



Full wwPDB Geometry-Only Validation Report ⓘ

Mar 10, 2026 – 03:28 AM UTC

PDB ID : 2MB5 / pdb_00002mb5
Title : HYDRATION IN PROTEIN CRYSTALS. A NEUTRON DIFFRACTION ANALYSIS OF CARBONMONOXYMYOGLOBIN
Authors : Schoenborn, B.P.; Cheng, X.
Deposited on : 1989-10-11
Resolution : 1.80 Å(reported)

This is a Full wwPDB Geometry-Only 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)
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

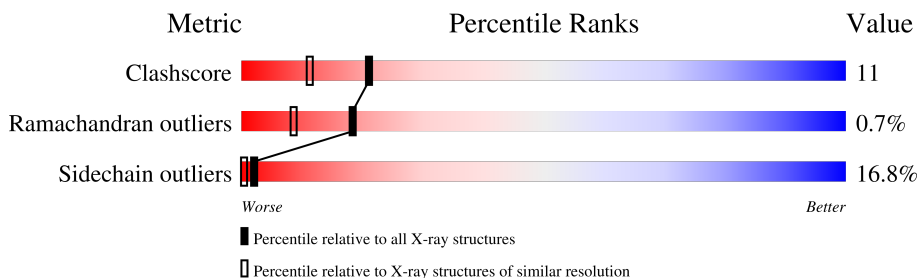
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

NEUTRON DIFFRACTION

The reported resolution of this entry is 1.80 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	8479 (1.80-1.80)
Ramachandran outliers	187476	8391 (1.80-1.80)
Sidechain outliers	187428	8390 (1.80-1.80)

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	153	

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 2842 atoms, of which 1004 are hydrogens and 475 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 MYOGLOBIN.

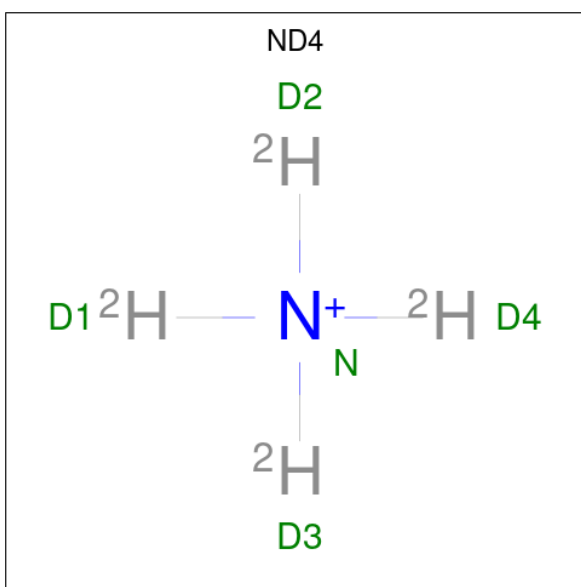
Mol	Chain	Residues	Atoms							ZeroOcc	AltConf	Trace
1	A	153	Total	C	D	H	N	O	S	0	0	0
			2468	783	277	974	216	216	2			

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



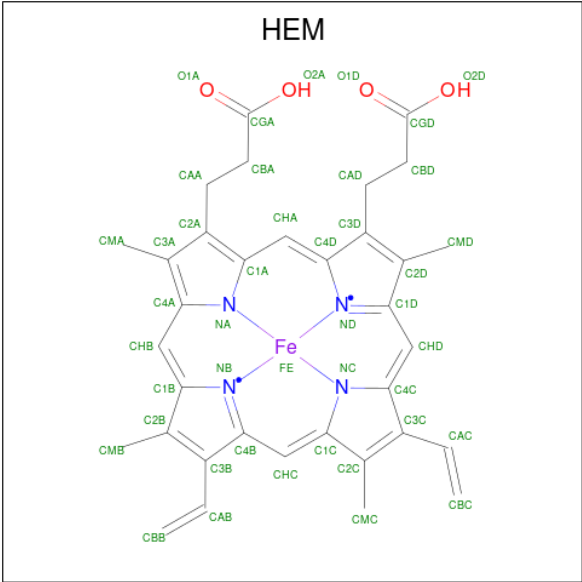
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is AMMONIUM CATION WITH D (CCD ID: ND4) (formula: N).



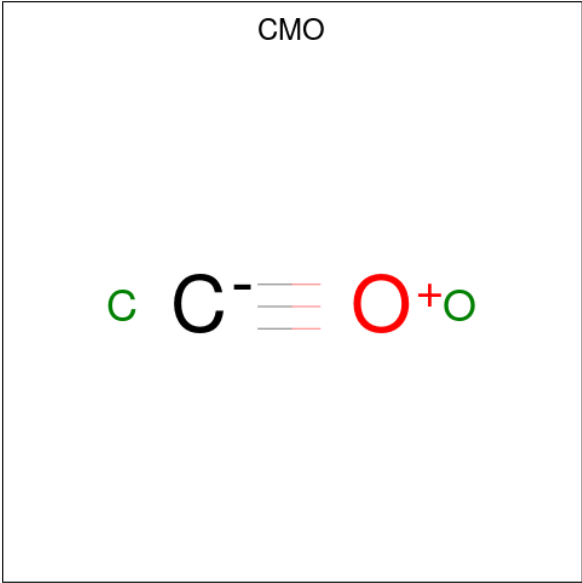
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	D	N	0	0
			5	4	1		
3	A	1	Total	D	N	0	0
			5	4	1		
3	A	1	Total	D	N	0	0
			5	4	1		
3	A	1	Total	D	N	0	0
			5	4	1		
3	A	1	Total	D	N	0	0
			5	4	1		

- Molecule 4 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
4	A	1	Total	C	Fe	H	N	O	0	0
			73	34	1	30	4	4		

- Molecule 5 is CARBON MONOXIDE (CCD ID: CMO) (formula: CO).



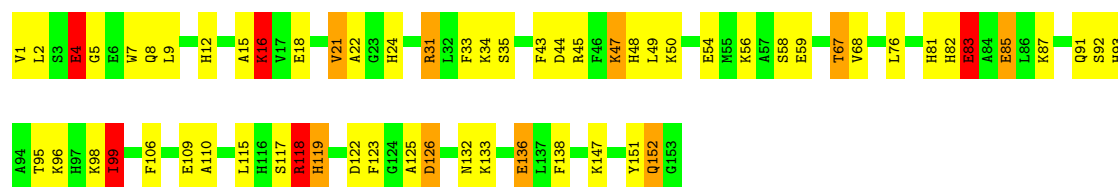
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	1
			4	2	2		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	89	Total	D	O	0	0
			267	178	89		

Note EDS was not executed.

Chain A: 59% 31% 6% 4%



4 Model quality ⓘ

4.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: CMO, DOD, HEM, SO4, ND4

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	0.93	0/1245	2.31	44/1671 (2.6%)

There are no bond length outliers.

All (44) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	126	ASP	CA-CB-CG	20.03	132.63	112.60
1	A	47	LYS	CD-CE-NZ	13.33	154.56	111.90
1	A	136	GLU	N-CA-CB	11.17	127.59	110.28
1	A	138	PHE	CA-CB-CG	10.21	124.01	113.80
1	A	91	GLN	CB-CA-C	10.03	127.90	110.85
1	A	56	LYS	CG-CD-CE	10.01	134.33	111.30
1	A	33	PHE	CA-CB-CG	9.74	123.54	113.80
1	A	118	ARG	N-CA-C	-8.83	98.63	110.55
1	A	15	ALA	N-CA-C	-8.42	102.19	111.36
1	A	12	HIS	N-CA-C	-7.40	103.14	111.14
1	A	35	SER	CA-CB-OG	7.38	125.85	111.10
1	A	132	ASN	CA-CB-CG	6.72	119.32	112.60
1	A	123	PHE	CA-CB-CG	6.72	120.52	113.80
1	A	68	VAL	CA-C-O	-6.62	114.15	121.17
1	A	22	ALA	N-CA-C	6.62	118.49	111.28
1	A	68	VAL	O-C-N	6.56	128.34	121.91
1	A	87	LYS	O-C-N	6.54	125.54	120.38
1	A	54	GLU	CB-CG-CD	6.32	123.34	112.60
1	A	106	PHE	CA-CB-CG	6.23	120.03	113.80
1	A	24	HIS	ND1-CE1-NE2	6.17	114.57	108.40
1	A	83	GLU	CA-CB-CG	6.00	126.10	114.10
1	A	4	GLU	CB-CG-CD	5.97	122.74	112.60
1	A	110	ALA	CA-C-N	5.90	128.21	120.60
1	A	110	ALA	C-N-CA	5.90	128.21	120.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	56	LYS	N-CA-CB	5.86	118.74	110.12
1	A	87	LYS	N-CA-CB	5.84	118.52	110.11
1	A	44	ASP	N-CA-C	-5.69	105.08	111.28
1	A	117	SER	CA-C-O	5.68	126.97	121.00
1	A	67	THR	CA-C-O	5.65	126.94	120.90
1	A	119	HIS	CA-C-N	5.62	124.82	118.97
1	A	119	HIS	C-N-CA	5.62	124.82	118.97
1	A	81	HIS	ND1-CE1-NE2	5.56	113.96	108.40
1	A	82	HIS	N-CA-C	5.46	119.25	112.59
1	A	48	HIS	CA-CB-CG	5.40	119.20	113.80
1	A	56	LYS	O-C-N	5.39	127.84	122.12
1	A	99	ILE	CB-CA-C	-5.38	104.99	111.18
1	A	4	GLU	N-CA-C	-5.20	105.69	111.36
1	A	125	ALA	CA-C-N	5.18	128.18	120.31
1	A	125	ALA	C-N-CA	5.18	128.18	120.31
1	A	16	LYS	CA-C-O	-5.12	115.12	120.55
1	A	85	GLU	CA-CB-CG	5.10	124.30	114.10
1	A	93	HIS	CA-CB-CG	-5.10	108.70	113.80
1	A	21	VAL	N-CA-CB	5.06	117.42	110.54
1	A	76	LEU	N-CA-C	5.03	118.19	111.75

There are no chirality outliers.

There are no planarity outliers.

4.2 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 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	1494	974	1242	28	2
2	A	5	0	0	0	0
3	A	25	0	0	1	0
4	A	43	30	30	5	0
5	A	4	0	0	0	0
6	A	267	0	0	9	0
All	All	1838	1004	1272	28	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 11.

All (28) 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)
1:A:118:ARG:HH11	1:A:118:ARG:HG2	1.24	0.91
1:A:118:ARG:HH11	1:A:118:ARG:CG	1.83	0.84
1:A:147:LYS:HB2	1:A:152:GLN:HG3	1.55	0.78
1:A:16:LYS:NZ	1:A:122:ASP:OD1	2.17	0.78
1:A:4:GLU:HB2	6:A:253:DOD:O	1.83	0.72
1:A:118:ARG:HG2	1:A:118:ARG:NH1	1.96	0.70
1:A:133:LYS:HD3	6:A:289:DOD:O	1.90	0.67
1:A:118:ARG:CG	1:A:118:ARG:NH1	2.52	0.63
1:A:126:ASP:OD2	3:A:178:ND4:N	2.34	0.59
1:A:43:PHE:O	1:A:47:LYS:HG3	1.99	0.58
1:A:1:VAL:HA	6:A:255:DOD:O	2.01	0.55
1:A:67:THR:HA	6:A:211:DOD:O	2.02	0.55
1:A:7:TRP:CD1	6:A:286:DOD:O	2.59	0.54
1:A:99:ILE:CD1	4:A:154:HEM:HHD	2.33	0.53
1:A:31:ARG:NH2	6:A:232:DOD:O	2.42	0.51
1:A:58:SER:HA	6:A:240:DOD:O	2.07	0.50
1:A:99:ILE:CD1	4:A:154:HEM:CHD	2.91	0.49
1:A:16:LYS:NZ	1:A:122:ASP:CG	2.70	0.49
1:A:99:ILE:HD11	4:A:154:HEM:HHD	1.84	0.48
1:A:5:GLY:O	6:A:225:DOD:O	2.24	0.48
1:A:133:LYS:CD	6:A:289:DOD:O	2.58	0.48
1:A:118:ARG:HB3	1:A:119:HIS:CD2	2.47	0.45
1:A:99:ILE:HD11	4:A:154:HEM:CHD	2.43	0.44
1:A:16:LYS:HZ2	1:A:122:ASP:CG	2.18	0.43
1:A:95:THR:HG22	1:A:151:TYR:CE2	2.50	0.41
1:A:83:GLU:H	1:A:83:GLU:CD	2.23	0.41
1:A:99:ILE:HD12	4:A:154:HEM:C3C	2.51	0.41
1:A:151:TYR:O	1:A:152:GLN:C	2.64	0.40

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)
1:A:96:LYS:HE2	1:A:109:GLU:OE2[1_565]	0.91	0.69
1:A:96:LYS:CE	1:A:109:GLU:OE2[1_565]	1.94	0.26

4.3 Torsion angles [i](#)

4.3.1 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	151/153 (99%)	144 (95%)	6 (4%)	1 (1%)	18 8

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	2	LEU

4.3.2 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	125/125 (100%)	104 (83%)	21 (17%)	2 0

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	GLU
1	A	8	GLN
1	A	9	LEU
1	A	16	LYS
1	A	18	GLU
1	A	21	VAL
1	A	31	ARG
1	A	34	LYS
1	A	45	ARG
1	A	49	LEU

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Mol	Chain	Res	Type
1	A	50	LYS
1	A	59	GLU
1	A	83	GLU
1	A	85	GLU
1	A	92	SER
1	A	98	LYS
1	A	99	ILE
1	A	115	LEU
1	A	118	ARG
1	A	136	GLU
1	A	152	GLN

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

Mol	Chain	Res	Type
1	A	91	GLN

4.3.3 RNA [i](#)

There are no RNA molecules in this entry.

4.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

4.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

4.6 Ligand geometry [i](#)

Of 9 ligands modelled in this entry, 5 are modelled with single atom - leaving 4 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	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
5	CMO	A	155[B]	4	0,1,1	-	-	-		
2	SO4	A	174	-	4,4,4	0.67	0	6,6,6	0.08	0
4	HEM	A	154	5,1	50,50,50	1.28	10 (20%)	67,82,82	1.44	9 (13%)
5	CMO	A	155[A]	4	0,1,1	-	-	-		

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	HEM	A	154	5,1	-	7/14/54/54	-

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	154	HEM	CAC-C3C	2.78	1.54	1.47
4	A	154	HEM	CAB-C3B	2.61	1.54	1.47
4	A	154	HEM	FE-ND	2.48	2.02	1.94
4	A	154	HEM	FE-NB	2.40	2.02	1.94
4	A	154	HEM	CMD-C2D	2.26	1.55	1.50
4	A	154	HEM	FE-NC	2.20	2.02	1.95
4	A	154	HEM	CMA-C3A	2.19	1.55	1.50
4	A	154	HEM	CMB-C2B	2.12	1.55	1.50
4	A	154	HEM	CMC-C2C	2.10	1.55	1.50
4	A	154	HEM	FE-NA	2.09	2.02	1.95

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	154	HEM	CBA-CAA-C2A	4.53	125.06	112.53
4	A	154	HEM	CAA-CBA-CGA	4.34	125.19	113.67
4	A	154	HEM	CHC-C4B-NB	-3.19	120.99	124.42
4	A	154	HEM	CMA-C3A-C4A	-3.06	120.76	125.42
4	A	154	HEM	C3B-C4B-NB	2.62	111.35	109.47
4	A	154	HEM	C1C-CHC-C4B	2.31	130.93	126.02
4	A	154	HEM	CMA-C3A-C2A	2.21	130.31	125.62
4	A	154	HEM	O2A-CGA-CBA	2.18	120.90	114.00
4	A	154	HEM	C4C-CHD-C1D	-2.11	121.53	126.02

There are no chirality outliers.

All (7) torsion outliers are listed below:

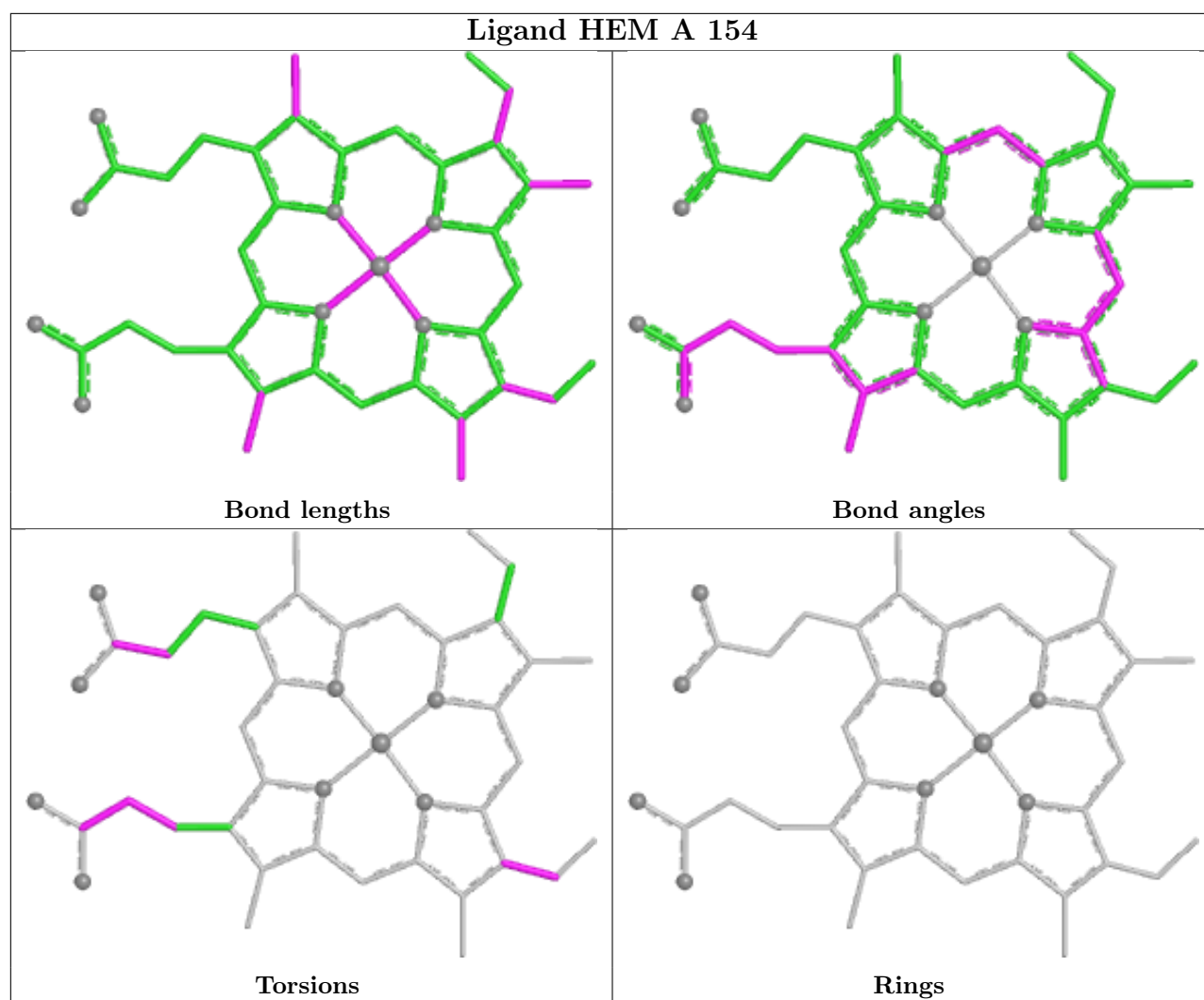
Mol	Chain	Res	Type	Atoms
4	A	154	HEM	C2A-CAA-CBA-CGA
4	A	154	HEM	C2B-C3B-CAB-CBB
4	A	154	HEM	C4B-C3B-CAB-CBB
4	A	154	HEM	CAD-CBD-CGD-O1D
4	A	154	HEM	CAD-CBD-CGD-O2D
4	A	154	HEM	CAA-CBA-CGA-O2A
4	A	154	HEM	CAA-CBA-CGA-O1A

There are no ring outliers.

1 monomer is involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	154	HEM	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.



4.7 Other polymers [i](#)

There are no such residues in this entry.

4.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.