



# Full wwPDB NMR Structure Validation Report ⓘ

Jun 12, 2024 – 11:04 PM EDT

PDB ID : 1GX7  
Title : Best model of the electron transfer complex between cytochrome c3 and [Fe]-hydrogenase  
Authors : Elantak, L.; Morelli, X.; Bornet, O.; Hatchikian, C.; Czjzek, M.; Dolla, A.; Guerlesquin, F.  
Deposited on : 2002-03-28

This is a Full wwPDB NMR Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto: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 ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
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)	:	2.36.2

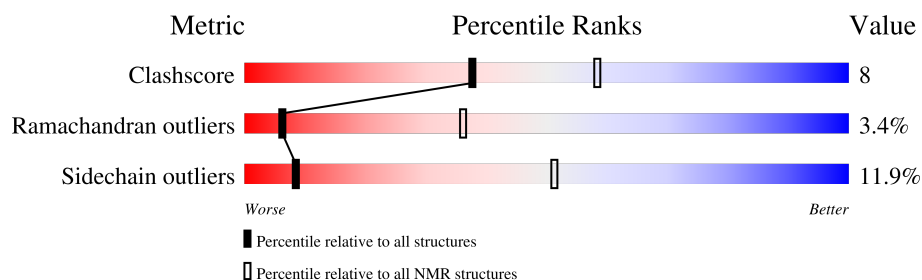
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*SOLUTION NMR, THEORETICAL MODEL*

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	158937	12864
Ramachandran outliers	154571	11451
Sidechain outliers	154315	11428

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  $\geq 3$ , 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  $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	371	
2	D	88	
3	E	107	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA and RNA chains that are outliers for geometric criteria:

Mol	Chain	Compound	Res	Total models with violations	
				Chirality	Geometry
5	A	PDT	4	-	1

## 2 Ensemble composition and analysis ⓘ

This entry contains 1 models. Identification of well-defined residues and clustering analysis are not possible.

### 3 Entry composition [i](#)

There are 9 unique types of molecules in this entry. The entry contains 5509 atoms, of which 968 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called PERIPLASMIC [FE] HYDROGENASE LARGE SUBUNIT.

Mol	Chain	Residues	Atoms						Trace
1	A	371	Total	C	H	N	O	S	0
			3394	1783	587	465	527	32	

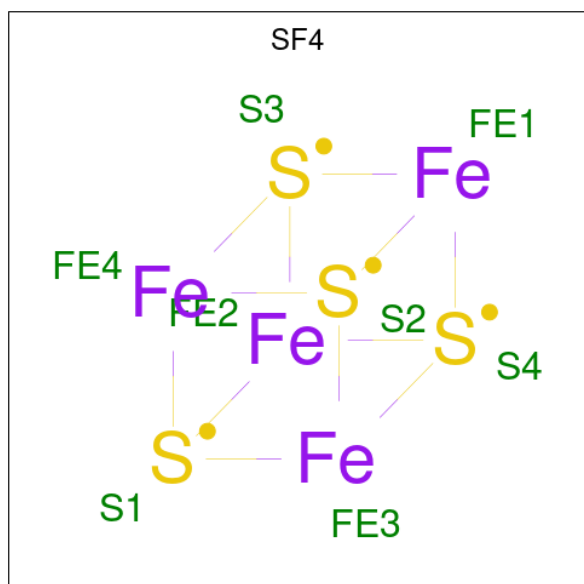
- Molecule 2 is a protein called PERIPLASMIC [FE] HYDROGENASE SMALL SUBUNIT.

Mol	Chain	Residues	Atoms						Trace
2	D	88	Total	C	H	N	O	S	0
			877	457	164	123	132	1	

- Molecule 3 is a protein called CYTOCHROME C3.

Mol	Chain	Residues	Atoms						Trace
3	E	107	Total	C	H	N	O	S	0
			1011	495	201	152	152	11	

- Molecule 4 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe<sub>4</sub>S<sub>4</sub>).



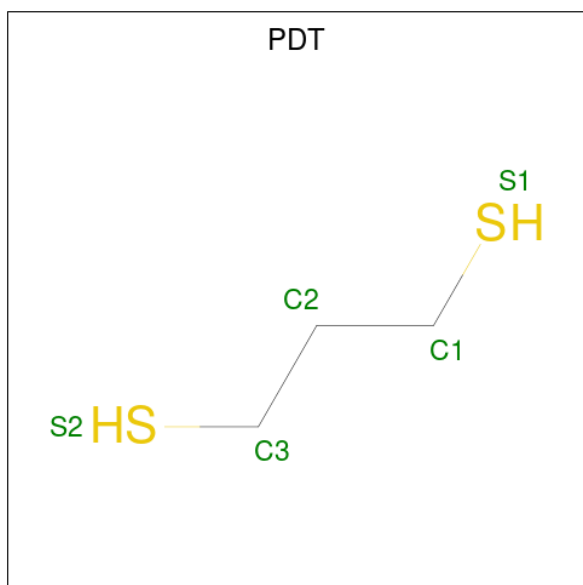
Mol	Chain	Residues	Atoms		
4	A	1	Total	Fe	S
			8	4	4

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Mol	Chain	Residues	Atoms		
4	A	1	Total	Fe	S
			8	4	4
4	A	1	Total	Fe	S
			8	4	4

- Molecule 5 is 1,3-PROPANEDITHIOL (three-letter code: PDT) (formula: C<sub>3</sub>H<sub>8</sub>S<sub>2</sub>).

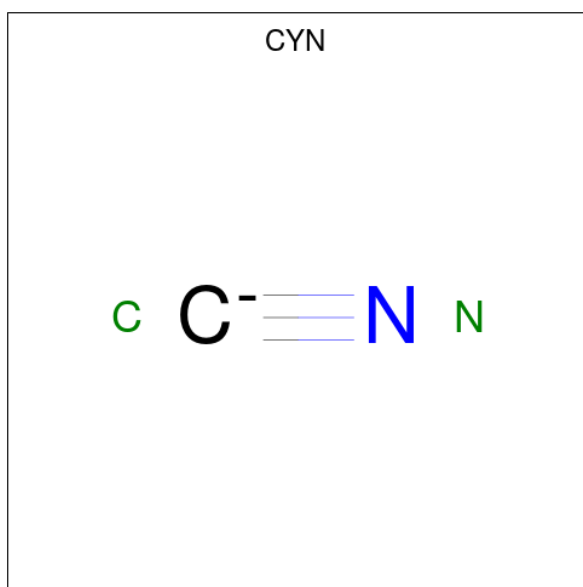


Mol	Chain	Residues	Atoms		
5	A	1	Total	C	S
			5	3	2

- Molecule 6 is FE (II) ION (three-letter code: FE2) (formula: Fe).

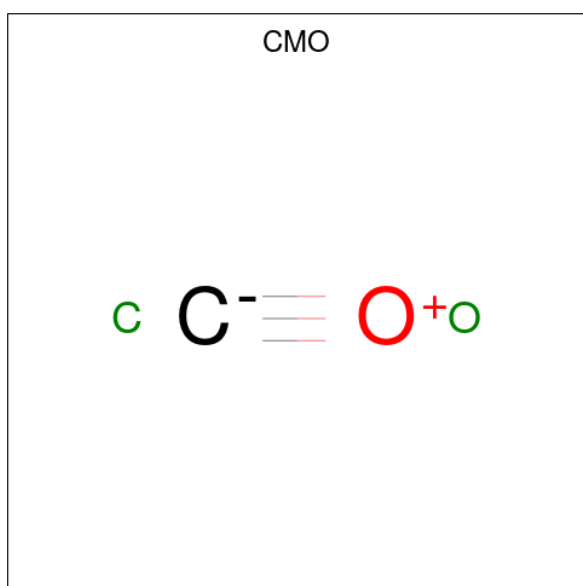
Mol	Chain	Residues	Atoms	
6	A	2	Total	Fe
			2	2

- Molecule 7 is CYANIDE ION (three-letter code: CYN) (formula: CN).



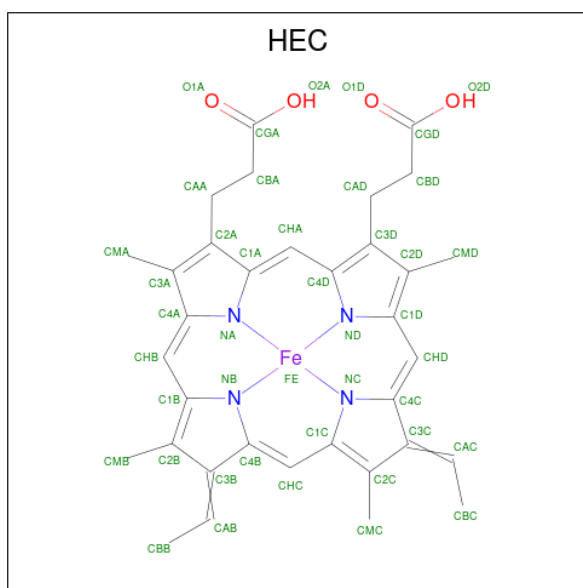
Mol	Chain	Residues	Atoms		
7	A	1	Total	C	N
			2	1	1
7	A	1	Total	C	N
			2	1	1

- Molecule 8 is CARBON MONOXIDE (three-letter code: CMO) (formula: CO).



Mol	Chain	Residues	Atoms		
8	A	1	Total	C	O
			2	1	1
8	A	1	Total	C	O
			2	1	1

- Molecule 9 is HEME C (three-letter code: HEC) (formula:  $\text{C}_{34}\text{H}_{34}\text{FeN}_4\text{O}_4$ ).

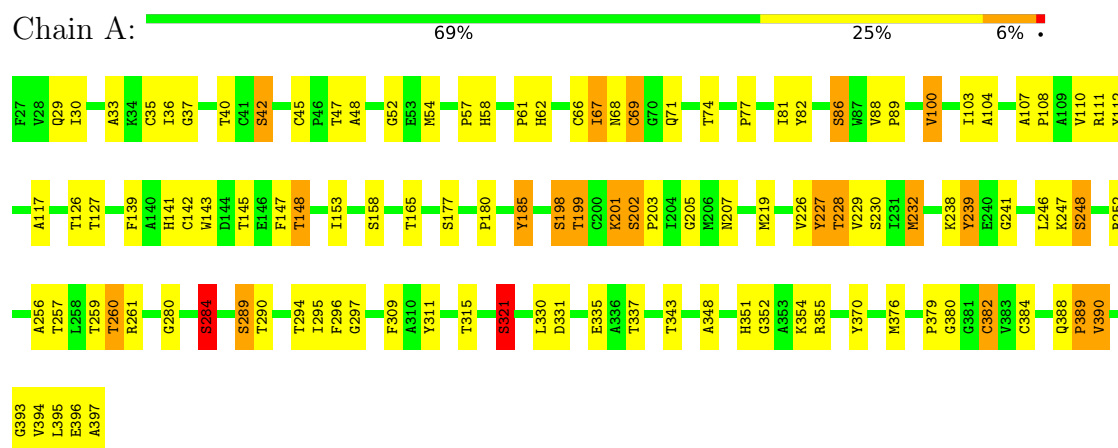


Mol	Chain	Residues	Atoms					
9	E	1	Total 47	C 34	Fe 1	H 4	N 4	O 4
9	E	1	Total 47	C 34	Fe 1	H 4	N 4	O 4
9	E	1	Total 47	C 34	Fe 1	H 4	N 4	O 4
9	E	1	Total 47	C 34	Fe 1	H 4	N 4	O 4

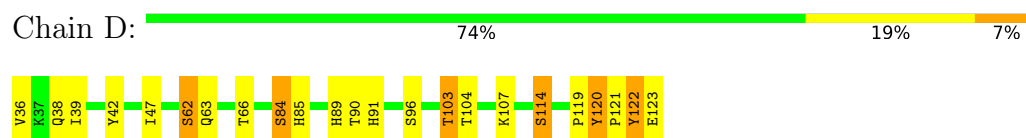
## 4 Residue-property plots

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.

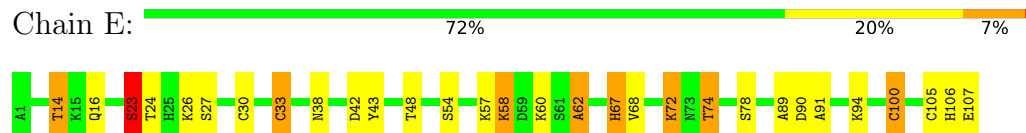
### • Molecule 1: PERIPLASMIC [FE] HYDROGENASE LARGE SUBUNIT



### • Molecule 2: PERIPLASMIC [FE] HYDROGENASE SMALL SUBUNIT



### • Molecule 3: CYTOCHROME C3





## 5 Refinement protocol and experimental data overview ⓘ

The models were refined using the following method: ?.

Of the ? calculated structures, 1 were deposited, based on the following criterion: ?.

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

Software name	Classification	Version
X-PLOR	refinement	

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: CYN, HEC, SF4, PDT, FE2, CMO

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 (average) 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	0.57	0/2874 ( 0.0%)	1.23	17/3885 ( 0.4%)
2	D	0.58	0/733 ( 0.0%)	1.16	5/988 ( 0.5%)
3	E	0.54	0/827 ( 0.0%)	1.29	4/1101 ( 0.4%)
All	All	0.57	0/4434 ( 0.0%)	1.23	26/5974 ( 0.4%)

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	Planarity
1	A	2	20
2	D	1	4
3	E	0	6
All	All	3	30

There are no bond-length outliers.

All angle outliers are listed below. They are sorted according to the Z-score.

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	107	GLU	N-CA-C	-6.77	92.71	111.00
1	A	382	CYS	CA-CB-SG	-6.63	102.06	114.00
2	D	123	GLU	N-CA-C	-6.61	93.14	111.00
1	A	397	ALA	N-CA-C	-6.60	93.18	111.00
1	A	321	SER	N-CA-CB	-6.14	101.30	110.50
1	A	311	TYR	CB-CG-CD2	-6.13	117.32	121.00
3	E	43	TYR	N-CA-C	-5.98	94.86	111.00
1	A	248	SER	N-CA-CB	-5.94	101.59	110.50
2	D	114	SER	N-CA-CB	-5.82	101.77	110.50
1	A	42	SER	N-CA-CB	-5.74	101.89	110.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	331	ASP	N-CA-C	-5.67	95.68	111.00
1	A	100	VAL	N-CA-C	-5.66	95.71	111.00
2	D	122	TYR	CB-CG-CD2	-5.59	117.65	121.00
2	D	120	TYR	N-CA-C	-5.58	95.94	111.00
3	E	58	LYS	N-CA-C	-5.47	96.23	111.00
1	A	280	GLY	N-CA-C	-5.44	99.49	113.10
1	A	239	TYR	CB-CG-CD2	-5.43	117.74	121.00
1	A	52	GLY	N-CA-C	-5.40	99.60	113.10
1	A	390	VAL	N-CA-C	-5.34	96.59	111.00
1	A	284	SER	N-CA-CB	-5.30	102.55	110.50
1	A	86	SER	N-CA-CB	-5.19	102.72	110.50
2	D	84	SER	N-CA-CB	-5.17	102.75	110.50
1	A	202	SER	N-CA-CB	-5.13	102.80	110.50
1	A	289	SER	N-CA-CB	-5.12	102.82	110.50
3	E	23	SER	N-CA-CB	-5.07	102.89	110.50
1	A	185	TYR	CB-CG-CD2	-5.06	117.96	121.00

All chiral outliers are listed below.

Mol	Chain	Res	Type	Atoms
1	A	50	ILE	CB
1	A	63	ILE	CB
2	D	39	ILE	CB

All planar outliers are listed below.

Mol	Chain	Res	Type	Group
1	A	36	ILE	Peptide
1	A	37	GLY	Peptide
1	A	68	ASN	Peptide
1	A	71	GLN	Peptide
1	A	82	TYR	Sidechain
1	A	111	ARG	Sidechain
1	A	112	TYR	Sidechain
1	A	147	PHE	Peptide
1	A	185	TYR	Sidechain
1	A	199	THR	Peptide
1	A	227	TYR	Sidechain
1	A	232	MET	Peptide
1	A	247	LYS	Peptide
1	A	252	ARG	Peptide
1	A	330	LEU	Peptide

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Mol	Chain	Res	Type	Group
1	A	370	TYR	Peptide,Sidechain
1	A	384	CYS	Peptide
1	A	388	GLN	Peptide
1	A	396	GLU	Peptide
2	D	42	TYR	Sidechain
2	D	119	PRO	Peptide
2	D	120	TYR	Sidechain
2	D	122	TYR	Sidechain
3	E	14	THR	Peptide
3	E	33	CYS	Peptide
3	E	42	ASP	Peptide
3	E	62	ALA	Peptide
3	E	72	LYS	Peptide
3	E	106	HIS	Peptide

## 6.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in 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	2807	587	2765	53
2	D	713	164	703	10
3	E	810	201	792	11
4	A	24	0	0	6
5	A	5	0	6	12
6	A	2	0	0	2
7	A	4	0	0	7
8	A	4	0	0	7
9	E	172	16	120	8
All	All	4541	968	4386	72

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

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)
1:A:238:LYS:HG2	1:A:257:THR:HB	0.90	1.44
1:A:232:MET:SD	8:A:9:CMO:C	0.81	2.68

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Atom-1	Atom-2	Clash(Å)	Distance(Å)
1:A:296:PHE:HB3	5:A:4:PDT:H11	0.80	1.51
1:A:232:MET:SD	7:A:7:CYN:C	0.78	2.70
1:A:104:ALA:HB2	1:A:139:PHE:HB3	0.75	1.58
1:A:232:MET:SD	6:A:6:FE2:FE	0.75	1.78
1:A:232:MET:SD	6:A:5:FE2:FE	0.74	1.78
1:A:180:PRO:HD2	4:A:3:SF4:S4	0.70	2.27
1:A:232:MET:SD	8:A:10:CMO:C	0.69	2.80
1:A:232:MET:SD	7:A:8:CYN:C	0.68	2.82
1:A:148:THR:HG21	1:A:207:ASN:HA	0.68	1.65
5:A:4:PDT:C3	8:A:9:CMO:C	0.67	2.71
1:A:201:LYS:HD3	2:D:90:THR:HB	0.66	1.68
3:E:16:GLN:HG2	9:E:109:HEC:HAA2	0.66	1.68
1:A:66:CYS:HA	4:A:2:SF4:S1	0.65	2.31
1:A:241:GLY:HA2	1:A:246:LEU:HD12	0.65	1.68
1:A:297:GLY:N	5:A:4:PDT:S1	0.65	2.70
1:A:117:ALA:HA	1:A:390:VAL:HB	0.63	1.69
1:A:35:CYS:HA	4:A:1:SF4:S2	0.61	2.35
1:A:296:PHE:HB3	5:A:4:PDT:C1	0.61	2.26
1:A:103:ILE:HG13	1:A:226:VAL:HG13	0.58	1.74
1:A:297:GLY:N	5:A:4:PDT:S2	0.58	2.77
1:A:390:VAL:HA	1:A:395:LEU:HD23	0.57	1.74
1:A:88:VAL:HB	1:A:89:PRO:HD3	0.57	1.76
2:D:85:HIS:HA	2:D:89:HIS:HD2	0.57	1.59
3:E:30:CYS:HA	9:E:111:HEC:HMC3	0.56	1.76
5:A:4:PDT:C1	7:A:7:CYN:C	0.56	2.83
5:A:4:PDT:H31	8:A:9:CMO:O	0.55	2.01
1:A:108:PRO:HD2	7:A:8:CYN:N	0.54	2.18
1:A:203:PRO:HD2	5:A:4:PDT:H12	0.52	1.81
1:A:382:CYS:HA	4:A:3:SF4:S2	0.52	2.44
1:A:100:VAL:HG12	1:A:227:TYR:HB2	0.52	1.80
5:A:4:PDT:H31	8:A:9:CMO:C	0.52	2.34
1:A:229:VAL:HA	1:A:256:ALA:HB3	0.51	1.81
1:A:382:CYS:SG	5:A:4:PDT:H32	0.51	2.46
1:A:393:GLY:HA3	2:D:36:VAL:HG21	0.49	1.83
1:A:352:GLY:HA3	1:A:355:ARG:HH21	0.49	1.67
2:D:121:PRO:HB3	3:E:58:LYS:HG2	0.49	1.84
1:A:110:VAL:HG13	1:A:260:THR:HG23	0.49	1.83
1:A:351:HIS:CE1	1:A:379:PRO:HA	0.48	2.43
1:A:232:MET:HB3	8:A:9:CMO:C	0.48	2.38
1:A:67:ILE:HG13	1:A:69:CYS:HB3	0.48	1.83
1:A:30:ILE:HG23	1:A:81:ILE:HG12	0.48	1.86
1:A:309:PHE:HA	2:D:63:GLN:NE2	0.48	2.24

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Atom-1	Atom-2	Clash(Å)	Distance(Å)
1:A:394:VAL:HA	3:E:72:LYS:HE3	0.48	1.84
5:A:4:PDT:H12	7:A:7:CYN:C	0.47	2.38
1:A:205:GLY:HA3	1:A:246:LEU:HD22	0.47	1.87
3:E:60:LYS:HA	3:E:67:HIS:CD2	0.47	2.44
3:E:74:THR:HB	9:E:110:HEC:O1A	0.47	2.10
9:E:111:HEC:HBD2	9:E:111:HEC:HMD1	0.47	1.84
1:A:107:ALA:HB1	7:A:8:CYN:N	0.47	2.25
1:A:261:ARG:HG2	1:A:389:PRO:HA	0.47	1.87
1:A:232:MET:HB3	8:A:9:CMO:O	0.46	2.11
3:E:26:LYS:HB2	9:E:111:HEC:HBB2	0.45	1.86
2:D:85:HIS:HA	2:D:89:HIS:CD2	0.45	2.43
1:A:77:PRO:HB3	3:E:94:LYS:HE2	0.45	1.89
3:E:68:VAL:HG12	9:E:110:HEC:HBA2	0.45	1.89
1:A:335:GLU:HA	1:A:348:ALA:HA	0.44	1.88
1:A:297:GLY:CA	5:A:4:PDT:S2	0.44	3.06
1:A:69:CYS:HB2	4:A:3:SF4:S3	0.43	2.53
3:E:26:LYS:HA	9:E:111:HEC:HMC2	0.43	1.90
2:D:38:GLN:NE2	2:D:38:GLN:HA	0.43	2.27
1:A:107:ALA:HB1	7:A:8:CYN:C	0.43	2.44
1:A:380:GLY:HA2	2:D:47:ILE:HD11	0.42	1.92
1:A:45:CYS:HA	4:A:2:SF4:S3	0.42	2.55
1:A:48:ALA:HB2	1:A:354:LYS:HG2	0.42	1.91
1:A:153:ILE:HG21	2:D:62:SER:HB2	0.42	1.90
3:E:100:CYS:HB3	9:E:109:HEC:HMB1	0.42	1.91
1:A:143:TRP:HZ2	1:A:219:MET:HG3	0.42	1.75
1:A:226:VAL:HG12	1:A:228:THR:HG23	0.41	1.92
2:D:103:THR:HA	2:D:107:LYS:HB2	0.41	1.92
1:A:230:SER:O	1:A:257:THR:HA	0.40	2.16

## 6.3 Torsion angles ⓘ

### 6.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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	369/371 (99%)	311 (84%)	49 (13%)	9 (2%)	9	46
2	D	86/88 (98%)	75 (87%)	10 (12%)	1 (1%)	17	64

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	E	105/107 (98%)	76 (72%)	20 (19%)	9 (9%)	2	12
All	All	560/566 (99%)	462 (82%)	79 (14%)	19 (3%)	6	36

All 19 Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type
1	A	33	ALA
1	A	57	PRO
1	A	61	PRO
1	A	67	ILE
1	A	198	SER
1	A	284	SER
1	A	295	ILE
1	A	321	SER
1	A	389	PRO
2	D	39	ILE
3	E	23	SER
3	E	33	CYS
3	E	38	ASN
3	E	62	ALA
3	E	89	ALA
3	E	90	ASP
3	E	91	ALA
3	E	100	CYS
3	E	105	CYS

### 6.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all 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	297/297 (100%)	260 (88%)	37 (12%)	8	50
2	D	76/76 (100%)	68 (89%)	8 (11%)	10	55
3	E	88/88 (100%)	78 (89%)	10 (11%)	9	52
All	All	461/461 (100%)	406 (88%)	55 (12%)	8	51

All 55 residues with a non-rotameric sidechain are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type
1	A	29	GLN
1	A	40	THR
1	A	42	SER
1	A	47	THR
1	A	54	MET
1	A	58	HIS
1	A	62	HIS
1	A	69	CYS
1	A	74	THR
1	A	86	SER
1	A	126	THR
1	A	127	THR
1	A	141	HIS
1	A	142	CYS
1	A	145	THR
1	A	148	THR
1	A	158	SER
1	A	165	THR
1	A	177	SER
1	A	198	SER
1	A	199	THR
1	A	201	LYS
1	A	202	SER
1	A	228	THR
1	A	239	TYR
1	A	248	SER
1	A	259	THR
1	A	260	THR
1	A	284	SER
1	A	289	SER
1	A	290	THR
1	A	294	THR
1	A	315	THR
1	A	321	SER
1	A	337	THR
1	A	343	THR
1	A	376	MET
2	D	62	SER
2	D	66	THR
2	D	84	SER
2	D	91	HIS

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Mol	Chain	Res	Type
2	D	96	SER
2	D	103	THR
2	D	104	THR
2	D	114	SER
3	E	14	THR
3	E	23	SER
3	E	24	THR
3	E	27	SER
3	E	48	THR
3	E	54	SER
3	E	57	LYS
3	E	67	HIS
3	E	74	THR
3	E	78	SER

### 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 monosaccharides in this entry.

## 6.6 Ligand geometry [i](#)

Of 14 ligands modelled in this entry, 2 are monoatomic - leaving 12 for Mogul analysis.

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
9	HEC	E	112	3	32,50,50	1.40	2 (6%)
7	CYN	A	7	8,6	0,1,1	0.00	-
4	SF4	A	1	1	0,12,12	0.00	-
4	SF4	A	2	1	0,12,12	0.00	-
4	SF4	A	3	1	0,12,12	0.00	-
7	CYN	A	8	8,6	0,1,1	0.00	-
9	HEC	E	109	3	32,50,50	1.30	2 (6%)
9	HEC	E	111	3	32,50,50	1.44	4 (12%)
5	PDT	A	4	6	4,4,4	2.55	2 (50%)
8	CMO	A	9	7,6	0,1,1	0.00	-
9	HEC	E	110	3	32,50,50	1.34	2 (6%)
8	CMO	A	10	7,6	0,1,1	0.00	-

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
9	HEC	E	112	3	24,82,82	1.47	4 (16%)
7	CYN	A	7	8,6	-	-	-
4	SF4	A	1	1	-	-	-
4	SF4	A	2	1	-	-	-
4	SF4	A	3	1	-	-	-
7	CYN	A	8	8,6	-	-	-
9	HEC	E	109	3	24,82,82	1.70	7 (29%)
9	HEC	E	111	3	24,82,82	1.82	7 (29%)
5	PDT	A	4	6	3,3,3	1.36	0 (0%)
8	CMO	A	9	7,6	-	-	-
9	HEC	E	110	3	24,82,82	1.28	4 (16%)
8	CMO	A	10	7,6	-	-	-

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
9	HEC	E	112	3	-	0,10,54,54	-
4	SF4	A	1	1	-	-	0,6,5,5
4	SF4	A	2	1	-	-	0,6,5,5
4	SF4	A	3	1	-	-	0,6,5,5
9	HEC	E	109	3	-	0,10,54,54	-
9	HEC	E	111	3	-	0,10,54,54	-
5	PDT	A	4	6	-	0,2,2,2	-
9	HEC	E	110	3	-	0,10,54,54	-

All bond outliers are listed below. They are sorted according to the Z-score.

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	E	111	HEC	C2B-C3B	4.61	1.35	1.40
9	E	112	HEC	C2B-C3B	4.42	1.36	1.40
5	A	4	PDT	C3-S2	4.12	1.95	1.80
9	E	110	HEC	C3C-C2C	4.12	1.36	1.40
9	E	109	HEC	C3C-C2C	3.70	1.36	1.40
9	E	109	HEC	C2B-C3B	3.50	1.37	1.40
9	E	111	HEC	C3C-C2C	3.32	1.37	1.40
9	E	112	HEC	C3C-C2C	3.31	1.37	1.40
9	E	110	HEC	C2B-C3B	3.28	1.37	1.40
5	A	4	PDT	C1-S1	2.87	1.90	1.80
9	E	111	HEC	C4B-C3B	2.25	1.47	1.43
9	E	111	HEC	C3C-C4C	2.19	1.47	1.43

All angle outliers are listed below. They are sorted according to the Z-score.

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	E	111	HEC	CBD-CAD-C3D	4.29	119.94	112.62
9	E	111	HEC	CMC-C2C-C1C	3.55	123.01	128.46
9	E	109	HEC	CBA-CAA-C2A	3.25	118.08	112.60
9	E	109	HEC	CMB-C2B-C1B	3.15	123.62	128.46
9	E	112	HEC	CMC-C2C-C1C	3.14	123.64	128.46
9	E	112	HEC	CBD-CAD-C3D	2.90	117.58	112.62
9	E	109	HEC	CMC-C2C-C1C	2.86	124.06	128.46
9	E	111	HEC	CMD-C2D-C1D	2.84	124.09	128.46
9	E	109	HEC	C2B-C3B-C4B	2.59	103.55	106.35
9	E	111	HEC	C4C-C3C-C2C	2.59	103.55	106.35
9	E	110	HEC	CBD-CAD-C3D	2.40	116.71	112.62
9	E	111	HEC	O1A-CGA-CBA	2.34	115.58	123.08
9	E	110	HEC	CMB-C2B-C1B	2.30	124.93	128.46
9	E	112	HEC	CMC-C2C-C3C	2.27	128.49	125.82
9	E	111	HEC	CMC-C2C-C3C	2.18	128.39	125.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	E	110	HEC	C4C-C3C-C2C	2.15	104.03	106.35
9	E	109	HEC	CMA-C3A-C2A	2.15	128.99	124.94
9	E	109	HEC	O1A-CGA-CBA	2.09	116.38	123.08
9	E	112	HEC	C4C-C3C-C2C	2.06	104.13	106.35
9	E	110	HEC	CMC-C2C-C1C	2.04	125.33	128.46
9	E	111	HEC	CMD-C2D-C3D	2.03	128.77	124.94
9	E	109	HEC	C4C-C3C-C2C	2.01	104.18	106.35

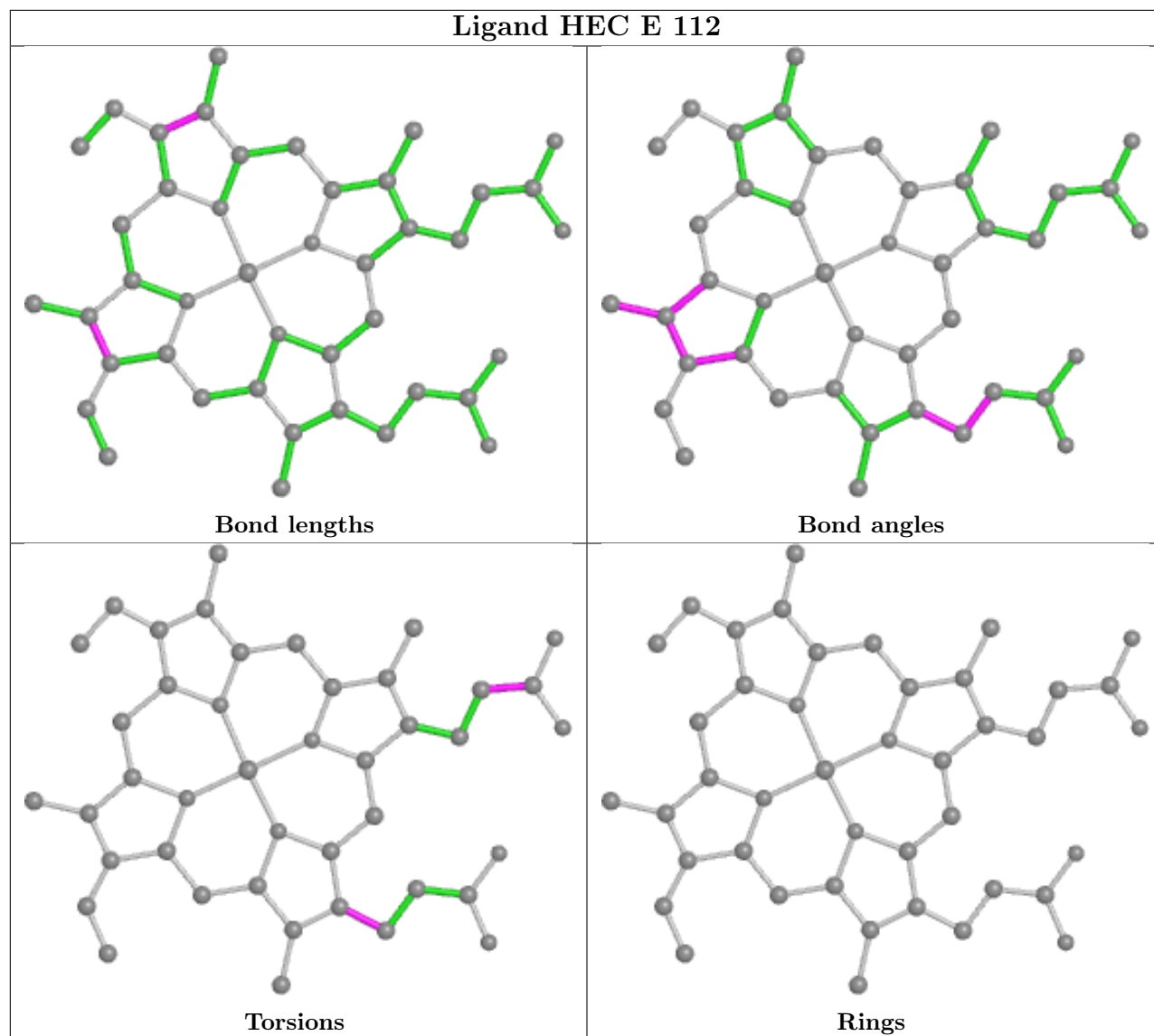
There are no chirality outliers.

There are no torsion outliers.

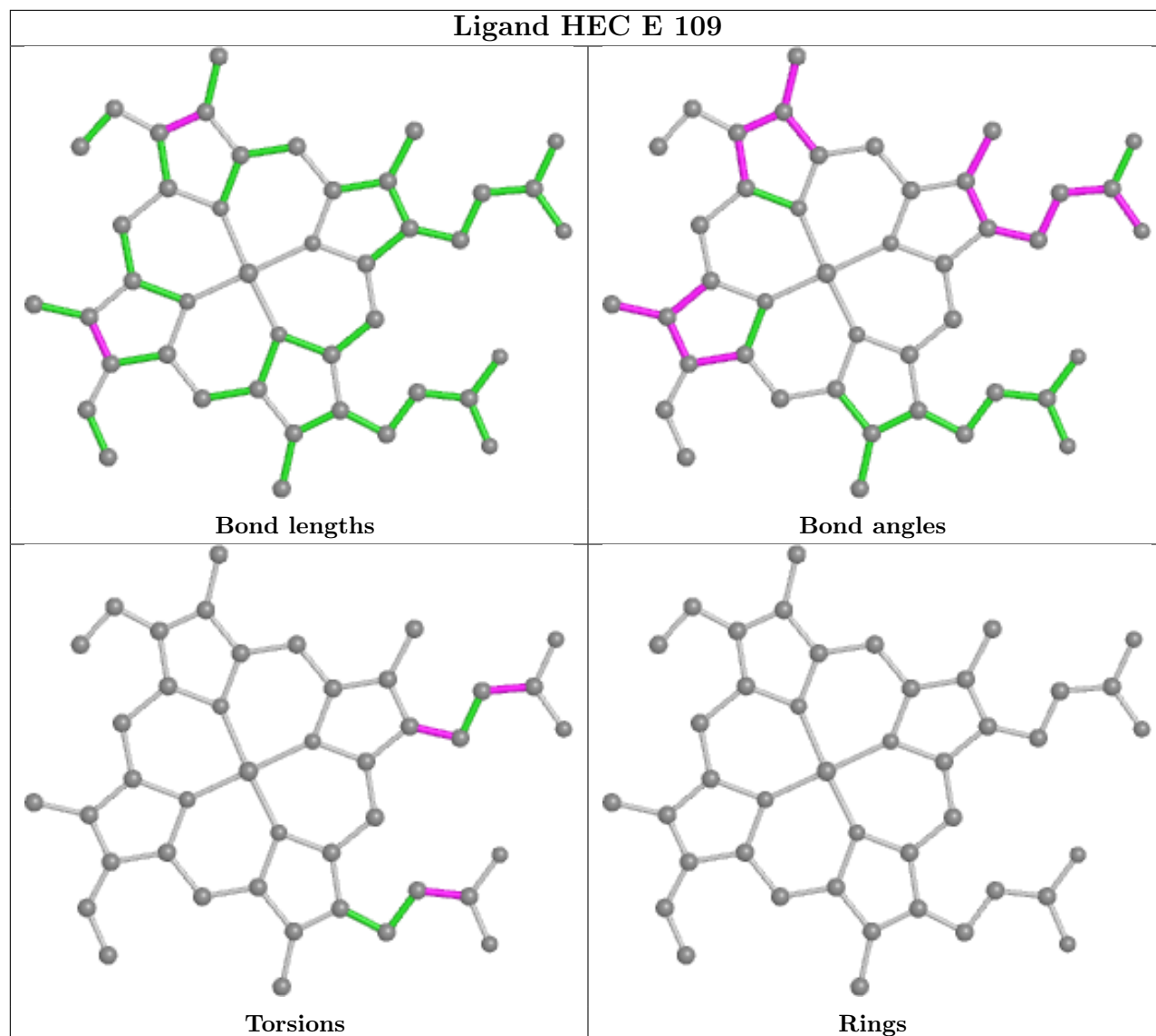
There are no ring outliers.

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 than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

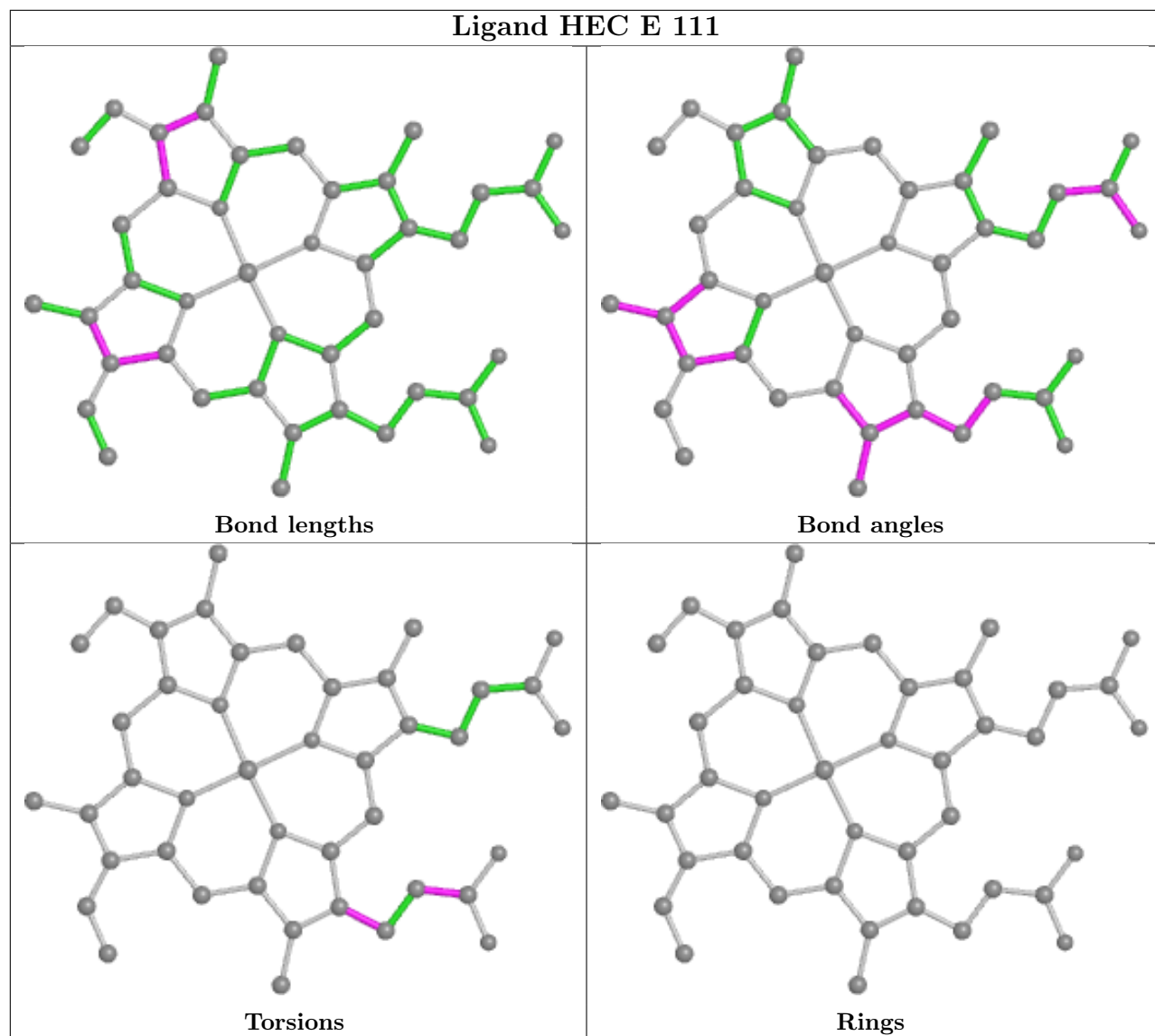
## Ligand HEC E 112

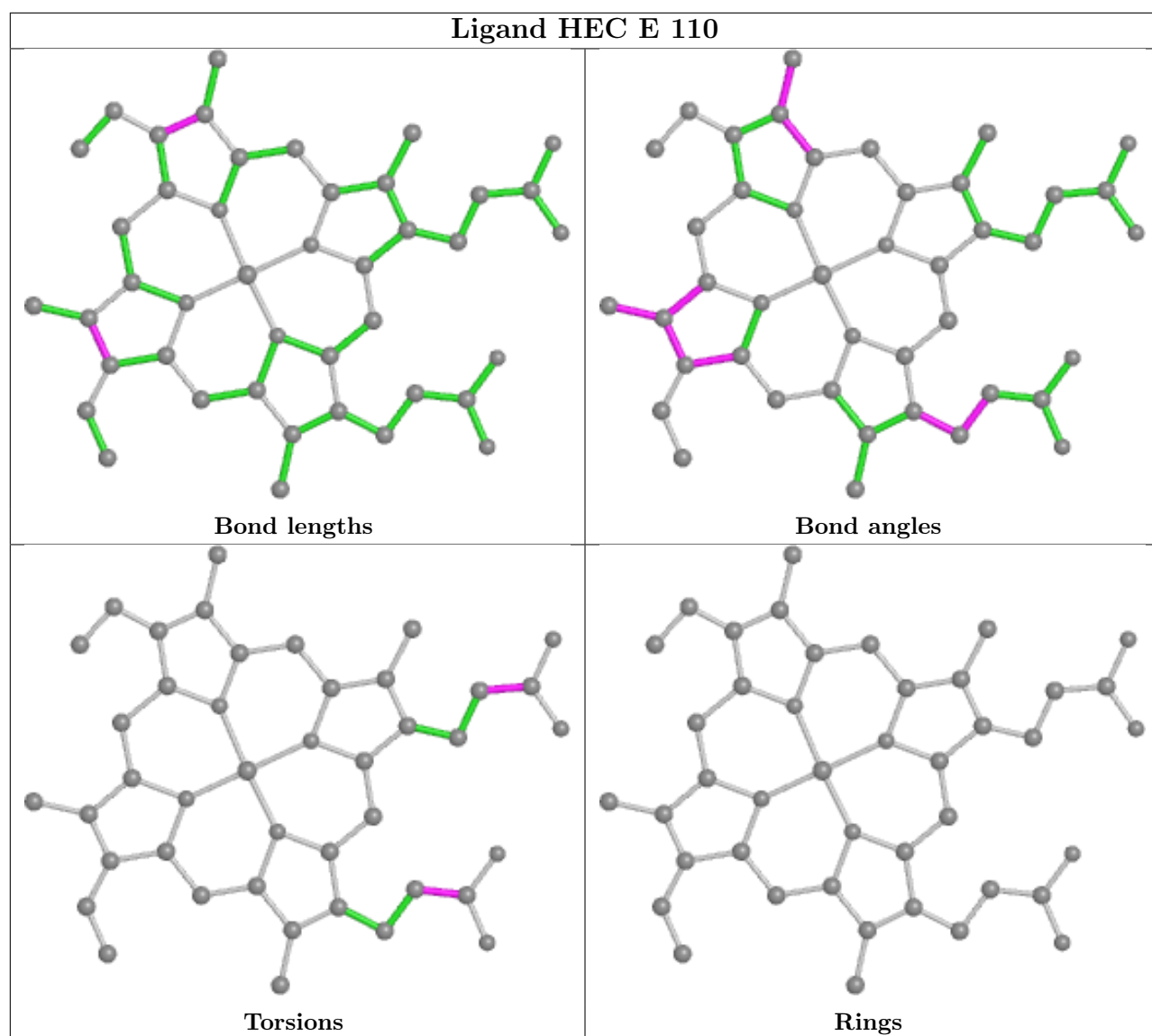


## Ligand HEC E 109



## Ligand HEC E 111





## 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

No chemical shift data were provided