



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 08:40 PM UTC

PDB ID : 1HJ5 / pdb_00001hj5
Title : Cytochrome cd1 Nitrite Reductase, reoxidised enzyme
Authors : Sjogren, T.; Hajdu, J.
Deposited on : 2001-01-08
Resolution : 1.46 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

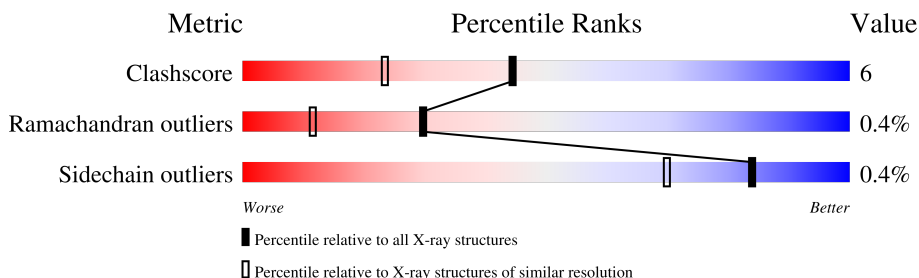
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.46 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))
Clashscore	190562	1795 (1.46-1.46)
Ramachandran outliers	187476	1776 (1.46-1.46)
Sidechain outliers	187428	1776 (1.46-1.46)

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

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	567	 89% 9% ..
1	B	567	 87% 11% .

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	DHE	A	602	X	-	-	-
3	DHE	B	602	X	-	-	-
4	GOL	A	611	-	X	X	-
4	GOL	A	612	-	-	X	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	GOL	A	613	-	-	X	-
4	GOL	B	611	-	X	X	-
5	SO4	B	623	-	-	X	-

2 Entry composition [i](#)

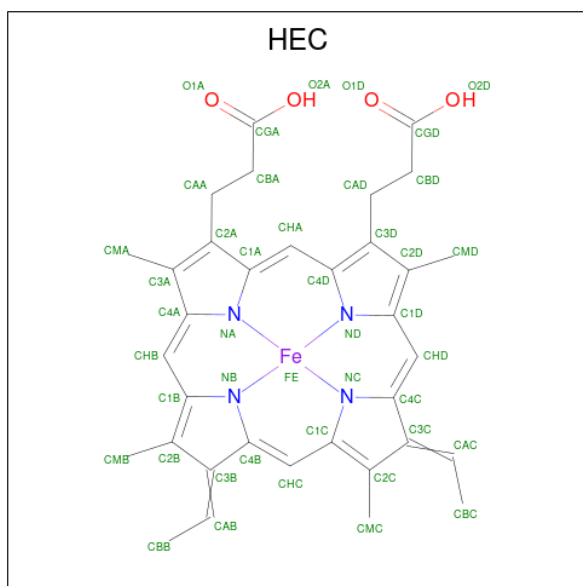
There are 6 unique types of molecules in this entry. The entry contains 9814 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Nitrite reductase.

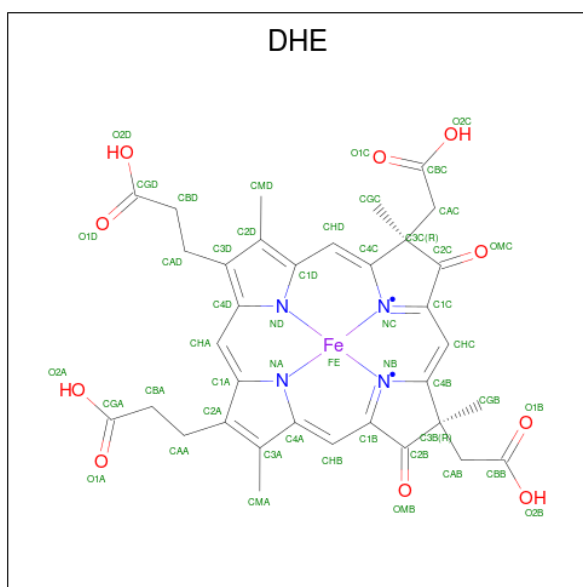
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	559	Total	C	N	O	S	0	0	0
			4345	2743	728	860	14			
1	B	559	Total	C	N	O	S	0	0	0
			4345	2743	728	860	14			

- Molecule 2 is HEME C (CCD ID: HEC) (formula: $C_{34}H_{34}FeN_4O_4$).



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

- Molecule 3 is HEME D (CCD ID: DHE) (formula: $C_{34}H_{32}FeN_4O_{10}$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total 49	C 34	Fe 1	N 4	O 10	0	0
3	B	1	Total 49	C 34	Fe 1	N 4	O 10	0	0

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula: $\text{C}_3\text{H}_8\text{O}_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 6 3 3	0	0
4	A	1	Total C O 6 3 3	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		

- Molecule 5 is SULFATE ION (CCD ID: SO4) (formula: O₄S).

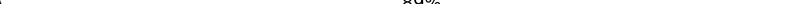


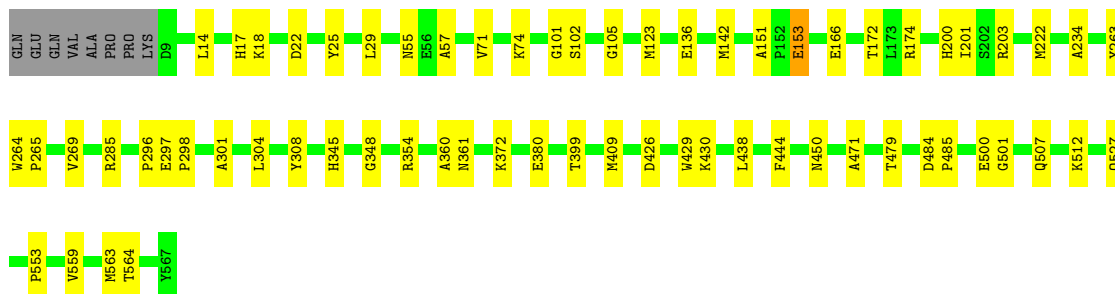
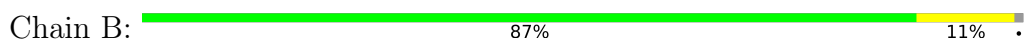
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	O	S	0	0
			5	4	1		
5	A	1	Total	O	S	0	0
			5	4	1		
5	B	1	Total	O	S	0	0
			5	4	1		
5	B	1	Total	O	S	0	0
			5	4	1		
5	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	440	Total	O	0	0
			440	440		
6	B	451	Total	O	0	0
			451	451		

Note EDS was not executed.

- Chain A:  89% 9% ..



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	106.82Å 60.97Å 100.33Å 90.00° 112.24° 90.00°	Depositor
Resolution (Å)	30.00 – 1.46	Depositor
% Data completeness (in resolution range)	91.2 (30.00-1.46)	Depositor
R_{merge}	0.05	Depositor
R_{sym}	0.05	Depositor
Refinement program	REFMAC	Depositor
R, R_{free}	0.195 , 0.215	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	9814	wwPDB-VP
Average B, all atoms (Å ²)	17.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: DHE, GOL, SO4, HEC

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.74	0/4451	0.97	2/6056 (0.0%)
1	B	0.73	1/4451 (0.0%)	0.97	2/6056 (0.0%)
All	All	0.73	1/8902 (0.0%)	0.97	4/12112 (0.0%)

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	1
1	B	0	1
All	All	0	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	301	ALA	N-CA	5.34	1.49	1.46

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	361	ASN	N-CA-C	6.29	118.66	111.11
1	A	200	HIS	CA-CB-CG	-5.54	108.26	113.80
1	B	361	ASN	N-CA-C	5.19	116.62	111.07
1	B	200	HIS	CA-CB-CG	-5.07	108.73	113.80

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	521	VAL	Mainchain
1	B	360	ALA	Mainchain

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	4345	0	4177	34	0
1	B	4345	0	4177	47	0
2	A	43	0	30	2	0
2	B	43	0	30	3	0
3	A	49	0	26	4	0
3	B	49	0	28	3	0
4	A	18	0	23	17	0
4	B	6	0	8	8	0
5	A	10	0	0	0	0
5	B	15	0	0	4	0
6	A	440	0	0	6	0
6	B	451	0	0	2	0
All	All	9814	0	8499	104	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 6.

All (104) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:613:GOL:C1	4:A:613:GOL:C2	1.86	1.52
4:B:611:GOL:C1	4:B:611:GOL:C2	1.87	1.51
4:A:612:GOL:C1	4:A:612:GOL:C2	1.89	1.49
4:A:611:GOL:C2	4:A:611:GOL:C1	1.87	1.49
1:B:57:ALA:HA	1:B:123:MET:HE1	1.36	1.06
1:B:354:ARG:HD2	5:B:623:SO4:O3	1.67	0.92
4:A:612:GOL:C1	4:A:612:GOL:C3	2.53	0.87
4:B:611:GOL:C1	4:B:611:GOL:C3	2.53	0.86
4:A:611:GOL:C1	4:A:611:GOL:C3	2.53	0.85
4:A:613:GOL:C1	4:A:613:GOL:C3	2.55	0.84

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:198:ALA:HB3	1:A:216:ARG:HD2	1.71	0.72
1:A:375:LYS:HE3	6:B:2254:HOH:O	1.94	0.66
4:A:611:GOL:C1	4:A:611:GOL:H31	2.26	0.65
4:A:612:GOL:C1	4:A:612:GOL:O2	2.46	0.64
4:A:612:GOL:C2	4:A:612:GOL:O1	2.46	0.64
4:B:611:GOL:C1	4:B:611:GOL:H31	2.27	0.64
1:B:426:ASP:O	1:B:430:LYS:HD3	1.97	0.64
4:A:612:GOL:C1	4:A:612:GOL:H31	2.27	0.64
1:B:57:ALA:CA	1:B:123:MET:HE1	2.22	0.63
1:A:105:GLY:HA2	4:A:611:GOL:H11	1.82	0.62
1:A:177:GLY:HA2	1:A:197:TYR:O	2.00	0.62
1:A:201:ILE:HD12	1:A:203:ARG:HG2	1.80	0.62
1:B:142:MET:HE1	1:B:269:VAL:HG21	1.81	0.62
1:B:153:GLU:H	1:B:153:GLU:CD	2.07	0.61
4:A:613:GOL:C1	4:A:613:GOL:H31	2.29	0.61
4:B:611:GOL:C2	4:B:611:GOL:O1	2.48	0.61
1:A:216:ARG:NH2	3:A:602:DHE:O2B	2.34	0.60
4:A:611:GOL:C1	4:A:611:GOL:O2	2.49	0.58
4:B:611:GOL:C1	4:B:611:GOL:O2	2.48	0.58
1:B:22:ASP:HA	1:B:409:MET:HE2	1.84	0.58
1:B:105:GLY:HA2	4:B:611:GOL:H11	1.86	0.57
1:A:537:LYS:HG2	6:A:2405:HOH:O	2.05	0.56
4:A:611:GOL:C2	4:A:611:GOL:O1	2.50	0.56
1:B:201:ILE:HD13	3:B:602:DHE:O2A	2.05	0.56
1:B:102:SER:HB3	2:B:601:HEC:HBB2	1.88	0.56
1:B:14:LEU:O	1:B:18:LYS:HB2	2.06	0.56
1:B:151:ALA:HB1	1:B:153:GLU:OE2	2.06	0.55
1:A:155:ARG:HG2	6:A:2179:HOH:O	2.06	0.55
1:B:142:MET:HE1	1:B:269:VAL:CG2	2.37	0.55
1:A:9:ASP:HB2	1:A:10:PRO:HD2	1.89	0.55
1:B:136:GLU:CD	1:B:285:ARG:HH22	2.16	0.54
1:B:438:LEU:HG	1:B:471:ALA:HB2	1.90	0.54
1:A:9:ASP:HB2	1:A:10:PRO:CD	2.38	0.54
1:B:308:TYR:HE2	5:B:623:SO4:O4	1.91	0.54
1:A:222:MET:HE1	1:A:274:GLU:HA	1.91	0.53
1:A:106:MET:HE1	1:A:460:LEU:HD21	1.90	0.52
1:A:500:GLU:HG2	6:A:2400:HOH:O	2.09	0.52
1:A:444:PHE:CE1	3:A:602:DHE:HBD1	2.45	0.52
1:A:18:LYS:HA	1:A:18:LYS:HE2	1.91	0.52
1:A:334:LYS:NZ	1:A:334:LYS:HB3	2.24	0.52
1:A:216:ARG:HH22	3:A:602:DHE:CBB	2.23	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:74:LYS:HG3	1:A:296:PRO:HG3	1.91	0.51
1:B:297:GLU:N	1:B:298:PRO:HD3	2.26	0.51
1:B:142:MET:CE	1:B:269:VAL:HG21	2.41	0.50
1:A:297:GLU:N	1:A:298:PRO:HD3	2.26	0.50
1:A:201:ILE:HD13	3:A:602:DHE:O2A	2.12	0.50
1:B:201:ILE:HD12	1:B:203:ARG:HG2	1.94	0.50
1:B:501:GLY:HA3	1:B:527:GLN:NE2	2.26	0.50
1:B:380:GLU:HG3	1:B:429:TRP:O	2.10	0.49
1:B:17:HIS:CE1	2:B:601:HEC:NB	2.81	0.49
4:A:613:GOL:H31	6:A:2437:HOH:O	2.12	0.49
1:A:108:ASN:O	1:A:109:TRP:HB3	2.13	0.48
1:B:372:LYS:HD2	5:B:623:SO4:O4	2.13	0.48
1:B:74:LYS:HG3	1:B:296:PRO:HG3	1.95	0.48
4:A:613:GOL:C1	4:A:613:GOL:O2	2.54	0.47
1:B:450:ASN:HB3	6:B:2397:HOH:O	2.13	0.47
1:A:102:SER:HB3	2:A:601:HEC:HBB2	1.96	0.47
1:B:17:HIS:HB3	1:B:101:GLY:O	2.15	0.47
1:B:559:VAL:O	1:B:563:MET:HG2	2.14	0.47
1:B:166:GLU:HB3	1:B:512:LYS:HD2	1.97	0.47
1:B:444:PHE:CE1	3:B:602:DHE:HBD1	2.50	0.47
1:A:304:LEU:HD21	1:A:348:GLY:HA2	1.97	0.46
1:A:470:VAL:HG22	1:A:490:LEU:HB2	1.98	0.46
1:B:222:MET:HG2	1:B:234:ALA:HB3	1.97	0.46
1:B:71:VAL:HG22	1:B:297:GLU:OE2	2.16	0.46
1:B:304:LEU:HD21	1:B:348:GLY:HA2	1.97	0.46
1:B:102:SER:CB	2:B:601:HEC:HBB2	2.46	0.46
1:B:123:MET:N	1:B:123:MET:HE2	2.32	0.45
4:B:611:GOL:C1	4:B:611:GOL:HO2	2.28	0.45
1:A:264:TRP:HA	1:A:265:PRO:C	2.41	0.45
1:B:105:GLY:HA2	4:B:611:GOL:C1	2.46	0.45
4:A:613:GOL:C2	4:A:613:GOL:O1	2.52	0.45
1:B:29:LEU:HD12	1:B:71:VAL:CG1	2.48	0.44
1:B:563:MET:HG3	1:B:564:THR:HG23	2.01	0.43
1:B:29:LEU:HD12	1:B:71:VAL:HG13	2.01	0.43
1:B:263:TYR:OH	3:B:602:DHE:HHB	2.18	0.43
2:A:601:HEC:HMC2	6:A:2043:HOH:O	2.19	0.43
1:A:263:TYR:CD1	1:A:299:ARG:HB3	2.53	0.43
1:A:309:ARG:HB3	1:A:310:PRO:HD2	2.01	0.43
1:A:200:HIS:HB2	6:A:2160:HOH:O	2.18	0.42
1:A:198:ALA:O	1:A:199:VAL:C	2.62	0.42
1:B:264:TRP:HA	1:B:265:PRO:C	2.43	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:142:MET:HE1	1:A:269:VAL:CG2	2.50	0.41
1:A:488:LYS:HE2	1:A:539:LEU:HD12	2.02	0.41
1:B:399:THR:HG21	1:B:479:THR:O	2.20	0.41
1:B:25:TYR:HE2	1:B:345:HIS:HE2	1.67	0.41
1:A:563:MET:HG3	1:A:564:THR:HG23	2.03	0.41
1:B:308:TYR:OH	5:B:623:SO4:O3	2.32	0.41
1:A:119:GLN:O	1:A:123:MET:HG2	2.20	0.41
1:B:500:GLU:O	1:B:501:GLY:C	2.61	0.41
1:B:22:ASP:HA	1:B:409:MET:CE	2.51	0.41
1:A:438:LEU:HG	1:A:471:ALA:HB2	2.04	0.40
1:B:484:ASP:HA	1:B:485:PRO:HD3	1.95	0.40
1:B:172:THR:O	1:B:553:PRO:HA	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	557/567 (98%)	532 (96%)	23 (4%)	2 (0%)	30	11
1	B	557/567 (98%)	532 (96%)	23 (4%)	2 (0%)	30	11
All	All	1114/1134 (98%)	1064 (96%)	46 (4%)	4 (0%)	30	11

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	109	TRP
1	A	507	GLN
1	B	507	GLN
1	B	174	ARG

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	462/469 (98%)	460 (100%)	2 (0%)	84	70
1	B	462/469 (98%)	460 (100%)	2 (0%)	84	70
All	All	924/938 (98%)	920 (100%)	4 (0%)	84	70

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	HIS
1	A	216	ARG
1	B	55	ASN
1	B	153	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	282	GLN
1	A	385	GLN
1	B	31	ASN
1	B	34	GLN
1	B	282	GLN
1	B	502	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

13 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	HEC	B	601	1	46,50,50	1.86	7 (15%)	58,82,82	1.56	4 (6%)
5	SO4	A	621	-	4,4,4	0.70	0	6,6,6	0.07	0
2	HEC	A	601	1	46,50,50	1.86	7 (15%)	58,82,82	1.60	3 (5%)
3	DHE	A	602	1	52,56,56	4.54	14 (26%)	68,94,94	3.11	20 (29%)
5	SO4	B	624	-	4,4,4	0.68	0	6,6,6	0.08	0
4	GOL	A	611	-	5,5,5	4.17	1 (20%)	5,5,5	2.66	3 (60%)
5	SO4	A	622	-	4,4,4	0.70	0	6,6,6	0.09	0
5	SO4	B	623	-	4,4,4	0.64	0	6,6,6	0.22	0
4	GOL	A	613	-	5,5,5	4.10	1 (20%)	5,5,5	2.19	1 (20%)
3	DHE	B	602	1	52,56,56	4.55	15 (28%)	68,94,94	3.24	23 (33%)
4	GOL	B	611	-	5,5,5	4.26	1 (20%)	5,5,5	2.81	3 (60%)
5	SO4	B	622	-	4,4,4	0.72	0	6,6,6	0.10	0
4	GOL	A	612	-	5,5,5	4.41	1 (20%)	5,5,5	3.12	3 (60%)

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	B	601	1	-	5/14/54/54	-
2	HEC	A	601	1	-	6/14/54/54	-
3	DHE	A	602	1	1/1/15/19	7/20/108/108	-
4	GOL	A	611	-	-	2/4/4/4	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GOL	A	613	-	-	2/4/4/4	-
3	DHE	B	602	1	1/1/15/19	7/20/108/108	-
4	GOL	B	611	-	-	2/4/4/4	-
4	GOL	A	612	-	-	1/4/4/4	-

All (47) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	602	DHE	OMC-C2C	18.38	1.54	1.22
3	B	602	DHE	OMB-C2B	18.25	1.54	1.22
3	B	602	DHE	OMC-C2C	17.99	1.53	1.22
3	A	602	DHE	OMB-C2B	17.97	1.53	1.22
3	A	602	DHE	C3C-C2C	-11.06	1.33	1.52
3	B	602	DHE	C3B-C2B	-10.90	1.34	1.52
3	B	602	DHE	C3C-C2C	-10.88	1.34	1.52
3	A	602	DHE	C3B-C2B	-10.64	1.34	1.52
4	A	612	GOL	C1-C2	9.82	1.89	1.51
4	B	611	GOL	C1-C2	9.48	1.87	1.51
4	A	611	GOL	C1-C2	9.28	1.87	1.51
4	A	613	GOL	C1-C2	8.97	1.86	1.51
3	A	602	DHE	CAC-CBC	-7.09	1.29	1.50
2	A	601	HEC	CAC-C3C	6.94	1.57	1.35
3	B	602	DHE	CAB-CBB	-6.86	1.29	1.50
2	B	601	HEC	CAB-C3B	6.80	1.57	1.35
2	B	601	HEC	CAC-C3C	6.77	1.57	1.35
2	A	601	HEC	CAB-C3B	6.77	1.57	1.35
3	B	602	DHE	CAC-CBC	-6.62	1.30	1.50
3	A	602	DHE	CAB-CBB	-6.60	1.30	1.50
3	B	602	DHE	CAB-C3B	-3.80	1.44	1.54
2	B	601	HEC	CBC-CAC	-3.30	1.37	1.49
2	A	601	HEC	CBC-CAC	-2.93	1.38	1.49
3	A	602	DHE	FE-NC	2.89	2.03	1.94
3	A	602	DHE	CAB-C3B	-2.68	1.47	1.54
3	A	602	DHE	CAC-C3C	-2.62	1.47	1.54
3	B	602	DHE	FE-NC	2.61	2.02	1.94
3	B	602	DHE	C1B-C2B	-2.58	1.43	1.47
2	A	601	HEC	CBB-CAB	-2.57	1.40	1.49
3	A	602	DHE	O1C-CBC	2.56	1.30	1.22
3	B	602	DHE	CMA-C3A	2.55	1.56	1.50
3	A	602	DHE	C1B-C2B	-2.48	1.43	1.47
3	A	602	DHE	CMA-C3A	2.36	1.55	1.50
3	B	602	DHE	O1B-CBB	2.30	1.29	1.22

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	602	DHE	CMD-C2D	2.29	1.55	1.50
2	B	601	HEC	CBB-CAB	-2.27	1.41	1.49
3	B	602	DHE	CAC-C3C	-2.23	1.48	1.54
2	A	601	HEC	C3C-C2C	-2.22	1.33	1.41
2	A	601	HEC	C3B-C2B	-2.21	1.33	1.41
2	B	601	HEC	C3C-C2C	-2.19	1.33	1.41
3	B	602	DHE	O1C-CBC	2.14	1.29	1.22
2	B	601	HEC	C3B-C2B	-2.14	1.33	1.41
3	B	602	DHE	FE-NB	2.13	2.01	1.94
3	A	602	DHE	O1B-CBB	2.11	1.29	1.22
3	A	602	DHE	CMD-C2D	2.10	1.55	1.50
2	A	601	HEC	CMB-C2B	2.01	1.54	1.50
2	B	601	HEC	CMC-C2C	2.01	1.54	1.50

All (60) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	602	DHE	C2C-C3C-C4C	14.50	108.04	100.35
3	A	602	DHE	C2B-C3B-C4B	14.27	107.92	100.35
3	A	602	DHE	C2C-C3C-C4C	14.22	107.89	100.35
3	B	602	DHE	C2B-C3B-C4B	14.22	107.89	100.35
2	B	601	HEC	CBB-CAB-C3B	-7.81	111.82	127.43
2	A	601	HEC	CBB-CAB-C3B	-7.48	112.49	127.43
3	B	602	DHE	CAB-C3B-C2B	7.11	120.14	112.22
2	A	601	HEC	CBC-CAC-C3C	-6.88	113.68	127.43
2	B	601	HEC	CBC-CAC-C3C	-5.65	116.15	127.43
3	A	602	DHE	C3B-C4B-CHC	4.95	126.84	122.44
3	B	602	DHE	CGB-C3B-C2B	-4.89	97.38	109.38
3	A	602	DHE	CGB-C3B-C2B	-4.81	97.58	109.38
4	A	612	GOL	C3-C2-C1	-4.78	94.26	111.80
4	B	611	GOL	C3-C2-C1	-4.56	95.09	111.80
4	A	611	GOL	C3-C2-C1	-4.48	95.36	111.80
3	B	602	DHE	C3C-C4C-CHD	4.46	126.41	122.44
3	B	602	DHE	CHB-C1B-C2B	4.37	127.11	122.21
3	A	602	DHE	CAB-C3B-C2B	4.32	117.03	112.22
3	B	602	DHE	C3B-C4B-CHC	4.24	126.21	122.44
3	A	602	DHE	CAC-C3C-C2C	4.20	116.90	112.22
3	B	602	DHE	CAC-C3C-C2C	4.13	116.82	112.22
3	A	602	DHE	C3C-C4C-CHD	3.94	125.94	122.44
3	A	602	DHE	CHB-C1B-C2B	3.85	126.53	122.21
4	A	613	GOL	C3-C2-C1	-3.70	98.22	111.80
4	A	612	GOL	O2-C2-C1	-3.64	94.09	109.18

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	602	DHE	OMC-C2C-C3C	3.64	130.21	125.93
3	A	602	DHE	OMC-C2C-C1C	-3.60	122.62	126.49
3	A	602	DHE	OMC-C2C-C3C	3.58	130.14	125.93
4	A	612	GOL	O1-C1-C2	-3.54	94.44	110.38
3	B	602	DHE	OMC-C2C-C1C	-3.38	122.85	126.49
3	A	602	DHE	O2C-CBC-O1C	-3.24	115.00	123.33
4	B	611	GOL	O2-C2-C1	-3.13	96.20	109.18
3	A	602	DHE	CAA-CBA-CGA	3.11	121.91	113.67
3	A	602	DHE	O2C-CBC-CAC	3.11	124.19	114.35
3	B	602	DHE	CAA-CBA-CGA	3.04	121.74	113.67
3	B	602	DHE	CGB-C3B-C4B	-3.03	98.19	109.93
3	A	602	DHE	OMB-C2B-C3B	3.03	129.49	125.93
3	B	602	DHE	OMB-C2B-C1B	-3.00	123.26	126.49
3	B	602	DHE	O2C-CBC-O1C	-2.98	115.66	123.33
3	A	602	DHE	OMB-C2B-C1B	-2.97	123.29	126.49
4	B	611	GOL	O1-C1-C2	-2.95	97.09	110.38
3	B	602	DHE	OMB-C2B-C3B	2.84	129.27	125.93
3	B	602	DHE	O2C-CBC-CAC	2.83	123.31	114.35
4	A	611	GOL	O2-C2-C1	-2.80	97.58	109.18
3	B	602	DHE	O2B-CBB-CAB	2.79	123.19	114.35
4	A	611	GOL	O1-C1-C2	-2.69	98.28	110.38
3	B	602	DHE	O2B-CBB-O1B	-2.62	116.59	123.33
3	A	602	DHE	CHC-C1C-C2C	2.59	125.12	122.21
3	A	602	DHE	O2B-CBB-O1B	-2.41	117.14	123.33
3	A	602	DHE	CGC-C3C-C4C	-2.33	100.92	109.93
3	B	602	DHE	CHB-C4A-NA	-2.29	121.96	124.45
3	A	602	DHE	O2B-CBB-CAB	2.28	121.58	114.35
3	A	602	DHE	CBD-CAD-C3D	2.23	118.71	112.53
3	B	602	DHE	CBD-CAD-C3D	2.23	118.69	112.53
2	B	601	HEC	O1A-CGA-CBA	-2.19	116.13	123.09
3	B	602	DHE	CGC-C3C-C4C	-2.14	101.63	109.93
2	A	601	HEC	O1D-CGD-CBD	-2.08	116.51	123.09
3	B	602	DHE	CGC-C3C-C2C	-2.06	104.32	109.38
2	B	601	HEC	O1D-CGD-CBD	-2.04	116.63	123.09
3	B	602	DHE	CHC-C1C-C2C	2.02	124.48	122.21

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	602	DHE	NA
3	B	602	DHE	NA

All (32) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	601	HEC	C2B-C3B-CAB-CBB
2	A	601	HEC	C4B-C3B-CAB-CBB
2	A	601	HEC	C4C-C3C-CAC-CBC
3	A	602	DHE	C2D-C3D-CAD-CBD
3	A	602	DHE	C4D-C3D-CAD-CBD
3	B	602	DHE	C4B-C3B-CAB-CBB
3	B	602	DHE	C2D-C3D-CAD-CBD
3	B	602	DHE	C4D-C3D-CAD-CBD
4	A	611	GOL	C1-C2-C3-O3
4	A	612	GOL	C1-C2-C3-O3
4	A	613	GOL	C1-C2-C3-O3
4	B	611	GOL	C1-C2-C3-O3
4	A	613	GOL	O2-C2-C3-O3
3	A	602	DHE	C3B-CAB-CBB-O2B
3	A	602	DHE	C3C-CAC-CBC-O2C
3	B	602	DHE	C3B-CAB-CBB-O2B
3	B	602	DHE	C3C-CAC-CBC-O2C
4	A	611	GOL	O2-C2-C3-O3
4	B	611	GOL	O2-C2-C3-O3
3	A	602	DHE	C3B-CAB-CBB-O1B
3	A	602	DHE	C3C-CAC-CBC-O1C
3	B	602	DHE	C3B-CAB-CBB-O1B
3	B	602	DHE	C3C-CAC-CBC-O1C
2	B	601	HEC	C4B-C3B-CAB-CBB
3	A	602	DHE	C4B-C3B-CAB-CBB
2	A	601	HEC	C2C-C3C-CAC-CBC
2	B	601	HEC	C2B-C3B-CAB-CBB
2	B	601	HEC	CAD-CBD-CGD-O1D
2	A	601	HEC	CAD-CBD-CGD-O1D
2	A	601	HEC	CAD-CBD-CGD-O2D
2	B	601	HEC	CAD-CBD-CGD-O2D
2	B	601	HEC	C4C-C3C-CAC-CBC

There are no ring outliers.

9 monomers are involved in 41 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	601	HEC	3	0
2	A	601	HEC	2	0
3	A	602	DHE	4	0
4	A	611	GOL	6	0

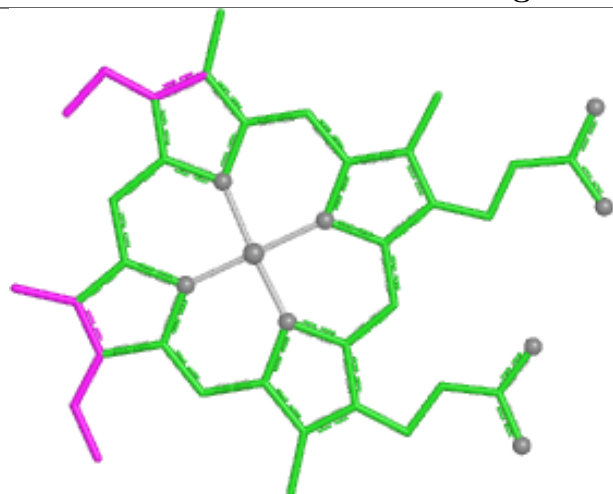
Continued on next page...

Continued from previous page...

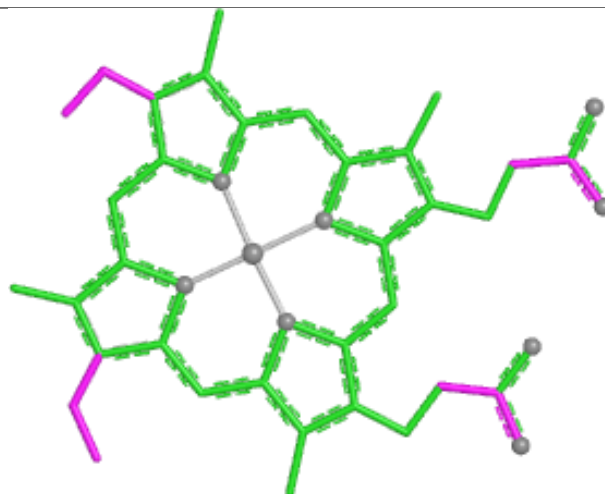
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	623	SO4	4	0
4	A	613	GOL	6	0
3	B	602	DHE	3	0
4	B	611	GOL	8	0
4	A	612	GOL	5	0

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

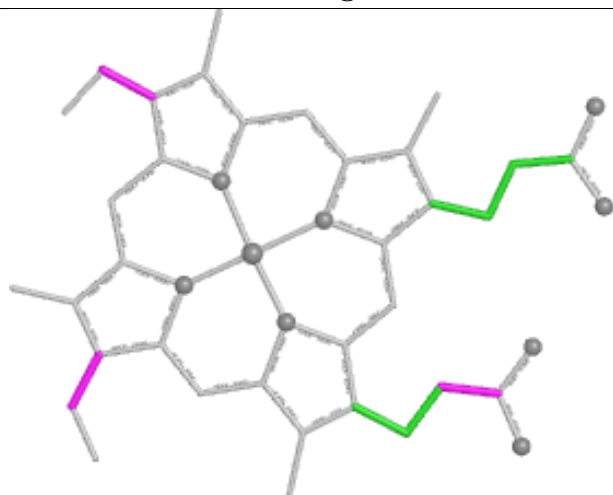
Ligand HEC B 601



Bond lengths



Bond angles

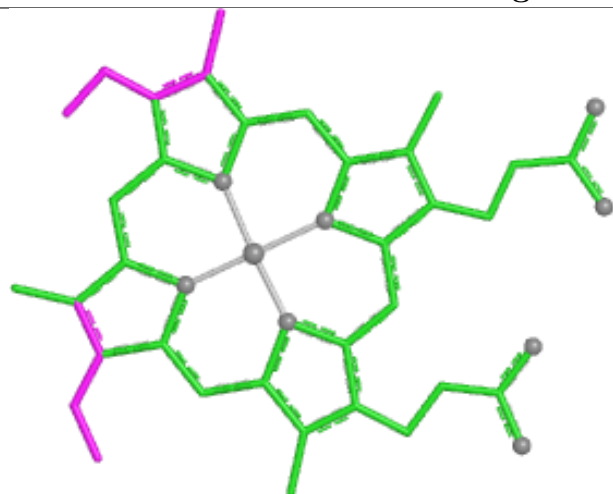


Torsions

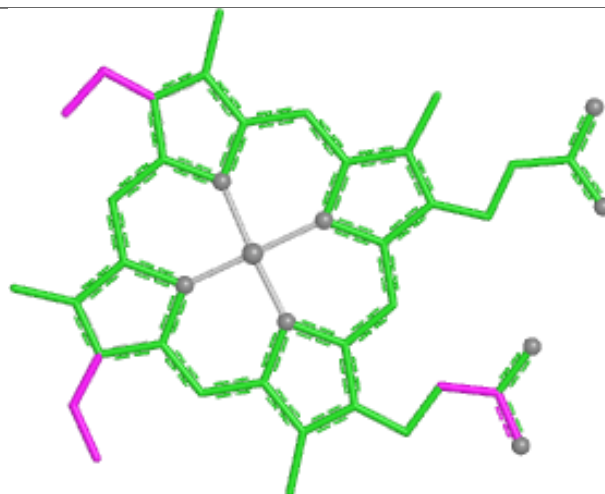


Rings

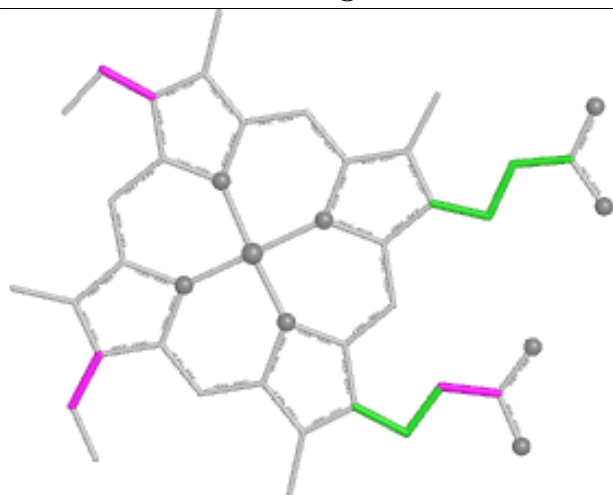
Ligand HEC A 601



Bond lengths



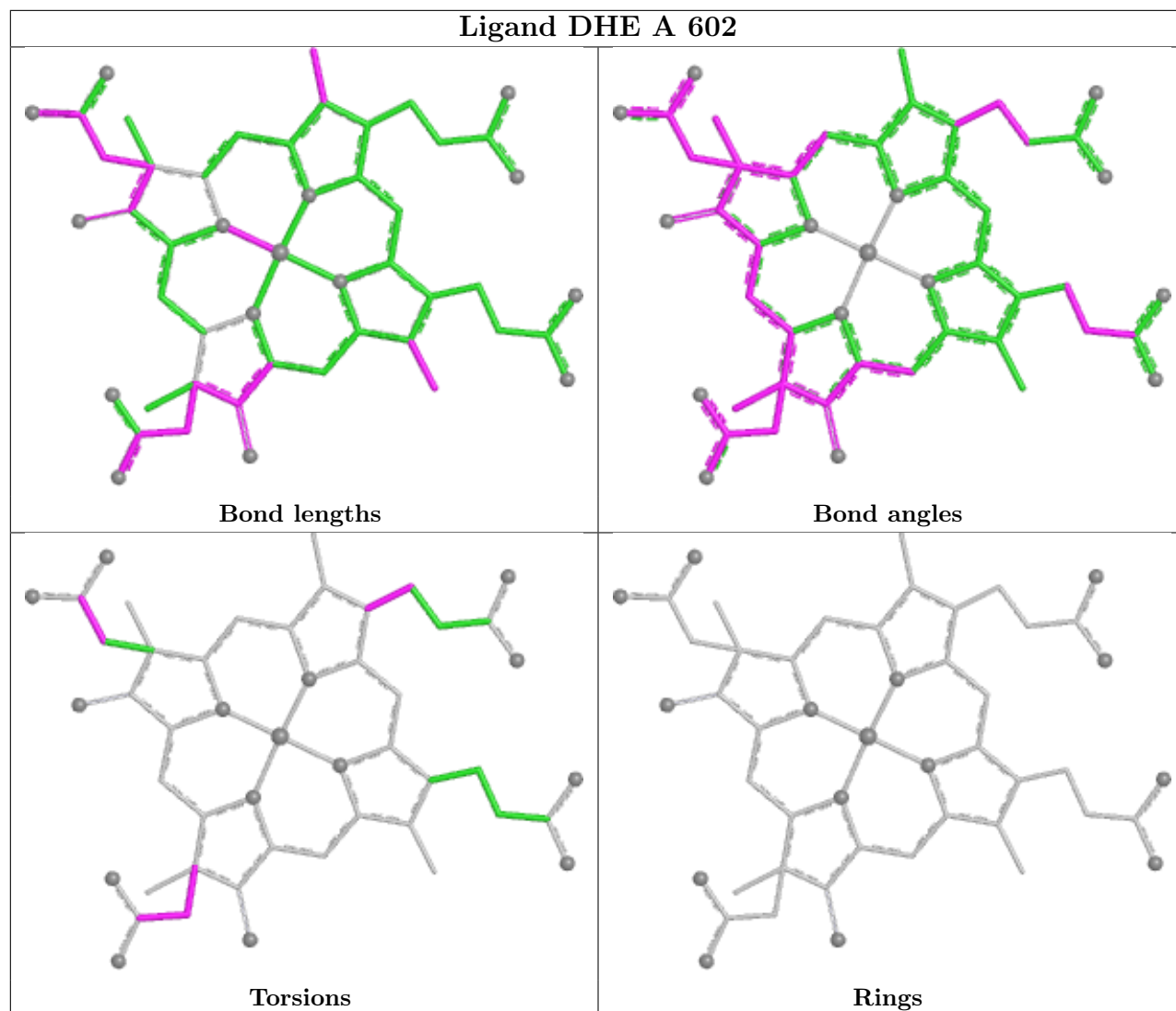
Bond angles

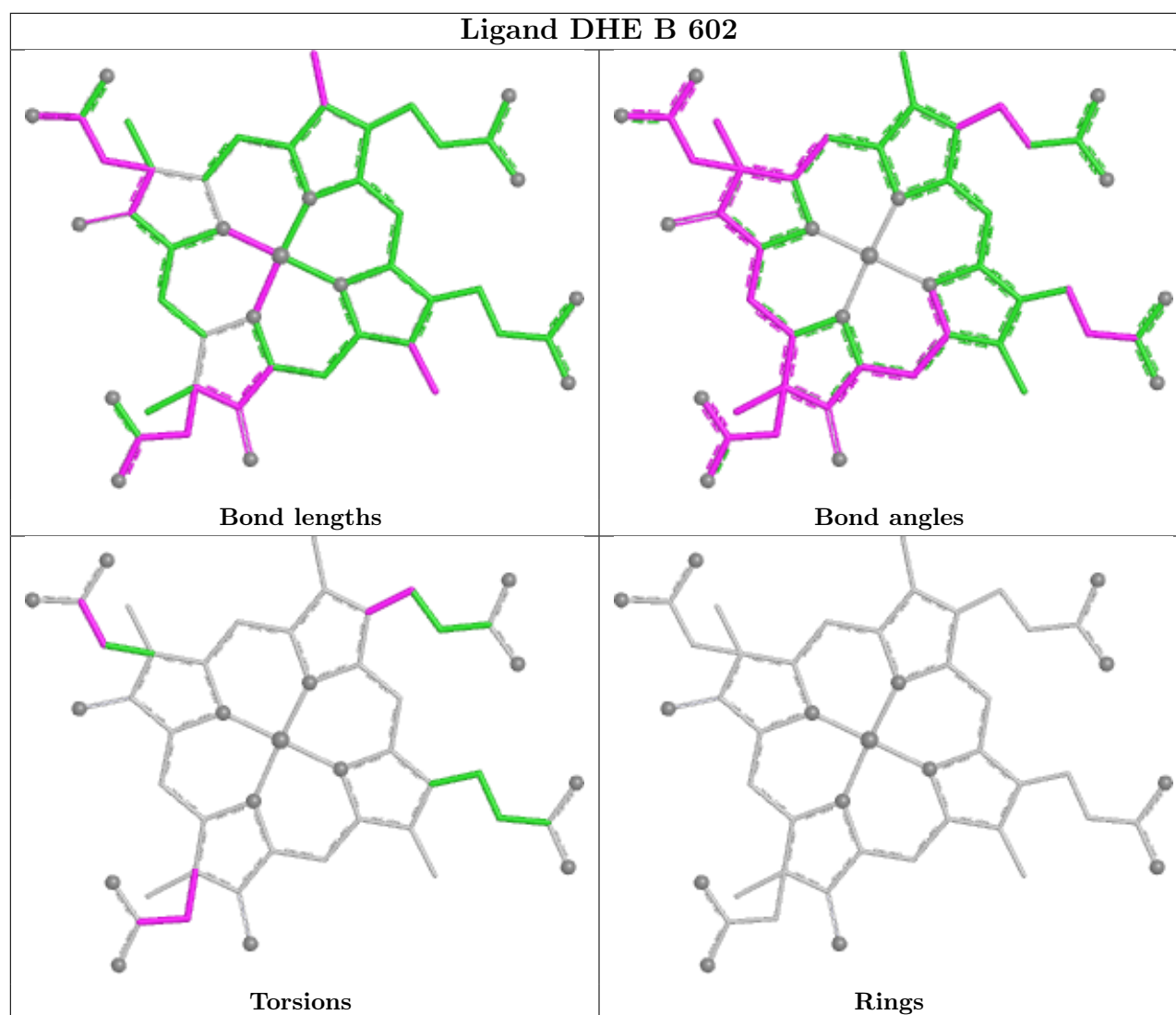


Torsions



Rings





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.