



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 5, 2026 – 02:09 PM EDT

PDB ID : 4FAS / pdb_00004fas
Title : Complex crystal structure of hydroxylamine oxidoreductase and NE1300 from *Nitrosomonas europaea*
Authors : Cedervall, P.E.; Wilmot, C.M.
Deposited on : 2012-05-22
Resolution : 2.10 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

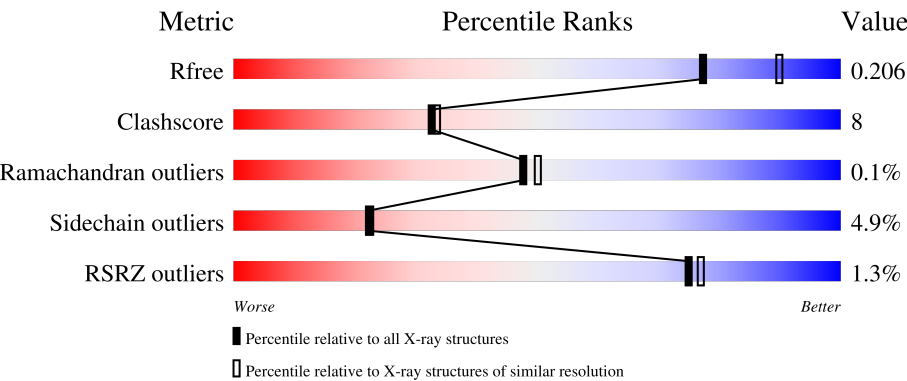
MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.015 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

1 Overall quality at a glance i

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

The reported resolution of this entry is 2.10 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	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	546	75%14%•8%
1	B	546	75%14%•8%
1	C	546	76%14%•8%
2	D	69	7% 62%9%29%
2	E	69	13% 52%14%•29%

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Mol	Chain	Length	Quality of chain
2	F	69	

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
3	HEC	A	601	X	-	-	-
3	HEC	A	602	X	-	-	-
3	HEC	A	603	X	-	-	-
3	HEC	A	604	X	-	-	-
3	HEC	A	605	X	-	-	-
3	HEC	A	606	X	-	-	-
3	HEC	A	607	X	-	-	-
3	HEC	B	601	X	-	-	-
3	HEC	B	602	X	-	-	-
3	HEC	B	603	X	-	-	-
3	HEC	B	604	X	-	-	-
3	HEC	B	605	X	-	-	-
3	HEC	B	606	X	-	-	-
3	HEC	B	607	X	-	-	-
3	HEC	C	602	X	-	-	-
3	HEC	C	603	X	-	-	-
3	HEC	C	604	X	-	-	-
3	HEC	C	605	X	-	-	-
3	HEC	C	606	X	-	-	-
3	HEC	C	607	X	-	-	-
3	HEC	C	608	X	-	-	-

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 15197 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.

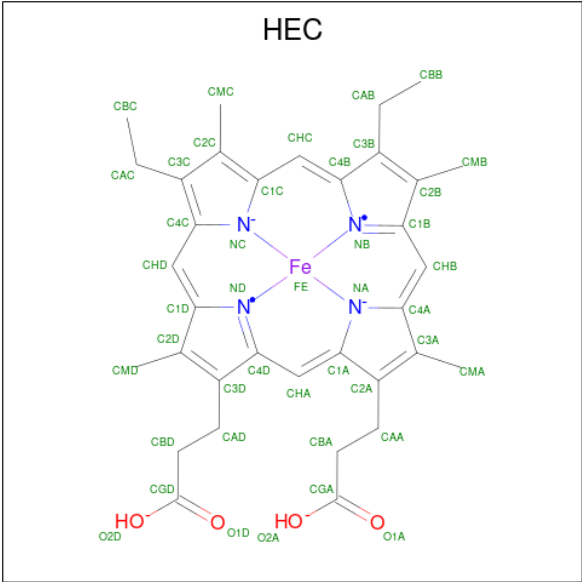
- Molecule 1 is a protein called Hydroxylamine oxidoreductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	502	Total	C	N	O	S	0	1	0
			4013	2495	711	775	32			
1	B	502	Total	C	N	O	S	0	1	0
			4005	2491	710	772	32			
1	C	502	Total	C	N	O	S	0	0	0
			4005	2491	710	772	32			

- Molecule 2 is a protein called NE1300.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	49	Total	C	N	O	S	0	0	0
			370	233	63	71	3			
2	E	49	Total	C	N	O	S	0	0	0
			370	233	63	71	3			
2	F	49	Total	C	N	O	S	0	0	0
			370	233	63	71	3			

- Molecule 3 is HEME C (CCD ID: HEC) (formula: $C_{34}H_{36}FeN_4O_4$).



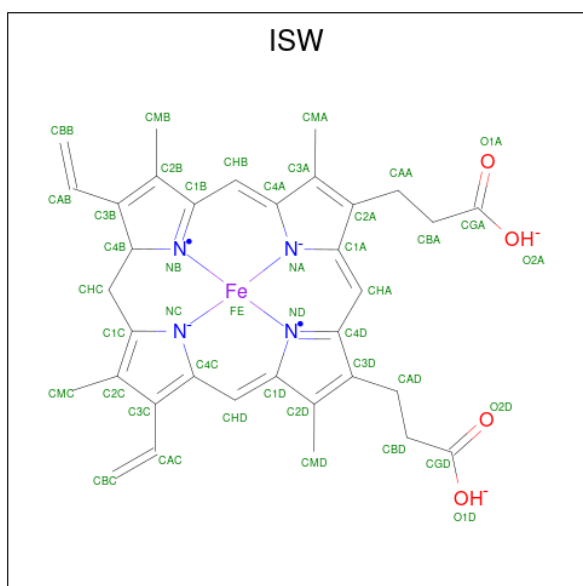
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	A	1	Total 43	C 34	Fe 1	N 4	O 4	0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

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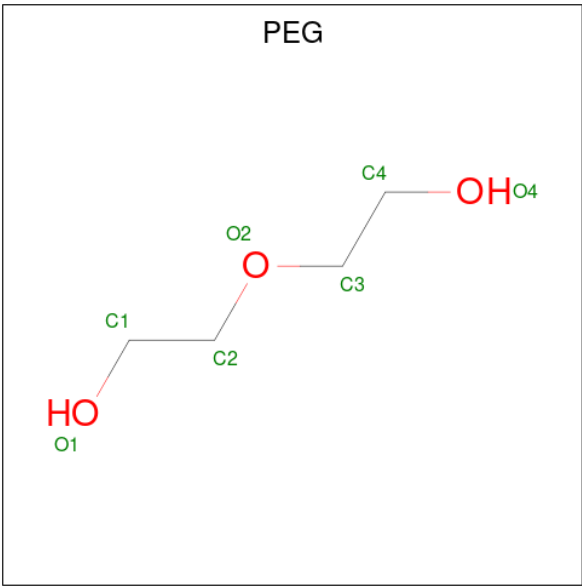
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	C	1	Total	C	Fe	N	O	
			43	34	1	4	4	
3	C	1	Total	C	Fe	N	O	
			43	34	1	4	4	
3	C	1	Total	C	Fe	N	O	
			43	34	1	4	4	
3	C	1	Total	C	Fe	N	O	
			43	34	1	4	4	
3	C	1	Total	C	Fe	N	O	
			43	34	1	4	4	
3	C	1	Total	C	Fe	N	O	
			43	34	1	4	4	

- Molecule 4 is {3,3'-[(9S)-8,13-diethenyl-3,7,12,17-tetramethyl-9,10-dihydroporphyrin-2,18-diyl-kappa 4 N 21 ,N 22 ,N 23 ,N 24]dipropanoato(2-)}iron (CCD ID: ISW) (formula: $C_{34}H_{34}FeN_4O_4$).



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

- Molecule 5 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: C₄H₁₀O₃).



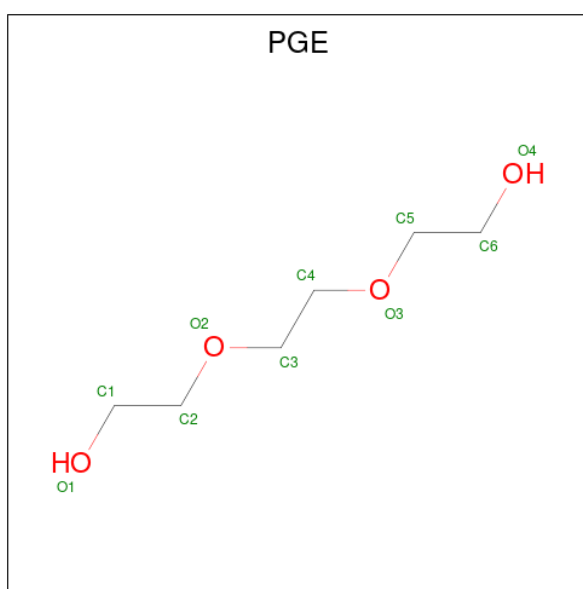
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			7	4	3		
5	A	1	Total	C	O	0	0
			7	4	3		
5	A	1	Total	C	O	0	0
			7	4	3		
5	A	1	Total	C	O	0	0
			7	4	3		
5	A	1	Total	C	O	0	0
			7	4	3		
5	B	1	Total	C	O	0	0
			7	4	3		
5	B	1	Total	C	O	0	0
			7	4	3		
5	B	1	Total	C	O	0	0
			7	4	3		
5	C	1	Total	C	O	0	0
			7	4	3		
5	C	1	Total	C	O	0	0
			7	4	3		
5	C	1	Total	C	O	0	0
			7	4	3		

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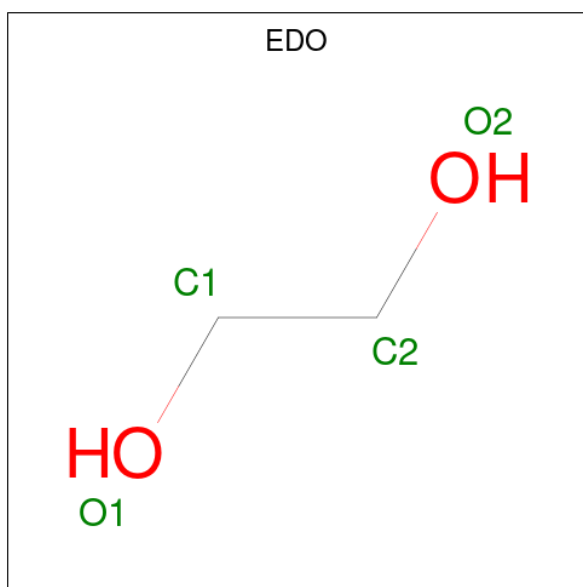
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	C	1	Total	C	O	0	0
			7	4	3		
5	C	1	Total	C	O	0	0
			7	4	3		
5	C	1	Total	C	O	0	0
			7	4	3		
5	F	1	Total	C	O	0	0
			7	4	3		

- Molecule 6 is TRIETHYLENE GLYCOL (CCD ID: PGE) (formula: $C_6H_{14}O_4$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			10	6	4		
6	C	1	Total	C	O	0	0
			10	6	4		

- Molecule 7 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



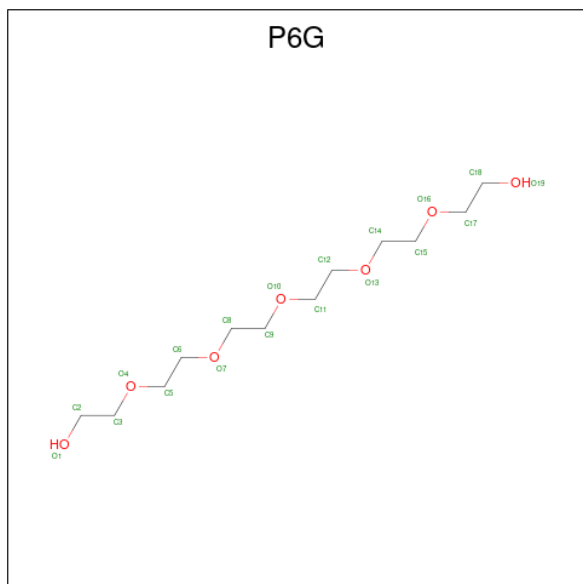
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			4	2	2		
7	A	1	Total	C	O	0	0
			4	2	2		
7	A	1	Total	C	O	0	0
			4	2	2		
7	A	1	Total	C	O	0	0
			4	2	2		
7	B	1	Total	C	O	0	0
			4	2	2		
7	B	1	Total	C	O	0	0
			4	2	2		
7	B	1	Total	C	O	0	0
			4	2	2		
7	B	1	Total	C	O	0	0
			4	2	2		
7	C	1	Total	C	O	0	0
			4	2	2		
7	C	1	Total	C	O	0	0
			4	2	2		
7	C	1	Total	C	O	0	0
			4	2	2		
7	C	1	Total	C	O	0	0
			4	2	2		

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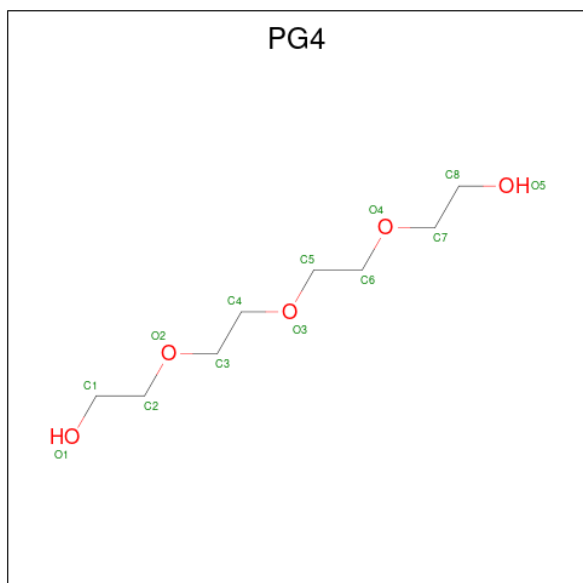
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	C	1	Total	C	O	0	0
			4	2	2		

- Molecule 8 is HEXAETHYLENE GLYCOL (CCD ID: P6G) (formula: $C_{12}H_{26}O_7$).



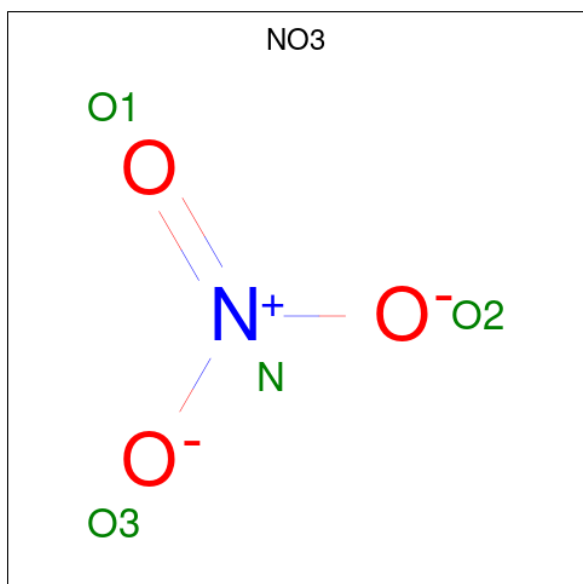
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	B	1	Total	C	O	0	0
			19	12	7		

- Molecule 9 is TETRAETHYLENE GLYCOL (CCD ID: PG4) (formula: $C_8H_{18}O_5$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	B	1	Total	C	O	0	0
			13	8	5		

- Molecule 10 is NITRATE ION (CCD ID: NO3) (formula: NO₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	B	1	Total	N	O	0	0
			4	1	3		
10	B	1	Total	N	O	0	0
			4	1	3		
10	C	1	Total	N	O	0	0
			4	1	3		
10	F	1	Total	N	O	0	0
			4	1	3		

- Molecule 11 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	A	237	Total	O	0	0
			237	237		
11	B	258	Total	O	0	0
			258	258		
11	C	244	Total	O	0	0
			244	244		
11	D	14	Total	O	0	0
			14	14		
11	E	10	Total	O	0	0
			10	10		

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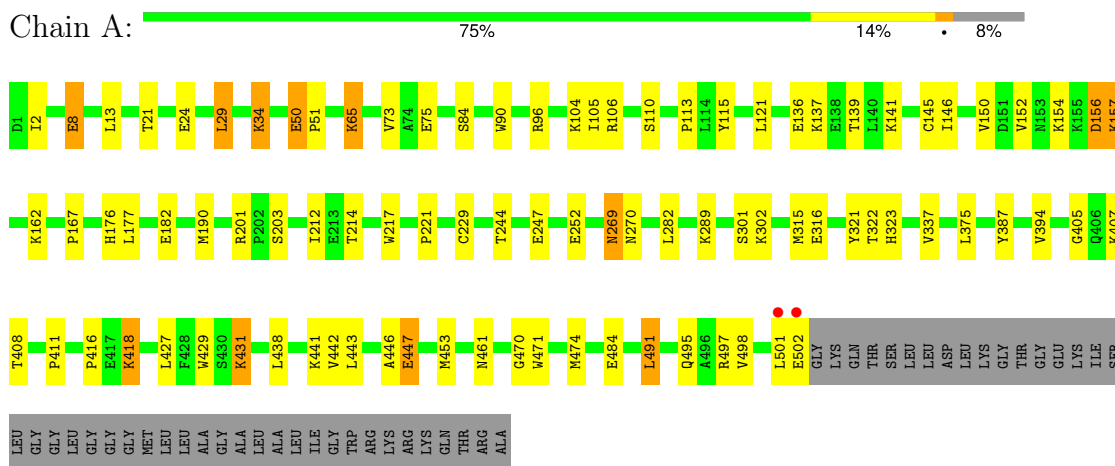
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	F	22	Total	O	0	0
			22	22		

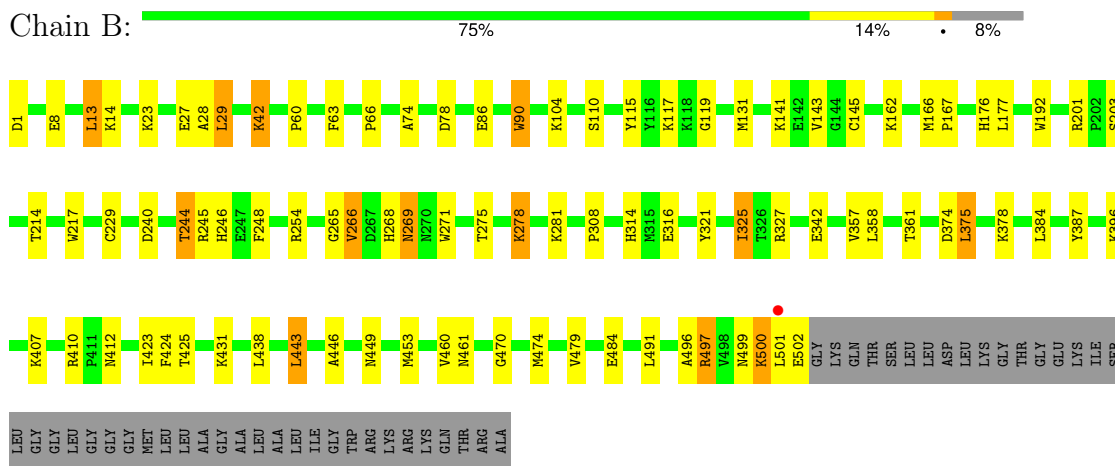
3 Residue-property plots

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.

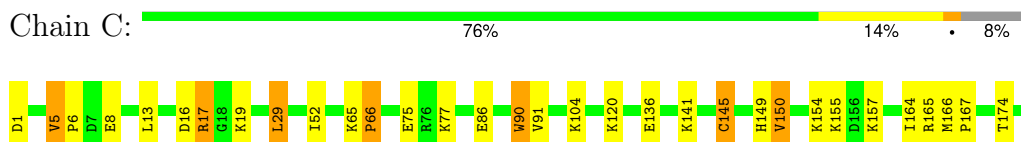
- Molecule 1: Hydroxylamine oxidoreductase

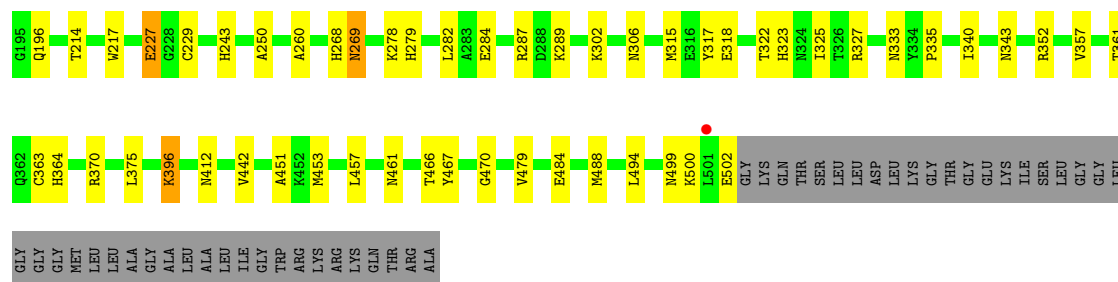


- Molecule 1: Hydroxylamine oxidoreductase



- Molecule 1: Hydroxylamine oxidoreductase





- Molecule 2: NE1300



- Molecule 2: NE1300



- Molecule 2: NE1300



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	140.73Å 142.62Å 107.38Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	42.89 – 2.10 42.89 – 2.10	Depositor EDS
% Data completeness (in resolution range)	79.9 (42.89-2.10) 79.9 (42.89-2.10)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.36 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.165 , 0.206 0.166 , 0.206	Depositor DCC
R_{free} test set	5071 reflections (4.03%)	wwPDB-VP
Wilson B-factor (Å ²)	23.6	Xtriage
Anisotropy	0.603	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 51.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.015 for k,h,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	15197	wwPDB-VP
Average B, all atoms (Å ²)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.74% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PGE, PG4, NO3, ISW, EDO, PEG, P6G, HEC

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	1.26	7/4116 (0.2%)	1.17	10/5578 (0.2%)
1	B	1.31	8/4108 (0.2%)	1.21	14/5567 (0.3%)
1	C	1.29	9/4108 (0.2%)	1.19	15/5567 (0.3%)
2	D	1.00	0/373	1.10	0/502
2	E	1.09	0/373	1.19	1/502 (0.2%)
2	F	1.16	0/373	1.18	0/502
All	All	1.27	24/13451 (0.2%)	1.19	40/18218 (0.2%)

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	466	THR	CA-C	8.99	1.56	1.52
1	C	91	VAL	CA-CB	6.34	1.62	1.54
1	C	363	CYS	C-O	-6.34	1.16	1.24
1	B	254	ARG	C-O	6.09	1.31	1.24
1	C	352	ARG	C-O	5.91	1.31	1.24
1	B	375	LEU	CA-C	5.64	1.60	1.52
1	B	314	HIS	N-CA	5.62	1.53	1.46
1	A	270	ASN	N-CA	5.59	1.53	1.46
1	A	162	LYS	C-O	-5.46	1.15	1.23
1	B	325	ILE	CA-CB	5.37	1.60	1.54
1	A	2	ILE	N-CA	5.36	1.52	1.46
1	A	50	GLU	CA-C	5.34	1.57	1.52
1	B	244	THR	CA-CB	5.32	1.62	1.53
1	C	457	LEU	C-O	5.32	1.30	1.24
1	A	51	PRO	N-CA	-5.29	1.40	1.47
1	A	461	ASN	C-O	5.21	1.30	1.24
1	C	250	ALA	CA-CB	5.20	1.61	1.53
1	B	66	PRO	CA-C	5.17	1.56	1.52
1	A	65	LYS	CA-C	5.16	1.57	1.52
1	C	165	ARG	CA-C	5.13	1.58	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	343	ASN	C-O	-5.09	1.17	1.24
1	B	117	LYS	C-O	-5.04	1.17	1.24
1	B	308	PRO	C-O	5.03	1.29	1.23
1	C	150	VAL	C-O	-5.01	1.18	1.24

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	66	PRO	CA-C-N	-7.87	112.60	120.31
1	C	66	PRO	C-N-CA	-7.87	112.60	120.31
1	C	5	VAL	CA-C-N	6.34	126.31	119.78
1	C	5	VAL	C-N-CA	6.34	126.31	119.78
1	B	443	LEU	N-CA-C	-6.30	104.33	111.14
1	C	461	ASN	CA-C-N	6.24	125.73	119.24
1	C	461	ASN	C-N-CA	6.24	125.73	119.24
1	B	265	GLY	N-CA-C	6.21	120.87	112.17
1	B	266	VAL	CB-CA-C	-6.06	100.22	111.79
1	B	410	ARG	CA-C-N	-6.01	113.78	119.85
1	B	410	ARG	C-N-CA	-6.01	113.78	119.85
2	E	47	CYS	N-CA-C	5.95	117.77	111.28
1	C	467	TYR	N-CA-C	5.87	117.35	111.07
1	B	412	ASN	CA-C-N	5.84	126.39	120.38
1	B	412	ASN	C-N-CA	5.84	126.39	120.38
1	B	449	ASN	N-CA-C	5.83	117.71	111.36
1	A	394	VAL	N-CA-C	-5.64	105.02	110.72
1	B	192	TRP	CA-C-N	-5.63	113.22	119.19
1	B	192	TRP	C-N-CA	-5.63	113.22	119.19
1	C	279	HIS	CA-C-N	5.53	126.12	119.98
1	C	279	HIS	C-N-CA	5.53	126.12	119.98
1	B	425	THR	N-CA-C	5.48	117.96	111.33
1	C	260	ALA	N-CA-C	5.46	117.31	111.36
1	C	412	ASN	CA-C-N	-5.46	114.75	120.38
1	C	412	ASN	C-N-CA	-5.46	114.75	120.38
1	B	461	ASN	CB-CA-C	-5.43	104.79	110.33
1	A	244	THR	N-CA-C	5.39	117.68	110.35
1	A	447	GLU	CB-CA-C	-5.34	102.49	110.88
1	C	174	THR	N-CA-C	-5.33	105.55	111.36
1	A	471	TRP	N-CA-C	5.29	117.46	111.11
1	A	337	VAL	CB-CA-C	5.27	116.74	110.68
1	A	105	ILE	CB-CA-C	-5.26	105.04	112.14
1	C	289	LYS	N-CA-C	-5.21	107.30	113.97
1	C	451	ALA	N-CA-C	-5.19	105.51	111.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	86	GLU	N-CA-C	5.14	116.96	111.36
1	A	418	LYS	CA-C-N	5.12	125.04	119.76
1	A	418	LYS	C-N-CA	5.12	125.04	119.76
1	A	84	SER	N-CA-C	-5.11	106.15	112.38
1	B	327	ARG	N-CA-C	5.08	118.73	112.54
1	A	156	ASP	N-CA-C	5.05	114.96	108.34

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4013	0	3811	62	0
1	B	4005	0	3807	64	0
1	C	4005	0	3808	61	0
2	D	370	0	391	1	0
2	E	370	0	391	9	0
2	F	370	0	391	8	0
3	A	301	0	210	8	0
3	B	301	0	210	10	0
3	C	301	0	210	13	0
4	A	43	0	28	10	0
4	B	43	0	28	10	0
4	C	43	0	28	11	0
5	A	42	0	60	6	0
5	B	28	0	40	4	0
5	C	42	0	60	4	0
5	F	7	0	10	1	0
6	A	10	0	14	1	0
6	C	10	0	14	4	0
7	A	16	0	24	3	0
7	B	20	0	30	0	0
7	C	24	0	36	3	0
8	B	19	0	26	1	0
9	B	13	0	18	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	B	8	0	0	0	0
10	C	4	0	0	0	0
10	F	4	0	0	0	0
11	A	237	0	0	4	0
11	B	258	0	0	1	0
11	C	244	0	0	3	0
11	D	14	0	0	0	0
11	E	10	0	0	0	0
11	F	22	0	0	1	0
All	All	15197	0	13645	221	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

All (221) 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)
4:A:608:ISW:HBAA	3:B:605:HEC:O1D	1.65	0.96
4:B:608:ISW:HBAA	3:C:606:HEC:O1D	1.66	0.95
1:B:497:ARG:HB2	1:B:497:ARG:HH11	1.31	0.95
1:B:497:ARG:HH11	1:B:497:ARG:CB	1.80	0.94
1:B:13:LEU:HD21	1:B:29:LEU:HD13	1.49	0.92
1:A:13:LEU:HD11	1:A:29:LEU:HD13	1.55	0.89
1:B:104:LYS:HE3	5:B:609:PEG:H22	1.54	0.87
1:A:495:GLN:HG2	1:C:494:LEU:HD13	1.61	0.81
1:C:13:LEU:HD11	1:C:29:LEU:HD13	1.64	0.80
1:B:104:LYS:CE	5:B:609:PEG:H22	2.12	0.79
2:E:30:VAL:HG22	2:E:46:LYS:HA	1.64	0.79
3:A:605:HEC:O1D	4:C:601:ISW:HBAA	1.83	0.77
1:B:497:ARG:HH11	1:B:497:ARG:CG	1.96	0.77
1:B:119:GLY:HA3	8:B:613:P6G:H61	1.68	0.75
1:A:407:LYS:HE3	5:A:613:PEG:H11	1.69	0.74
4:A:608:ISW:HBB	4:A:608:ISW:HMB	1.70	0.74
1:B:497:ARG:HB2	1:B:497:ARG:NH1	2.03	0.73
1:A:315:MET:HE2	1:A:323:HIS:HA	1.69	0.72
1:C:269:ASN:HD22	1:C:269:ASN:H	1.36	0.71
1:A:405:GLY:HA2	1:A:408:THR:CG2	2.21	0.70
1:A:407:LYS:CE	5:A:613:PEG:H11	2.21	0.70
2:D:46:LYS:HB3	2:D:49:ASP:OD2	1.90	0.70
1:A:405:GLY:HA2	1:A:408:THR:HG22	1.73	0.69
1:B:497:ARG:CB	1:B:497:ARG:NH1	2.56	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:396:LYS:HE2	1:C:396:LYS:HA	1.74	0.69
1:A:8:GLU:N	1:A:8:GLU:OE1	2.28	0.67
1:A:431:LYS:HE3	11:F:212:HOH:O	1.95	0.66
1:B:8:GLU:OE1	1:B:8:GLU:N	2.20	0.66
1:C:104:LYS:NZ	6:C:614:PGE:H42	2.11	0.65
1:A:498:VAL:O	1:A:502:GLU:HG3	1.96	0.64
1:B:248:PHE:O	3:B:603:HEC:HBA1	1.98	0.64
1:A:214:THR:HG21	4:C:601:ISW:HMBA	1.81	0.63
1:C:13:LEU:CD1	1:C:29:LEU:HD13	2.28	0.62
1:B:13:LEU:CD2	1:B:29:LEU:HD13	2.27	0.62
1:C:90:TRP:HA	1:C:90:TRP:CE3	2.33	0.62
3:A:605:HEC:O2A	4:C:601:ISW:O2D	2.18	0.62
4:B:608:ISW:HBB	4:B:608:ISW:HMB	1.81	0.62
1:B:374:ASP:OD1	1:B:378:LYS:HE2	2.01	0.61
1:A:316:GLU:HB2	1:A:321:TYR:CE2	2.36	0.60
1:A:269:ASN:HD22	1:A:269:ASN:H	1.48	0.60
1:C:333:ASN:O	1:C:335:PRO:HD3	2.01	0.60
1:C:19:LYS:NZ	7:C:617:EDO:H21	2.17	0.59
4:A:608:ISW:HHC	1:B:229:CYS:SG	2.42	0.59
5:A:614:PEG:H42	4:C:601:ISW:HMA	1.84	0.59
4:B:608:ISW:HMBA	1:C:214:THR:HG21	1.84	0.59
1:C:13:LEU:HD11	1:C:29:LEU:CD1	2.31	0.59
1:B:387:TYR:CE1	1:B:446:ALA:HB2	2.38	0.58
1:B:269:ASN:H	1:B:269:ASN:HD22	1.50	0.58
1:A:34:LYS:NZ	11:A:832:HOH:O	2.32	0.58
1:C:315:MET:HE3	1:C:323:HIS:HA	1.85	0.58
1:C:194:ASN:HB3	2:F:7:SER:HB3	1.86	0.57
1:A:201:ARG:NE	4:C:601:ISW:O1A	2.29	0.57
1:A:229:CYS:SG	4:C:601:ISW:HHC	2.45	0.57
1:C:90:TRP:HA	1:C:90:TRP:HE3	1.71	0.56
2:F:11:ILE:HD13	2:F:54:VAL:HG22	1.87	0.56
1:B:23:LYS:HG3	1:B:131:MET:HA	1.88	0.55
4:C:601:ISW:HMB	4:C:601:ISW:HBB	1.87	0.55
1:A:495:GLN:HG2	1:C:494:LEU:CD1	2.32	0.55
3:C:606:HEC:HBA2	3:C:607:HEC:HMA3	1.87	0.55
3:C:608:HEC:HBB3	3:C:608:HEC:CMB	2.37	0.55
1:A:190:MET:HE3	1:A:190:MET:HA	1.89	0.55
1:B:501:LEU:HD11	1:C:502:GLU:HG2	1.88	0.54
4:B:608:ISW:HHC	1:C:229:CYS:SG	2.46	0.54
1:A:407:LYS:NZ	5:A:613:PEG:H11	2.21	0.54
1:A:501:LEU:HD11	1:B:502:GLU:HG3	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:302:LYS:HZ3	7:A:617:EDO:H12	1.72	0.54
1:B:90:TRP:HA	1:B:90:TRP:CE3	2.43	0.54
3:B:605:HEC:HBA2	3:B:606:HEC:HMA3	1.89	0.54
1:C:19:LYS:HZ2	7:C:617:EDO:H21	1.70	0.54
4:A:608:ISW:O2A	1:B:201:ARG:NE	2.35	0.53
1:B:497:ARG:HH11	1:B:497:ARG:HG3	1.71	0.53
1:A:75:GLU:OE2	1:A:157:LYS:HE2	2.09	0.53
4:B:608:ISW:C3A	5:C:610:PEG:H32	2.39	0.53
5:A:614:PEG:H42	4:C:601:ISW:CMA	2.39	0.52
1:B:316:GLU:HB2	1:B:321:TYR:CE2	2.43	0.52
4:A:608:ISW:HMBA	1:B:214:THR:HG21	1.92	0.52
1:B:357:VAL:O	1:B:361:THR:HG23	2.10	0.52
1:C:1:ASP:HB3	1:C:17:ARG:O	2.10	0.52
4:A:608:ISW:HBB	4:A:608:ISW:CMB	2.38	0.51
1:B:1:ASP:OD2	9:B:614:PG4:O1	2.27	0.51
1:C:75:GLU:HG3	1:C:157:LYS:HG2	1.93	0.51
1:B:453:MET:SD	1:B:474:MET:CE	2.99	0.51
4:A:608:ISW:HMB	4:A:608:ISW:CBB	2.40	0.50
1:B:453:MET:HB2	1:B:470:GLY:HA2	1.93	0.50
1:C:375:LEU:HD23	1:C:375:LEU:C	2.36	0.50
1:A:104:LYS:NZ	6:A:615:PGE:H1	2.26	0.50
1:C:104:LYS:HZ3	6:C:614:PGE:H42	1.76	0.50
2:F:32:LYS:HD2	5:F:102:PEG:H22	1.94	0.50
1:B:90:TRP:HA	1:B:90:TRP:HE3	1.77	0.50
1:A:427:LEU:HD11	1:A:447:GLU:HG3	1.92	0.49
1:B:479:VAL:HG22	11:C:726:HOH:O	2.11	0.49
2:E:50:ILE:HD13	2:E:50:ILE:O	2.12	0.49
1:B:203:SER:O	3:B:605:HEC:HBD1	2.13	0.49
1:A:217:TRP:HB2	4:C:601:ISW:HMB	1.94	0.49
1:C:484:GLU:OE2	1:C:488:MET:HE2	2.12	0.49
1:B:496:ALA:O	1:B:500:LYS:HE2	2.13	0.48
1:C:184:GLU:OE1	1:C:187:ARG:NE	2.43	0.48
4:A:608:ISW:O1A	1:B:201:ARG:NH1	2.35	0.48
1:C:453:MET:HB2	1:C:470:GLY:HA2	1.95	0.48
4:A:608:ISW:HMB	1:B:217:TRP:HB2	1.95	0.48
3:B:601:HEC:CAA	3:B:602:HEC:HMA3	2.43	0.48
1:A:387:TYR:CE1	1:A:446:ALA:HB2	2.49	0.48
1:B:60:PRO:HB3	1:B:166:MET:HB2	1.95	0.48
1:C:488:MET:HE1	11:C:877:HOH:O	2.13	0.48
1:C:484:GLU:HG2	1:C:488:MET:CE	2.44	0.48
1:C:8:GLU:OE1	1:C:8:GLU:N	2.46	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:66:PRO:HB3	1:C:164:ILE:HB	1.96	0.47
2:E:22:CYS:O	2:E:23:LYS:C	2.57	0.47
1:B:431:LYS:NZ	11:B:914:HOH:O	2.44	0.47
1:C:104:LYS:HZ2	6:C:614:PGE:H42	1.79	0.47
3:C:602:HEC:CAA	3:C:603:HEC:HMA3	2.44	0.47
1:A:453:MET:SD	1:A:474:MET:CE	3.03	0.47
1:B:271:TRP:O	1:B:275:THR:HG23	2.14	0.47
1:A:453:MET:HB2	1:A:470:GLY:HA2	1.96	0.47
1:C:141:LYS:HB3	5:C:612:PEG:H22	1.97	0.47
1:A:495:GLN:CG	1:C:494:LEU:HD13	2.39	0.47
3:A:601:HEC:HBC3	3:A:601:HEC:HMC1	1.95	0.47
3:A:604:HEC:HHA	3:A:604:HEC:HAA2	1.69	0.47
1:C:269:ASN:HD22	1:C:269:ASN:N	2.05	0.47
2:F:50:ILE:O	2:F:50:ILE:HD13	2.14	0.47
1:C:120:LYS:HE2	3:C:605:HEC:HAA1	1.97	0.46
1:C:284:GLU:O	1:C:287:ARG:HG2	2.15	0.46
1:A:150:VAL:HG11	1:A:154:LYS:HD3	1.97	0.46
3:C:602:HEC:HBC3	3:C:602:HEC:HMC3	1.96	0.46
2:F:19:TYR:CE2	2:F:23:LYS:HE2	2.50	0.46
3:A:603:HEC:CAA	3:A:604:HEC:HBA1	2.46	0.46
1:B:110:SER:HA	1:B:115:TYR:CG	2.51	0.46
1:C:317:TYR:O	1:C:318:GLU:C	2.57	0.46
1:A:13:LEU:CD1	1:A:29:LEU:HD13	2.38	0.46
3:B:601:HEC:HAA2	3:B:602:HEC:HMA3	1.98	0.46
1:A:106:ARG:NH2	1:A:139:THR:HB	2.31	0.45
1:A:106:ARG:HG3	1:A:121:LEU:HD21	1.97	0.45
1:A:411:PRO:HG3	1:A:431:LYS:HG3	1.98	0.45
1:B:74:ALA:HB1	1:B:78:ASP:HB2	1.99	0.45
1:C:86:GLU:HG3	3:C:602:HEC:HMD3	1.98	0.45
1:A:50:GLU:OE1	2:F:32:LYS:NZ	2.48	0.45
1:C:196:GLN:HG2	1:C:340:ILE:HD13	1.98	0.45
2:E:55:GLN:CD	2:E:55:GLN:N	2.74	0.45
1:A:21:THR:OG1	1:A:24:GLU:HG3	2.17	0.45
1:B:13:LEU:HG	1:B:28:ALA:HB1	1.98	0.45
1:B:407:LYS:HD3	1:B:407:LYS:HA	1.71	0.45
1:C:1:ASP:OD1	1:C:17:ARG:NE	2.40	0.45
1:A:375:LEU:HD23	1:A:375:LEU:C	2.42	0.45
2:F:47:CYS:O	2:F:51:VAL:HG23	2.17	0.44
1:A:302:LYS:NZ	7:A:617:EDO:H12	2.32	0.44
4:B:608:ISW:O2D	3:C:606:HEC:O2A	2.35	0.44
2:E:30:VAL:HG22	2:E:46:LYS:CA	2.42	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:146:ILE:O	1:A:150:VAL:HB	2.18	0.44
1:B:269:ASN:HD22	1:B:269:ASN:N	2.12	0.44
3:A:605:HEC:HBA2	3:A:606:HEC:HMA3	2.00	0.44
1:B:162:LYS:HB2	1:B:162:LYS:HE3	1.77	0.44
4:B:608:ISW:C3A	5:C:610:PEG:C3	2.96	0.44
1:C:52:ILE:HD11	1:C:227:GLU:HG2	2.00	0.44
1:A:156:ASP:OD1	1:A:156:ASP:N	2.49	0.44
1:B:167:PRO:HG2	3:B:602:HEC:CHD	2.48	0.44
1:B:438:LEU:HG	1:B:484:GLU:CD	2.42	0.44
1:C:302:LYS:HZ3	5:C:622:PEG:C3	2.31	0.44
1:B:384:LEU:HD23	2:E:13:ALA:HB2	2.00	0.43
1:C:243:HIS:CE1	3:C:605:HEC:NB	2.85	0.43
4:B:608:ISW:HMB	1:C:217:TRP:HB2	2.00	0.43
1:C:361:THR:HA	1:C:364:HIS:O	2.18	0.43
1:A:176:HIS:HA	11:A:804:HOH:O	2.18	0.43
1:A:221:PRO:HB3	2:F:42:ILE:HG12	2.00	0.43
11:A:775:HOH:O	1:C:479:VAL:HG22	2.17	0.43
1:B:491:LEU:O	1:B:491:LEU:HD13	2.18	0.43
1:C:396:LYS:HE2	1:C:396:LYS:CA	2.34	0.43
1:C:453:MET:HB2	1:C:470:GLY:CA	2.48	0.43
1:A:96:ARG:HH22	1:C:306:ASN:HB3	1.83	0.43
1:B:104:LYS:NZ	5:B:609:PEG:H22	2.34	0.43
1:A:157:LYS:CD	1:A:157:LYS:H	2.31	0.43
1:B:23:LYS:O	1:B:27:GLU:HG3	2.19	0.43
1:B:42:LYS:HD2	1:B:63:PHE:CZ	2.53	0.43
1:B:375:LEU:C	1:B:375:LEU:HD23	2.44	0.43
1:A:110:SER:HA	1:A:115:TYR:CG	2.54	0.43
1:A:203:SER:O	3:A:605:HEC:HBD1	2.18	0.43
1:B:275:THR:O	1:B:281:LYS:HG2	2.18	0.43
1:C:166:MET:HA	1:C:167:PRO:HD3	1.93	0.42
1:C:278:LYS:HA	1:C:278:LYS:HD3	1.80	0.42
1:A:113:PRO:HA	5:A:612:PEG:H21	2.00	0.42
1:A:167:PRO:HG2	3:A:602:HEC:CHD	2.49	0.42
2:E:47:CYS:O	2:E:51:VAL:HB	2.19	0.42
1:C:145:CYS:O	1:C:149:HIS:HB2	2.20	0.42
3:C:602:HEC:HMC3	3:C:602:HEC:CBC	2.49	0.42
2:E:20:LEU:HD23	2:E:20:LEU:HA	1.68	0.42
1:C:150:VAL:HG11	1:C:154:LYS:HE2	2.01	0.42
1:A:96:ARG:NH2	1:C:306:ASN:HB3	2.34	0.42
1:A:438:LEU:HG	1:A:484:GLU:CD	2.45	0.42
1:B:176:HIS:CD2	3:B:603:HEC:NB	2.86	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:327:ARG:HB2	11:C:727:HOH:O	2.19	0.42
1:C:370:ARG:HB3	7:C:616:EDO:H21	2.02	0.42
1:B:423:ILE:O	1:B:424:PHE:C	2.61	0.41
1:C:104:LYS:HD2	6:C:614:PGE:H2	2.00	0.41
1:A:214:THR:CG2	4:C:601:ISW:HMBA	2.50	0.41
1:B:278:LYS:HA	1:B:278:LYS:HD3	1.60	0.41
1:B:245:ARG:HA	1:B:246:HIS:HA	1.87	0.41
4:B:608:ISW:HMBA	1:C:214:THR:CG2	2.50	0.41
1:C:357:VAL:O	1:C:361:THR:HG23	2.20	0.41
2:E:18:ASP:HB2	2:E:50:ILE:HG13	2.02	0.41
1:B:143:VAL:HG22	3:B:603:HEC:HBC2	2.02	0.41
3:C:608:HEC:HBB3	3:C:608:HEC:HMB1	2.02	0.41
1:A:252:GLU:OE2	1:C:282:LEU:HD21	2.20	0.41
4:B:608:ISW:HBAA	3:C:606:HEC:CGD	2.44	0.41
5:B:612:PEG:H41	5:B:612:PEG:H21	1.59	0.41
1:A:429:TRP:CZ2	1:A:431:LYS:HB3	2.56	0.41
1:A:416:PRO:O	7:A:619:EDO:H11	2.21	0.41
1:B:143:VAL:HG21	3:B:603:HEC:CHD	2.51	0.41
1:A:152:VAL:HG23	11:A:720:HOH:O	2.21	0.41
1:A:182:GLU:CD	1:A:322:THR:HB	2.46	0.41
1:A:491:LEU:CD2	1:B:491:LEU:HD21	2.51	0.41
4:A:608:ISW:O1A	4:A:608:ISW:HMAB	2.21	0.41
1:A:8:GLU:H	1:A:8:GLU:CD	2.22	0.40
1:B:42:LYS:HD2	1:B:63:PHE:HZ	1.85	0.40
1:B:240:ASP:O	1:B:244:THR:HA	2.21	0.40
1:C:325:ILE:HD13	3:C:606:HEC:C3A	2.51	0.40
1:A:441:LYS:HE3	1:A:441:LYS:HB2	1.90	0.40
1:C:5:VAL:HA	1:C:6:PRO:HD3	1.83	0.40
1:A:491:LEU:HD21	1:B:491:LEU:HD21	2.03	0.40
1:A:201:ARG:HH21	4:C:601:ISW:CGA	2.33	0.40
1:B:271:TRP:CZ2	1:B:275:THR:HG21	2.57	0.40
1:A:282:LEU:HD23	1:A:282:LEU:HA	1.87	0.40
1:B:13:LEU:HD21	1:B:29:LEU:CD1	2.34	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	501/546 (92%)	482 (96%)	19 (4%)	0	100	100
1	B	500/546 (92%)	483 (97%)	16 (3%)	1 (0%)	43	44
1	C	500/546 (92%)	478 (96%)	21 (4%)	1 (0%)	43	44
2	D	47/69 (68%)	45 (96%)	2 (4%)	0	100	100
2	E	47/69 (68%)	44 (94%)	3 (6%)	0	100	100
2	F	47/69 (68%)	45 (96%)	2 (4%)	0	100	100
All	All	1642/1845 (89%)	1577 (96%)	63 (4%)	2 (0%)	48	50

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	268	HIS
1	C	268	HIS

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	430/459 (94%)	407 (95%)	23 (5%)	20	19
1	B	429/459 (94%)	409 (95%)	20 (5%)	23	24
1	C	429/459 (94%)	413 (96%)	16 (4%)	30	33
2	D	43/57 (75%)	39 (91%)	4 (9%)	8	6
2	E	43/57 (75%)	39 (91%)	4 (9%)	8	6

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	F	43/57 (75%)	40 (93%)	3 (7%)	14	11
All	All	1417/1548 (92%)	1347 (95%)	70 (5%)	22	22

All (70) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	GLU
1	A	29	LEU
1	A	34	LYS
1	A	65	LYS
1	A	73	VAL
1	A	90	TRP
1	A	136	GLU
1	A	137	LYS
1	A	141	LYS
1	A	145	CYS
1	A	157	LYS
1	A	177	LEU
1	A	212	ILE
1	A	247	GLU
1	A	269	ASN
1	A	289	LYS
1	A	301	SER
1	A	418	LYS
1	A	431	LYS
1	A	442	VAL
1	A	443	LEU
1	A	491	LEU
1	A	497	ARG
1	B	13	LEU
1	B	14	LYS
1	B	29	LEU
1	B	42	LYS
1	B	90	TRP
1	B	141	LYS
1	B	145	CYS
1	B	177	LEU
1	B	266	VAL
1	B	269	ASN
1	B	278	LYS
1	B	325	ILE
1	B	342	GLU

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Mol	Chain	Res	Type
1	B	358	LEU
1	B	396	LYS
1	B	443	LEU
1	B	460	VAL
1	B	497	ARG
1	B	499	ASN
1	B	500	LYS
1	C	16	ASP
1	C	17	ARG
1	C	29	LEU
1	C	65	LYS
1	C	77	LYS
1	C	90	TRP
1	C	136	GLU
1	C	145	CYS
1	C	155	LYS
1	C	227	GLU
1	C	269	ASN
1	C	322	THR
1	C	396	LYS
1	C	442	VAL
1	C	499	ASN
1	C	500	LYS
2	D	17	LEU
2	D	44	ARG
2	D	45	VAL
2	D	50	ILE
2	E	25	LYS
2	E	50	ILE
2	E	51	VAL
2	E	53	LEU
2	F	17	LEU
2	F	24	ASP
2	F	50	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	211	ASN
1	A	269	ASN
1	A	343	ASN
1	A	461	ASN

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Mol	Chain	Res	Type
1	B	211	ASN
1	B	233	HIS
1	B	269	ASN
1	B	362	GLN
1	B	448	ASN
1	B	449	ASN
1	B	461	ASN
1	C	211	ASN
1	C	233	HIS
1	C	269	ASN
1	C	449	ASN
1	C	461	ASN
1	C	495	GLN
1	C	499	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

64 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	EDO	B	615	-	3,3,3	0.60	0	2,2,2	0.08	0
10	NO3	C	619	-	1,3,3	3.37	1 (100%)	0,3,3	-	-
5	PEG	A	613	-	6,6,6	0.56	0	5,5,5	0.52	0
3	HEC	C	602	1	50,50,50	2.37	23 (46%)	68,82,82	1.57	13 (19%)
3	HEC	C	608	1	50,50,50	2.26	21 (42%)	68,82,82	2.06	22 (32%)
10	NO3	B	617	-	1,3,3	2.76	1 (100%)	0,3,3	-	-
4	ISW	B	608	11,1	47,50,50	3.40	25 (53%)	53,82,82	2.49	21 (39%)
7	EDO	B	620	-	3,3,3	0.70	0	2,2,2	0.42	0
3	HEC	A	601	1	50,50,50	2.38	22 (44%)	68,82,82	1.76	16 (23%)
3	HEC	C	605	1	50,50,50	2.26	23 (46%)	68,82,82	1.56	17 (25%)
3	HEC	A	607	1	50,50,50	2.38	23 (46%)	68,82,82	1.79	17 (25%)
3	HEC	B	602	1	50,50,50	2.16	20 (40%)	68,82,82	1.40	9 (13%)
3	HEC	B	605	1	50,50,50	2.15	23 (46%)	68,82,82	1.52	14 (20%)
3	HEC	A	606	1	50,50,50	2.37	22 (44%)	68,82,82	1.49	11 (16%)
7	EDO	C	618	-	3,3,3	0.70	0	2,2,2	0.14	0
7	EDO	A	616	-	3,3,3	0.61	0	2,2,2	1.00	0
6	PGE	A	615	-	9,9,9	0.68	0	8,8,8	0.79	0
4	ISW	C	601	11,1	47,50,50	3.23	27 (57%)	53,82,82	2.40	19 (35%)
10	NO3	F	101	-	1,3,3	3.53	1 (100%)	0,3,3	-	-
7	EDO	C	616	-	3,3,3	0.18	0	2,2,2	0.76	0
5	PEG	B	609	-	6,6,6	0.47	0	5,5,5	0.93	0
7	EDO	C	615	-	3,3,3	0.41	0	2,2,2	0.28	0
4	ISW	A	608	11,1	47,50,50	3.27	25 (53%)	53,82,82	2.76	24 (45%)
8	P6G	B	613	-	18,18,18	0.49	0	17,17,17	0.74	0
3	HEC	C	607	1	50,50,50	2.23	25 (50%)	68,82,82	1.57	13 (19%)
5	PEG	C	612	-	6,6,6	0.47	0	5,5,5	0.83	0
5	PEG	C	613	-	6,6,6	0.65	0	5,5,5	0.90	0
3	HEC	C	603	1	50,50,50	2.15	19 (38%)	68,82,82	1.70	15 (22%)
5	PEG	C	611	-	6,6,6	0.56	0	5,5,5	0.61	0
3	HEC	A	604	1	50,50,50	2.28	20 (40%)	68,82,82	1.73	14 (20%)
7	EDO	A	618	-	3,3,3	0.44	0	2,2,2	0.24	0
7	EDO	A	619	-	3,3,3	0.54	0	2,2,2	0.36	0
7	EDO	B	621	-	3,3,3	0.46	0	2,2,2	0.20	0
5	PEG	A	610	-	6,6,6	0.28	0	5,5,5	1.04	0
5	PEG	C	610	-	6,6,6	0.75	0	5,5,5	0.68	0
3	HEC	B	603	1	50,50,50	2.31	22 (44%)	68,82,82	1.64	14 (20%)
3	HEC	C	604	1	50,50,50	2.19	23 (46%)	68,82,82	1.81	15 (22%)
3	HEC	A	605	1	50,50,50	2.14	20 (40%)	68,82,82	1.75	20 (29%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	PEG	C	622	-	6,6,6	0.97	0	5,5,5	1.20	0
3	HEC	A	602	1	50,50,50	2.30	21 (42%)	68,82,82	1.63	16 (23%)
3	HEC	A	603	1	50,50,50	2.14	22 (44%)	68,82,82	1.63	12 (17%)
3	HEC	C	606	1	50,50,50	2.07	20 (40%)	68,82,82	1.55	14 (20%)
5	PEG	A	612	-	6,6,6	0.53	0	5,5,5	0.35	0
10	NO3	B	618	-	1,3,3	3.79	1 (100%)	0,3,3	-	-
5	PEG	B	610	-	6,6,6	0.50	0	5,5,5	0.48	0
5	PEG	F	102	-	6,6,6	0.60	0	5,5,5	0.67	0
7	EDO	C	621	-	3,3,3	0.53	0	2,2,2	0.47	0
3	HEC	B	601	1	50,50,50	2.58	22 (44%)	68,82,82	1.85	19 (27%)
5	PEG	B	612	-	6,6,6	0.69	0	5,5,5	0.70	0
6	PGE	C	614	-	9,9,9	0.36	0	8,8,8	1.00	0
5	PEG	A	614	-	6,6,6	0.76	0	5,5,5	0.84	0
5	PEG	B	611	-	6,6,6	0.35	0	5,5,5	0.95	0
7	EDO	A	617	-	3,3,3	0.65	0	2,2,2	0.38	0
7	EDO	B	619	-	3,3,3	0.23	0	2,2,2	0.73	0
7	EDO	C	620	-	3,3,3	0.81	0	2,2,2	0.38	0
3	HEC	B	607	1	50,50,50	2.07	19 (38%)	68,82,82	1.47	13 (19%)
7	EDO	C	617	-	3,3,3	0.49	0	2,2,2	0.36	0
9	PG4	B	614	-	12,12,12	0.61	0	11,11,11	0.90	0
5	PEG	C	609	-	6,6,6	0.49	0	5,5,5	0.41	0
3	HEC	B	604	1	50,50,50	2.24	21 (42%)	68,82,82	1.40	9 (13%)
7	EDO	B	616	-	3,3,3	0.45	0	2,2,2	0.44	0
3	HEC	B	606	1	50,50,50	2.39	23 (46%)	68,82,82	1.49	13 (19%)
5	PEG	A	611	-	6,6,6	0.65	0	5,5,5	0.48	0
5	PEG	A	609	-	6,6,6	0.22	0	5,5,5	1.00	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
7	EDO	B	615	-	-	1/1/1/1	-
5	PEG	A	613	-	-	4/4/4/4	-
3	HEC	C	602	1	1/1/3/7	4/14/54/54	-
3	HEC	C	608	1	1/1/3/7	6/14/54/54	-
4	ISW	B	608	11,1	-	4/14/74/74	-
7	EDO	B	620	-	-	0/1/1/1	-
3	HEC	A	601	1	1/1/3/7	6/14/54/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	HEC	C	605	1	1/1/3/7	4/14/54/54	-
3	HEC	A	607	1	1/1/3/7	6/14/54/54	-
3	HEC	B	602	1	1/1/3/7	7/14/54/54	-
3	HEC	B	605	1	1/1/3/7	4/14/54/54	-
3	HEC	A	606	1	1/1/3/7	7/14/54/54	-
7	EDO	C	618	-	-	0/1/1/1	-
7	EDO	A	616	-	-	0/1/1/1	-
6	PGE	A	615	-	-	5/7/7/7	-
4	ISW	C	601	11,1	-	3/14/74/74	-
7	EDO	C	616	-	-	1/1/1/1	-
5	PEG	B	609	-	-	2/4/4/4	-
7	EDO	C	615	-	-	0/1/1/1	-
4	ISW	A	608	11,1	-	3/14/74/74	-
8	P6G	B	613	-	-	10/16/16/16	-
3	HEC	C	607	1	1/1/3/7	9/14/54/54	-
5	PEG	C	612	-	-	2/4/4/4	-
5	PEG	C	613	-	-	3/4/4/4	-
3	HEC	C	603	1	1/1/3/7	7/14/54/54	-
5	PEG	C	611	-	-	4/4/4/4	-
3	HEC	A	604	1	1/1/3/7	8/14/54/54	-
7	EDO	A	618	-	-	1/1/1/1	-
7	EDO	A	619	-	-	1/1/1/1	-
7	EDO	B	621	-	-	1/1/1/1	-
5	PEG	A	610	-	-	1/4/4/4	-
5	PEG	C	610	-	-	4/4/4/4	-
3	HEC	B	603	1	1/1/3/7	8/14/54/54	-
3	HEC	C	604	1	1/1/3/7	6/14/54/54	-
3	HEC	A	605	1	1/1/3/7	6/14/54/54	-
5	PEG	C	622	-	-	3/4/4/4	-
3	HEC	A	602	1	1/1/3/7	6/14/54/54	-
3	HEC	A	603	1	1/1/3/7	8/14/54/54	-
3	HEC	C	606	1	1/1/3/7	6/14/54/54	-
5	PEG	A	612	-	-	1/4/4/4	-
5	PEG	B	610	-	-	1/4/4/4	-
5	PEG	F	102	-	-	3/4/4/4	-
7	EDO	C	621	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	HEC	B	601	1	1/1/3/7	6/14/54/54	-
5	PEG	B	612	-	-	4/4/4/4	-
6	PGE	C	614	-	-	6/7/7/7	-
5	PEG	A	614	-	-	3/4/4/4	-
5	PEG	B	611	-	-	2/4/4/4	-
7	EDO	A	617	-	-	1/1/1/1	-
7	EDO	B	619	-	-	1/1/1/1	-
7	EDO	C	620	-	-	1/1/1/1	-
3	HEC	B	607	1	1/1/3/7	6/14/54/54	-
7	EDO	C	617	-	-	1/1/1/1	-
9	PG4	B	614	-	-	4/10/10/10	-
5	PEG	C	609	-	-	1/4/4/4	-
3	HEC	B	604	1	1/1/3/7	5/14/54/54	-
7	EDO	B	616	-	-	0/1/1/1	-
3	HEC	B	606	1	1/1/3/7	8/14/54/54	-
5	PEG	A	611	-	-	2/4/4/4	-
5	PEG	A	609	-	-	3/4/4/4	-

All (535) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	608	ISW	C2A-C3A	7.48	1.52	1.36
4	A	608	ISW	C3D-C2D	6.66	1.51	1.36
4	A	608	ISW	C2A-C3A	6.64	1.51	1.36
3	A	601	HEC	FE-NC	6.58	2.16	1.95
4	C	601	ISW	CHB-C4A	6.55	1.51	1.38
3	B	601	HEC	FE-NC	6.46	2.16	1.95
4	C	601	ISW	C2A-C3A	6.15	1.50	1.36
4	B	608	ISW	CHA-C4D	6.14	1.53	1.39
4	C	601	ISW	FE-NC	6.13	2.15	1.95
4	B	608	ISW	CHB-C4A	5.97	1.50	1.38
4	B	608	ISW	C1C-C2C	5.93	1.52	1.37
3	A	606	HEC	FE-ND	5.92	2.13	1.94
3	B	602	HEC	C4B-NB	-5.76	1.30	1.40
3	B	604	HEC	FE-ND	5.73	2.12	1.94
4	A	608	ISW	FE-NC	5.73	2.14	1.95
4	B	608	ISW	CHA-C1A	5.70	1.49	1.38
4	A	608	ISW	CHA-C4D	5.62	1.52	1.39
3	B	604	HEC	FE-NB	5.53	2.11	1.94
3	A	602	HEC	C4B-C3B	-5.52	1.35	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	608	ISW	CHB-C4A	5.50	1.49	1.38
4	B	608	ISW	FE-NC	5.45	2.13	1.95
4	C	601	ISW	C3D-C2D	5.37	1.48	1.36
3	B	601	HEC	CHD-C1D	5.37	1.49	1.38
4	A	608	ISW	CHD-C1D	5.34	1.49	1.38
4	B	608	ISW	C3D-C2D	5.33	1.48	1.36
3	A	604	HEC	FE-NB	5.32	2.11	1.94
3	A	605	HEC	CHB-C4A	5.29	1.48	1.38
4	C	601	ISW	C1C-C2C	5.19	1.50	1.37
4	C	601	ISW	CHD-C1D	5.17	1.48	1.38
4	C	601	ISW	CBC-CAC	5.17	1.55	1.30
3	C	604	HEC	FE-NC	5.16	2.12	1.95
4	C	601	ISW	CHA-C4D	5.14	1.50	1.39
3	A	606	HEC	FE-NB	5.12	2.10	1.94
3	A	606	HEC	CHB-C4A	5.11	1.48	1.38
4	C	601	ISW	FE-NA	5.05	2.11	1.95
3	A	607	HEC	CHC-C4B	5.03	1.48	1.38
4	B	608	ISW	CBC-CAC	4.98	1.54	1.30
3	C	602	HEC	FE-ND	4.98	2.10	1.94
4	A	608	ISW	CBB-CAB	4.96	1.54	1.30
4	A	608	ISW	CHD-C4C	4.95	1.50	1.39
3	B	601	HEC	CHB-C4A	4.95	1.48	1.38
4	B	608	ISW	FE-ND	4.85	2.09	1.94
3	B	603	HEC	FE-NC	4.85	2.11	1.95
3	B	606	HEC	FE-NC	4.84	2.11	1.95
3	B	603	HEC	CHB-C4A	4.83	1.47	1.38
3	C	608	HEC	C4D-C3D	-4.80	1.36	1.45
3	A	605	HEC	FE-NA	4.72	2.10	1.95
3	A	604	HEC	FE-ND	4.72	2.09	1.94
3	B	601	HEC	CHC-C4B	4.72	1.47	1.38
4	C	601	ISW	CBB-CAB	4.70	1.53	1.30
4	B	608	ISW	CAB-C3B	4.65	1.52	1.46
4	A	608	ISW	CAB-C3B	4.62	1.51	1.46
4	B	608	ISW	FE-NA	4.61	2.10	1.95
3	C	607	HEC	CHD-C1D	4.60	1.47	1.38
3	C	603	HEC	C4B-C3B	-4.58	1.37	1.45
4	B	608	ISW	CHD-C1D	4.56	1.47	1.38
3	B	602	HEC	C1C-NC	-4.54	1.31	1.39
3	C	602	HEC	FE-NA	4.54	2.10	1.95
3	A	603	HEC	FE-NC	4.53	2.10	1.95
4	C	601	ISW	CHA-C1A	4.53	1.47	1.38
3	A	604	HEC	C4B-NB	-4.53	1.32	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	608	ISW	CHD-C4C	4.52	1.49	1.39
3	C	603	HEC	CHA-C1A	4.52	1.47	1.38
3	A	604	HEC	C1A-NA	-4.52	1.31	1.39
3	A	602	HEC	FE-ND	4.48	2.08	1.94
4	B	608	ISW	C1B-NB	4.47	1.33	1.29
4	A	608	ISW	C1C-C2C	4.47	1.48	1.37
3	A	607	HEC	FE-NB	4.46	2.08	1.94
3	B	601	HEC	FE-NB	4.46	2.08	1.94
3	B	603	HEC	CHD-C1D	4.44	1.47	1.38
3	C	605	HEC	FE-ND	4.43	2.08	1.94
4	C	601	ISW	FE-ND	4.40	2.08	1.94
4	A	608	ISW	FE-ND	4.40	2.08	1.94
3	B	604	HEC	C4B-NB	-4.33	1.32	1.40
4	A	608	ISW	CHA-C1A	4.31	1.46	1.38
4	A	608	ISW	C1A-C2A	4.30	1.52	1.45
4	C	601	ISW	C1B-NB	4.28	1.32	1.29
3	B	603	HEC	FE-NA	4.27	2.09	1.95
3	C	606	HEC	CHB-C4A	4.25	1.46	1.38
3	B	605	HEC	CHC-C4B	4.24	1.47	1.38
3	C	608	HEC	C1B-NB	-4.23	1.30	1.38
3	B	606	HEC	FE-ND	4.23	2.07	1.94
3	A	601	HEC	CHC-C4B	4.22	1.46	1.38
3	A	604	HEC	CHB-C4A	4.21	1.46	1.38
3	B	603	HEC	C1A-NA	-4.20	1.31	1.39
3	C	602	HEC	FE-NB	4.19	2.07	1.94
3	B	606	HEC	CHC-C4B	4.18	1.46	1.38
3	A	602	HEC	C3D-C2D	4.17	1.45	1.36
3	C	607	HEC	FE-ND	4.10	2.07	1.94
3	B	601	HEC	FE-ND	4.08	2.07	1.94
3	C	608	HEC	CHA-C1A	4.06	1.46	1.38
3	C	602	HEC	CHB-C4A	4.05	1.46	1.38
3	B	606	HEC	FE-NB	4.05	2.07	1.94
3	C	603	HEC	CHB-C4A	4.04	1.46	1.38
3	A	603	HEC	C4B-NB	-4.03	1.33	1.40
4	A	608	ISW	FE-NA	4.02	2.08	1.95
3	A	606	HEC	C1B-NB	-4.02	1.31	1.38
3	A	606	HEC	CHD-C1D	4.02	1.46	1.38
3	A	603	HEC	CHD-C1D	4.01	1.46	1.38
4	B	608	ISW	C4D-C3D	4.00	1.51	1.45
3	A	603	HEC	FE-NA	4.00	2.08	1.95
3	A	601	HEC	CHD-C1D	3.99	1.46	1.38
4	C	601	ISW	C1D-ND	-3.99	1.33	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	608	ISW	CBB-CAB	3.97	1.49	1.30
3	B	606	HEC	C3D-C2D	3.96	1.45	1.36
3	B	602	HEC	FE-NA	3.96	2.08	1.95
3	C	608	HEC	FE-NC	3.94	2.08	1.95
3	A	607	HEC	C4D-ND	-3.94	1.31	1.38
3	B	605	HEC	FE-NB	3.93	2.07	1.94
3	B	601	HEC	CHA-C1A	3.93	1.46	1.38
3	C	604	HEC	CHD-C1D	3.92	1.46	1.38
3	A	607	HEC	CHC-C1C	3.89	1.48	1.39
3	C	605	HEC	C1C-NC	-3.87	1.32	1.39
3	C	605	HEC	CHC-C4B	3.87	1.46	1.38
4	A	608	ISW	CBC-CAC	3.86	1.48	1.30
3	C	602	HEC	FE-NC	3.85	2.07	1.95
3	B	605	HEC	FE-ND	3.84	2.06	1.94
3	B	606	HEC	CHC-C1C	3.83	1.48	1.39
3	C	606	HEC	C1D-ND	-3.82	1.33	1.40
3	B	603	HEC	CHC-C4B	3.82	1.46	1.38
3	A	605	HEC	C1D-ND	-3.80	1.33	1.40
10	B	618	NO3	O1-N	3.79	1.43	1.24
3	A	607	HEC	FE-NC	3.79	2.07	1.95
3	C	602	HEC	CHD-C1D	3.78	1.46	1.38
3	B	601	HEC	C4A-NA	-3.78	1.32	1.39
3	A	602	HEC	C1B-NB	-3.77	1.31	1.38
3	B	606	HEC	C4D-C3D	-3.77	1.38	1.45
4	B	608	ISW	C1D-ND	-3.76	1.33	1.40
3	C	608	HEC	C4A-NA	-3.76	1.32	1.39
3	C	606	HEC	FE-NC	3.74	2.07	1.95
3	A	607	HEC	FE-ND	3.74	2.06	1.94
4	B	608	ISW	CHB-C1B	3.74	1.47	1.39
3	C	607	HEC	CHB-C4A	3.73	1.45	1.38
3	C	602	HEC	CHD-C4C	3.70	1.47	1.39
3	C	605	HEC	FE-NC	3.70	2.07	1.95
4	A	608	ISW	C4A-C3A	3.69	1.52	1.45
3	C	605	HEC	CHA-C4D	3.68	1.47	1.39
3	C	607	HEC	C4A-C3A	-3.67	1.38	1.45
3	A	606	HEC	C4D-ND	-3.67	1.31	1.38
3	C	603	HEC	FE-ND	3.65	2.06	1.94
3	B	607	HEC	C3D-C2D	3.64	1.44	1.36
3	C	605	HEC	C1D-ND	-3.63	1.34	1.40
4	A	608	ISW	CHC-C1C	3.62	1.54	1.50
3	B	603	HEC	FE-ND	3.61	2.06	1.94
3	B	607	HEC	C4B-C3B	-3.61	1.38	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	605	HEC	FE-NC	3.61	2.07	1.95
3	C	608	HEC	C1C-NC	-3.60	1.32	1.39
3	C	608	HEC	CHD-C1D	3.60	1.45	1.38
3	B	605	HEC	C1D-ND	-3.60	1.34	1.40
3	A	601	HEC	C4B-C3B	-3.60	1.38	1.45
3	C	604	HEC	FE-NA	3.59	2.07	1.95
3	C	605	HEC	C4B-C3B	-3.59	1.38	1.45
3	A	601	HEC	C4D-C3D	-3.58	1.39	1.45
3	C	603	HEC	CHA-C4D	3.57	1.47	1.39
3	B	604	HEC	C3D-C2D	3.56	1.44	1.36
3	B	601	HEC	CHD-C4C	3.56	1.47	1.39
3	A	602	HEC	FE-NB	3.56	2.05	1.94
3	C	605	HEC	C1A-NA	-3.54	1.32	1.39
3	A	602	HEC	CHC-C4B	3.54	1.45	1.38
3	A	602	HEC	FE-NA	3.54	2.06	1.95
3	B	606	HEC	C4A-C3A	-3.54	1.38	1.45
3	C	604	HEC	CHC-C4B	3.54	1.45	1.38
10	F	101	NO3	O1-N	3.53	1.41	1.24
3	A	601	HEC	C1B-C2B	-3.52	1.37	1.44
3	B	602	HEC	FE-ND	3.52	2.05	1.94
3	A	606	HEC	CHC-C4B	3.50	1.45	1.38
3	C	605	HEC	FE-NA	3.50	2.06	1.95
4	B	608	ISW	C1A-C2A	3.50	1.51	1.45
3	A	605	HEC	FE-NC	3.50	2.06	1.95
3	A	604	HEC	C4D-C3D	-3.49	1.39	1.45
3	C	604	HEC	CHB-C1B	3.49	1.47	1.39
3	B	606	HEC	CHB-C4A	3.49	1.45	1.38
3	C	602	HEC	CHC-C4B	3.48	1.45	1.38
3	C	606	HEC	FE-ND	3.48	2.05	1.94
3	C	603	HEC	C4A-C3A	-3.47	1.38	1.45
3	C	607	HEC	C1D-ND	-3.46	1.34	1.40
3	C	604	HEC	CHA-C1A	3.46	1.45	1.38
3	B	607	HEC	C1A-NA	-3.46	1.33	1.39
3	C	607	HEC	FE-NA	3.46	2.06	1.95
3	C	602	HEC	CHC-C1C	3.46	1.47	1.39
3	B	607	HEC	FE-NB	3.45	2.05	1.94
3	C	603	HEC	FE-NB	3.44	2.05	1.94
3	B	601	HEC	CHC-C1C	3.44	1.47	1.39
3	A	604	HEC	C4B-C3B	-3.43	1.39	1.45
3	C	602	HEC	C4A-NA	-3.43	1.33	1.39
3	C	604	HEC	C4D-C3D	-3.41	1.39	1.45
3	C	607	HEC	C1A-NA	-3.41	1.33	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	603	HEC	CHA-C1A	3.40	1.45	1.38
3	C	606	HEC	C4A-NA	-3.40	1.33	1.39
10	C	619	NO3	O1-N	3.37	1.40	1.24
3	B	606	HEC	C4C-C3C	-3.37	1.37	1.44
3	C	606	HEC	C1B-NB	-3.36	1.32	1.38
3	A	607	HEC	CHD-C1D	3.36	1.45	1.38
3	A	601	HEC	FE-NA	3.35	2.06	1.95
3	B	603	HEC	CHB-C1B	3.35	1.46	1.39
4	C	601	ISW	C4C-NC	-3.35	1.33	1.39
3	C	605	HEC	CHD-C1D	3.35	1.45	1.38
4	C	601	ISW	CHB-C1B	3.34	1.46	1.39
3	C	606	HEC	CHC-C4B	3.33	1.45	1.38
3	B	607	HEC	CHA-C1A	3.33	1.44	1.38
3	C	602	HEC	C4B-NB	-3.33	1.34	1.40
3	C	604	HEC	C4B-C3B	-3.33	1.39	1.45
3	C	603	HEC	FE-NC	3.33	2.06	1.95
3	A	605	HEC	CHC-C4B	3.32	1.45	1.38
3	B	601	HEC	FE-NA	3.32	2.06	1.95
3	B	607	HEC	CHD-C1D	3.32	1.45	1.38
3	A	605	HEC	CHA-C4D	3.31	1.46	1.39
3	A	607	HEC	C4D-C3D	-3.31	1.39	1.45
3	A	605	HEC	C4B-NB	-3.28	1.34	1.40
3	C	607	HEC	C4B-NB	-3.28	1.34	1.40
3	B	604	HEC	CHC-C4B	3.27	1.45	1.38
3	A	605	HEC	C4B-C3B	-3.26	1.39	1.45
3	A	601	HEC	C1A-NA	-3.26	1.33	1.39
3	B	604	HEC	C4C-NC	-3.26	1.33	1.39
3	A	601	HEC	C4C-C3C	-3.26	1.38	1.44
3	A	601	HEC	C1D-ND	-3.26	1.34	1.40
3	C	605	HEC	C4D-C3D	-3.25	1.39	1.45
3	A	602	HEC	CHD-C1D	3.25	1.45	1.38
3	B	602	HEC	C4B-C3B	-3.24	1.39	1.45
3	C	603	HEC	CHB-C1B	3.24	1.46	1.39
3	A	604	HEC	C1B-C2B	-3.24	1.37	1.44
3	B	607	HEC	C4C-NC	-3.22	1.33	1.39
3	A	606	HEC	C1D-ND	-3.19	1.34	1.40
3	B	601	HEC	C1A-C2A	-3.19	1.39	1.45
3	C	607	HEC	C4D-C3D	-3.19	1.39	1.45
3	A	607	HEC	CHA-C1A	3.18	1.44	1.38
3	B	606	HEC	C4C-NC	-3.18	1.33	1.39
3	B	603	HEC	CHD-C4C	3.18	1.46	1.39
3	A	607	HEC	CHA-C4D	3.18	1.46	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	608	HEC	FE-ND	3.18	2.04	1.94
3	B	604	HEC	C1D-ND	-3.18	1.34	1.40
4	B	608	ISW	FE-NB	3.18	2.12	1.96
3	B	607	HEC	CHA-C4D	3.17	1.46	1.39
4	A	608	ISW	C4D-C3D	3.13	1.50	1.45
3	A	601	HEC	C1C-NC	-3.12	1.33	1.39
3	B	602	HEC	CHB-C4A	3.12	1.44	1.38
3	B	606	HEC	O1A-CGA	3.12	1.32	1.22
3	C	604	HEC	C4A-C3A	-3.11	1.39	1.45
4	C	601	ISW	FE-NB	3.11	2.12	1.96
3	B	605	HEC	CHB-C4A	3.11	1.44	1.38
3	C	608	HEC	C4B-C3B	-3.11	1.39	1.45
3	B	605	HEC	CHA-C1A	3.09	1.44	1.38
3	B	605	HEC	C4A-NA	-3.08	1.33	1.39
3	B	607	HEC	CHC-C1C	3.08	1.46	1.39
3	A	607	HEC	C4B-NB	-3.08	1.34	1.40
3	C	604	HEC	C1A-NA	-3.07	1.33	1.39
3	B	605	HEC	C1A-NA	-3.07	1.33	1.39
3	C	603	HEC	FE-NA	3.07	2.05	1.95
3	A	606	HEC	CMD-C2D	3.05	1.57	1.50
4	A	608	ISW	C1B-NB	3.04	1.31	1.29
3	B	604	HEC	CHB-C1B	3.03	1.46	1.39
3	A	604	HEC	C1D-ND	-3.03	1.35	1.40
3	B	607	HEC	CHB-C4A	3.02	1.44	1.38
3	A	602	HEC	FE-NC	3.02	2.05	1.95
3	B	606	HEC	CHA-C1A	3.02	1.44	1.38
3	C	608	HEC	C1B-C2B	-3.02	1.38	1.44
3	B	603	HEC	CHC-C1C	3.02	1.46	1.39
3	A	603	HEC	CHB-C4A	3.02	1.44	1.38
3	A	607	HEC	C4A-NA	-3.01	1.33	1.39
3	A	604	HEC	CHA-C4D	3.01	1.46	1.39
3	B	602	HEC	C1B-NB	-3.01	1.32	1.38
3	A	607	HEC	CMD-C2D	3.01	1.56	1.50
3	B	605	HEC	C4C-NC	-3.00	1.34	1.39
3	B	602	HEC	C1A-NA	-3.00	1.34	1.39
3	C	603	HEC	CHD-C1D	3.00	1.44	1.38
3	B	607	HEC	FE-NA	2.99	2.05	1.95
3	A	602	HEC	CHD-C4C	2.99	1.46	1.39
3	A	606	HEC	CHC-C1C	2.98	1.46	1.39
3	C	606	HEC	CHA-C4D	2.97	1.46	1.39
3	B	602	HEC	C4A-NA	-2.97	1.34	1.39
3	B	601	HEC	CHA-C4D	2.96	1.45	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	607	HEC	C1B-NB	-2.96	1.33	1.38
3	C	608	HEC	C4B-NB	-2.96	1.35	1.40
3	A	607	HEC	CHB-C4A	2.95	1.44	1.38
3	A	606	HEC	C3D-C2D	2.95	1.43	1.36
3	A	605	HEC	C4A-NA	-2.94	1.34	1.39
3	A	605	HEC	CAB-C3B	2.94	1.58	1.51
3	A	604	HEC	CHD-C1D	2.94	1.44	1.38
3	A	601	HEC	CHB-C1B	2.94	1.45	1.39
3	C	604	HEC	FE-ND	2.93	2.03	1.94
3	A	601	HEC	C1B-NB	-2.93	1.33	1.38
3	A	607	HEC	C4C-NC	-2.92	1.34	1.39
3	B	603	HEC	FE-NB	2.91	2.03	1.94
3	B	606	HEC	C1D-ND	-2.91	1.35	1.40
3	B	601	HEC	C3D-C2D	2.91	1.43	1.36
3	A	605	HEC	C1C-NC	-2.91	1.34	1.39
3	B	605	HEC	C4D-C3D	-2.91	1.40	1.45
3	B	602	HEC	CHD-C1D	2.91	1.44	1.38
3	C	602	HEC	CHA-C4D	2.90	1.45	1.39
3	A	605	HEC	C3D-C2D	2.89	1.43	1.36
3	B	601	HEC	C1B-C2B	-2.89	1.38	1.44
4	A	608	ISW	C4C-NC	-2.89	1.34	1.39
3	B	602	HEC	C1D-ND	-2.88	1.35	1.40
3	A	603	HEC	C1B-C2B	-2.88	1.38	1.44
3	A	603	HEC	C1B-NB	-2.88	1.33	1.38
3	A	601	HEC	CHA-C1A	2.87	1.44	1.38
3	B	601	HEC	C4B-C3B	-2.86	1.40	1.45
3	C	603	HEC	C4C-NC	-2.86	1.34	1.39
3	A	603	HEC	C4C-NC	-2.86	1.34	1.39
3	A	603	HEC	C1A-C2A	-2.85	1.40	1.45
3	A	602	HEC	CHB-C1B	2.85	1.45	1.39
3	A	607	HEC	C1D-ND	-2.84	1.35	1.40
3	A	602	HEC	CHB-C4A	2.84	1.43	1.38
3	C	607	HEC	C3D-C2D	2.84	1.42	1.36
3	C	605	HEC	CHB-C4A	2.84	1.43	1.38
3	C	607	HEC	C1A-C2A	-2.84	1.40	1.45
3	A	603	HEC	CHC-C4B	2.84	1.44	1.38
3	C	607	HEC	CHC-C4B	2.83	1.44	1.38
3	C	608	HEC	CHA-C4D	2.83	1.45	1.39
3	A	603	HEC	C4A-NA	-2.83	1.34	1.39
3	B	604	HEC	CHB-C4A	2.83	1.43	1.38
3	B	603	HEC	C4B-C3B	-2.81	1.40	1.45
3	C	608	HEC	CHD-C4C	2.81	1.45	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	603	HEC	C1D-ND	-2.81	1.35	1.40
3	B	601	HEC	CHB-C1B	2.79	1.45	1.39
3	C	602	HEC	C1B-C2B	-2.79	1.38	1.44
3	B	601	HEC	C4D-C3D	-2.79	1.40	1.45
4	B	608	ISW	C1A-NA	-2.79	1.34	1.39
3	A	601	HEC	CHB-C4A	2.79	1.43	1.38
3	B	604	HEC	C1A-NA	-2.78	1.34	1.39
3	A	606	HEC	C4C-NC	-2.78	1.34	1.39
3	B	605	HEC	C4A-C3A	-2.78	1.39	1.45
3	B	603	HEC	CHA-C1A	2.77	1.43	1.38
3	B	604	HEC	C1B-NB	-2.77	1.33	1.38
4	C	601	ISW	C4A-C3A	2.77	1.50	1.45
3	A	606	HEC	CMA-C3A	2.77	1.56	1.50
3	B	607	HEC	C1B-C2B	-2.76	1.38	1.44
3	C	606	HEC	FE-NA	2.76	2.04	1.95
10	B	617	NO3	O1-N	2.76	1.37	1.24
3	B	606	HEC	CHA-C4D	2.76	1.45	1.39
3	C	607	HEC	CHB-C1B	2.75	1.45	1.39
3	B	605	HEC	C1A-C2A	-2.75	1.40	1.45
4	B	608	ISW	C4B-C3B	-2.75	1.48	1.52
4	A	608	ISW	CHB-C1B	2.75	1.45	1.39
4	C	601	ISW	CHD-C4C	2.74	1.45	1.39
3	C	604	HEC	CHD-C4C	2.74	1.45	1.39
3	A	603	HEC	C1D-ND	-2.73	1.35	1.40
3	A	606	HEC	C4B-C3B	-2.73	1.40	1.45
3	C	607	HEC	CHA-C1A	2.72	1.43	1.38
3	A	604	HEC	C4D-ND	-2.71	1.33	1.38
3	C	607	HEC	C4A-NA	-2.71	1.34	1.39
3	C	604	HEC	C1D-ND	-2.71	1.35	1.40
3	B	605	HEC	C1D-C2D	-2.71	1.39	1.44
3	B	606	HEC	FE-NA	2.71	2.04	1.95
3	C	604	HEC	CHA-C4D	2.70	1.45	1.39
3	C	604	HEC	C1D-C2D	-2.69	1.39	1.44
3	B	602	HEC	FE-NC	2.69	2.04	1.95
4	C	601	ISW	CHC-C1C	2.69	1.53	1.50
3	A	604	HEC	C4C-NC	-2.69	1.34	1.39
3	A	604	HEC	CHA-C1A	2.68	1.43	1.38
3	B	601	HEC	C1D-C2D	-2.68	1.39	1.44
3	C	602	HEC	C1D-ND	-2.68	1.35	1.40
3	C	606	HEC	O1A-CGA	2.68	1.30	1.22
3	A	602	HEC	C4C-NC	-2.67	1.34	1.39
3	B	602	HEC	CHD-C4C	2.67	1.45	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	607	HEC	CHC-C4B	2.67	1.43	1.38
3	B	603	HEC	CHA-C4D	2.67	1.45	1.39
3	B	602	HEC	C4C-NC	-2.67	1.34	1.39
3	C	605	HEC	C4A-C3A	-2.67	1.40	1.45
4	A	608	ISW	C1B-C2B	2.67	1.49	1.44
3	A	605	HEC	CHC-C1C	2.66	1.45	1.39
3	C	605	HEC	C4C-NC	-2.66	1.34	1.39
4	C	601	ISW	C1A-C2A	2.65	1.49	1.45
4	A	608	ISW	FE-NB	2.65	2.10	1.96
3	B	602	HEC	CHA-C1A	2.64	1.43	1.38
3	A	602	HEC	CHA-C1A	2.64	1.43	1.38
3	C	604	HEC	CHB-C4A	2.64	1.43	1.38
3	B	604	HEC	CHD-C4C	2.63	1.45	1.39
3	A	605	HEC	CHA-C1A	2.62	1.43	1.38
3	C	606	HEC	C4A-C3A	-2.62	1.40	1.45
3	A	603	HEC	CHA-C4D	2.61	1.45	1.39
3	B	604	HEC	C4B-C3B	-2.61	1.40	1.45
3	A	605	HEC	C4C-NC	-2.61	1.34	1.39
3	C	608	HEC	FE-NA	2.61	2.03	1.95
3	C	602	HEC	C4C-C3C	-2.61	1.39	1.44
3	C	607	HEC	C4C-NC	-2.61	1.34	1.39
3	C	603	HEC	C3D-C2D	2.60	1.42	1.36
3	B	606	HEC	CHD-C1D	2.60	1.43	1.38
3	C	604	HEC	C4A-NA	-2.59	1.34	1.39
3	A	607	HEC	CMA-C3A	2.59	1.56	1.50
3	B	602	HEC	C1B-C2B	-2.59	1.39	1.44
3	A	602	HEC	C1D-ND	-2.57	1.35	1.40
3	C	604	HEC	C4B-NB	-2.57	1.35	1.40
3	B	606	HEC	CHB-C1B	2.57	1.45	1.39
3	B	604	HEC	CHA-C1A	2.56	1.43	1.38
3	C	605	HEC	C4C-C3C	-2.56	1.39	1.44
4	C	601	ISW	C1B-C2B	2.56	1.49	1.44
3	C	605	HEC	CHB-C1B	2.56	1.45	1.39
3	C	602	HEC	C4D-ND	-2.56	1.33	1.38
3	C	602	HEC	C1C-NC	-2.56	1.34	1.39
3	C	608	HEC	C1A-C2A	-2.56	1.40	1.45
3	C	608	HEC	C4D-ND	-2.55	1.33	1.38
3	C	607	HEC	FE-NC	2.54	2.03	1.95
3	A	601	HEC	C4A-C3A	-2.54	1.40	1.45
3	A	601	HEC	CHD-C4C	2.53	1.45	1.39
3	A	601	HEC	C4B-NB	-2.53	1.35	1.40
3	B	607	HEC	CHB-C1B	2.53	1.44	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	603	HEC	C1B-NB	-2.52	1.33	1.38
3	C	607	HEC	CHD-C4C	2.52	1.45	1.39
3	B	607	HEC	FE-ND	2.52	2.02	1.94
3	B	607	HEC	C4B-NB	-2.52	1.35	1.40
3	A	602	HEC	CHC-C1C	2.52	1.45	1.39
3	B	604	HEC	O2A-CGA	-2.51	1.22	1.30
3	A	603	HEC	C1A-NA	-2.50	1.34	1.39
3	C	602	HEC	C4A-C3A	-2.50	1.40	1.45
3	A	601	HEC	C4C-NC	-2.50	1.34	1.39
3	C	604	HEC	C1B-NB	-2.49	1.34	1.38
3	C	606	HEC	CHA-C1A	2.48	1.43	1.38
3	C	607	HEC	C1D-C2D	-2.48	1.39	1.44
3	B	603	HEC	C3D-C2D	2.47	1.42	1.36
3	A	606	HEC	FE-NC	2.47	2.03	1.95
4	B	608	ISW	C3C-C2C	2.47	1.49	1.41
3	A	601	HEC	FE-NB	2.46	2.02	1.94
3	B	605	HEC	C4B-NB	-2.46	1.36	1.40
3	A	602	HEC	C1C-NC	-2.45	1.35	1.39
3	C	605	HEC	C1A-C2A	-2.45	1.40	1.45
3	B	604	HEC	C1A-C2A	-2.44	1.40	1.45
3	C	602	HEC	C1D-C2D	-2.44	1.39	1.44
3	C	608	HEC	CHB-C4A	2.44	1.43	1.38
3	C	602	HEC	CHA-C1A	2.43	1.43	1.38
3	B	605	HEC	CHD-C1D	2.43	1.43	1.38
3	B	603	HEC	CAC-C3C	2.42	1.57	1.51
3	A	601	HEC	CMD-C2D	2.41	1.55	1.50
3	C	606	HEC	C4D-ND	-2.41	1.34	1.38
3	C	608	HEC	CHC-C4B	2.40	1.43	1.38
3	B	602	HEC	C4A-C3A	-2.39	1.40	1.45
3	C	606	HEC	CHC-C1C	2.38	1.44	1.39
3	B	607	HEC	CMC-C2C	2.37	1.55	1.50
3	A	605	HEC	FE-NB	2.37	2.02	1.94
3	A	607	HEC	FE-NA	2.36	2.02	1.95
3	A	603	HEC	CHD-C4C	2.36	1.44	1.39
3	C	606	HEC	C1A-C2A	-2.36	1.41	1.45
3	B	607	HEC	C4D-C3D	-2.35	1.41	1.45
3	C	605	HEC	CHD-C4C	2.35	1.44	1.39
3	A	607	HEC	C4A-C3A	-2.35	1.40	1.45
3	C	602	HEC	C1A-C2A	-2.35	1.41	1.45
3	A	604	HEC	C1C-NC	-2.35	1.35	1.39
3	C	607	HEC	C1B-C2B	-2.34	1.39	1.44
3	C	603	HEC	CHC-C1C	2.34	1.44	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	605	HEC	CHD-C4C	2.34	1.44	1.39
3	B	605	HEC	CHB-C1B	2.33	1.44	1.39
3	C	606	HEC	C4D-C3D	-2.33	1.41	1.45
3	C	603	HEC	C4A-NA	-2.33	1.35	1.39
3	A	602	HEC	O1D-CGD	2.33	1.29	1.22
3	A	604	HEC	C4A-C3A	-2.33	1.40	1.45
3	A	602	HEC	CHA-C4D	2.32	1.44	1.39
3	B	604	HEC	C4C-C3C	-2.32	1.39	1.44
3	B	605	HEC	C4D-ND	-2.32	1.34	1.38
3	B	604	HEC	C1C-NC	-2.32	1.35	1.39
3	C	608	HEC	FE-NB	2.32	2.02	1.94
4	A	608	ISW	CBA-CGA	2.31	1.55	1.50
3	A	601	HEC	C3D-C2D	2.31	1.41	1.36
3	B	603	HEC	C1C-NC	-2.31	1.35	1.39
3	B	605	HEC	CHC-C1C	2.31	1.44	1.39
3	C	607	HEC	O1A-CGA	2.29	1.29	1.22
3	C	606	HEC	CHD-C1D	2.29	1.43	1.38
3	C	607	HEC	CHA-C4D	2.28	1.44	1.39
3	C	608	HEC	CMB-C2B	2.27	1.55	1.50
3	C	606	HEC	CHD-C4C	2.27	1.44	1.39
3	B	605	HEC	C3D-C2D	2.27	1.41	1.36
3	C	607	HEC	CMA-C3A	2.26	1.55	1.50
3	B	606	HEC	C1D-C2D	-2.25	1.39	1.44
3	C	602	HEC	C4C-NC	-2.25	1.35	1.39
3	B	606	HEC	C4B-NB	-2.25	1.36	1.40
3	A	607	HEC	O2A-CGA	-2.24	1.23	1.30
4	B	608	ISW	O1D-CGD	-2.24	1.23	1.30
3	C	605	HEC	CHA-C1A	2.24	1.42	1.38
3	B	603	HEC	C4B-NB	-2.23	1.36	1.40
3	B	601	HEC	C4A-C3A	-2.23	1.40	1.45
3	B	602	HEC	CHB-C1B	2.22	1.44	1.39
3	B	603	HEC	C4A-C3A	-2.22	1.40	1.45
3	A	606	HEC	CHB-C1B	2.20	1.44	1.39
3	C	608	HEC	C1D-ND	-2.20	1.36	1.40
3	B	601	HEC	C4B-NB	-2.19	1.36	1.40
3	C	604	HEC	C4D-ND	-2.19	1.34	1.38
4	A	608	ISW	C1D-ND	-2.19	1.36	1.40
3	A	602	HEC	C4A-C3A	-2.19	1.41	1.45
3	C	603	HEC	C4D-ND	-2.18	1.34	1.38
3	A	604	HEC	C1D-C2D	-2.18	1.40	1.44
3	A	607	HEC	CHB-C1B	2.18	1.44	1.39
3	C	602	HEC	C1A-NA	-2.18	1.35	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	605	HEC	C4D-ND	-2.17	1.34	1.38
3	A	606	HEC	C1C-C2C	-2.17	1.38	1.43
3	B	606	HEC	CBA-CGA	2.17	1.55	1.50
3	B	607	HEC	O1D-CGD	2.16	1.29	1.22
3	B	604	HEC	C1B-C2B	-2.15	1.40	1.44
3	C	604	HEC	C1C-NC	-2.15	1.35	1.39
3	A	605	HEC	C1A-NA	-2.15	1.35	1.39
3	B	606	HEC	C1C-C2C	-2.15	1.38	1.43
3	C	603	HEC	CHC-C4B	2.14	1.42	1.38
3	B	605	HEC	C1C-NC	-2.14	1.35	1.39
3	A	604	HEC	C3D-C2D	2.13	1.41	1.36
4	C	601	ISW	C4D-C3D	2.13	1.48	1.45
3	A	606	HEC	C4A-NA	-2.13	1.35	1.39
3	B	603	HEC	C4D-C3D	-2.12	1.41	1.45
3	B	601	HEC	C1B-NB	-2.12	1.34	1.38
3	A	606	HEC	CHA-C4D	2.12	1.44	1.39
3	C	607	HEC	C4B-C3B	-2.12	1.41	1.45
3	A	606	HEC	CAA-C2A	2.11	1.56	1.51
3	B	604	HEC	C4D-ND	-2.11	1.34	1.38
3	B	604	HEC	FE-NC	2.11	2.02	1.95
3	A	603	HEC	C1C-NC	-2.10	1.35	1.39
3	C	604	HEC	C3D-C2D	2.10	1.41	1.36
3	A	602	HEC	CAC-C3C	2.10	1.56	1.51
3	B	602	HEC	FE-NB	2.10	2.01	1.94
3	C	603	HEC	C1D-ND	-2.10	1.36	1.40
3	C	607	HEC	FE-NB	2.09	2.01	1.94
3	A	603	HEC	CHB-C1B	2.09	1.44	1.39
3	C	605	HEC	FE-NB	2.09	2.01	1.94
4	C	601	ISW	C3C-C2C	2.09	1.48	1.41
3	A	604	HEC	C1A-C2A	-2.08	1.41	1.45
3	C	606	HEC	C1C-NC	-2.08	1.35	1.39
3	A	605	HEC	C1B-NB	-2.07	1.34	1.38
3	B	605	HEC	O2D-CGD	-2.06	1.24	1.30
4	B	608	ISW	C4A-C3A	2.05	1.49	1.45
3	A	606	HEC	CHD-C4C	2.05	1.44	1.39
4	C	601	ISW	C1A-NA	-2.05	1.35	1.39
4	C	601	ISW	CAC-C3C	2.05	1.52	1.47
4	C	601	ISW	CAB-C3B	2.05	1.48	1.46
3	C	604	HEC	C4C-NC	-2.04	1.35	1.39
3	B	606	HEC	C1B-C2B	-2.04	1.40	1.44
3	A	606	HEC	CHA-C1A	2.04	1.42	1.38
3	A	603	HEC	C4B-C3B	-2.04	1.41	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	603	HEC	FE-ND	2.04	2.01	1.94
3	A	605	HEC	CHB-C1B	2.04	1.43	1.39
3	A	605	HEC	C1B-C2B	-2.03	1.40	1.44
3	A	607	HEC	C1A-NA	-2.03	1.35	1.39
3	C	605	HEC	C3D-C2D	2.03	1.41	1.36
3	C	606	HEC	CMC-C2C	2.02	1.54	1.50
3	B	603	HEC	C4A-NA	-2.02	1.35	1.39
3	A	604	HEC	CHC-C1C	2.02	1.43	1.39
3	A	603	HEC	CMB-C2B	2.01	1.54	1.50
3	C	605	HEC	C4A-NA	-2.01	1.35	1.39
3	B	602	HEC	C1A-C2A	-2.00	1.41	1.45
3	A	603	HEC	C1D-C2D	-2.00	1.40	1.44

All (370) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	601	ISW	C4B-CHC-C1C	6.87	121.22	108.94
4	A	608	ISW	C4B-CHC-C1C	6.49	120.55	108.94
4	A	608	ISW	CHB-C4A-NA	-6.35	117.54	124.45
4	A	608	ISW	C1B-C2B-C3B	-6.27	99.53	106.80
4	B	608	ISW	C4B-CHC-C1C	6.17	119.97	108.94
4	A	608	ISW	CHA-C1A-NA	-6.03	117.89	124.45
3	C	608	HEC	CAB-C3B-C4B	5.89	132.45	124.79
3	A	607	HEC	C1D-C2D-C3D	-5.81	100.87	106.98
3	C	608	HEC	CHD-C1D-ND	5.75	131.48	124.37
4	C	601	ISW	C3C-C4C-NC	5.61	114.52	109.80
3	A	603	HEC	CHB-C1B-NB	5.58	130.43	124.42
4	B	608	ISW	C3C-C4C-NC	5.58	114.50	109.80
3	B	601	HEC	CAC-C3C-C4C	5.57	132.57	124.91
4	C	601	ISW	C1B-C2B-C3B	-5.50	100.42	106.80
3	B	601	HEC	CHD-C1D-ND	5.35	130.98	124.37
4	B	608	ISW	CHA-C1A-NA	-5.32	118.66	124.45
3	C	604	HEC	CHD-C1D-ND	5.30	130.93	124.37
3	A	605	HEC	CHB-C1B-NB	5.21	130.03	124.42
3	A	604	HEC	CHA-C1A-NA	5.14	130.05	124.45
3	A	601	HEC	CHC-C4B-NB	4.93	130.47	124.37
4	B	608	ISW	C1B-C2B-C3B	-4.56	101.52	106.80
4	B	608	ISW	C4C-C3C-C2C	-4.55	101.65	107.30
3	C	604	HEC	C1A-CHA-C4D	-4.52	116.41	126.02
4	A	608	ISW	CHA-C4D-ND	-4.52	119.56	124.42
3	A	601	HEC	CHD-C1D-ND	4.52	129.96	124.37
3	B	603	HEC	CAA-CBA-CGA	-4.51	101.70	113.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	601	ISW	C4C-C3C-C2C	-4.46	101.76	107.30
3	C	608	HEC	C4C-CHD-C1D	-4.43	115.82	126.25
4	C	601	ISW	CBC-CAC-C3C	-4.42	105.42	127.53
4	B	608	ISW	C1D-C2D-C3D	-4.34	102.42	106.98
3	A	603	HEC	CHB-C1B-C2B	-4.32	118.20	125.03
4	B	608	ISW	CBC-CAC-C3C	-4.30	106.02	127.53
3	A	604	HEC	CBD-CAD-C3D	-4.30	100.64	112.53
4	B	608	ISW	CAD-CBD-CGD	-4.26	102.37	113.67
4	A	608	ISW	CHB-C1B-NB	-4.23	119.88	124.44
3	C	607	HEC	CAB-C3B-C4B	4.20	130.26	124.79
3	B	604	HEC	CBD-CAD-C3D	-4.20	100.92	112.53
4	A	608	ISW	C1D-C2D-C3D	-4.17	102.60	106.98
3	C	602	HEC	O2A-CGA-CBA	4.11	126.99	114.00
4	A	608	ISW	CBC-CAC-C3C	-4.06	107.25	127.53
4	A	608	ISW	CAD-CBD-CGD	-4.02	103.01	113.67
3	A	607	HEC	CHB-C4A-NA	3.99	128.80	124.45
3	B	605	HEC	CHB-C4A-NA	3.98	128.79	124.45
3	A	602	HEC	CHC-C4B-NB	3.98	129.29	124.37
3	B	607	HEC	C1D-C2D-C3D	-3.94	102.84	106.98
4	C	601	ISW	CAD-CBD-CGD	-3.91	103.31	113.67
3	B	606	HEC	CHB-C4A-NA	3.88	128.68	124.45
3	A	603	HEC	CHD-C1D-ND	3.87	129.15	124.37
3	C	608	HEC	CMC-C2C-C3C	3.82	133.72	125.62
3	C	605	HEC	CBD-CAD-C3D	-3.80	102.02	112.53
3	C	604	HEC	CHB-C1B-NB	3.77	128.49	124.42
3	A	606	HEC	CHC-C1C-NC	3.77	130.70	123.86
4	B	608	ISW	C2D-C1D-ND	3.74	114.14	109.84
3	B	606	HEC	C1D-ND-C4D	3.73	109.62	105.21
3	C	604	HEC	CHC-C4B-NB	3.72	128.97	124.37
3	A	604	HEC	CHA-C1A-C2A	-3.70	119.01	124.86
3	A	607	HEC	CAC-C3C-C2C	3.68	132.72	126.89
3	C	606	HEC	CHB-C1B-C2B	-3.63	119.29	125.03
3	A	606	HEC	CAC-C3C-C4C	3.61	129.88	124.91
3	C	608	HEC	C2A-C1A-NA	3.59	113.79	110.32
3	C	608	HEC	CMC-C2C-C1C	-3.57	119.98	125.42
3	C	604	HEC	C1C-CHC-C4B	-3.56	117.87	126.25
3	C	603	HEC	CAA-C2A-C1A	3.56	132.10	124.85
3	B	602	HEC	CHB-C1B-NB	3.55	128.24	124.42
3	B	601	HEC	CHA-C1A-NA	3.54	128.31	124.45
4	A	608	ISW	C1A-C2A-C3A	-3.54	102.45	107.11
4	A	608	ISW	CHA-C4D-C3D	3.53	129.91	124.77
3	B	603	HEC	CHB-C4A-NA	3.50	128.26	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	607	HEC	CHB-C1B-NB	3.50	128.19	124.42
4	C	601	ISW	C2A-C1A-NA	3.49	113.69	110.32
3	A	605	HEC	CHB-C1B-C2B	-3.48	119.53	125.03
3	A	606	HEC	C1D-C2D-C3D	-3.46	103.34	106.98
3	B	603	HEC	CHC-C4B-NB	3.45	128.63	124.37
3	A	606	HEC	C1C-CHC-C4B	-3.41	118.23	126.25
3	C	606	HEC	CBC-CAC-C3C	3.40	121.63	112.42
4	C	601	ISW	C1A-C2A-C3A	-3.40	102.64	107.11
4	A	608	ISW	C1D-ND-C4D	3.37	109.19	105.21
4	C	601	ISW	C1D-ND-C4D	3.36	109.18	105.21
3	B	603	HEC	O2D-CGD-CBD	3.35	124.60	114.00
3	C	608	HEC	CAA-C2A-C1A	3.35	131.67	124.85
3	C	607	HEC	C3C-C4C-NC	3.35	113.87	110.15
3	A	601	HEC	CMC-C2C-C3C	3.34	132.71	125.62
3	A	601	HEC	CHA-C4D-ND	3.31	127.98	124.42
3	B	606	HEC	CAB-C3B-C4B	-3.30	120.50	124.79
4	C	601	ISW	CHB-C4A-NA	-3.29	120.87	124.45
4	C	601	ISW	C1D-C2D-C3D	-3.27	103.54	106.98
3	A	604	HEC	C3D-C4D-ND	3.26	113.50	110.35
3	A	604	HEC	CAA-C2A-C3A	3.26	133.97	127.87
3	B	603	HEC	CHB-C1B-NB	3.24	127.91	124.42
3	B	605	HEC	C3C-C4C-NC	3.24	113.75	110.15
3	A	605	HEC	CHA-C4D-ND	3.24	127.91	124.42
3	C	608	HEC	CHA-C4D-ND	3.23	127.90	124.42
3	C	603	HEC	CHC-C4B-C3B	-3.22	119.29	125.23
3	B	601	HEC	CBA-CAA-C2A	-3.21	103.67	112.53
3	A	607	HEC	CMC-C2C-C3C	3.21	132.43	125.62
3	C	603	HEC	CBC-CAC-C3C	3.20	121.08	112.42
3	C	604	HEC	CMC-C2C-C3C	3.19	132.39	125.62
3	A	602	HEC	CAA-C2A-C1A	3.19	131.34	124.85
4	B	608	ISW	C1D-ND-C4D	3.19	108.98	105.21
4	A	608	ISW	O2A-CGA-CBA	3.18	124.05	114.00
4	A	608	ISW	C2A-C1A-NA	3.18	113.39	110.32
3	C	603	HEC	C1D-C2D-C3D	-3.18	103.64	106.98
3	C	605	HEC	CHB-C1B-NB	3.14	127.80	124.42
3	A	607	HEC	CAA-C2A-C1A	3.14	131.23	124.85
3	B	603	HEC	CAD-CBD-CGD	-3.11	105.41	113.67
3	A	601	HEC	CAC-C3C-C2C	3.09	131.78	126.89
3	C	603	HEC	CHC-C4B-NB	3.09	128.19	124.37
3	B	603	HEC	C4A-CHB-C1B	-3.08	119.48	126.02
4	B	608	ISW	C1A-C2A-C3A	-3.07	103.06	107.11
3	A	601	HEC	O2D-CGD-CBD	3.07	123.69	114.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	601	HEC	CAD-CBD-CGD	-3.06	105.54	113.67
3	C	605	HEC	CHA-C4D-ND	3.06	127.72	124.42
3	B	601	HEC	CBC-CAC-C3C	3.04	120.67	112.42
4	C	601	ISW	CHA-C1A-NA	-3.02	121.16	124.45
3	C	603	HEC	CMD-C2D-C1D	3.01	129.74	125.03
3	C	603	HEC	CAA-C2A-C3A	-3.00	122.25	127.87
3	A	605	HEC	C4A-CHB-C1B	-2.99	119.66	126.02
3	C	604	HEC	CHC-C4B-C3B	-2.99	119.71	125.23
3	C	602	HEC	C1D-ND-C4D	2.99	108.75	105.21
3	C	606	HEC	C2B-C1B-NB	2.99	113.36	109.90
3	B	603	HEC	CHC-C4B-C3B	-2.99	119.72	125.23
3	A	601	HEC	C1D-ND-C4D	2.99	108.75	105.21
3	A	605	HEC	CBA-CAA-C2A	-2.97	104.31	112.53
3	C	603	HEC	O2A-CGA-CBA	2.95	123.32	114.00
3	C	602	HEC	CAC-C3C-C2C	2.93	131.53	126.89
3	C	608	HEC	CMA-C3A-C4A	2.91	129.86	124.73
3	C	607	HEC	CBD-CAD-C3D	-2.90	104.52	112.53
3	B	601	HEC	CHC-C4B-NB	2.89	127.94	124.37
3	B	605	HEC	CHD-C1D-ND	2.88	127.93	124.37
3	C	602	HEC	CHB-C1B-NB	2.87	127.51	124.42
3	C	608	HEC	CAC-C3C-C2C	2.87	131.43	126.89
3	A	602	HEC	CMD-C2D-C1D	2.87	129.51	125.03
3	A	603	HEC	CHC-C4B-NB	2.86	127.91	124.37
3	A	607	HEC	C2D-C1D-ND	2.86	113.13	109.84
4	B	608	ISW	C4A-C3A-C2A	-2.86	102.73	106.97
3	B	601	HEC	C1A-CHA-C4D	-2.86	119.94	126.02
3	B	605	HEC	CAD-C3D-C4D	2.86	129.68	124.70
3	C	606	HEC	CHC-C4B-NB	2.84	127.88	124.37
3	C	608	HEC	CHA-C4D-C3D	-2.84	120.64	124.77
3	A	604	HEC	CHB-C4A-NA	2.84	127.54	124.45
3	B	606	HEC	CHC-C4B-NB	2.83	127.87	124.37
4	B	608	ISW	CHA-C4D-C3D	2.83	128.90	124.77
3	A	601	HEC	C4A-CHB-C1B	-2.81	120.04	126.02
4	B	608	ISW	CHB-C1B-NB	-2.80	121.42	124.44
3	B	601	HEC	O1A-CGA-CBA	-2.80	114.21	123.09
3	C	604	HEC	CAD-C3D-C4D	2.79	129.56	124.70
3	C	605	HEC	O2D-CGD-CBD	2.78	122.79	114.00
3	B	602	HEC	CAD-C3D-C4D	2.78	129.54	124.70
3	A	604	HEC	CBA-CAA-C2A	2.78	120.22	112.53
3	C	604	HEC	CAA-CBA-CGA	-2.78	106.30	113.67
3	C	603	HEC	C1D-ND-C4D	2.77	108.49	105.21
3	A	602	HEC	C1D-C2D-C3D	-2.77	104.07	106.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	603	HEC	C1A-CHA-C4D	-2.77	120.13	126.02
3	C	605	HEC	C2A-C1A-NA	2.76	112.99	110.32
3	B	606	HEC	C1A-CHA-C4D	-2.76	120.16	126.02
3	B	605	HEC	O2D-CGD-CBD	2.75	122.69	114.00
3	C	604	HEC	C1D-ND-C4D	2.75	108.46	105.21
3	A	605	HEC	C3C-C4C-NC	2.74	113.19	110.15
3	B	606	HEC	CAB-C3B-C2B	2.73	132.58	127.56
3	A	601	HEC	CMC-C2C-C1C	-2.73	121.26	125.42
3	C	607	HEC	C1D-ND-C4D	2.73	108.44	105.21
4	B	608	ISW	CHB-C4A-NA	-2.71	121.50	124.45
3	A	605	HEC	CAA-C2A-C1A	2.71	130.36	124.85
3	A	604	HEC	CAA-C2A-C1A	-2.70	119.36	124.85
3	C	602	HEC	CBD-CAD-C3D	2.70	119.99	112.53
3	A	601	HEC	CHC-C4B-C3B	-2.69	120.27	125.23
4	A	608	ISW	C2D-C1D-ND	2.69	112.93	109.84
3	A	602	HEC	CAA-C2A-C3A	-2.69	122.83	127.87
3	C	605	HEC	O1D-CGD-CBD	-2.69	114.57	123.09
4	A	608	ISW	CMB-C2B-C1B	2.68	129.23	125.03
3	A	602	HEC	CHB-C1B-NB	2.68	127.31	124.42
3	A	601	HEC	O2D-CGD-O1D	-2.67	116.46	123.33
3	C	608	HEC	C1D-ND-C4D	2.67	108.37	105.21
3	C	606	HEC	CHB-C1B-NB	2.66	127.28	124.42
3	C	608	HEC	C4A-CHB-C1B	-2.65	120.38	126.02
3	C	608	HEC	CHA-C1A-C2A	-2.65	120.69	124.86
3	A	603	HEC	CMA-C3A-C4A	2.64	129.38	124.73
4	C	601	ISW	CAD-C3D-C4D	2.64	129.30	124.70
3	A	605	HEC	C4C-C3C-C2C	-2.64	102.79	106.87
3	C	607	HEC	CBC-CAC-C3C	2.63	119.54	112.42
3	C	603	HEC	CHC-C1C-C2C	-2.62	119.81	127.43
3	A	605	HEC	C1C-CHC-C4B	-2.62	120.08	126.25
3	A	604	HEC	CAC-C3C-C4C	2.62	128.51	124.91
3	B	604	HEC	C4D-C3D-C2D	-2.61	103.09	106.89
3	C	602	HEC	O1A-CGA-CBA	-2.61	114.81	123.09
3	B	601	HEC	C1D-ND-C4D	2.61	108.30	105.21
3	B	605	HEC	CBA-CAA-C2A	-2.61	105.32	112.53
3	A	602	HEC	CBA-CAA-C2A	2.61	119.75	112.53
3	A	602	HEC	C4B-NB-C1B	2.60	108.29	105.21
3	A	602	HEC	C2D-C1D-ND	2.60	112.83	109.84
3	B	607	HEC	C4A-CHB-C1B	-2.59	120.51	126.02
3	A	607	HEC	C4A-CHB-C1B	-2.59	120.52	126.02
3	A	602	HEC	CHD-C4C-C3C	-2.58	119.64	125.30
3	B	601	HEC	CAC-C3C-C2C	-2.58	122.81	126.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	604	HEC	CAB-C3B-C4B	2.58	128.15	124.79
3	A	602	HEC	CHA-C4D-ND	2.58	127.20	124.42
3	A	605	HEC	C1D-ND-C4D	2.58	108.26	105.21
4	B	608	ISW	CHA-C4D-ND	-2.57	121.66	124.42
3	A	607	HEC	CAD-C3D-C4D	-2.57	120.22	124.70
3	B	607	HEC	CHB-C1B-C2B	-2.57	120.97	125.03
3	A	607	HEC	CHB-C4A-C3A	-2.56	120.16	125.49
3	A	607	HEC	CAA-C2A-C3A	-2.56	123.08	127.87
3	B	605	HEC	CAC-C3C-C2C	2.55	130.92	126.89
4	B	608	ISW	C2A-C1A-NA	2.54	112.78	110.32
3	A	601	HEC	CHB-C1B-NB	2.54	127.16	124.42
3	A	602	HEC	C1C-CHC-C4B	-2.53	120.30	126.25
3	A	601	HEC	CHB-C4A-NA	2.52	127.19	124.45
3	B	605	HEC	C1A-CHA-C4D	-2.51	120.68	126.02
3	B	607	HEC	C2D-C1D-ND	2.51	112.72	109.84
3	C	605	HEC	C4A-CHB-C1B	-2.50	120.70	126.02
3	B	603	HEC	CHD-C1D-ND	2.50	127.45	124.37
3	A	604	HEC	CMB-C2B-C3B	2.49	132.90	126.15
3	A	603	HEC	C1C-CHC-C4B	-2.49	120.39	126.25
3	C	602	HEC	CMC-C2C-C3C	2.49	130.90	125.62
3	B	605	HEC	CAD-CBD-CGD	-2.48	107.08	113.67
3	C	603	HEC	CHD-C1D-ND	2.48	127.44	124.37
3	A	605	HEC	CMC-C2C-C1C	-2.48	121.64	125.42
3	C	604	HEC	CHA-C4D-ND	2.48	127.09	124.42
3	A	606	HEC	CHC-C1C-C2C	-2.48	120.23	127.43
3	B	603	HEC	O1D-CGD-CBD	-2.48	115.24	123.09
3	C	602	HEC	C1A-C2A-C3A	-2.47	103.85	107.11
3	B	603	HEC	CAD-C3D-C4D	2.47	129.00	124.70
3	C	608	HEC	C1A-C2A-C3A	-2.47	103.86	107.11
3	C	606	HEC	C1C-CHC-C4B	-2.46	120.45	126.25
4	B	608	ISW	CMD-C2D-C3D	2.46	132.80	126.15
4	A	608	ISW	C3C-C2C-C1C	-2.46	103.62	107.09
3	A	603	HEC	C3C-C4C-NC	2.46	112.88	110.15
3	B	606	HEC	CHD-C1D-ND	2.45	127.40	124.37
3	B	606	HEC	CHB-C4A-C3A	-2.45	120.39	125.49
3	A	606	HEC	CAB-C3B-C4B	2.45	127.98	124.79
3	C	603	HEC	C3C-C4C-NC	2.45	112.87	110.15
3	B	607	HEC	CHB-C1B-NB	2.45	127.06	124.42
4	A	608	ISW	CHA-C1A-C2A	2.44	128.72	124.86
3	B	607	HEC	CHC-C1C-NC	2.43	128.26	123.86
4	C	601	ISW	O1D-CGD-CBD	2.42	121.66	114.00
3	C	604	HEC	C1C-C2C-C3C	-2.42	104.04	106.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	607	HEC	CAC-C3C-C4C	-2.42	121.58	124.91
3	A	607	HEC	O2D-CGD-CBD	2.41	121.62	114.00
3	B	601	HEC	CHD-C1D-C2D	-2.41	120.09	126.95
3	A	605	HEC	CBC-CAC-C3C	2.41	118.94	112.42
3	A	604	HEC	C1B-C2B-C3B	-2.41	104.45	106.98
4	A	608	ISW	CMD-C2D-C3D	2.40	132.65	126.15
3	A	607	HEC	CHB-C1B-C2B	-2.40	121.24	125.03
3	C	607	HEC	O2D-CGD-CBD	2.39	121.56	114.00
3	C	605	HEC	CHA-C4D-C3D	-2.39	121.28	124.77
3	C	603	HEC	CHA-C4D-ND	2.39	127.00	124.42
3	C	606	HEC	CMD-C2D-C1D	2.39	128.77	125.03
3	B	601	HEC	CHB-C4A-NA	2.39	127.05	124.45
3	B	601	HEC	CMD-C2D-C1D	-2.39	121.31	125.03
3	C	602	HEC	CHB-C1B-C2B	-2.38	121.26	125.03
3	A	604	HEC	O2A-CGA-CBA	2.38	121.53	114.00
3	A	607	HEC	O1D-CGD-CBD	-2.37	115.58	123.09
3	C	605	HEC	C1C-CHC-C4B	-2.37	120.68	126.25
3	C	606	HEC	CHC-C4B-C3B	-2.35	120.89	125.23
3	C	605	HEC	CHB-C4A-C3A	-2.35	120.61	125.49
3	C	607	HEC	CAC-C3C-C2C	2.33	130.58	126.89
3	C	608	HEC	CHB-C1B-NB	2.33	126.93	124.42
3	A	603	HEC	CHC-C4B-C3B	-2.33	120.94	125.23
4	B	608	ISW	CHA-C1A-C2A	2.32	128.52	124.86
3	B	606	HEC	CMB-C2B-C3B	2.32	132.41	126.15
3	B	607	HEC	CHA-C1A-NA	2.31	126.97	124.45
3	A	601	HEC	CHB-C4A-C3A	-2.30	120.69	125.49
3	A	605	HEC	CHC-C4B-NB	2.30	127.22	124.37
3	B	601	HEC	CHB-C1B-NB	2.30	126.90	124.42
3	A	605	HEC	CMC-C2C-C3C	2.30	130.51	125.62
3	A	603	HEC	O1A-CGA-CBA	-2.29	115.82	123.09
4	A	608	ISW	C4A-C3A-C2A	-2.29	103.58	106.97
3	A	606	HEC	CAC-C3C-C2C	-2.29	123.27	126.89
3	B	607	HEC	CHC-C1C-C2C	-2.28	120.80	127.43
3	A	606	HEC	CHA-C4D-ND	-2.28	121.97	124.42
3	C	608	HEC	O1D-CGD-CBD	-2.28	115.87	123.09
3	C	605	HEC	CHB-C4A-NA	2.28	126.93	124.45
3	C	607	HEC	C4B-NB-C1B	2.27	107.90	105.21
3	B	606	HEC	C1C-CHC-C4B	-2.27	120.91	126.25
4	C	601	ISW	C2D-C1D-ND	2.27	112.45	109.84
3	A	606	HEC	C1D-ND-C4D	2.27	107.89	105.21
3	A	602	HEC	C3C-C4C-NC	2.26	112.66	110.15
3	B	604	HEC	CHC-C1C-NC	2.26	127.96	123.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	602	HEC	CAA-CBA-CGA	-2.25	107.69	113.67
3	B	606	HEC	CMD-C2D-C1D	2.25	128.56	125.03
3	C	607	HEC	C4A-CHB-C1B	-2.25	121.23	126.02
3	B	602	HEC	C3C-C4C-NC	2.25	112.65	110.15
3	B	607	HEC	CHB-C4A-NA	2.25	126.91	124.45
3	B	602	HEC	C4A-CHB-C1B	-2.25	121.24	126.02
4	B	608	ISW	C4A-CHB-C1B	-2.25	121.25	126.02
3	B	607	HEC	CHA-C1A-C2A	-2.24	121.33	124.86
3	A	602	HEC	CHC-C4B-C3B	-2.23	121.12	125.23
3	C	608	HEC	C4B-C3B-C2B	-2.22	103.66	106.89
3	C	603	HEC	C1C-CHC-C4B	-2.22	121.03	126.25
3	C	605	HEC	CHD-C4C-NC	2.21	127.86	123.86
3	C	602	HEC	CHD-C1D-ND	2.20	127.09	124.37
3	C	605	HEC	CMD-C2D-C1D	2.20	128.48	125.03
4	A	608	ISW	O2A-CGA-O1A	-2.20	117.67	123.33
3	A	606	HEC	CMB-C2B-C1B	-2.20	121.59	125.03
3	A	605	HEC	CMD-C2D-C1D	2.20	128.47	125.03
3	C	604	HEC	CHD-C1D-C2D	-2.19	120.72	126.95
3	B	602	HEC	CHB-C1B-C2B	-2.19	121.58	125.03
3	B	601	HEC	CHA-C1A-C2A	-2.18	121.42	124.86
3	B	605	HEC	O2D-CGD-O1D	-2.17	117.75	123.33
3	C	602	HEC	CAD-CBD-CGD	-2.17	107.92	113.67
3	B	604	HEC	CHB-C4A-NA	2.17	126.81	124.45
4	A	608	ISW	O2D-CGD-CBD	-2.16	116.23	123.09
3	B	605	HEC	C4C-C3C-C2C	-2.16	103.52	106.87
3	B	607	HEC	C1A-CHA-C4D	-2.16	121.42	126.02
3	B	601	HEC	O2A-CGA-CBA	2.16	120.81	114.00
3	B	601	HEC	C3C-C4C-NC	2.15	112.54	110.15
3	B	602	HEC	CAC-C3C-C4C	2.15	127.87	124.91
3	A	604	HEC	C4A-CHB-C1B	-2.15	121.45	126.02
3	C	608	HEC	CHD-C1D-C2D	-2.15	120.84	126.95
3	B	604	HEC	CHA-C1A-C2A	-2.15	121.47	124.86
4	C	601	ISW	CMD-C2D-C1D	2.15	128.39	125.03
3	C	606	HEC	C4A-CHB-C1B	-2.15	121.46	126.02
3	B	604	HEC	C4B-NB-C1B	2.14	107.75	105.21
3	A	607	HEC	CHB-C1B-NB	2.14	126.72	124.42
3	C	605	HEC	CAD-C3D-C2D	2.14	131.87	127.87
3	B	602	HEC	C3B-C4B-NB	2.13	112.51	110.17
3	C	605	HEC	CHC-C4B-NB	2.13	127.00	124.37
3	B	605	HEC	CMD-C2D-C1D	2.13	128.36	125.03
4	C	601	ISW	CHB-C1B-NB	-2.13	122.15	124.44
3	B	604	HEC	CHD-C4C-C3C	-2.12	120.65	125.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	603	HEC	CHD-C1D-C2D	-2.11	120.94	126.95
3	B	607	HEC	C1B-C2B-C3B	-2.11	104.76	106.98
3	B	604	HEC	C3D-C4D-ND	2.11	112.39	110.35
3	B	605	HEC	CBB-CAB-C3B	2.11	118.14	112.42
3	B	605	HEC	CHB-C4A-C3A	-2.11	121.10	125.49
3	C	608	HEC	CHC-C1C-C2C	-2.11	121.31	127.43
3	B	603	HEC	C4D-C3D-C2D	-2.11	103.83	106.89
3	A	607	HEC	CMA-C3A-C4A	2.10	128.43	124.73
3	C	607	HEC	CHB-C4A-C3A	-2.10	121.11	125.49
3	A	605	HEC	C1A-C2A-C3A	-2.10	104.35	107.11
3	A	605	HEC	CHA-C1A-NA	-2.10	122.17	124.45
4	A	608	ISW	C2B-C1B-NB	2.09	112.32	109.90
3	A	601	HEC	O2A-CGA-CBA	2.09	120.61	114.00
3	C	606	HEC	CAD-C3D-C4D	2.09	128.34	124.70
3	C	605	HEC	CAB-C3B-C4B	2.09	127.51	124.79
3	C	602	HEC	CAD-C3D-C4D	2.09	128.34	124.70
3	A	605	HEC	C2A-C1A-NA	2.09	112.34	110.32
3	C	608	HEC	CBC-CAC-C3C	2.09	118.08	112.42
3	C	604	HEC	CHB-C1B-C2B	-2.09	121.73	125.03
3	C	606	HEC	O1D-CGD-CBD	-2.09	116.48	123.09
3	B	607	HEC	C4C-CHD-C1D	-2.08	121.36	126.25
3	B	606	HEC	CAA-C2A-C1A	2.08	129.07	124.85
3	C	608	HEC	CAB-C3B-C2B	-2.07	123.75	127.56
3	B	603	HEC	C1C-CHC-C4B	-2.06	121.39	126.25
3	A	601	HEC	C4B-NB-C1B	2.06	107.65	105.21
4	A	608	ISW	C4C-C3C-C2C	-2.06	104.74	107.30
3	A	605	HEC	O1D-CGD-CBD	-2.06	116.57	123.09
3	A	605	HEC	CHC-C4B-C3B	-2.05	121.44	125.23
4	C	601	ISW	C4A-C3A-C2A	-2.05	103.93	106.97
3	C	607	HEC	C1A-CHA-C4D	-2.05	121.66	126.02
3	B	601	HEC	O2D-CGD-CBD	2.05	120.48	114.00
3	C	606	HEC	CAD-CBD-CGD	-2.05	108.23	113.67
3	C	602	HEC	CBA-CAA-C2A	-2.05	106.87	112.53
3	C	607	HEC	CHD-C1D-ND	2.04	126.89	124.37
3	A	607	HEC	CMC-C2C-C1C	-2.04	122.31	125.42
3	A	606	HEC	CBD-CAD-C3D	-2.04	106.89	112.53
3	C	603	HEC	C3B-C4B-NB	2.04	112.40	110.17
3	B	604	HEC	C2A-C1A-NA	2.03	112.28	110.32
3	C	606	HEC	CAC-C3C-C2C	2.03	130.10	126.89
3	B	603	HEC	CBA-CAA-C2A	-2.03	106.93	112.53
3	C	606	HEC	CHA-C4D-ND	2.03	126.60	124.42
3	C	605	HEC	CHD-C4C-C3C	-2.03	120.86	125.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	602	HEC	CHC-C4B-C3B	-2.02	121.50	125.23
3	B	606	HEC	CMB-C2B-C1B	-2.02	121.88	125.03
3	A	602	HEC	CHA-C4D-C3D	-2.02	121.83	124.77
4	C	601	ISW	O2A-CGA-CBA	2.01	120.36	114.00
3	A	604	HEC	O1D-CGD-CBD	-2.01	116.71	123.09
4	B	608	ISW	CHB-C1B-C2B	2.01	128.20	125.03
3	B	602	HEC	CAD-CBD-CGD	-2.01	108.34	113.67
3	A	603	HEC	CAB-C3B-C4B	2.00	127.39	124.79

All (21) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	601	HEC	NA
3	A	602	HEC	NA
3	A	603	HEC	NA
3	A	604	HEC	NA
3	A	605	HEC	NA
3	A	606	HEC	NA
3	A	607	HEC	NA
3	B	601	HEC	NA
3	B	602	HEC	NA
3	B	603	HEC	NA
3	B	604	HEC	NA
3	B	605	HEC	NA
3	B	606	HEC	NA
3	B	607	HEC	NA
3	C	602	HEC	NA
3	C	603	HEC	NA
3	C	604	HEC	NA
3	C	605	HEC	NA
3	C	606	HEC	NA
3	C	607	HEC	NA
3	C	608	HEC	NA

All (221) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	604	HEC	C1A-C2A-CAA-CBA
3	C	602	HEC	C2C-C3C-CAC-CBC
3	B	606	HEC	C4C-C3C-CAC-CBC
3	C	602	HEC	C4C-C3C-CAC-CBC
3	A	601	HEC	C4C-C3C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
3	B	606	HEC	C2B-C3B-CAB-CBB
3	B	607	HEC	C2B-C3B-CAB-CBB
3	A	601	HEC	C2C-C3C-CAC-CBC
3	B	606	HEC	C2C-C3C-CAC-CBC
3	C	604	HEC	C4C-C3C-CAC-CBC
3	C	606	HEC	C2C-C3C-CAC-CBC
3	A	607	HEC	C4C-C3C-CAC-CBC
3	C	603	HEC	C2B-C3B-CAB-CBB
3	C	608	HEC	C2B-C3B-CAB-CBB
3	A	607	HEC	C2C-C3C-CAC-CBC
3	A	604	HEC	C3A-C2A-CAA-CBA
3	C	604	HEC	C2C-C3C-CAC-CBC
5	B	612	PEG	C4-C3-O2-C2
3	B	601	HEC	C2B-C3B-CAB-CBB
3	B	605	HEC	C2C-C3C-CAC-CBC
3	A	603	HEC	C2B-C3B-CAB-CBB
3	B	605	HEC	C4C-C3C-CAC-CBC
3	C	606	HEC	C4C-C3C-CAC-CBC
3	A	602	HEC	C2C-C3C-CAC-CBC
8	B	613	P6G	O4-C5-C6-O7
3	C	606	HEC	C2B-C3B-CAB-CBB
3	C	603	HEC	C2C-C3C-CAC-CBC
3	C	603	HEC	C4B-C3B-CAB-CBB
3	B	607	HEC	C2C-C3C-CAC-CBC
3	C	607	HEC	C2C-C3C-CAC-CBC
3	C	603	HEC	C4C-C3C-CAC-CBC
3	B	606	HEC	C4B-C3B-CAB-CBB
3	A	601	HEC	C2B-C3B-CAB-CBB
5	B	610	PEG	O1-C1-C2-O2
8	B	613	P6G	O16-C17-C18-O19
9	B	614	PG4	O1-C1-C2-O2
3	A	605	HEC	C2C-C3C-CAC-CBC
3	C	605	HEC	C2C-C3C-CAC-CBC
3	A	607	HEC	C2B-C3B-CAB-CBB
3	A	605	HEC	C4C-C3C-CAC-CBC
3	C	608	HEC	C2C-C3C-CAC-CBC
8	B	613	P6G	O7-C8-C9-O10
3	B	607	HEC	C4C-C3C-CAC-CBC
3	C	607	HEC	C4C-C3C-CAC-CBC
5	B	611	PEG	O1-C1-C2-O2
3	B	604	HEC	C2C-C3C-CAC-CBC
3	A	605	HEC	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
3	A	606	HEC	C2B-C3B-CAB-CBB
3	B	602	HEC	C2B-C3B-CAB-CBB
3	A	602	HEC	C2B-C3B-CAB-CBB
3	B	604	HEC	C4C-C3C-CAC-CBC
5	A	610	PEG	O2-C3-C4-O4
5	B	611	PEG	O2-C3-C4-O4
5	C	622	PEG	O2-C3-C4-O4
5	F	102	PEG	O2-C3-C4-O4
6	A	615	PGE	O1-C1-C2-O2
6	C	614	PGE	O1-C1-C2-O2
3	B	601	HEC	C2C-C3C-CAC-CBC
3	A	602	HEC	C4C-C3C-CAC-CBC
3	C	608	HEC	C4C-C3C-CAC-CBC
9	B	614	PG4	O3-C5-C6-O4
3	B	603	HEC	C2B-C3B-CAB-CBB
5	A	613	PEG	O2-C3-C4-O4
5	A	614	PEG	O1-C1-C2-O2
5	B	612	PEG	O1-C1-C2-O2
5	C	609	PEG	O1-C1-C2-O2
5	C	611	PEG	O1-C1-C2-O2
5	C	622	PEG	O1-C1-C2-O2
3	A	605	HEC	C4B-C3B-CAB-CBB
3	C	607	HEC	C2B-C3B-CAB-CBB
5	A	613	PEG	O1-C1-C2-O2
5	A	614	PEG	O2-C3-C4-O4
5	C	610	PEG	O1-C1-C2-O2
5	C	612	PEG	O1-C1-C2-O2
3	C	608	HEC	C4B-C3B-CAB-CBB
7	B	615	EDO	O1-C1-C2-O2
7	C	616	EDO	O1-C1-C2-O2
3	B	601	HEC	C4B-C3B-CAB-CBB
3	B	602	HEC	C4B-C3B-CAB-CBB
3	A	603	HEC	C2C-C3C-CAC-CBC
5	C	611	PEG	O2-C3-C4-O4
3	B	607	HEC	C4B-C3B-CAB-CBB
3	A	601	HEC	C4B-C3B-CAB-CBB
3	C	606	HEC	C4B-C3B-CAB-CBB
5	B	609	PEG	O2-C3-C4-O4
5	B	612	PEG	O2-C3-C4-O4
5	F	102	PEG	O1-C1-C2-O2
6	C	614	PGE	O3-C5-C6-O4
8	B	613	P6G	O13-C14-C15-O16

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Mol	Chain	Res	Type	Atoms
3	B	601	HEC	C4C-C3C-CAC-CBC
7	A	617	EDO	O1-C1-C2-O2
7	C	621	EDO	O1-C1-C2-O2
3	B	602	HEC	C4C-C3C-CAC-CBC
3	A	602	HEC	C1A-C2A-CAA-CBA
3	A	607	HEC	C4B-C3B-CAB-CBB
3	B	603	HEC	C2C-C3C-CAC-CBC
3	C	603	HEC	C1A-C2A-CAA-CBA
3	B	603	HEC	C4B-C3B-CAB-CBB
7	A	618	EDO	O1-C1-C2-O2
7	A	619	EDO	O1-C1-C2-O2
7	B	621	EDO	O1-C1-C2-O2
7	C	617	EDO	O1-C1-C2-O2
3	A	603	HEC	C4C-C3C-CAC-CBC
5	A	611	PEG	O1-C1-C2-O2
6	A	615	PGE	O2-C3-C4-O3
3	C	602	HEC	C2B-C3B-CAB-CBB
5	C	611	PEG	C4-C3-O2-C2
5	C	613	PEG	O2-C3-C4-O4
6	A	615	PGE	O3-C5-C6-O4
3	A	604	HEC	C4C-C3C-CAC-CBC
5	A	609	PEG	C4-C3-O2-C2
5	B	609	PEG	C1-C2-O2-C3
5	C	622	PEG	C1-C2-O2-C3
4	A	608	ISW	C2A-CAA-CBA-CGA
8	B	613	P6G	C6-C5-O4-C3
6	C	614	PGE	C4-C3-O2-C2
3	C	605	HEC	C2B-C3B-CAB-CBB
3	C	605	HEC	C4C-C3C-CAC-CBC
5	A	613	PEG	C1-C2-O2-C3
5	B	612	PEG	C1-C2-O2-C3
5	A	612	PEG	O1-C1-C2-O2
7	B	619	EDO	O1-C1-C2-O2
5	C	612	PEG	C1-C2-O2-C3
6	A	615	PGE	C1-C2-O2-C3
5	A	611	PEG	C4-C3-O2-C2
3	C	607	HEC	C2A-CAA-CBA-CGA
3	B	602	HEC	C2C-C3C-CAC-CBC
3	A	604	HEC	C2B-C3B-CAB-CBB
8	B	613	P6G	C9-C8-O7-C6
3	A	603	HEC	C4B-C3B-CAB-CBB
5	C	610	PEG	C1-C2-O2-C3

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Mol	Chain	Res	Type	Atoms
3	C	607	HEC	C4B-C3B-CAB-CBB
3	A	602	HEC	C4B-C3B-CAB-CBB
5	F	102	PEG	C4-C3-O2-C2
9	B	614	PG4	O4-C7-C8-O5
3	B	603	HEC	C4C-C3C-CAC-CBC
6	A	615	PGE	C6-C5-O3-C4
7	C	620	EDO	O1-C1-C2-O2
5	A	613	PEG	C4-C3-O2-C2
6	C	614	PGE	C3-C4-O3-C5
3	A	604	HEC	C2C-C3C-CAC-CBC
6	C	614	PGE	C6-C5-O3-C4
3	B	604	HEC	C2B-C3B-CAB-CBB
8	B	613	P6G	C12-C11-O10-C9
8	B	613	P6G	C8-C9-O10-C11
4	C	601	ISW	CAD-CBD-CGD-O1D
3	C	605	HEC	C4B-C3B-CAB-CBB
5	C	613	PEG	C4-C3-O2-C2
3	A	606	HEC	C4B-C3B-CAB-CBB
3	C	604	HEC	CAA-CBA-CGA-O1A
4	B	608	ISW	C2A-CAA-CBA-CGA
8	B	613	P6G	C14-C15-O16-C17
3	B	603	HEC	CAD-CBD-CGD-O1D
3	A	603	HEC	CAA-CBA-CGA-O1A
4	C	601	ISW	CAD-CBD-CGD-O2D
3	A	607	HEC	CAD-CBD-CGD-O1D
3	B	607	HEC	CAD-CBD-CGD-O1D
3	C	604	HEC	CAD-CBD-CGD-O2D
3	B	605	HEC	CAD-CBD-CGD-O2D
3	C	604	HEC	CAD-CBD-CGD-O1D
4	C	601	ISW	C2A-CAA-CBA-CGA
3	A	603	HEC	CAD-CBD-CGD-O2D
3	B	603	HEC	CAA-CBA-CGA-O2A
3	B	603	HEC	CAD-CBD-CGD-O2D
3	C	604	HEC	CAA-CBA-CGA-O2A
3	A	606	HEC	CAD-CBD-CGD-O2D
3	C	608	HEC	CAD-CBD-CGD-O1D
3	A	602	HEC	C3A-C2A-CAA-CBA
3	A	603	HEC	CAD-CBD-CGD-O1D
3	A	605	HEC	CAD-CBD-CGD-O2D
3	C	606	HEC	CAD-CBD-CGD-O2D
3	B	601	HEC	CAD-CBD-CGD-O2D
3	B	603	HEC	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
3	A	607	HEC	CAD-CBD-CGD-O2D
3	C	608	HEC	CAD-CBD-CGD-O2D
4	A	608	ISW	CAD-CBD-CGD-O1D
5	A	609	PEG	C1-C2-O2-C3
3	A	606	HEC	CAA-CBA-CGA-O2A
3	A	603	HEC	CAA-CBA-CGA-O2A
3	B	601	HEC	CAD-CBD-CGD-O1D
3	B	606	HEC	CAD-CBD-CGD-O2D
3	B	607	HEC	CAD-CBD-CGD-O2D
3	C	607	HEC	CAD-CBD-CGD-O1D
5	C	610	PEG	C4-C3-O2-C2
3	B	605	HEC	CAD-CBD-CGD-O1D
3	A	604	HEC	C4B-C3B-CAB-CBB
3	C	602	HEC	C4B-C3B-CAB-CBB
3	C	606	HEC	CAD-CBD-CGD-O1D
3	A	606	HEC	CAD-CBD-CGD-O1D
4	B	608	ISW	CAD-CBD-CGD-O1D
3	A	605	HEC	CAD-CBD-CGD-O1D
3	B	606	HEC	CAD-CBD-CGD-O1D
5	A	614	PEG	C4-C3-O2-C2
3	A	606	HEC	CAA-CBA-CGA-O1A
3	B	606	HEC	CAA-CBA-CGA-O2A
5	C	611	PEG	C1-C2-O2-C3
3	C	607	HEC	CAA-CBA-CGA-O2A
4	A	608	ISW	CAD-CBD-CGD-O2D
4	B	608	ISW	CAD-CBD-CGD-O2D
3	C	603	HEC	C3A-C2A-CAA-CBA
3	B	606	HEC	CAA-CBA-CGA-O1A
3	C	607	HEC	CAD-CBD-CGD-O2D
3	C	607	HEC	CAA-CBA-CGA-O1A
5	C	610	PEG	O2-C3-C4-O4
9	B	614	PG4	C8-C7-O4-C6
3	A	606	HEC	C2A-CAA-CBA-CGA
6	C	614	PGE	O2-C3-C4-O3
5	C	613	PEG	O1-C1-C2-O2
4	B	608	ISW	C4C-C3C-CAC-CBC
3	B	602	HEC	CAD-CBD-CGD-O2D
3	A	604	HEC	CAD-CBD-CGD-O1D
8	B	613	P6G	C15-C14-O13-C12
3	B	602	HEC	C1A-C2A-CAA-CBA
3	B	602	HEC	CAD-CBD-CGD-O1D
3	A	601	HEC	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
3	A	601	HEC	CAD-CBD-CGD-O2D
3	B	604	HEC	C4B-C3B-CAB-CBB
3	A	604	HEC	CAD-CBD-CGD-O2D
3	C	603	HEC	CAA-CBA-CGA-O2A
5	A	609	PEG	O2-C3-C4-O4
3	B	604	HEC	CAA-CBA-CGA-O2A

There are no ring outliers.

37 monomers are involved in 80 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	613	PEG	3	0
3	C	602	HEC	4	0
3	C	608	HEC	2	0
4	B	608	ISW	10	0
3	A	601	HEC	1	0
3	C	605	HEC	2	0
3	B	602	HEC	3	0
3	B	605	HEC	3	0
3	A	606	HEC	1	0
6	A	615	PGE	1	0
4	C	601	ISW	11	0
7	C	616	EDO	1	0
5	B	609	PEG	3	0
4	A	608	ISW	10	0
8	B	613	P6G	1	0
3	C	607	HEC	1	0
5	C	612	PEG	1	0
3	C	603	HEC	1	0
3	A	604	HEC	2	0
7	A	619	EDO	1	0
5	C	610	PEG	2	0
3	B	603	HEC	4	0
3	A	605	HEC	4	0
5	C	622	PEG	1	0
3	A	602	HEC	1	0
3	A	603	HEC	1	0
3	C	606	HEC	5	0
5	A	612	PEG	1	0
5	F	102	PEG	1	0
3	B	601	HEC	2	0
5	B	612	PEG	1	0

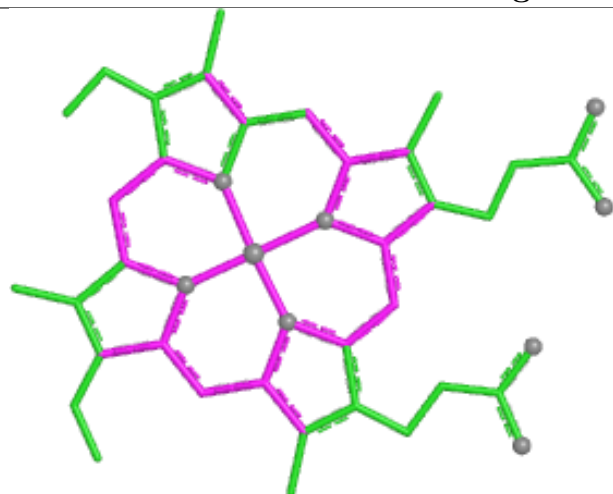
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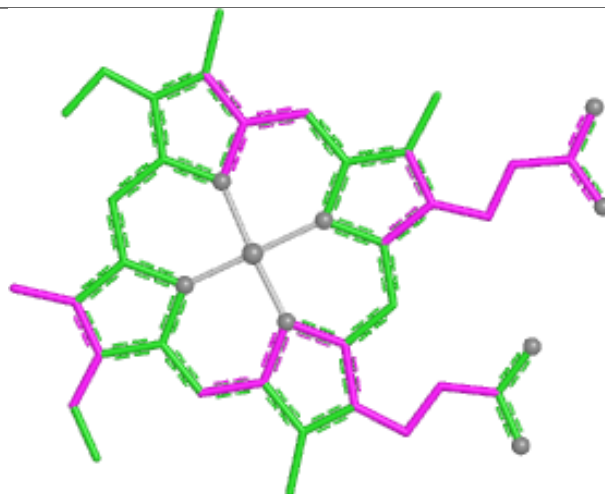
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	C	614	PGE	4	0
5	A	614	PEG	2	0
7	A	617	EDO	2	0
7	C	617	EDO	2	0
9	B	614	PG4	1	0
3	B	606	HEC	1	0

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.

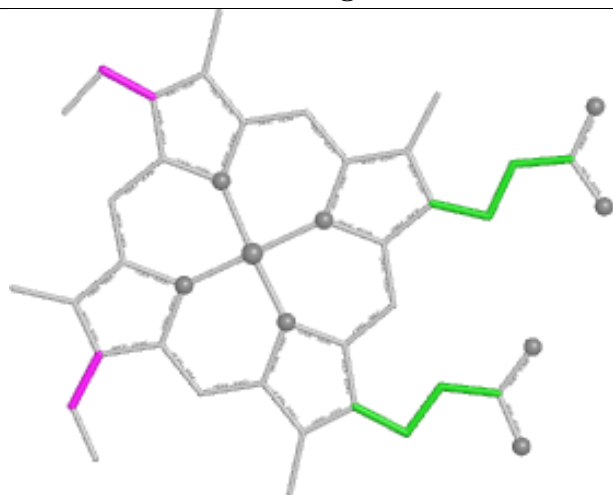
Ligand HEC C 602



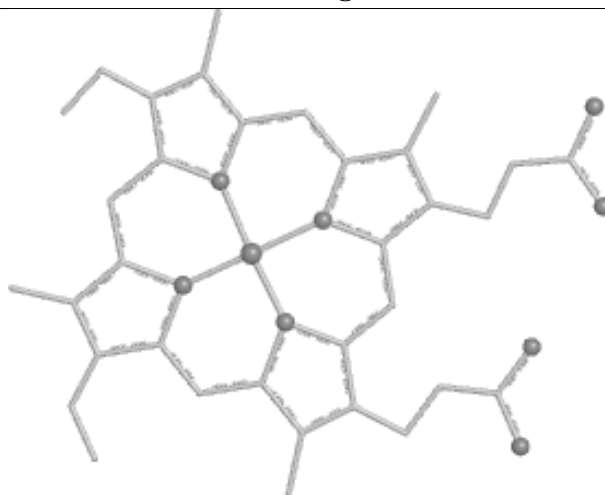
Bond lengths



Bond angles

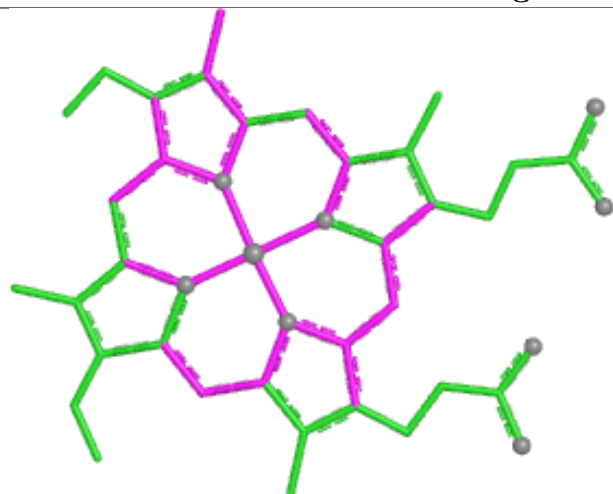


Torsions

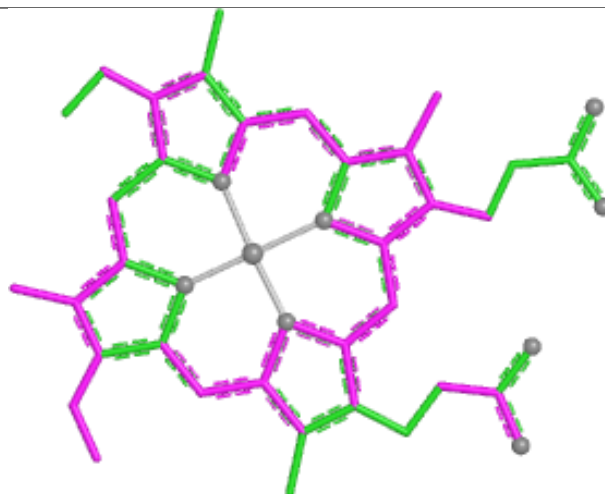


Rings

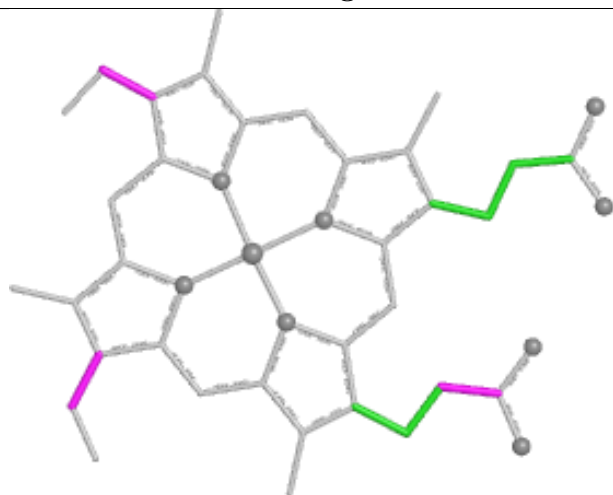
Ligand HEC C 608



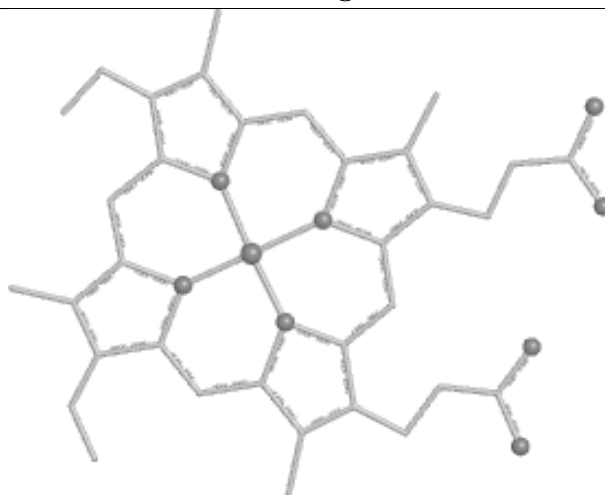
Bond lengths



Bond angles

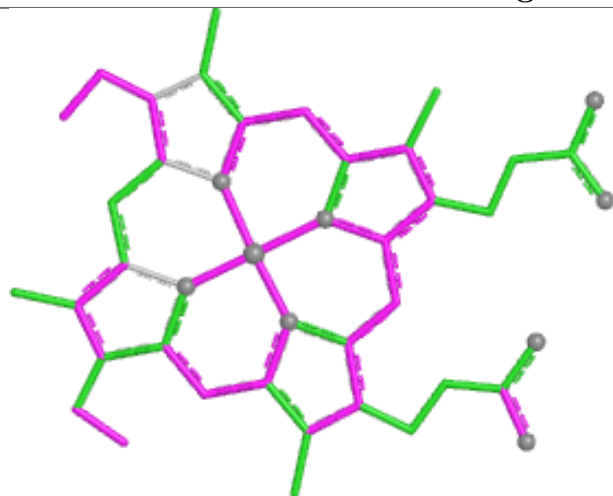


Torsions

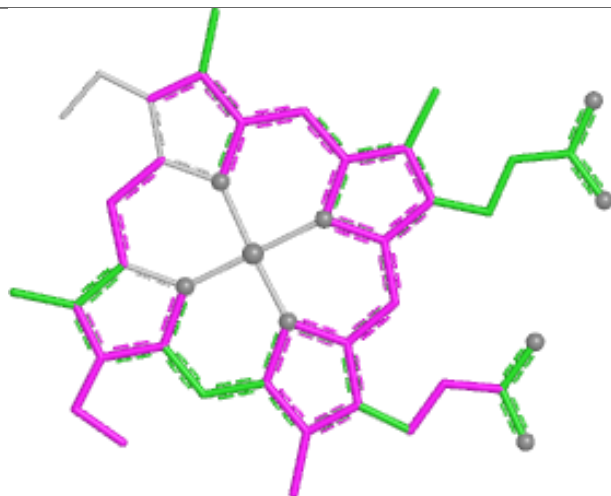


Rings

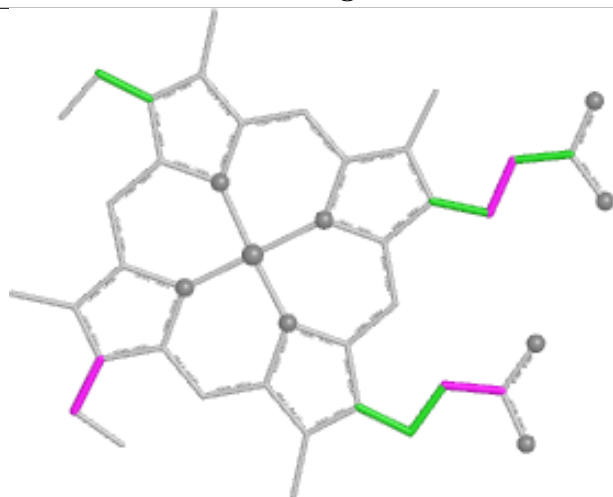
Ligand ISW B 608



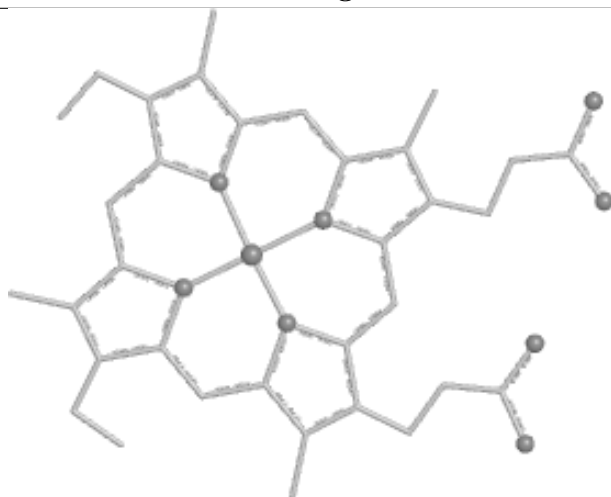
Bond lengths



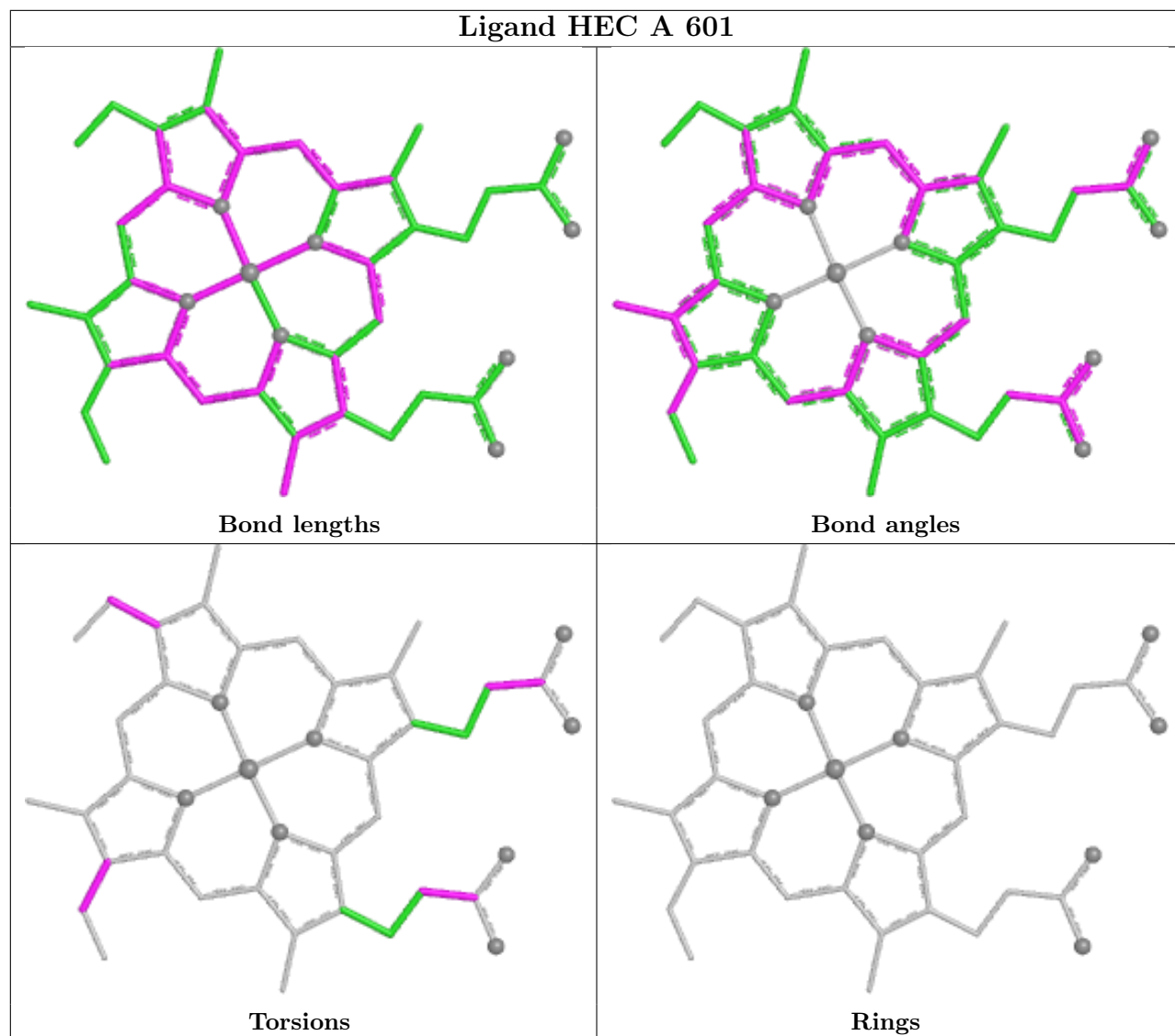
Bond angles

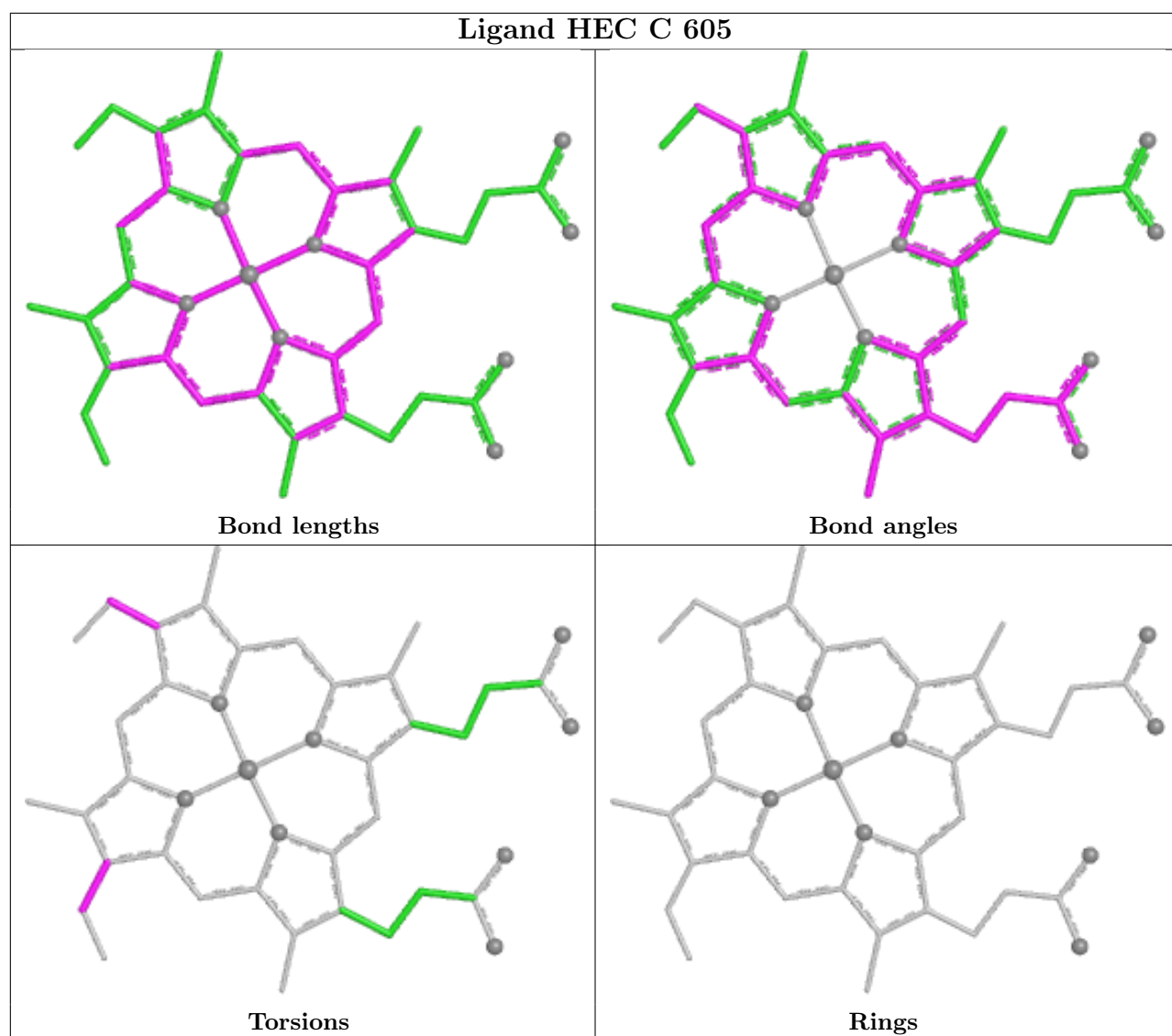


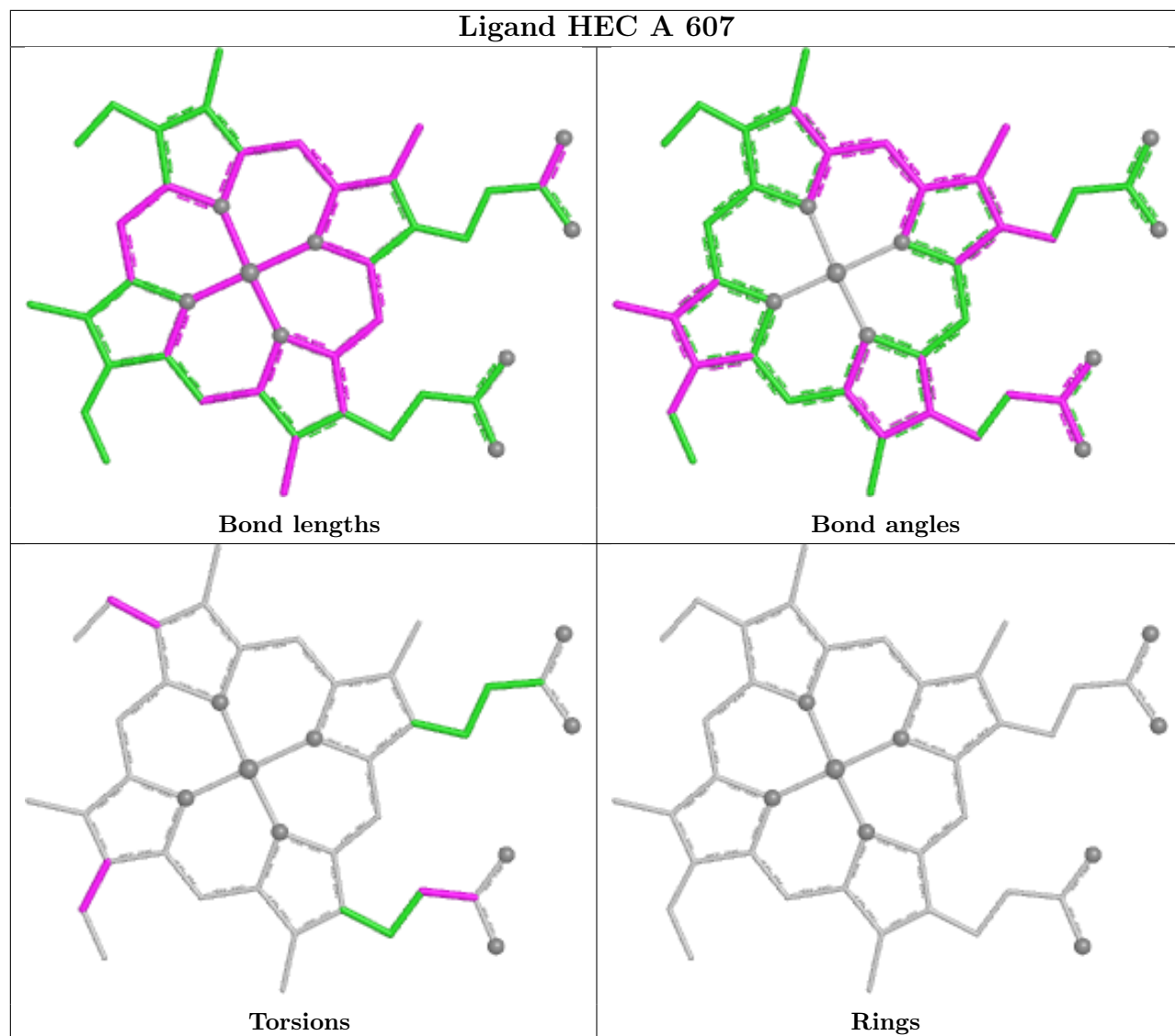
Torsions



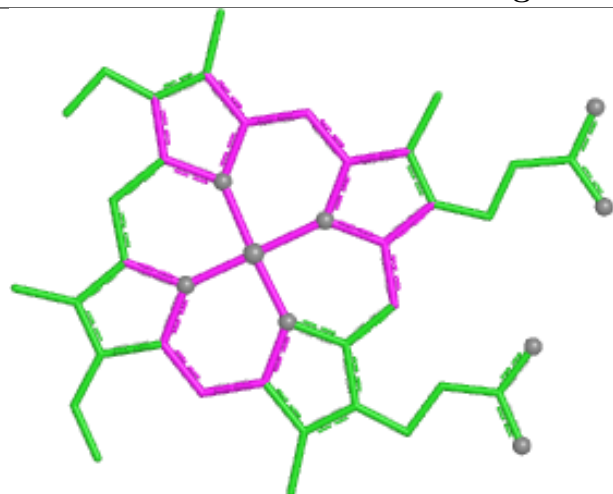
Rings



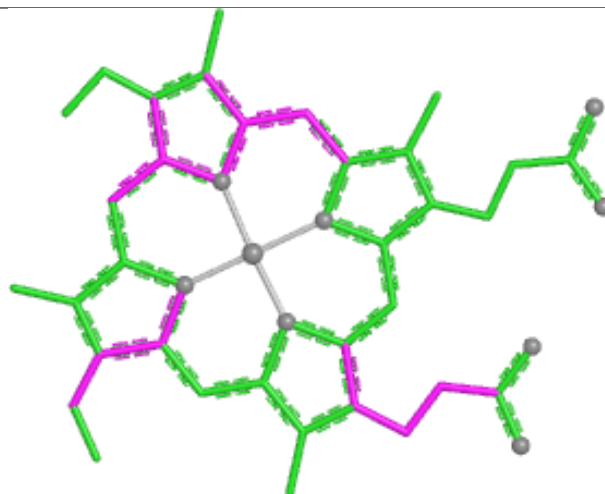




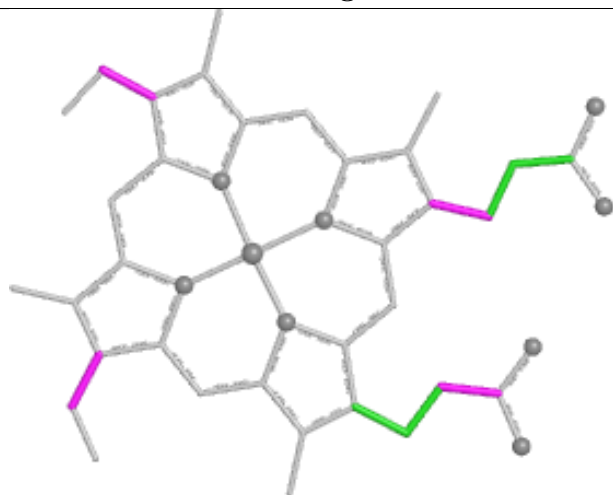
Ligand HEC B 602



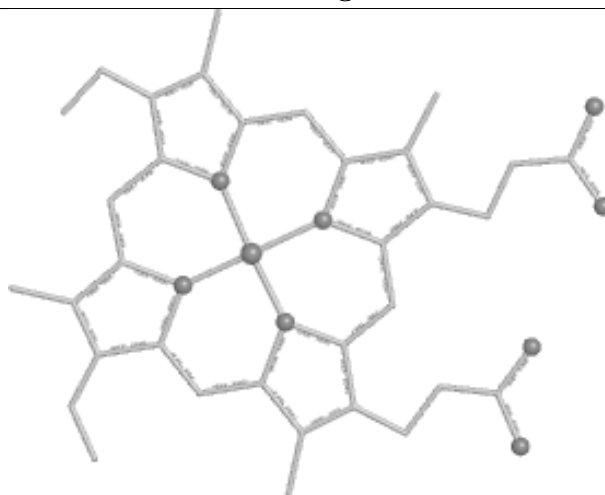
Bond lengths



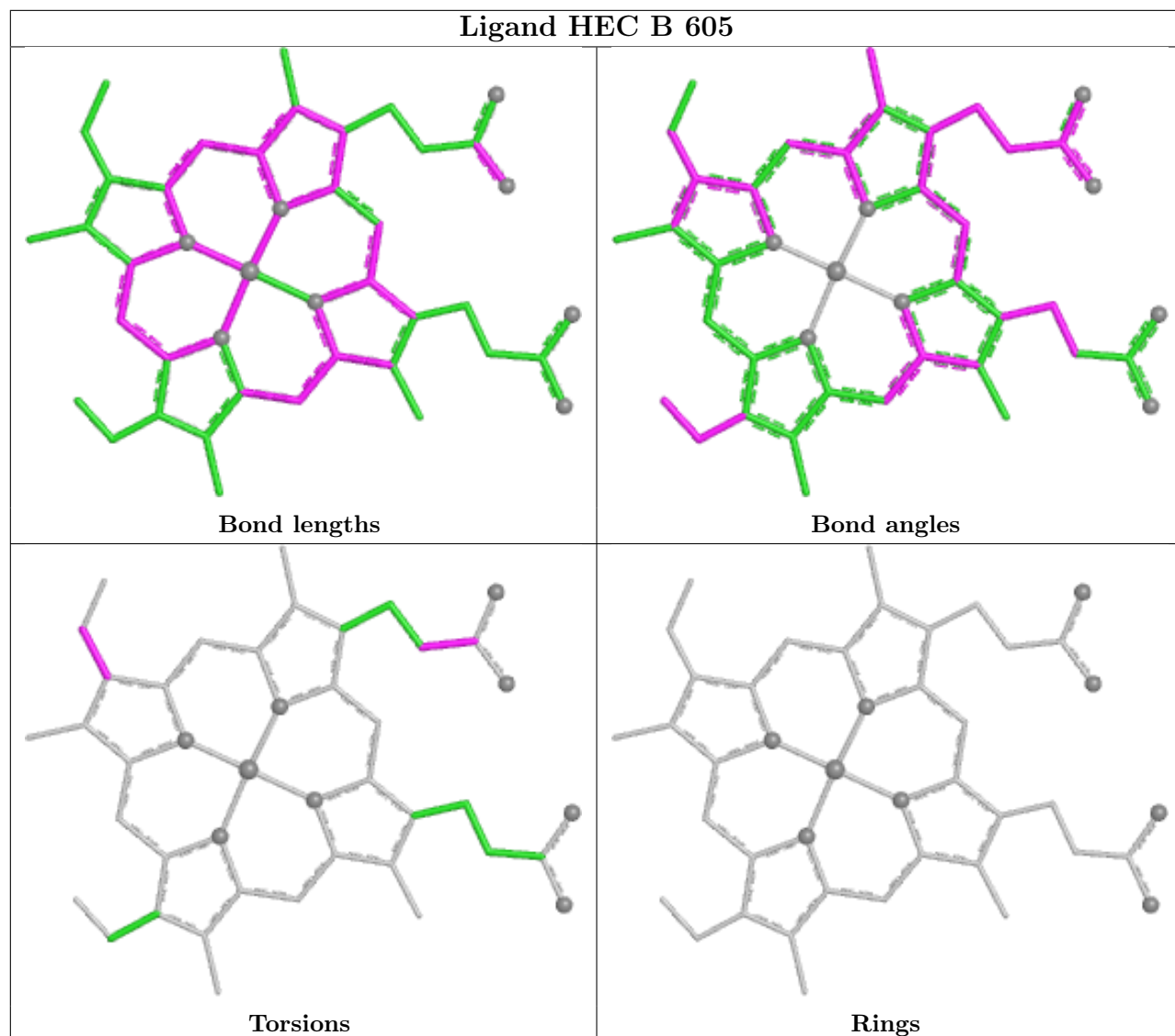
Bond angles

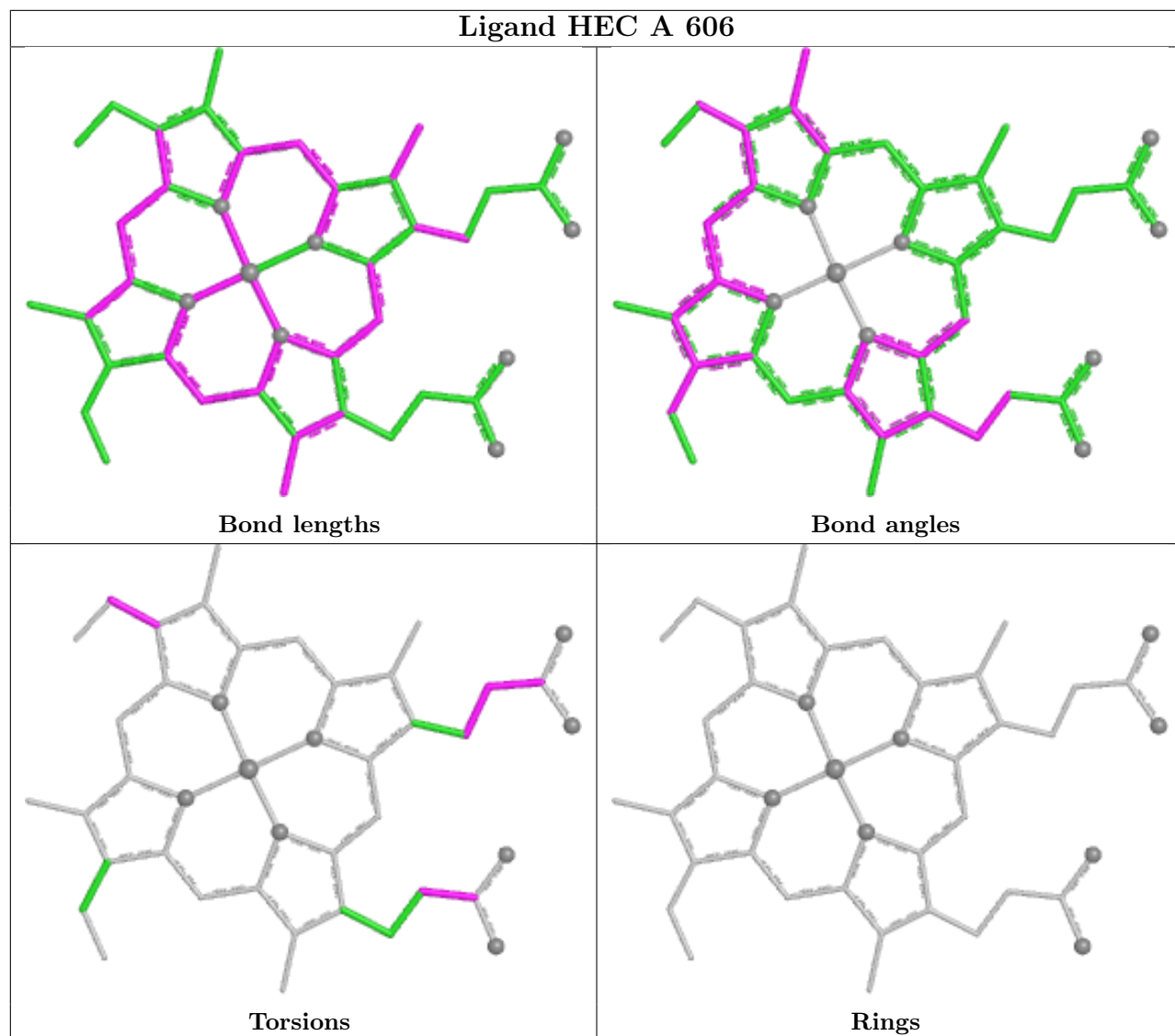


Torsions

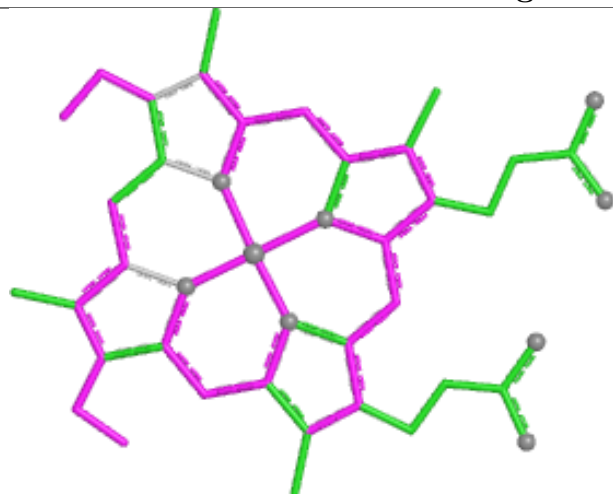


Rings

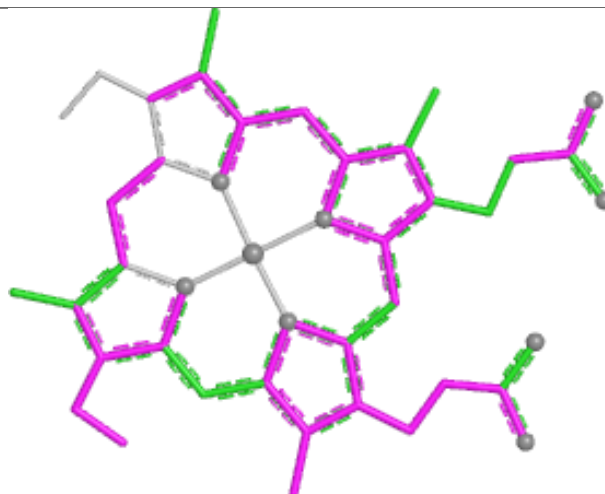




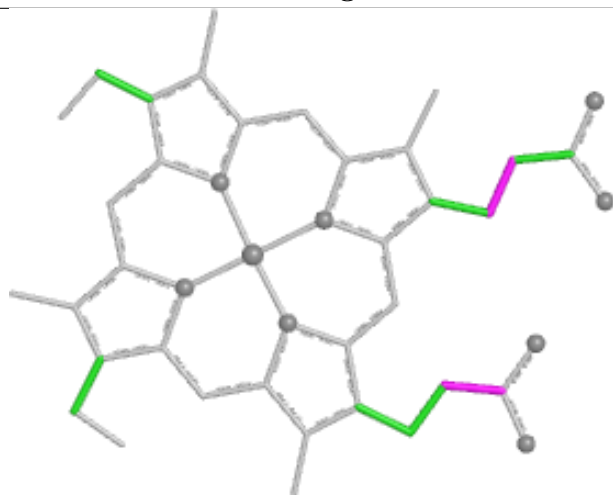
Ligand ISW C 601



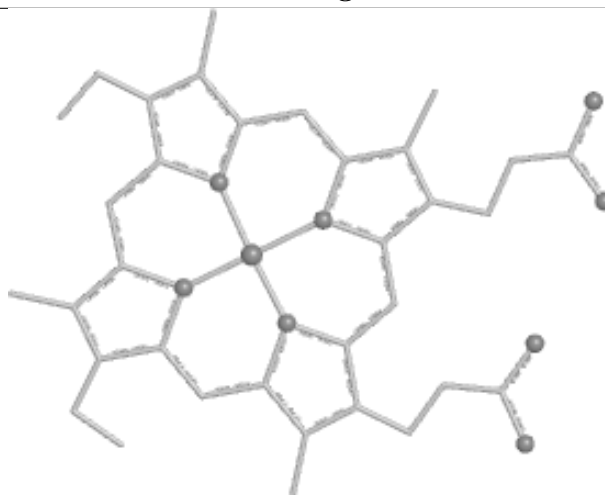
Bond lengths



Bond angles

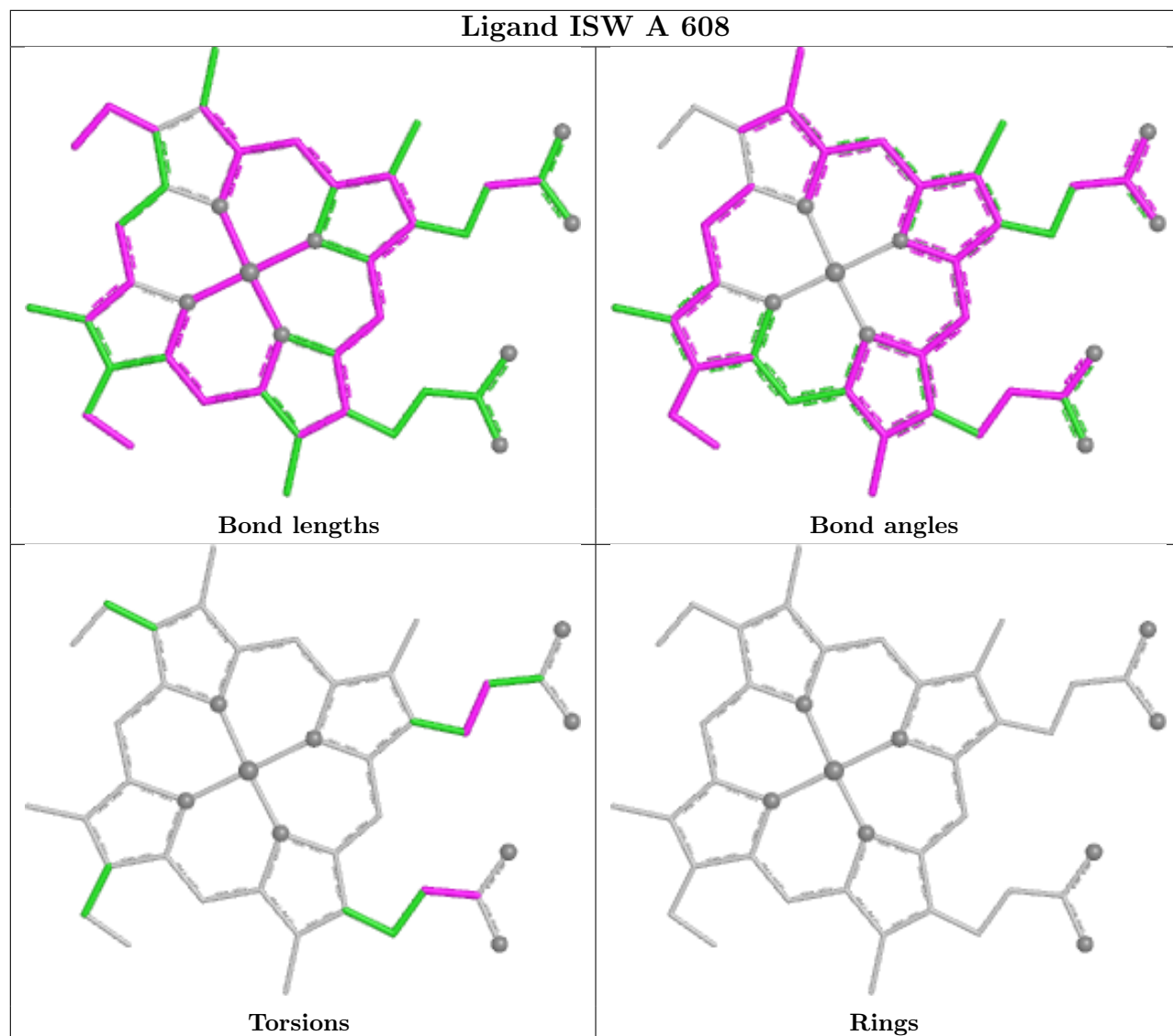


Torsions

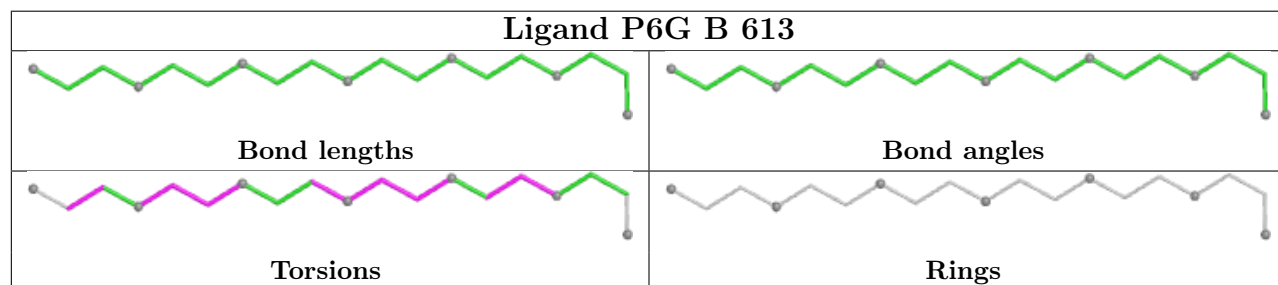


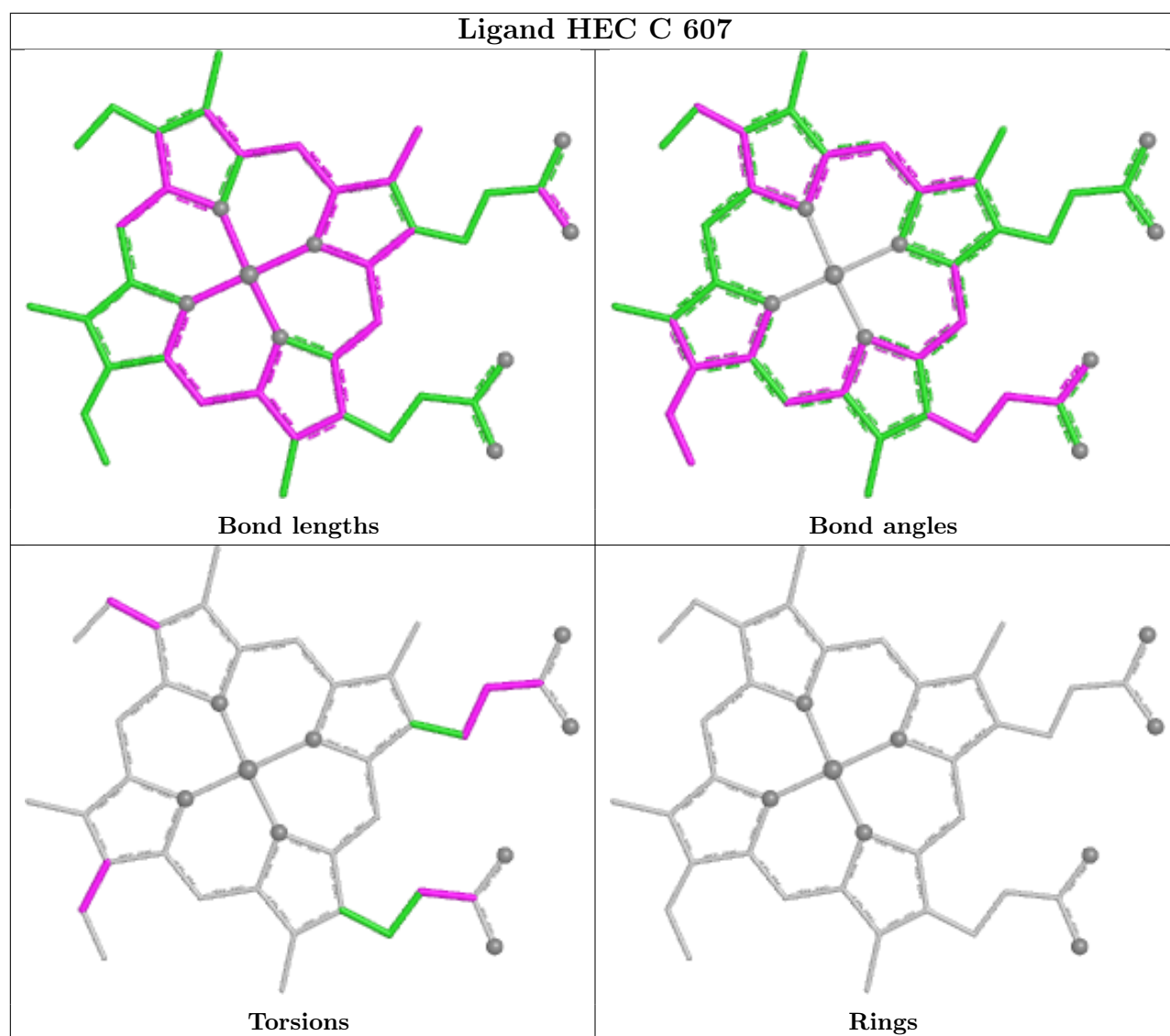
Rings

Ligand ISW A 608

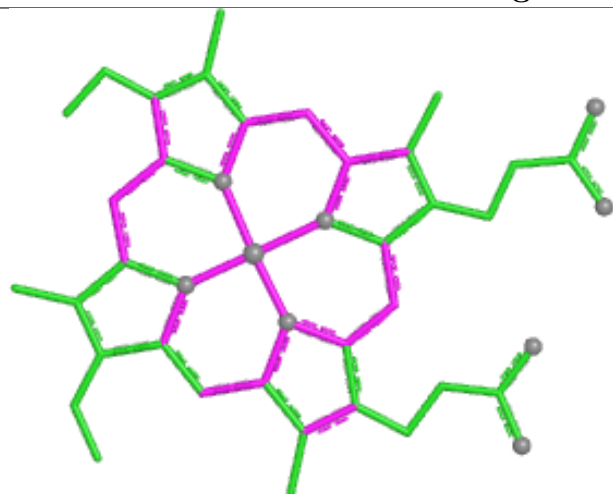


Ligand P6G B 613

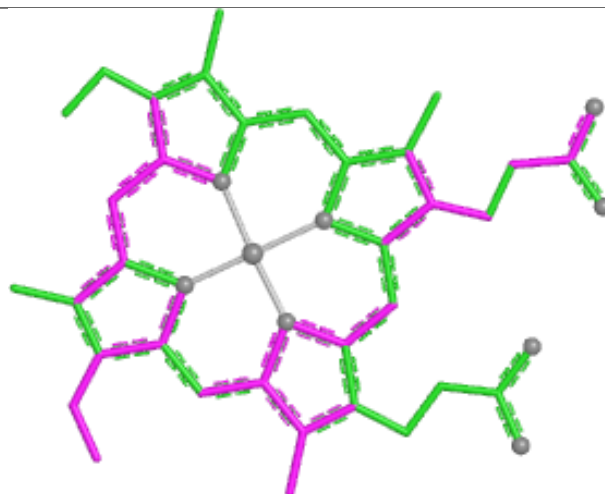




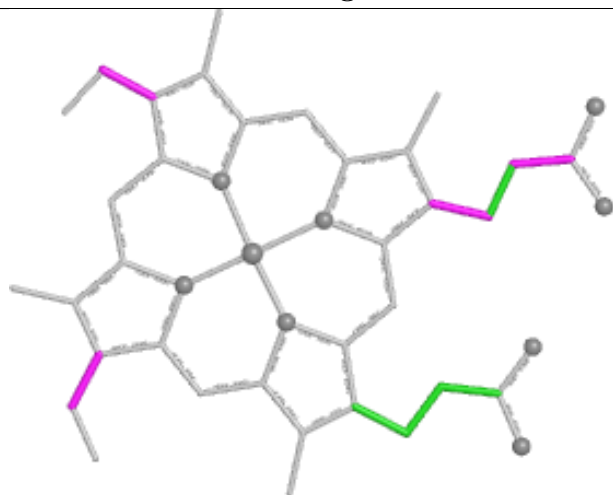
Ligand HEC C 603



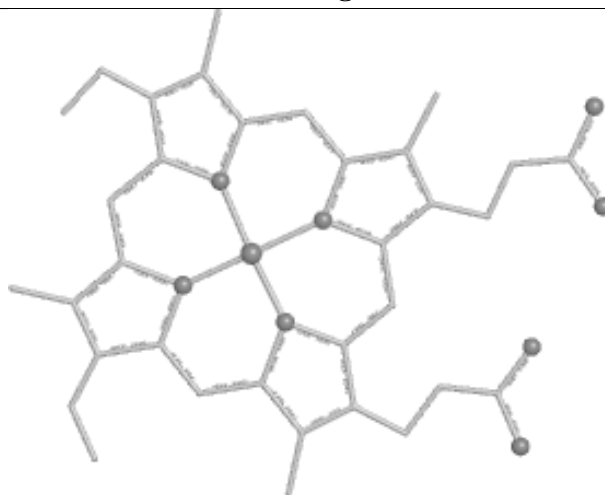
Bond lengths



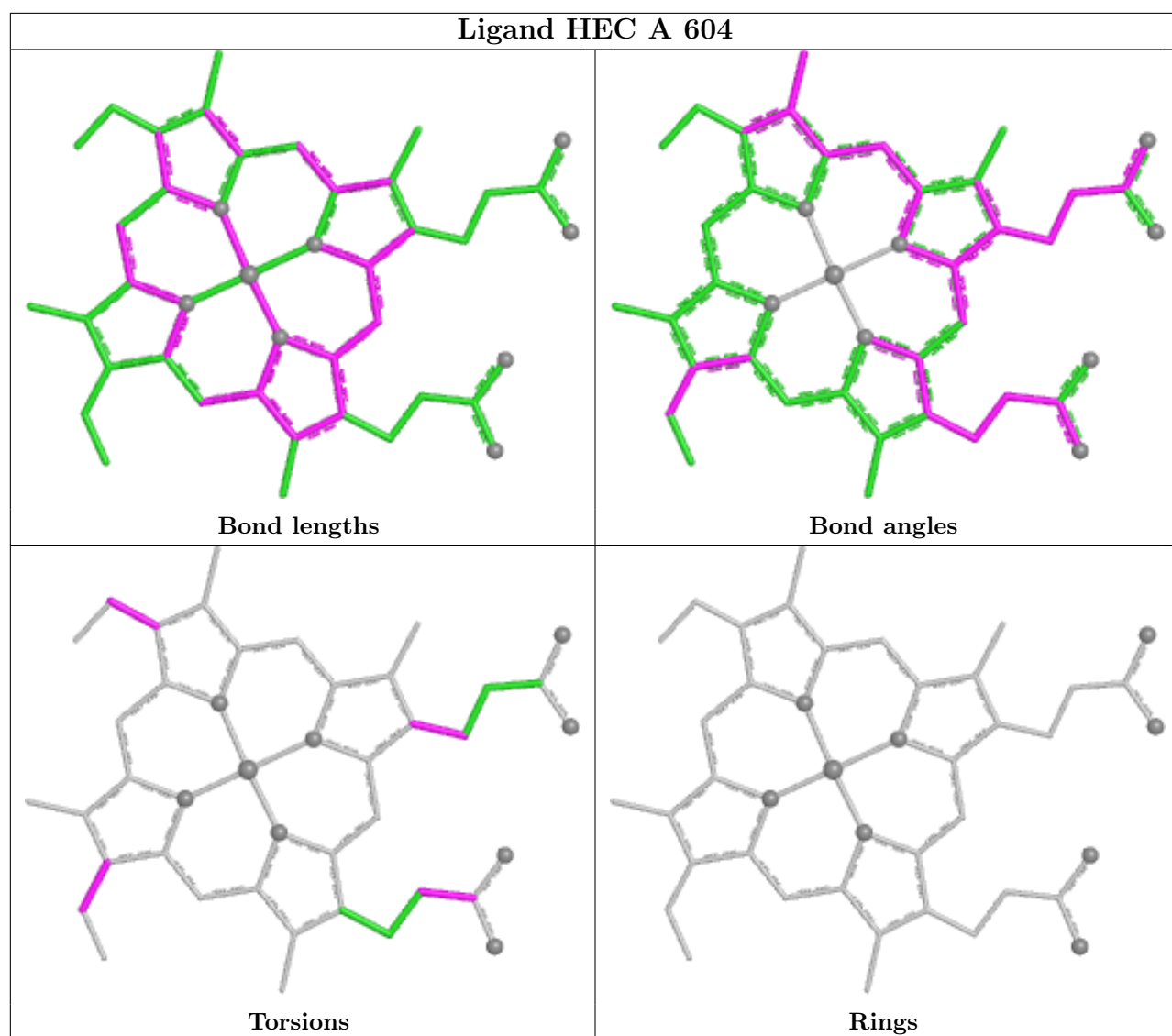
Bond angles



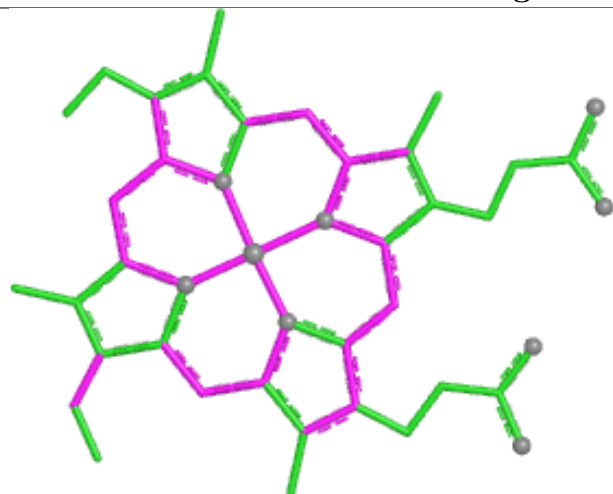
Torsions



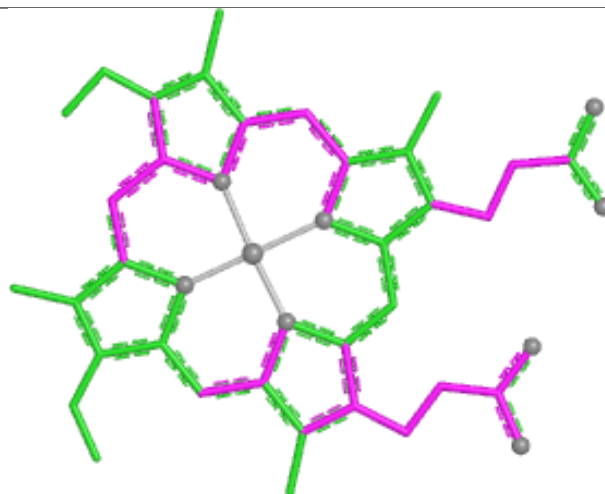
Rings



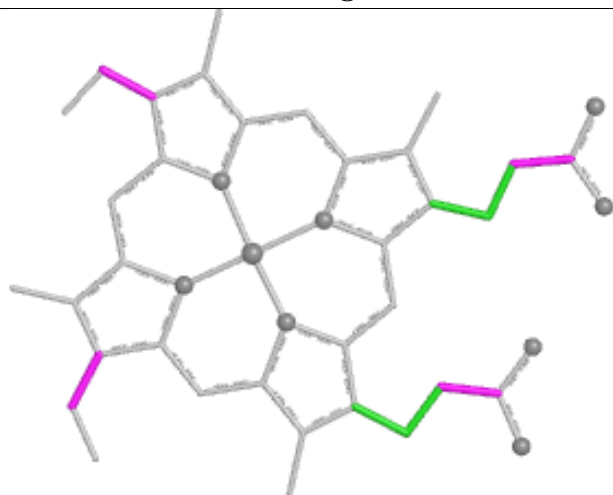
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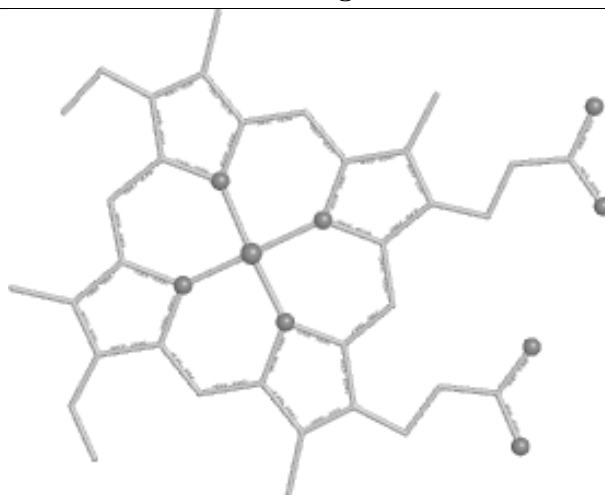
Bond lengths



Bond angles

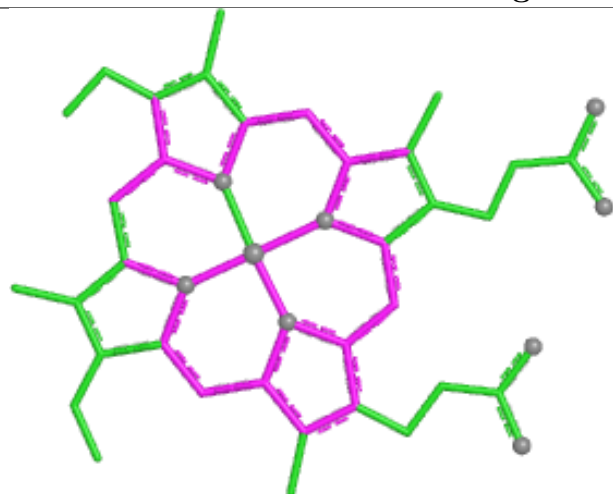


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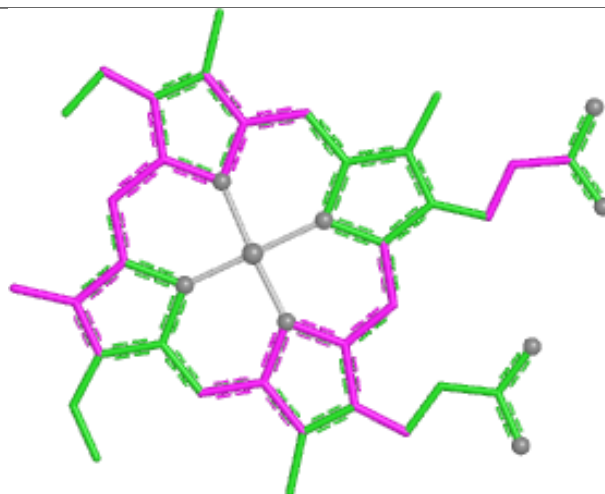


Rings

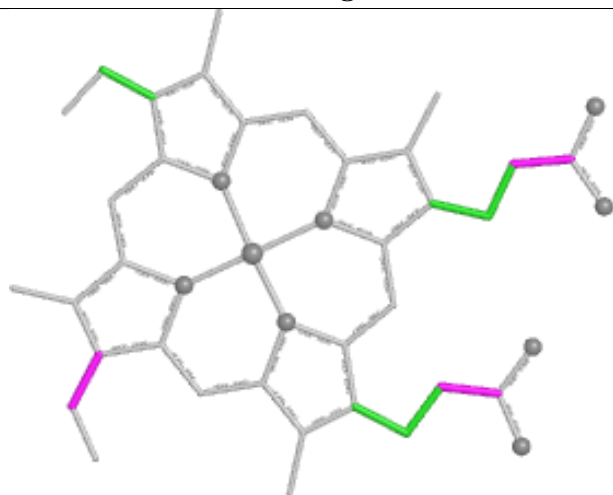
Ligand HEC C 604



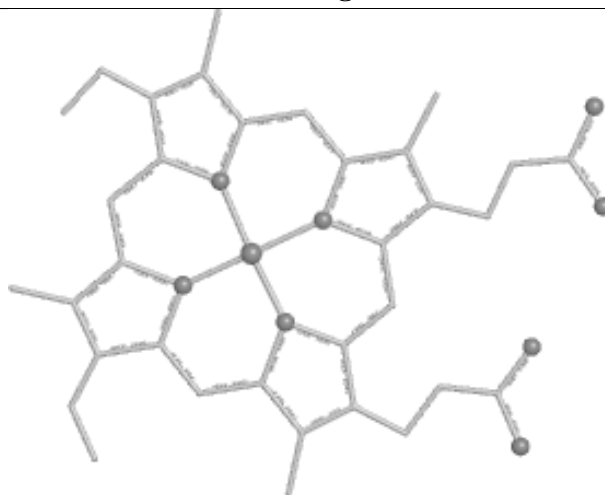
Bond lengths



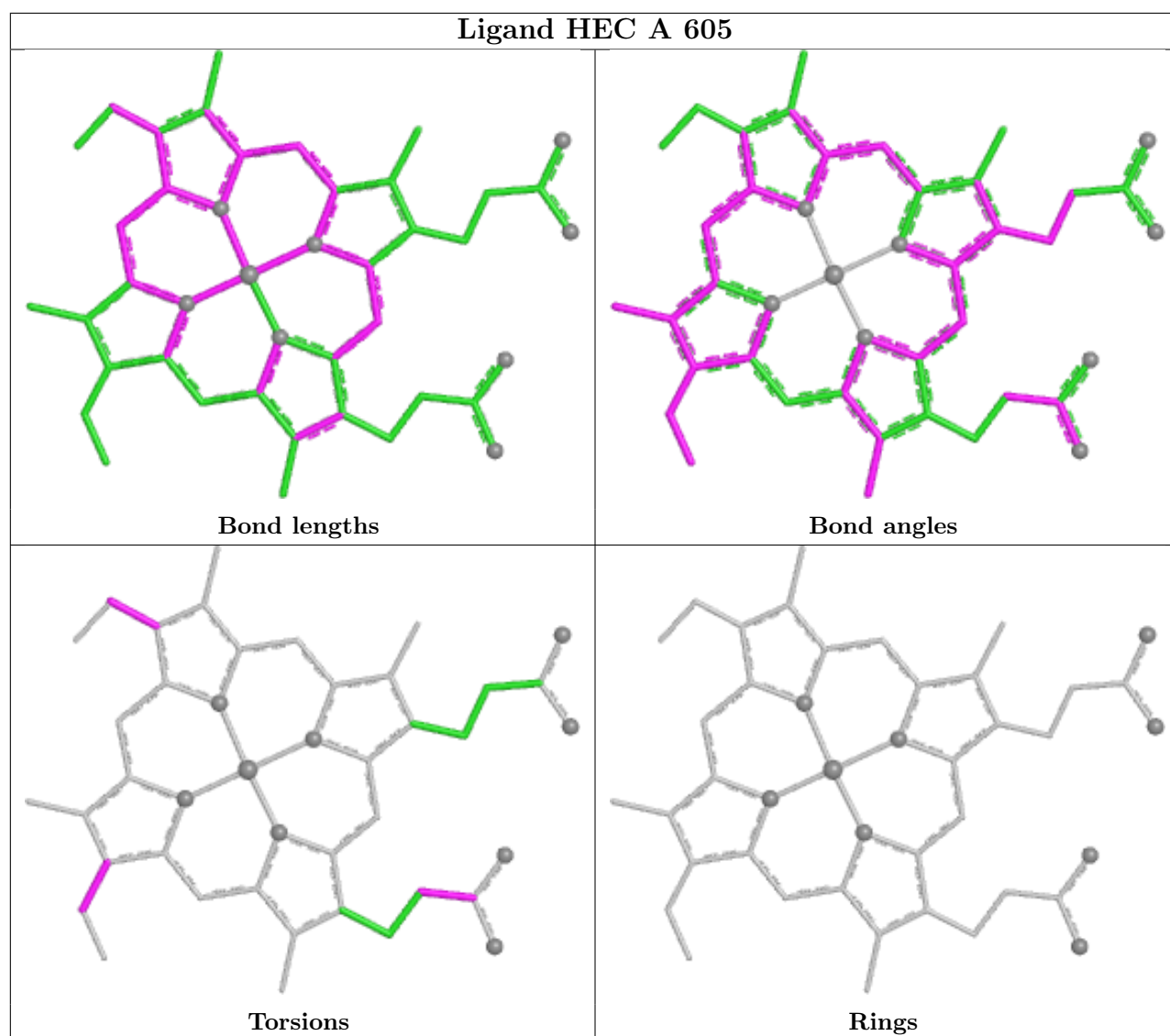
Bond angles

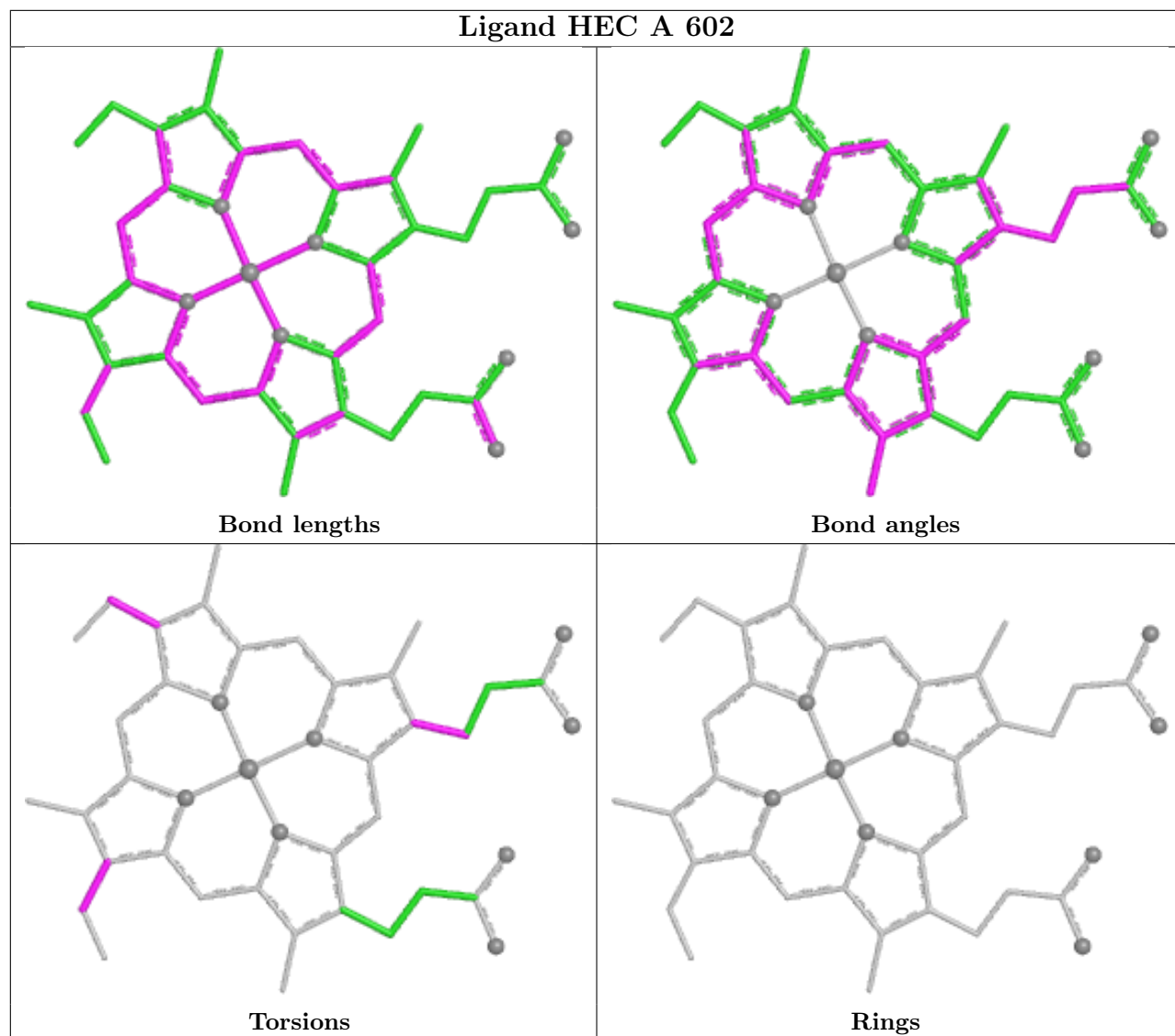


Torsions

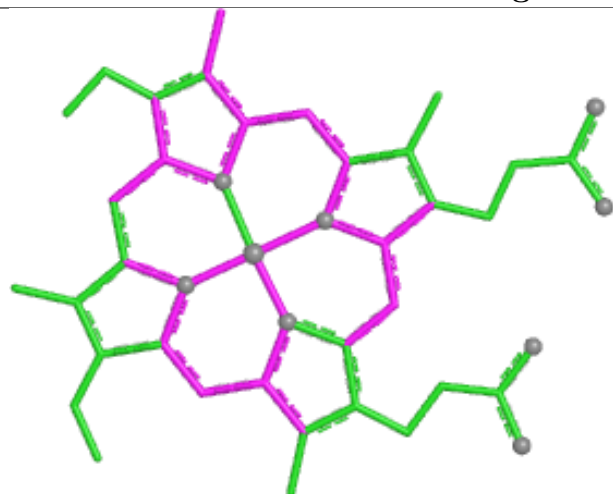


Rings

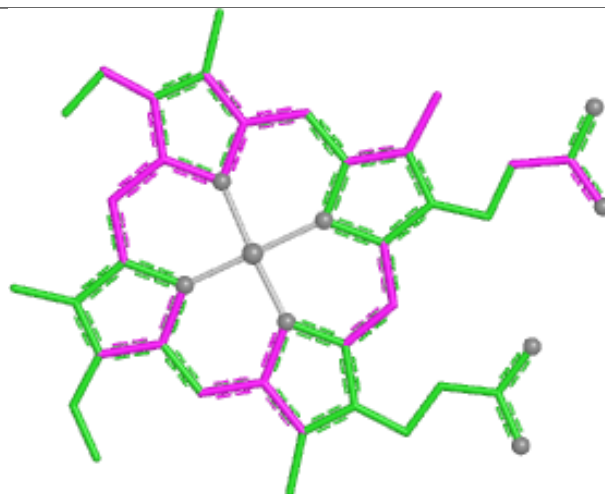




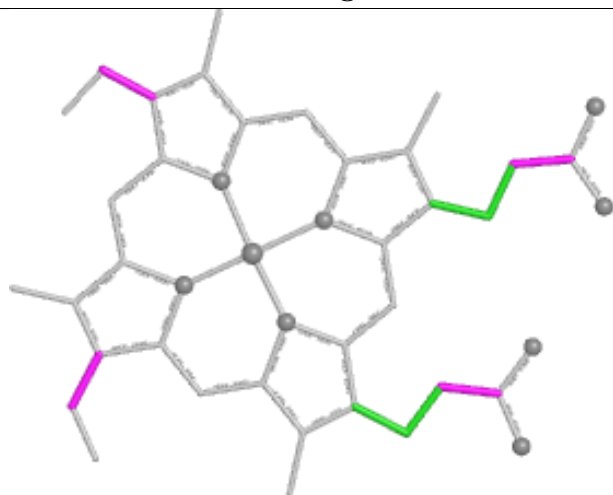
Ligand HEC A 603



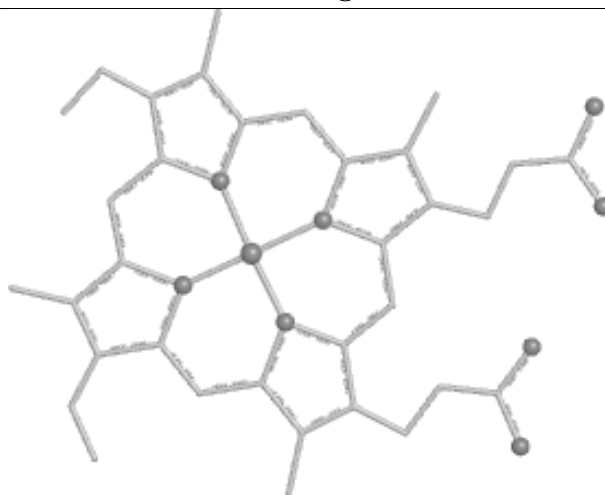
Bond lengths



Bond angles

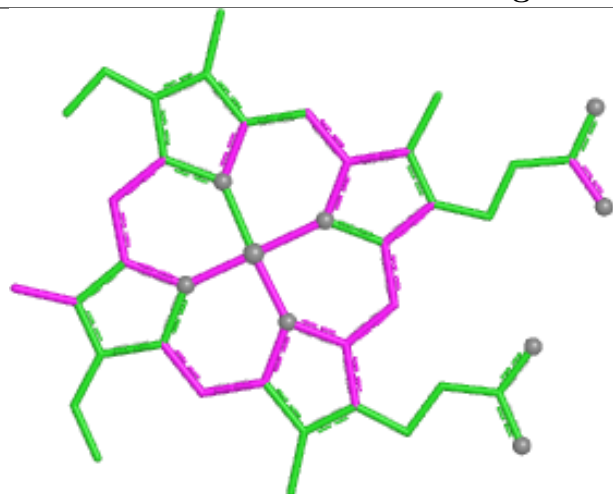


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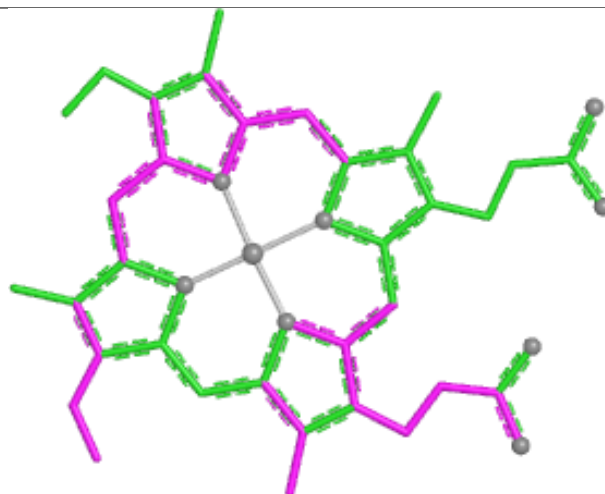


Rings

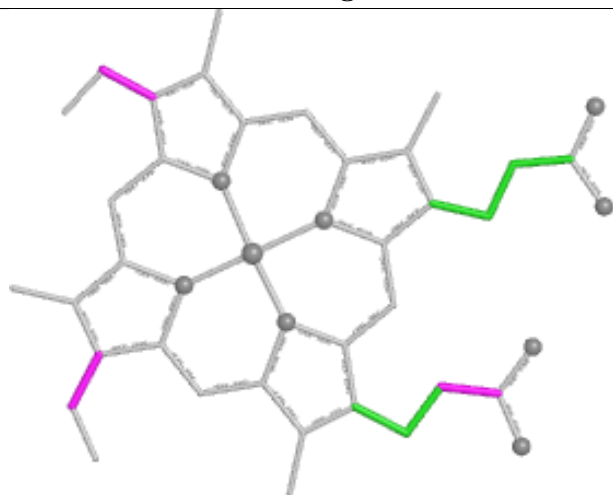
Ligand HEC C 606



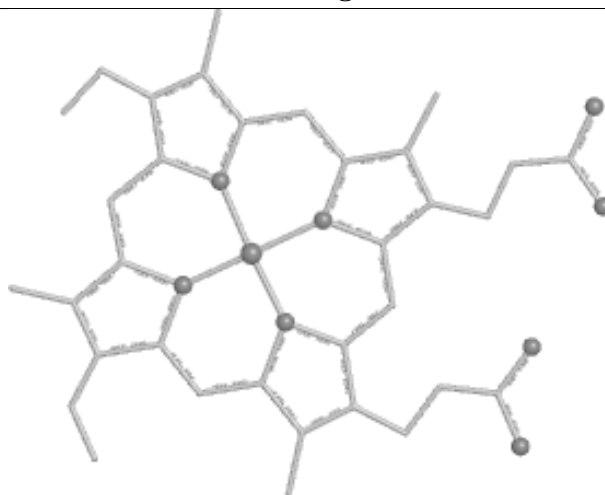
Bond lengths



Bond angles

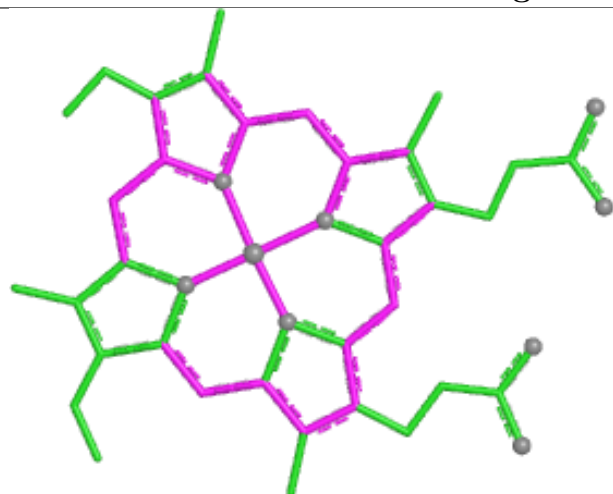


Torsions

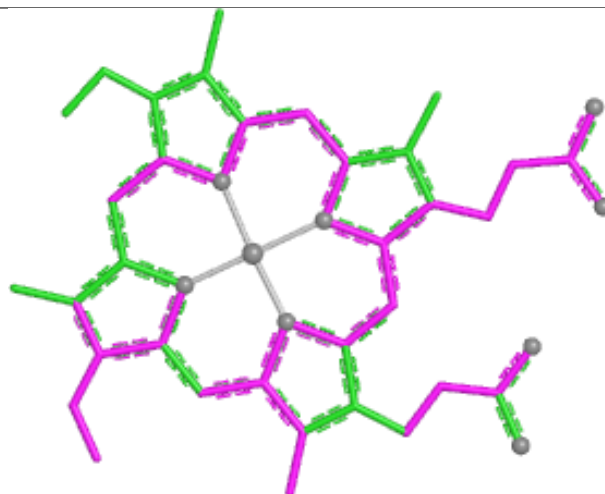


Rings

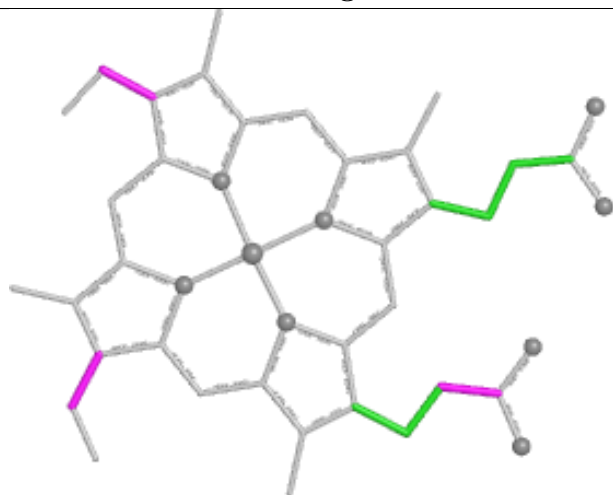
Ligand HEC B 601



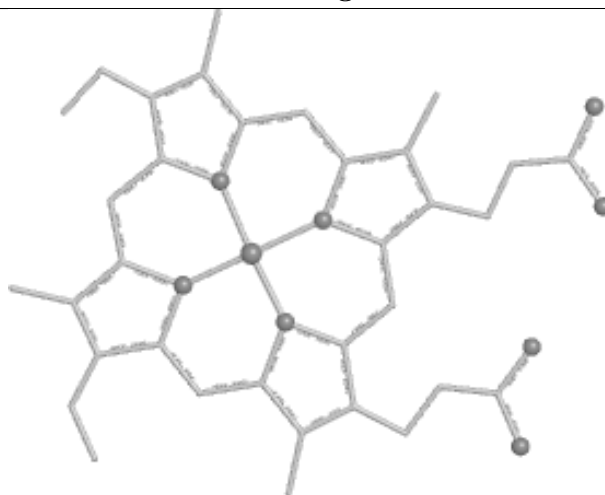
Bond lengths



Bond angles

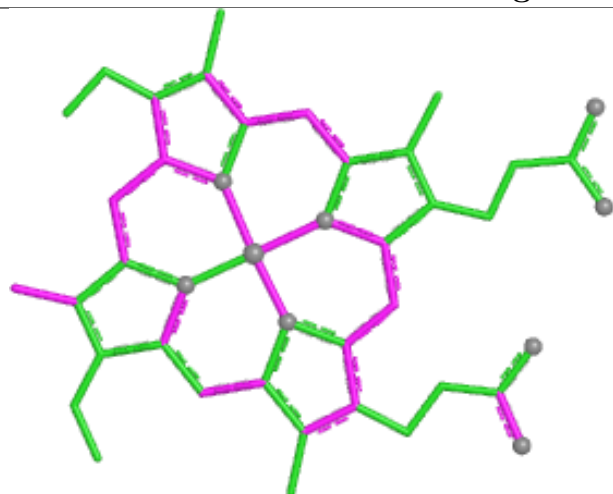


Torsions

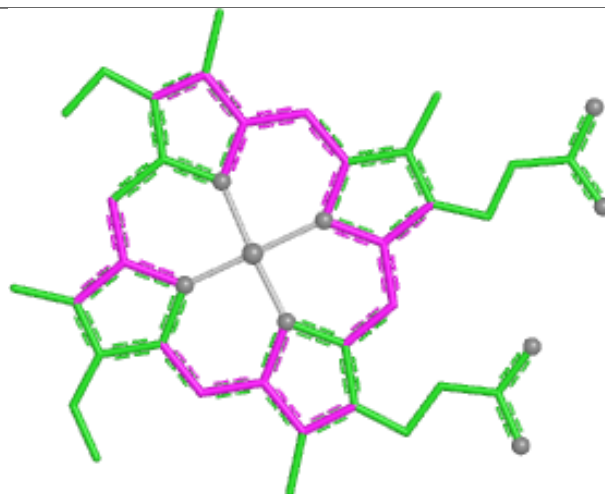


Rings

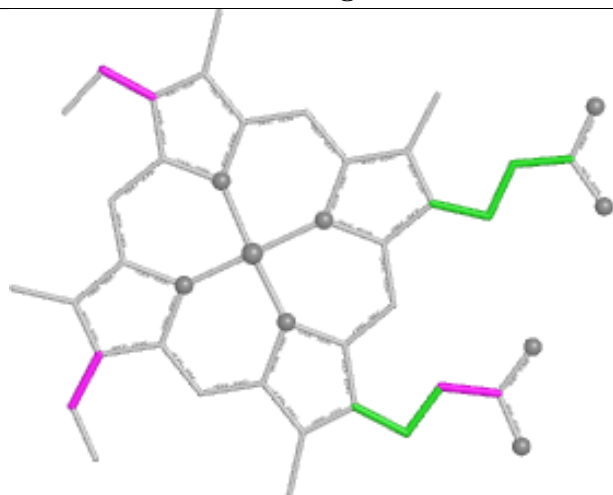
Ligand HEC B 607



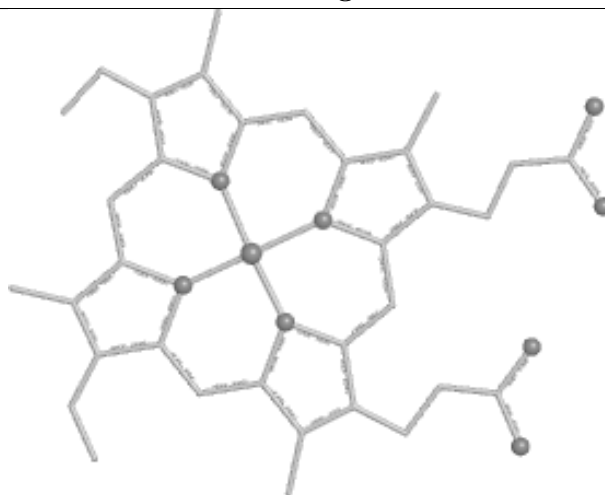
Bond lengths



Bond angles

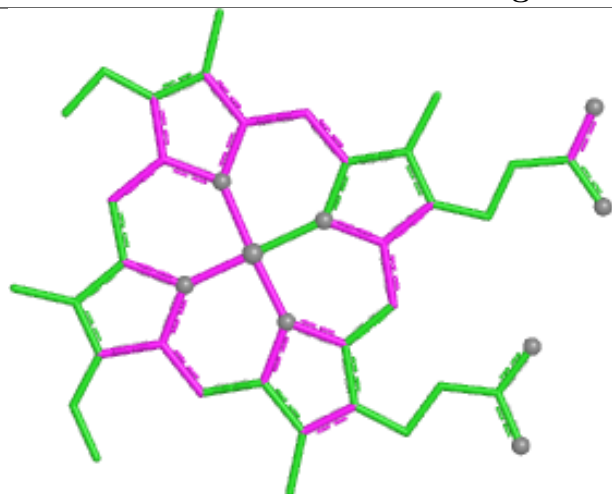


Torsions

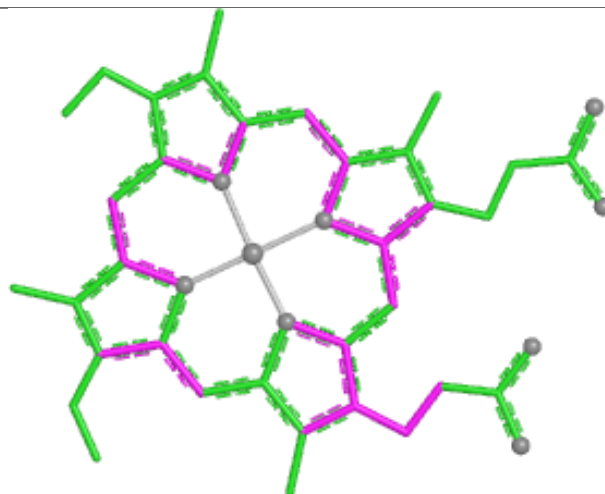


Rings

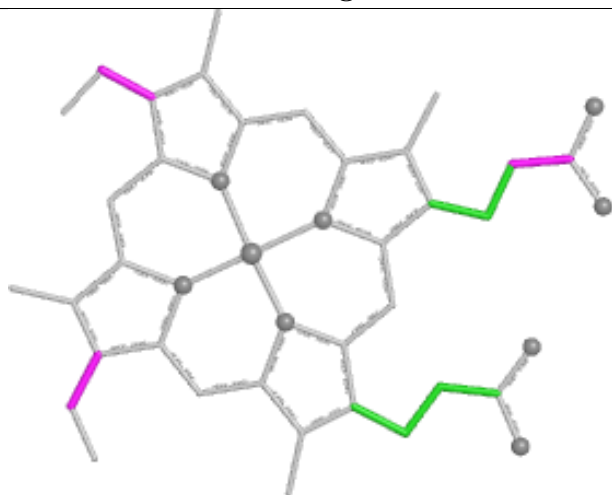
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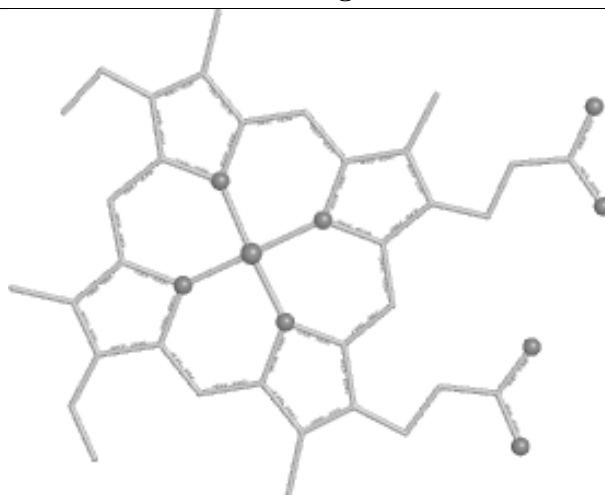
Bond lengths



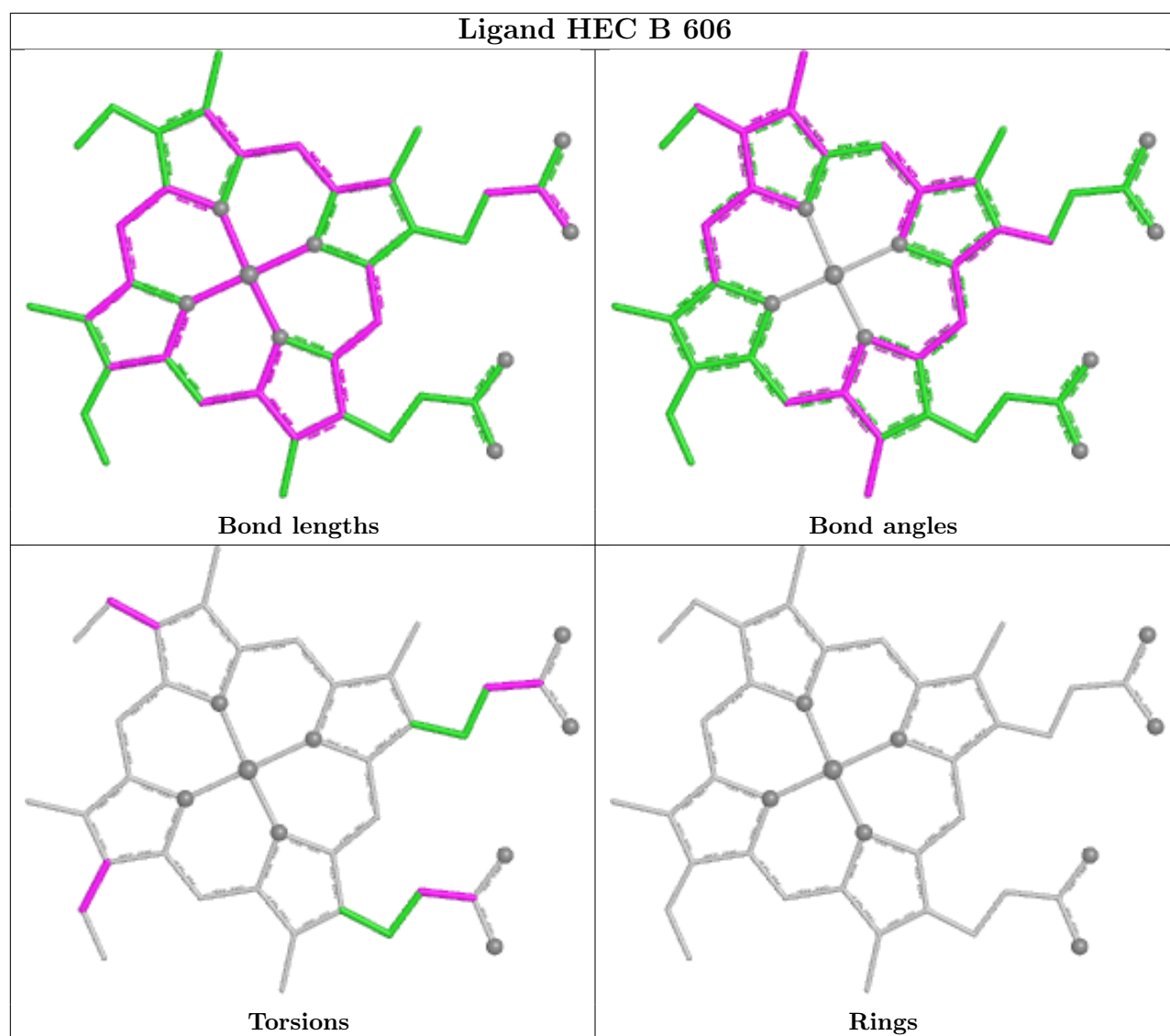
Bond angles



Torsions



Rings



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2		OWAB(Å ²)	Q < 0.9
1	A	502/546 (91%)	-0.36	2 (0%)	88 90	16, 33, 52, 88	1 (0%)
1	B	502/546 (91%)	-0.34	1 (0%)	91 92	18, 34, 53, 80	0
1	C	502/546 (91%)	-0.30	1 (0%)	91 92	18, 35, 55, 82	0
2	D	49/69 (71%)	0.90	5 (10%)	12 12	39, 58, 89, 96	0
2	E	49/69 (71%)	1.12	9 (18%)	3 3	36, 64, 94, 101	0
2	F	49/69 (71%)	0.42	4 (8%)	17 18	35, 48, 72, 84	0
All	All	1653/1845 (89%)	-0.23	22 (1%)	75 77	16, 35, 63, 101	1 (0%)

All (22) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	501	LEU	4.3
2	E	54	VAL	4.1
2	E	50	ILE	3.3
2	D	54	VAL	3.2
2	F	53	LEU	3.1
1	B	501	LEU	3.0
2	D	51	VAL	3.0
2	E	52	ALA	2.9
2	F	24	ASP	2.8
2	D	53	LEU	2.7
2	E	8	LEU	2.7
2	E	51	VAL	2.6
2	E	53	LEU	2.6
2	E	11	ILE	2.6
1	A	502	GLU	2.4
2	F	54	VAL	2.4
2	E	27	PRO	2.4
2	D	50	ILE	2.3
1	C	501	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
2	E	55	GLN	2.2
2	F	55	GLN	2.2
2	D	28	THR	2.1

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
10	NO3	F	101	4/4	0.78	0.13	70,71,71,71	0
10	NO3	B	618	4/4	0.81	0.16	67,68,68,69	0
7	EDO	B	616	4/4	0.83	0.16	60,61,62,63	0
5	PEG	A	614	7/7	0.83	0.19	54,61,63,64	0
7	EDO	A	617	4/4	0.83	0.17	63,63,63,65	0
6	PGE	A	615	10/10	0.84	0.14	52,55,62,62	0
7	EDO	A	616	4/4	0.84	0.15	44,46,46,50	0
10	NO3	C	619	4/4	0.84	0.10	72,72,72,72	0
5	PEG	B	612	7/7	0.84	0.18	63,68,69,71	0
7	EDO	C	618	4/4	0.86	0.14	51,52,53,55	0
8	P6G	B	613	19/19	0.87	0.14	54,60,64,65	0
5	PEG	C	611	7/7	0.87	0.14	54,60,63,64	0
7	EDO	B	620	4/4	0.89	0.14	46,51,52,55	0
7	EDO	B	621	4/4	0.89	0.14	51,52,52,53	0
5	PEG	B	610	7/7	0.89	0.13	58,59,63,66	0
5	PEG	A	613	7/7	0.89	0.13	56,57,58,60	0
5	PEG	A	611	7/7	0.89	0.14	53,55,57,59	0
7	EDO	B	615	4/4	0.89	0.13	50,51,51,55	0
5	PEG	C	622	7/7	0.89	0.12	43,48,50,51	0
5	PEG	F	102	7/7	0.90	0.11	50,51,54,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
9	PG4	B	614	13/13	0.90	0.13	43,50,64,65	0
5	PEG	B	611	7/7	0.90	0.12	60,61,61,62	0
7	EDO	C	616	4/4	0.90	0.11	40,45,46,50	0
5	PEG	C	610	7/7	0.90	0.14	54,58,61,63	0
5	PEG	A	609	7/7	0.91	0.10	44,45,51,51	0
6	PGE	C	614	10/10	0.91	0.11	49,52,54,57	0
5	PEG	C	613	7/7	0.91	0.11	50,55,60,61	0
5	PEG	A	610	7/7	0.92	0.11	56,57,64,67	0
7	EDO	C	615	4/4	0.92	0.15	50,51,52,55	0
10	NO3	B	617	4/4	0.92	0.09	51,53,54,56	0
7	EDO	A	619	4/4	0.93	0.09	44,45,48,49	0
5	PEG	C	612	7/7	0.93	0.09	54,56,58,60	0
7	EDO	C	620	4/4	0.93	0.10	48,48,49,51	0
7	EDO	C	621	4/4	0.93	0.08	41,42,44,45	0
5	PEG	A	612	7/7	0.93	0.10	56,58,61,64	0
5	PEG	B	609	7/7	0.94	0.09	46,48,52,52	0
7	EDO	B	619	4/4	0.94	0.08	45,47,49,50	0
7	EDO	C	617	4/4	0.94	0.08	42,45,46,49	0
5	PEG	C	609	7/7	0.95	0.09	55,59,59,61	0
7	EDO	A	618	4/4	0.95	0.08	42,46,46,52	0
4	ISW	B	608	43/43	0.96	0.08	22,34,51,56	0
4	ISW	C	601	43/43	0.96	0.09	20,32,47,50	0
4	ISW	A	608	43/43	0.96	0.08	21,32,46,47	0
3	HEC	A	607	43/43	0.98	0.05	20,24,30,32	0
3	HEC	B	601	43/43	0.98	0.07	26,34,43,48	0
3	HEC	B	602	43/43	0.98	0.05	21,26,31,33	0
3	HEC	B	603	43/43	0.98	0.06	23,29,33,35	0
3	HEC	C	602	43/43	0.98	0.06	25,34,39,43	0
3	HEC	C	603	43/43	0.98	0.06	18,25,28,31	0
3	HEC	C	604	43/43	0.98	0.05	20,25,29,31	0
3	HEC	A	601	43/43	0.98	0.06	21,29,33,44	0
3	HEC	A	602	43/43	0.98	0.06	20,24,29,34	0
3	HEC	A	603	43/43	0.98	0.06	20,28,32,34	0
3	HEC	C	608	43/43	0.99	0.05	16,21,32,33	0
3	HEC	B	604	43/43	0.99	0.05	15,24,28,33	0
3	HEC	B	605	43/43	0.99	0.06	17,24,30,36	0
3	HEC	B	606	43/43	0.99	0.05	15,21,25,26	0
3	HEC	B	607	43/43	0.99	0.05	15,21,31,36	0
3	HEC	A	605	43/43	0.99	0.05	17,23,37,39	0
3	HEC	A	606	43/43	0.99	0.05	17,23,29,30	0
3	HEC	A	604	43/43	0.99	0.05	20,25,31,36	0
3	HEC	C	605	43/43	0.99	0.05	17,25,30,32	0

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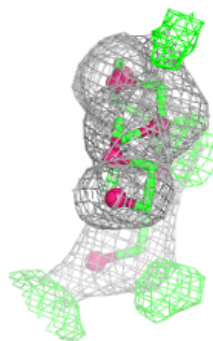
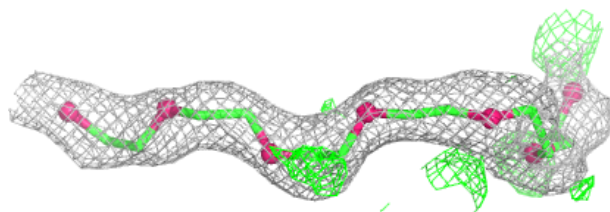
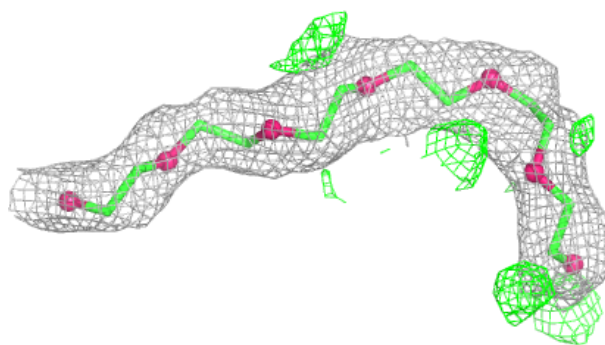
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	HEC	C	606	43/43	0.99	0.05	17,22,33,44	0
3	HEC	C	607	43/43	0.99	0.05	16,22,28,32	0

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.

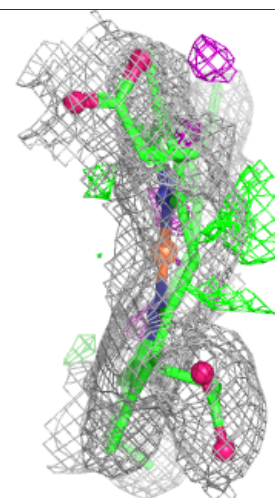
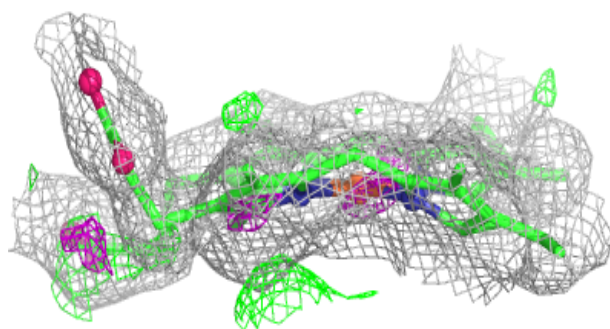
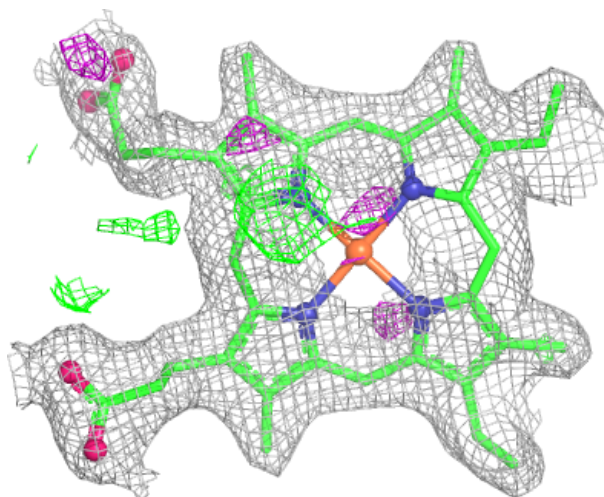
Electron density around P6G B 613:

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



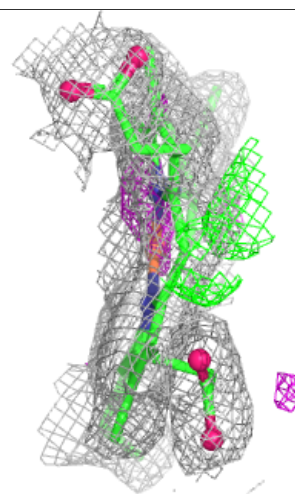
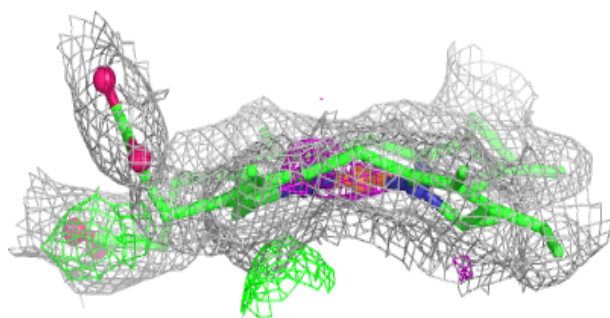
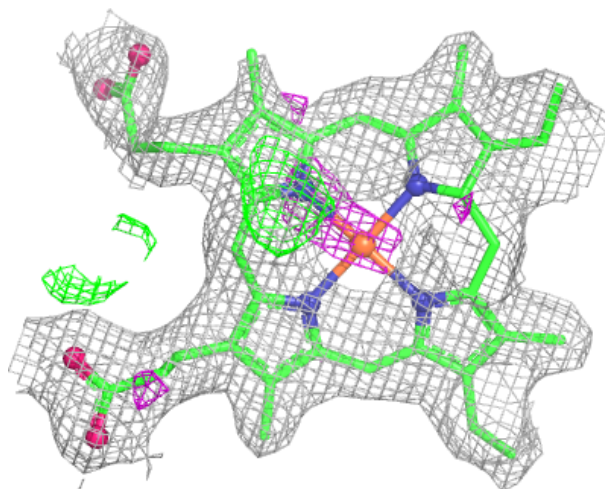
Electron density around ISW B 608:

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



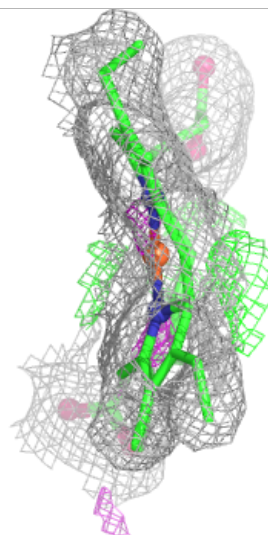
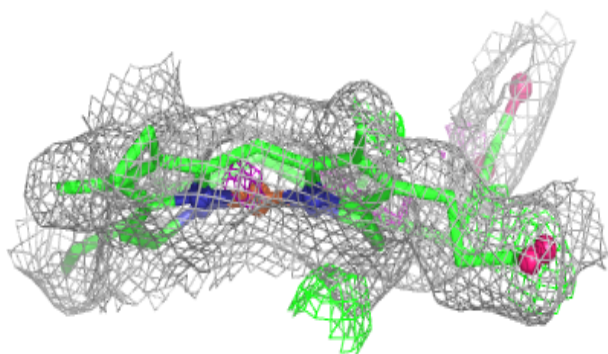
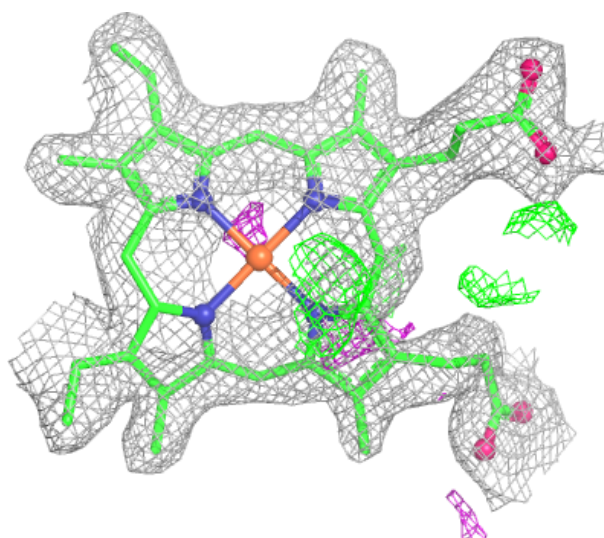
Electron density around ISW C 601:

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and green (positive)



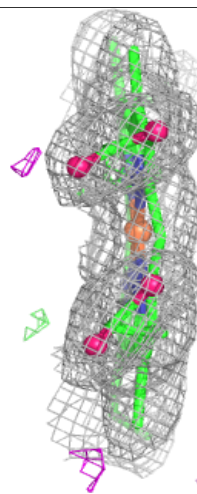
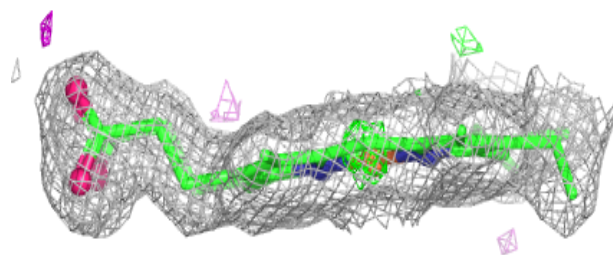
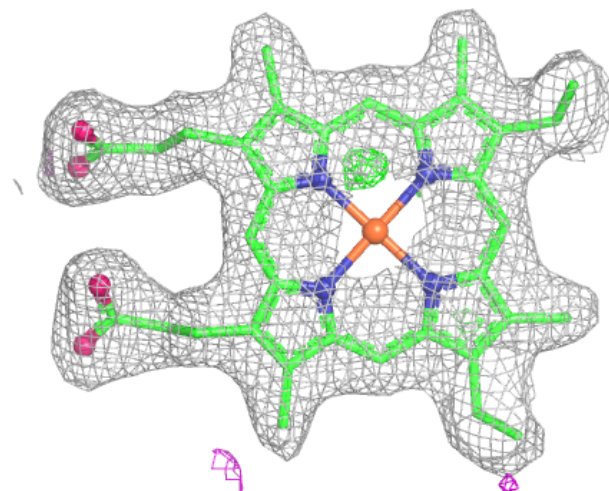
Electron density around ISW A 608:

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and green (positive)



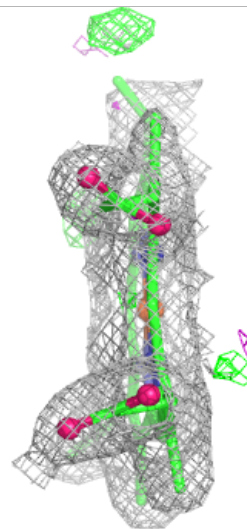
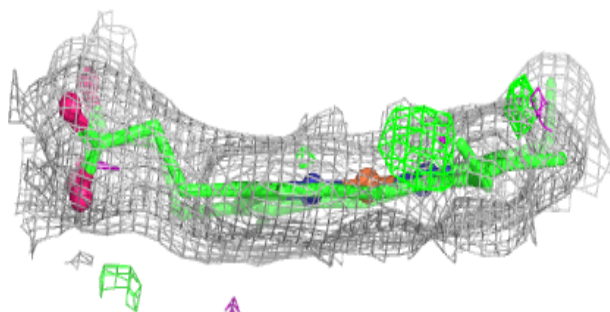
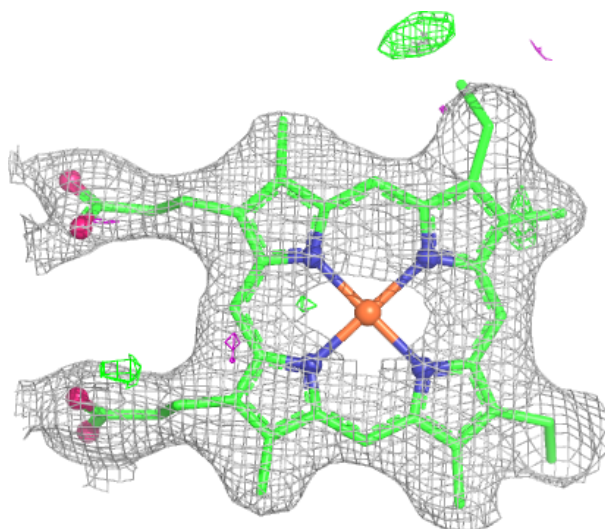
Electron density around HEC A 607:

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and green (positive)



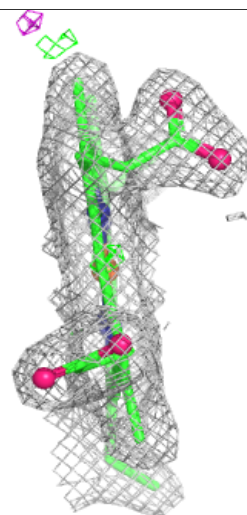
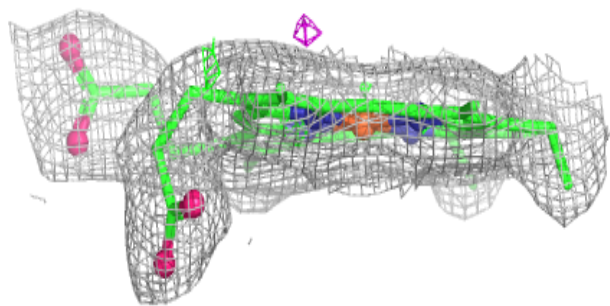
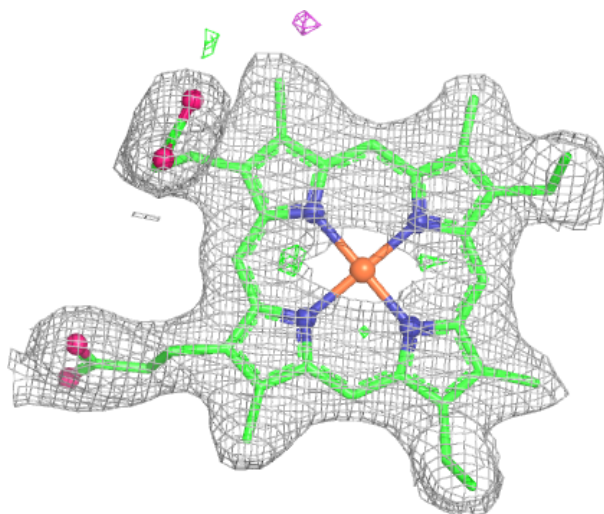
Electron density around HEC B 601:

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and green (positive)



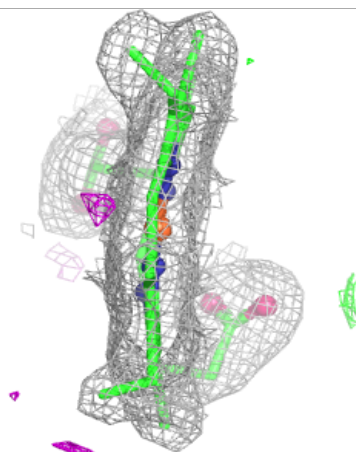
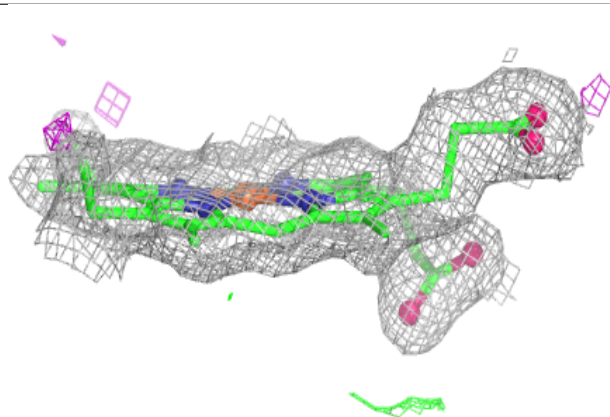
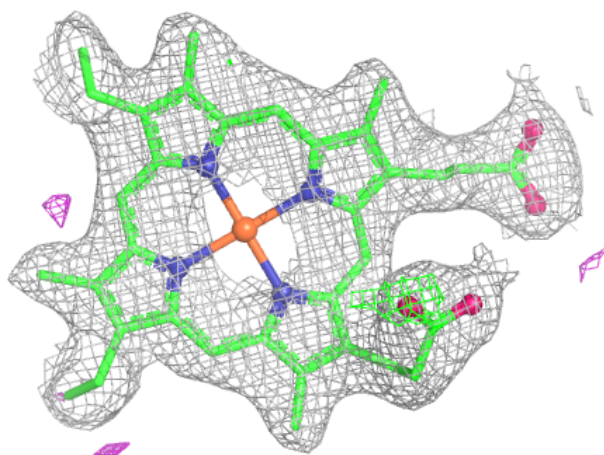
Electron density around HEC B 602:

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and green (positive)



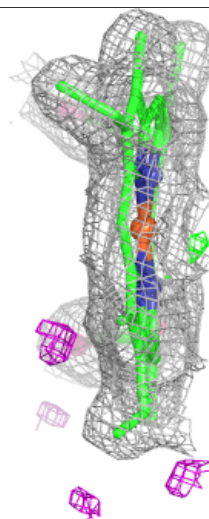
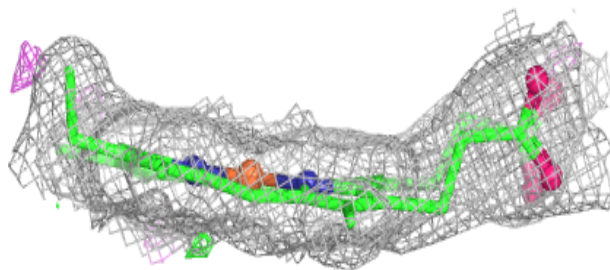
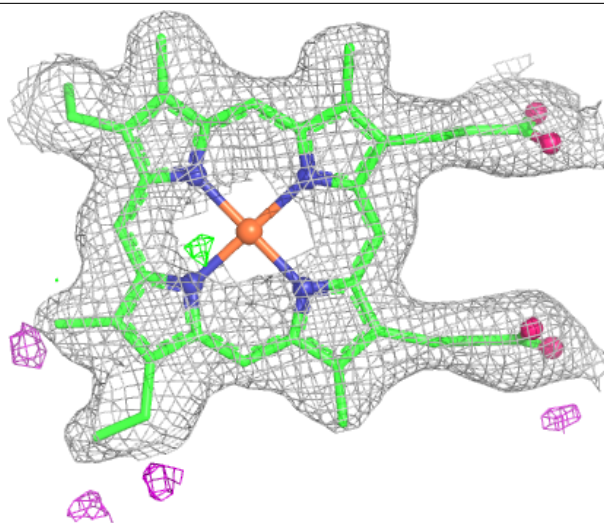
Electron density around HEC B 603:

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and green (positive)



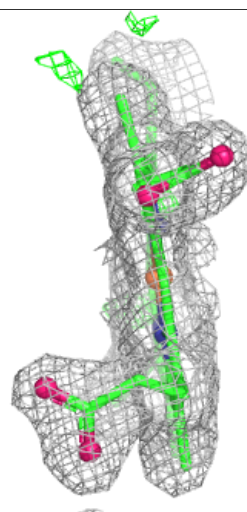
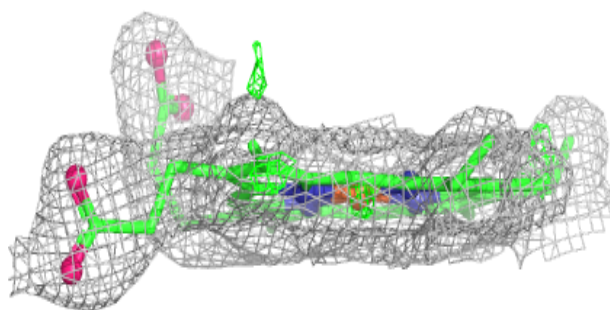
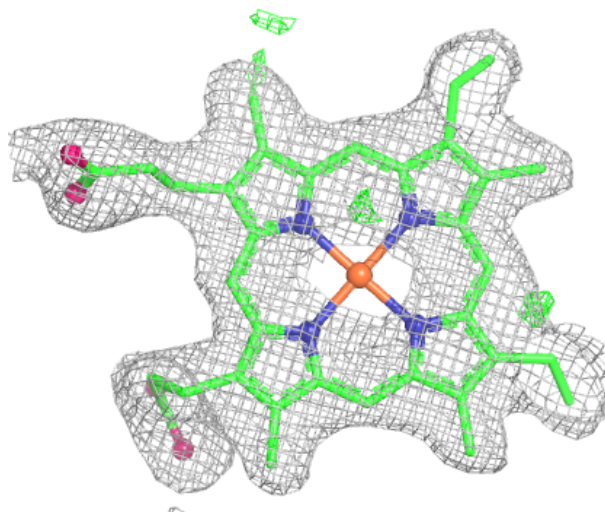
Electron density around HEC C 602:

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and green (positive)



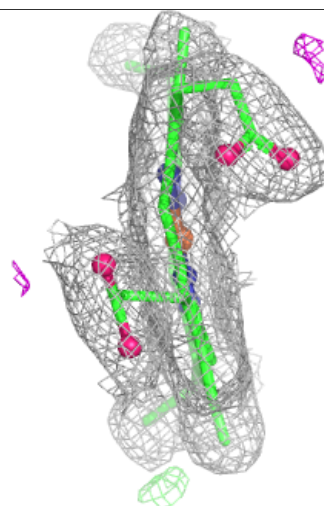
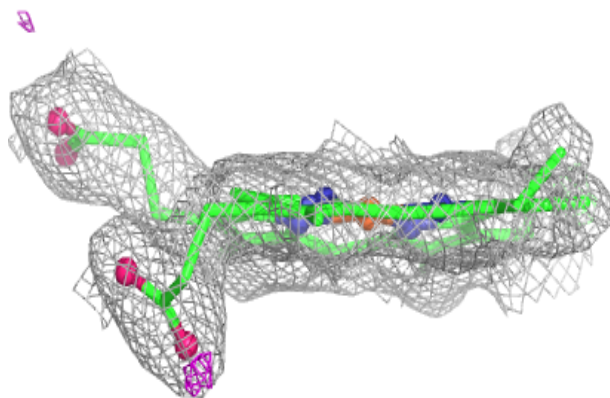
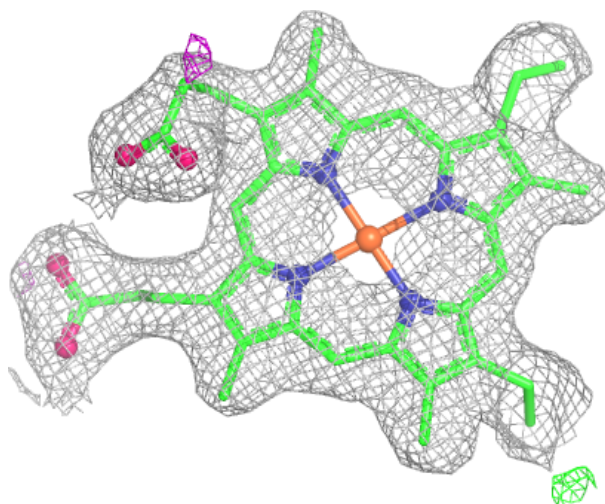
Electron density around HEC C 603:

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and green (positive)



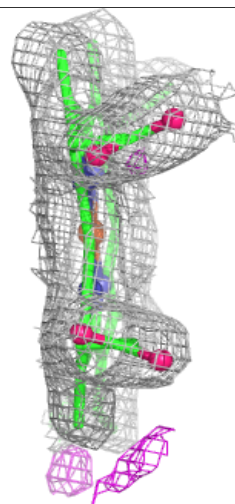
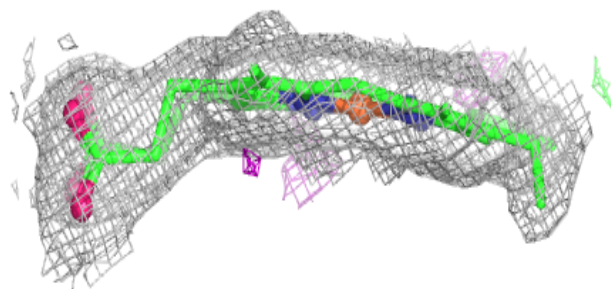
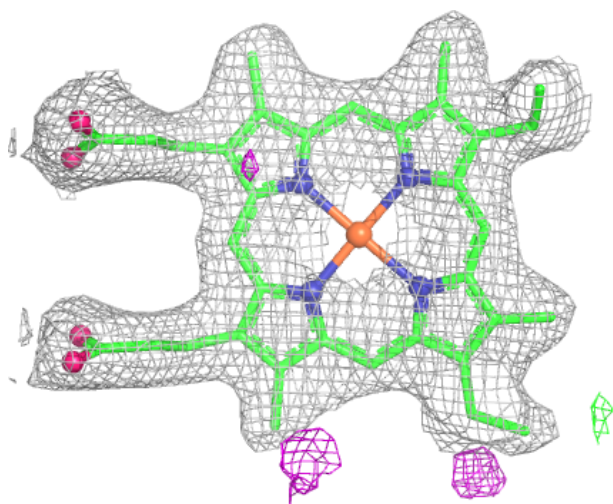
Electron density around HEC C 604:

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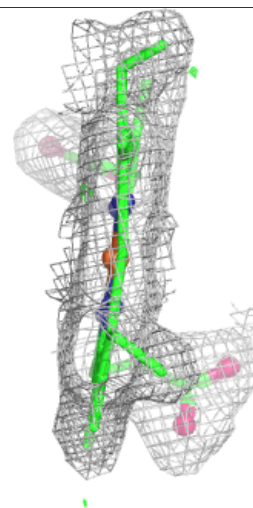
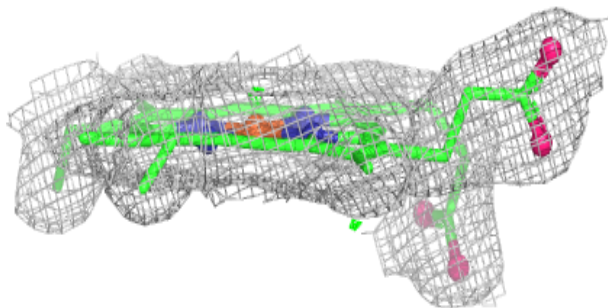
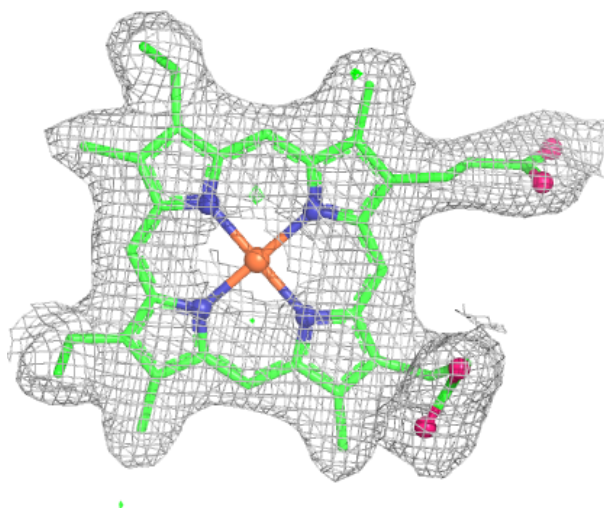
Electron density around HEC A 601:

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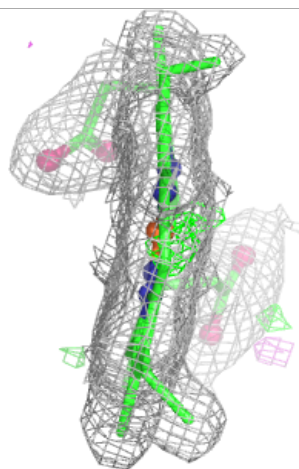
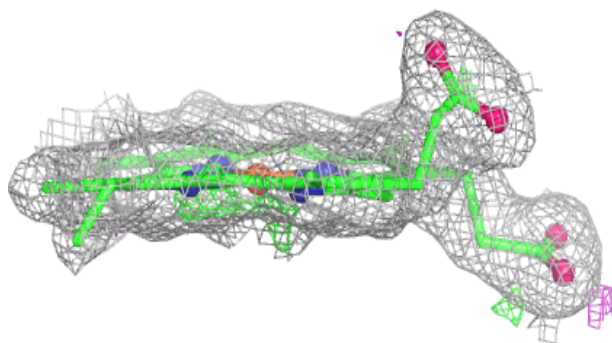
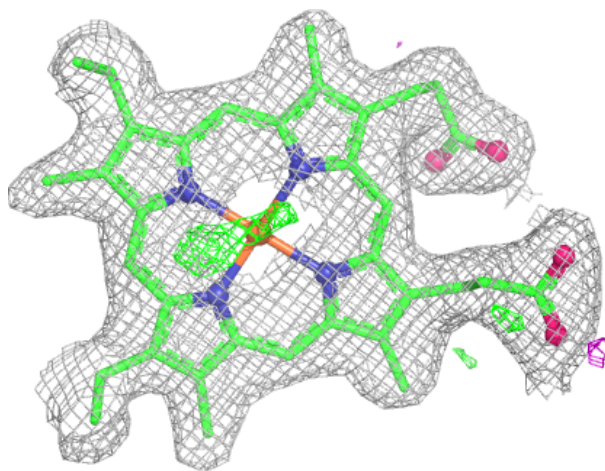
Electron density around HEC A 602:

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and green (positive)



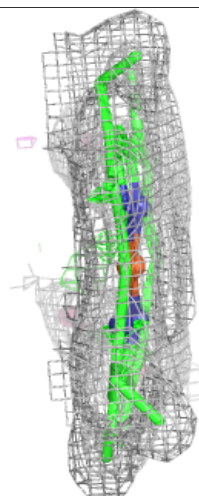
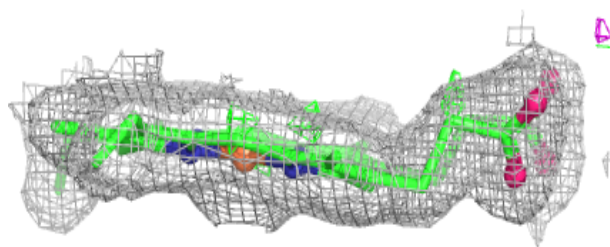
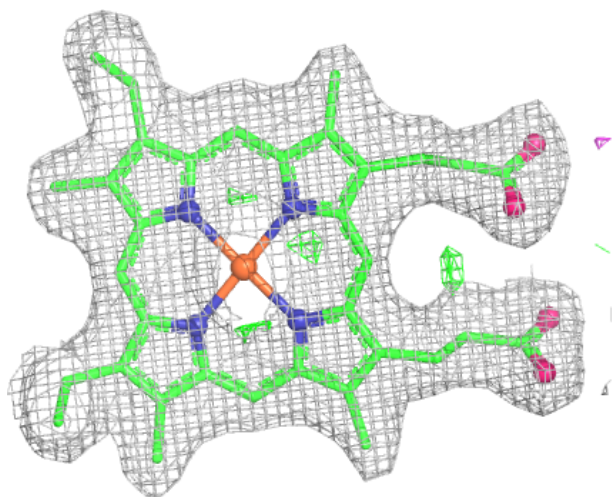
Electron density around HEC A 603:

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and green (positive)



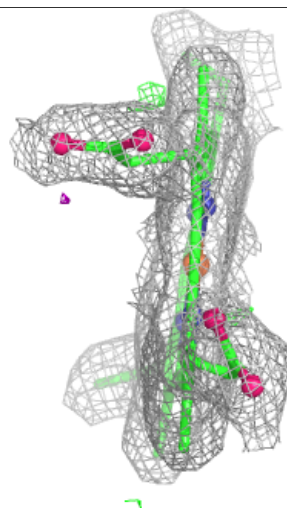
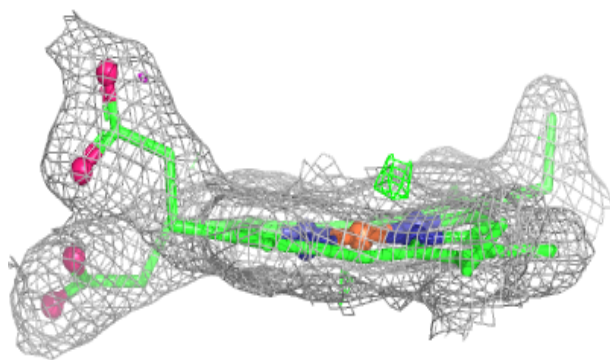
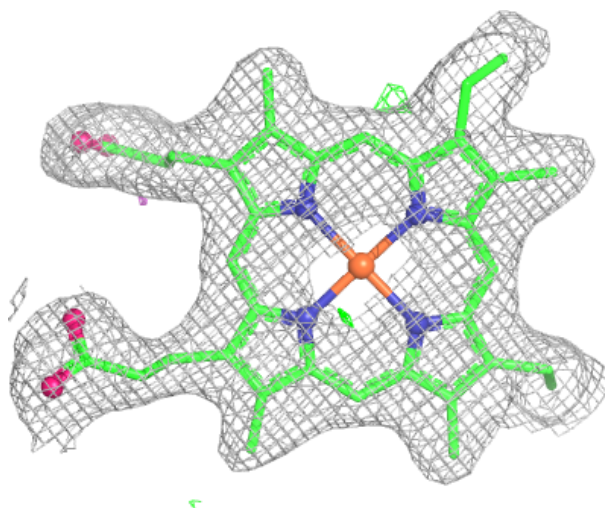
Electron density around HEC C 608:

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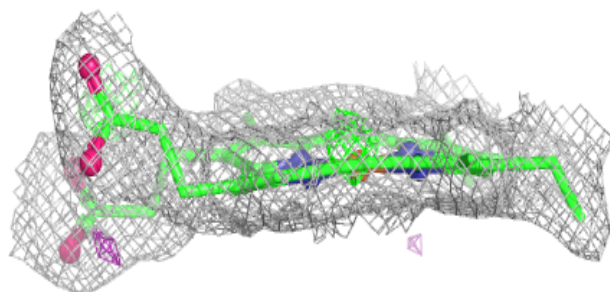
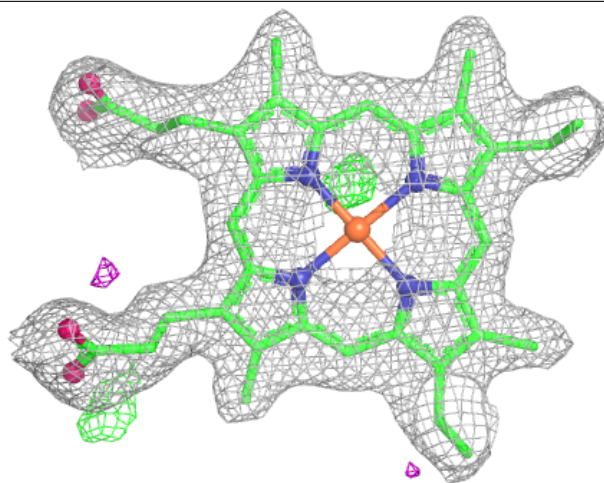
Electron density around HEC B 604:

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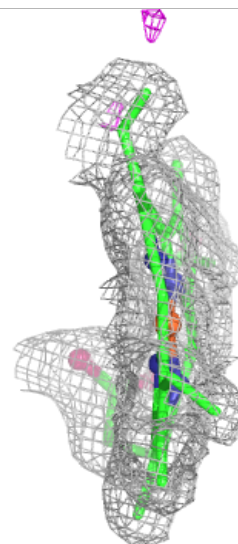
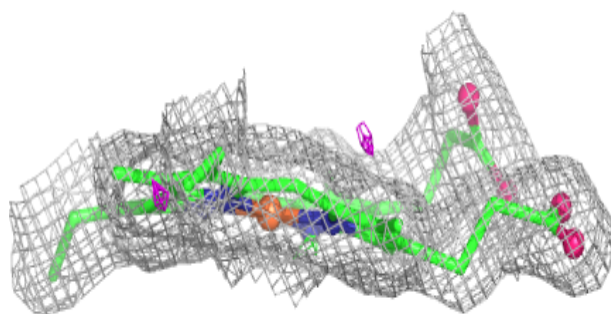
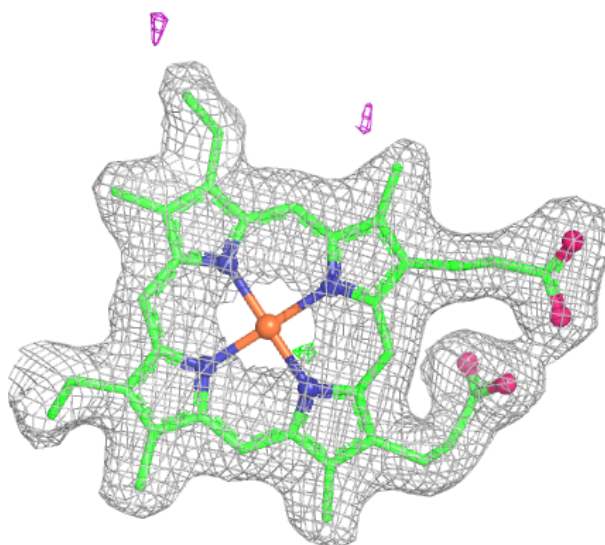
Electron density around HEC B 605:

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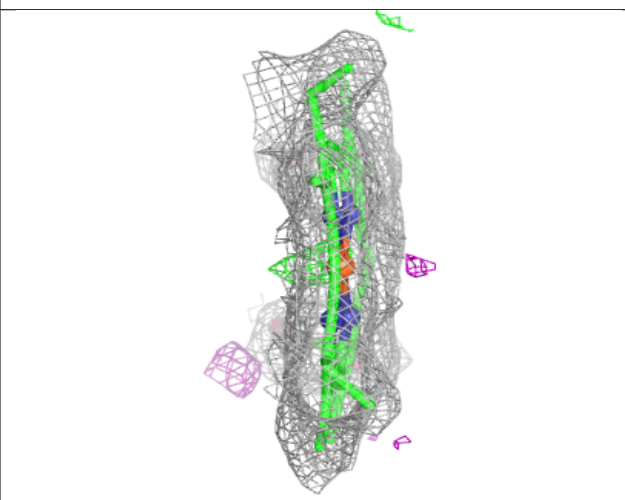
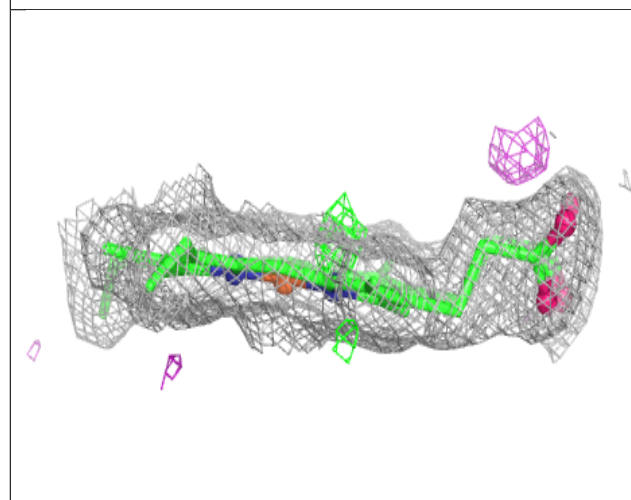
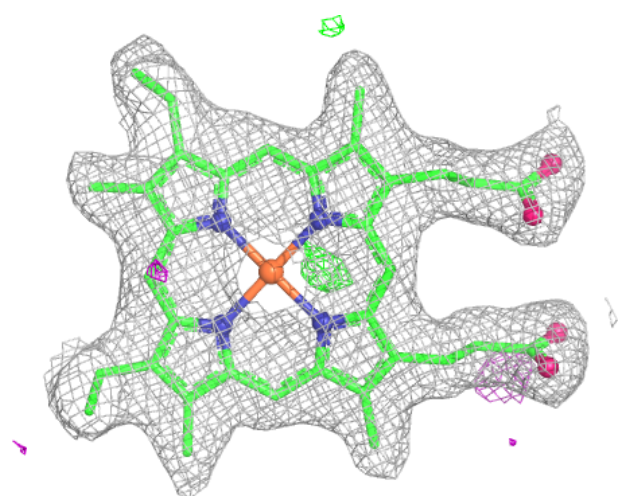
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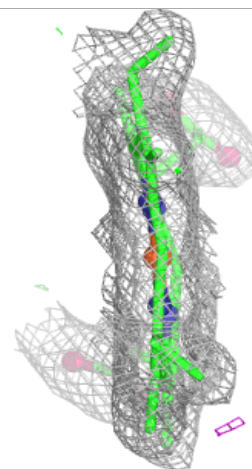
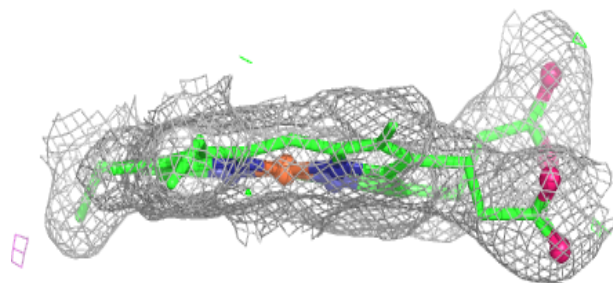
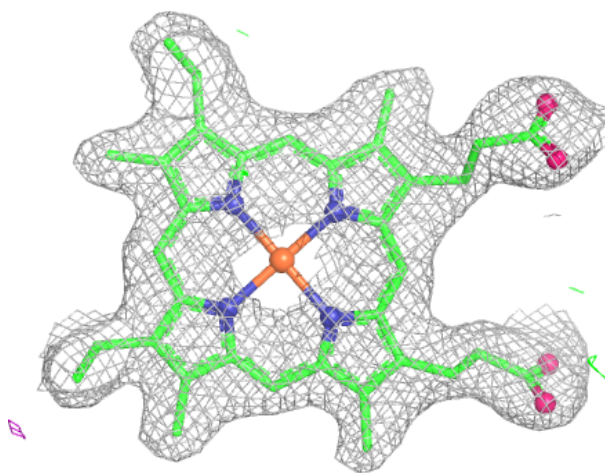
Electron density around HEC B 607:

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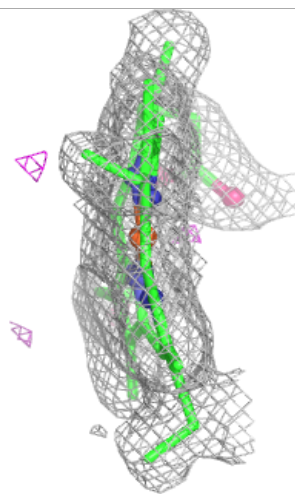
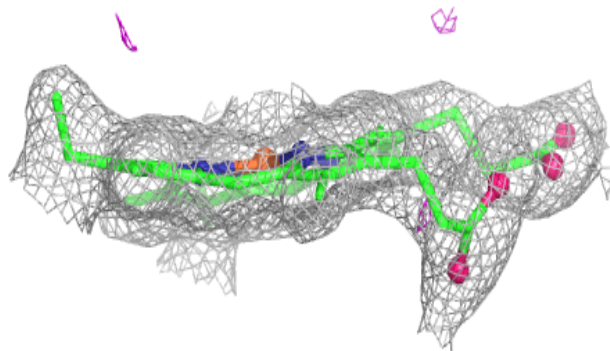
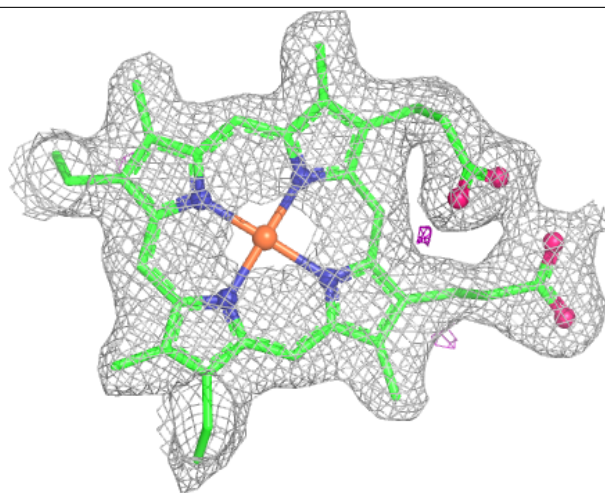
Electron density around HEC A 605:

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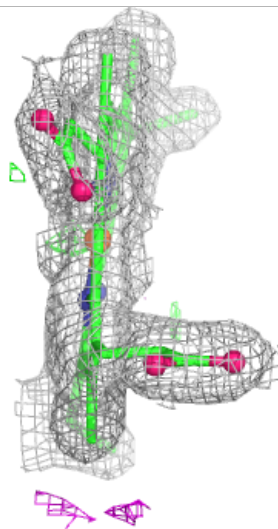
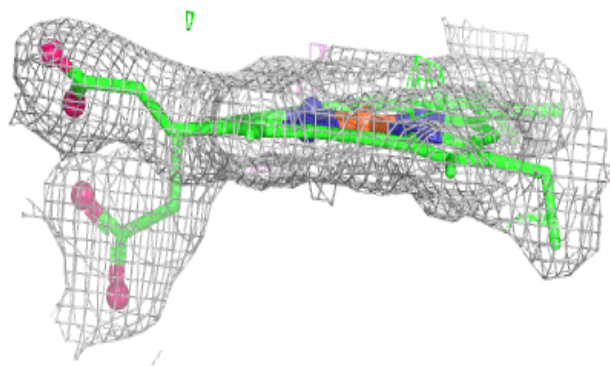
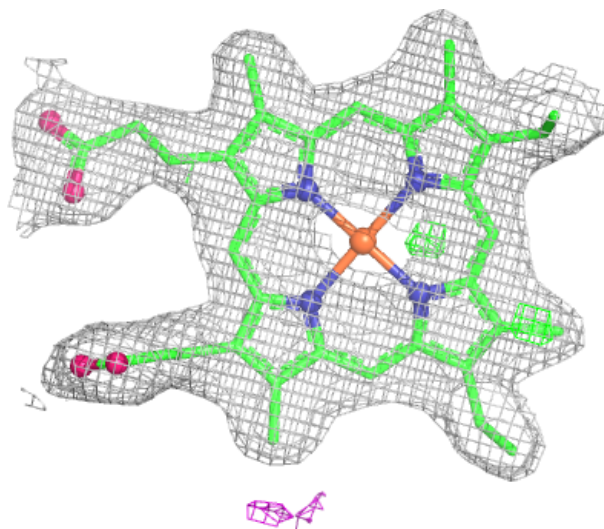
Electron density around HEC A 606:

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and green (positive)



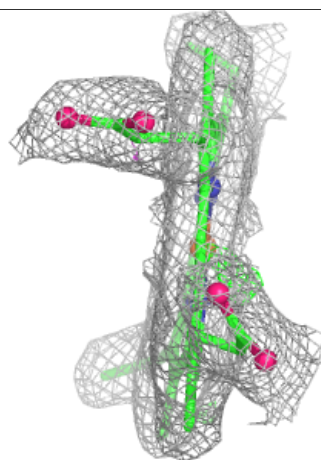
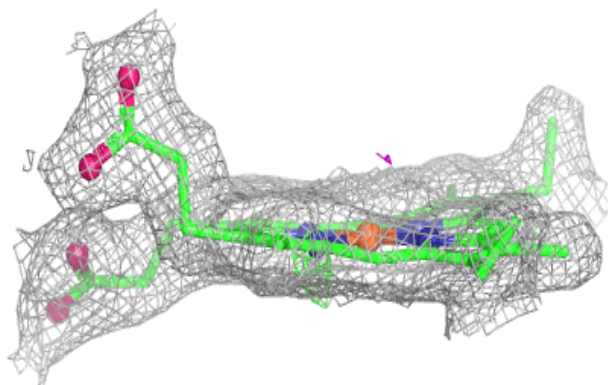
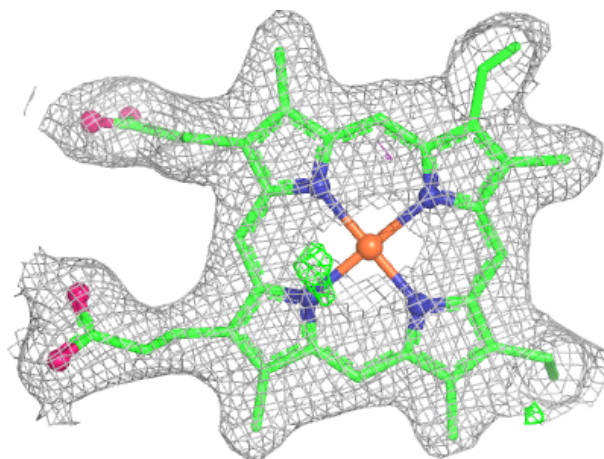
Electron density around HEC A 604:

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



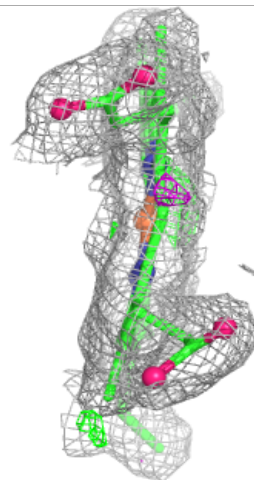
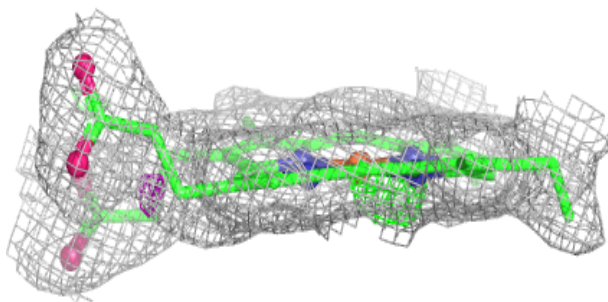
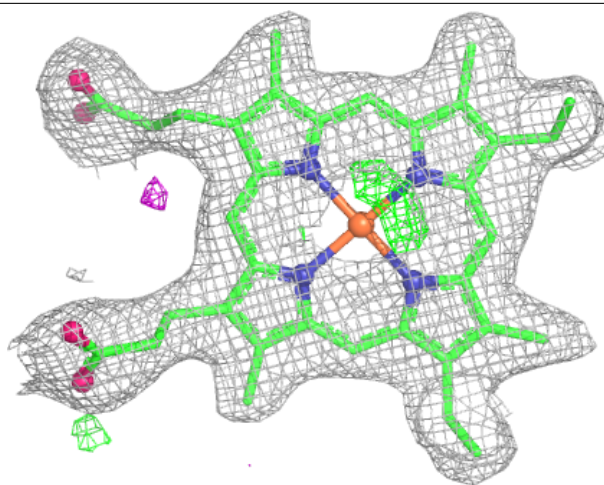
Electron density around HEC C 605:

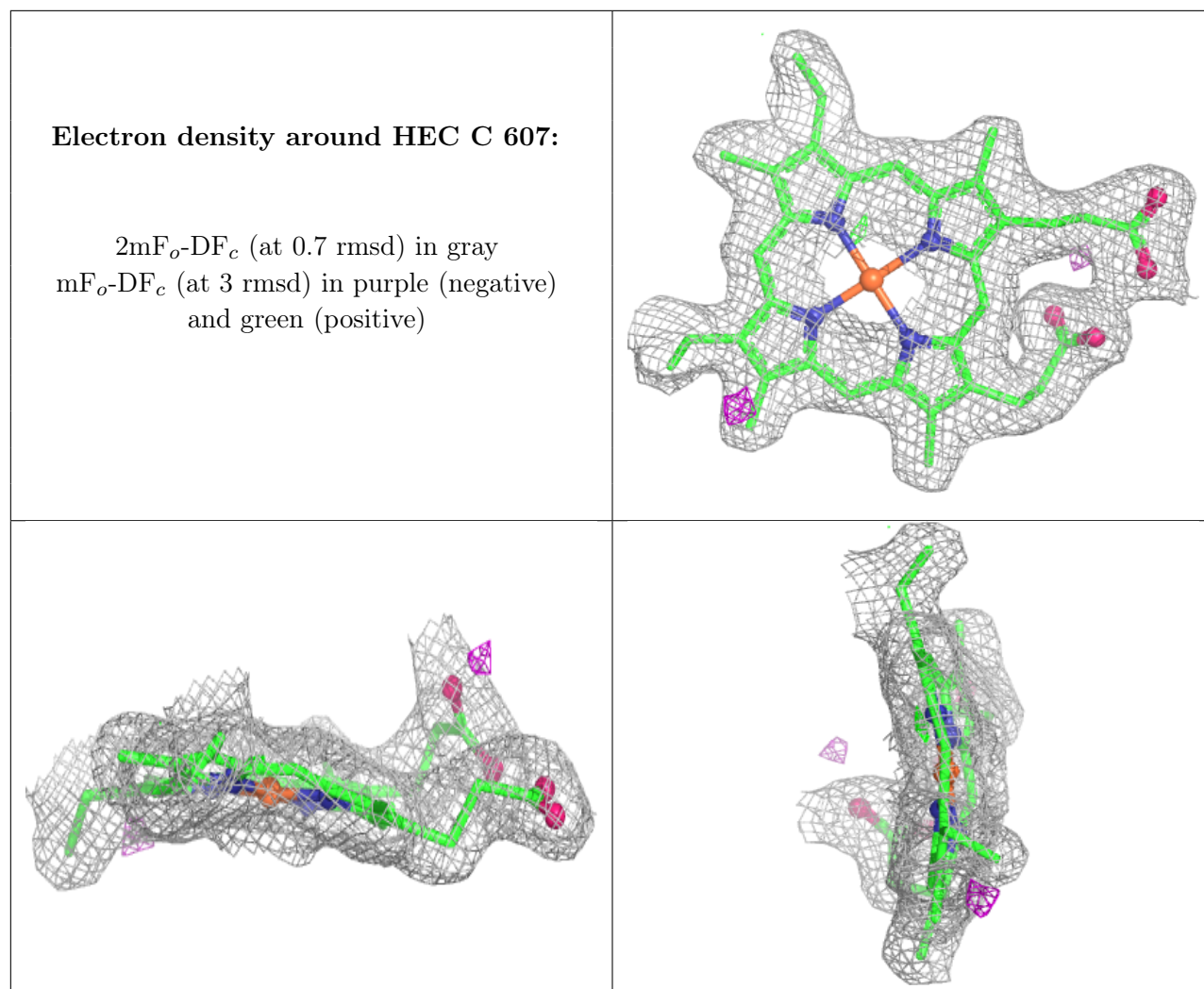
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around HEC C 606:

$2mF_o-DF_c$ (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.