

wwPDB X-ray Structure Validation Summary Report (i)

Dec 6, 2023 - 02:36 am GMT

PDB ID : 2C1V

Title : CRYSTAL STRUCTURE OF THE DI-HAEM CYTOCHROME C PEROXI-

DASE FROM PARACOCCUS PANTOTROPHUS - Mixed VALENCE FORM

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Deposited on : 2005-09-21

Resolution : 1.20 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 (1)) were used in the production of this report:

MolProbity: 4.02b-467

Mogul : 1.8.4, CSD as541be (2020)

Xtriage (Phenix) : NOT EXECUTED

EDS : NOT EXECUTED

buster-report : 1.1.7 (2018)

Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)

Ideal geometry (proteins) : Engh & Huber (2001) Ideal geometry (DNA, RNA) : Parkinson et al. (1996)

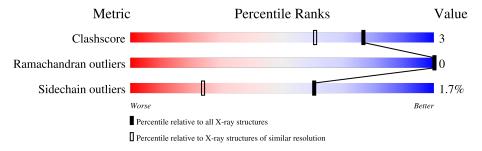
Validation Pipeline (wwPDB-VP) : 2.36

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 1.20 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	Similar resolution
Metric	$(\# \mathrm{Entries})$	$(\# ext{Entries}, ext{ resolution range}(ext{Å}))$
Clashscore	141614	1286 (1.22-1.18)
Ramachandran outliers	138981	1240 (1.22-1.18)
Sidechain outliers	138945	1239 (1.22-1.18)

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%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain					
1	A	338	95%					
1	В	338	93%	5%•				

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:

\mathbf{Mol}	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	EDO	В	1340	-	-	X	-



2 Entry composition (i)

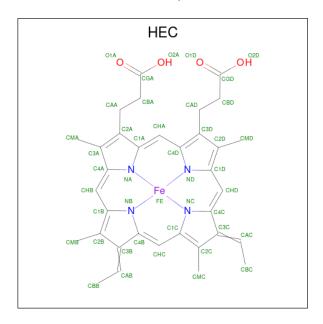
There are 5 unique types of molecules in this entry. The entry contains 6305 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 DI-HAEM CYTOCHROME C PEROXIDASE.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
1	A	335	Total 2528	C 1594	N 422	O 499	S 13	0	0	0
1	В	335	Total 2528	C 1594	N 422	O 499	S 13	0	0	0

• Molecule 2 is HEME C (three-letter code: HEC) (formula: C₃₄H₃₄FeN₄O₄).



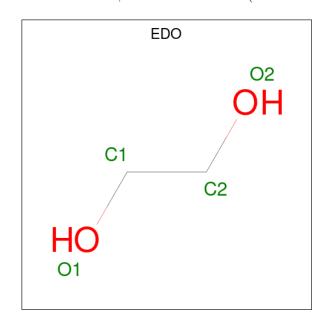
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf			
2	A	1	Total	С	Fe	N	О	0	0	
	Λ	1	43	34	1	4	4	U	U	
2	Λ	1	Total	С	Fe	N	О	0	0	
	A	1	43	34	1	4	4	0		
2	В	1	Total	С	Fe	N	О	0	0	
	Б	1	43	34	1	4	4	0	0	
2	D	1	Total	С	Fe	N	О	0	0	
	Б	1	43	34	1	4	4	0	0	



• Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Ca 1 1	0	0
3	В	1	Total Ca 1 1	0	0

 \bullet Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $\mathrm{C_2H_6O_2}).$



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 6 3 3	0	1
4	A	1	Total C O 4 2 2	0	0
4	В	1	Total C O 6 3 3	0	1
4	В	1	Total C O 4 2 2	0	0

• Molecule 5 is water.

\mathbf{N}	/Iol	Chain	Residues	Atoms	ZeroOcc	AltConf
	5	A	509	Total O 509 509	0	0
	5	В	546	Total O 546 546	0	0

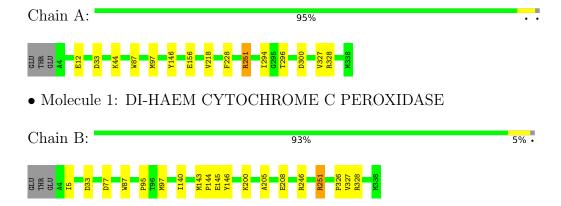


3 Residue-property plots (i)

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. 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. 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.

Note EDS was not executed.

• Molecule 1: DI-HAEM CYTOCHROME C PEROXIDASE





4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants	101.37Å 141.20Å 51.58Å	Depositor
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.22 - 1.20	Depositor
% Data completeness	92.5 (48.22-1.20)	Depositor
(in resolution range)	32.9 (10.22 1.20)	Беровног
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	REFMAC 5.1.9999	Depositor
R, R_{free}	0.173 , 0.188	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6305	wwPDB-VP
Average B, all atoms (Å ²)	18.0	wwPDB-VP



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: CA, HEC, EDO

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	Bo	nd angles
IVIOI	Chain	RMSZ	# Z > 5	RMSZ	# Z > 5
1	A	0.61	0/2587	0.82	$2/3523 \ (0.1\%)$
1	В	0.62	0/2587	0.82	4/3523 (0.1%)
All	All	0.61	0/5174	0.82	6/7046 (0.1%)

There are no bond length outliers.

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^o)$	$\operatorname{Ideal}({}^{o})$
1	В	328	ARG	NE-CZ-NH2	-12.22	114.19	120.30
1	A	328	ARG	NE-CZ-NH2	-8.00	116.30	120.30
1	В	328	ARG	NE-CZ-NH1	6.52	123.56	120.30
1	В	33	ASP	CB-CG-OD2	5.35	123.12	118.30
1	A	300	ASP	CB-CG-OD2	5.33	123.09	118.30

There are no chirality outliers.

There are no planarity outliers.

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	2528	0	2432	10	0
1	В	2528	0	2432	18	0
2	A	86	0	60	2	0
2	В	86	0	60	2	0



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Continueu	110111	predidus	puyc

Mol	Chain	Non-H	H(model)	$\mathbf{H}(\mathbf{added})$	Clashes	Symm-Clashes
3	A	1	0	0	0	0
3	В	1	0	0	0	0
4	A	10	0	18	2	0
4	В	10	0	18	11	0
5	A	509	0	0	3	0
5	В	546	0	0	3	1
All	All	6305	0	5020	31	1

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 3.

The worst 5 of 31 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	$\begin{array}{c} {\rm Interatomic} \\ {\rm distance} \ ({\rm \AA}) \end{array}$	Clash overlap (Å)
1:A:251:ARG:HH11	1:A:251:ARG:HG2	1.29	0.97
1:A:294:ILE:HG22	1:A:296:THR:HG23	1.58	0.86
1:B:327:VAL:O	4:B:1340:EDO:H12	1.85	0.77
1:B:143:MET:HA	4:B:1340:EDO:H11	1.68	0.75
1:A:251:ARG:HG2	1:A:251:ARG:NH1	1.97	0.74

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	$\begin{array}{c} {\rm Interatomic} \\ {\rm distance} \ ({\rm \AA}) \end{array}$	Clash overlap (Å)
5:B:2193:HOH:O	5:B:2193:HOH:O[2_565]	2.06	0.14

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	Perce	entiles
1	A	333/338 (98%)	326 (98%)	7 (2%)	0	100	100



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Mol	Chain	Analysed Favoured		Allowed	Outliers	Perce	ntiles
1	В	333/338 (98%)	326 (98%)	7 (2%)	0	100	100
All	All	666/676 (98%)	652 (98%)	14 (2%)	0	100	100

There are no Ramachandran outliers to report.

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		Outliers	Percentiles
1	A	264/267 (99%)	258 (98%)	6 (2%)	50 14
1	В	264/267 (99%)	261 (99%)	3 (1%)	73 41
All	All	528/534 (99%)	519 (98%)	9 (2%)	60 24

5 of 9 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	В	246	ARG
1	В	251	ARG
1	A	156	GLU
1	A	228	PHE
1	A	251	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

\mathbf{Mol}	Chain	Res	Type
1	В	30	GLN

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 12 ligands modelled in this entry, 2 are monoatomic - leaving 10 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	Во	ond leng	ths	В	ond ang	gles
MIOI	Type	Chain	nes	Lilik	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	EDO	A	1340	-	3,3,3	0.36	0	2,2,2	0.31	0
4	EDO	A	1339[B]	-	3,3,3	0.51	0	2,2,2	0.05	0
4	EDO	В	1339[A]	-	3,3,3	0.47	0	2,2,2	0.30	0
2	HEC	В	401	5,1	32,50,50	1.81	3 (9%)	24,82,82	2.00	10 (41%)
4	EDO	В	1339[B]	-	3,3,3	0.40	0	2,2,2	0.25	0
4	EDO	В	1340	-	3,3,3	0.23	0	2,2,2	0.37	0
2	HEC	A	402	1	32,50,50	1.82	4 (12%)	24,82,82	1.98	8 (33%)
2	HEC	A	401	5,1	32,50,50	2.08	5 (15%)	24,82,82	1.72	6 (25%)
4	EDO	A	1339[A]	-	3,3,3	0.46	0	2,2,2	0.35	0
2	HEC	В	402	1	32,50,50	2.09	3 (9%)	24,82,82	2.34	9 (37%)

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
4	EDO	A	1340	-	-	1/1/1/1	-
4	EDO	A	1339[B]	-	-	1/1/1/1	-
4	EDO	В	1339[A]	-	-	0/1/1/1	-
2	HEC	В	401	5,1	-	0/10/54/54	-



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COHABABACA		DIEUIUU	DUIUE
0 0 1000100000			

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	EDO	В	1339[B]	_	-	0/1/1/1	-
4	EDO	В	1340	-	-	0/1/1/1	-
2	HEC	A	402	1	-	4/10/54/54	-
2	HEC	A	401	5,1	-	0/10/54/54	-
4	EDO	A	1339[A]	-	-	0/1/1/1	-
2	HEC	В	402	1	-	2/10/54/54	-

The worst 5 of 15 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$\operatorname{Observed}(\text{\AA})$	Ideal(Å)
2	A	401	HEC	C2B-C3B	-7.35	1.33	1.40
2	В	402	HEC	C2B-C3B	-6.77	1.33	1.40
2	A	401	HEC	C3C-C2C	-6.33	1.34	1.40
2	В	402	HEC	C3C-C2C	-6.25	1.34	1.40
2	В	401	HEC	C2B-C3B	-6.20	1.34	1.40

The worst 5 of 33 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$\mathbf{Observed}(^o)$	$\operatorname{Ideal}({}^{o})$
2	В	402	HEC	CBD-CAD-C3D	-5.67	102.94	112.62
2	A	401	HEC	CMB-C2B-C1B	-4.75	121.17	128.46
2	A	402	HEC	CBD-CAD-C3D	-4.62	104.74	112.62
2	В	401	HEC	CMB-C2B-C1B	-4.10	122.17	128.46
2	В	402	HEC	C1D-C2D-C3D	-3.80	104.35	107.00

There are no chirality outliers.

5 of 8 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1340	EDO	O1-C1-C2-O2
2	A	402	HEC	CAD-CBD-CGD-O1D
2	A	402	HEC	CAD-CBD-CGD-O2D
2	В	402	HEC	CAD-CBD-CGD-O1D
2	В	402	HEC	CAD-CBD-CGD-O2D

There are no ring outliers.

5 monomers are involved in 17 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1340	EDO	2	0

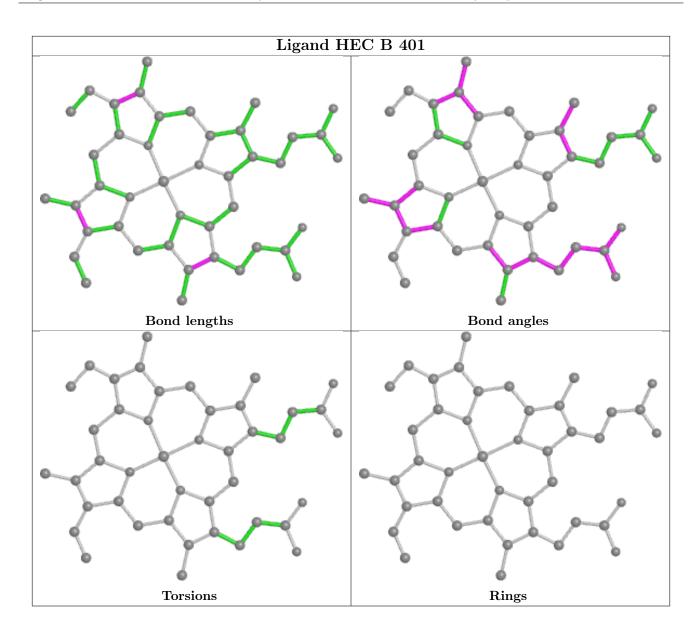


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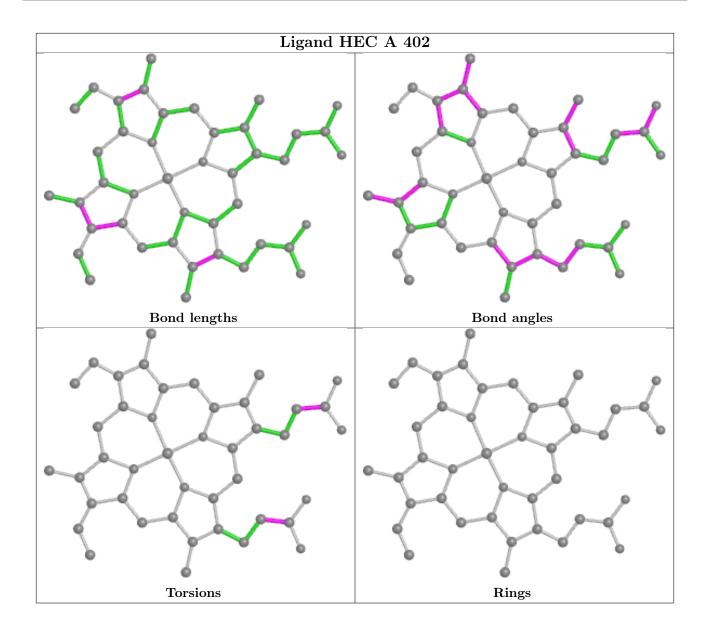
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	В	401	HEC	1	0
4	В	1340	EDO	11	0
2	A	402	HEC	2	0
2	В	402	HEC	1	0

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

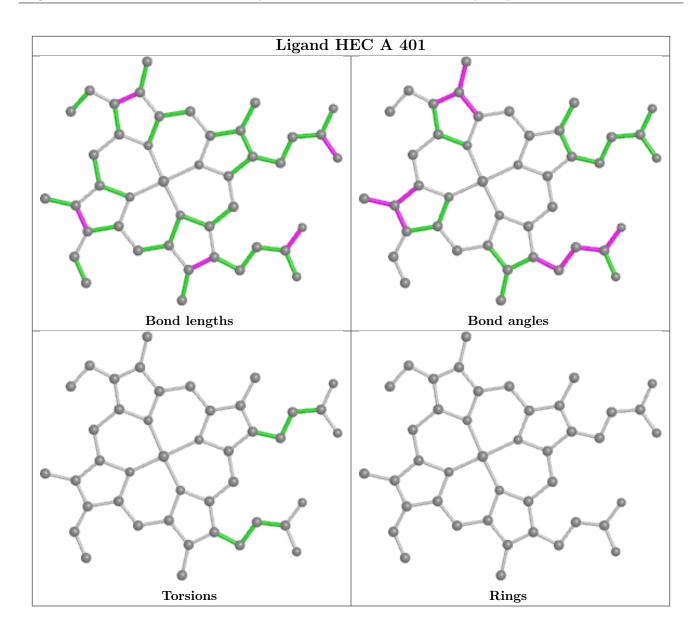




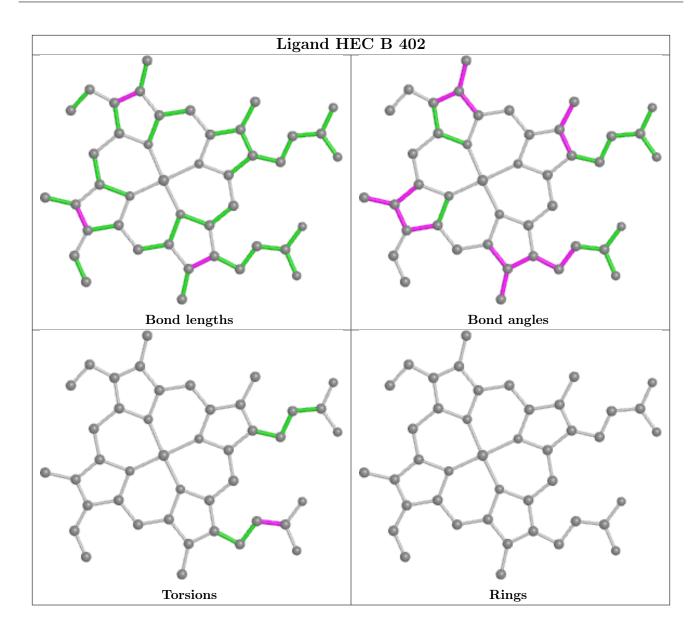












5.7 Other polymers (i)

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)

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates (i)

EDS was not executed - this section is therefore empty.

6.4 Ligands (i)

EDS was not executed - this section is therefore empty.

6.5 Other polymers (i)

EDS was not executed - this section is therefore empty.

