Full wwPDB NMR Structure Validation Report (i)

Sep 28, 2024 – 07:19 pm BST

PDB ID	:	2BPN
BMRB ID	:	5625
Title	:	SOLUTION STRUCTURE OF DESULFOVIBRIO VULGARIS (HILDENBOROUGH) FERRICYTOCHROME C3, NMR, 20 STRUCTURES
Authors	:	Messias, A.C.; Aguiar, A.P.; Brennan, L.; Xavier, A.V.; Turner, D.L.
Deposited on	:	2005-04-21

This is a Full wwPDB NMR 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/NMRValidationReportHelp
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:

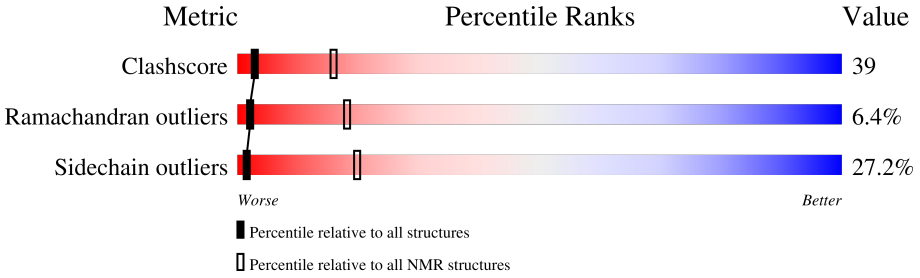
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
SOLUTION NMR

The overall completeness of chemical shifts assignment was not calculated.

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)	NMR archive (#Entries)
Clashscore	210492	14027
Ramachandran outliers	207382	12486
Sidechain outliers	206894	12463

The table below summarises the geometric issues observed across the polymeric chains and their fit to the experimental data. The red, orange, yellow and green segments indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A cyan segment indicates the fraction of residues that are not part of the well-defined cores, and 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%

Mol	Chain	Length	Quality of chain
1	A	107	34% 45% 12% • 8%

2 Ensemble composition and analysis (i)

This entry contains 20 models. Model 8 is the overall representative, medoid model (most similar to other models).

The following residues are included in the computation of the global validation metrics.

Well-defined (core) protein residues			
Well-defined core	**Residue range (total)**	**Backbone RMSD (Å)**	**Medoid model**
1	A:4-A:86, A:93-A:107 (98)	0.40	8

Ill-defined regions of proteins are excluded from the global statistics.

Ligands and non-protein polymers are included in the analysis.

The models can be grouped into 5 clusters. No single-model clusters were found.

Cluster number	Models
1	1, 2, 3, 4, 5, 8, 12, 15, 17
2	6, 9, 13, 19
3	10, 14, 20
4	7, 16
5	11, 18

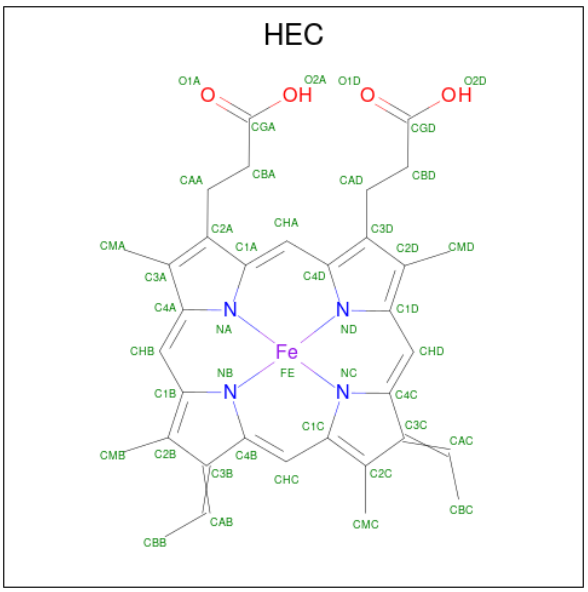
3 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 1900 atoms, of which 919 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called CYTOCHROME C3.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	107	1600	495	791	152	151	11	0

- Molecule 2 is HEME C (three-letter code: HEC) (formula: $C_{34}H_{34}FeN_4O_4$).



Mol	Chain	Residues	Atoms					
			Total	C	Fe	H	N	O
2	A	1	75	34	1	32	4	4
			Total	C	Fe	H	N	O
2	A	1	75	34	1	32	4	4
			Total	C	Fe	H	N	O
2	A	1	75	34	1	32	4	4
			Total	C	Fe	H	N	O
2	A	1	75	34	1	32	4	4

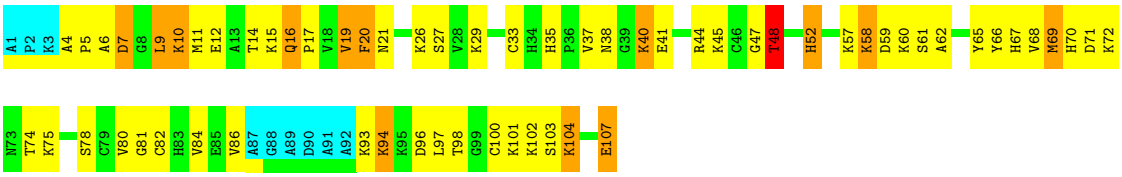
4 Residue-property plots (i)

4.1 Average score per residue in the NMR ensemble

These plots are provided for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic is the same as shown in the summary in section 1 of this report. The second graphic shows the sequence where residues are colour-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. Stretches of 2 or more consecutive residues without any outliers are shown as green connectors. Residues which are classified as ill-defined in the NMR ensemble, are shown in cyan with an underline colour-coded according to the previous scheme. Residues which were present in the experimental sample, but not modelled in the final structure are shown in grey.

• Molecule 1: CYTOCHROME C3

Chain A: 34% 45% 12% • 8%



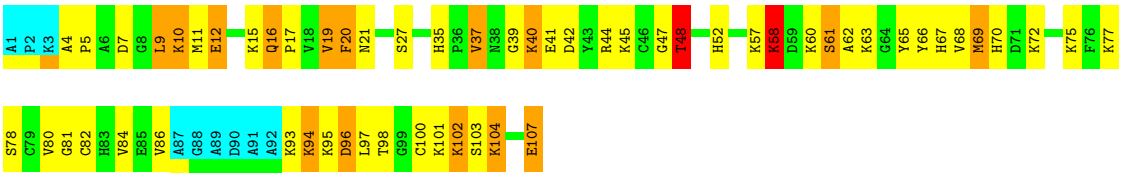
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

• Molecule 1: CYTOCHROME C3

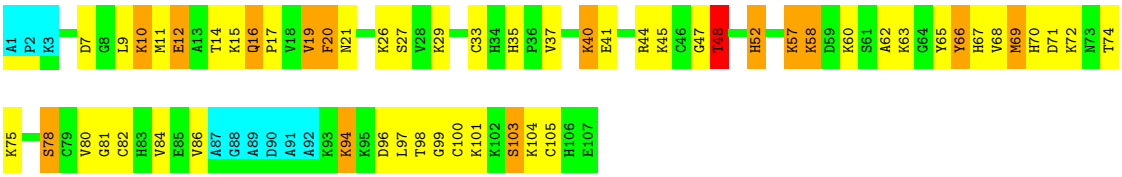
Chain A: 37% 38% 14% • 8%



4.2.2 Score per residue for model 2

• Molecule 1: CYTOCHROME C3

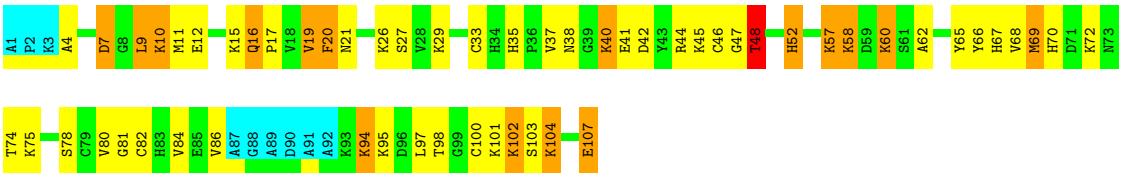
Chain A: 39% 38% 13% • 8%



4.2.3 Score per residue for model 3

- Molecule 1: CYTOCHROME C3

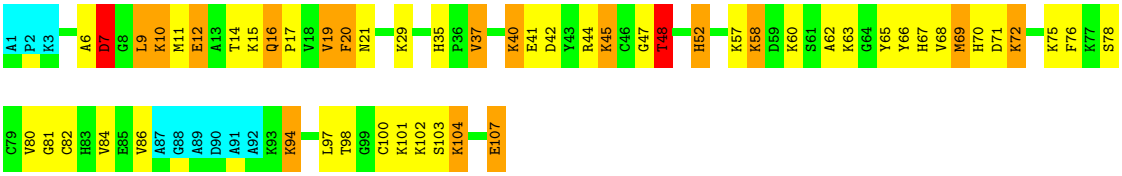
Chain A: 38% 37% 15% • 8%



4.2.4 Score per residue for model 4

- Molecule 1: CYTOCHROME C3

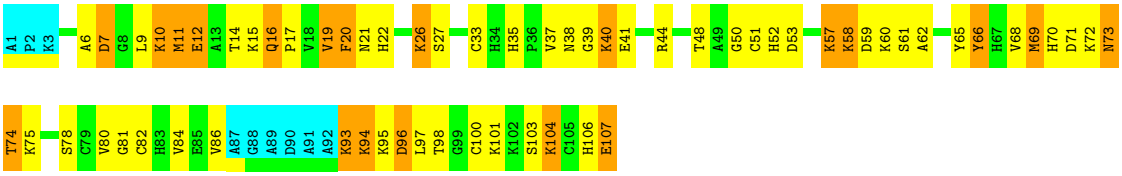
Chain A: 41% 34% 15% • 8%



4.2.5 Score per residue for model 5

- Molecule 1: CYTOCHROME C3

Chain A: 33% 40% 19% 8%



4.2.6 Score per residue for model 6

- Molecule 1: CYTOCHROME C3

Chain A: 36% 40% 15% • 8%

A1 P2 K3 A4 P5 A6 D7 G8 L9 K10 M11 E12 A13 T14 K15 Q16 P17 V18 V19 F20 K26 K29 C30 G31 D32 C33 H34 H35 P36 V37 N38 G39 K40 E41 D42 Y43 R44 K45 C46 G47 T48 C51 H52 D53 S54 M55 D56 K57 K58 D59 K60 S61 A62 Y65 Y66 H67

V68 M69 H70 D71 K77 S78 C79 V80 G81 C82 H83 V84 E85 V86 A87 G88 A89 D90 A91 A92 K93 K94 L97 T98 G99 C100 K101 K102 S103 K104 E107

4.2.7 Score per residue for model 7

- Molecule 1: CYTOCHROME C3

Chain A: 37% 38% 13% • 8%

A1 P2 K3 A6 D7 G8 L9 K10 M11 E12 K15 Q16 V19 F20 N21 K26 K29 H35 P36 V37 N38 G39 K40 E41 D42 Y43 R44 K45 C46 G47 T48 H52 K57 K58 D59 K60 S61 A62 Y65 Y66 H67 V68 M69 H70 T74 K75 S78 C79 V80

G81 C82 H83 V84 E85 V86 A87 G88 A89 D90 A91 A92 K93 K94 K95 D96 L97 T98 G99 C100 K101 K102 S103 K104 C105 H106 E107

4.2.8 Score per residue for model 8 (medoid)

- Molecule 1: CYTOCHROME C3

Chain A: 36% 38% 15% • 8%

A1 P2 K3 A4 P5 A6 D7 G8 L9 K10 M11 E12 A13 T14 K15 Q16 P17 V18 V19 F20 S27 V28 K29 H35 P36 V37 N38 G39 K40 E41 D42 Y43 R44 K45 C46 G47 T48 H52 K58 D59 K60 S61 A62 K63 G64 Y65 Y66 H67 V68 M69 H70 D71 K72 K75

V80 G81 C82 H83 V84 E85 V86 A87 G88 A89 D90 A91 A92 K93 K94 K95 D96 L97 T98 G99 C100 K101 K102 S103 K104 E107

4.2.9 Score per residue for model 9

- Molecule 1: CYTOCHROME C3

Chain A: 35% 40% 16% • 8%

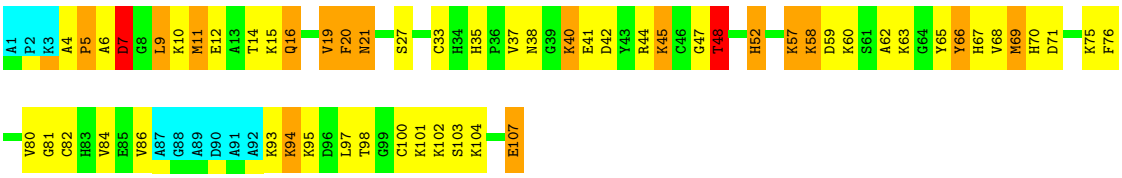
A1 P2 K3 A4 P5 A6 D7 G8 L9 K10 M11 E12 A13 T14 K15 Q16 P17 V18 V19 F20 N21 T24 H25 K26 S27 V28 K29 V37 N38 G39 K40 E41 D42 Y43 R44 K45 C46 G47 T48 C51 H52 D53 K57 K58 D59 K60 S61 A62 Y65 Y66 H67 V68 M69 H70 D71

K72 N73 T74 K75 V80 G81 V84 E85 V86 A87 G88 A89 D90 A91 A92 K93 K94 K95 D96 L97 T98 G99 C100 K101 K102 S103 K104 E107

4.2.10 Score per residue for model 10

- Molecule 1: CYTOCHROME C3

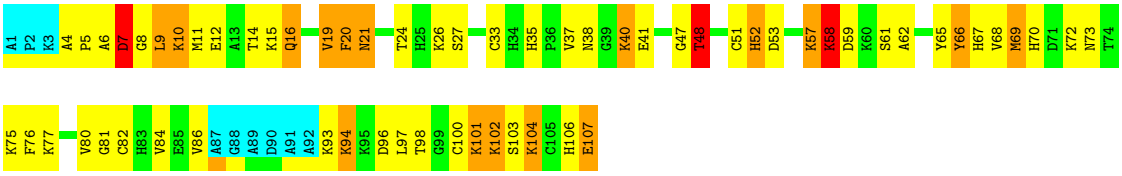
Chain A: 37% 37% 15% • 8%



4.2.11 Score per residue for model 11

- Molecule 1: CYTOCHROME C3

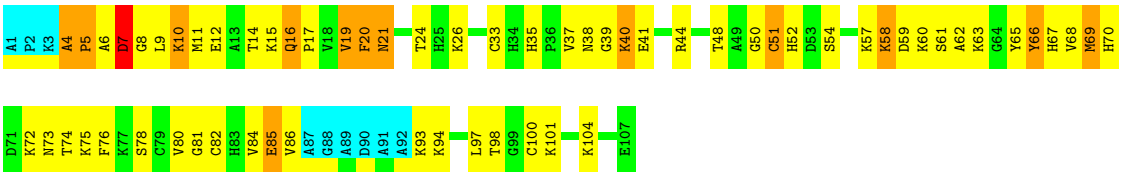
Chain A: 34% 40% 15% • 8%



4.2.12 Score per residue for model 12

- Molecule 1: CYTOCHROME C3

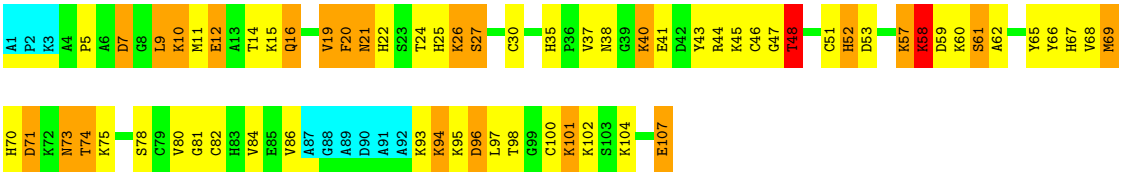
Chain A: 33% 46% 12% • 8%



4.2.13 Score per residue for model 13

- Molecule 1: CYTOCHROME C3

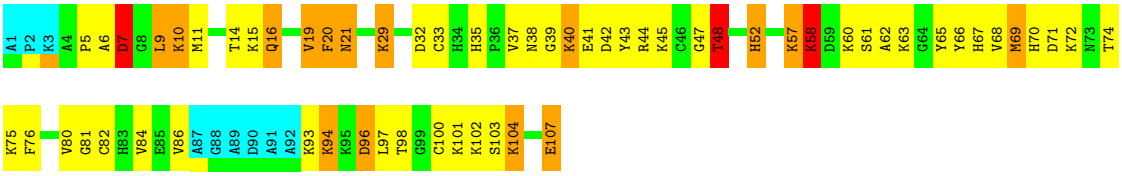
Chain A: 31% 38% 21% • 8%



4.2.14 Score per residue for model 14

- Molecule 1: CYTOCHROME C3

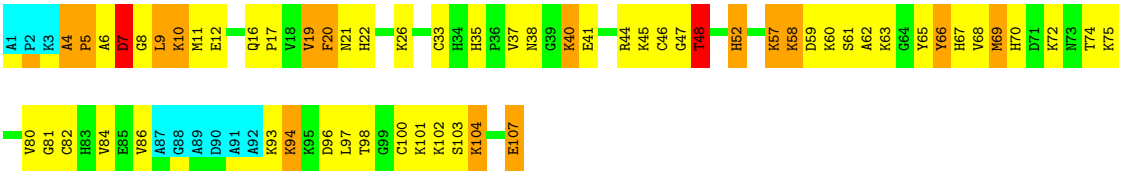
Chain A: 35% 40% 14% • 8%



4.2.15 Score per residue for model 15

- Molecule 1: CYTOCHROME C3

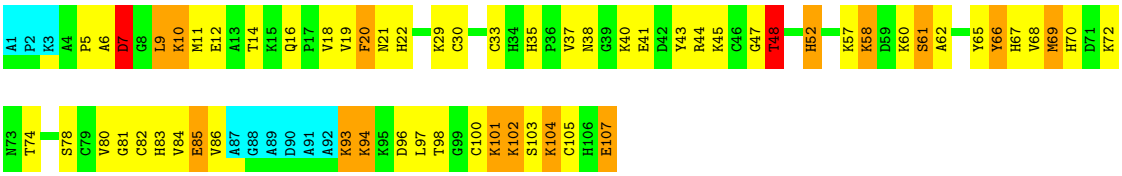
Chain A: 36% 40% 14% • 8%



4.2.16 Score per residue for model 16

- Molecule 1: CYTOCHROME C3

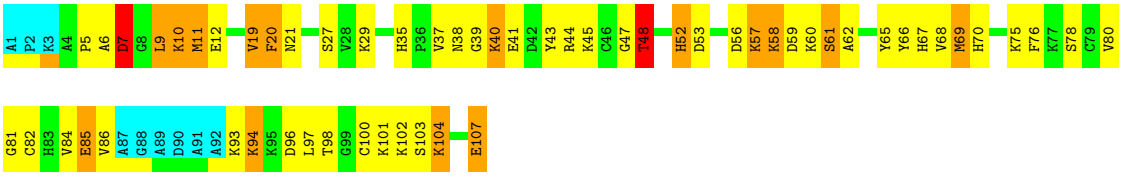
Chain A: 35% 41% 14% • 8%



4.2.17 Score per residue for model 17

- Molecule 1: CYTOCHROME C3

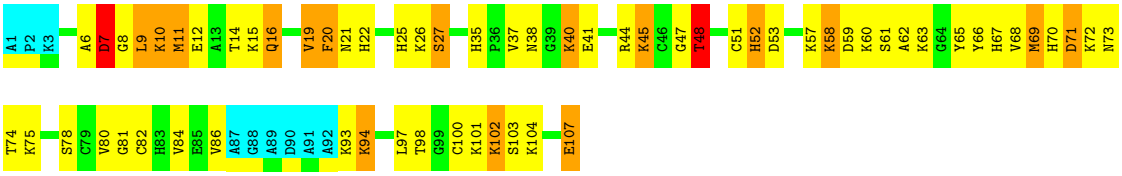
Chain A: 37% 38% 14% • 8%



4.2.18 Score per residue for model 18

- Molecule 1: CYTOCHROME C3

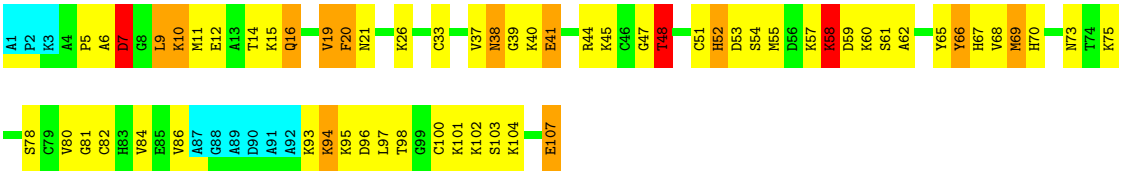
Chain A: 33% 42% 15% • 8%



4.2.19 Score per residue for model 19

- Molecule 1: CYTOCHROME C3

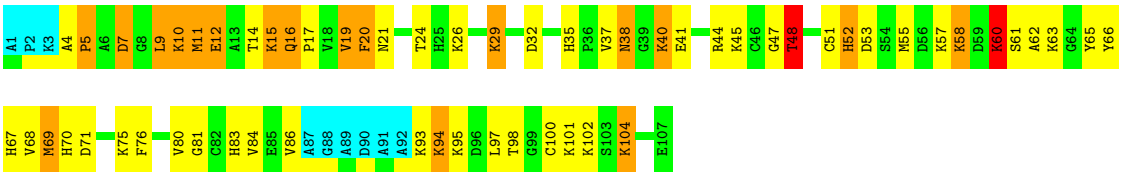
Chain A: 35% 43% 11% • 8%



4.2.20 Score per residue for model 20

- Molecule 1: CYTOCHROME C3

Chain A: 36% 37% 17% • 8%



5 Refinement protocol and experimental data overview (i)

The models were refined using the following method: *TORSION ANGLE DYNAMICS WITH SIMULATED ANNEALING*.

Of the 155 calculated structures, 20 were deposited, based on the following criterion: *LEAST RESTRAINT VIOLATION*.

The following table shows the software used for structure solution, optimisation and refinement.

Software name	Classification	Version
PARADYANA	refinement	
PARADYANA	structure solution	

No chemical shift data was provided.

6 Model quality (i)

6.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: HEC

There are no covalent bond-length or bond-angle outliers.

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

6.2 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 each 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 averaged over the ensemble.

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	756	737	738	60±5
2	A	172	128	120	30±4
All	All	18560	17300	17160	1400

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 39.

All unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:37:VAL:HG11	2:A:109:HEC:HBC2	1.09	1.22	7	12
1:A:80:VAL:HG22	2:A:111:HEC:HMC2	0.97	1.37	20	19
1:A:80:VAL:O	1:A:84:VAL:HG23	0.96	1.61	16	20
1:A:52:HIS:CE1	1:A:68:VAL:HG11	0.94	1.96	1	20
1:A:82:CYS:O	1:A:86:VAL:HG23	0.92	1.64	4	18
1:A:37:VAL:HG11	2:A:109:HEC:CBC	0.90	1.96	19	12
2:A:108:HEC:HBC3	2:A:108:HEC:HMC1	0.88	1.46	16	20
2:A:108:HEC:HBB3	2:A:108:HEC:HMB1	0.88	1.46	14	20
2:A:110:HEC:HMC1	2:A:110:HEC:HBC3	0.88	1.46	3	20
1:A:66:TYR:CD2	1:A:70:HIS:CE1	0.81	2.68	16	18
1:A:57:LYS:NZ	2:A:111:HEC:HMA2	0.81	1.91	14	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:10:LYS:HB3	1:A:19:VAL:HG23	0.81	1.52	8	16
1:A:104:LYS:HB3	2:A:110:HEC:HMA3	0.80	1.53	15	18
1:A:37:VAL:CG1	2:A:109:HEC:HBC2	0.80	2.06	20	12
1:A:100:CYS:SG	2:A:111:HEC:HMB1	0.80	2.15	14	18
1:A:9:LEU:HD21	1:A:20:PHE:CE1	0.78	2.13	16	10
2:A:108:HEC:HMC1	2:A:108:HEC:CBC	0.77	2.09	14	20
1:A:20:PHE:CE2	2:A:110:HEC:HBB2	0.77	2.15	9	1
1:A:78:SER:O	2:A:110:HEC:HMC3	0.76	1.80	4	10
1:A:10:LYS:CB	1:A:19:VAL:HG23	0.76	2.09	15	17
2:A:111:HEC:HMC1	2:A:111:HEC:HBC3	0.76	1.55	20	19
1:A:66:TYR:CE2	1:A:70:HIS:CD2	0.74	2.75	4	12
2:A:110:HEC:HMB1	2:A:110:HEC:HBB3	0.73	1.59	17	20
1:A:80:VAL:HG22	2:A:111:HEC:CMC	0.73	2.13	20	12
1:A:20:PHE:CZ	2:A:108:HEC:CHD	0.72	2.71	16	19
1:A:35:HIS:CE1	1:A:37:VAL:HG22	0.72	2.19	3	18
2:A:108:HEC:HMB1	2:A:108:HEC:CBB	0.71	2.16	14	3
1:A:9:LEU:HD21	1:A:20:PHE:CD1	0.71	2.20	16	11
1:A:57:LYS:HZ1	2:A:111:HEC:HMA2	0.69	1.45	14	1
1:A:37:VAL:HG11	2:A:109:HEC:CAC	0.69	2.17	6	9
1:A:66:TYR:CD1	1:A:66:TYR:O	0.68	2.47	10	18
1:A:86:VAL:HG11	2:A:110:HEC:O1D	0.66	1.89	10	4
2:A:108:HEC:CGD	2:A:108:HEC:CMD	0.65	2.74	15	3
1:A:104:LYS:O	2:A:110:HEC:HMA3	0.65	1.90	2	1
1:A:93:LYS:HD2	1:A:97:LEU:HD11	0.65	1.69	19	4
1:A:20:PHE:CD1	1:A:20:PHE:O	0.64	2.51	16	19
1:A:5:PRO:HG2	2:A:108:HEC:C3A	0.64	2.23	9	2
2:A:110:HEC:HMC1	2:A:110:HEC:CBC	0.64	2.21	3	20
2:A:108:HEC:HMA2	2:A:108:HEC:O1A	0.63	1.94	5	2
1:A:26:LYS:O	1:A:27:SER:CB	0.63	2.46	13	4
1:A:33:CYS:O	2:A:109:HEC:HBB2	0.63	1.93	3	11
1:A:65:TYR:CE2	2:A:111:HEC:O2D	0.63	2.51	17	11
1:A:65:TYR:CE1	1:A:69:MET:CE	0.63	2.82	18	18
1:A:21:ASN:HD22	1:A:21:ASN:N	0.62	1.90	12	1
1:A:66:TYR:CD1	1:A:66:TYR:C	0.62	2.73	12	15
1:A:65:TYR:CE2	2:A:111:HEC:O1D	0.61	2.53	7	6
1:A:9:LEU:HD13	2:A:108:HEC:HAD2	0.61	1.73	11	3
1:A:40:LYS:O	1:A:41:GLU:C	0.60	2.39	19	20
2:A:108:HEC:CGD	2:A:108:HEC:HMD1	0.60	2.25	15	3
1:A:60:LYS:O	1:A:67:HIS:CE1	0.60	2.55	18	8
2:A:109:HEC:HMD1	2:A:109:HEC:O2D	0.60	1.97	6	1
1:A:65:TYR:O	1:A:69:MET:CG	0.60	2.49	6	20

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:61:SER:O	1:A:67:HIS:CD2	0.60	2.55	20	10
1:A:45:LYS:HD3	1:A:48:THR:HG23	0.58	1.75	19	3
1:A:10:LYS:CD	1:A:10:LYS:N	0.58	2.66	16	2
1:A:93:LYS:NZ	1:A:97:LEU:HD11	0.58	2.14	20	1
1:A:20:PHE:CD2	2:A:110:HEC:HBB2	0.57	2.34	9	1
1:A:62:ALA:CB	2:A:109:HEC:CBD	0.57	2.82	4	1
1:A:97:LEU:O	2:A:111:HEC:HMC1	0.57	2.00	4	19
1:A:45:LYS:O	2:A:109:HEC:HMC3	0.56	2.01	20	12
1:A:66:TYR:O	1:A:66:TYR:CG	0.56	2.59	16	18
1:A:9:LEU:HD21	1:A:20:PHE:HD1	0.56	1.60	11	4
2:A:108:HEC:C2D	2:A:108:HEC:O2D	0.56	2.54	9	1
1:A:71:ASP:HB3	1:A:74:THR:HG23	0.55	1.77	9	2
1:A:16:GLN:OE1	2:A:111:HEC:C1A	0.55	2.55	10	3
1:A:75:LYS:NZ	1:A:76:PHE:CE1	0.55	2.73	14	2
1:A:42:ASP:OD2	2:A:109:HEC:HMC2	0.55	2.01	1	1
1:A:97:LEU:O	2:A:111:HEC:CMC	0.55	2.55	4	20
1:A:60:LYS:O	1:A:67:HIS:CG	0.55	2.60	10	4
1:A:20:PHE:CE1	2:A:108:HEC:CHD	0.55	2.91	11	4
1:A:66:TYR:C	1:A:66:TYR:CD1	0.55	2.81	7	2
1:A:10:LYS:CG	1:A:19:VAL:HG23	0.54	2.33	3	1
2:A:108:HEC:O2A	2:A:108:HEC:HMA2	0.54	2.02	12	1
1:A:52:HIS:CE1	1:A:62:ALA:O	0.54	2.60	19	11
1:A:66:TYR:O	1:A:70:HIS:ND1	0.54	2.41	7	7
1:A:35:HIS:CG	1:A:76:PHE:CE2	0.54	2.96	17	2
1:A:47:GLY:O	1:A:48:THR:O	0.53	2.26	3	18
1:A:101:LYS:O	1:A:102:LYS:CB	0.53	2.56	3	14
1:A:60:LYS:O	1:A:67:HIS:CD2	0.53	2.62	10	7
1:A:20:PHE:CZ	2:A:108:HEC:C4C	0.52	2.93	11	18
1:A:65:TYR:CE1	1:A:69:MET:HE3	0.52	2.39	13	9
1:A:12:GLU:O	1:A:12:GLU:CG	0.52	2.56	16	6
1:A:60:LYS:O	1:A:61:SER:CB	0.52	2.58	1	4
1:A:9:LEU:HD21	1:A:20:PHE:HE1	0.52	1.64	16	3
1:A:62:ALA:CB	2:A:109:HEC:O2A	0.52	2.58	12	1
2:A:108:HEC:O1D	2:A:108:HEC:C2D	0.52	2.57	15	1
1:A:62:ALA:CB	2:A:109:HEC:O1A	0.52	2.58	5	1
1:A:57:LYS:NZ	1:A:66:TYR:CE1	0.52	2.77	20	2
1:A:57:LYS:O	1:A:58:LYS:CB	0.51	2.58	1	17
1:A:52:HIS:ND1	1:A:62:ALA:O	0.51	2.44	15	20
1:A:76:PHE:O	2:A:109:HEC:HMA2	0.51	2.06	10	2
1:A:57:LYS:HE2	1:A:66:TYR:CE1	0.51	2.41	20	2
2:A:108:HEC:CGD	2:A:108:HEC:C2D	0.50	2.89	9	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:16:GLN:HG2	1:A:106:HIS:CE1	0.50	2.42	7	2
1:A:66:TYR:CE2	1:A:70:HIS:CG	0.50	2.99	4	8
1:A:5:PRO:CG	1:A:22:HIS:CE1	0.50	2.95	16	1
1:A:65:TYR:CD1	1:A:69:MET:HE3	0.50	2.42	18	8
1:A:67:HIS:CE1	1:A:74:THR:HG22	0.50	2.41	15	4
1:A:103:SER:O	1:A:107:GLU:CB	0.50	2.60	1	10
1:A:52:HIS:ND1	1:A:68:VAL:HG11	0.49	2.21	7	6
1:A:57:LYS:O	1:A:58:LYS:CG	0.49	2.60	7	9
1:A:66:TYR:CE2	2:A:111:HEC:C4A	0.49	2.95	4	6
1:A:57:LYS:N	1:A:57:LYS:CD	0.49	2.75	15	1
1:A:66:TYR:CE2	1:A:70:HIS:NE2	0.49	2.80	4	5
2:A:109:HEC:HBB3	2:A:109:HEC:HMB1	0.49	1.83	3	3
1:A:72:LYS:N	1:A:72:LYS:CD	0.49	2.74	4	1
1:A:104:LYS:O	2:A:110:HEC:CMA	0.49	2.61	2	1
1:A:5:PRO:HG3	1:A:22:HIS:CE1	0.49	2.42	16	1
2:A:110:HEC:C2D	2:A:110:HEC:O2D	0.49	2.60	3	1
1:A:66:TYR:CD2	1:A:70:HIS:ND1	0.49	2.80	13	16
1:A:37:VAL:HG11	2:A:109:HEC:CHD	0.49	2.38	3	1
1:A:94:LYS:O	1:A:98:THR:OG1	0.49	2.30	7	20
1:A:9:LEU:O	1:A:19:VAL:HG22	0.49	2.08	7	2
1:A:65:TYR:O	1:A:68:VAL:HG22	0.49	2.07	17	6
1:A:81:GLY:O	1:A:84:VAL:N	0.48	2.46	1	20
1:A:97:LEU:HD23	1:A:97:LEU:N	0.48	2.22	15	3
1:A:11:MET:SD	2:A:108:HEC:CGD	0.48	3.01	5	7
1:A:85:GLU:O	1:A:85:GLU:CG	0.48	2.61	8	1
1:A:46:CYS:SG	2:A:108:HEC:CGD	0.48	3.02	15	2
1:A:14:THR:HG23	2:A:111:HEC:O2D	0.48	2.08	6	5
1:A:16:GLN:OE1	2:A:111:HEC:C2A	0.48	2.62	4	2
1:A:66:TYR:CE2	1:A:70:HIS:CE1	0.48	3.01	6	12
2:A:110:HEC:CHA	2:A:110:HEC:CGD	0.48	2.92	8	2
1:A:11:MET:HE3	2:A:108:HEC:HMD1	0.48	1.84	14	2
1:A:101:LYS:CD	1:A:102:LYS:N	0.48	2.77	16	3
1:A:35:HIS:ND1	1:A:37:VAL:HG22	0.48	2.23	3	3
1:A:99:GLY:O	1:A:103:SER:CB	0.47	2.62	2	1
2:A:108:HEC:O2D	2:A:108:HEC:C3D	0.47	2.61	9	1
1:A:7:ASP:N	1:A:7:ASP:OD1	0.47	2.47	10	1
2:A:111:HEC:HMC1	2:A:111:HEC:CBC	0.47	2.34	20	2
1:A:14:THR:HG23	2:A:111:HEC:O1D	0.47	2.09	19	8
1:A:10:LYS:HB2	1:A:19:VAL:HG23	0.47	1.85	15	2
1:A:68:VAL:HB	2:A:109:HEC:CHB	0.47	2.40	3	20
1:A:33:CYS:O	2:A:109:HEC:CBB	0.47	2.62	11	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:80:VAL:HG22	2:A:111:HEC:C2C	0.47	2.40	14	4
1:A:67:HIS:CE1	1:A:71:ASP:OD2	0.47	2.68	9	1
1:A:14:THR:HG23	2:A:111:HEC:CGD	0.47	2.39	12	2
1:A:76:PHE:CE2	2:A:109:HEC:O2D	0.47	2.67	12	1
1:A:11:MET:CE	2:A:108:HEC:O1D	0.47	2.62	6	7
1:A:30:CYS:CB	1:A:43:TYR:OH	0.47	2.63	13	3
1:A:51:CYS:O	1:A:53:ASP:N	0.47	2.48	9	7
1:A:35:HIS:CD2	1:A:76:PHE:CD2	0.46	3.02	4	1
1:A:57:LYS:HZ1	1:A:66:TYR:HE1	0.46	1.50	6	1
1:A:75:LYS:HD3	1:A:76:PHE:CE1	0.46	2.45	11	1
1:A:103:SER:O	1:A:107:GLU:N	0.46	2.49	11	13
1:A:100:CYS:SG	2:A:111:HEC:CMB	0.46	3.00	18	3
1:A:99:GLY:C	1:A:103:SER:CB	0.46	2.83	2	1
2:A:108:HEC:CBB	2:A:108:HEC:CMB	0.46	2.91	14	3
1:A:80:VAL:O	1:A:84:VAL:CG2	0.46	2.57	4	2
1:A:70:HIS:N	1:A:78:SER:OG	0.46	2.49	13	1
2:A:108:HEC:CMD	2:A:108:HEC:O1D	0.46	2.63	15	1
1:A:15:LYS:O	1:A:16:GLN:NE2	0.46	2.48	19	1
2:A:109:HEC:O1A	2:A:109:HEC:CHA	0.46	2.63	5	1
2:A:110:HEC:CHA	2:A:110:HEC:O1D	0.46	2.64	8	1
1:A:37:VAL:HG12	1:A:38:ASN:ND2	0.46	2.26	20	1
1:A:103:SER:O	1:A:107:GLU:CA	0.46	2.64	11	3
1:A:62:ALA:CB	2:A:109:HEC:HBD1	0.46	2.41	4	1
2:A:109:HEC:O1D	2:A:109:HEC:C2D	0.46	2.64	9	1
1:A:85:GLU:OE1	1:A:85:GLU:CA	0.46	2.64	17	3
2:A:108:HEC:CBC	2:A:108:HEC:CMC	0.45	2.90	19	17
1:A:22:HIS:O	1:A:26:LYS:N	0.45	2.49	18	2
1:A:69:MET:O	1:A:70:HIS:ND1	0.45	2.49	17	1
1:A:11:MET:CE	2:A:108:HEC:O2D	0.45	2.63	2	6
1:A:9:LEU:O	1:A:19:VAL:CG2	0.45	2.64	10	2
1:A:102:LYS:O	1:A:107:GLU:CG	0.45	2.64	8	3
1:A:57:LYS:HE2	1:A:66:TYR:CD1	0.45	2.46	6	1
1:A:67:HIS:ND1	1:A:71:ASP:OD2	0.45	2.50	6	3
1:A:67:HIS:NE2	2:A:109:HEC:O2A	0.45	2.49	13	3
1:A:80:VAL:O	1:A:84:VAL:N	0.45	2.49	7	5
1:A:38:ASN:ND2	1:A:38:ASN:N	0.45	2.64	20	1
1:A:58:LYS:O	1:A:60:LYS:CD	0.45	2.64	16	1
1:A:58:LYS:O	1:A:60:LYS:CE	0.45	2.65	16	1
1:A:44:ARG:O	1:A:45:LYS:C	0.45	2.55	8	17
2:A:109:HEC:O1D	2:A:109:HEC:C3D	0.45	2.64	9	1
1:A:82:CYS:O	1:A:86:VAL:N	0.45	2.49	12	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:96:ASP:N	1:A:96:ASP:OD1	0.45	2.50	8	4
2:A:109:HEC:O2A	2:A:109:HEC:CHA	0.45	2.64	12	1
1:A:37:VAL:C	1:A:39:GLY:N	0.45	2.70	8	5
1:A:62:ALA:CB	2:A:109:HEC:HBD2	0.44	2.40	4	1
1:A:68:VAL:C	1:A:69:MET:HG2	0.44	2.31	17	1
1:A:6:ALA:O	1:A:7:ASP:C	0.44	2.56	12	6
1:A:21:ASN:N	1:A:21:ASN:OD1	0.44	2.51	14	1
1:A:58:LYS:O	1:A:60:LYS:NZ	0.44	2.50	16	1
1:A:57:LYS:HZ1	2:A:111:HEC:CMA	0.44	2.22	14	1
1:A:11:MET:HE3	2:A:108:HEC:O2D	0.44	2.12	2	2
1:A:45:LYS:O	1:A:48:THR:OG1	0.44	2.35	8	10
1:A:21:ASN:OD1	1:A:21:ASN:N	0.44	2.49	10	1
1:A:21:ASN:N	1:A:21:ASN:ND2	0.44	2.63	12	1
1:A:103:SER:OG	1:A:104:LYS:N	0.43	2.49	2	1
2:A:110:HEC:O2D	2:A:110:HEC:CMD	0.43	2.65	3	1
1:A:14:THR:HG22	1:A:55:MET:SD	0.43	2.53	6	3
1:A:9:LEU:HD13	2:A:108:HEC:CAD	0.43	2.43	7	1
1:A:74:THR:HG22	2:A:109:HEC:O2A	0.43	2.13	9	2
1:A:68:VAL:HB	2:A:109:HEC:C4A	0.43	2.42	17	1
1:A:74:THR:HG22	2:A:109:HEC:O1A	0.43	2.13	2	2
1:A:11:MET:HE3	2:A:108:HEC:O1D	0.43	2.12	6	3
1:A:15:LYS:C	1:A:16:GLN:CG	0.43	2.86	5	3
1:A:11:MET:HE2	2:A:108:HEC:O2D	0.43	2.13	13	1
1:A:69:MET:CA	1:A:78:SER:OG	0.43	2.67	13	1
1:A:57:LYS:CE	1:A:66:TYR:CE1	0.43	3.02	20	1
1:A:62:ALA:HB1	2:A:109:HEC:CBD	0.43	2.43	4	1
1:A:16:GLN:OE1	1:A:106:HIS:CE1	0.43	2.72	5	1
1:A:20:PHE:CZ	2:A:108:HEC:C1D	0.43	3.02	16	1
1:A:72:LYS:C	1:A:74:THR:N	0.43	2.72	5	2
2:A:108:HEC:C2D	2:A:108:HEC:O1D	0.43	2.67	13	1
1:A:5:PRO:HG2	1:A:22:HIS:ND1	0.43	2.28	16	1
1:A:18:VAL:HG22	1:A:105:CYS:O	0.43	2.14	16	1
1:A:12:GLU:CB	1:A:17:PRO:HB3	0.43	2.44	2	11
1:A:22:HIS:O	1:A:26:LYS:CG	0.43	2.67	5	1
1:A:62:ALA:HB1	2:A:109:HEC:O1A	0.43	2.13	5	1
2:A:110:HEC:CGD	2:A:110:HEC:HHA	0.43	2.44	8	2
2:A:110:HEC:HMB1	2:A:110:HEC:CBB	0.43	2.40	17	3
1:A:15:LYS:C	1:A:16:GLN:CD	0.42	2.78	14	8
2:A:110:HEC:CBC	2:A:110:HEC:CMC	0.42	2.95	3	6
1:A:62:ALA:HB1	2:A:109:HEC:O2A	0.42	2.13	12	1
1:A:96:ASP:HB3	1:A:104:LYS:CE	0.42	2.45	2	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:32:ASP:OD2	2:A:110:HEC:CBC	0.42	2.67	6	1
1:A:37:VAL:O	1:A:39:GLY:N	0.42	2.53	1	3
2:A:109:HEC:O1D	2:A:109:HEC:CMD	0.42	2.67	9	1
1:A:80:VAL:CG2	2:A:111:HEC:C2C	0.42	2.97	16	1
1:A:65:TYR:O	1:A:69:MET:SD	0.42	2.78	12	1
1:A:57:LYS:N	1:A:57:LYS:HD3	0.42	2.30	15	1
1:A:15:LYS:O	1:A:16:GLN:CD	0.42	2.58	11	2
1:A:26:LYS:O	1:A:27:SER:OG	0.42	2.38	9	2
1:A:62:ALA:HA	2:A:109:HEC:CGA	0.42	2.45	5	2
1:A:69:MET:O	1:A:70:HIS:CG	0.42	2.73	12	1
1:A:20:PHE:CE1	2:A:108:HEC:C1D	0.42	3.03	7	1
1:A:46:CYS:SG	2:A:108:HEC:O1D	0.41	2.78	9	2
1:A:38:ASN:O	1:A:39:GLY:C	0.41	2.58	19	1
1:A:40:LYS:O	1:A:42:ASP:OD1	0.41	2.38	3	1
1:A:22:HIS:O	1:A:25:HIS:C	0.41	2.58	18	2
1:A:73:ASN:O	1:A:74:THR:O	0.41	2.39	5	3
1:A:35:HIS:O	1:A:37:VAL:HG23	0.41	2.15	14	1
1:A:104:LYS:O	1:A:105:CYS:SG	0.41	2.78	2	1
2:A:110:HEC:O2D	2:A:110:HEC:C3D	0.41	2.68	3	1
1:A:65:TYR:O	1:A:69:MET:HG2	0.41	2.15	19	2
1:A:5:PRO:CG	2:A:108:HEC:C3A	0.41	2.96	9	1
1:A:11:MET:SD	2:A:108:HEC:O1D	0.41	2.78	9	1
1:A:21:ASN:O	1:A:24:THR:OG1	0.41	2.39	9	5
1:A:67:HIS:NE2	2:A:109:HEC:O1A	0.41	2.52	11	1
1:A:4:ALA:O	1:A:5:PRO:O	0.41	2.39	15	5
1:A:26:LYS:O	1:A:26:LYS:CD	0.41	2.69	9	1
1:A:29:LYS:O	1:A:32:ASP:N	0.41	2.48	14	2
1:A:6:ALA:O	1:A:7:ASP:O	0.41	2.38	8	8
1:A:93:LYS:O	1:A:96:ASP:N	0.41	2.47	16	2
1:A:45:LYS:O	1:A:46:CYS:C	0.41	2.59	3	1
1:A:50:GLY:O	1:A:51:CYS:SG	0.41	2.79	12	2
1:A:20:PHE:CD1	1:A:20:PHE:C	0.41	2.93	9	1
1:A:93:LYS:CD	1:A:97:LEU:HD11	0.41	2.45	10	1
1:A:54:SER:O	1:A:65:TYR:CB	0.41	2.69	12	1
1:A:46:CYS:SG	2:A:108:HEC:O2D	0.41	2.79	13	2
1:A:68:VAL:C	1:A:78:SER:OG	0.41	2.59	18	2
1:A:15:LYS:O	1:A:16:GLN:OE1	0.41	2.39	1	4
1:A:58:LYS:O	1:A:59:ASP:C	0.41	2.60	8	4
1:A:97:LEU:HD22	2:A:110:HEC:O1D	0.40	2.16	8	1
1:A:65:TYR:CZ	2:A:111:HEC:O2D	0.40	2.74	17	1
1:A:39:GLY:O	1:A:40:LYS:CB	0.40	2.68	14	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:A:109:HEC:HBC3	2:A:109:HEC:HMC1	0.40	1.92	14	1
1:A:9:LEU:CD2	1:A:22:HIS:CE1	0.40	3.04	15	1
1:A:12:GLU:HB3	1:A:17:PRO:CB	0.40	2.46	2	1
1:A:9:LEU:HD12	1:A:9:LEU:C	0.40	2.37	6	1

6.3 Torsion angles (i)

6.3.1 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 PDB entries followed by that with respect to all NMR entries. 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	97/107 (91%)	70±2 (72±2%)	21±2 (22±2%)	6±1 (6±2%)	2	18
All	All	1940/2140 (91%)	1395 (72%)	420 (22%)	125 (6%)	2	18

All 15 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	7	ASP	20
1	A	58	LYS	20
1	A	48	THR	18
1	A	52	HIS	17
1	A	40	LYS	13
1	A	5	PRO	11
1	A	74	THR	5
1	A	8	GLY	5
1	A	71	ASP	5
1	A	61	SER	3
1	A	27	SER	3
1	A	4	ALA	2
1	A	51	CYS	1
1	A	41	GLU	1
1	A	60	LYS	1

6.3.2 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 PDB entries followed by that with respect to all NMR entries. 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	85/88 (97%)	62±2 (73±3%)	23±2 (27±3%)	1 20
All	All	1700/1760 (97%)	1237 (73%)	463 (27%)	1 20

All 48 unique residues with a non-rotameric sidechain are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	9	LEU	20
1	A	10	LYS	20
1	A	19	VAL	20
1	A	20	PHE	20
1	A	48	THR	20
1	A	69	MET	20
1	A	94	LYS	19
1	A	16	GLN	18
1	A	21	ASN	17
1	A	7	ASP	17
1	A	38	ASN	17
1	A	107	GLU	16
1	A	75	LYS	15
1	A	104	LYS	15
1	A	72	LYS	11
1	A	26	LYS	11
1	A	29	LYS	11
1	A	57	LYS	11
1	A	93	LYS	11
1	A	12	GLU	10
1	A	63	LYS	10
1	A	102	LYS	10
1	A	95	LYS	9
1	A	101	LYS	9
1	A	66	TYR	8
1	A	27	SER	7
1	A	61	SER	7
1	A	96	ASP	7
1	A	60	LYS	7

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Mol	Chain	Res	Type	Models (Total)
1	A	11	MET	7
1	A	59	ASP	7
1	A	58	LYS	6
1	A	42	ASP	6
1	A	73	ASN	6
1	A	40	LYS	6
1	A	71	ASP	5
1	A	45	LYS	4
1	A	44	ARG	4
1	A	37	VAL	3
1	A	77	LYS	3
1	A	85	GLU	3
1	A	78	SER	2
1	A	100	CYS	2
1	A	53	ASP	2
1	A	103	SER	1
1	A	56	ASP	1
1	A	54	SER	1
1	A	15	LYS	1

6.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

6.6 Ligand geometry (i)

4 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds for which Mogul statistics could be retrieved, the number of bonds that are observed in the model and the number of bonds 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 is the number of standard deviations the observed value is removed from the expected value. A bond length with $|Z| > 2$ is

considered an outlier worth inspection. RMSZ is the average root-mean-square of all Z scores of the bond lengths.

Mol	Type	Chain	Res	Link	Bond lengths		
					Counts	RMSZ	#Z>2
2	HEC	A	108	1	32,50,50	1.57±0.01	2±0 (6±0%)
2	HEC	A	111	1	32,50,50	1.61±0.01	3±0 (9±0%)
2	HEC	A	109	1	32,50,50	1.59±0.01	2±0 (6±1%)
2	HEC	A	110	1	32,50,50	1.59±0.01	2±0 (7±1%)

In the following table, the Counts columns list the number of angles for which Mogul statistics could be retrieved, the number of angles that are observed in the model and the number of 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 angle is the number of standard deviations the observed value is removed from the expected value. A bond angle with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the average root-mean-square of all Z scores of the bond angles.

Mol	Type	Chain	Res	Link	Bond angles		
					Counts	RMSZ	#Z>2
2	HEC	A	108	1	24,82,82	1.36±0.00	3±0 (12±0%)
2	HEC	A	111	1	24,82,82	1.36±0.00	3±0 (12±0%)
2	HEC	A	109	1	24,82,82	1.35±0.00	3±0 (12±0%)
2	HEC	A	110	1	24,82,82	1.35±0.00	3±0 (12±0%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	HEC	A	111	1	-	0±0,10,54,54	-
2	HEC	A	108	1	-	0±0,10,54,54	-
2	HEC	A	109	1	-	0±0,10,54,54	-
2	HEC	A	110	1	-	0±0,10,54,54	-

All unique bond outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
2	A	108	HEC	C3C-C2C	5.19	1.35	1.40	11	20
2	A	109	HEC	C2B-C3B	5.18	1.35	1.40	5	20

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
2	A	110	HEC	C2B-C3B	5.17	1.35	1.40	19	20
2	A	111	HEC	C2B-C3B	5.17	1.35	1.40	12	20
2	A	109	HEC	C3C-C2C	5.17	1.35	1.40	20	20
2	A	111	HEC	C3C-C2C	5.17	1.35	1.40	4	20
2	A	108	HEC	C2B-C3B	5.16	1.35	1.40	4	20
2	A	110	HEC	C3C-C2C	5.16	1.35	1.40	2	20
2	A	111	HEC	C1C-CHC	2.90	1.49	1.41	7	20
2	A	110	HEC	C1C-CHC	2.38	1.47	1.41	11	6
2	A	109	HEC	C1C-CHC	2.09	1.46	1.41	20	3
2	A	108	HEC	C1C-CHC	2.07	1.46	1.41	2	1

All unique angle outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
2	A	111	HEC	CMB-C2B-C1B	2.37	124.82	128.46	12	20
2	A	109	HEC	CMC-C2C-C1C	2.36	124.84	128.46	9	20
2	A	108	HEC	CMB-C2B-C1B	2.36	124.84	128.46	10	20
2	A	111	HEC	CMD-C2D-C1D	2.36	124.84	128.46	10	20
2	A	108	HEC	CMC-C2C-C1C	2.35	124.84	128.46	18	20
2	A	109	HEC	CMB-C2B-C1B	2.35	124.85	128.46	5	20
2	A	110	HEC	CMD-C2D-C1D	2.35	124.85	128.46	2	20
2	A	110	HEC	CMB-C2B-C1B	2.35	124.85	128.46	17	20
2	A	110	HEC	CMC-C2C-C1C	2.35	124.86	128.46	2	20
2	A	111	HEC	CMC-C2C-C1C	2.35	124.85	128.46	4	20
2	A	109	HEC	CMD-C2D-C1D	2.34	124.86	128.46	19	20
2	A	108	HEC	CMD-C2D-C1D	2.34	124.87	128.46	20	20

There are no chirality outliers.

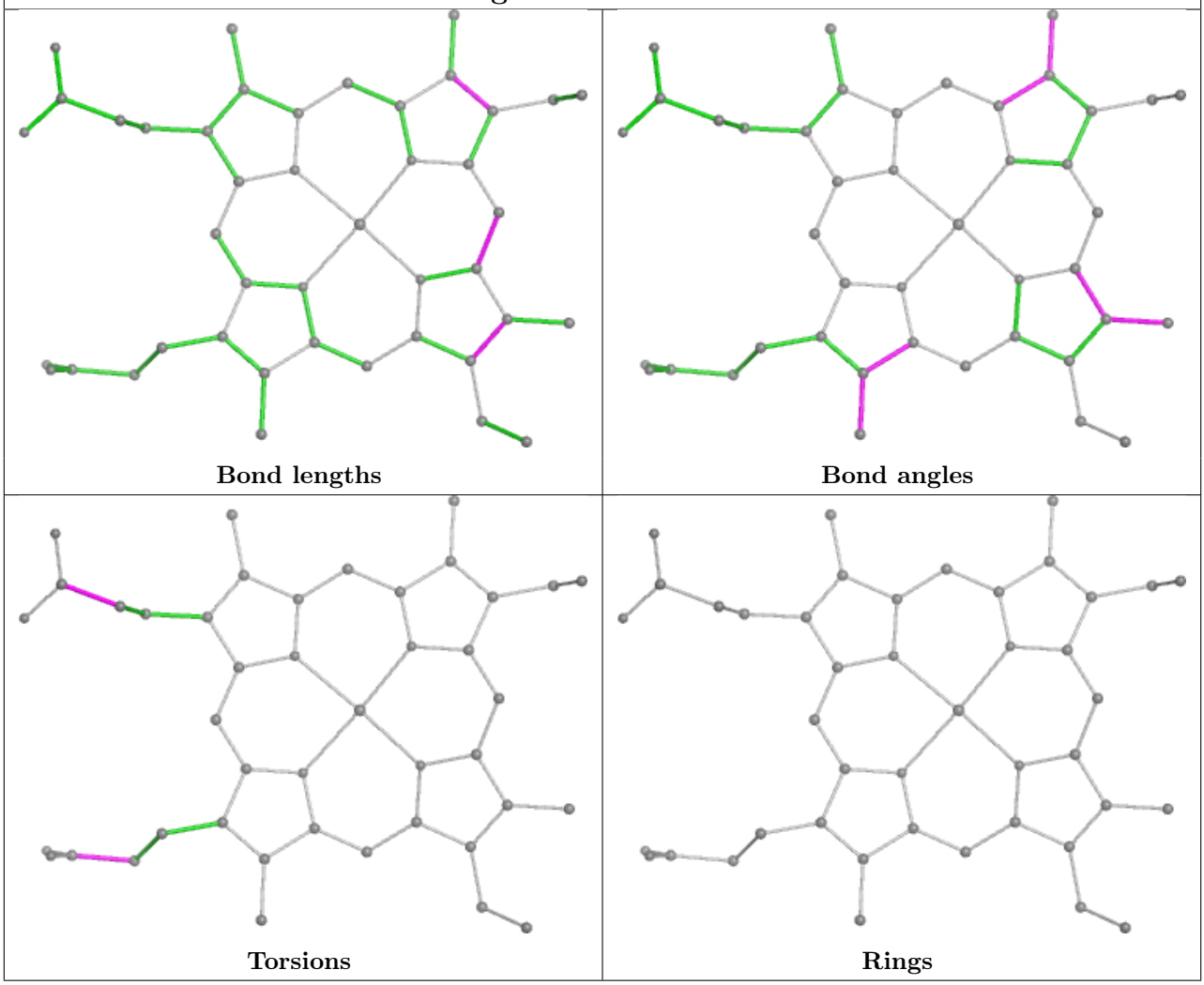
There are no torsion outliers.

There are no ring outliers.

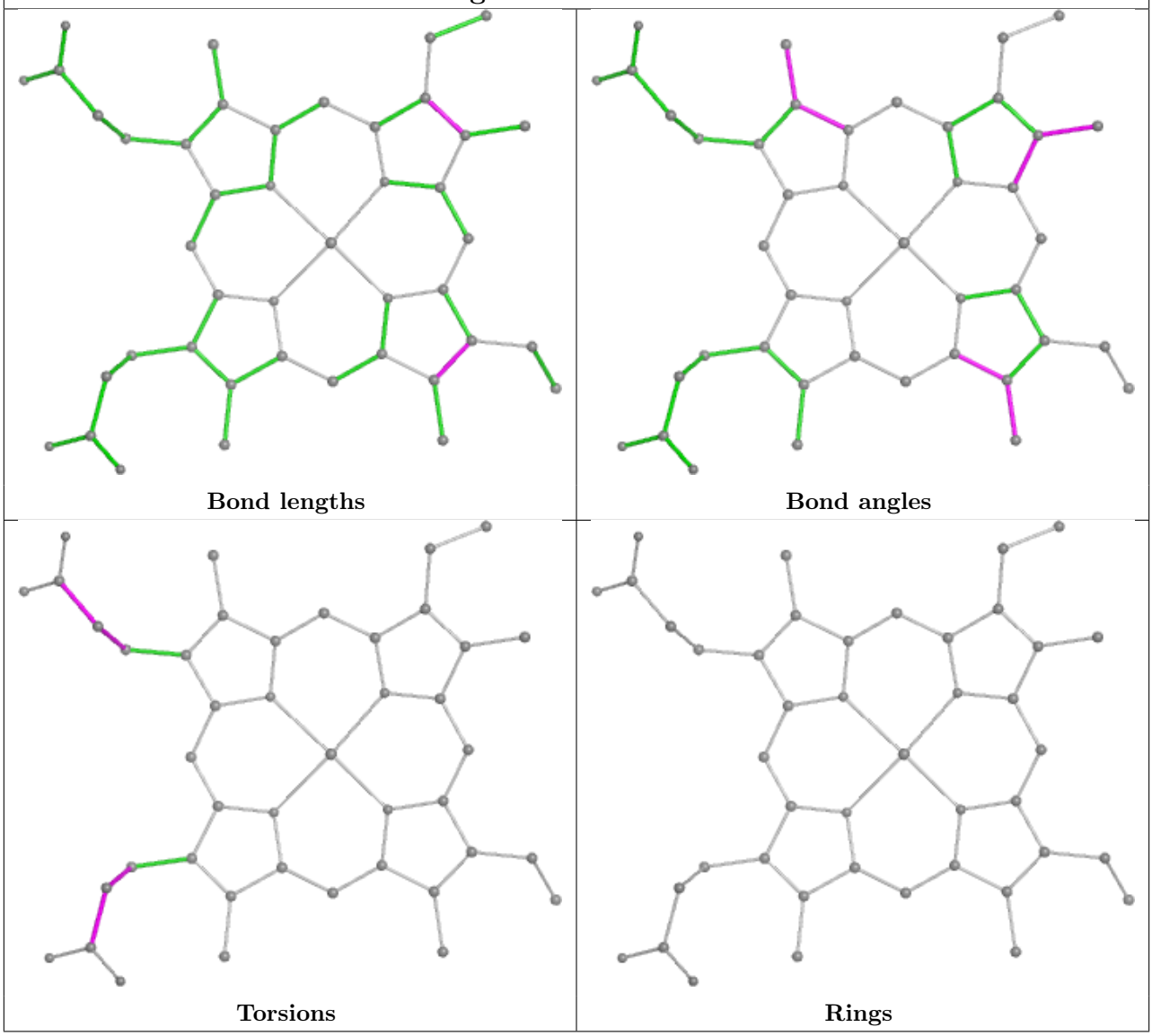
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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 A 111



Ligand HEC A 108



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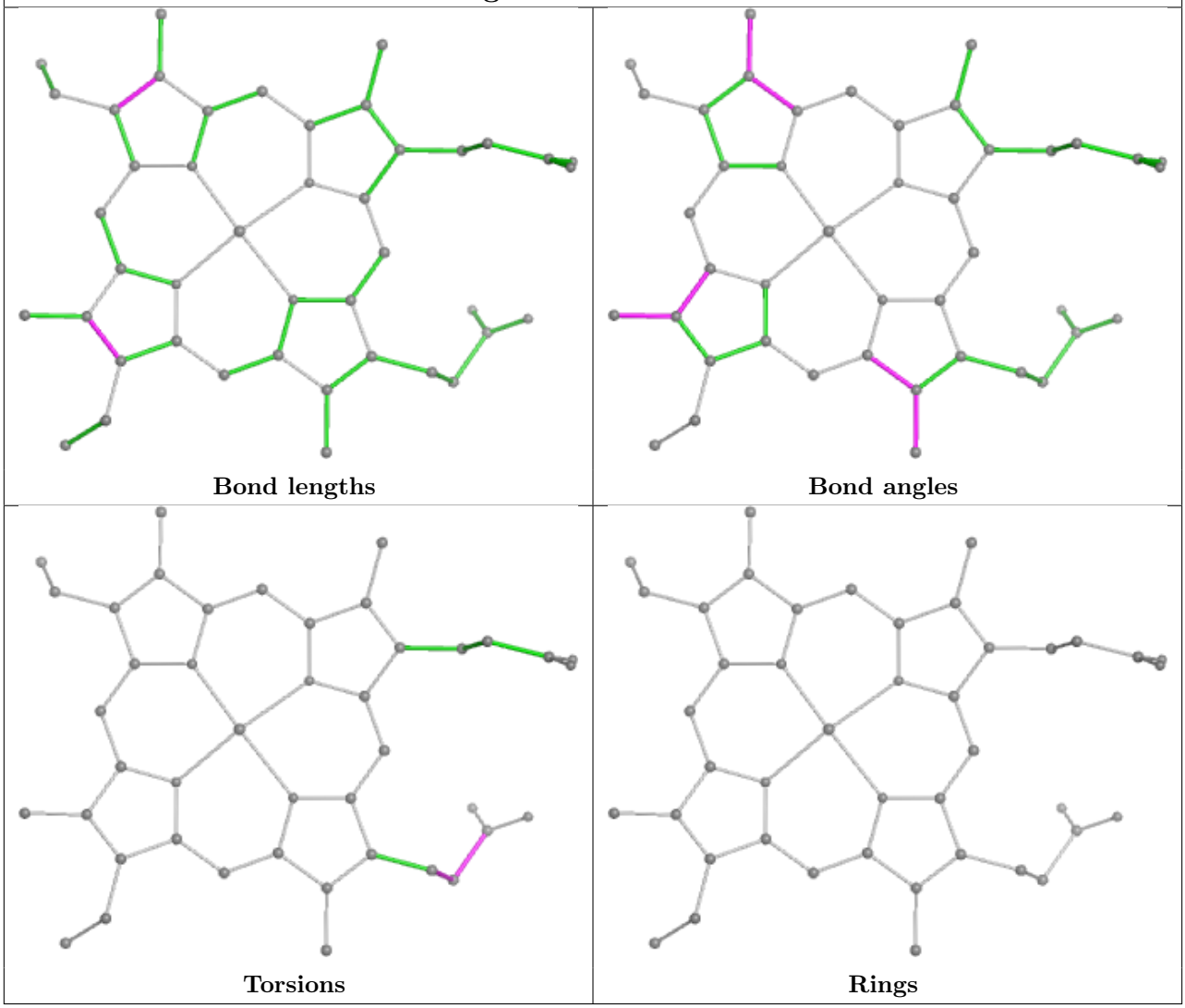
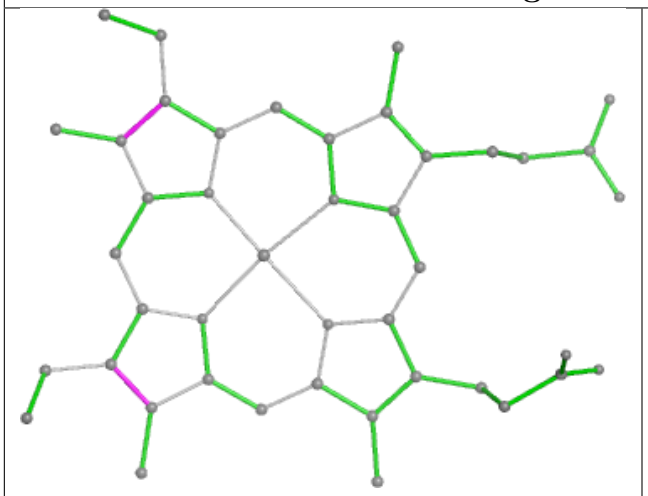
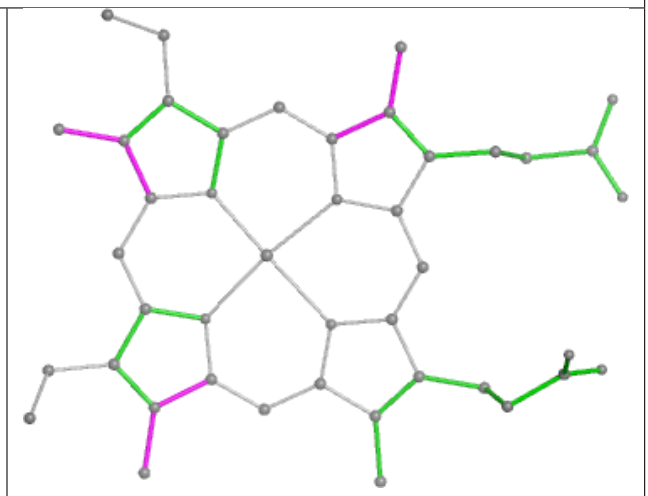


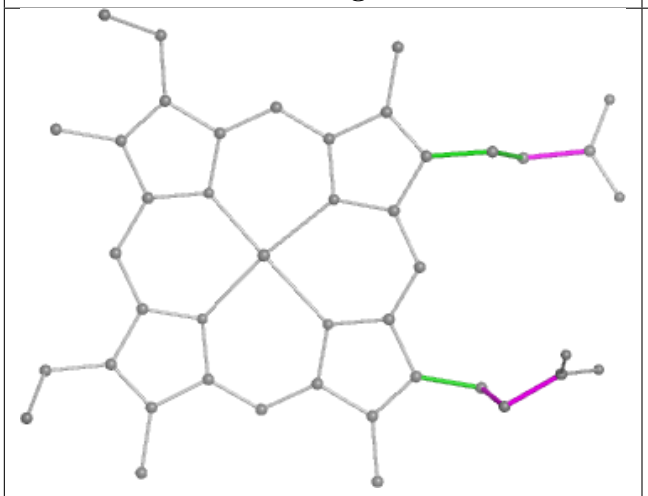
Ligand HEC A 110



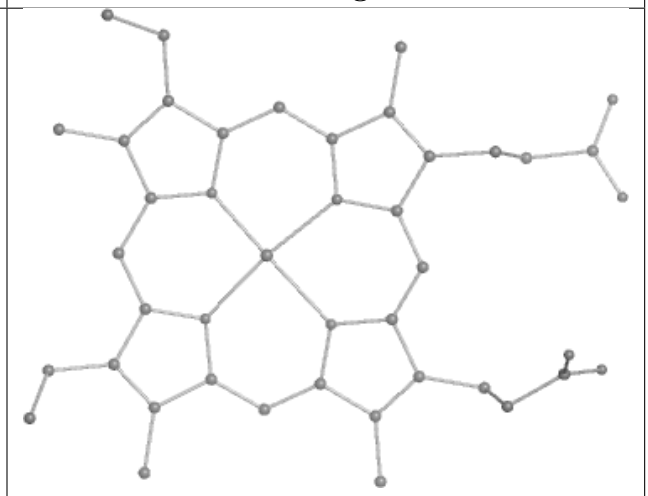
Bond lengths



Bond angles



Torsions



Rings

6.7 Other polymers (i)

There are no such molecules in this entry.

6.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

7 Chemical shift validation (i)

No chemical shift data were provided