wwPDB X-ray Structure Validation Summary Report (i)

Mar 8, 2023 – 12:56 AM EST

PDB ID	:	1B86
Title	:	HUMAN DEOXYHAEMOGLOBIN-2,3-DIPHOSPHOGLYCERATE COMPLEX
Authors	:	Richard, V.; Dodson, G.G.; Mauguen, Y.
Deposited on	:	1999-02-08
Resolution	:	2.50 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:

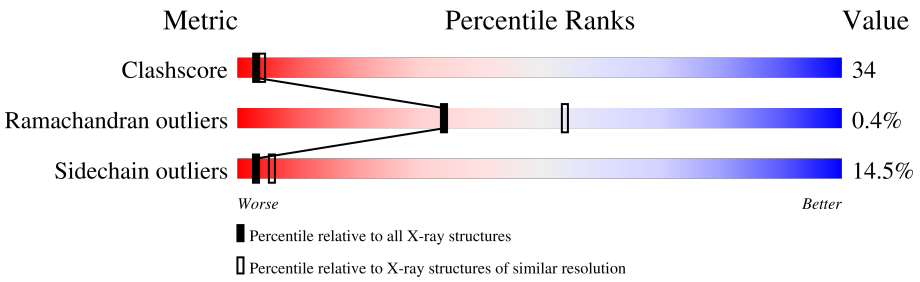
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.32.1

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 2.50 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	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)

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	141	32% 44% 18% 6%
1	C	141	33% 48% 15% •
2	B	146	32% 40% 23% 5%
2	D	146	25% 36% 32% 7%

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
5	DG2	D	701	X	-	-	-

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 4715 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.

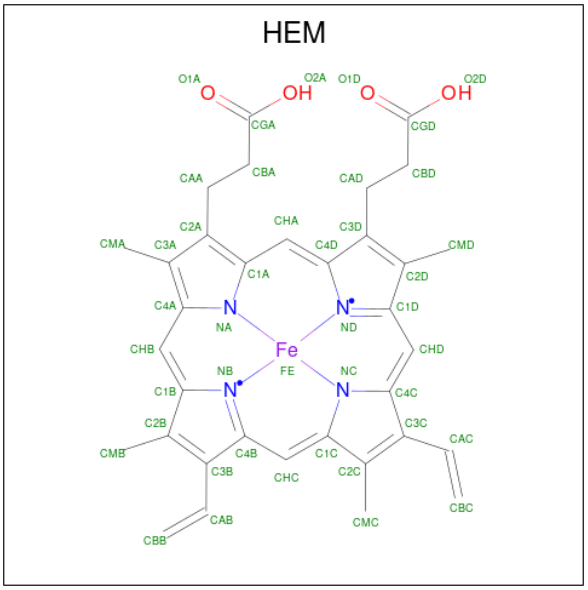
- Molecule 1 is a protein called PROTEIN (HEMOGLOBIN; ALPHA CHAIN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	141	1069	685	187	194	3	0	0	0
1	C	141	1069	685	187	194	3	0	0	0

- Molecule 2 is a protein called PROTEIN (HEMOGLOBIN; BETA CHAIN).

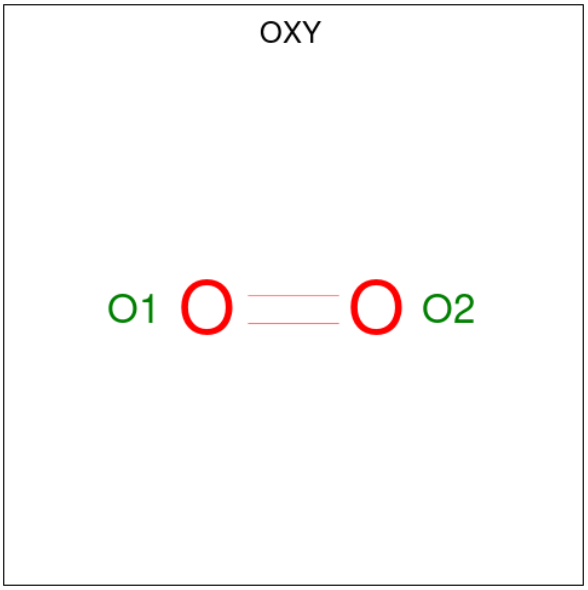
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	146	1123	724	195	201	3	0	0	0
2	D	146	1127	727	196	201	3	0	1	0

- Molecule 3 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



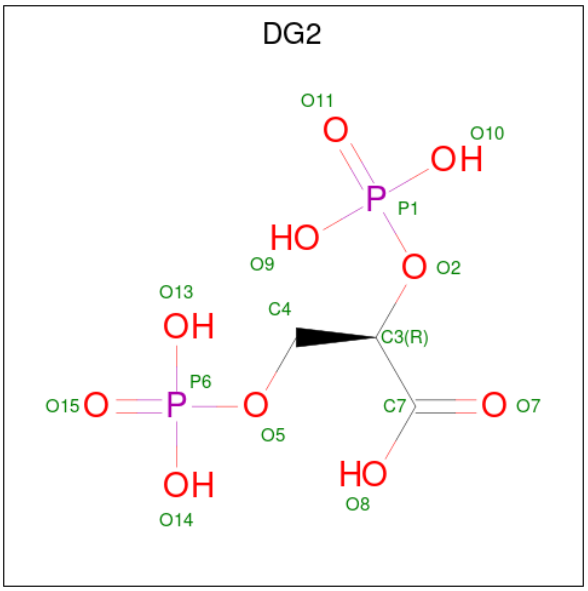
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Fe	N	O		
3	A	1	43	34	1	4	4	0	0
3	B	1	43	34	1	4	4	0	0
3	C	1	43	34	1	4	4	0	0
3	D	1	43	34	1	4	4	0	0

- Molecule 4 is OXYGEN MOLECULE (three-letter code: OXY) (formula: O_2).



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

- Molecule 5 is (2R)-2,3-diphosphoglyceric acid (three-letter code: DG2) (formula: $C_3H_8O_{10}P_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O	P		
5	D	1	15	3	10	2	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
6	A	29	29	29	0	0
			Total	O		
6	B	46	46	46	0	0
			Total	O		
6	C	16	16	16	0	0
			Total	O		
6	D	45	45	45	0	0

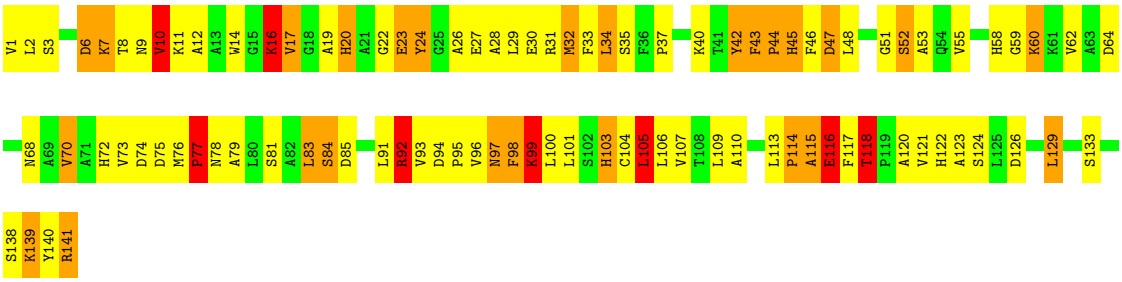
3 Residue-property plots (i)

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.

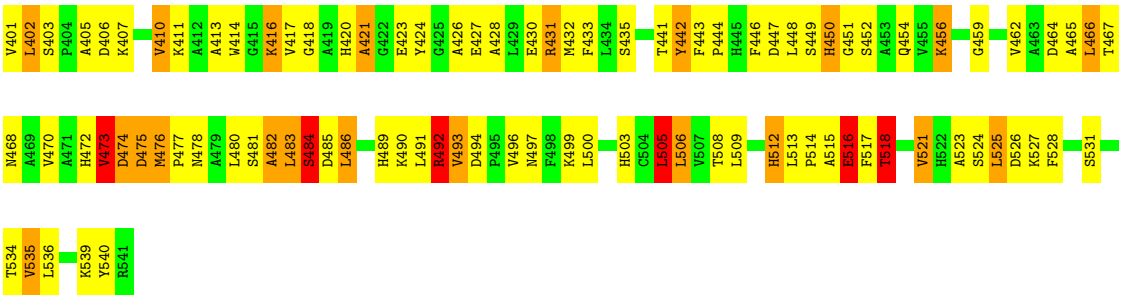
• Molecule 1: PROTEIN (HEMOGLOBIN; ALPHA CHAIN)

Chain A: 32% 44% 18% 6%



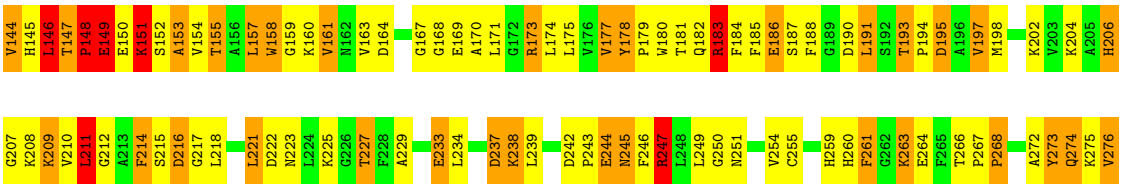
• Molecule 1: PROTEIN (HEMOGLOBIN; ALPHA CHAIN)

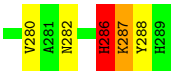
Chain C: 33% 48% 15% •



• Molecule 2: PROTEIN (HEMOGLOBIN; BETA CHAIN)

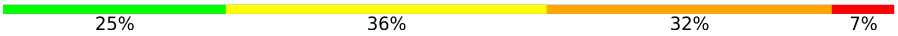
Chain B: 32% 40% 23% 5%





• Molecule 2: PROTEIN (HEMOGLOBIN; BETA CHAIN)

Chain D:



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 a, b, c, α, β, γ	96.30Å 98.08Å 65.76Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 2.50	Depositor
% Data completeness (in resolution range)	96.0 (10.00-2.50)	Depositor
R_{merge}	0.10	Depositor
R_{sym}	0.13	Depositor
Refinement program	PROLSQ	Depositor
R, R_{free}	0.169 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	4715	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: HEM, OXY, DG2

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	1.10	2/1097 (0.2%)	2.97	120/1491 (8.0%)
1	C	1.10	0/1097	2.83	98/1491 (6.6%)
2	B	1.13	1/1153 (0.1%)	2.85	112/1566 (7.2%)
2	D	1.14	2/1162 (0.2%)	2.85	118/1577 (7.5%)
All	All	1.12	5/4509 (0.1%)	2.88	448/6125 (7.3%)

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	C	0	1
2	B	0	2
2	D	1	0
All	All	1	4

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	626	GLY	N-CA	6.77	1.56	1.46
2	B	212	GLY	N-CA	6.00	1.55	1.46
2	D	650	GLY	N-CA	5.55	1.54	1.46
1	A	27	GLU	CD-OE2	-5.35	1.19	1.25
1	A	124	SER	CB-OG	5.03	1.48	1.42

The worst 5 of 448 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	92	ARG	NE-CZ-NH2	25.57	133.09	120.30
1	C	492	ARG	NE-CZ-NH2	-22.38	109.11	120.30
1	C	526	ASP	CB-CG-OD1	18.50	134.95	118.30
2	B	286	HIS	CA-CB-CG	18.29	144.69	113.60
1	C	431	ARG	NE-CZ-NH2	-17.40	111.60	120.30

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	D	545	HIS	CA

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	141	ARG	Sidechain
2	B	183	ARG	Sidechain
2	B	247	ARG	Sidechain
1	C	492	ARG	Sidechain

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	1069	0	1073	58	1
1	C	1069	0	1070	54	0
2	B	1123	0	1115	92	0
2	D	1127	0	1124	107	0
3	A	43	0	30	2	0
3	B	43	0	30	6	0
3	C	43	0	30	0	0
3	D	43	0	30	12	0
4	A	2	0	0	0	0
4	C	2	0	0	0	0
5	D	15	0	3	2	0
6	A	29	0	0	1	1
6	B	46	0	0	9	1
6	C	16	0	0	0	0
6	D	45	0	0	9	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	4715	0	4505	308	2

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 34.

The worst 5 of 308 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)
2:D:686:HIS:NE2	6:D:102:HOH:O	1.57	1.28
2:D:571:LEU:HD22	6:D:128:HOH:O	1.12	1.24
2:B:153:ALA:HA	6:B:49:HOH:O	1.38	1.17
2:D:649:LEU:HD23	3:D:691:HEM:HBB2	1.25	1.14
1:A:118:THR:HG22	1:A:121:VAL:H	1.09	1.13

All (2) 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	Interatomic distance (Å)	Clash overlap (Å)
6:A:170:HOH:O	6:D:132:HOH:O[4_554]	0.01	2.19
1:A:23:GLU:OE1	6:B:28:HOH:O[3_445]	1.65	0.55

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	139/141 (99%)	129 (93%)	10 (7%)	0	100	100
1	C	139/141 (99%)	129 (93%)	10 (7%)	0	100	100
2	B	144/146 (99%)	137 (95%)	7 (5%)	0	100	100
2	D	145/146 (99%)	133 (92%)	10 (7%)	2 (1%)	11	20
All	All	567/574 (99%)	528 (93%)	37 (6%)	2 (0%)	34	54

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	662	GLY
2	D	564	ASP

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	113/113 (100%)	98 (87%)	15 (13%)	4 7
1	C	113/113 (100%)	104 (92%)	9 (8%)	12 23
2	B	118/118 (100%)	98 (83%)	20 (17%)	2 3
2	D	119/118 (101%)	95 (80%)	24 (20%)	1 2
All	All	463/462 (100%)	395 (85%)	68 (15%)	3 5

5 of 68 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	D	620	HIS
2	D	622	ASP
2	D	663	LYS
2	B	183	ARG
2	B	175	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 12 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	497	ASN
1	C	503	HIS
2	D	645	ASN
2	D	620	HIS
2	B	223	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

7 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	$\#\|Z\| > 2$
3	HEM	A	143	1,4	41,50,50	1.57	5 (12%)	45,82,82	2.48	19 (42%)
3	HEM	C	543	1,4	41,50,50	1.52	9 (21%)	45,82,82	2.18	14 (31%)
5	DG2	D	701	-	13,14,14	2.00	3 (23%)	18,21,21	5.67	9 (50%)
3	HEM	D	691	2,6	41,50,50	1.54	8 (19%)	45,82,82	2.32	15 (33%)
4	OXY	A	144	3	1,1,1	0.39	0	-		
3	HEM	B	291	2,6	41,50,50	1.66	8 (19%)	45,82,82	1.80	9 (20%)
4	OXY	C	544	3	1,1,1	0.54	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
3	HEM	A	143	1,4	-	2/12/54/54	-
3	HEM	C	543	1,4	-	6/12/54/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	DG2	D	701	-	1/1/4/4	7/15/15/15	-
3	HEM	D	691	2,6	-	4/12/54/54	-
3	HEM	B	291	2,6	-	3/12/54/54	-

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	291	HEM	C3C-C2C	-5.32	1.33	1.40
5	D	701	DG2	O5-C4	-4.79	1.26	1.44
3	A	143	HEM	C3C-C2C	-4.71	1.33	1.40
3	D	691	HEM	C3C-C2C	-4.67	1.33	1.40
3	C	543	HEM	C3C-C2C	-4.40	1.34	1.40

The worst 5 of 66 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	D	701	DG2	O2-C3-C4	18.31	136.61	106.56
5	D	701	DG2	O13-P6-O5	7.57	126.89	106.73
5	D	701	DG2	P6-O5-C4	7.34	138.50	118.30
3	A	143	HEM	CAD-CBD-CGD	7.32	129.36	113.60
5	D	701	DG2	P1-O2-C3	-7.30	106.30	123.04

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	D	701	DG2	C3

5 of 22 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	D	701	DG2	C7-C3-C4-O5
5	D	701	DG2	C7-C3-O2-P1
5	D	701	DG2	O2-C3-C7-O7
5	D	701	DG2	C3-C4-O5-P6
5	D	701	DG2	C4-O5-P6-O15

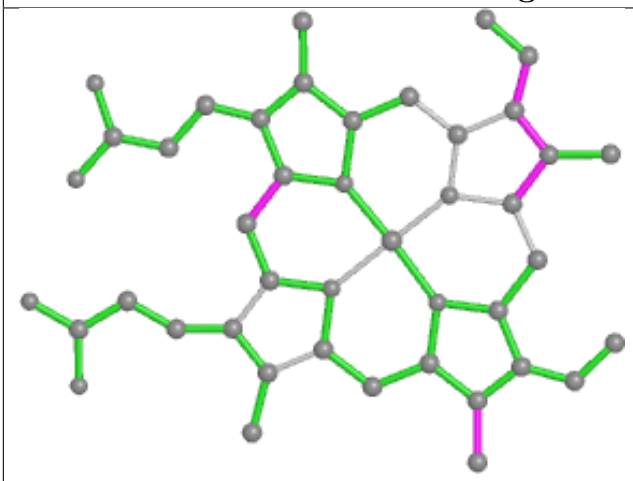
There are no ring outliers.

4 monomers are involved in 22 short contacts:

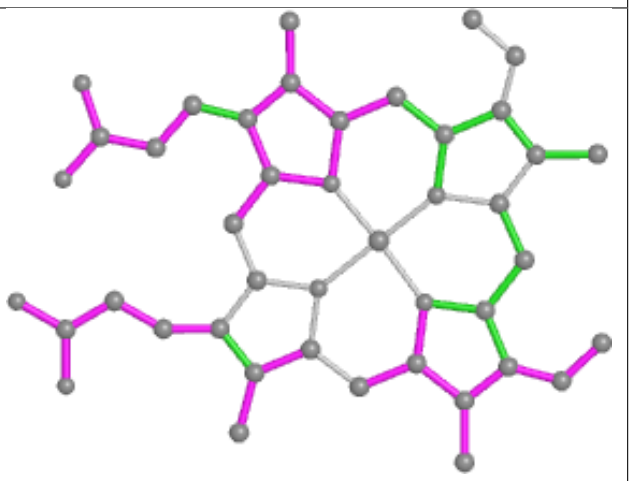
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	143	HEM	2	0
5	D	701	DG2	2	0
3	D	691	HEM	12	0
3	B	291	HEM	6	0

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.

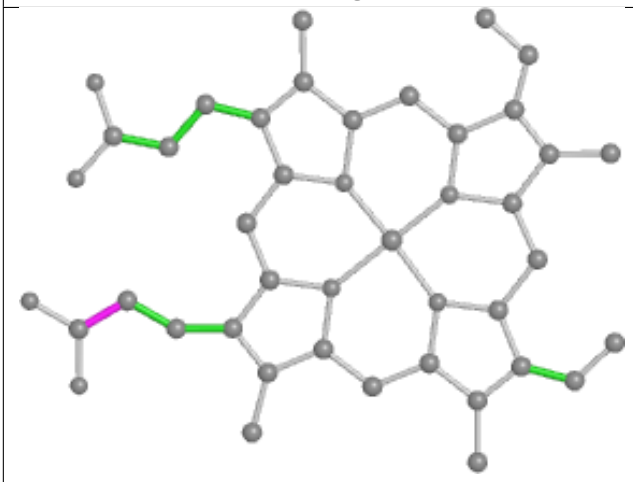
Ligand HEM A 143



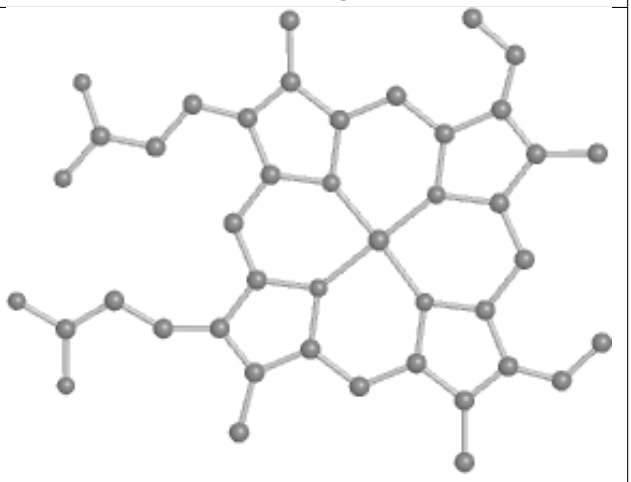
Bond lengths



Bond angles

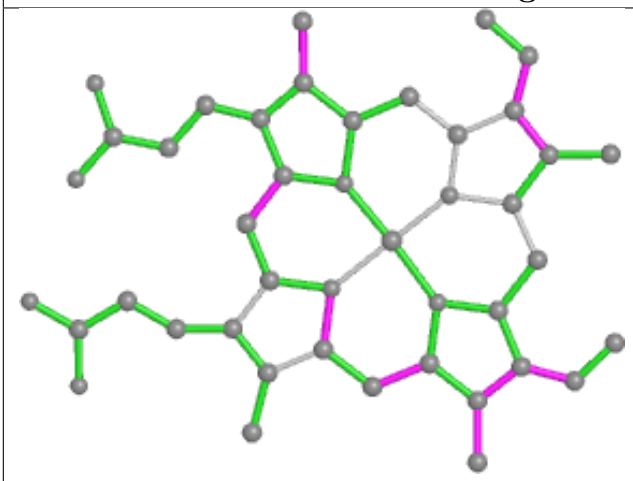


Torsions

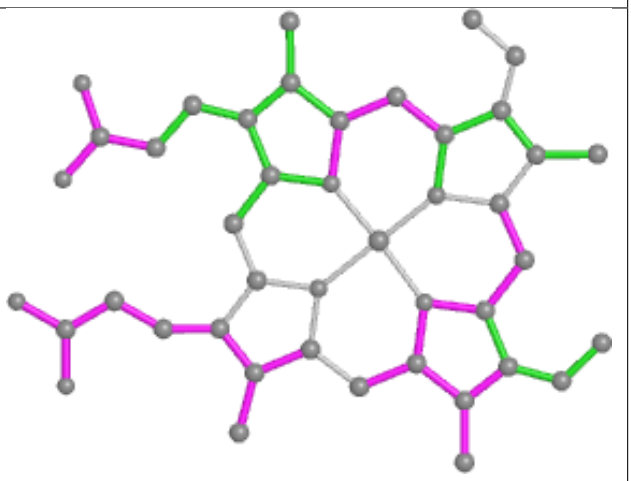


Rings

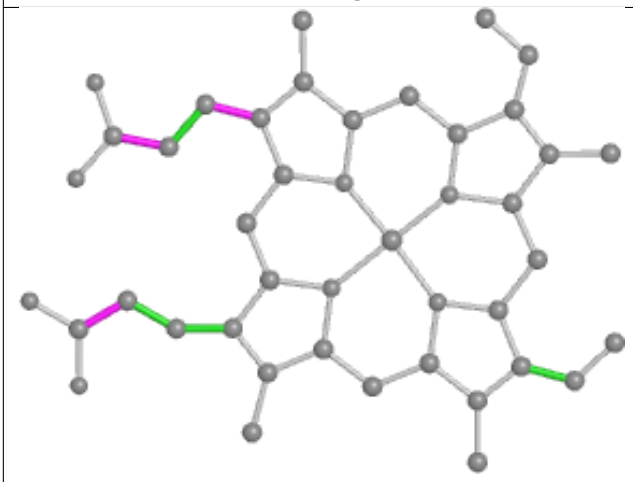
Ligand HEM C 543



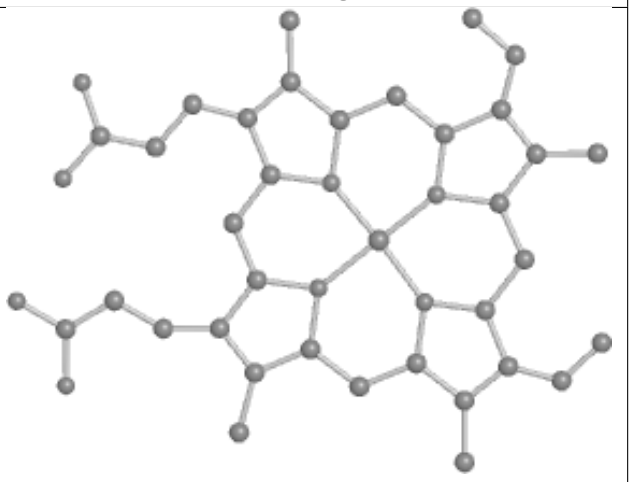
Bond lengths



Bond angles

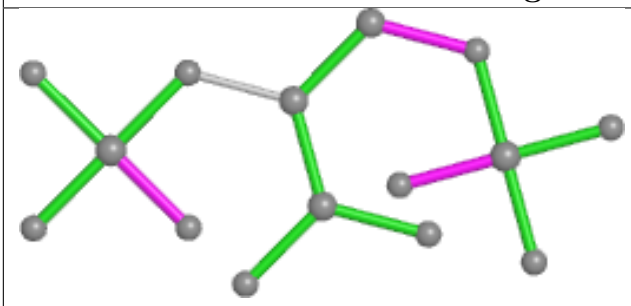


Torsions



Rings

Ligand DG2 D 701



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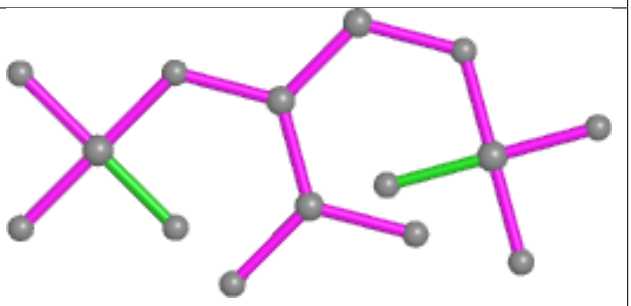
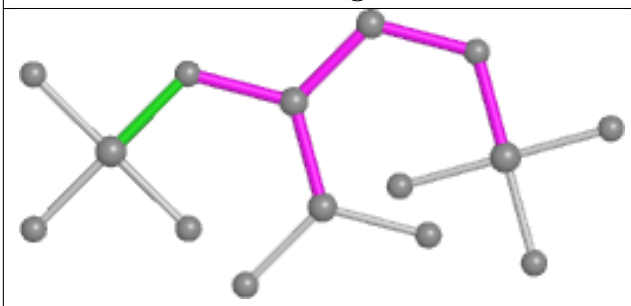
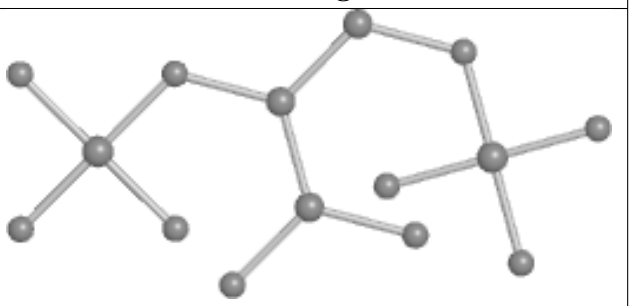


Bond angles

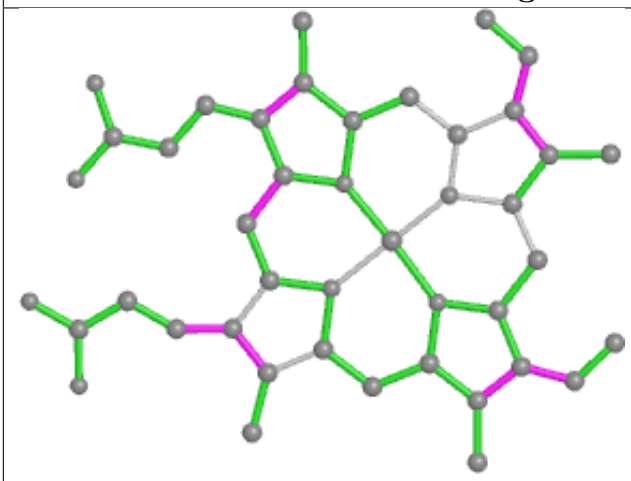


Torsions

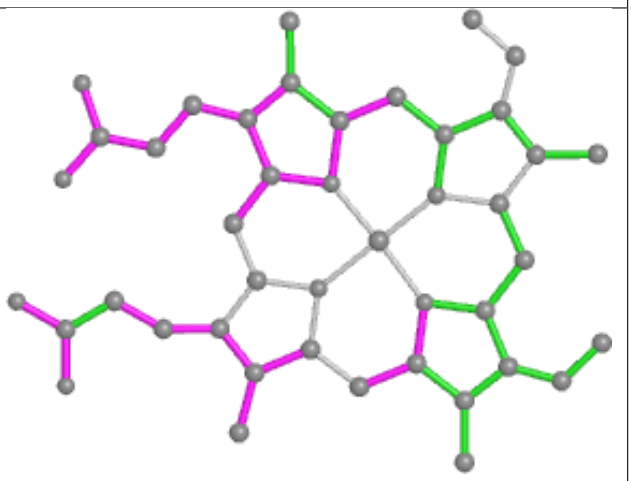


Rings

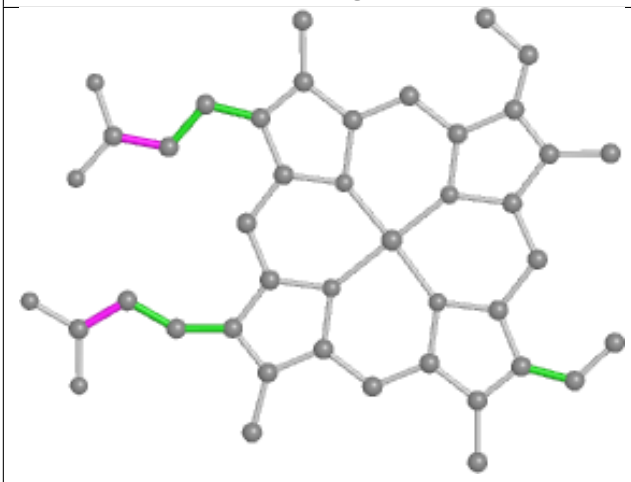
Ligand HEM D 691



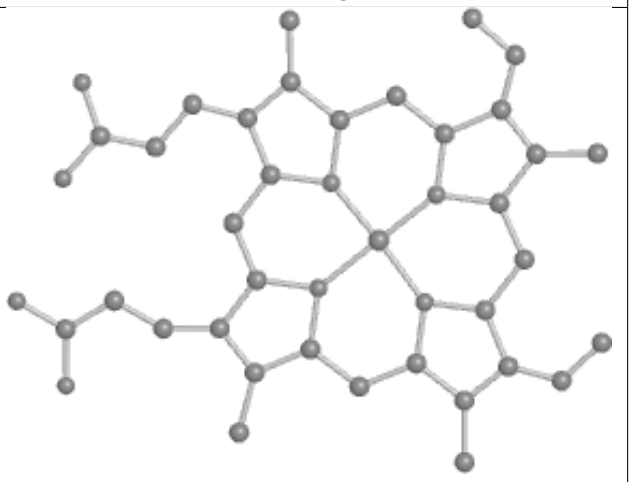
Bond lengths



Bond angles

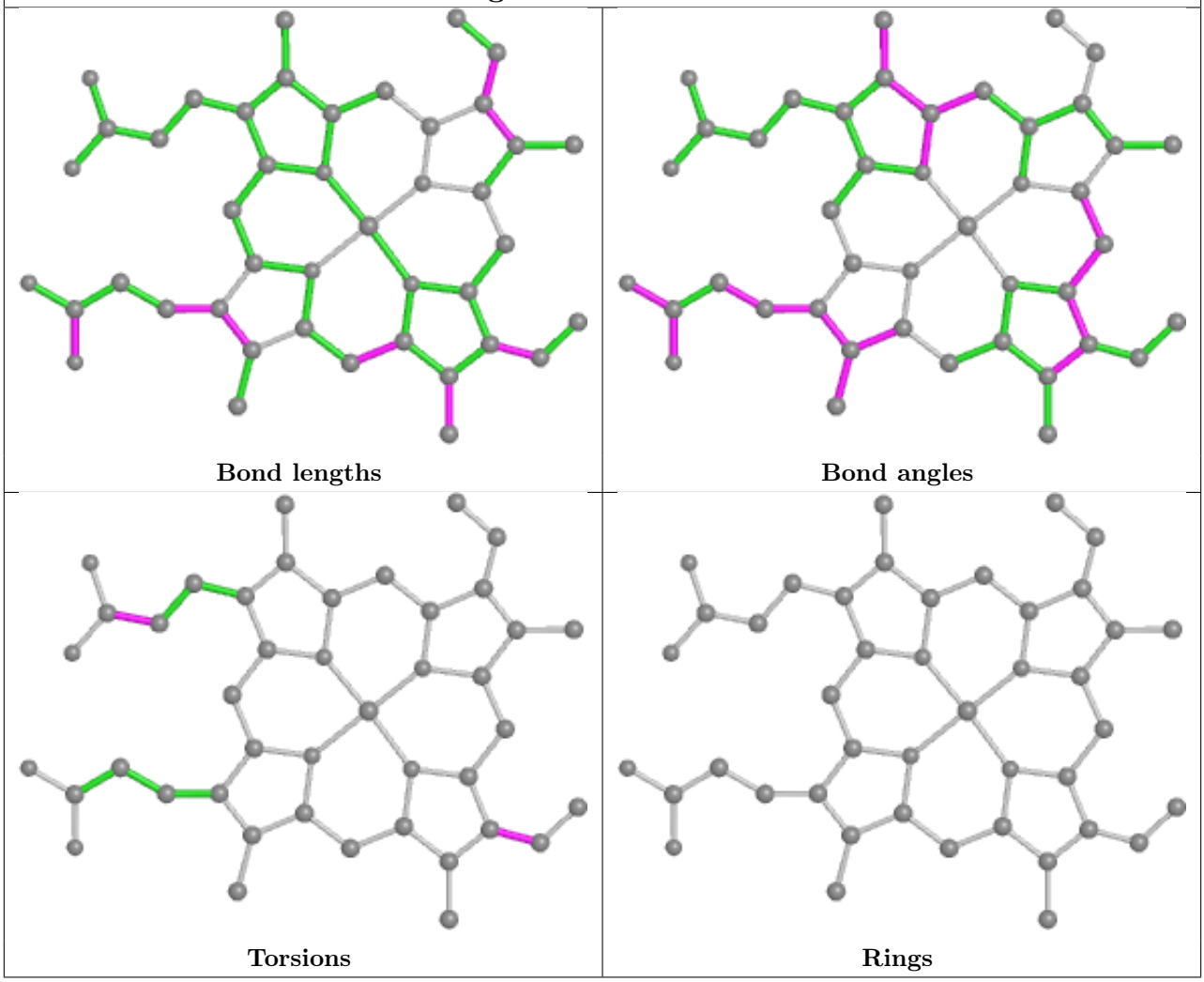


Torsions



Rings

Ligand HEM B 291



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.