wwPDB X-ray Structure Validation Summary Report (i)

Aug 23, 2026 – 06:22 am BST

PDB ID	:	1HJ3 / pdb_00001hj3
Title	:	Cytochrome cd1 Nitrite Reductase, dioxygen complex
Authors	:	Sjogren, T.; Hajdu, J.
Deposited on	:	2001-01-08
Resolution	:	1.60 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:

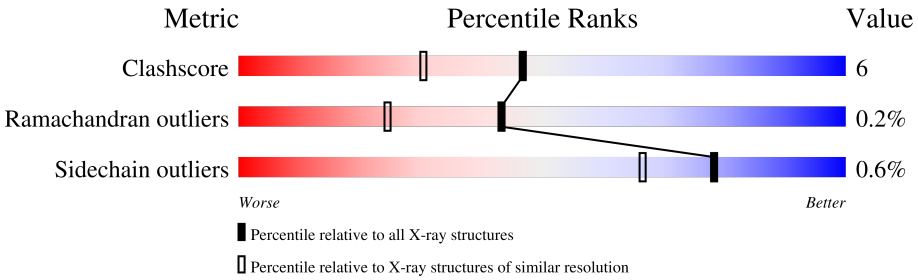
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

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 1.60 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	4931 (1.60-1.60)
Ramachandran outliers	187476	4831 (1.60-1.60)
Sidechain outliers	187428	4830 (1.60-1.60)

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	567	89% 7% .
1	B	567	84% 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
2	HEC	A	601	X	-	-	-
2	HEC	B	601	X	-	-	-
3	DHE	A	602	X	-	-	-
3	DHE	B	602	X	-	-	-

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

2 Entry composition

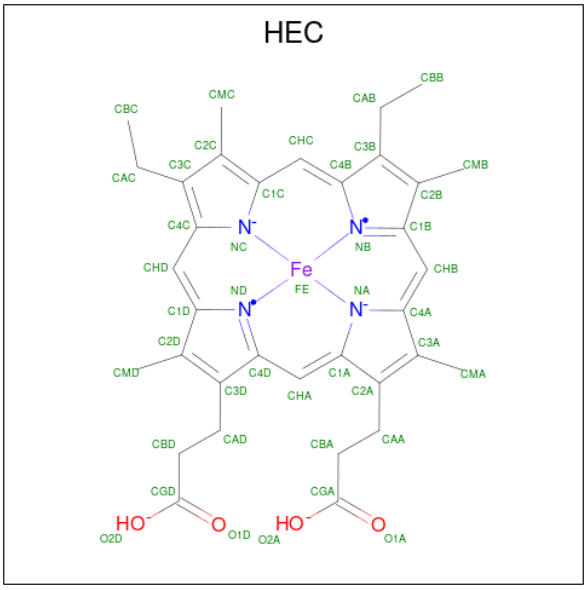
There are 7 unique types of molecules in this entry. The entry contains 9453 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

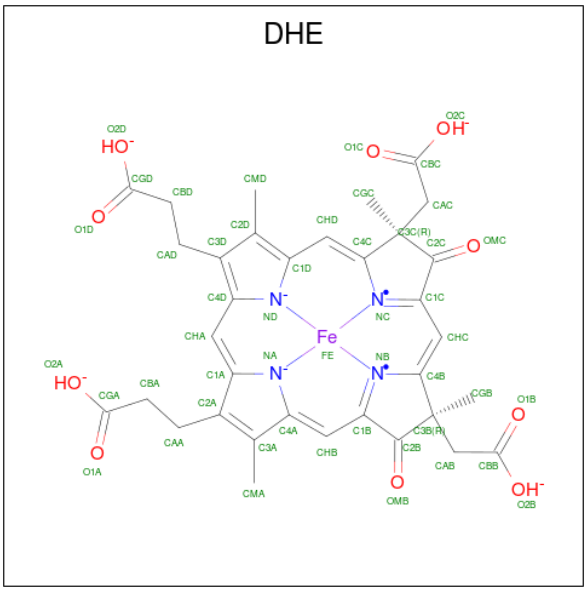
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	544	Total	C	N	O	S	0	0	0
			4238	2679	711	834	14			
1	B	542	Total	C	N	O	S	0	0	0
			4207	2661	701	831	14			

- Molecule 2 is HEME C (CCD ID: HEC) (formula: $C_{34}H_{36}FeN_4O_4$).



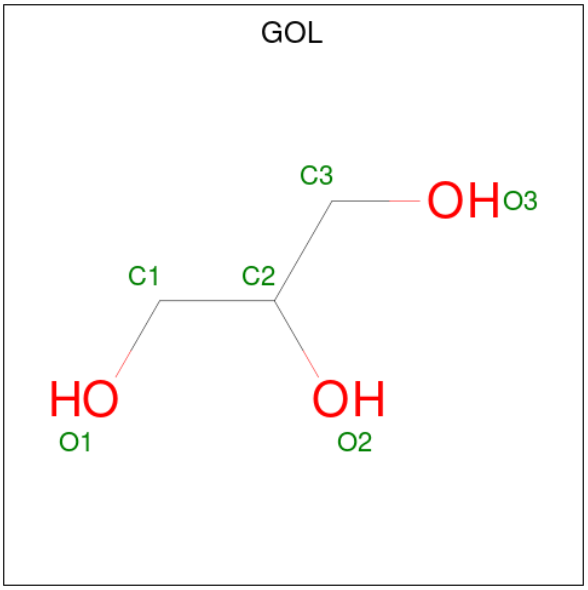
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

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



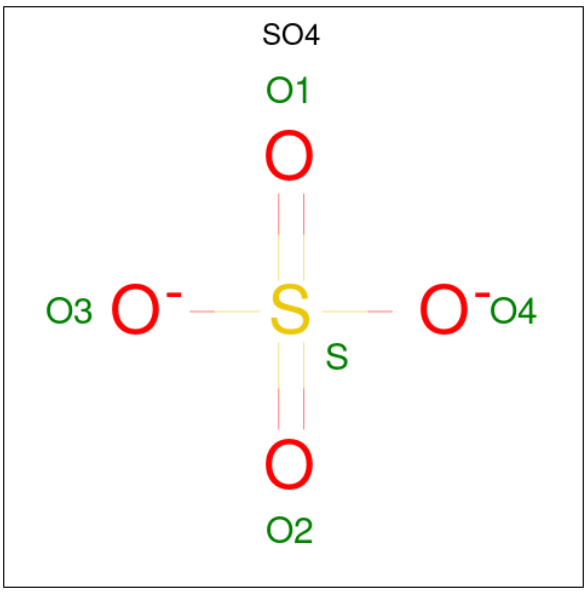
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	Fe	N	O	0	0
			49	34	1	4	10		
3	B	1	Total	C	Fe	N	O	0	0
			49	34	1	4	10		

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



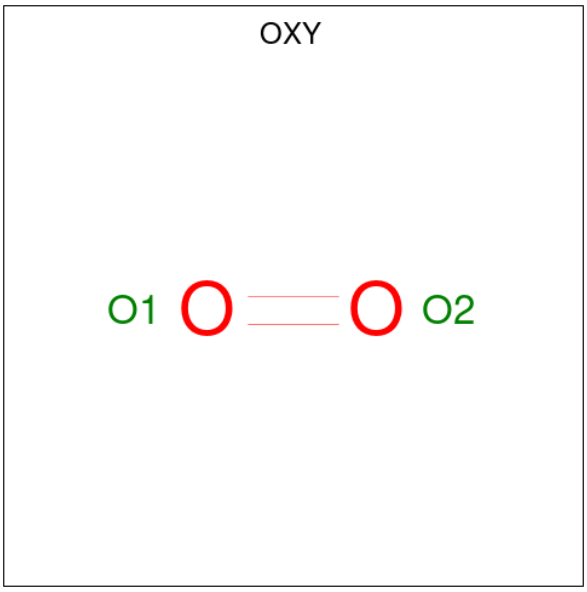
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	O		0	0
			6	3	3			
4	B	1	Total	C	O		0	0
			6	3	3			

- Molecule 5 is SULFATE ION (CCD ID: SO4) (formula: O_4S).



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

- Molecule 6 is OXYGEN MOLECULE (CCD ID: OXY) (formula: O_2).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	B	1	Total O 2 2	0	0

- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	388	Total O 388 388	0	0
7	B	407	Total O 407 407	0	0

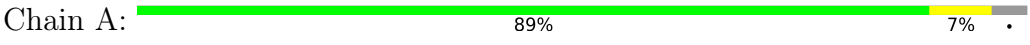
3 Residue-property plots (i)

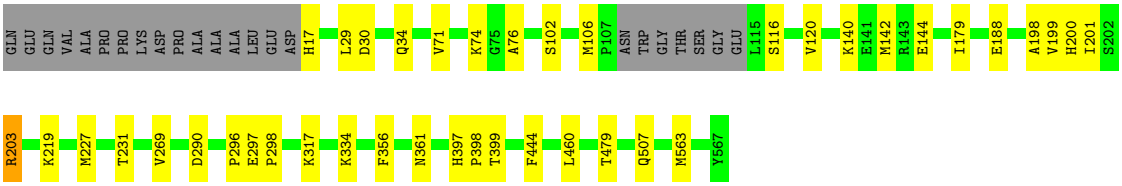
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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: Nitrite reductase

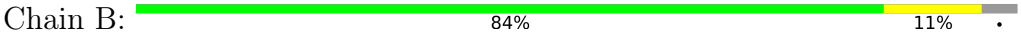
Chain A:

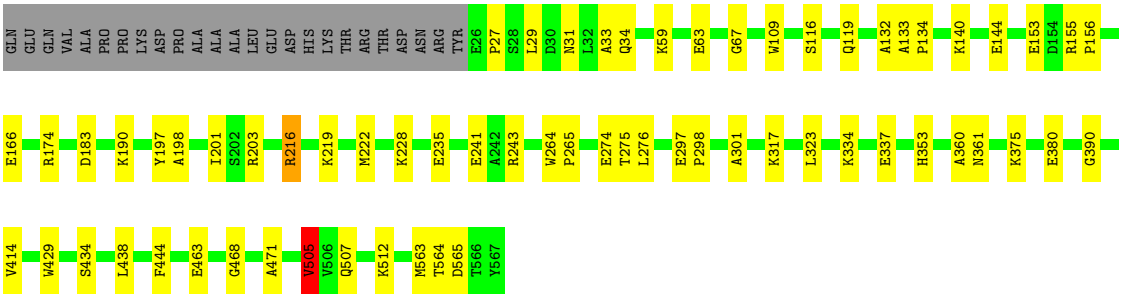




- Molecule 1: Nitrite reductase

Chain B:





4 Data and refinement statistics (i)

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	107.19Å 61.17Å 100.52Å 90.00° 112.19° 90.00°	Depositor
Resolution (Å)	30.00 – 1.60	Depositor
% Data completeness (in resolution range)	85.3 (30.00-1.60)	Depositor
R_{merge}	0.05	Depositor
R_{sym}	0.05	Depositor
Refinement program	REFMAC	Depositor
R, R_{free}	0.196 , 0.219	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	9453	wwPDB-VP
Average B, all atoms (Å^2)	21.0	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, OXY, 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	0.88	0/4340	1.10	7/5901 (0.1%)
1	B	0.85	1/4310 (0.0%)	1.10	5/5864 (0.1%)
All	All	0.87	1/8650 (0.0%)	1.10	12/11765 (0.1%)

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	B	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	5.38	1.49	1.46

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	216	ARG	CD-NE-CZ	7.97	135.56	124.40
1	A	361	ASN	N-CA-C	7.46	119.05	111.07
1	B	317	LYS	N-CA-C	7.34	118.97	110.97
1	B	505	VAL	N-CA-CB	5.99	118.83	110.56
1	A	188	GLU	CA-CB-CG	5.87	125.84	114.10

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	360	ALA	Mainchain
1	B	390	GLY	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	4238	0	4089	27	0
1	B	4207	0	4052	56	0
2	A	43	0	30	3	0
2	B	43	0	30	2	0
3	A	49	0	26	3	0
3	B	49	0	28	6	0
4	A	6	0	8	6	0
4	B	6	0	8	12	0
5	A	5	0	0	0	0
5	B	10	0	0	0	0
6	B	2	0	0	0	0
7	A	388	0	0	5	0
7	B	407	0	0	7	0
All	All	9453	0	8271	97	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.

The worst 5 of 97 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:611:GOL:C2	4:A:611:GOL:C1	1.85	1.51
4:B:612:GOL:C1	4:B:612:GOL:C2	1.88	1.51
1:B:174:ARG:HH22	4:B:612:GOL:H31	1.28	0.97
4:B:612:GOL:C1	4:B:612:GOL:C3	2.53	0.86
1:B:174:ARG:HH12	4:B:612:GOL:H11	1.40	0.83

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	540/567 (95%)	516 (96%)	23 (4%)	1 (0%)	43 24
1	B	540/567 (95%)	513 (95%)	26 (5%)	1 (0%)	43 24
All	All	1080/1134 (95%)	1029 (95%)	49 (4%)	2 (0%)	43 24

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	507	GLN
1	A	507	GLN

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	452/469 (96%)	449 (99%)	3 (1%)	76 63
1	B	448/469 (96%)	446 (100%)	2 (0%)	84 75
All	All	900/938 (96%)	895 (99%)	5 (1%)	78 66

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	HIS
1	A	219	LYS
1	A	563	MET
1	B	228	LYS

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Mol	Chain	Res	Type
1	B	505	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 10 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	119	GLN
1	B	282	GLN
1	B	353	HIS
1	A	385	GLN
1	B	31	ASN

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 oligosaccharides in this entry.

5.6 Ligand geometry (i)

10 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	$\#\|Z\| > 2$
5	SO4	A	621	-	4,4,4	0.60	0	6,6,6	0.14	0
3	DHE	A	602	1	52,56,56	4.57	13 (25%)	53,94,94	1.90	11 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	HEC	B	601	1	50,50,50	1.27	7 (14%)	68,82,82	0.95	3 (4%)
4	GOL	B	612	-	5,5,5	3.97	1 (20%)	5,5,5	2.74	3 (60%)
2	HEC	A	601	1	50,50,50	1.27	4 (8%)	68,82,82	0.94	2 (2%)
5	SO4	B	621	-	4,4,4	0.66	0	6,6,6	0.14	0
6	OXY	B	603	3	1,1,1	0.40	0	-		
5	SO4	B	622	-	4,4,4	0.60	0	6,6,6	0.04	0
4	GOL	A	611	-	5,5,5	3.72	1 (20%)	5,5,5	1.98	1 (20%)
3	DHE	B	602	6,1	52,56,56	4.40	8 (15%)	53,94,94	1.65	12 (22%)

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
3	DHE	A	602	1	1/1/15/19	9/20/108/108	-
2	HEC	B	601	1	1/1/3/7	5/14/54/54	-
4	GOL	B	612	-	-	2/4/4/4	-
2	HEC	A	601	1	1/1/3/7	2/14/54/54	-
4	GOL	A	611	-	-	2/4/4/4	-
3	DHE	B	602	6,1	1/1/15/19	6/20/108/108	-

The worst 5 of 34 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	602	DHE	OMC-C2C	17.66	1.53	1.22
3	B	602	DHE	OMB-C2B	17.56	1.53	1.22
3	B	602	DHE	OMC-C2C	17.48	1.53	1.22
3	A	602	DHE	OMB-C2B	16.93	1.52	1.22
3	A	602	DHE	C3C-C2C	-12.20	1.34	1.52

The worst 5 of 32 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	602	DHE	CGB-C3B-C2B	-5.67	94.47	109.47
3	A	602	DHE	O2C-CBC-O1C	-4.98	110.90	123.30
3	A	602	DHE	CGC-C3C-C2C	-4.54	97.45	109.47
4	B	612	GOL	C3-C2-C1	-4.24	95.24	111.70
3	A	602	DHE	O2C-CBC-CAC	4.13	127.61	114.35

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	601	HEC	NA
2	B	601	HEC	NA
3	A	602	DHE	NA
3	B	602	DHE	NA

5 of 26 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	602	DHE	C4B-C3B-CAB-CBB
3	A	602	DHE	C2D-C3D-CAD-CBD
3	A	602	DHE	C4D-C3D-CAD-CBD
4	B	612	GOL	C1-C2-C3-O3
3	B	602	DHE	C4D-C3D-CAD-CBD

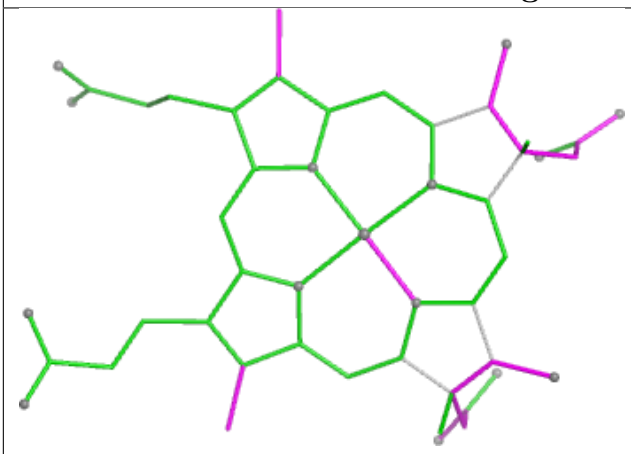
There are no ring outliers.

6 monomers are involved in 32 short contacts:

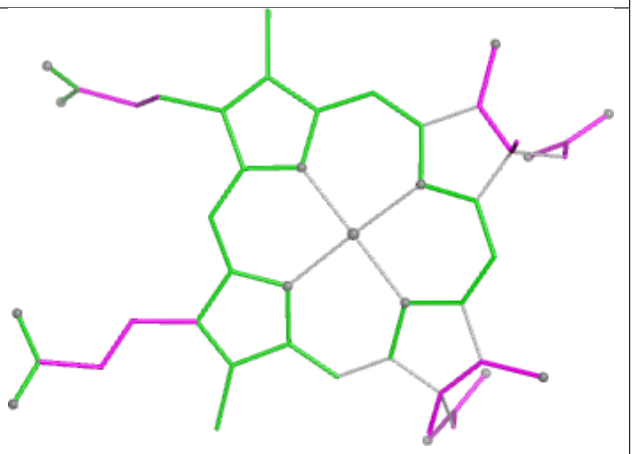
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	602	DHE	3	0
2	B	601	HEC	2	0
4	B	612	GOL	12	0
2	A	601	HEC	3	0
4	A	611	GOL	6	0
3	B	602	DHE	6	0

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

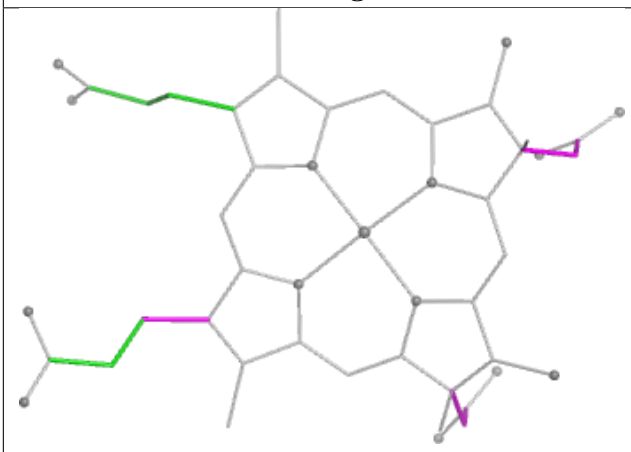
Ligand DHE A 602



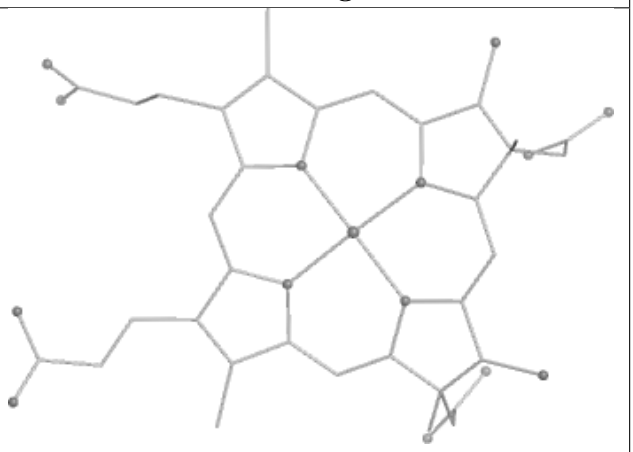
Bond lengths



Bond angles

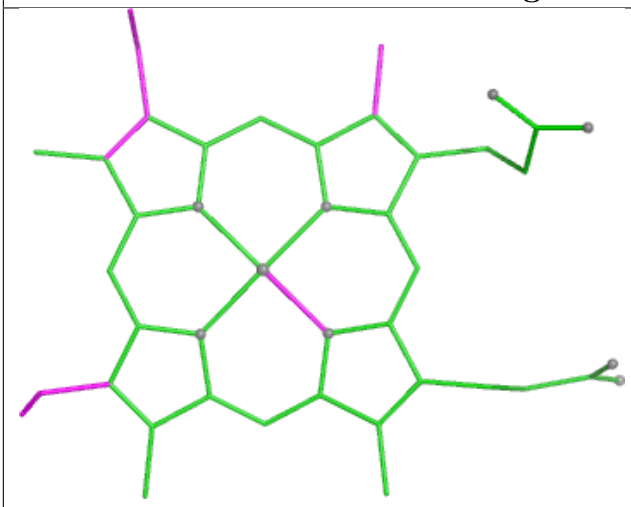


Torsions

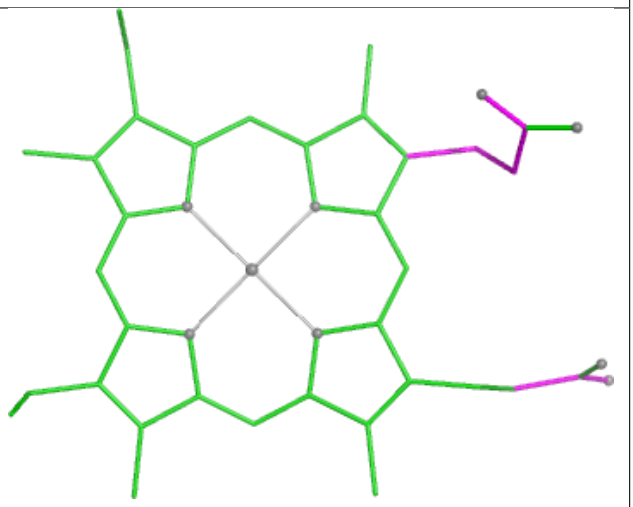


Rings

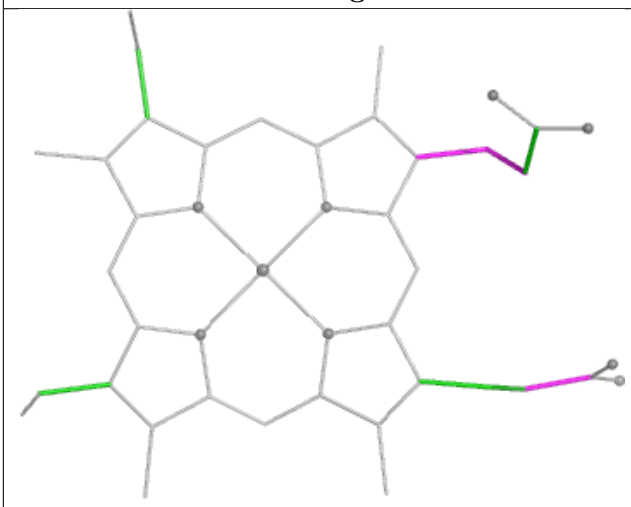
Ligand HEC B 601



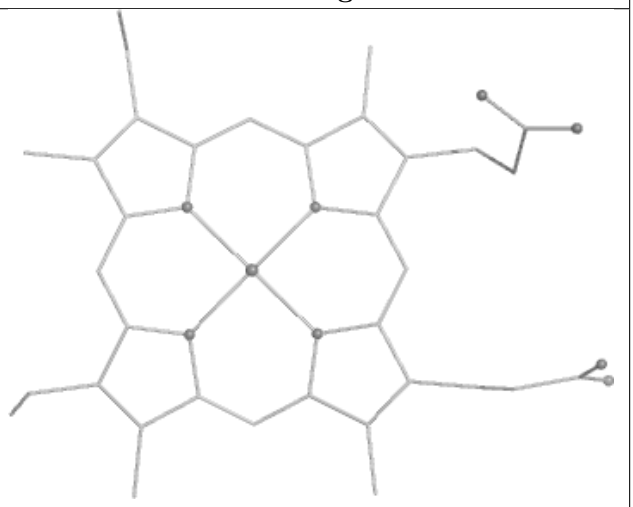
Bond lengths



Bond angles

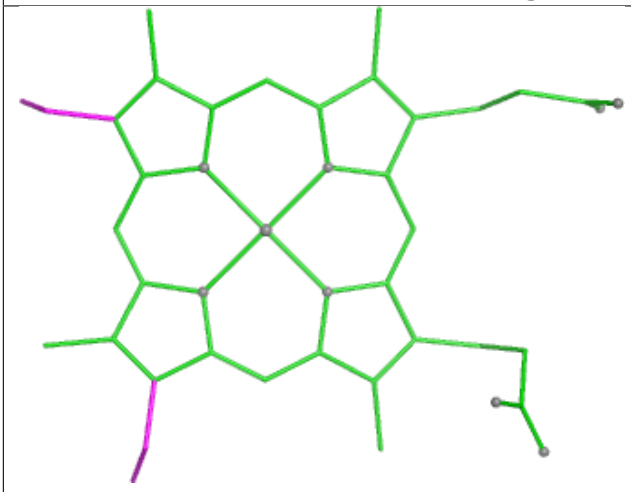


Torsions

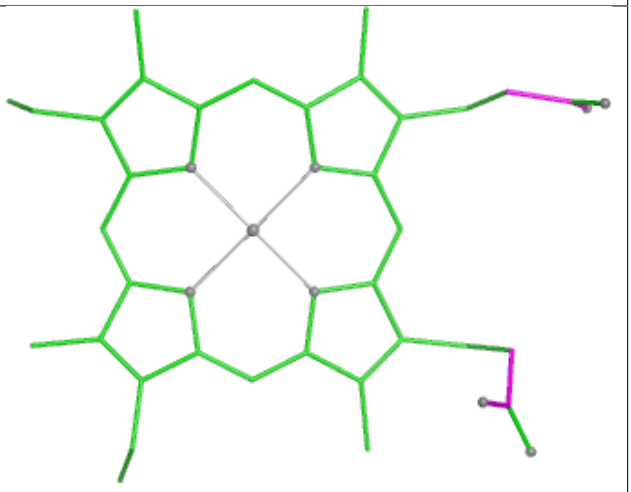


Rings

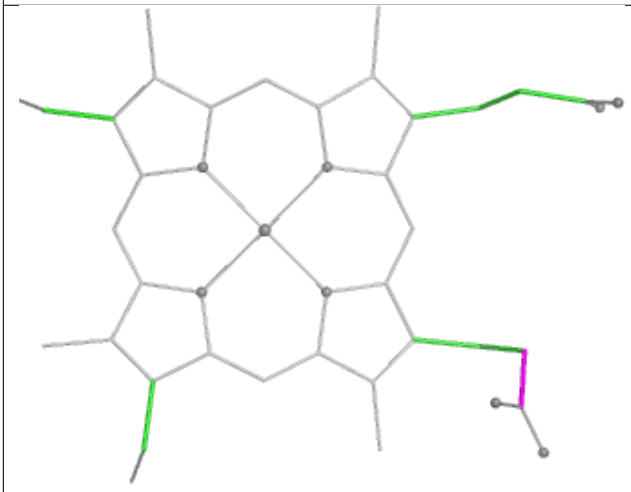
Ligand HEC A 601



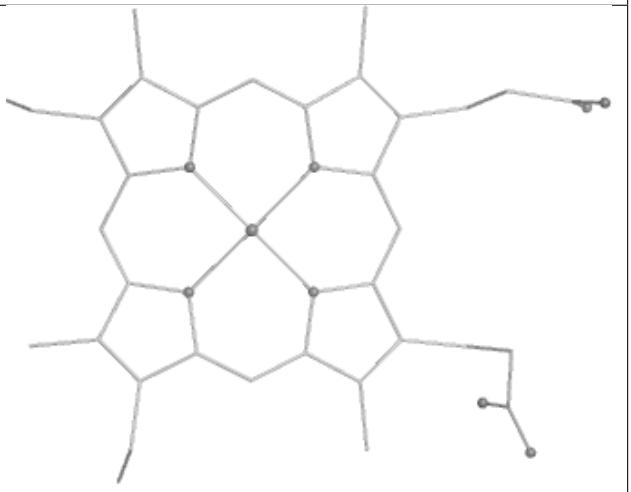
Bond lengths



Bond angles

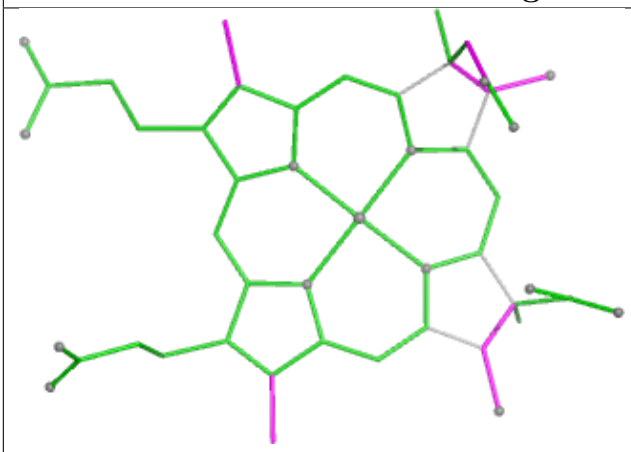


Torsions

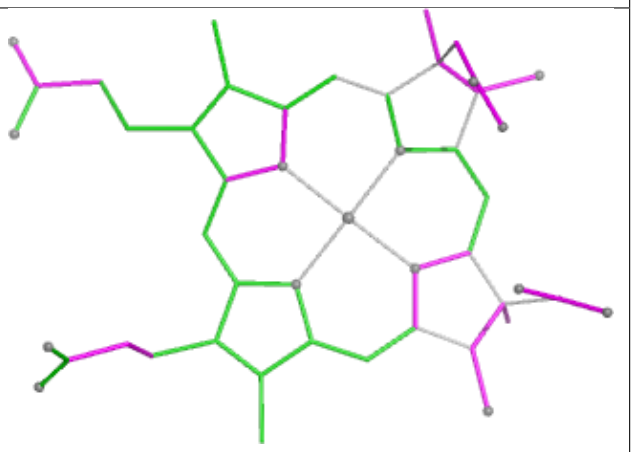


Rings

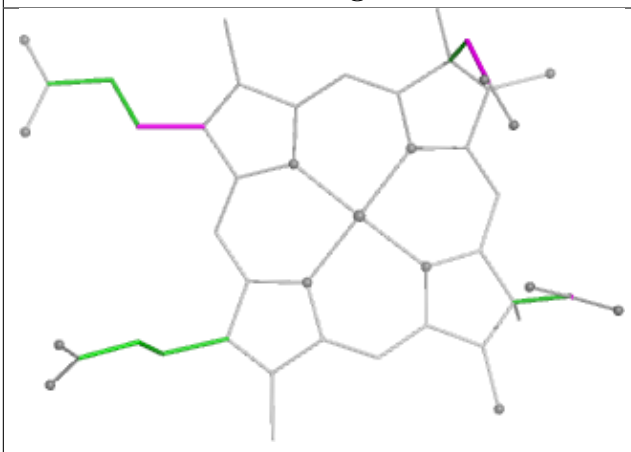
Ligand DHE B 602



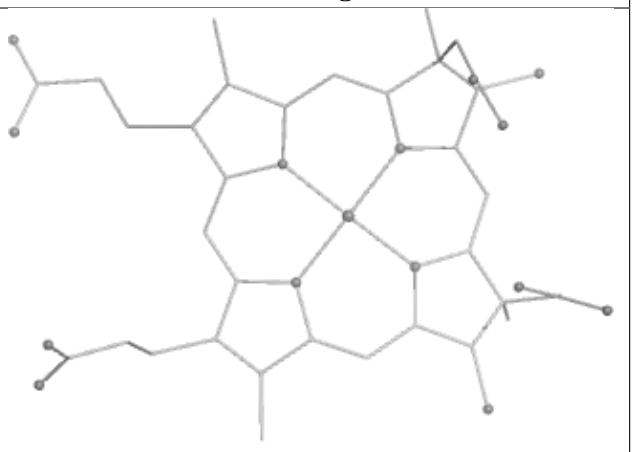
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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.