Full wwPDB X-ray Structure Validation Report (i)

Nov 6, 2023 – 02:50 pm GMT

PDB ID	:	5C2V
Title	:	Kuenenia stuttgartiensis Hydrazine Synthase
Authors	:	Dietl, A.; Ferousi, C.; Maalcke, W.J.; Menzel, A.; de Vries, S.; Keltjens, J.T.; Jetten, M.S.M.; Kartal, B.; Barends, T.R.M.
Deposited on	:	2015-06-16
Resolution	:	2.70 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 (i) 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 (i)) were used in the production of this report:

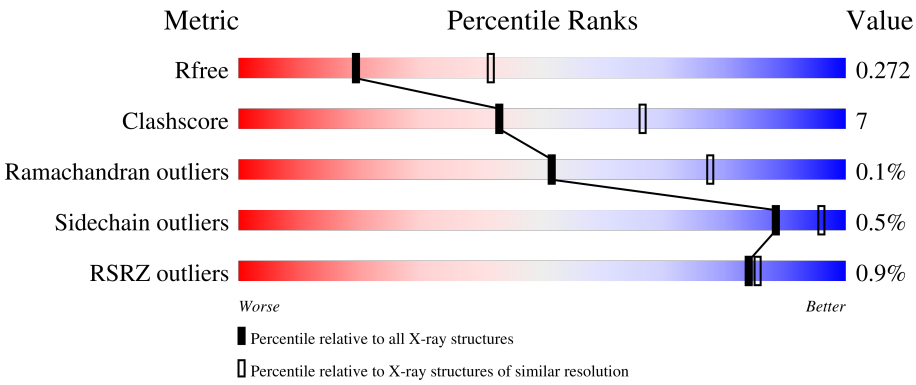
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.70 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}	130704	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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 <=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	782	85% 13% •
1	D	782	% 85% 14% •
2	B	352	79% 21%
2	E	352	% 78% 22%
3	C	314	2% 84% 15% •

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Mol	Chain	Length	Quality of chain
3	F	314	3% 78% 21%

2 Entry composition (i)

There are 10 unique types of molecules in this entry. The entry contains 23385 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 HYDRAZINE SYNTHASE ALPHA SUBUNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	768	6081	3867	1045	1144	25	0	0	0
1	D	770	6087	3871	1044	1147	25	0	0	0

- Molecule 2 is a protein called HYDRAZINE SYNTHASE BETA SUBUNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	352	2706	1697	464	531	14	0	1	0
2	E	352	2692	1688	459	531	14	0	1	0

- Molecule 3 is a protein called HYDRAZINE SYNTHASE GAMMA SUBUNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	314	2457	1543	432	472	10	0	0	0
3	F	314	2443	1534	427	472	10	0	0	0

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Cl		
4	A	1	2	2	0	1
4	D	1	1	1	0	0

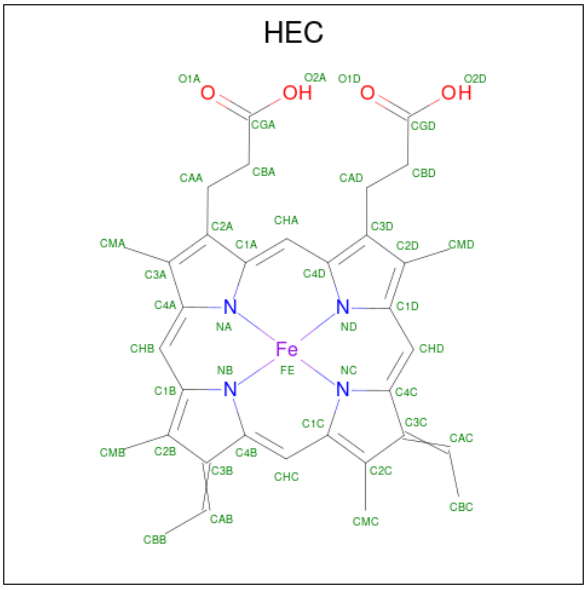
- Molecule 5 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Ca		
5	A	2	2	2	0	0
5	B	1	1	1	0	0
5	C	3	3	3	0	0
5	D	2	2	2	0	0
5	E	1	1	1	0	0
5	F	3	3	3	0	0

- Molecule 6 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Zn		
6	A	1	1	1	0	0
6	D	1	1	1	0	0

- Molecule 7 is HEME C (three-letter code: HEC) (formula: $C_{34}H_{34}FeN_4O_4$).



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

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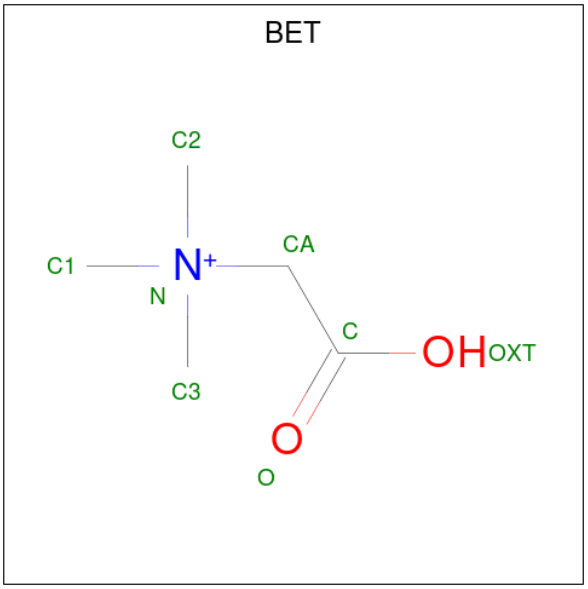
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Fe	N	O		
7	C	1	43	34	1	4	4	0	0
			Total	C	Fe	N	O		
7	C	1	43	34	1	4	4	0	0
			Total	C	Fe	N	O		
7	D	1	43	34	1	4	4	0	0
			Total	C	Fe	N	O		
7	D	1	43	34	1	4	4	0	0
			Total	C	Fe	N	O		
7	F	1	43	34	1	4	4	0	0
			Total	C	Fe	N	O		
7	F	1	43	34	1	4	4	0	0

- Molecule 8 is TRIMETHYL GLYCINE (three-letter code: BET) (formula: $C_5H_{12}NO_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
8	A	1	8	5	1	2	0	0
			Total	C	N	O		
8	A	1	8	5	1	2	0	0
			Total	C	N	O		
8	A	1	8	5	1	2	0	0
			Total	C	N	O		
8	B	1	8	5	1	2	0	0
			Total	C	N	O		
8	C	1	8	5	1	2	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
8	D	1	8	5	1	2	0	0
			Total	C	N	O		
8	E	1	8	5	1	2	0	0

- Molecule 9 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
9	B	1	1	1	0	0
			Total	Mg		
9	E	1	1	1	0	0

- Molecule 10 is water.

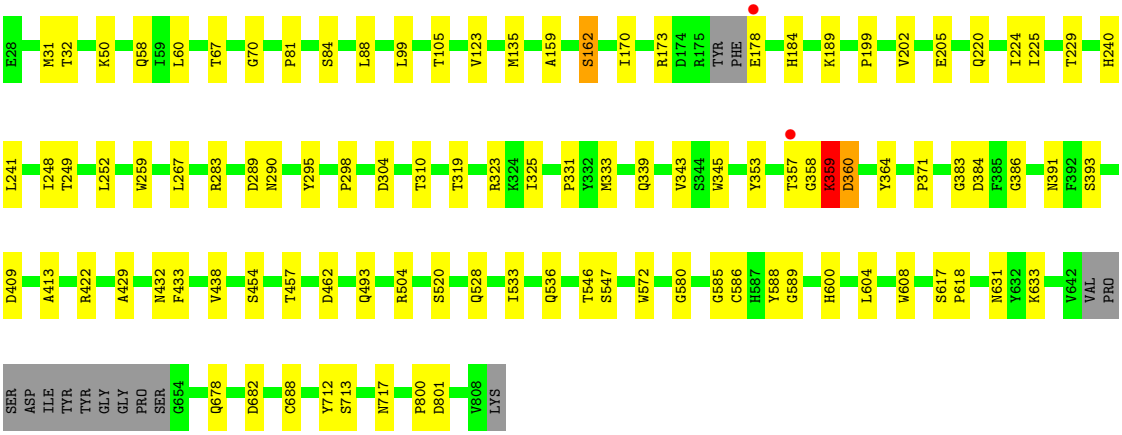
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
10	A	168	168	168	0	0
			Total	O		
10	B	60	60	60	0	0
			Total	O		
10	C	84	84	84	0	0
			Total	O		
10	D	112	112	112	0	0
			Total	O		
10	E	30	30	30	0	0
			Total	O		
10	F	46	46	46	0	0

3 Residue-property plots (i)

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.

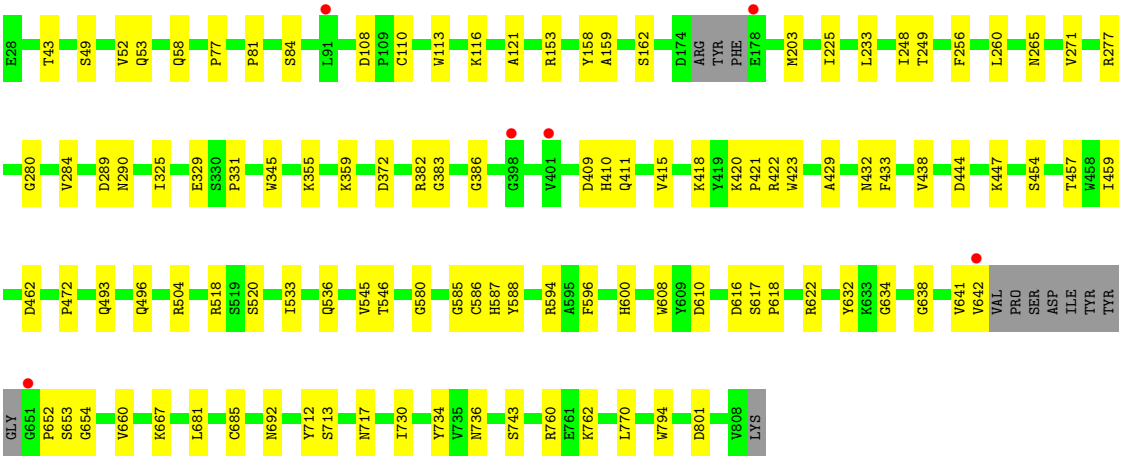
• Molecule 1: HYDRAZINE SYNTHASE ALPHA SUBUNIT

Chain A:



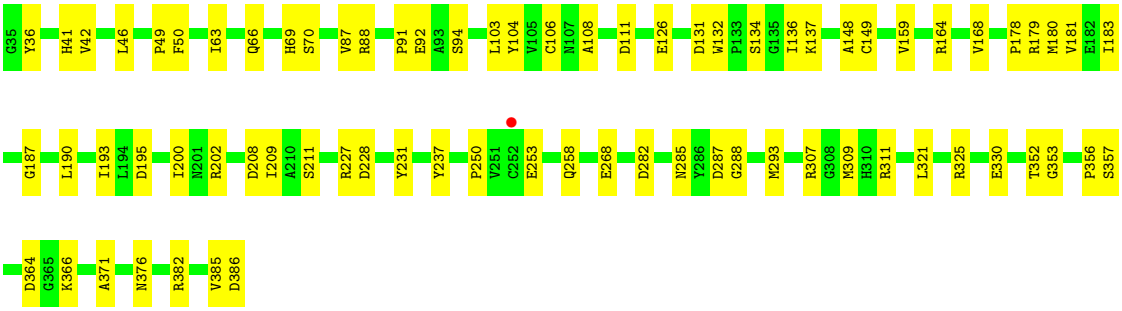
• Molecule 1: HYDRAZINE SYNTHASE ALPHA SUBUNIT

Chain D:



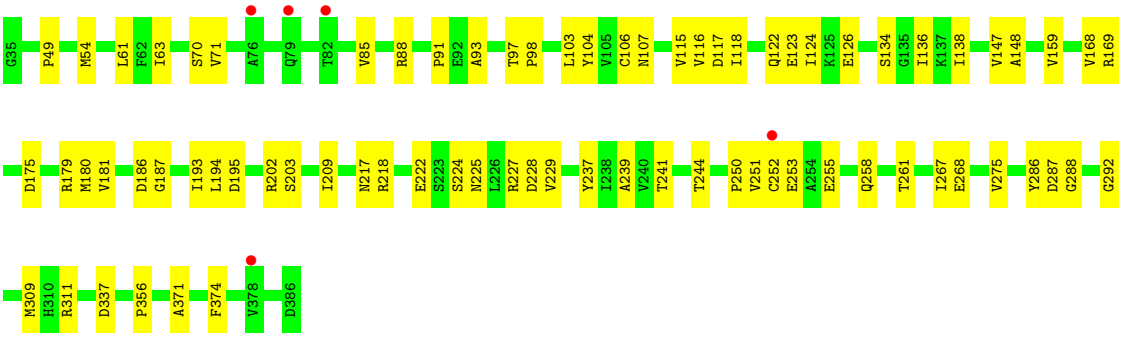
• Molecule 2: HYDRAZINE SYNTHASE BETA SUBUNIT

Chain B:



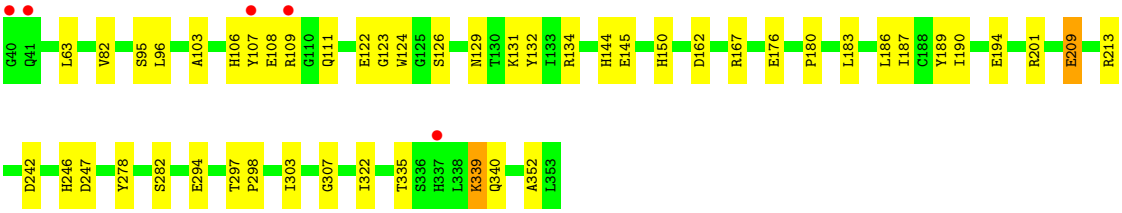
- Molecule 2: HYDRAZINE SYNTHASE BETA SUBUNIT

Chain E:



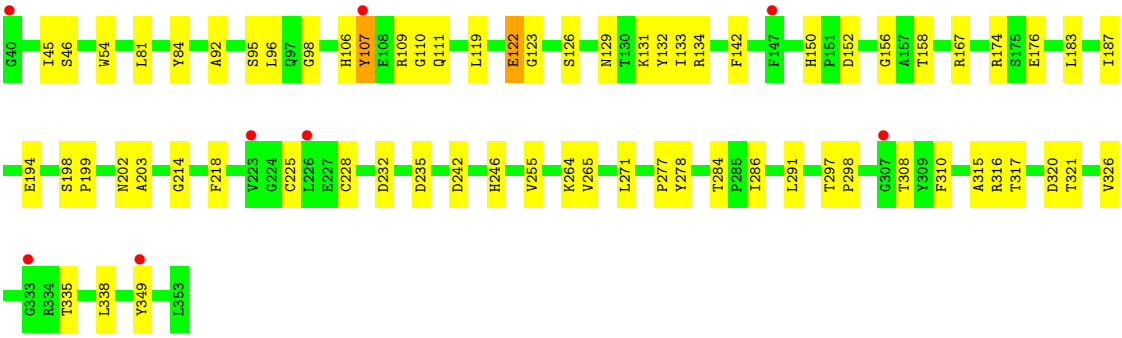
- Molecule 3: HYDRAZINE SYNTHASE GAMMA SUBUNIT

Chain C:



- Molecule 3: HYDRAZINE SYNTHASE GAMMA SUBUNIT

Chain F:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, α, β, γ	464.54Å 464.54Å 145.75Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	40.00 – 2.70 48.98 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.8 (40.00-2.70) 99.8 (48.98-2.70)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.68 (at 2.69Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.234 , 0.271 0.237 , 0.272	Depositor DCC
R_{free} test set	8147 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	57.0	Xtriage
Anisotropy	0.402	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 49.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	23385	wwPDB-VP
Average B, all atoms (Å^2)	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.80% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: BET, CL, CA, HEC, ZN, MG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
1	A	0.23	0/6259	0.44	0/8503
1	D	0.22	0/6266	0.43	0/8514
2	B	0.24	0/2758	0.49	0/3752
2	E	0.23	0/2744	0.49	0/3737
3	C	0.26	0/2522	0.46	0/3421
3	F	0.24	0/2508	0.45	0/3406
All	All	0.23	0/23057	0.45	0/31333

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

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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	359	LYS	Peptide
1	A	360	ASP	Peptide
3	C	339	LYS	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	6081	0	5783	72	0
1	D	6087	0	5784	72	0
2	B	2706	0	2675	49	0
2	E	2692	0	2642	52	0
3	C	2457	0	2324	41	0
3	F	2443	0	2291	45	0
4	A	2	0	0	2	0
4	D	1	0	0	1	0
5	A	2	0	0	0	0
5	B	1	0	0	0	0
5	C	3	0	0	0	0
5	D	2	0	0	0	0
5	E	1	0	0	0	0
5	F	3	0	0	0	0
6	A	1	0	0	0	0
6	D	1	0	0	0	0
7	A	86	0	61	10	0
7	C	86	0	59	6	0
7	D	86	0	60	7	0
7	F	86	0	59	4	0
8	A	24	0	33	0	0
8	B	8	0	11	0	0
8	C	8	0	11	0	0
8	D	8	0	11	0	0
8	E	8	0	11	0	0
9	B	1	0	0	0	0
9	E	1	0	0	0	0
10	A	168	0	0	1	0
10	B	60	0	0	1	0
10	C	84	0	0	3	0
10	D	112	0	0	4	0
10	E	30	0	0	1	0
10	F	46	0	0	2	0
All	All	23385	0	21815	303	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 7.

All (303) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:688:CYS:SG	7:A:906:HEC:CAC	2.16	1.32
1:A:688:CYS:SG	7:A:906:HEC:HBC1	1.83	1.07
1:A:688:CYS:CB	7:A:906:HEC:HBC2	1.84	1.06
1:A:688:CYS:SG	7:A:906:HEC:HBC2	0.51	1.04
1:A:688:CYS:SG	7:A:906:HEC:CBC	1.04	1.03
3:C:339:LYS:HG3	3:C:340:GLN:H	1.34	0.93
1:A:688:CYS:HG	7:A:906:HEC:HBC3	1.18	0.91
1:A:688:CYS:SG	7:A:906:HEC:C3C	2.61	0.88
1:D:520:SER:O	1:D:712:TYR:OH	2.01	0.78
2:B:288:GLY:H	2:B:309:MET:HG2	1.49	0.76
3:F:122:GLU:OE2	3:F:126:SER:OG	2.03	0.76
3:F:123:GLY:O	3:F:126:SER:OG	2.03	0.75
1:D:429:ALA:HB3	1:D:433:PHE:HB3	1.67	0.75
2:E:288:GLY:H	2:E:309:MET:HG2	1.53	0.74
1:A:688:CYS:SG	7:A:906:HEC:HBC3	1.32	0.73
3:C:122:GLU:OE2	10:C:501:HOH:O	2.06	0.73
2:E:122:GLN:NE2	2:E:123:GLU:O	2.24	0.71
3:C:339:LYS:HG3	3:C:340:GLN:N	2.06	0.71
1:D:642:VAL:HG12	1:D:652:PRO:HG3	1.71	0.70
1:D:608:TRP:NE1	1:D:610:ASP:O	2.24	0.70
1:D:438:VAL:O	3:F:167:ARG:NH2	2.24	0.69
3:F:129:ASN:ND2	10:F:501:HOH:O	2.26	0.69
1:A:422:ARG:NH1	3:C:95:SER:O	2.26	0.68
3:C:129:ASN:ND2	10:C:504:HOH:O	2.27	0.67
1:D:280:GLY:O	1:D:518:ARG:NH1	2.26	0.67
1:A:386:GLY:HA2	1:A:409:ASP:HB2	1.77	0.67
1:A:429:ALA:HB3	1:A:433:PHE:HB3	1.76	0.67
2:E:195:ASP:OD1	2:E:202:ARG:NH1	2.27	0.66
1:A:589:GLY:N	4:A:901[B]:CL:CL	2.66	0.66
2:B:250:PRO:O	2:B:258:GLN:NE2	2.29	0.66
3:C:307:GLY:O	10:C:502:HOH:O	2.12	0.65
1:A:32:THR:OG1	2:B:309:MET:O	2.12	0.64
1:D:418:LYS:NZ	10:D:1002:HOH:O	2.30	0.64
2:B:36:TYR:H	2:B:69:HIS:HE2	1.44	0.64
2:E:252:CYS:H	2:E:258:GLN:HE22	1.45	0.64
1:D:496:GLN:NE2	10:D:1003:HOH:O	2.31	0.64
1:D:622:ARG:NH2	1:D:667:LYS:O	2.31	0.63
1:A:422:ARG:HB2	3:C:176:GLU:HB2	1.80	0.62
1:D:386:GLY:HA2	1:D:409:ASP:HB2	1.80	0.62
1:D:248:ILE:HG13	1:D:249:THR:HG23	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:98:PRO:HD3	2:E:138:ILE:HD11	1.81	0.61
2:B:195:ASP:OD1	2:B:202:ARG:NH1	2.33	0.61
3:C:322:ILE:HG23	3:C:335:THR:HG21	1.82	0.61
1:D:203:MET:O	1:D:496:GLN:NE2	2.33	0.61
1:D:108:ASP:OD1	1:D:411:GLN:NE2	2.33	0.61
1:D:622:ARG:HD2	1:D:638:GLY:HA3	1.83	0.60
2:B:227:ARG:NH2	3:C:107:TYR:HE1	2.00	0.60
3:C:106:HIS:CD2	7:C:404:HEC:NB	2.70	0.60
1:D:422:ARG:HB3	3:F:176:GLU:HB2	1.84	0.59
1:D:760:ARG:NE	1:D:762:LYS:O	2.24	0.59
1:A:438:VAL:O	3:C:167:ARG:NH2	2.36	0.59
2:E:228:ASP:HB2	2:E:292:GLY:HA2	1.85	0.58
2:E:287:ASP:OD1	2:E:311:ARG:NH2	2.31	0.58
3:C:297:THR:HG22	7:C:405:HEC:HMD3	1.85	0.58
2:E:218:ARG:NH1	2:E:268:GLU:O	2.37	0.57
2:B:228:ASP:HB3	2:B:293:MET:HE2	1.85	0.57
1:A:162:SER:HB3	1:A:189:LYS:HB3	1.86	0.56
1:A:432:ASN:ND2	1:A:454:SER:OG	2.34	0.56
2:B:159:VAL:HG23	2:B:168:VAL:HB	1.87	0.56
3:F:106:HIS:CD2	7:F:404:HEC:NB	2.74	0.56
1:D:504:ARG:NH2	1:D:801:ASP:O	2.38	0.56
1:D:457:THR:O	1:D:580:GLY:HA2	2.06	0.55
1:A:248:ILE:HG13	1:A:249:THR:HG23	1.88	0.55
2:B:183:ILE:HG12	2:B:190:LEU:HD23	1.88	0.55
3:C:111:GLN:HB3	3:C:132:TYR:CE1	2.42	0.55
2:E:70:SER:OG	2:E:71:VAL:N	2.39	0.55
1:A:588:TYR:HB3	4:A:901[A]:CL:CL	2.45	0.54
3:F:142:PHE:HB2	3:F:158:THR:HB	1.88	0.54
1:A:283:ARG:NH2	1:A:304:ASP:OD1	2.40	0.54
1:A:162:SER:CB	1:A:189:LYS:HB3	2.38	0.54
1:A:462:ASP:O	1:A:585:GLY:HA2	2.08	0.54
3:F:315:ALA:HB2	3:F:326:VAL:HG21	1.90	0.54
1:D:770:LEU:HD21	7:D:906:HEC:HBC2	1.90	0.54
2:B:287:ASP:OD1	2:B:311:ARG:NH2	2.35	0.54
2:B:111:ASP:OD2	2:B:131:ASP:HA	2.07	0.54
1:A:631:ASN:ND2	10:A:1007:HOH:O	2.40	0.54
3:F:335:THR:HA	3:F:338:LEU:HD13	1.88	0.54
1:D:159:ALA:HB1	1:D:162:SER:O	2.07	0.54
3:C:145:GLU:OE1	3:C:150:HIS:NE2	2.32	0.53
1:D:359:LYS:NZ	10:D:1005:HOH:O	2.35	0.53
3:C:82:VAL:HG23	3:C:189:TYR:HA	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:148:ALA:HB2	2:E:181:VAL:HG13	1.89	0.53
1:A:170:ILE:HB	1:A:184:HIS:O	2.09	0.52
1:A:520:SER:O	1:A:712:TYR:OH	2.22	0.52
3:F:132:TYR:CE2	3:F:134:ARG:HB2	2.44	0.52
3:C:144:HIS:ND1	7:C:404:HEC:O2D	2.34	0.52
3:C:132:TYR:CE2	3:C:134:ARG:HB2	2.45	0.52
7:D:906:HEC:HBD2	7:D:906:HEC:HHA	1.91	0.52
2:B:42:VAL:HG11	3:C:82:VAL:HG11	1.92	0.51
1:A:159:ALA:HB1	1:A:162:SER:O	2.10	0.51
3:C:63:LEU:HD21	3:C:180:PRO:HG3	1.92	0.51
1:D:325:ILE:HD11	1:D:345:TRP:HE3	1.75	0.51
1:D:493:GLN:HB2	1:D:533:ILE:HG13	1.93	0.51
1:D:462:ASP:O	1:D:585:GLY:HA2	2.11	0.51
3:F:202:ASN:OD1	3:F:203:ALA:N	2.43	0.51
2:B:70:SER:HA	2:B:87:VAL:HG22	1.92	0.51
2:B:307:ARG:HE	2:B:357:SER:HB3	1.75	0.51
2:B:88:ARG:NE	2:B:126:GLU:OE2	2.44	0.51
1:D:265:ASN:OD1	1:D:290:ASN:ND2	2.44	0.51
1:D:713:SER:O	1:D:717:ASN:ND2	2.39	0.51
1:A:678:GLN:NE2	1:A:682:ASP:OD1	2.44	0.50
1:D:422:ARG:NH1	3:F:95:SER:O	2.43	0.50
3:F:81:LEU:HA	3:F:84:TYR:HD2	1.76	0.50
1:D:329:GLU:OE2	1:D:355:LYS:NZ	2.31	0.50
1:D:608:TRP:CE3	3:F:123:GLY:HA2	2.47	0.50
3:F:317:THR:OG1	3:F:320:ASP:OD2	2.26	0.50
2:B:49:PRO:HB3	2:B:63:ILE:CG2	2.41	0.50
3:C:186:LEU:HD21	7:C:404:HEC:HMB1	1.94	0.50
2:E:251:VAL:HG12	10:F:518:HOH:O	2.10	0.50
2:B:94:SER:HB2	2:B:103:LEU:HD11	1.94	0.50
2:E:71:VAL:HG23	2:E:85:VAL:HB	1.92	0.50
1:A:339:GLN:HB3	1:A:357:THR:O	2.12	0.50
2:E:168:VAL:HG12	2:E:169:ARG:HG3	1.94	0.50
2:E:91:PRO:HA	2:E:106:CYS:O	2.11	0.49
3:F:109:ARG:HG2	3:F:109:ARG:HH11	1.77	0.49
1:D:536:GLN:HG2	1:D:546:THR:HB	1.93	0.49
3:F:284:THR:HG21	3:F:308:THR:HG21	1.93	0.49
3:C:242:ASP:OD2	3:C:246:HIS:NE2	2.41	0.49
1:A:604:LEU:HD13	2:B:250:PRO:HG3	1.93	0.49
1:D:225:ILE:HG13	1:D:233:LEU:HB2	1.94	0.49
1:A:504:ARG:NH1	1:A:801:ASP:O	2.40	0.49
2:E:88:ARG:NE	2:E:126:GLU:OE1	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:359:LYS:HE3	1:A:360:ASP:H	1.77	0.49
1:A:713:SER:O	1:A:717:ASN:ND2	2.35	0.49
2:E:202:ARG:HD2	2:E:224:SER:HA	1.93	0.49
2:E:225:ASN:HA	2:E:227:ARG:NH2	2.28	0.48
3:F:228:CYS:HA	3:F:242:ASP:HB2	1.94	0.48
1:D:432:ASN:HD22	1:D:454:SER:HB3	1.76	0.48
3:F:255:VAL:HA	3:F:264:LYS:HG3	1.95	0.48
1:A:608:TRP:CE3	3:C:123:GLY:HA2	2.49	0.48
2:B:92:GLU:OE1	2:B:132:TRP:NE1	2.42	0.48
1:A:58:GLN:HB3	1:A:88:LEU:HD11	1.95	0.48
2:E:203:SER:HB3	2:E:217:ASN:OD1	2.13	0.48
3:F:277:PRO:HA	3:F:286:ILE:HD11	1.95	0.48
1:A:81:PRO:HB2	1:A:84:SER:OG	2.14	0.48
1:A:383:GLY:HA3	1:D:383:GLY:HA3	1.96	0.48
2:B:46:LEU:HD13	2:B:376:ASN:HD21	1.78	0.48
1:D:444:ASP:OD1	1:D:447:LYS:N	2.46	0.48
2:B:91:PRO:HA	2:B:106:CYS:O	2.14	0.48
1:D:736:ASN:HD22	1:D:743:SER:HA	1.79	0.47
2:E:97:THR:HA	2:E:138:ILE:HD11	1.96	0.47
2:B:352:THR:HG22	2:B:353:GLY:H	1.79	0.47
2:B:382:ARG:NH1	2:B:385:VAL:O	2.41	0.47
3:C:131:LYS:HB3	7:C:404:HEC:HBA1	1.97	0.47
2:E:356:PRO:HA	2:E:371:ALA:O	2.15	0.47
3:F:111:GLN:HB3	3:F:132:TYR:CE1	2.50	0.47
3:C:107:TYR:CG	3:C:108:GLU:N	2.83	0.47
1:A:325:ILE:HD11	1:A:345:TRP:HE3	1.78	0.46
3:F:92:ALA:O	3:F:98:GLY:HA2	2.15	0.46
2:E:159:VAL:HG22	2:E:169:ARG:H	1.79	0.46
2:B:208:ASP:HB3	2:B:211:SER:HB3	1.97	0.46
1:D:260:LEU:HD13	1:D:421:PRO:HG2	1.97	0.46
2:E:93:ALA:HB3	2:E:106:CYS:HB2	1.98	0.46
3:F:119:LEU:HB2	3:F:122:GLU:OE1	2.15	0.46
1:D:81:PRO:HB2	1:D:84:SER:OG	2.16	0.46
1:D:110:CYS:SG	10:D:1002:HOH:O	2.61	0.46
1:D:382:ARG:HA	1:D:382:ARG:HD3	1.42	0.46
1:D:472:PRO:HB2	1:D:730:ILE:HD13	1.97	0.46
1:A:31:MET:O	2:B:311:ARG:NH1	2.46	0.46
3:F:45:ILE:HG23	3:F:46:SER:H	1.80	0.46
3:F:214:GLY:HA3	3:F:349:TYR:HB2	1.98	0.46
1:A:173:ARG:HH21	1:A:178:GLU:HG3	1.81	0.46
2:B:50:PHE:HB2	2:B:66:GLN:HB2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:227:ARG:NH2	3:C:107:TYR:CE1	2.82	0.46
1:A:310:THR:O	1:A:333:MET:HG3	2.16	0.46
1:A:391:ASN:OD1	1:A:393:SER:OG	2.27	0.46
2:E:186:ASP:OD1	2:E:187:GLY:N	2.48	0.46
1:D:653:SER:OG	1:D:654:GLY:N	2.48	0.45
2:E:116:VAL:HG22	2:E:123:GLU:HA	1.97	0.45
1:A:60:LEU:O	1:A:413:ALA:N	2.43	0.45
1:A:240:HIS:CD2	1:A:241:LEU:HG	2.51	0.45
1:A:225:ILE:O	1:A:229:THR:OG1	2.18	0.45
2:B:108:ALA:HB1	2:B:132:TRP:CE2	2.51	0.45
1:D:432:ASN:HA	1:D:454:SER:HB3	1.99	0.45
2:E:49:PRO:HB3	2:E:63:ILE:CG2	2.47	0.45
1:A:319:THR:O	1:A:323:ARG:HA	2.16	0.45
1:A:331:PRO:HB2	1:D:331:PRO:HB3	1.98	0.45
1:A:586:CYS:SG	7:A:905:HEC:HHD	2.57	0.45
2:B:200:ILE:HD12	3:C:282:SER:O	2.17	0.45
1:A:504:ARG:HD3	1:A:800:PRO:HB3	1.99	0.45
2:B:187:GLY:O	2:B:209:ILE:HD12	2.17	0.45
3:C:209:GLU:O	3:C:213:ARG:HB2	2.16	0.45
2:E:253[B]:GLU:HA	3:F:174:ARG:HG3	1.98	0.45
3:F:150:HIS:CD2	3:F:156:GLY:H	2.34	0.45
1:A:99:LEU:HB3	1:A:135:MET:HE1	1.99	0.45
1:D:77:PRO:HB3	1:D:256:PHE:CG	2.52	0.45
1:A:536:GLN:HG2	1:A:546:THR:HB	1.97	0.44
2:B:227:ARG:NH2	10:B:507:HOH:O	2.50	0.44
1:D:271:VAL:HG22	1:D:284:VAL:HG22	1.99	0.44
2:E:267:ILE:HG12	2:E:275:VAL:HG13	1.98	0.44
3:C:303:ILE:HG12	7:C:405:HEC:HMA3	2.00	0.44
3:C:183:LEU:O	3:C:187:ILE:HG12	2.17	0.44
2:E:88:ARG:HB2	2:E:107:ASN:CG	2.38	0.44
3:F:134:ARG:NH1	3:F:194:GLU:O	2.44	0.44
2:E:103:LEU:HD23	2:E:104:TYR:N	2.32	0.44
2:B:149:CYS:O	2:B:178:PRO:HD2	2.18	0.44
2:E:286:TYR:O	2:E:311:ARG:NH2	2.50	0.44
1:A:493:GLN:HB2	1:A:533:ILE:HG13	1.99	0.44
1:D:681:LEU:O	1:D:685:CYS:HB2	2.17	0.44
2:B:104:TYR:HB3	2:B:136:ILE:HD13	2.00	0.44
2:B:227:ARG:NH1	3:C:108:GLU:OE2	2.51	0.44
2:B:250:PRO:HB3	3:C:124:TRP:CZ3	2.52	0.44
3:F:297:THR:HA	3:F:298:PRO:HD3	1.80	0.44
1:A:633:LYS:HD2	1:A:633:LYS:HA	1.73	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:586:CYS:SG	7:D:905:HEC:HHD	2.58	0.44
1:D:641:VAL:HA	1:D:660:VAL:O	2.17	0.44
3:F:131:LYS:HB3	7:F:404:HEC:HBA1	1.99	0.44
1:D:53:GLN:NE2	1:D:372:ASP:OD1	2.51	0.43
1:D:113:TRP:CG	1:D:420:LYS:HE2	2.53	0.43
1:A:50:LYS:HG2	1:A:371:PRO:O	2.18	0.43
3:C:297:THR:HA	3:C:298:PRO:HD3	1.80	0.43
3:C:247:ASP:HB2	3:C:294:GLU:HG2	2.01	0.43
2:E:374:PHE:HB3	3:F:54:TRP:CZ3	2.53	0.43
3:F:232:ASP:HB3	3:F:235:ASP:HB2	2.00	0.43
3:C:103:ALA:O	3:C:107:TYR:HA	2.18	0.43
3:C:187:ILE:HA	3:C:190:ILE:HD12	2.00	0.43
1:D:289:ASP:OD1	1:D:290:ASN:N	2.51	0.43
2:E:244:THR:HB	2:E:261:THR:OG1	2.19	0.43
1:A:547:SER:OG	1:A:617:SER:OG	2.32	0.43
1:D:43:THR:O	1:D:422:ARG:NH2	2.46	0.43
2:E:134:SER:OG	2:E:179:ARG:O	2.36	0.43
1:A:289:ASP:OD1	1:A:290:ASN:N	2.52	0.43
1:A:298:PRO:HD3	7:A:905:HEC:HMA2	1.99	0.43
1:A:358:GLY:C	1:A:359:LYS:HG3	2.39	0.43
1:A:457:THR:O	1:A:580:GLY:HA2	2.19	0.43
1:D:734:TYR:HE1	7:D:906:HEC:HBA2	1.84	0.43
2:E:180:MET:HB3	2:E:193:ILE:HD11	2.01	0.43
2:E:237:TYR:CE1	2:E:268:GLU:HG2	2.54	0.43
1:A:259:TRP:N	1:A:267:LEU:O	2.50	0.42
1:D:121:ALA:HB2	1:D:153:ARG:HA	2.00	0.42
3:C:107:TYR:HE2	3:C:109:ARG:CG	2.33	0.42
3:F:242:ASP:OD2	3:F:246:HIS:NE2	2.42	0.42
2:B:41:HIS:CD2	3:C:194:GLU:HG3	2.55	0.42
1:D:158:TYR:OH	1:D:423:TRP:HA	2.20	0.42
1:D:459:ILE:HB	1:D:545:VAL:HG23	2.01	0.42
1:D:587:HIS:HB2	7:D:905:HEC:C1D	2.49	0.42
1:D:617:SER:HA	1:D:618:PRO:HD3	1.90	0.42
2:E:237:TYR:HE1	2:E:268:GLU:HG2	1.84	0.42
1:A:81:PRO:HB2	1:A:84:SER:HG	1.85	0.42
1:A:343:VAL:HG12	1:A:353:TYR:HA	2.01	0.42
3:C:201:ARG:HD3	3:C:352:ALA:HB1	2.01	0.42
1:D:712:TYR:HD1	1:D:794:TRP:CG	2.38	0.42
3:F:265:VAL:HB	3:F:271:LEU:HD12	2.02	0.42
2:B:164:ARG:HG2	2:B:164:ARG:HH11	1.84	0.42
1:D:277:ARG:HG3	7:D:905:HEC:O1D	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:111:GLN:O	3:F:132:TYR:HA	2.19	0.42
1:A:357:THR:HG21	1:A:364:TYR:CE2	2.55	0.42
2:B:136:ILE:O	2:B:137:LYS:HG3	2.20	0.42
3:F:310:PHE:N	7:F:405:HEC:O1A	2.53	0.42
1:A:67:THR:HB	1:A:70:GLY:H	1.85	0.42
1:D:49:SER:HA	1:D:52:VAL:HG12	2.02	0.42
1:D:588:TYR:HB3	4:D:901:CL:CL	2.57	0.41
1:D:632:TYR:CZ	1:D:634:GLY:HA2	2.55	0.41
2:B:180:MET:HB3	2:B:193:ILE:HD11	2.02	0.41
2:B:364:ASP:CG	2:B:366:LYS:HG3	2.41	0.41
2:E:228:ASP:CB	2:E:292:GLY:HA2	2.50	0.41
2:E:115:VAL:O	2:E:124:ILE:N	2.50	0.41
2:E:288:GLY:H	2:E:309:MET:CG	2.27	0.41
2:B:325:ARG:HD3	1:D:692:ASN:HA	2.02	0.41
2:B:386:ASP:N	2:B:386:ASP:OD1	2.54	0.41
2:E:117:ASP:OD1	2:E:118:ILE:N	2.53	0.41
2:E:136:ILE:HG22	2:E:147:VAL:HG22	2.03	0.41
2:E:175:ASP:H	2:E:194:LEU:HD13	1.85	0.41
3:F:183:LEU:O	3:F:187:ILE:HG12	2.20	0.41
3:F:218:PHE:O	3:F:225:CYS:HB2	2.21	0.41
1:A:173:ARG:NH2	1:A:178:GLU:OE2	2.54	0.41
1:A:252:LEU:HD12	1:A:572:TRP:CZ2	2.55	0.41
1:D:600:HIS:HB3	3:F:278:TYR:O	2.21	0.41
2:E:54:MET:HE2	2:E:61:LEU:HD21	2.02	0.41
1:D:596:PHE:HB2	2:E:258:GLN:HA	2.02	0.41
2:E:179:ARG:NH1	3:F:107:TYR:OH	2.54	0.41
3:F:198:SER:HA	3:F:199:PRO:HD3	1.85	0.41
3:F:321:THR:HG21	7:F:405:HEC:HMA2	2.02	0.41
1:A:205:GLU:HA	1:A:528:GLN:NE2	2.35	0.41
3:C:123:GLY:O	3:C:126:SER:OG	2.32	0.41
1:D:116:LYS:HA	1:D:116:LYS:HD3	1.89	0.41
1:D:410:HIS:CD2	1:D:411:GLN:HG3	2.56	0.41
2:E:255:GLU:OE1	2:E:255:GLU:N	2.54	0.41
2:B:237:TYR:CE1	2:B:268:GLU:HG2	2.55	0.41
1:D:58:GLN:O	1:D:415:VAL:HG22	2.20	0.41
2:E:229:VAL:HA	2:E:239:ALA:O	2.21	0.41
3:F:122:GLU:O	3:F:291:LEU:HD22	2.20	0.41
1:A:600:HIS:HB3	3:C:278:TYR:O	2.21	0.41
1:A:617:SER:HA	1:A:618:PRO:HD3	1.93	0.41
2:B:134:SER:OG	2:B:179:ARG:O	2.19	0.41
2:B:148:ALA:HB2	2:B:181:VAL:HG13	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:282:ASP:N	2:B:285:ASN:O	2.50	0.41
2:B:356:PRO:HA	2:B:371:ALA:O	2.21	0.41
1:D:594:ARG:NH2	2:E:337:ASP:HB2	2.36	0.41
2:E:253[A]:GLU:HB3	2:E:255:GLU:OE1	2.20	0.41
2:E:222:GLU:OE2	10:E:501:HOH:O	2.22	0.41
2:E:250:PRO:O	2:E:258:GLN:NE2	2.54	0.41
1:A:105:THR:HB	1:A:123:VAL:HG12	2.02	0.40
2:E:187:GLY:O	2:E:209:ILE:HD12	2.21	0.40
1:A:199:PRO:HG2	1:A:202:VAL:HG21	2.03	0.40
1:A:295:TYR:CE1	2:B:253[A]:GLU:HG3	2.56	0.40
3:C:131:LYS:HE2	3:C:144:HIS:CE1	2.57	0.40
3:F:110:GLY:HA2	3:F:133:ILE:HD11	2.03	0.40
3:F:308:THR:HG23	3:F:316:ARG:HA	2.03	0.40
1:A:220:GLN:HB2	1:A:224:ILE:HG12	2.03	0.40
2:B:321:LEU:O	2:B:325:ARG:HG3	2.22	0.40
1:D:277:ARG:NH1	7:D:905:HEC:O2D	2.55	0.40
1:D:608:TRP:HD1	1:D:616:ASP:OD2	2.05	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	762/782 (97%)	731 (96%)	31 (4%)	0	100	100
1	D	764/782 (98%)	739 (97%)	25 (3%)	0	100	100
2	B	351/352 (100%)	343 (98%)	8 (2%)	0	100	100
2	E	351/352 (100%)	342 (97%)	9 (3%)	0	100	100
3	C	312/314 (99%)	295 (95%)	16 (5%)	1 (0%)	41	66
3	F	312/314 (99%)	298 (96%)	13 (4%)	1 (0%)	41	66
All	All	2852/2896 (98%)	2748 (96%)	102 (4%)	2 (0%)	51	78

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	96	LEU
3	F	96	LEU

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	641/653 (98%)	638 (100%)	3 (0%)	88	96
1	D	642/653 (98%)	642 (100%)	0	100	100
2	B	303/302 (100%)	301 (99%)	2 (1%)	84	94
2	E	300/302 (99%)	299 (100%)	1 (0%)	92	98
3	C	262/264 (99%)	260 (99%)	2 (1%)	81	93
3	F	259/264 (98%)	256 (99%)	3 (1%)	71	88
All	All	2407/2438 (99%)	2396 (100%)	11 (0%)	88	96

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	162	SER
1	A	359	LYS
1	A	384	ASP
2	B	231	TYR
2	B	330	GLU
3	C	162	ASP
3	C	209	GLU
2	E	241	THR
3	F	107	TYR
3	F	122	GLU
3	F	152	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	41	HIS
3	C	340	GLN
3	C	344	GLN
1	D	184	HIS
1	D	290	ASN
1	D	432	ASN
1	D	468	GLN
1	D	496	GLN
1	D	606	ASN
2	E	90	GLN
2	E	122	GLN
3	F	150	HIS

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 34 ligands modelled in this entry, 19 are monoatomic - leaving 15 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
8	BET	A	908	-	7,7,7	2.52	1 (14%)	10,10,10	1.96	2 (20%)
8	BET	E	403	-	7,7,7	2.47	1 (14%)	10,10,10	1.96	2 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
7	HEC	F	405	3	32,50,50	2.18	3 (9%)	24,82,82	1.51	4 (16%)
8	BET	A	909	-	7,7,7	2.49	1 (14%)	10,10,10	1.96	2 (20%)
8	BET	B	403	-	7,7,7	2.51	1 (14%)	10,10,10	1.96	2 (20%)
7	HEC	C	405	3	32,50,50	2.16	3 (9%)	24,82,82	1.46	3 (12%)
7	HEC	D	905	6,1	32,50,50	2.24	3 (9%)	24,82,82	1.41	3 (12%)
7	HEC	C	404	10,3	32,50,50	2.17	3 (9%)	24,82,82	1.45	4 (16%)
8	BET	A	907	-	7,7,7	2.49	1 (14%)	10,10,10	1.88	2 (20%)
7	HEC	A	906	1	32,50,50	2.16	3 (9%)	24,82,82	1.45	5 (20%)
7	HEC	F	404	10,3	32,50,50	2.17	3 (9%)	24,82,82	1.44	3 (12%)
8	BET	C	406	-	7,7,7	2.57	1 (14%)	10,10,10	1.86	2 (20%)
7	HEC	D	906	1	32,50,50	2.20	4 (12%)	24,82,82	1.35	2 (8%)
8	BET	D	907	-	7,7,7	2.47	1 (14%)	10,10,10	1.98	2 (20%)
7	HEC	A	905	6,1	32,50,50	2.24	3 (9%)	24,82,82	1.35	2 (8%)

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
8	BET	A	908	-	-	5/5/5/5	-
8	BET	E	403	-	-	5/5/5/5	-
7	HEC	F	405	3	-	0/10/54/54	-
8	BET	A	909	-	-	5/5/5/5	-
8	BET	B	403	-	-	5/5/5/5	-
7	HEC	C	405	3	-	2/10/54/54	-
7	HEC	D	905	6,1	-	2/10/54/54	-
7	HEC	C	404	10,3	-	2/10/54/54	-
8	BET	A	907	-	-	5/5/5/5	-
7	HEC	A	906	1	-	0/10/54/54	-
7	HEC	F	404	10,3	-	0/10/54/54	-
8	BET	C	406	-	-	5/5/5/5	-
7	HEC	D	906	1	-	6/10/54/54	-
8	BET	D	907	-	-	5/5/5/5	-
7	HEC	A	905	6,1	-	4/10/54/54	-

All (32) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	D	905	HEC	C2B-C3B	-6.61	1.33	1.40
7	A	905	HEC	C2B-C3B	-6.60	1.33	1.40
7	D	905	HEC	C3C-C2C	-6.48	1.34	1.40
7	A	905	HEC	C3C-C2C	-6.48	1.34	1.40
8	C	406	BET	CA-C	6.21	1.63	1.52
7	F	405	HEC	C3C-C2C	-6.21	1.34	1.40
7	D	906	HEC	C2B-C3B	-6.19	1.34	1.40
7	A	906	HEC	C2B-C3B	-6.19	1.34	1.40
7	F	405	HEC	C2B-C3B	-6.19	1.34	1.40
7	C	405	HEC	C3C-C2C	-6.16	1.34	1.40
7	F	404	HEC	C2B-C3B	-6.15	1.34	1.40
7	C	404	HEC	C2B-C3B	-6.11	1.34	1.40
7	D	906	HEC	C3C-C2C	-6.07	1.34	1.40
7	C	404	HEC	C3C-C2C	-6.05	1.34	1.40
8	A	908	BET	CA-C	6.05	1.62	1.52
8	A	909	BET	CA-C	6.05	1.62	1.52
8	B	403	BET	CA-C	6.04	1.62	1.52
8	A	907	BET	CA-C	6.02	1.62	1.52
7	A	906	HEC	C3C-C2C	-6.01	1.34	1.40
8	E	403	BET	CA-C	5.99	1.62	1.52
7	F	404	HEC	C3C-C2C	-5.96	1.34	1.40
8	D	907	BET	CA-C	5.96	1.62	1.52
7	C	405	HEC	C2B-C3B	-5.95	1.34	1.40
7	C	405	HEC	C3D-C2D	5.53	1.54	1.37
7	F	404	HEC	C3D-C2D	5.50	1.54	1.37
7	A	906	HEC	C3D-C2D	5.50	1.54	1.37
7	F	405	HEC	C3D-C2D	5.49	1.53	1.37
7	D	906	HEC	C3D-C2D	5.48	1.53	1.37
7	C	404	HEC	C3D-C2D	5.48	1.53	1.37
7	A	905	HEC	C3D-C2D	5.44	1.53	1.37
7	D	905	HEC	C3D-C2D	5.41	1.53	1.37
7	D	906	HEC	CAD-C3D	2.47	1.55	1.52

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	D	907	BET	C-CA-N	-4.85	109.67	116.34
8	A	909	BET	C-CA-N	-4.85	109.68	116.34
8	E	403	BET	C-CA-N	-4.81	109.73	116.34
8	A	908	BET	C-CA-N	-4.79	109.75	116.34
8	B	403	BET	C-CA-N	-4.75	109.80	116.34
8	A	907	BET	C-CA-N	-4.58	110.04	116.34
8	C	406	BET	C-CA-N	-4.48	110.19	116.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	E	403	BET	OXT-C-O	3.32	131.57	123.30
8	D	907	BET	OXT-C-O	3.31	131.55	123.30
8	A	909	BET	OXT-C-O	3.31	131.54	123.30
8	C	406	BET	OXT-C-O	3.29	131.51	123.30
8	A	907	BET	OXT-C-O	3.28	131.48	123.30
8	B	403	BET	OXT-C-O	3.28	131.47	123.30
8	A	908	BET	OXT-C-O	3.28	131.47	123.30
7	F	404	HEC	CMC-C2C-C1C	-3.12	123.67	128.46
7	D	906	HEC	CMC-C2C-C1C	-3.01	123.84	128.46
7	C	404	HEC	CMC-C2C-C1C	-2.99	123.87	128.46
7	F	405	HEC	CMC-C2C-C1C	-2.90	124.01	128.46
7	F	405	HEC	CBA-CAA-C2A	-2.68	108.09	112.60
7	D	905	HEC	C1D-C2D-C3D	-2.67	105.14	107.00
7	C	405	HEC	CMC-C2C-C1C	-2.65	124.40	128.46
7	F	405	HEC	C1D-C2D-C3D	-2.59	105.19	107.00
7	A	905	HEC	C1D-C2D-C3D	-2.56	105.21	107.00
7	C	405	HEC	C1D-C2D-C3D	-2.47	105.28	107.00
7	A	906	HEC	CMC-C2C-C1C	-2.45	124.69	128.46
7	C	404	HEC	CBD-CAD-C3D	-2.42	108.50	112.62
7	C	404	HEC	CMB-C2B-C1B	-2.36	124.84	128.46
7	C	405	HEC	CMB-C2B-C1B	-2.33	124.89	128.46
7	F	404	HEC	CMB-C2B-C1B	-2.31	124.91	128.46
7	D	905	HEC	CBD-CAD-C3D	-2.30	108.69	112.62
7	A	906	HEC	C1D-C2D-C3D	-2.28	105.41	107.00
7	F	405	HEC	CMB-C2B-C1B	-2.23	125.04	128.46
7	A	906	HEC	CMB-C2B-C1B	-2.20	125.09	128.46
7	A	906	HEC	CBD-CAD-C3D	-2.16	108.93	112.62
7	A	905	HEC	CMC-C2C-C1C	-2.16	125.15	128.46
7	C	404	HEC	C1D-C2D-C3D	-2.13	105.52	107.00
7	D	905	HEC	CMC-C2C-C1C	-2.08	125.27	128.46
7	A	906	HEC	CBA-CAA-C2A	-2.06	109.13	112.60
7	F	404	HEC	C1D-C2D-C3D	-2.02	105.59	107.00
7	D	906	HEC	CMB-C2B-C1B	-2.01	125.38	128.46

There are no chirality outliers.

All (51) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	D	906	HEC	C2D-C3D-CAD-CBD
7	D	906	HEC	C4D-C3D-CAD-CBD
8	A	907	BET	C-CA-N-C2
8	A	907	BET	O-C-CA-N

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Mol	Chain	Res	Type	Atoms
8	A	907	BET	OXT-C-CA-N
8	A	908	BET	O-C-CA-N
8	A	908	BET	OXT-C-CA-N
8	A	909	BET	O-C-CA-N
8	A	909	BET	OXT-C-CA-N
8	B	403	BET	O-C-CA-N
8	B	403	BET	OXT-C-CA-N
8	C	406	BET	O-C-CA-N
8	C	406	BET	OXT-C-CA-N
8	D	907	BET	O-C-CA-N
8	D	907	BET	OXT-C-CA-N
8	E	403	BET	O-C-CA-N
8	E	403	BET	OXT-C-CA-N
8	B	403	BET	C-CA-N-C1
8	B	403	BET	C-CA-N-C3
8	D	907	BET	C-CA-N-C1
8	D	907	BET	C-CA-N-C3
8	A	908	BET	C-CA-N-C1
8	C	406	BET	C-CA-N-C2
8	E	403	BET	C-CA-N-C1
8	A	907	BET	C-CA-N-C1
8	B	403	BET	C-CA-N-C2
8	D	907	BET	C-CA-N-C2
8	A	907	BET	C-CA-N-C3
8	A	908	BET	C-CA-N-C2
8	A	908	BET	C-CA-N-C3
8	A	909	BET	C-CA-N-C1
8	C	406	BET	C-CA-N-C1
8	E	403	BET	C-CA-N-C2
8	E	403	BET	C-CA-N-C3
8	A	909	BET	C-CA-N-C2
8	A	909	BET	C-CA-N-C3
8	C	406	BET	C-CA-N-C3
7	D	905	HEC	CAA-CBA-CGA-O1A
7	A	905	HEC	CAA-CBA-CGA-O1A
7	A	905	HEC	CAA-CBA-CGA-O2A
7	D	905	HEC	CAA-CBA-CGA-O2A
7	C	404	HEC	CAD-CBD-CGD-O2D
7	A	905	HEC	CAD-CBD-CGD-O2D
7	C	404	HEC	CAD-CBD-CGD-O1D
7	A	905	HEC	CAD-CBD-CGD-O1D
7	C	405	HEC	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
7	C	405	HEC	CAD-CBD-CGD-O1D
7	D	906	HEC	CAA-CBA-CGA-O2A
7	D	906	HEC	CAD-CBD-CGD-O2D
7	D	906	HEC	CAA-CBA-CGA-O1A
7	D	906	HEC	CAD-CBD-CGD-O1D

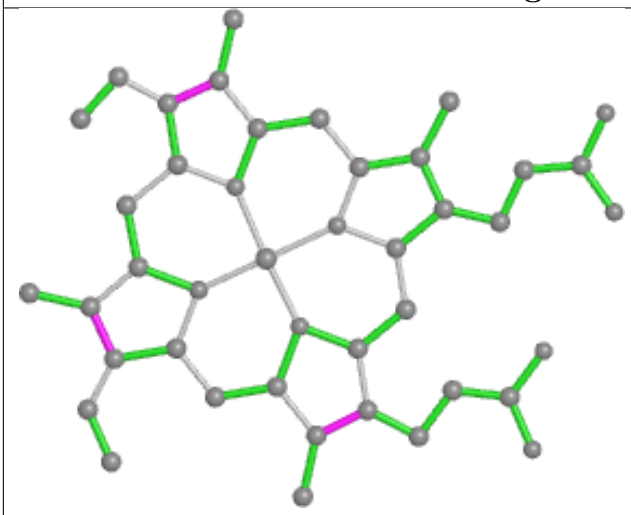
There are no ring outliers.

8 monomers are involved in 27 short contacts:

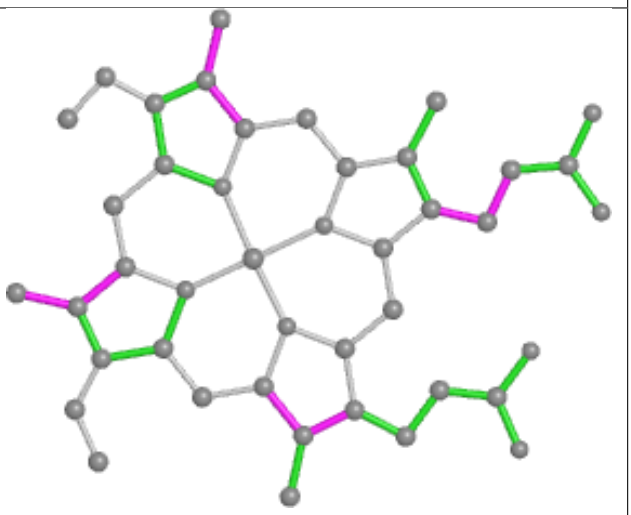
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	F	405	HEC	2	0
7	C	405	HEC	2	0
7	D	905	HEC	4	0
7	C	404	HEC	4	0
7	A	906	HEC	8	0
7	F	404	HEC	2	0
7	D	906	HEC	3	0
7	A	905	HEC	2	0

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 then 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.

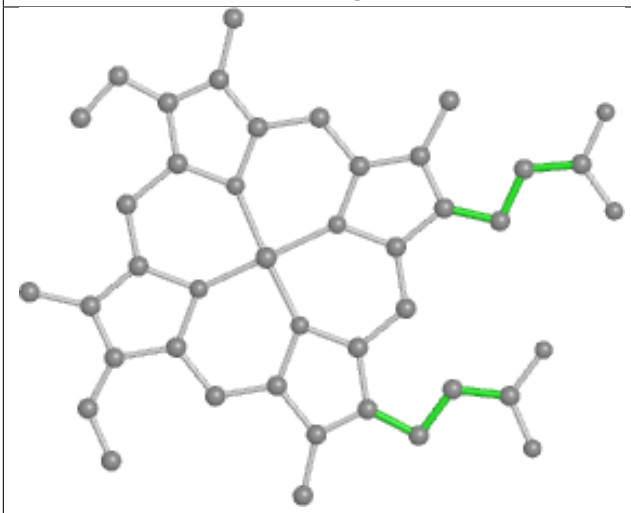
Ligand HEC F 405



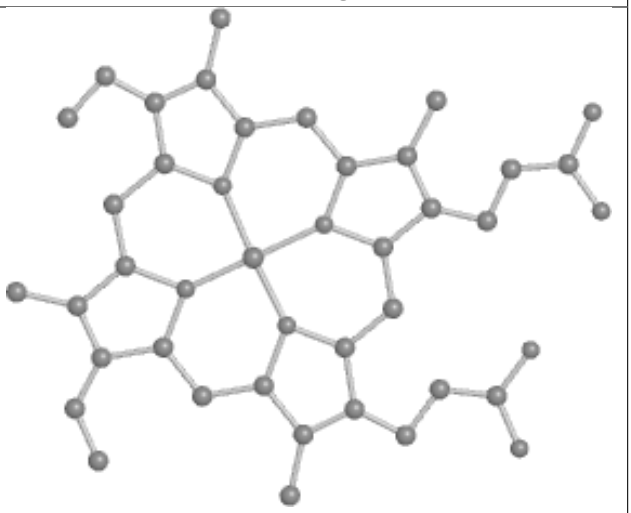
Bond lengths



Bond angles

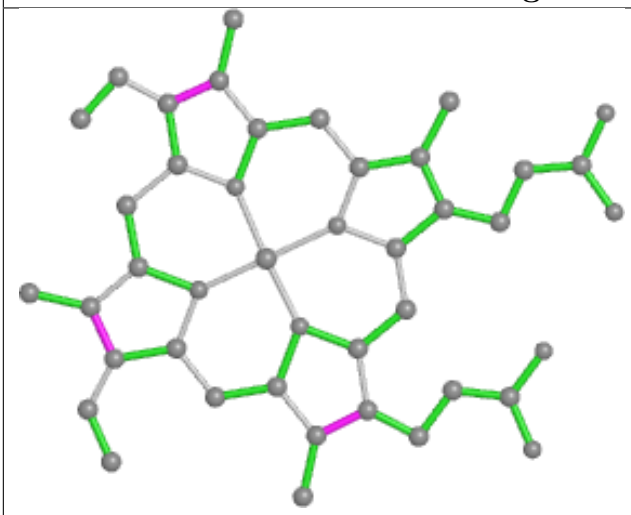


Torsions



Rings

Ligand HEC C 405



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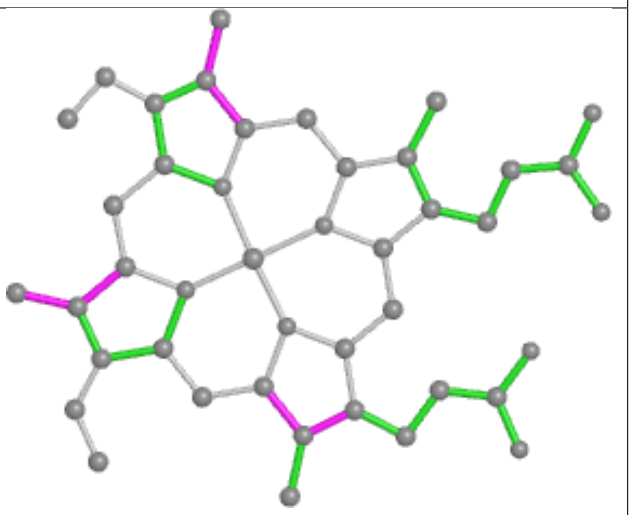
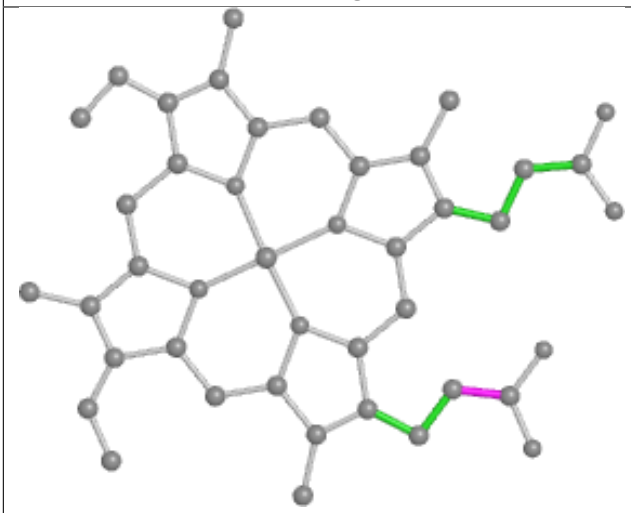


Bond angles



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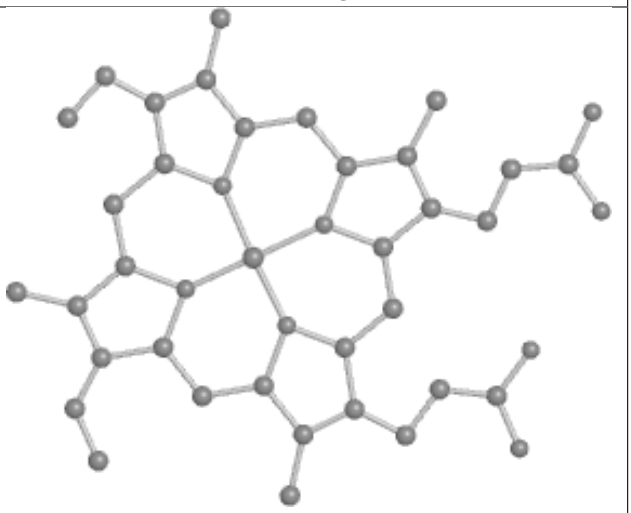
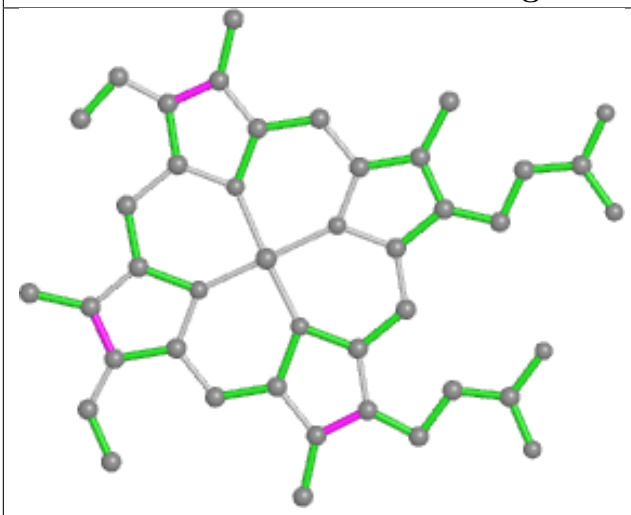
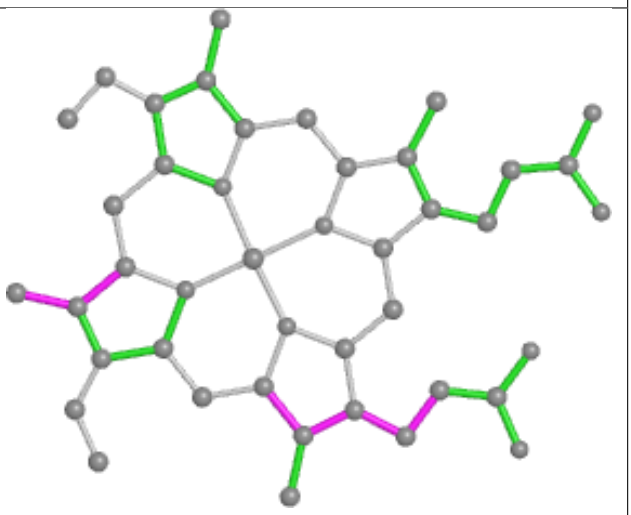


Rings

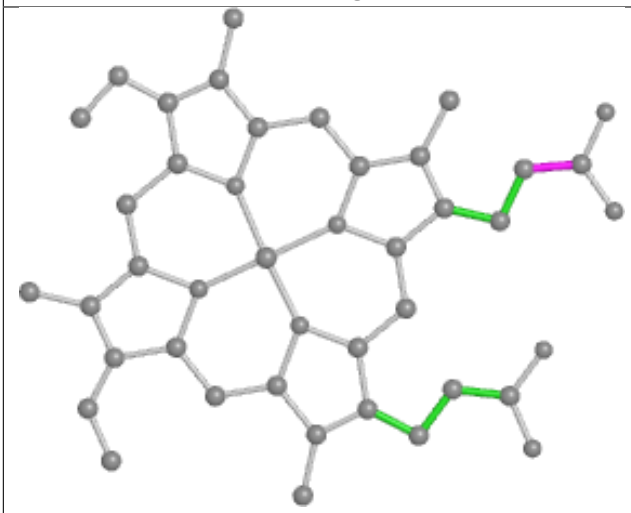
Ligand HEC D 905



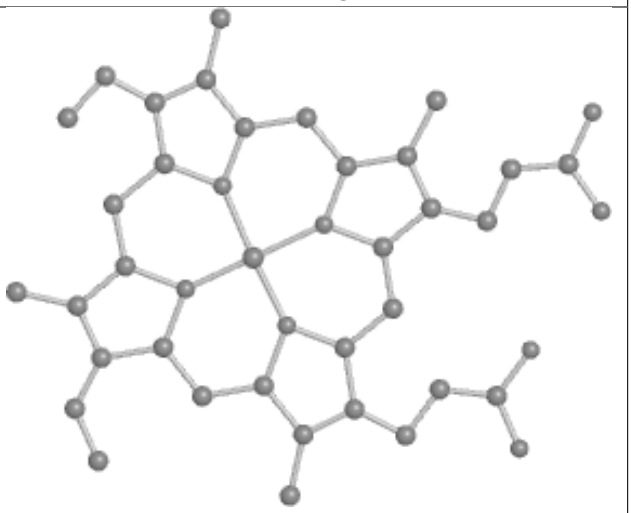
Bond lengths



Bond angles

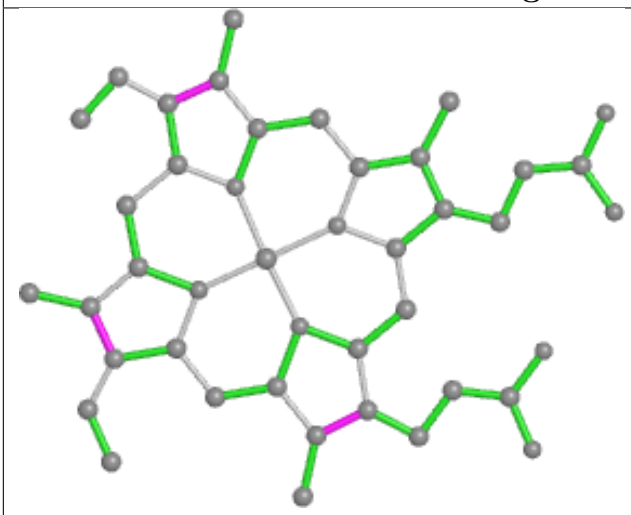


Torsions

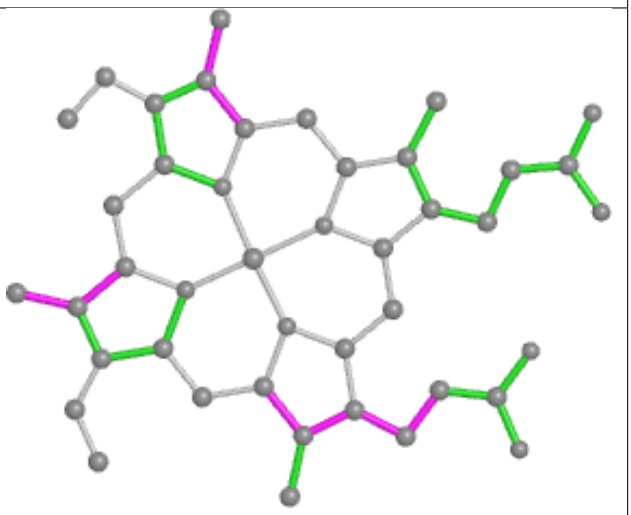


Rings

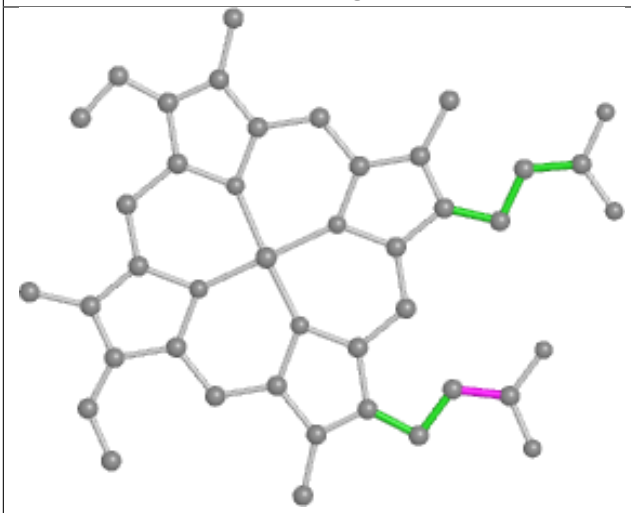
Ligand HEC C 404



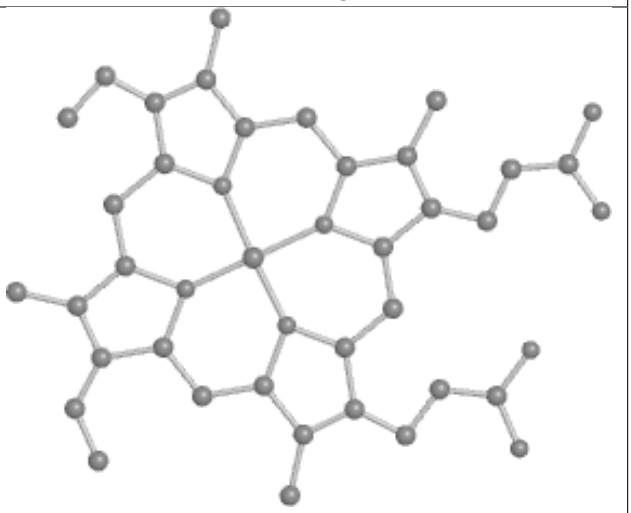
Bond lengths



Bond angles

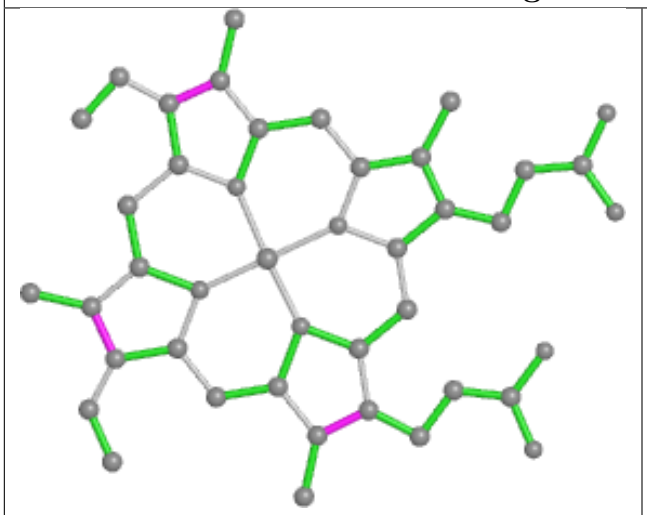


Torsions

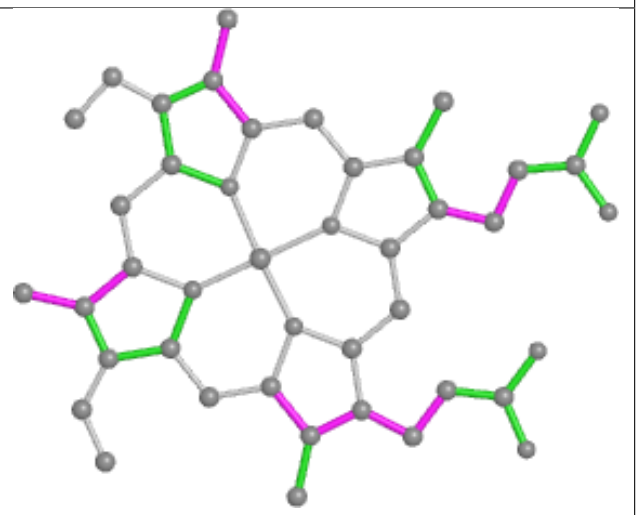


Rings

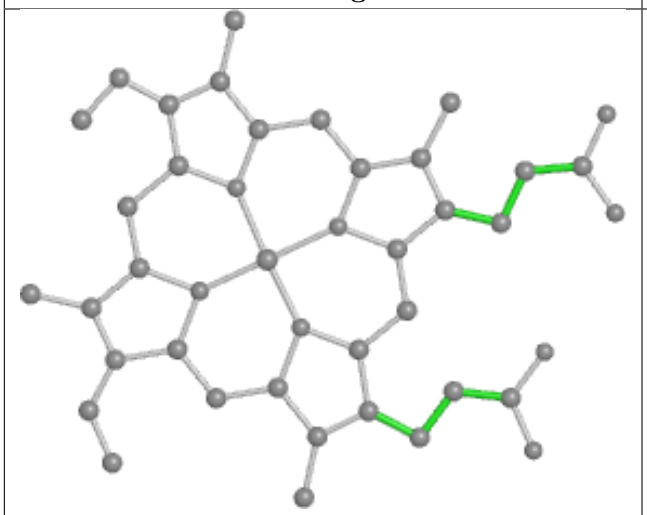
Ligand HEC A 906



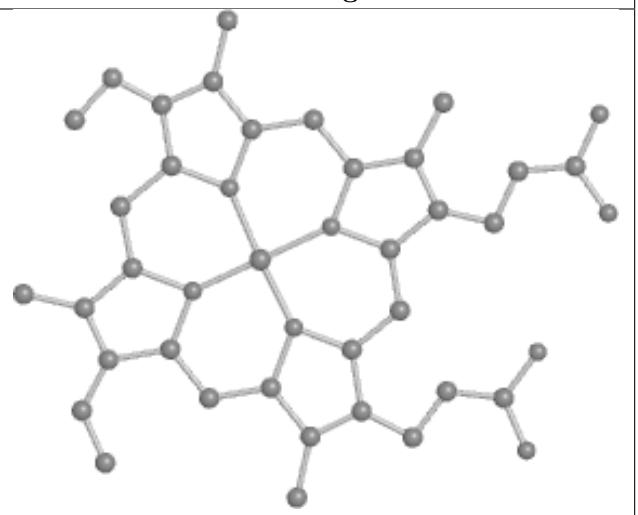
Bond lengths



Bond angles

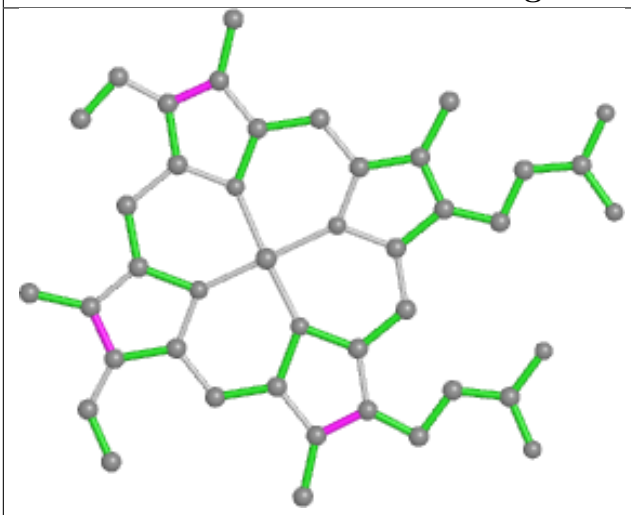


Torsions

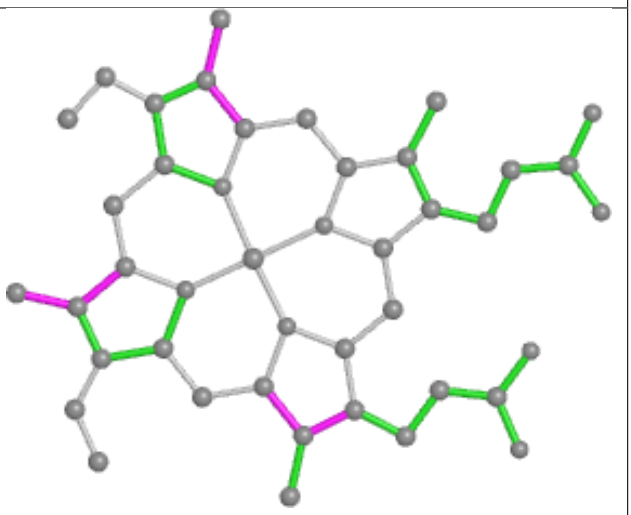


Rings

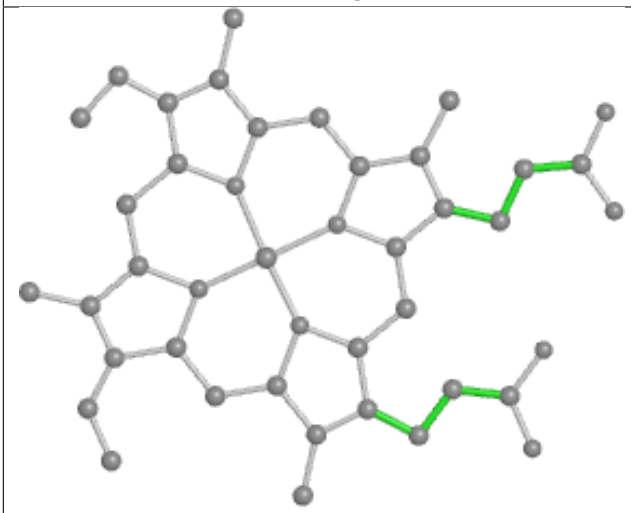
Ligand HEC F 404



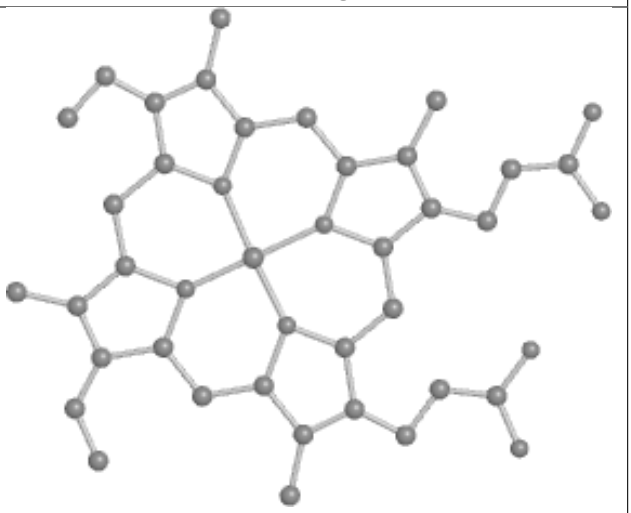
Bond lengths



Bond angles

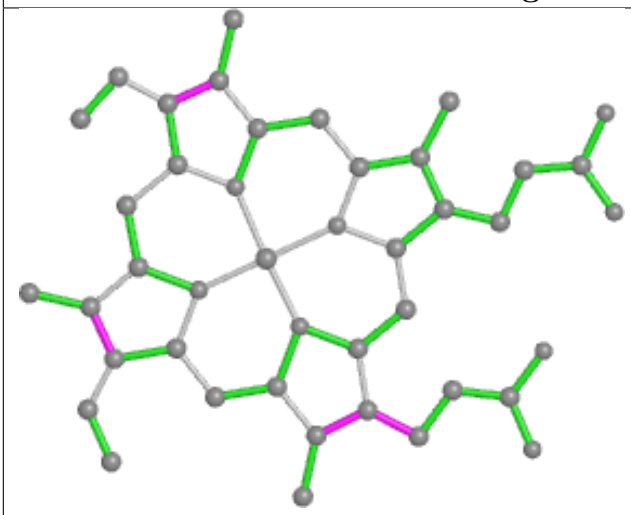


Torsions

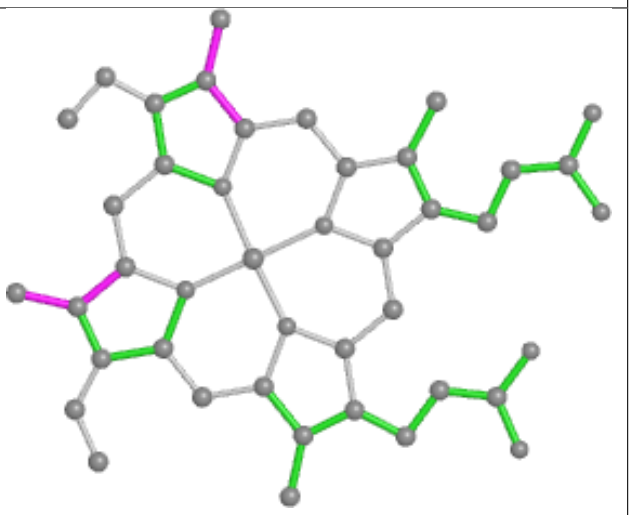


Rings

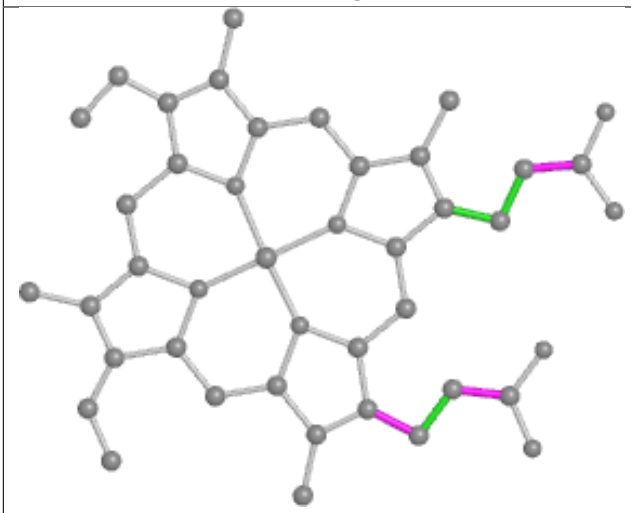
Ligand HEC D 906



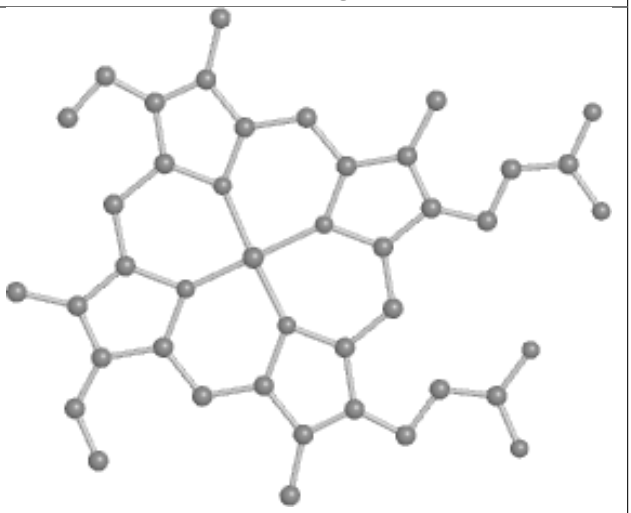
Bond lengths



Bond angles

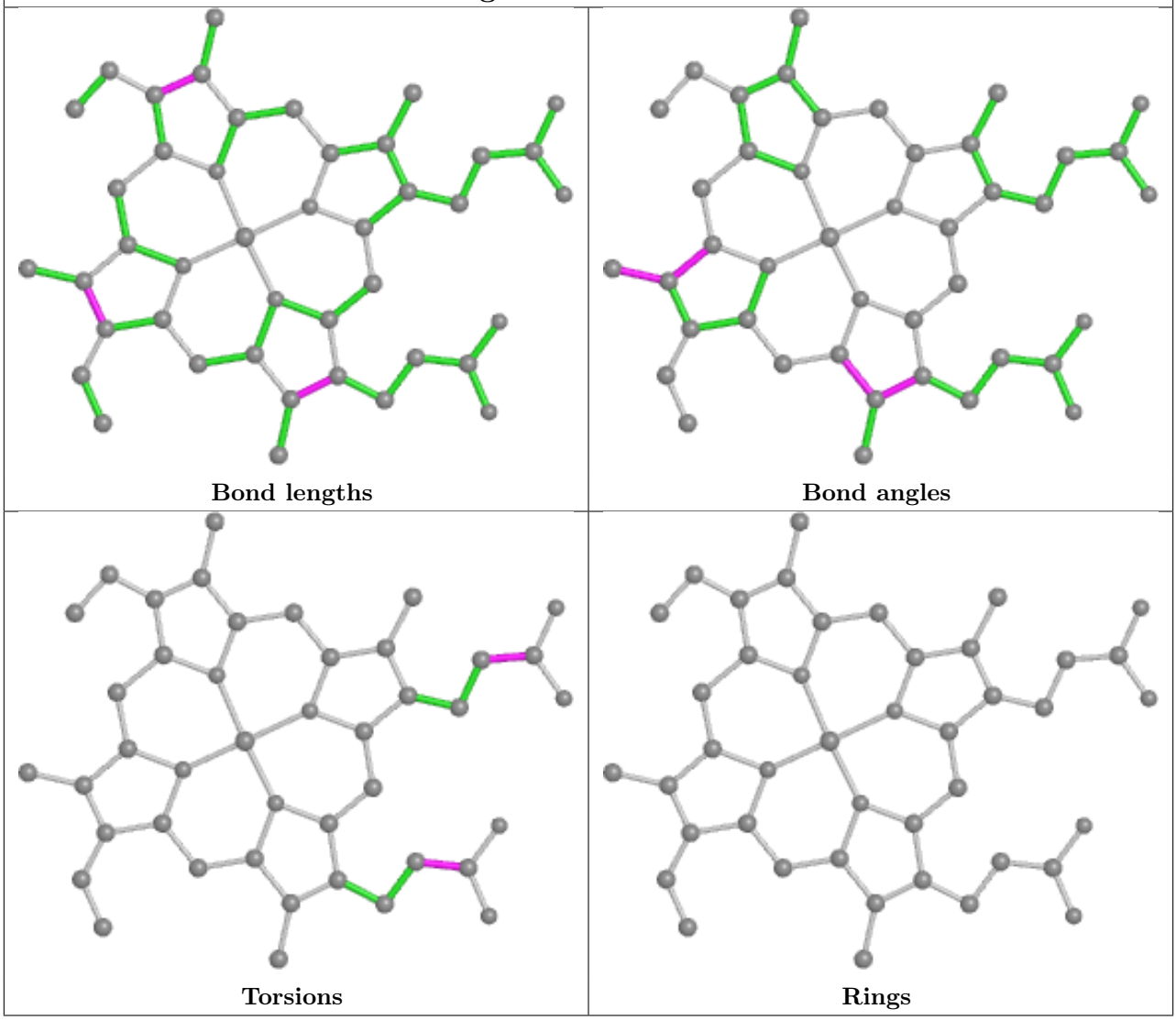


Torsions



Rings

Ligand HEC A 905



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	768/782 (98%)	-0.23	2 (0%)	94	95	32, 54, 77, 111	0
1	D	770/782 (98%)	-0.04	6 (0%)	86	87	37, 61, 83, 119	0
2	B	352/352 (100%)	-0.00	1 (0%)	94	95	38, 60, 80, 96	0
2	E	352/352 (100%)	0.28	5 (1%)	75	77	46, 77, 99, 113	0
3	C	314/314 (100%)	-0.04	5 (1%)	72	74	36, 57, 79, 97	0
3	F	314/314 (100%)	0.35	8 (2%)	57	59	46, 74, 91, 103	0
All	All	2870/2896 (99%)	-0.00	27 (0%)	84	85	32, 62, 87, 119	0

All (27) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	107	TYR	4.1
3	F	107	TYR	4.1
3	F	223	VAL	3.2
3	F	333	GLY	3.1
1	D	178	GLU	2.9
3	C	109	ARG	2.7
2	E	378	VAL	2.6
3	F	40	GLY	2.6
2	E	76	ALA	2.5
3	C	337	HIS	2.5
1	D	91	LEU	2.4
1	D	401	VAL	2.4
3	F	307	GLY	2.3
2	B	252	CYS	2.3
3	C	40	GLY	2.3
3	F	226	LEU	2.3
1	A	357	THR	2.3
2	E	252	CYS	2.2
2	E	79	GLN	2.2

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Mol	Chain	Res	Type	RSRZ
2	E	82	THR	2.2
3	C	41	GLN	2.2
1	D	651	GLY	2.1
1	D	398	GLY	2.1
3	F	349	TYR	2.1
1	D	642	VAL	2.1
1	A	178	GLU	2.1
3	F	147	PHE	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides 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
5	CA	F	401	1/1	0.35	0.18	79,79,79,79	0
5	CA	C	403	1/1	0.56	0.20	48,48,48,48	0
5	CA	C	401	1/1	0.70	0.15	54,54,54,54	0
9	MG	B	401	1/1	0.79	0.26	33,33,33,33	0
5	CA	F	403	1/1	0.83	0.12	88,88,88,88	0
5	CA	B	402	1/1	0.85	0.13	68,68,68,68	0
8	BET	A	907	8/8	0.85	0.24	62,75,83,86	0
5	CA	C	402	1/1	0.85	0.09	59,59,59,59	0
5	CA	E	402	1/1	0.87	0.06	76,76,76,76	0
5	CA	A	903	1/1	0.89	0.09	68,68,68,68	0
8	BET	C	406	8/8	0.90	0.33	65,74,80,81	0
9	MG	E	401	1/1	0.90	0.29	47,47,47,47	0
4	CL	D	901	1/1	0.91	0.11	60,60,60,60	0
8	BET	D	907	8/8	0.92	0.31	64,72,84,86	0
4	CL	A	901[B]	1/1	0.92	0.40	40,40,40,40	1

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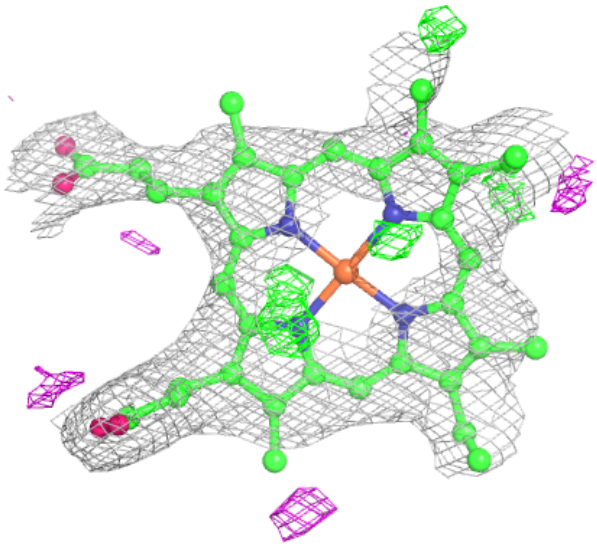
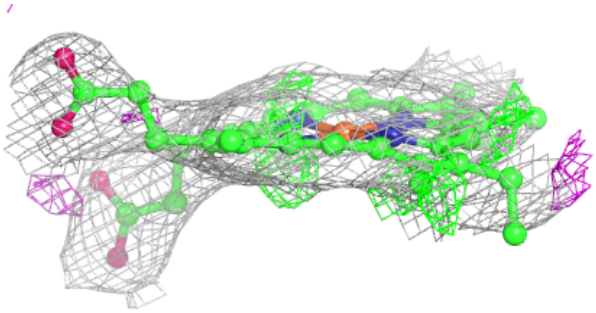
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	CL	A	901[A]	1/1	0.92	0.40	14,14,14,14	1
8	BET	A	909	8/8	0.93	0.38	72,80,84,89	0
5	CA	D	903	1/1	0.94	0.06	65,65,65,65	0
5	CA	D	902	1/1	0.94	0.06	68,68,68,68	0
6	ZN	D	904	1/1	0.94	0.18	53,53,53,53	0
5	CA	F	402	1/1	0.95	0.13	70,70,70,70	0
7	HEC	F	404	43/43	0.95	0.20	47,62,77,82	0
7	HEC	F	405	43/43	0.96	0.20	64,77,87,93	0
8	BET	E	403	8/8	0.96	0.21	63,66,71,74	0
8	BET	B	403	8/8	0.96	0.20	52,58,69,69	0
8	BET	A	908	8/8	0.96	0.20	62,69,72,77	0
7	HEC	C	405	43/43	0.97	0.17	42,61,70,75	0
7	HEC	D	905	43/43	0.97	0.18	38,53,67,71	0
7	HEC	D	906	43/43	0.97	0.15	36,46,58,74	0
5	CA	A	902	1/1	0.97	0.04	59,59,59,59	0
7	HEC	A	905	43/43	0.97	0.16	23,37,49,54	0
7	HEC	A	906	43/43	0.97	0.16	37,55,69,94	0
7	HEC	C	404	43/43	0.97	0.18	26,44,61,66	0
6	ZN	A	904	1/1	0.98	0.18	46,46,46,46	0

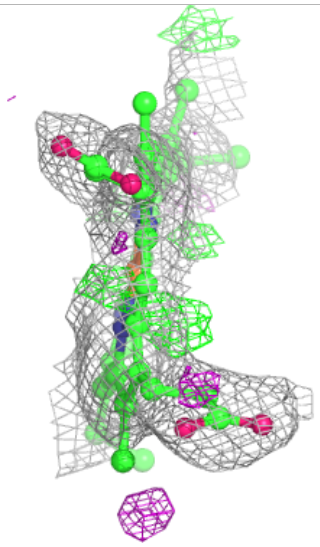
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around HEC F 404:

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

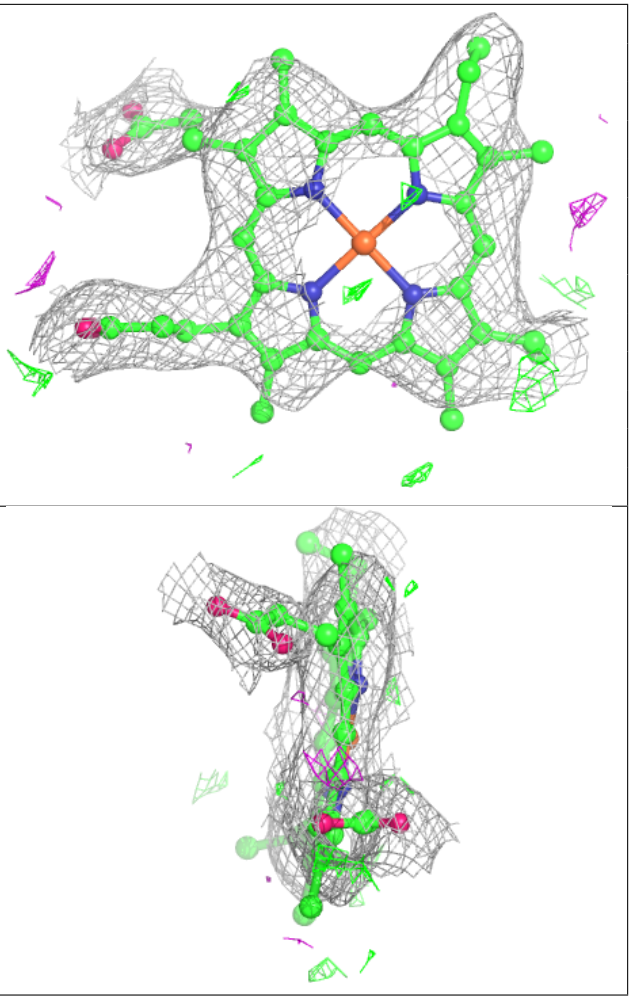






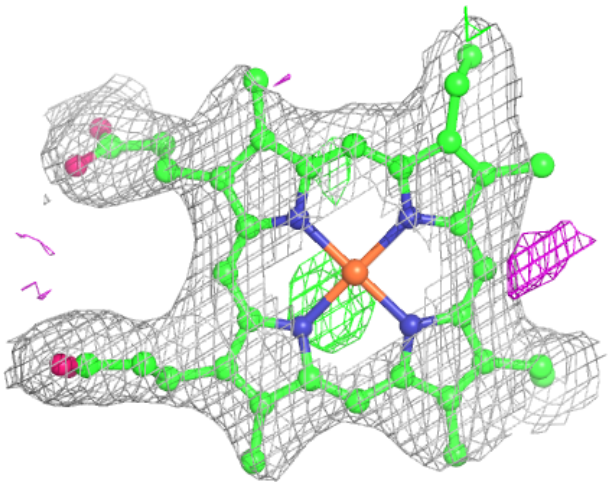
Electron density around HEC F 405:

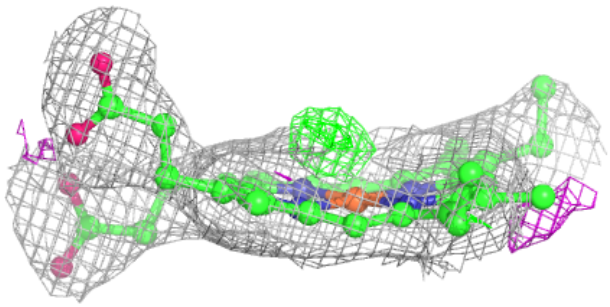
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

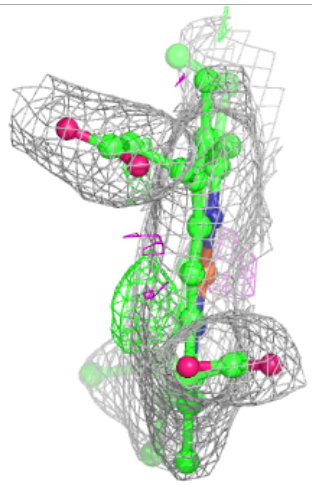


Electron density around HEC C 405:

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

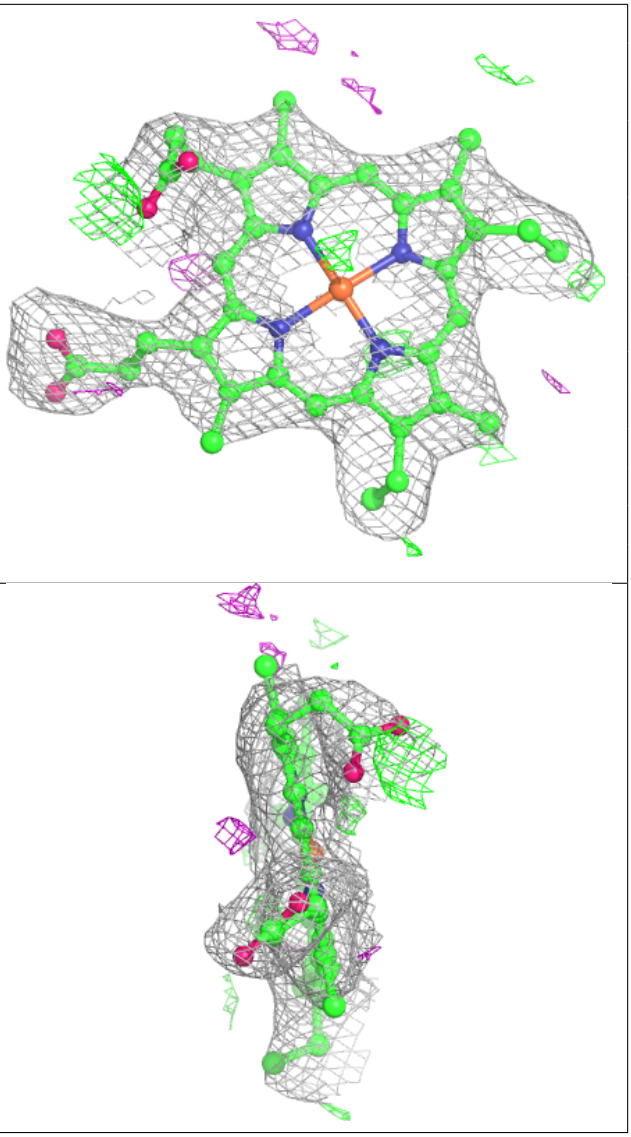






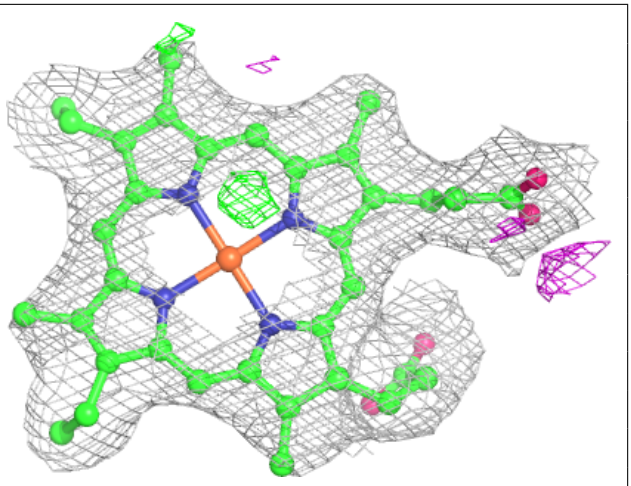
Electron density around HEC D 905:

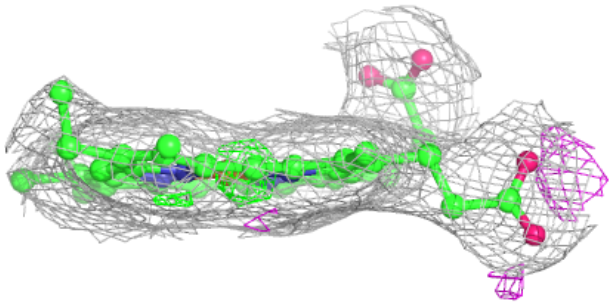
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around HEC D 906:

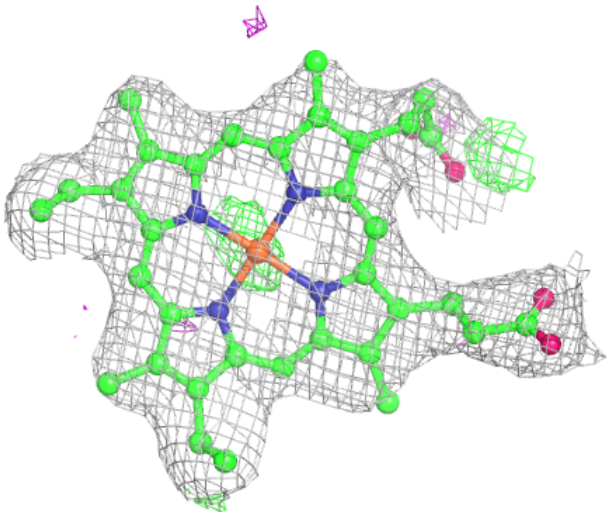
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

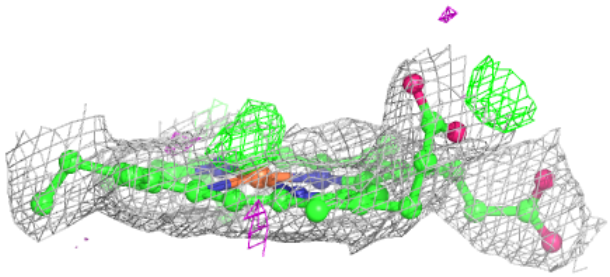


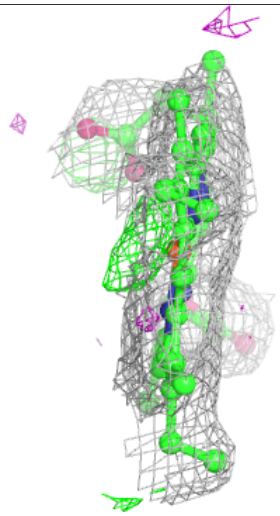


Electron density around HEC A 905:

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

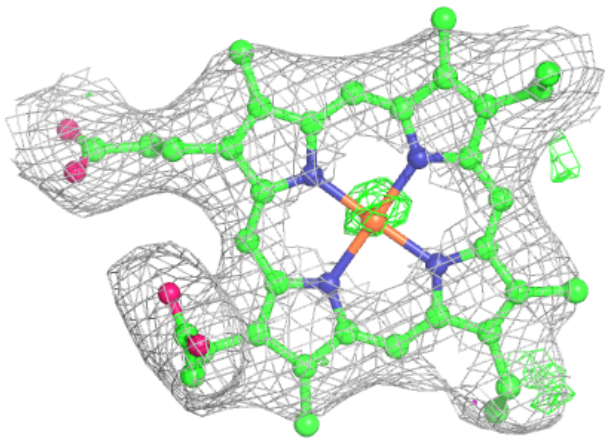


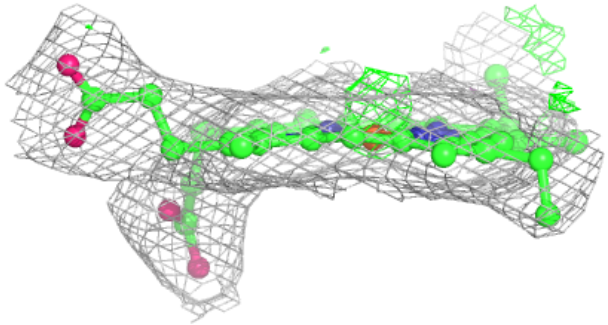




Electron density around HEC A 906:

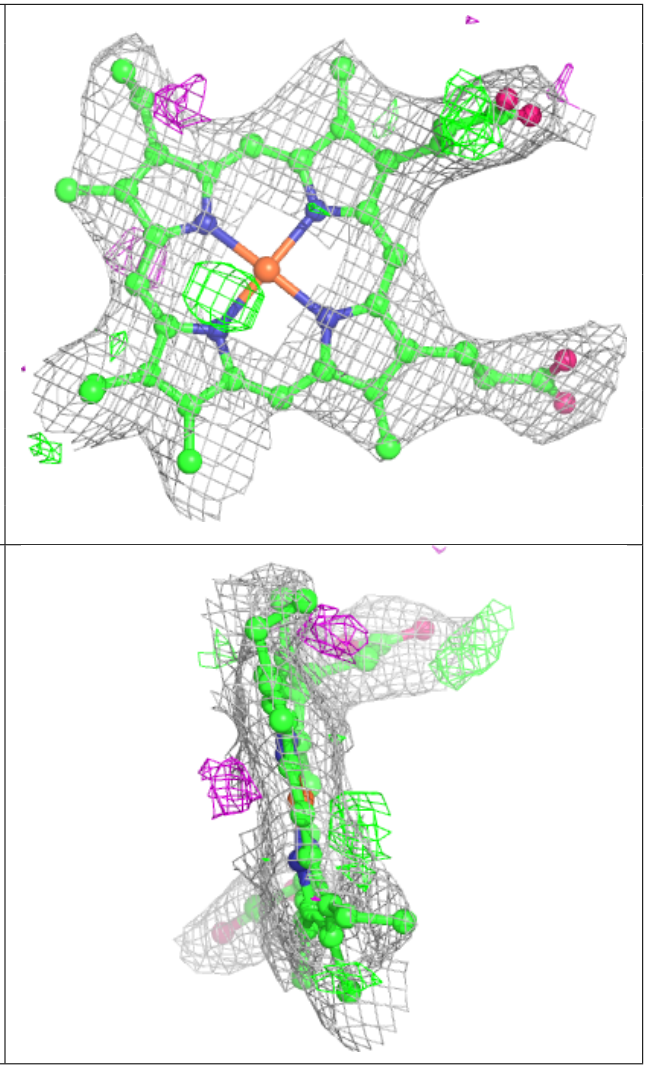
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





Electron density around HEC C 404:

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



6.5 Other polymers (i)

There are no such residues in this entry.