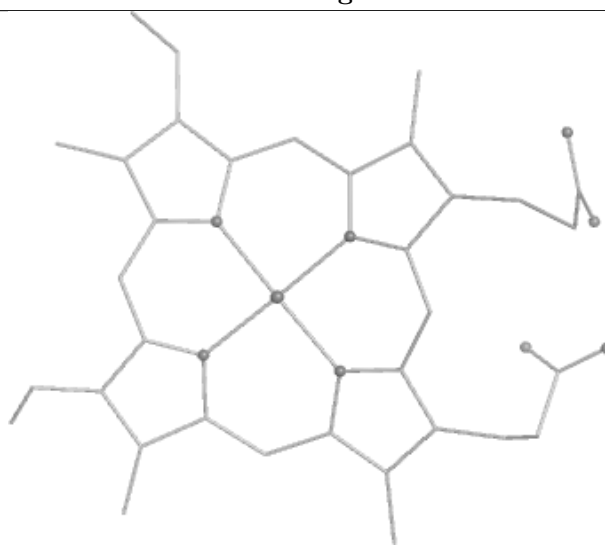
Bond lengths



Bond angles

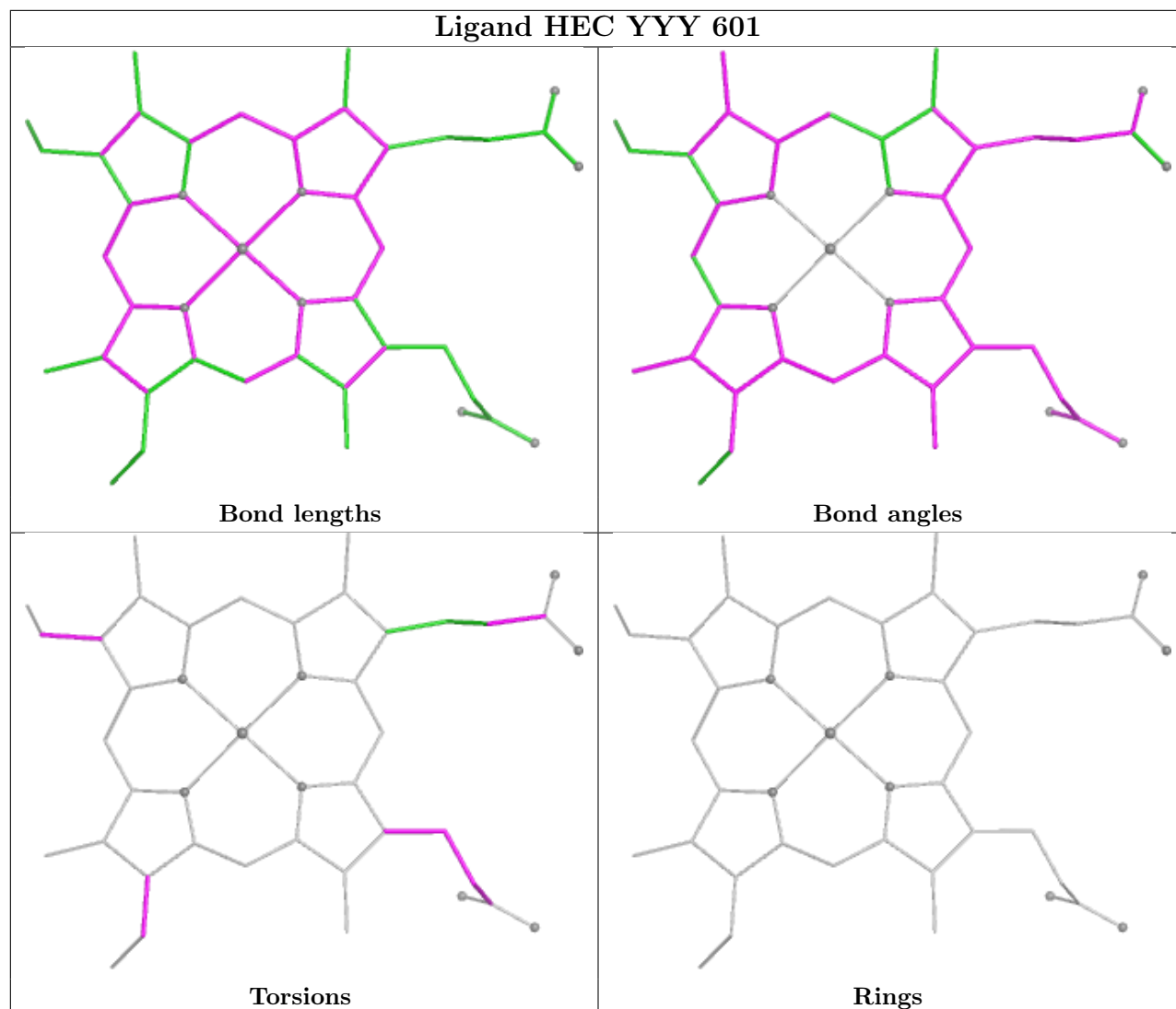


Torsions

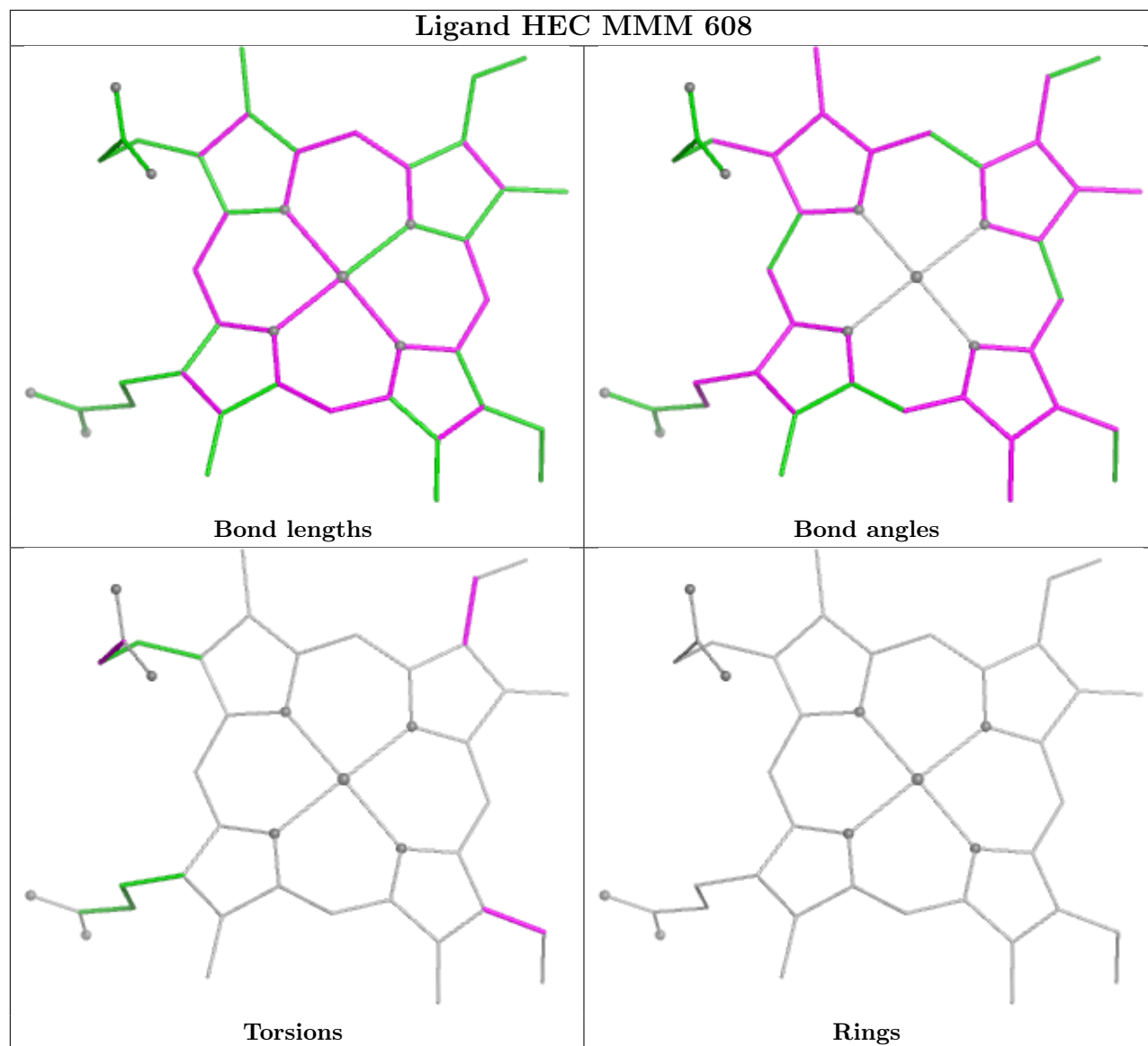


Rings

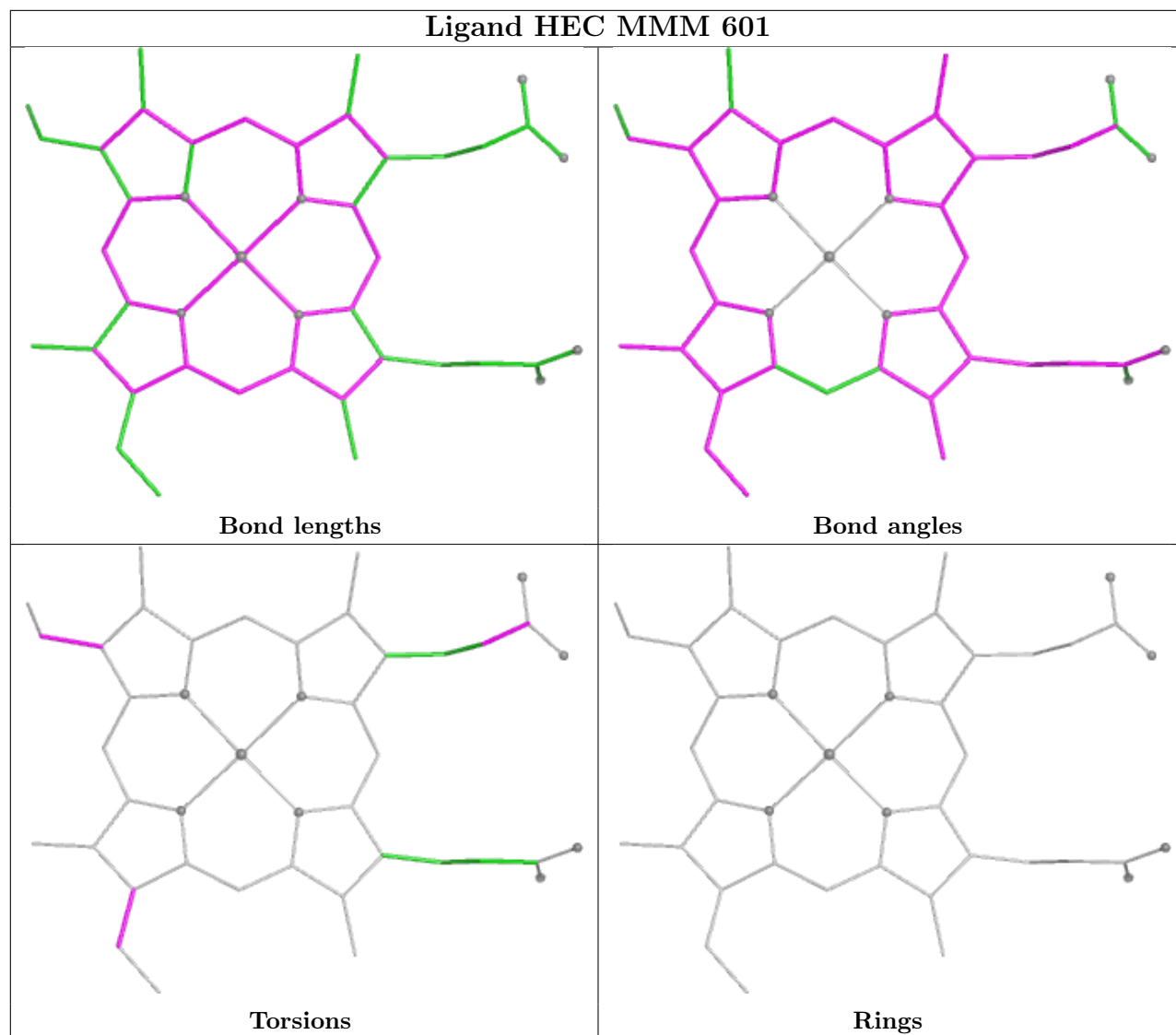
Ligand HEC YYY 601

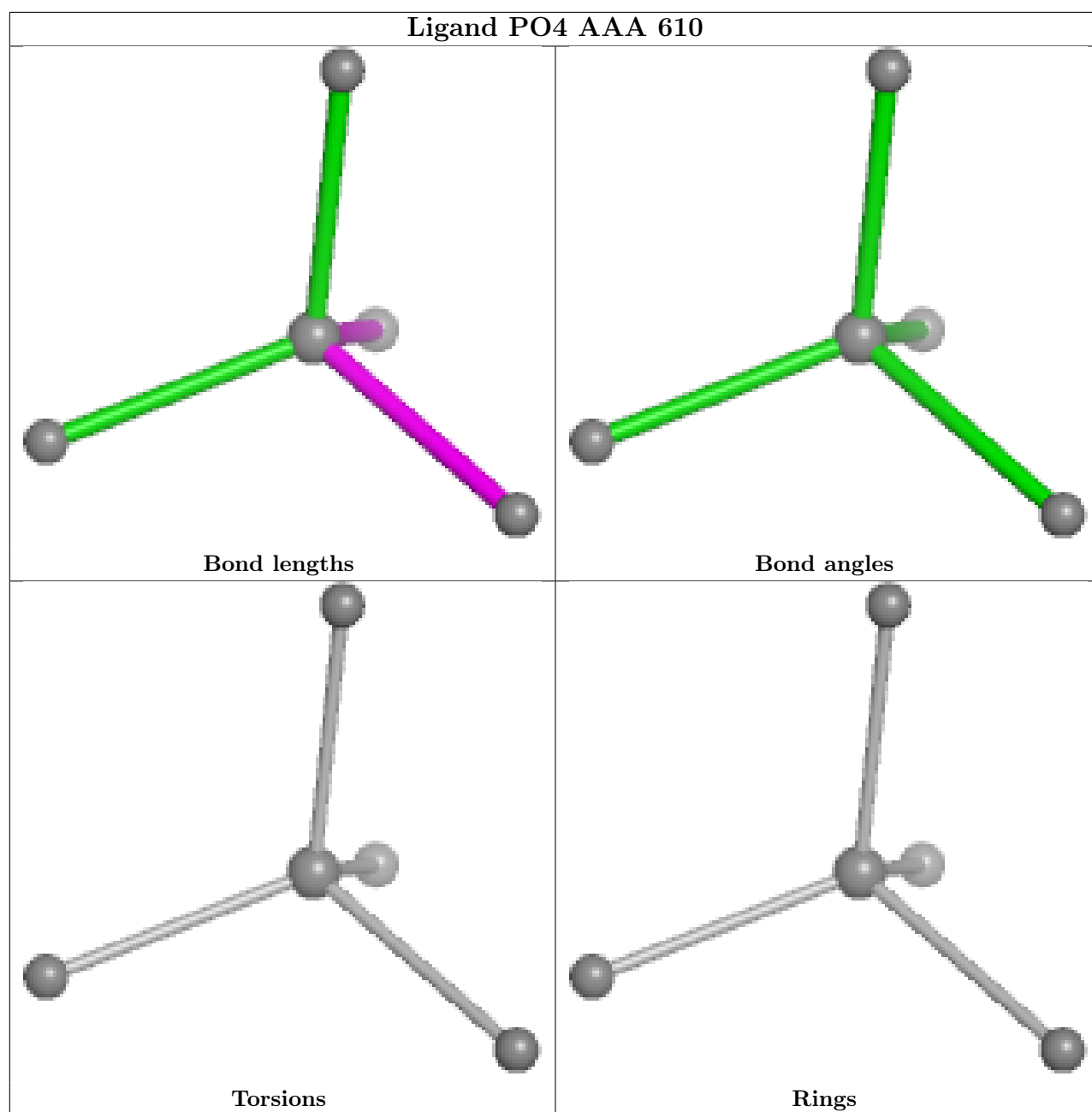


Ligand HEC MMM 608



Ligand HEC MMM 601





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	AAA	495/495 (100%)	-1.07	0 100 100	12, 22, 36, 55	2 (0%)
1	MMM	495/495 (100%)	-1.06	0 100 100	10, 21, 37, 69	3 (0%)
1	YYY	495/495 (100%)	-1.06	0 100 100	9, 22, 38, 53	2 (0%)
All	All	1485/1485 (100%)	-1.07	0 100 100	9, 22, 38, 69	7 (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(Å ²)	Q<0.9
2	HEC	AAA	601	43/43	0.99	0.04	16,23,32,38	0
2	HEC	AAA	602	43/43	0.99	0.04	19,22,25,32	0
2	HEC	AAA	603	43/43	0.99	0.04	22,28,32,33	0
2	HEC	AAA	604	43/43	0.99	0.03	10,15,18,19	0
2	HEC	AAA	605	43/43	0.99	0.04	17,22,25,27	0

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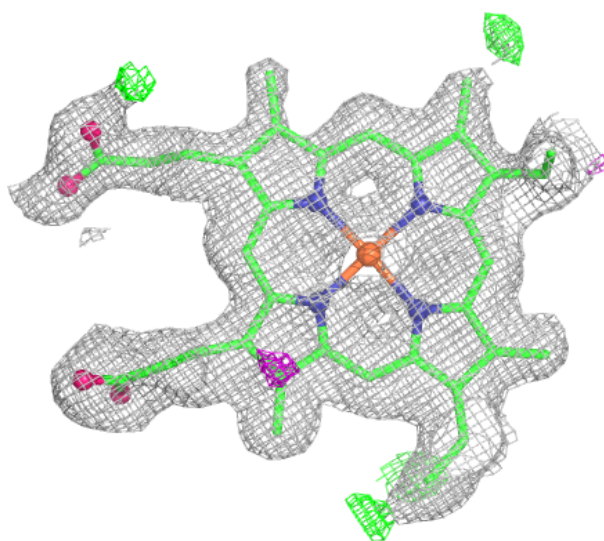
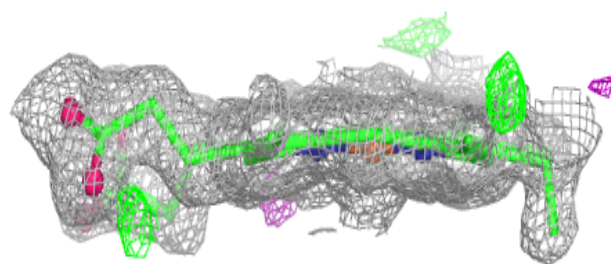
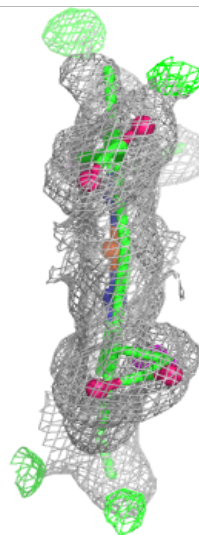
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	HEC	AAA	606	43/43	0.99	0.03	12,15,18,21	0
2	HEC	AAA	607[A]	43/43	0.99	0.03	11,14,18,18	3
2	HEC	AAA	607[B]	43/43	0.99	0.03	11,14,18,18	3
2	HEC	AAA	608	43/43	0.99	0.03	13,18,27,34	0
2	HEC	MMM	601	43/43	0.99	0.04	22,26,30,39	0
2	HEC	MMM	602	43/43	0.99	0.04	16,21,23,26	0
2	HEC	MMM	603	43/43	0.99	0.04	24,26,35,42	0
2	HEC	MMM	604	43/43	0.99	0.03	11,15,17,22	0
2	HEC	MMM	605	43/43	0.99	0.04	14,21,29,30	0
2	HEC	MMM	606	43/43	0.99	0.03	11,14,16,21	0
2	HEC	MMM	607	43/43	0.99	0.03	12,15,20,23	0
2	HEC	MMM	608	43/43	0.99	0.03	13,17,27,35	0
2	HEC	YYY	601	43/43	0.99	0.04	20,25,31,40	0
2	HEC	YYY	602	43/43	0.99	0.04	17,24,27,29	0
2	HEC	YYY	603	43/43	0.99	0.04	20,27,29,31	0
2	HEC	YYY	604	43/43	0.99	0.03	12,16,20,23	0
2	HEC	YYY	605	43/43	0.99	0.03	14,22,27,36	0
2	HEC	YYY	606	43/43	0.99	0.03	13,16,18,20	0
2	HEC	YYY	608	43/43	0.99	0.03	14,22,28,31	0
3	CA	MMM	609	1/1	0.99	0.02	21,21,21,21	0
4	PO4	AAA	610	5/5	0.99	0.03	17,18,20,21	0
4	PO4	MMM	610	5/5	0.99	0.03	19,21,23,24	0
4	PO4	YYY	610	5/5	0.99	0.04	16,20,23,23	0
3	CA	AAA	609	1/1	1.00	0.01	21,21,21,21	0
2	HEC	YYY	607	43/43	1.00	0.03	13,16,20,22	0
3	CA	YYY	609	1/1	1.00	0.02	18,18,18,18	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.

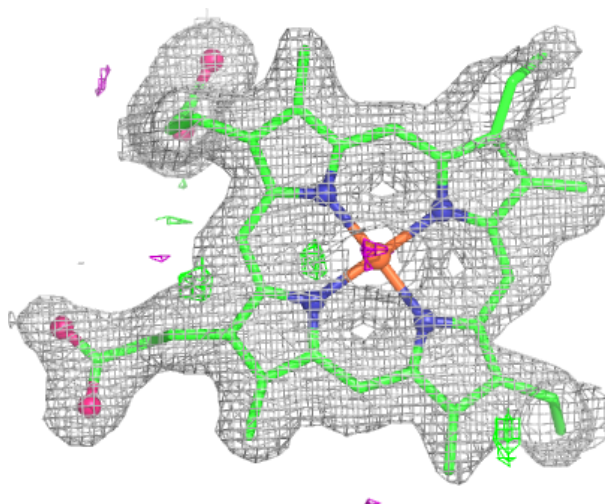
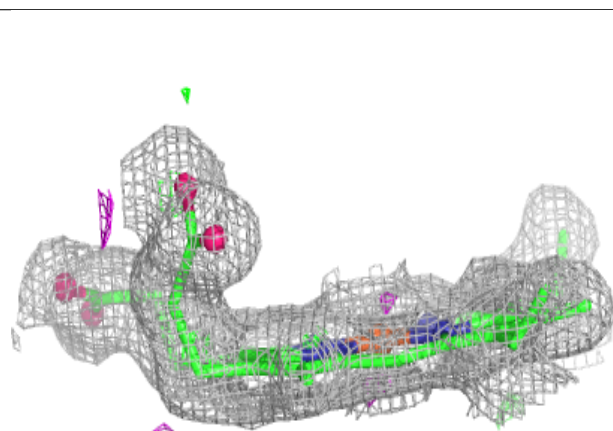
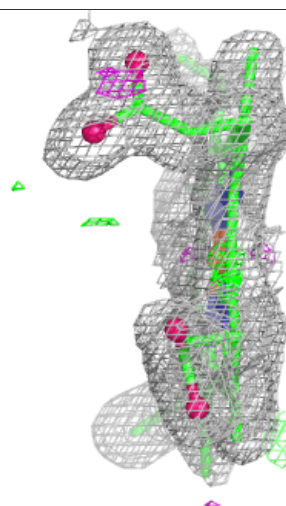
Electron density around HEC AAA 601:

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



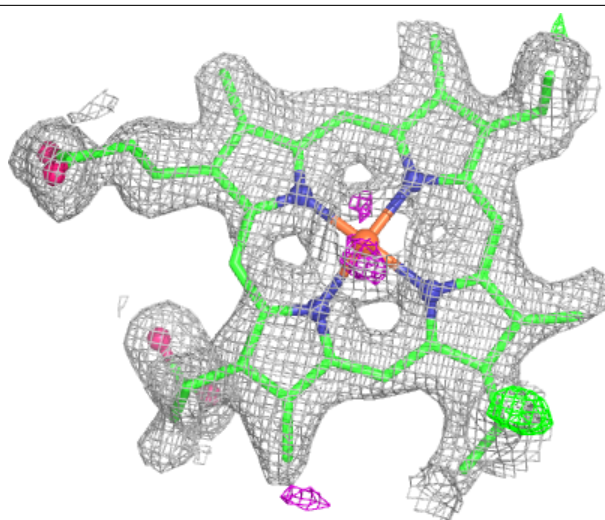
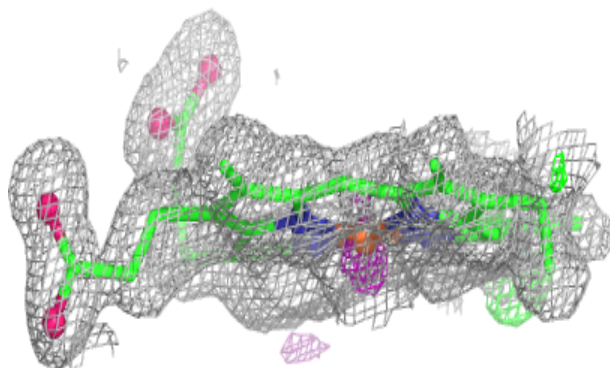
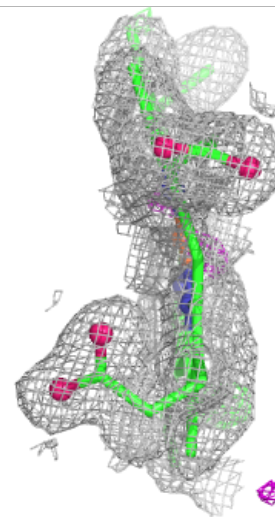
Electron density around HEC AAA 602:

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and green (positive)



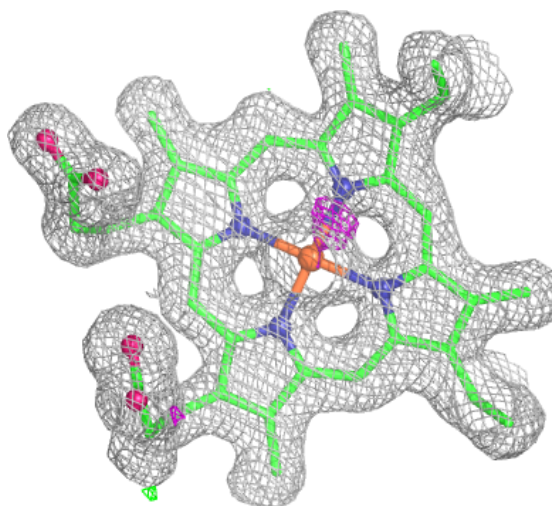
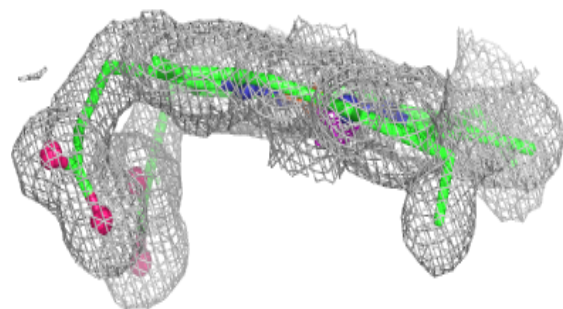
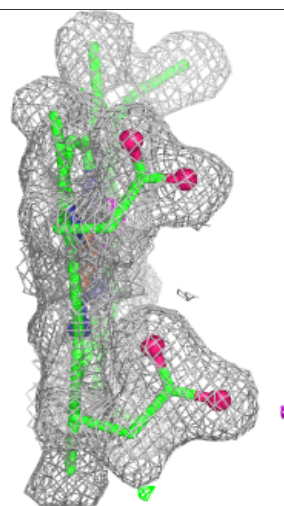
Electron density around HEC AAA 603:

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



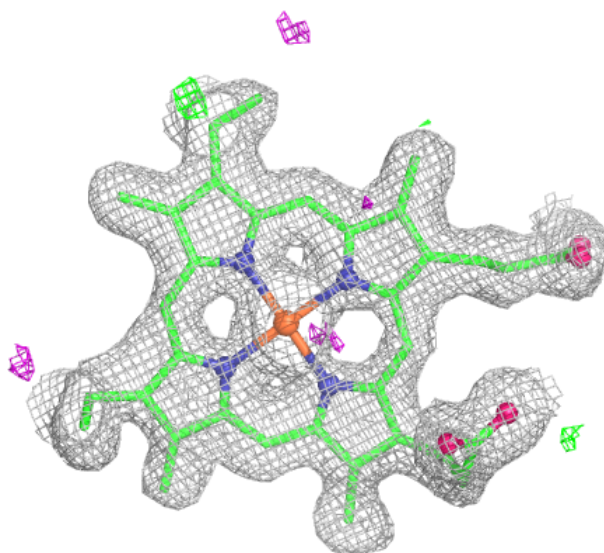
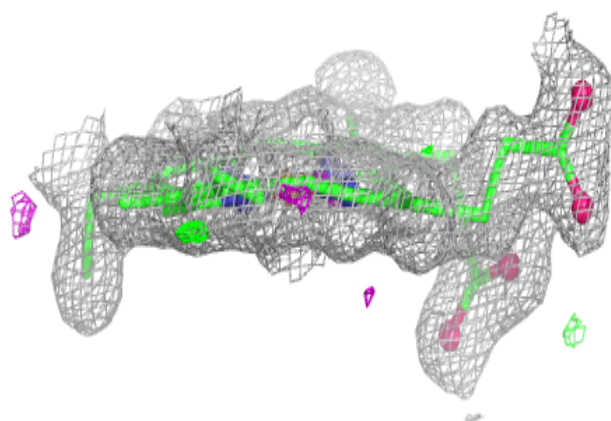
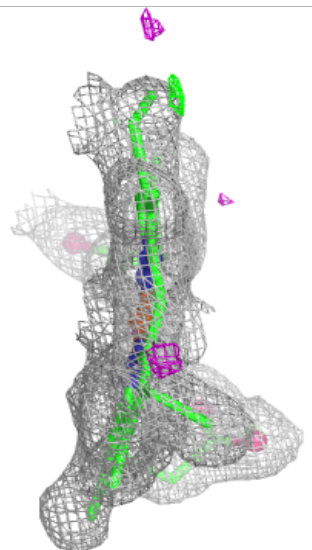
Electron density around HEC AAA 604:

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and green (positive)



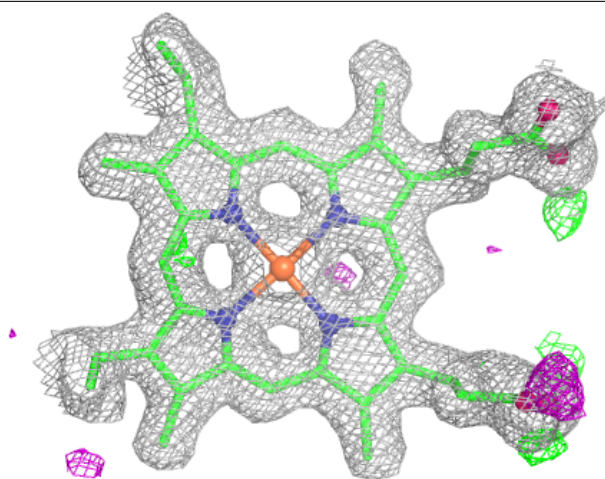
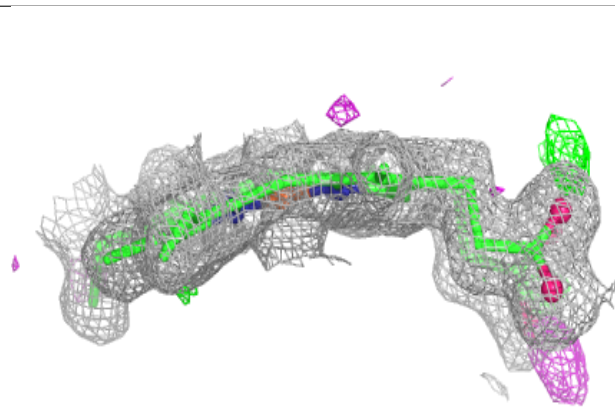
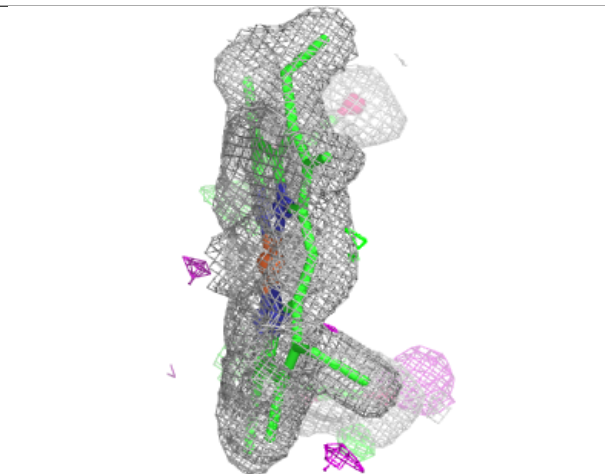
Electron density around HEC AAA 605:

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



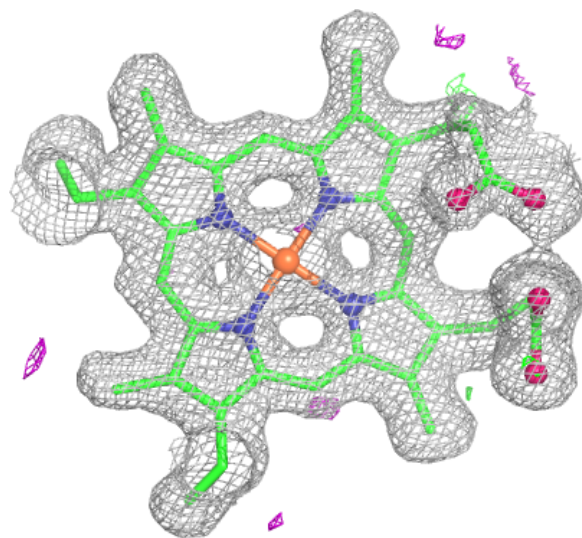
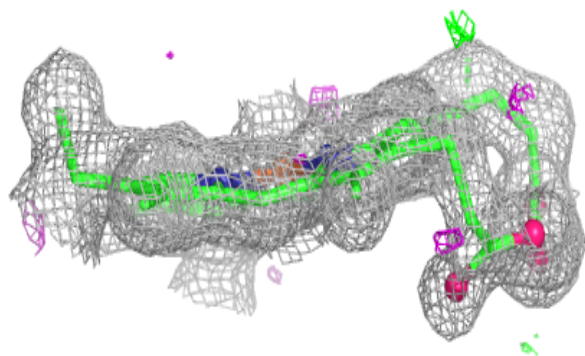
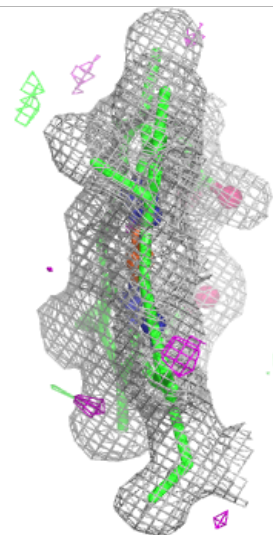
Electron density around HEC AAA 606:

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



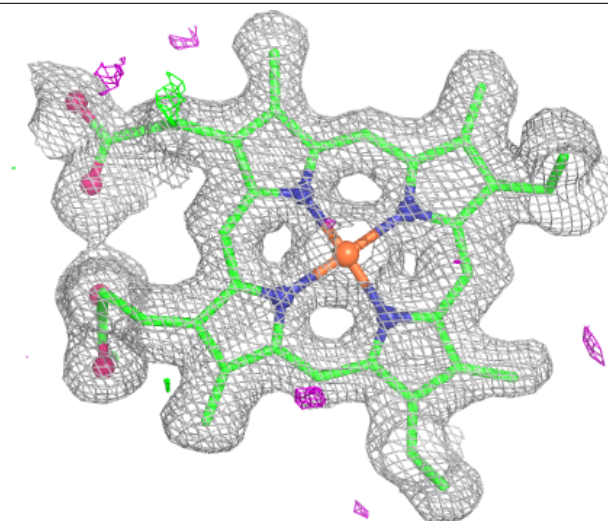
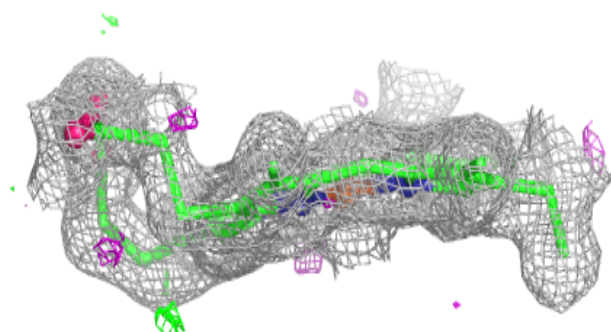
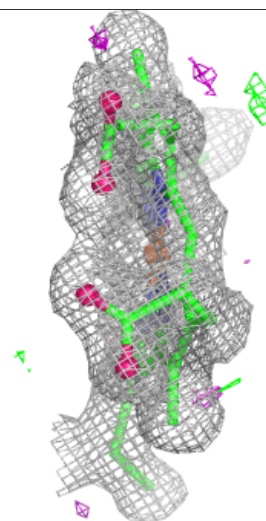
Electron density around HEC AAA 607 (A):

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



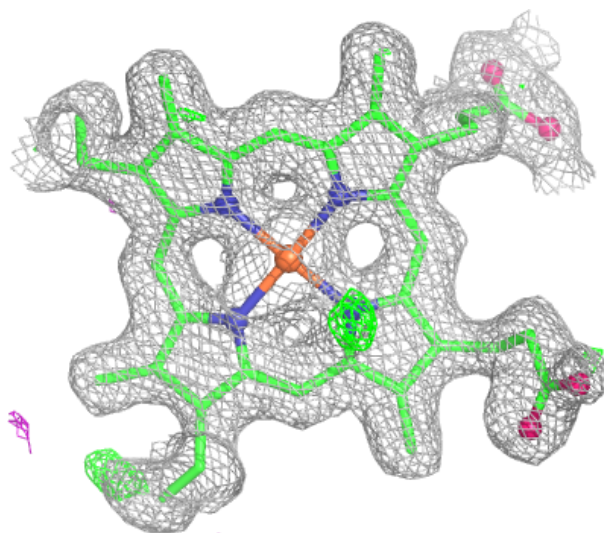
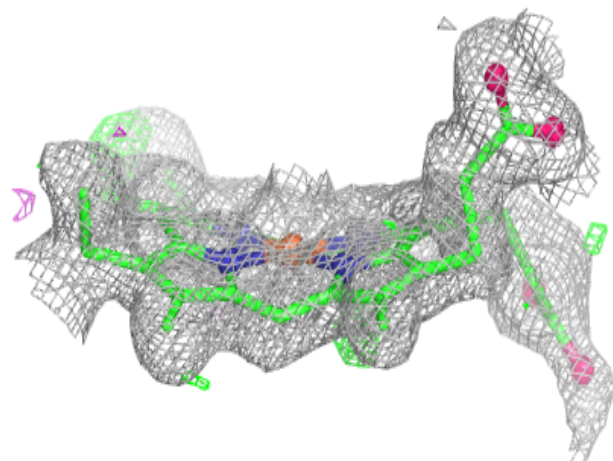
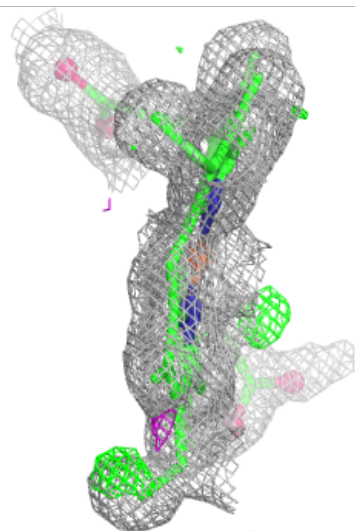
Electron density around HEC AAA 607 (B):

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



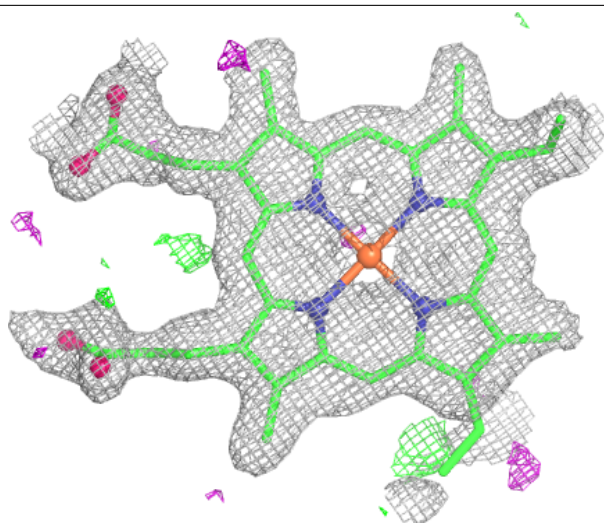
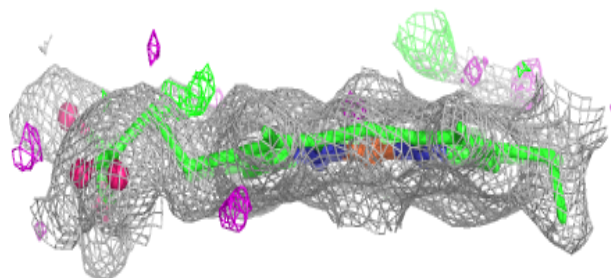
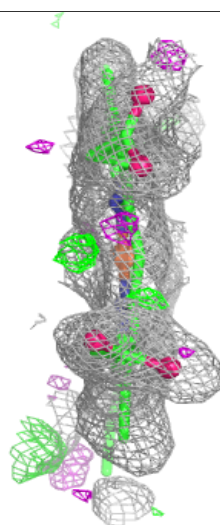
Electron density around HEC AAA 608:

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and green (positive)



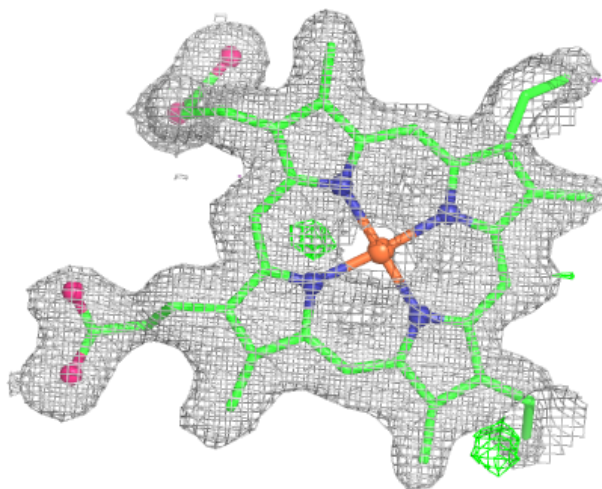
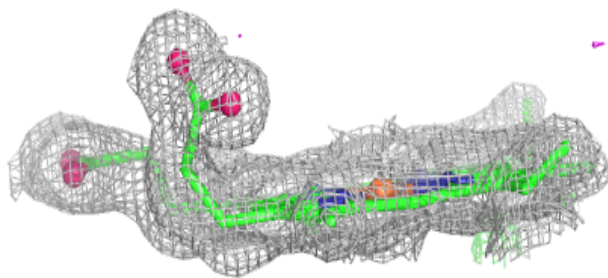
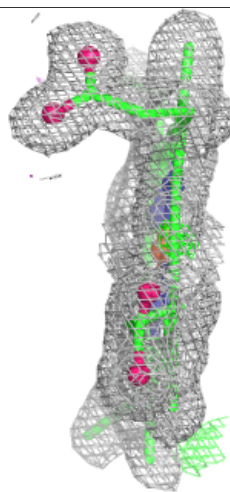
Electron density around HEC MMM 601:

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



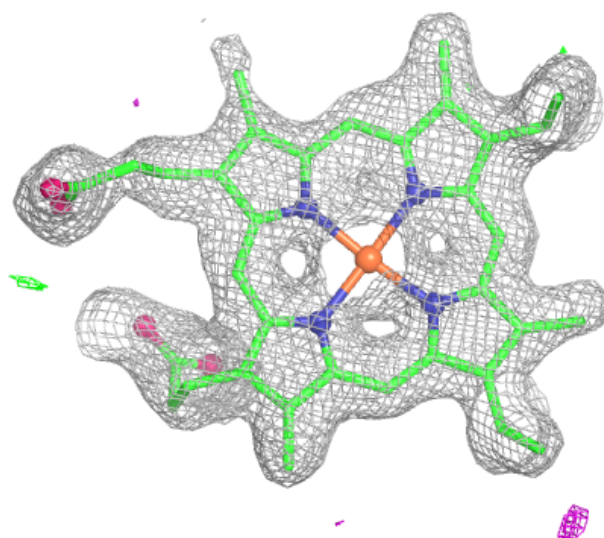
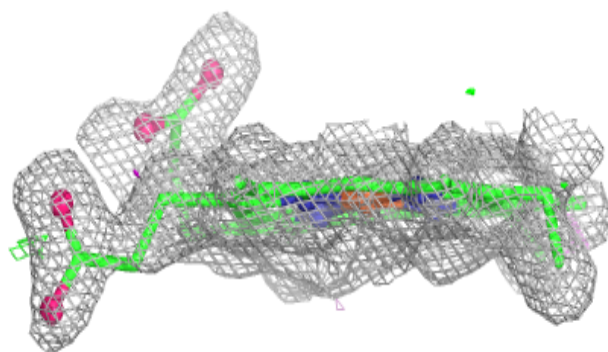
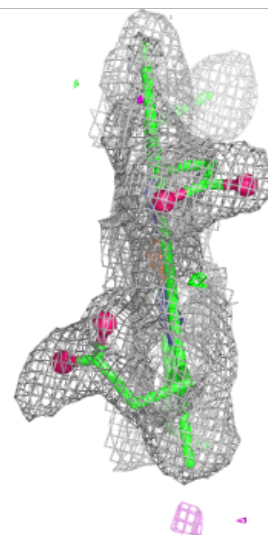
Electron density around HEC MMM 602:

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and green (positive)



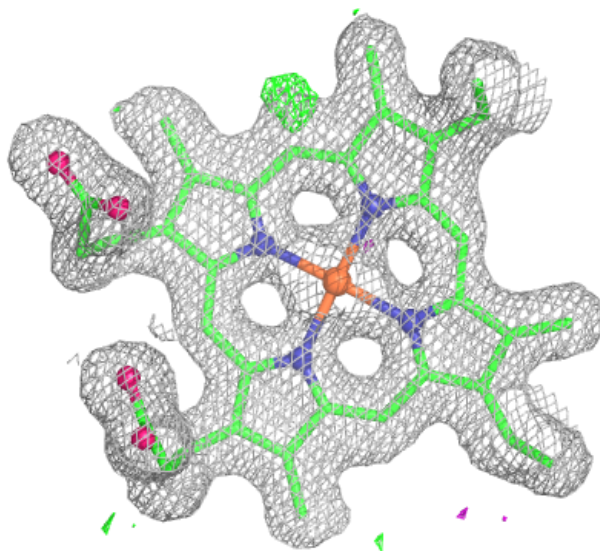
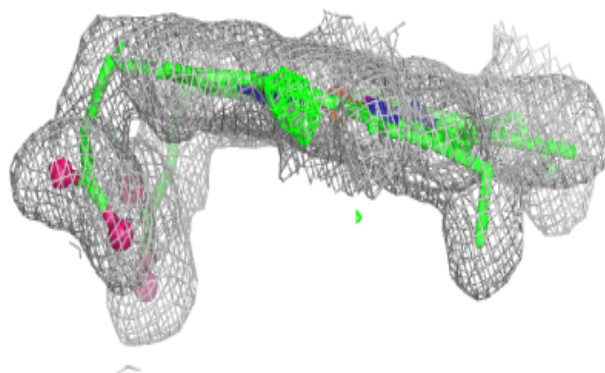
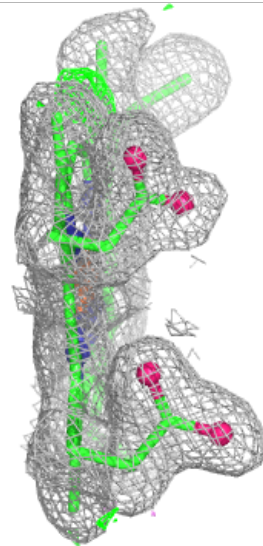
Electron density around HEC MMM 603:

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and green (positive)



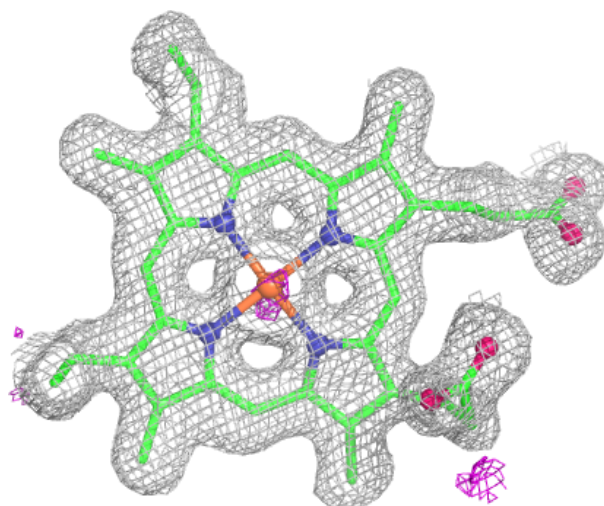
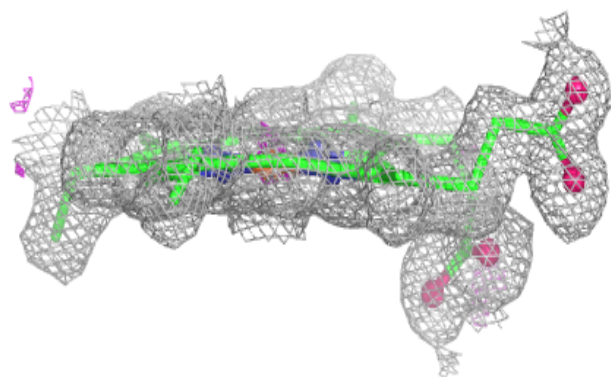
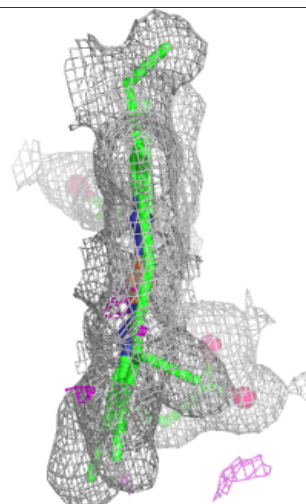
Electron density around HEC MMM 604:

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



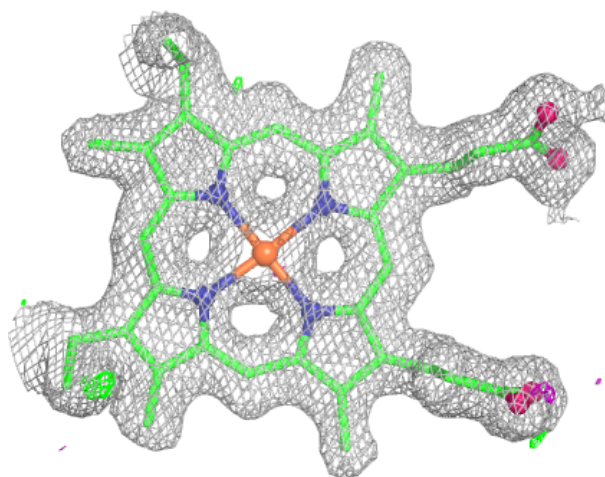
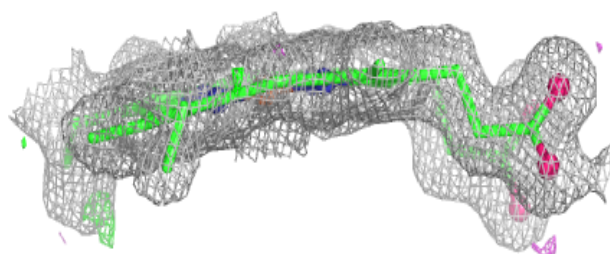
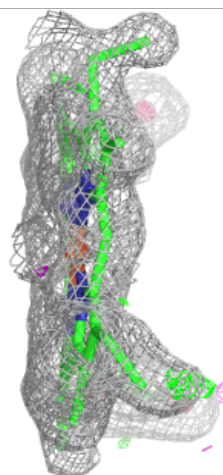
Electron density around HEC MMM 605:

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



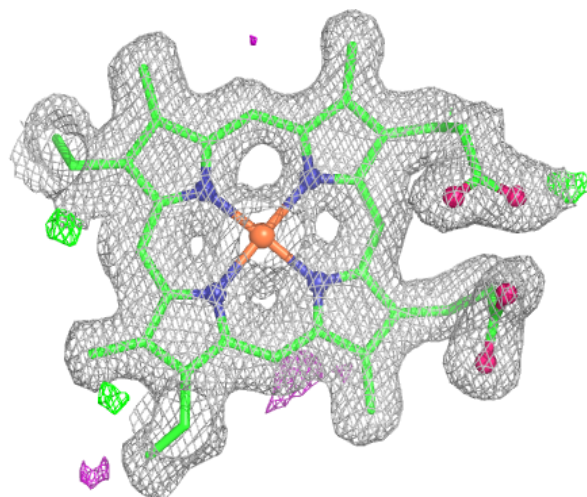
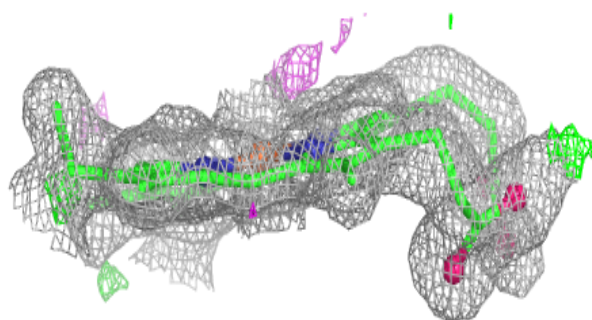
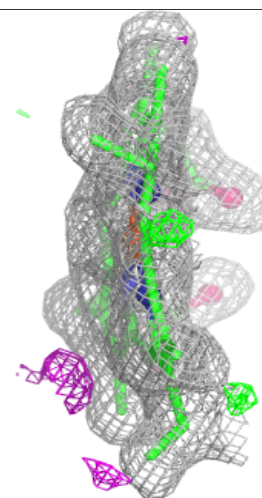
Electron density around HEC MMM 606:

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and green (positive)



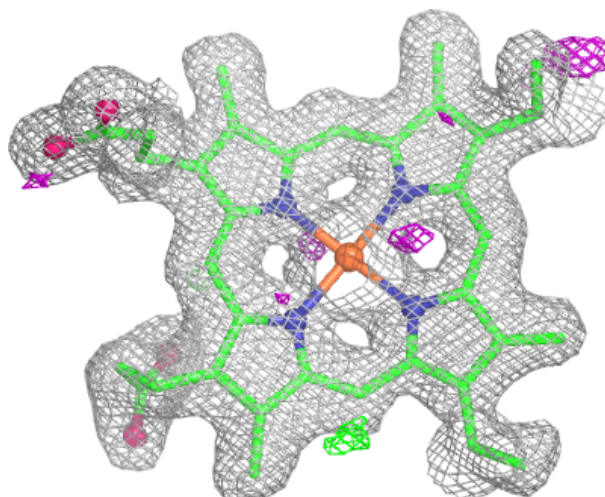
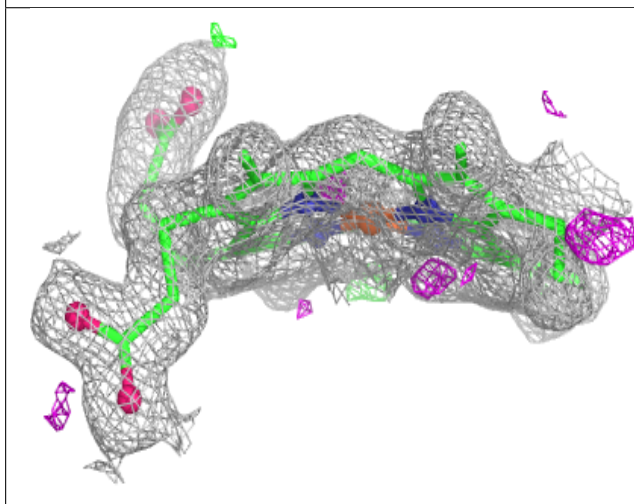
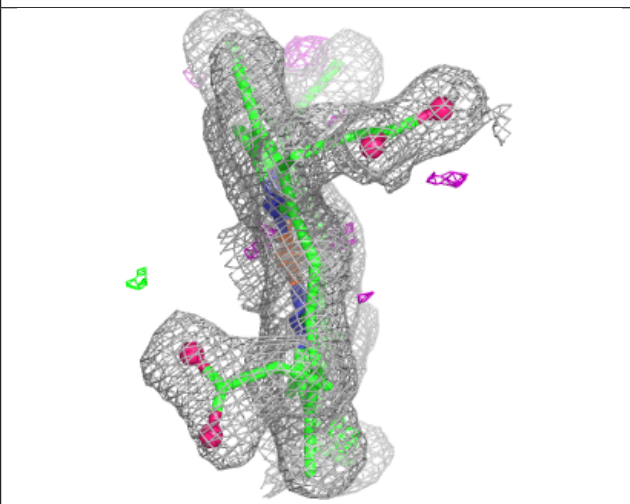
Electron density around HEC MMM 607:

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and green (positive)



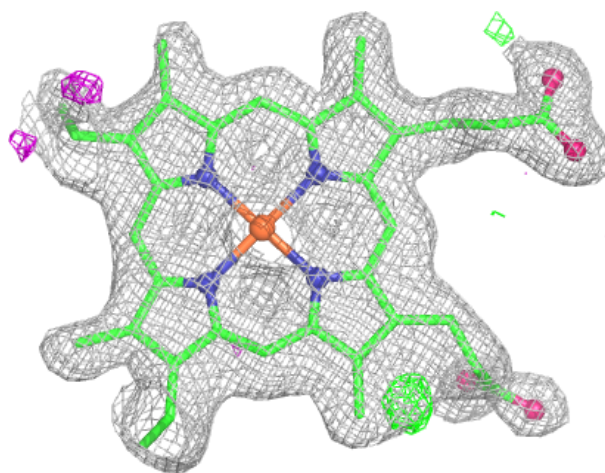
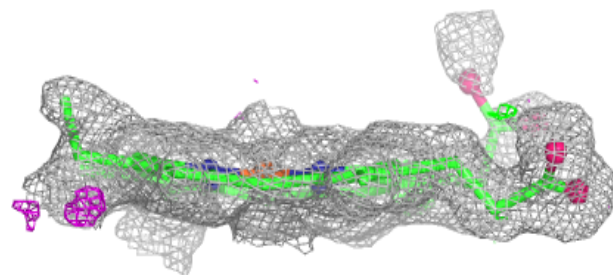
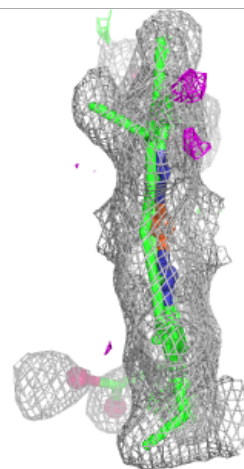
Electron density around HEC MMM 608:

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and green (positive)



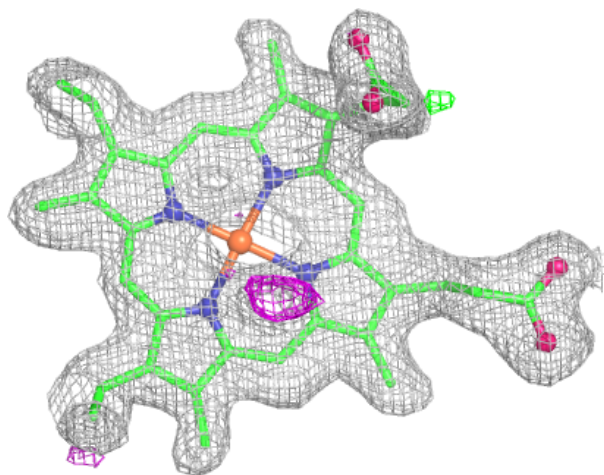
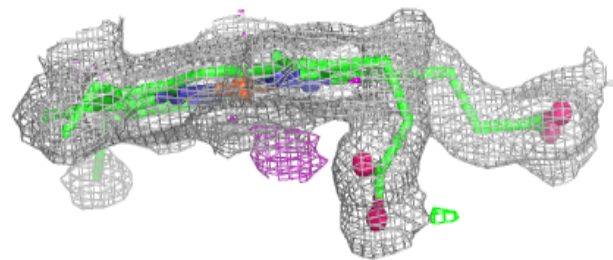
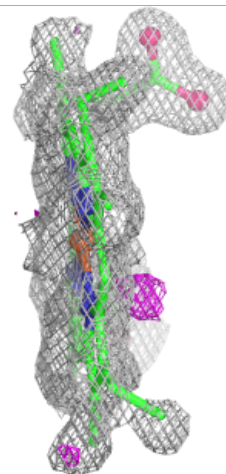
Electron density around HEC YYY 601:

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



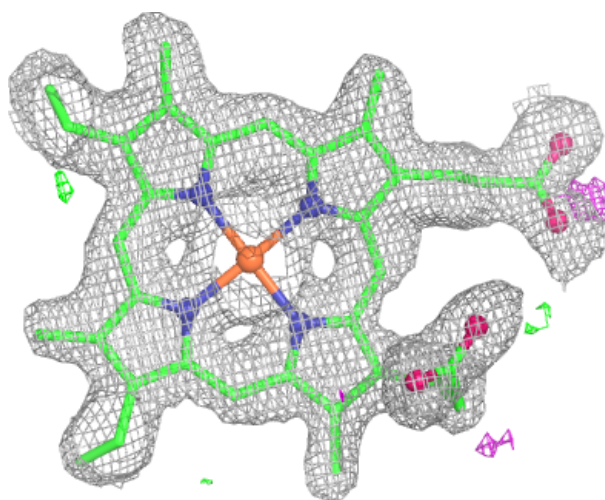
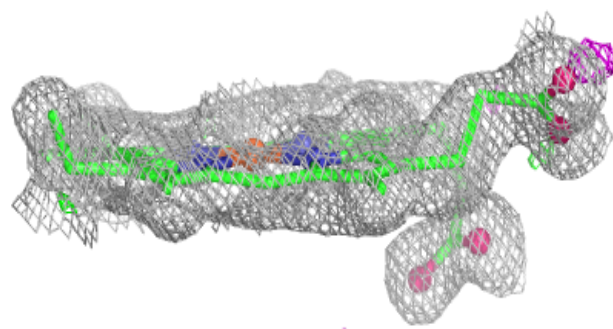
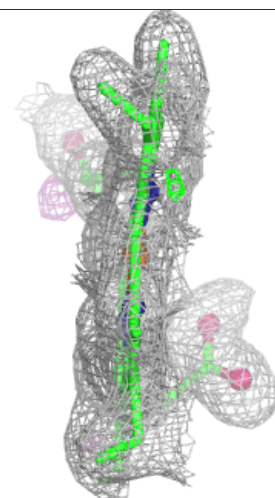
Electron density around HEC YYY 602:

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and green (positive)



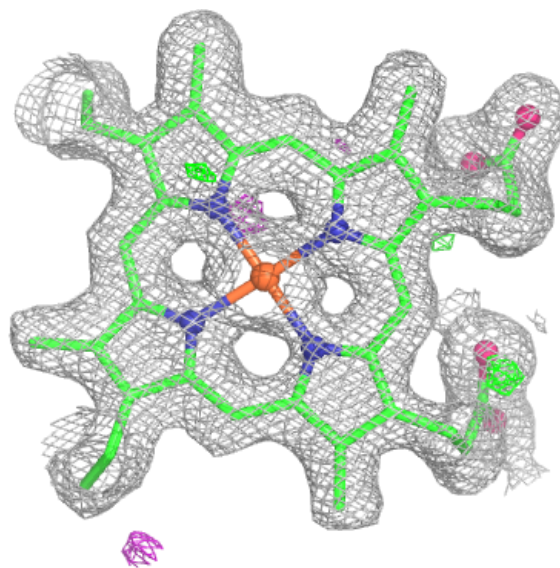
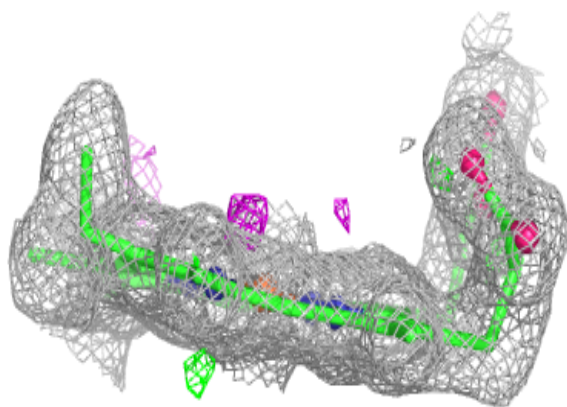
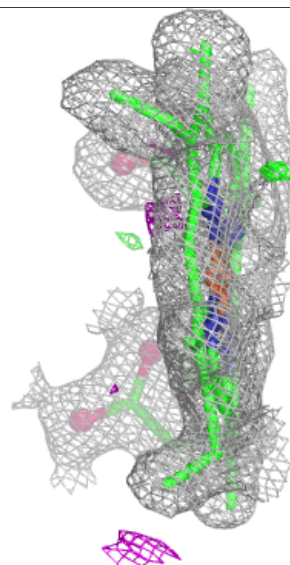
Electron density around HEC YYY 603:

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and green (positive)



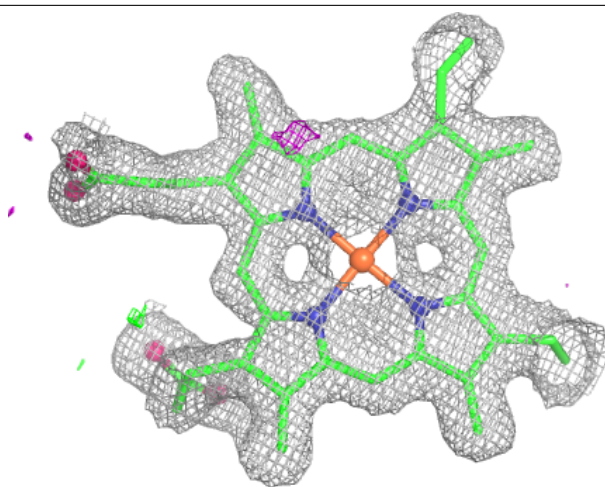
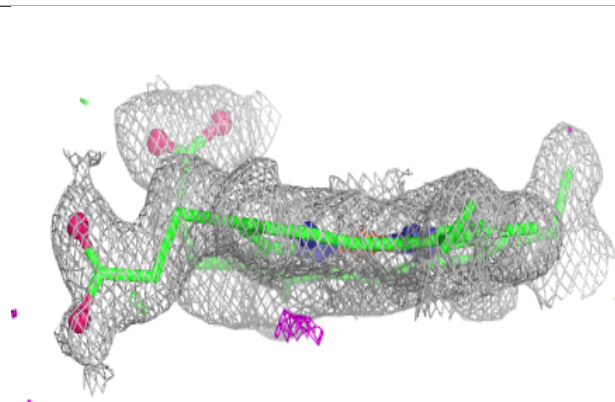
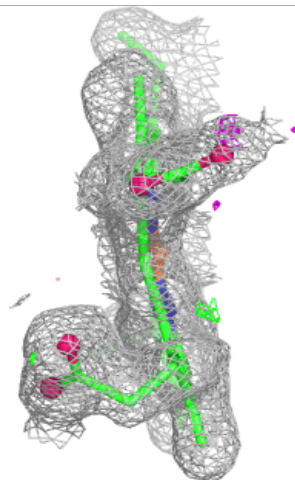
Electron density around HEC YYY 604:

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and green (positive)



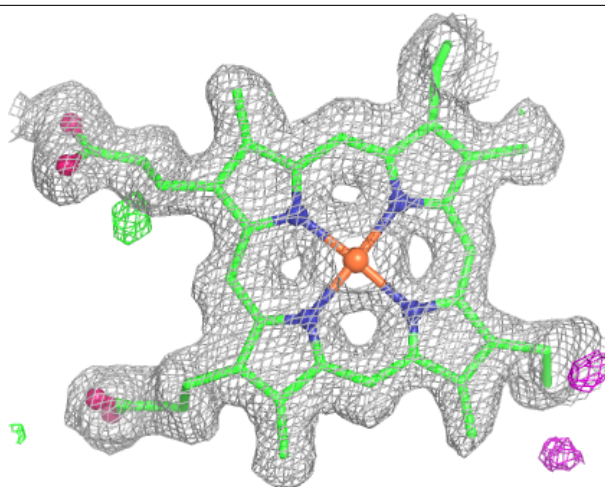
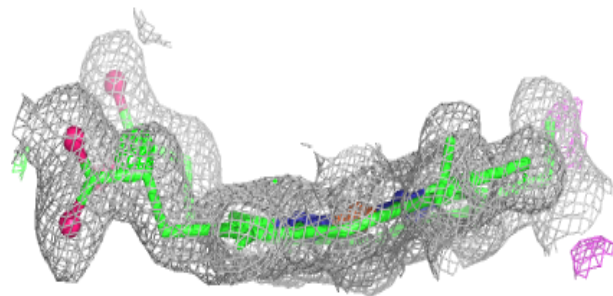
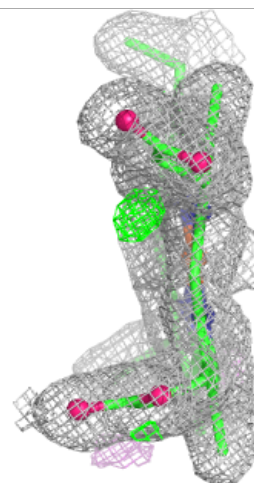
Electron density around HEC YYY 605:

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



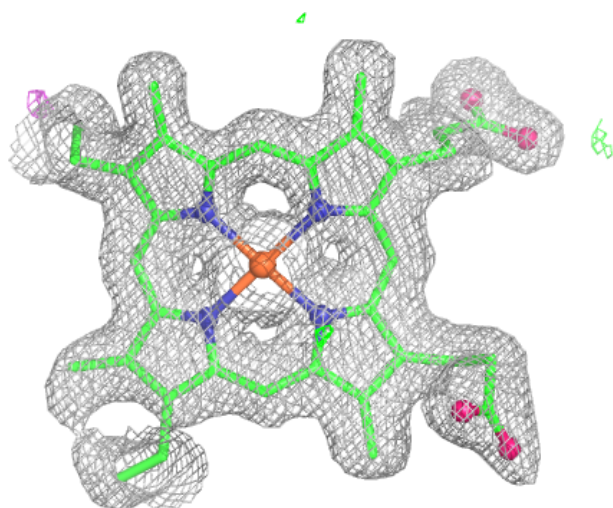
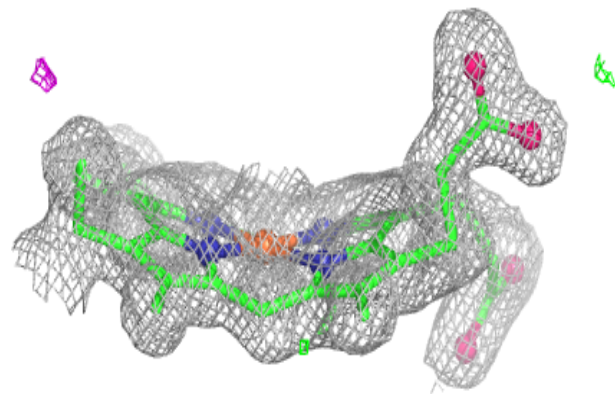
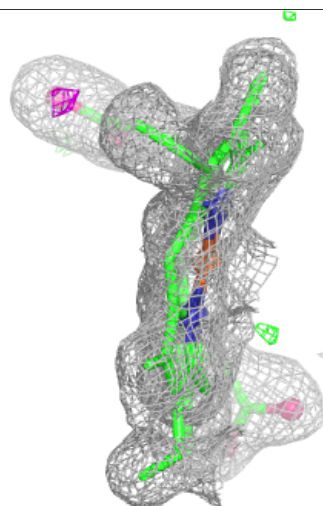
Electron density around HEC YYY 606:

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



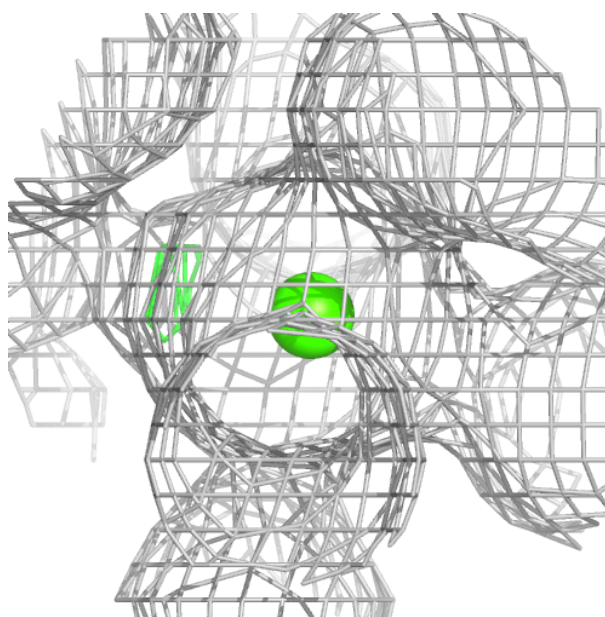
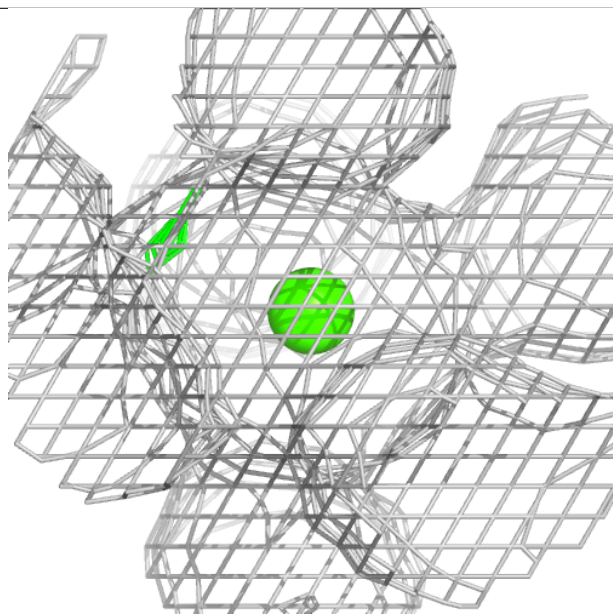
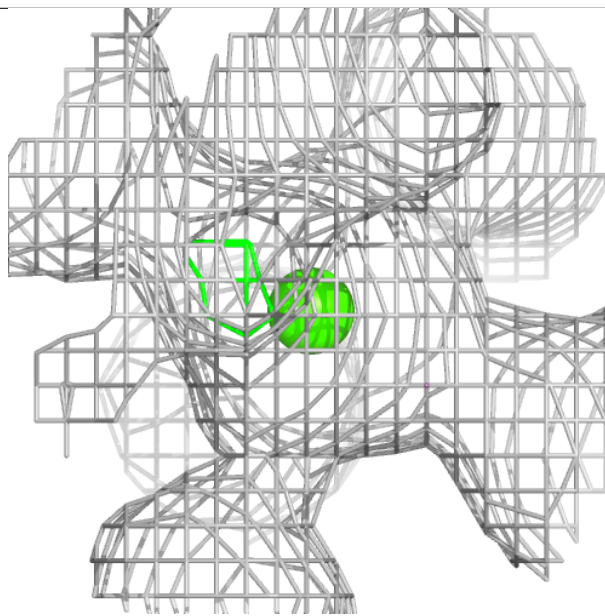
Electron density around HEC YYY 608:

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



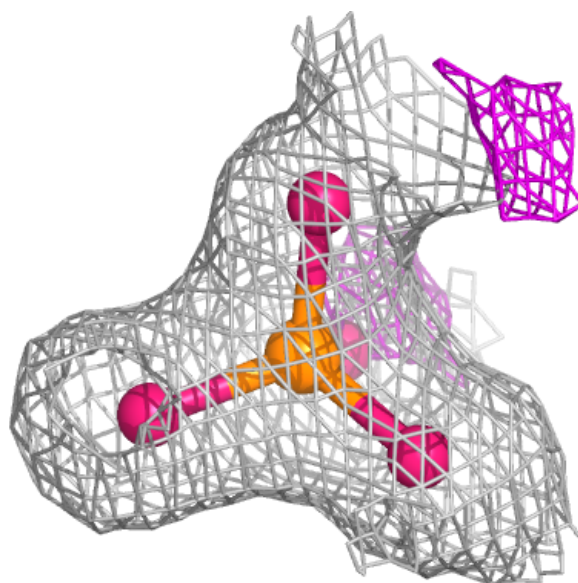
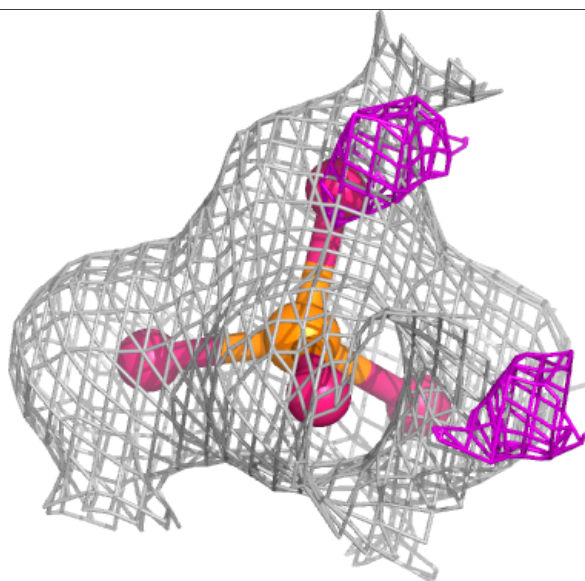
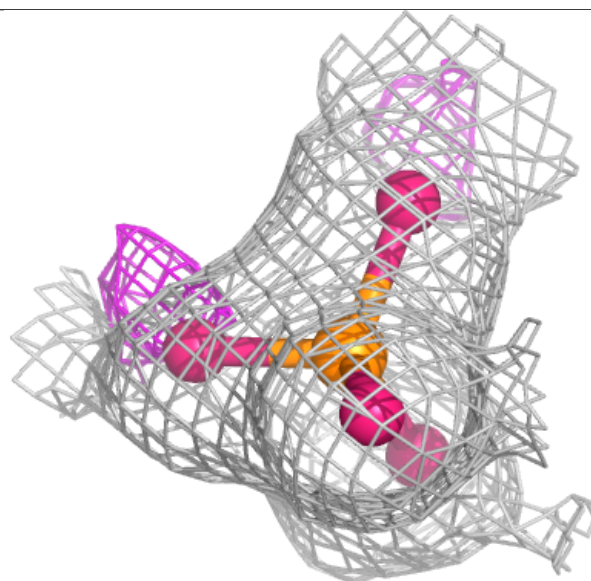
Electron density around CA MMM 609:

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



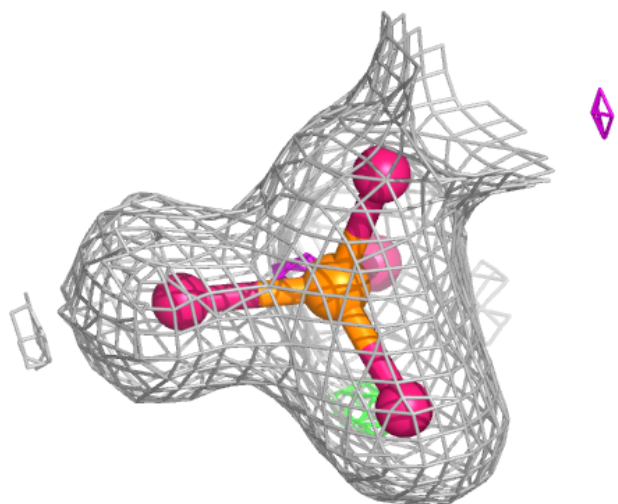
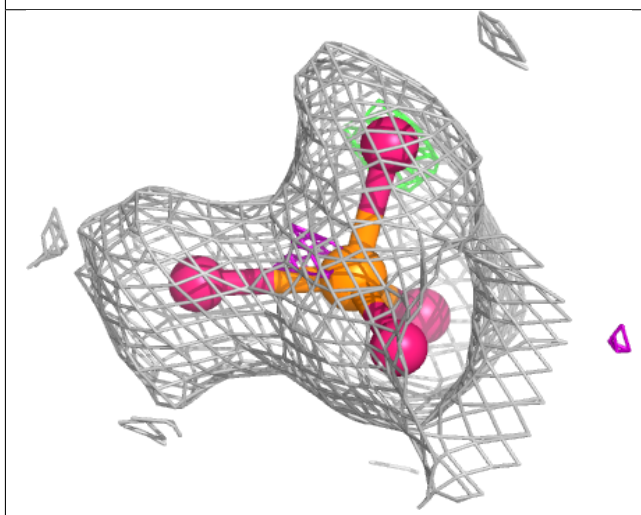
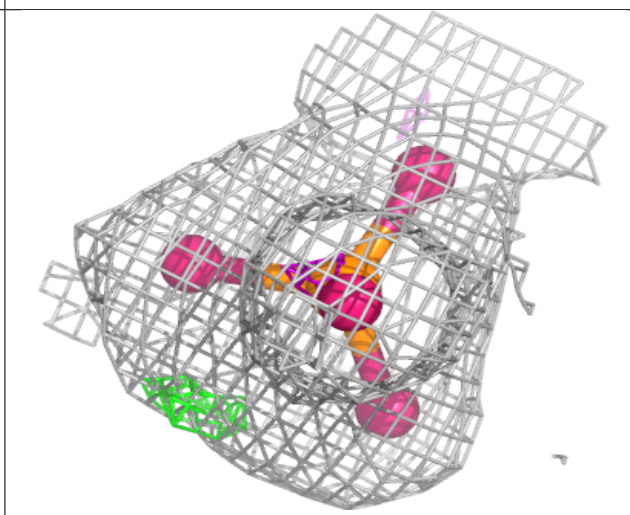
Electron density around PO4 AAA 610:

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



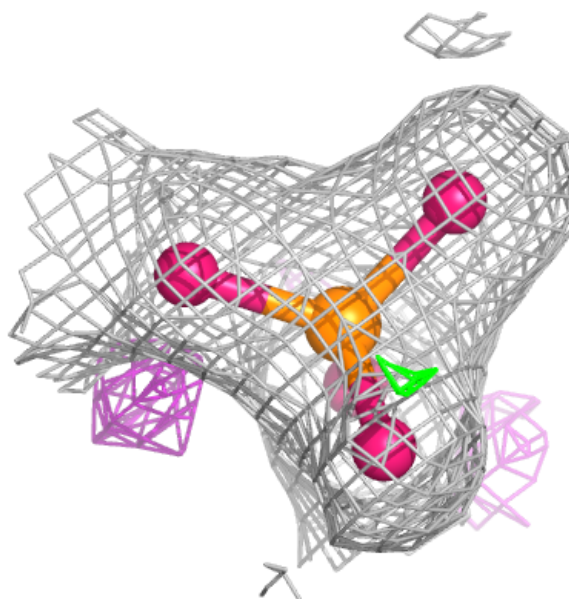
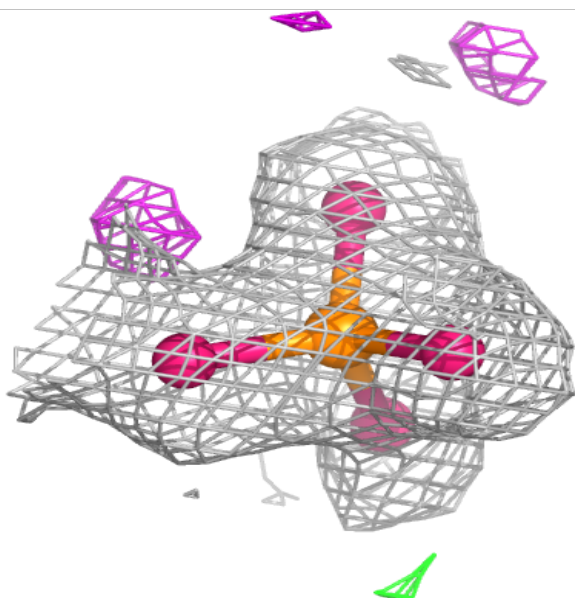
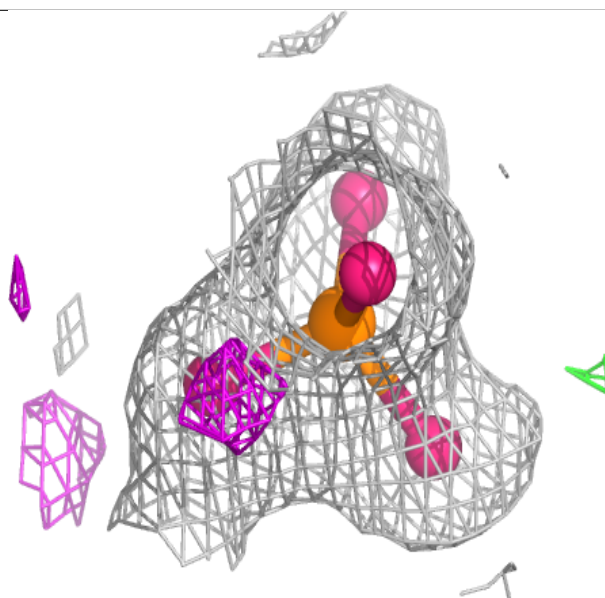
Electron density around PO4 MMM 610:

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



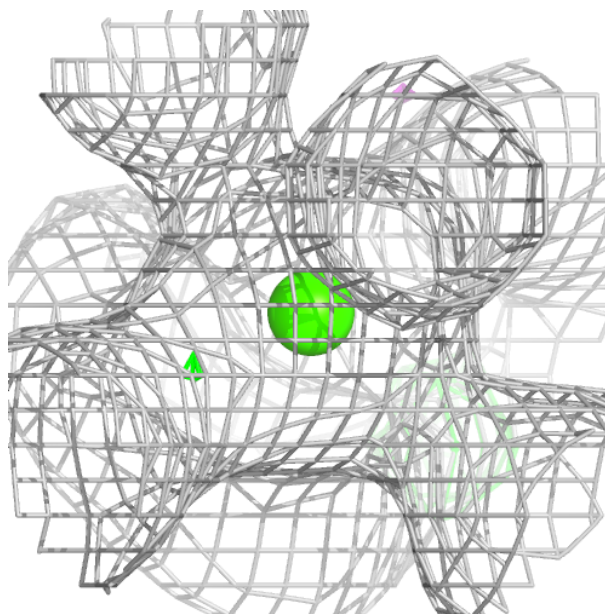
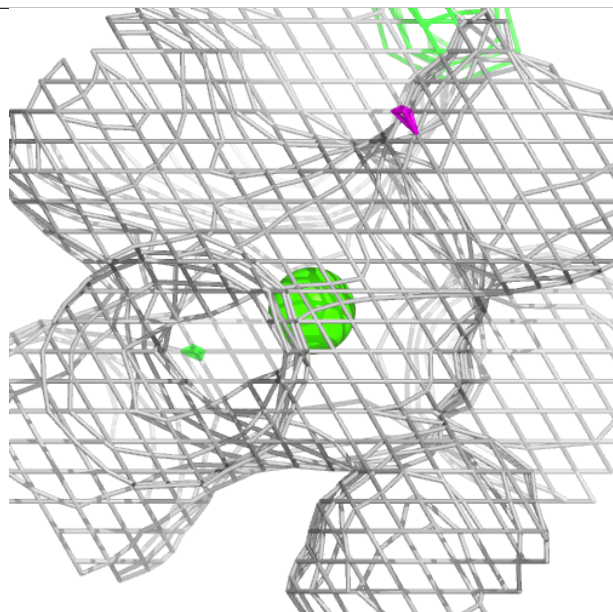
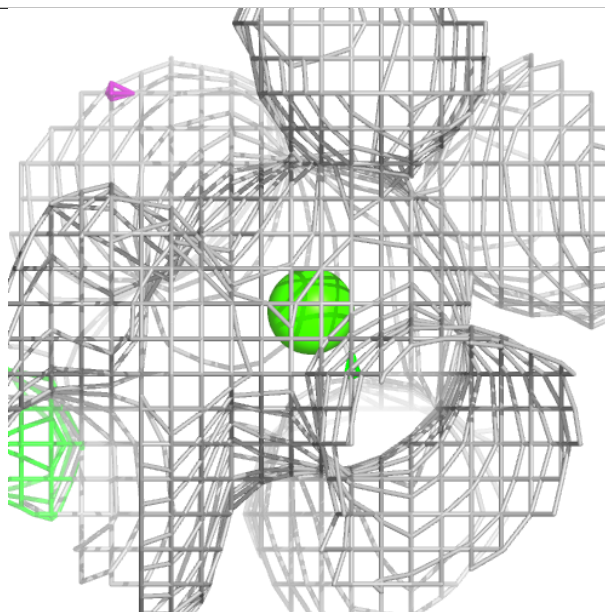
Electron density around PO4 YYY 610:

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



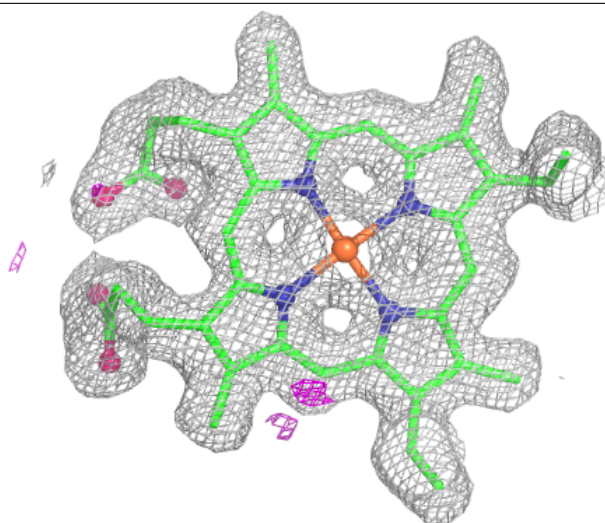
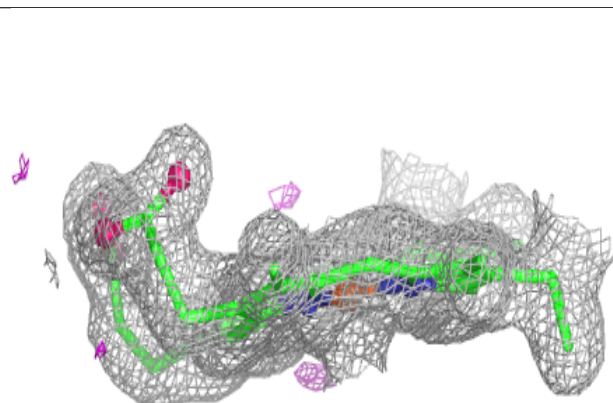
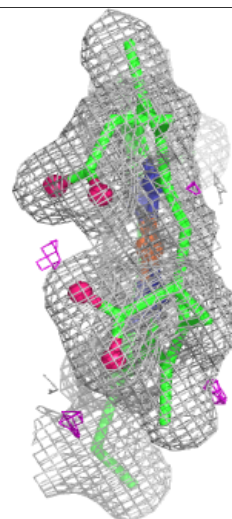
Electron density around CA AAA 609:

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



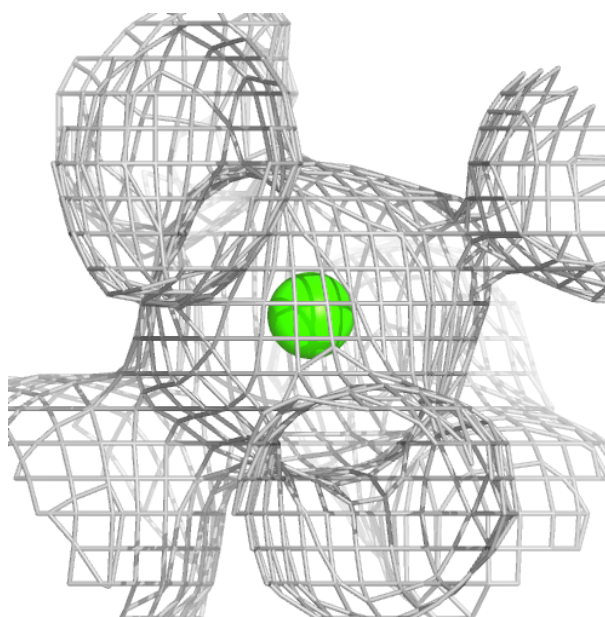
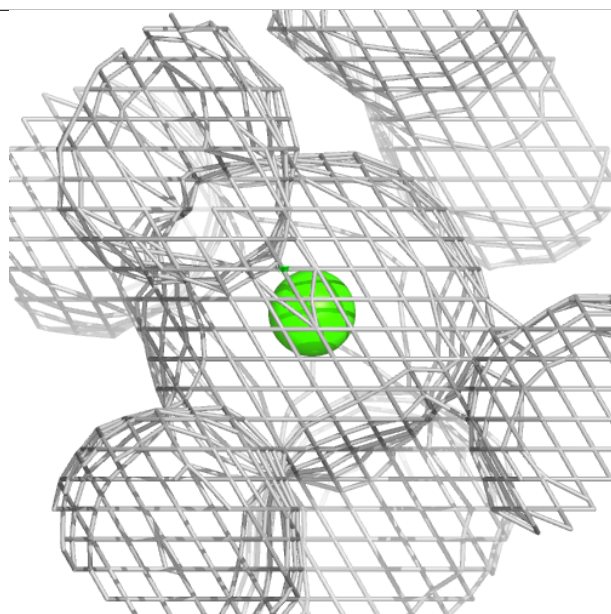
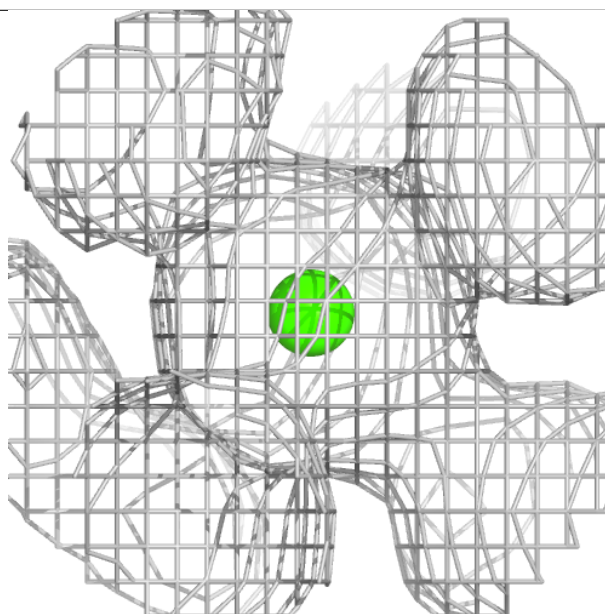
Electron density around HEC YYY 607:

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



Electron density around CA YYY 609:

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



6.5 Other polymers ⓘ

There are no such residues in this entry.