



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 4, 2026 – 08:51 AM EDT

PDB ID : 1COH / pdb_00001coh
Title : STRUCTURE OF HAEMOGLOBIN IN THE DEOXY QUATERNARY
STATE WITH LIGAND BOUND AT THE ALPHA HAEMS
Authors : Luisi, B.
Deposited on : 1989-01-13
Resolution : 2.90 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)	:	2.50

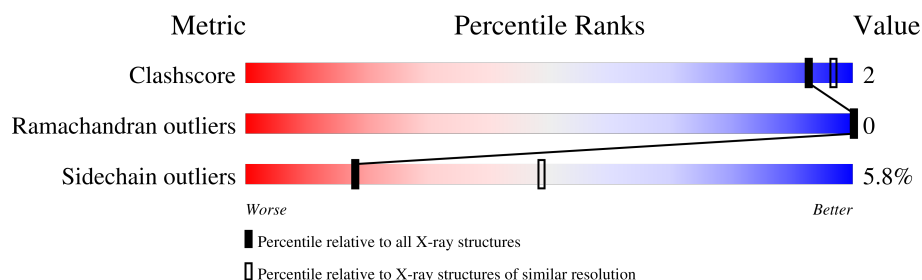
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)

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	141	 82% 16% ..
1	C	141	 74% 23% .
2	B	146	 79% 18% .
2	D	146	 76% 18% 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:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	COH	B	147	X	-	-	-
5	COH	D	147	X	-	-	-

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 4757 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.

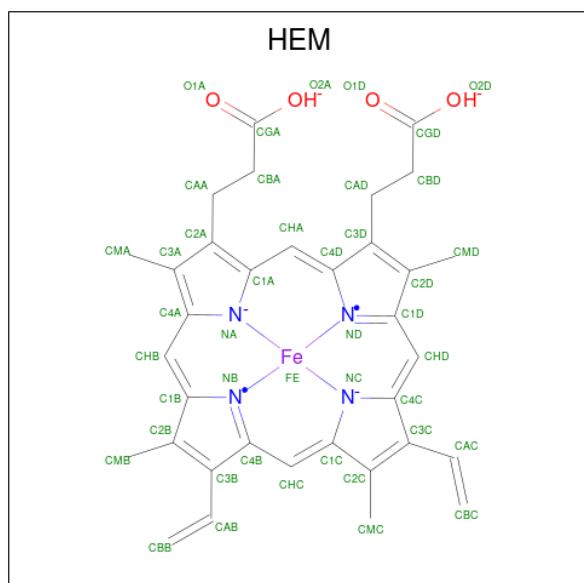
- Molecule 1 is a protein called HEMOGLOBIN (FERROUS CARBONMONOXY) (ALPHA CHAIN).

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

- Molecule 2 is a protein called HEMOGLOBIN (COBALTOUS DEOXY) (BETA CHAIN).

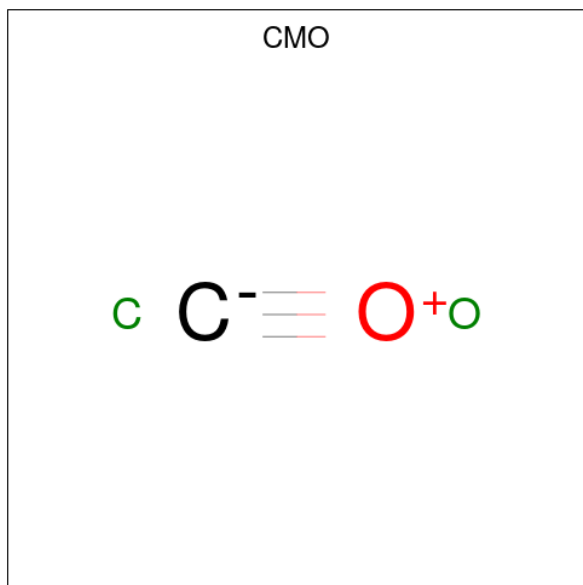
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	146	Total	C	N	O	S	0	0	0
			1123	724	195	201	3			
2	D	146	Total	C	N	O	S	0	0	0
			1123	724	195	201	3			

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



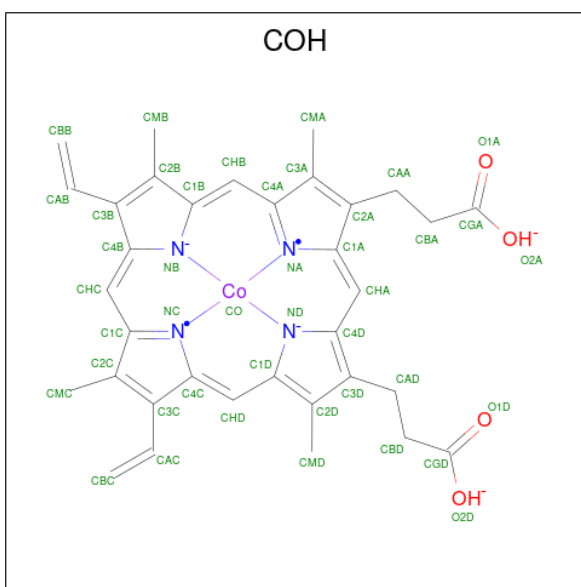
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 4 is CARBON MONOXIDE (CCD ID: CMO) (formula: CO).



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

- Molecule 5 is PROTOPORPHYRIN IX CONTAINING CO (CCD ID: COH) (formula: C₃₄H₃₂CoN₄O₄).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	B	1	Total 43	C 34	Co 1	N 4	O 4	0	0
5	D	1	Total 43	C 34	Co 1	N 4	O 4	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	46	Total O 46 46	0	0
6	B	50	Total O 50 50	0	0
6	C	52	Total O 52 52	0	0
6	D	49	Total O 49 49	0	0

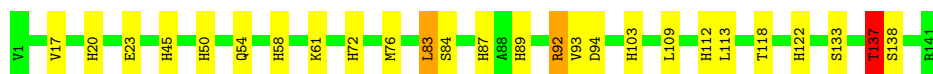
3 Residue-property plots [i](#)

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.

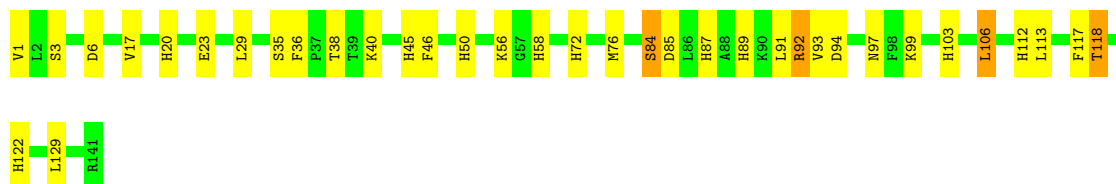
- Molecule 1: HEMOGLOBIN (FERROUS CARBONMONOXY) (ALPHA CHAIN)

Chain A: 



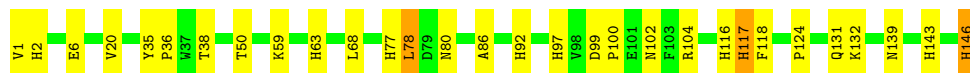
- Molecule 1: HEMOGLOBIN (FERROUS CARBONMONOXY) (ALPHA CHAIN)

Chain C: 



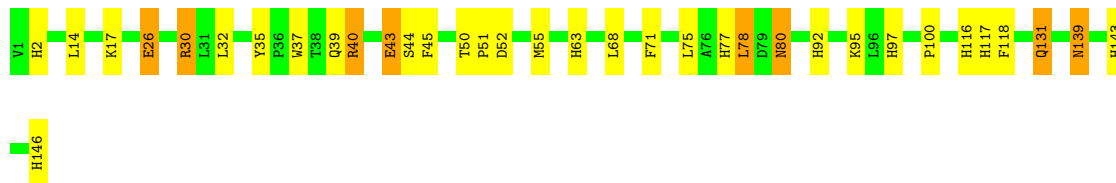
- Molecule 2: HEMOGLOBIN (COBALTOUS DEOXY) (BETA CHAIN)

Chain B: 



- Molecule 2: HEMOGLOBIN (COBALTOUS DEOXY) (BETA CHAIN)

Chain D: 



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	63.09 Å 83.06 Å 53.67 Å 90.00° 99.63° 90.00°	Depositor
Resolution (Å)	(Not available) – 2.90	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-2.90)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	EREF	Depositor
R, R_{free}	(Not available) , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	4757	wwPDB-VP
Average B, all atoms (Å ²)	24.0	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: COH, HEM, CMO

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	1.39	17/1097 (1.5%)	1.77	19/1491 (1.3%)
1	C	1.39	15/1097 (1.4%)	1.82	26/1491 (1.7%)
2	B	1.37	16/1153 (1.4%)	1.77	21/1566 (1.3%)
2	D	1.34	16/1153 (1.4%)	1.87	22/1566 (1.4%)
All	All	1.37	64/4500 (1.4%)	1.81	88/6114 (1.4%)

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	C	0	1
2	D	0	2
All	All	0	3

All (64) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	20	HIS	CE1-NE2	10.50	1.43	1.32
1	C	50	HIS	ND1-CE1	10.20	1.42	1.32
1	A	45	HIS	ND1-CE1	9.82	1.42	1.32
2	B	116	HIS	ND1-CE1	9.57	1.42	1.32
1	A	89	HIS	CE1-NE2	9.38	1.42	1.32
2	B	143	HIS	CE1-NE2	9.37	1.42	1.32
2	D	77	HIS	CE1-NE2	9.32	1.41	1.32
2	B	77	HIS	CE1-NE2	9.18	1.41	1.32
2	B	146	HIS	ND1-CE1	9.16	1.41	1.32
2	D	2	HIS	CE1-NE2	8.92	1.41	1.32
2	B	2	HIS	CE1-NE2	8.85	1.41	1.32
1	C	72	HIS	ND1-CE1	8.78	1.41	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	97	HIS	ND1-CE1	8.46	1.41	1.32
2	D	117	HIS	ND1-CE1	8.43	1.41	1.32
2	D	2	HIS	ND1-CE1	8.40	1.41	1.32
1	C	50	HIS	CE1-NE2	8.37	1.41	1.32
2	D	143	HIS	CE1-NE2	8.36	1.41	1.32
1	A	89	HIS	ND1-CE1	8.35	1.40	1.32
2	B	146	HIS	CE1-NE2	8.25	1.40	1.32
1	A	122	HIS	CE1-NE2	8.20	1.40	1.32
1	C	45	HIS	ND1-CE1	8.14	1.40	1.32
2	D	146	HIS	CE1-NE2	8.12	1.40	1.32
1	C	20	HIS	CE1-NE2	8.09	1.40	1.32
1	A	72	HIS	ND1-CE1	8.08	1.40	1.32
1	C	122	HIS	ND1-CE1	7.94	1.40	1.32
1	A	72	HIS	CE1-NE2	7.92	1.40	1.32
2	D	97	HIS	CE1-NE2	7.87	1.40	1.32
2	B	143	HIS	ND1-CE1	7.83	1.40	1.32
1	C	72	HIS	CE1-NE2	7.80	1.40	1.32
2	B	97	HIS	CE1-NE2	7.79	1.40	1.32
1	A	45	HIS	CE1-NE2	7.79	1.40	1.32
1	C	45	HIS	CE1-NE2	7.67	1.40	1.32
2	D	146	HIS	ND1-CE1	7.67	1.40	1.32
1	A	112	HIS	ND1-CE1	7.65	1.40	1.32
1	A	50	HIS	CE1-NE2	7.64	1.40	1.32
2	D	77	HIS	ND1-CE1	7.63	1.40	1.32
2	B	77	HIS	ND1-CE1	7.53	1.40	1.32
2	D	117	HIS	CE1-NE2	7.45	1.40	1.32
2	B	2	HIS	ND1-CE1	7.30	1.39	1.32
2	D	143	HIS	ND1-CE1	7.21	1.39	1.32
1	A	20	HIS	ND1-CE1	7.12	1.39	1.32
2	B	116	HIS	CE1-NE2	7.10	1.39	1.32
1	C	20	HIS	ND1-CE1	7.07	1.39	1.32
1	A	112	HIS	CE1-NE2	6.92	1.39	1.32
2	D	63	HIS	CE1-NE2	6.89	1.39	1.32
2	D	116	HIS	ND1-CE1	6.78	1.39	1.32
2	B	97	HIS	ND1-CE1	6.66	1.39	1.32
1	A	122	HIS	ND1-CE1	6.64	1.39	1.32
1	A	50	HIS	ND1-CE1	6.63	1.39	1.32
2	B	117	HIS	CE1-NE2	6.47	1.39	1.32
1	C	89	HIS	CE1-NE2	6.46	1.39	1.32
2	D	116	HIS	CE1-NE2	6.42	1.39	1.32
2	B	92	HIS	CE1-NE2	6.22	1.38	1.32
2	B	117	HIS	ND1-CE1	6.19	1.38	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	122	HIS	CE1-NE2	6.14	1.38	1.32
1	C	112	HIS	CE1-NE2	6.02	1.38	1.32
1	C	87	HIS	CE1-NE2	5.87	1.38	1.32
1	A	58	HIS	CE1-NE2	5.84	1.38	1.32
2	D	92	HIS	CE1-NE2	5.74	1.38	1.32
1	C	89	HIS	ND1-CE1	5.67	1.38	1.32
1	A	87	HIS	ND1-CE1	5.59	1.38	1.32
2	B	63	HIS	CE1-NE2	5.45	1.38	1.32
1	A	87	HIS	CE1-NE2	5.43	1.38	1.32
1	C	58	HIS	CE1-NE2	5.28	1.37	1.32

All (88) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	139	ASN	CA-CB-CG	-12.88	99.72	112.60
2	D	43	GLU	CB-CG-CD	-10.95	93.99	112.60
2	D	80	ASN	CA-CB-CG	10.45	123.05	112.60
2	D	30	ARG	NE-CZ-NH2	-9.52	110.63	119.20
1	A	122	HIS	CA-CB-CG	8.79	122.59	113.80
2	D	30	ARG	NE-CZ-NH1	8.53	130.03	121.50
1	C	94	ASP	CA-C-N	8.34	129.15	119.47
1	C	94	ASP	C-N-CA	8.34	129.15	119.47
1	C	92	ARG	CD-NE-CZ	-7.86	113.40	124.40
2	B	118	PHE	CA-CB-CG	-7.68	106.12	113.80
1	A	94	ASP	CA-C-N	7.43	128.09	119.47
1	A	94	ASP	C-N-CA	7.43	128.09	119.47
1	A	58	HIS	CA-CB-CG	-7.36	106.44	113.80
2	D	52	ASP	CA-CB-CG	-7.24	105.36	112.60
1	C	58	HIS	CA-CB-CG	-7.09	106.71	113.80
1	C	117	PHE	CA-C-N	6.92	131.18	120.60
1	C	117	PHE	C-N-CA	6.92	131.18	120.60
1	C	122	HIS	CA-CB-CG	6.87	120.67	113.80
2	B	50	THR	CA-C-N	6.81	126.33	119.24
2	B	50	THR	C-N-CA	6.81	126.33	119.24
1	C	36	PHE	CA-C-N	6.75	126.45	119.56
1	C	36	PHE	C-N-CA	6.75	126.45	119.56
1	A	93	VAL	CA-C-O	-6.63	113.29	120.85
1	C	113	LEU	CA-C-O	-6.62	112.06	120.80
2	D	39	GLN	CA-C-N	6.45	133.86	121.54
2	D	39	GLN	C-N-CA	6.45	133.86	121.54
1	C	84	SER	CA-C-O	-6.27	113.77	120.42
2	D	131	GLN	CA-C-O	-6.25	113.80	120.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	137	THR	CA-CB-CG2	6.20	121.04	110.50
1	C	46	PHE	CA-CB-CG	6.13	119.93	113.80
2	B	132	LYS	CA-C-O	-6.10	113.95	120.42
1	A	92	ARG	CD-NE-CZ	-6.03	115.96	124.40
1	A	17	VAL	O-C-N	5.99	127.78	121.91
2	D	118	PHE	CA-CB-CG	-5.97	107.83	113.80
2	B	80	ASN	CA-CB-CG	5.96	118.56	112.60
1	A	61	LYS	CA-C-O	-5.94	114.12	120.42
1	A	23	GLU	CB-CG-CD	-5.92	102.54	112.60
2	B	146	HIS	CA-CB-CG	5.91	119.71	113.80
1	C	118	THR	CA-CB-CG2	5.87	120.48	110.50
1	A	113	LEU	CA-C-N	5.86	125.55	119.05
1	A	113	LEU	C-N-CA	5.86	125.55	119.05
1	A	76	MET	CA-C-O	-5.84	112.16	120.16
2	D	40	ARG	CG-CD-NE	-5.77	99.30	112.00
2	B	99	ASP	CA-C-O	-5.77	114.57	119.59
2	B	20	VAL	CA-C-O	-5.76	114.96	120.95
1	A	113	LEU	CA-C-O	-5.70	113.28	120.80
1	A	58	HIS	ND1-CG-CD2	5.64	111.74	106.10
2	D	26	GLU	CA-C-O	-5.64	114.44	120.42
2	B	139	ASN	CA-CB-CG	-5.62	106.98	112.60
2	B	35	TYR	CA-C-N	5.56	125.23	119.56
2	B	35	TYR	C-N-CA	5.56	125.23	119.56
1	C	29	LEU	CA-C-O	-5.55	114.99	120.82
2	B	139	ASN	O-C-N	5.53	127.77	122.07
2	B	86	ALA	CA-C-O	-5.53	115.02	120.82
1	C	106	LEU	CA-C-O	-5.52	115.02	120.82
2	B	99	ASP	CA-CB-CG	5.51	118.11	112.60
2	D	26	GLU	CB-CG-CD	-5.50	103.24	112.60
2	D	100	PRO	N-CA-CB	5.50	108.75	103.52
2	B	99	ASP	CA-C-N	5.49	125.20	119.82
2	B	99	ASP	C-N-CA	5.49	125.20	119.82
2	D	17	LYS	CB-CG-CD	-5.46	98.75	111.30
1	C	58	HIS	ND1-CG-CD2	5.44	111.54	106.10
1	C	97	ASN	CA-CB-CG	-5.44	107.16	112.60
1	A	118	THR	CA-C-N	5.42	124.88	119.24
1	A	118	THR	C-N-CA	5.42	124.88	119.24
1	C	6	ASP	CA-C-O	-5.40	114.82	120.55
1	C	17	VAL	O-C-N	5.38	127.50	121.90
1	A	94	ASP	CA-CB-CG	-5.37	107.23	112.60
1	C	76	MET	CA-C-O	-5.36	112.82	120.16
1	A	54	GLN	CA-C-O	-5.33	115.23	120.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	93	VAL	CA-C-O	-5.28	114.52	120.74
2	D	50	THR	CA-C-N	5.26	125.31	119.32
2	D	50	THR	C-N-CA	5.26	125.31	119.32
2	B	124	PRO	CA-C-O	-5.22	113.00	120.56
2	D	45	PHE	CA-C-N	-5.22	111.19	121.41
2	D	45	PHE	C-N-CA	-5.22	111.19	121.41
2	B	36	PRO	N-CA-CB	5.18	108.66	103.48
2	B	100	PRO	N-CA-CB	5.14	108.41	103.52
2	D	71	PHE	CA-C-O	-5.12	115.12	120.55
1	C	56	LYS	CA-C-N	5.11	125.62	120.00
1	C	56	LYS	C-N-CA	5.11	125.62	120.00
2	D	35	TYR	CA-C-N	5.06	125.13	119.87
2	D	35	TYR	C-N-CA	5.06	125.13	119.87
1	C	3	SER	CA-C-N	5.03	125.06	119.32
1	C	3	SER	C-N-CA	5.03	125.06	119.32
2	B	78	LEU	CA-C-N	5.03	128.64	120.60
2	B	78	LEU	C-N-CA	5.03	128.64	120.60
1	C	23	GLU	CB-CG-CD	-5.00	104.09	112.60

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	92	ARG	Sidechain
2	D	30	ARG	Sidechain
2	D	40	ARG	Sidechain

5.2 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	1069	0	1073	4	0
1	C	1069	0	1073	5	2
2	B	1123	0	1118	4	0
2	D	1123	0	1118	5	0
3	A	43	0	30	0	0
3	C	43	0	30	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	2	0	0	0	0
4	C	2	0	0	0	0
5	B	43	0	30	0	0
5	D	43	0	30	0	0
6	A	46	0	0	0	0
6	B	50	0	0	1	4
6	C	52	0	0	1	2
6	D	49	0	0	0	0
All	All	4757	0	4502	14	4

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 2.

All (14) 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:133:SER:O	1:A:137:THR:HB	2.15	0.46
1:A:103:HIS:HE1	2:B:131:GLN:OE1	2.00	0.44
2:D:95:LYS:HD3	2:D:95:LYS:HA	1.74	0.44
1:C:129:LEU:HD23	1:C:129:LEU:HA	1.79	0.43
2:D:51:PRO:O	2:D:55:MET:HG2	2.19	0.42
1:A:92:ARG:HB3	2:D:37:TRP:HB2	2.02	0.41
2:D:78:LEU:HD12	2:D:78:LEU:HA	1.89	0.41
1:C:35:SER:OG	6:C:879:HOH:O	2.20	0.41
1:C:103:HIS:HE1	2:D:131:GLN:OE1	2.04	0.41
2:B:38:THR:HG22	2:B:102:ASN:OD1	2.21	0.40
2:B:146:HIS:OXT	1:C:40:LYS:NZ	2.45	0.40
1:A:83:LEU:HD12	1:A:83:LEU:HA	1.60	0.40
2:B:104:ARG:HD3	6:B:998:HOH:O	2.20	0.40
1:C:91:LEU:HD23	1:C:91:LEU:HA	1.89	0.40

All (4) 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:C:85:ASP:OD2	6:B:1008:HOH:O[2_657]	1.18	1.02
6:B:1008:HOH:O	6:C:865:HOH:O[2_647]	1.90	0.30
1:C:85:ASP:CG	6:B:1008:HOH:O[2_657]	1.96	0.24
6:B:920:HOH:O	6:C:829:HOH:O[2_647]	2.14	0.06

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	139/141 (99%)	137 (99%)	2 (1%)	0	100	100
1	C	139/141 (99%)	136 (98%)	3 (2%)	0	100	100
2	B	144/146 (99%)	143 (99%)	1 (1%)	0	100	100
2	D	144/146 (99%)	141 (98%)	3 (2%)	0	100	100
All	All	566/574 (99%)	557 (98%)	9 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	113/113 (100%)	108 (96%)	5 (4%)	25	59
1	C	113/113 (100%)	107 (95%)	6 (5%)	20	52
2	B	118/118 (100%)	112 (95%)	6 (5%)	21	53
2	D	118/118 (100%)	108 (92%)	10 (8%)	10	31
All	All	462/462 (100%)	435 (94%)	27 (6%)	18	49

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	83	LEU
1	A	84	SER

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Mol	Chain	Res	Type
1	A	109	LEU
1	A	137	THR
1	A	138	SER
2	B	1	VAL
2	B	6	GLU
2	B	59	LYS
2	B	68	LEU
2	B	78	LEU
2	B	117	HIS
1	C	1	VAL
1	C	38	THR
1	C	84	SER
1	C	99	LYS
1	C	106	LEU
1	C	118	THR
2	D	14	LEU
2	D	26	GLU
2	D	32	LEU
2	D	43	GLU
2	D	44	SER
2	D	68	LEU
2	D	75	LEU
2	D	78	LEU
2	D	80	ASN
2	D	139	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	103	HIS
2	B	80	ASN
2	B	143	HIS
1	C	50	HIS
1	C	68	ASN
1	C	72	HIS
1	C	103	HIS
2	D	2	HIS
2	D	80	ASN
2	D	139	ASN

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 ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

6 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	$\# Z > 2$
4	CMO	A	143	-	0,1,1	-	-	-		
5	COH	D	147	2	50,50,50	0.92	2 (4%)	66,82,82	1.10	4 (6%)
3	HEM	C	142	1	50,50,50	1.16	7 (14%)	67,82,82	1.04	2 (2%)
3	HEM	A	142	1	50,50,50	1.27	3 (6%)	67,82,82	1.00	3 (4%)
5	COH	B	147	2	50,50,50	1.12	4 (8%)	66,82,82	1.18	5 (7%)
4	CMO	C	143	-	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
5	COH	D	147	2	1/1/3/9	6/14/54/54	-
3	HEM	C	142	1	-	4/14/54/54	-
3	HEM	A	142	1	-	2/14/54/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	COH	B	147	2	1/1/3/9	4/14/54/54	-

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	142	HEM	FE-NB	4.22	2.07	1.94
3	C	142	HEM	FE-NA	3.88	2.08	1.95
3	A	142	HEM	FE-NC	3.68	2.07	1.95
5	B	147	COH	CO-ND	3.21	2.08	1.96
3	C	142	HEM	FE-NB	2.90	2.03	1.94
3	C	142	HEM	FE-NC	-2.55	1.86	1.95
3	C	142	HEM	O2D-CGD	-2.31	1.23	1.30
5	B	147	COH	CO-NC	-2.28	1.88	1.96
5	B	147	COH	CO-NB	-2.27	1.87	1.96
3	A	142	HEM	CBB-CAB	2.18	1.40	1.30
3	C	142	HEM	CBC-CAC	2.12	1.40	1.30
5	B	147	COH	CBB-CAB	2.11	1.40	1.30
5	D	147	COH	CBB-CAB	2.11	1.40	1.30
3	C	142	HEM	CBB-CAB	2.08	1.40	1.30
3	C	142	HEM	O2A-CGA	-2.06	1.24	1.30
5	D	147	COH	O2D-CGD	-2.02	1.24	1.30

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	147	COH	C2B-C1B-NB	3.20	113.36	110.88
3	C	142	HEM	C3B-C4B-NB	3.08	111.68	109.47
5	B	147	COH	CHC-C1C-C2C	-3.00	120.29	125.03
3	C	142	HEM	C4C-C3C-C2C	-2.77	104.41	106.81
5	D	147	COH	CAA-CBA-CGA	2.46	120.20	113.67
5	D	147	COH	C2D-C1D-ND	2.43	112.06	109.69
5	D	147	COH	C4C-C3C-C2C	-2.32	105.14	107.28
3	A	142	HEM	CAA-CBA-CGA	2.31	119.80	113.67
5	B	147	COH	O1D-CGD-CBD	-2.29	115.83	123.09
5	B	147	COH	C4B-NB-C1B	-2.28	101.76	105.11
3	A	142	HEM	CMC-C2C-C1C	-2.18	120.89	124.73
5	B	147	COH	CMC-C2C-C1C	-2.11	121.74	125.03
5	D	147	COH	CBD-CAD-C3D	2.07	118.26	112.53
3	A	142	HEM	O2D-CGD-CBD	2.07	120.53	114.00

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	B	147	COH	NB
5	D	147	COH	NB

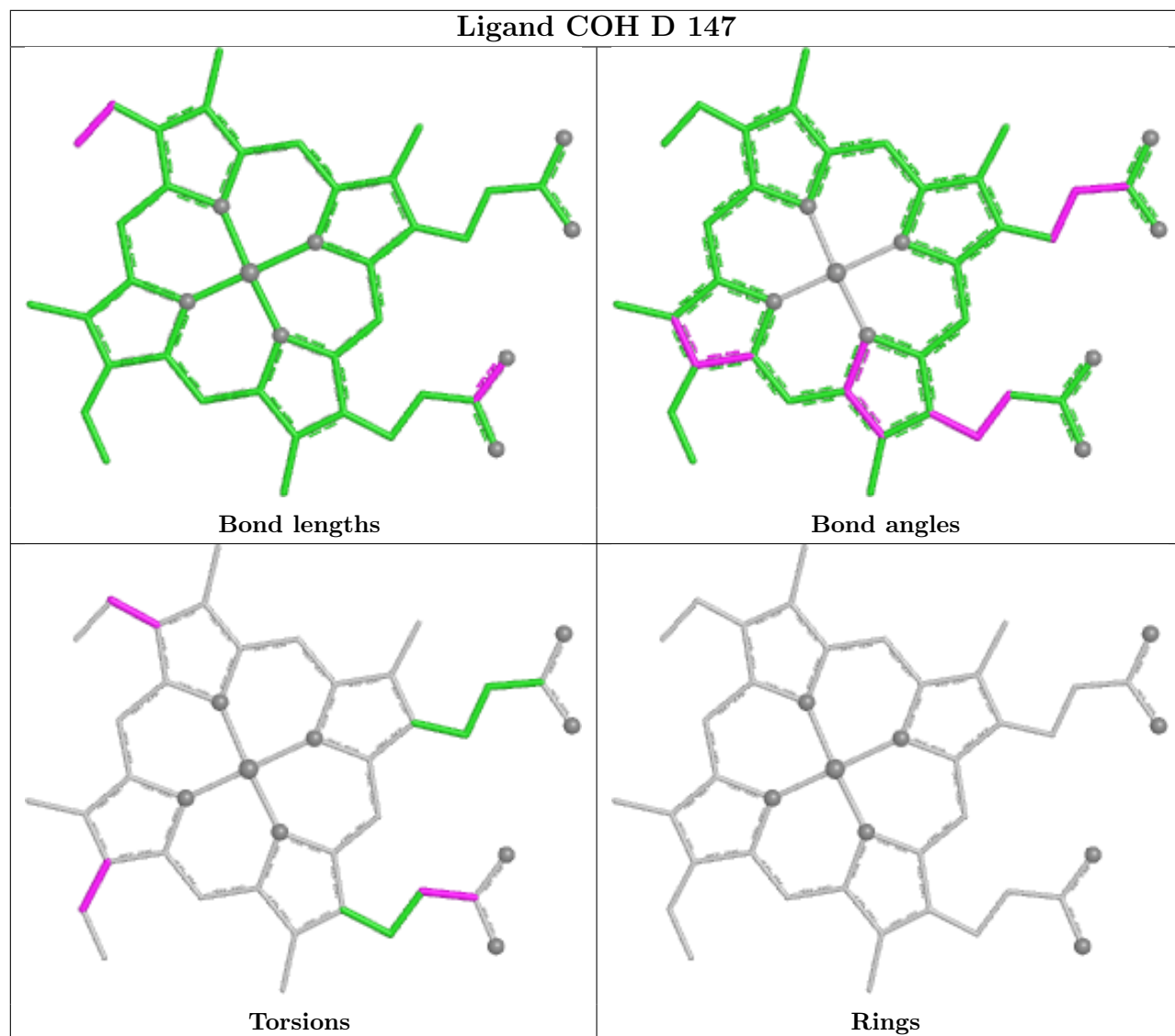
All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	142	HEM	C2B-C3B-CAB-CBB
5	D	147	COH	C2C-C3C-CAC-CBC
5	D	147	COH	C2B-C3B-CAB-CBB
5	D	147	COH	C4B-C3B-CAB-CBB
5	B	147	COH	C2C-C3C-CAC-CBC
3	C	142	HEM	CAD-CBD-CGD-O1D
5	D	147	COH	CAD-CBD-CGD-O1D
5	D	147	COH	CAD-CBD-CGD-O2D
3	C	142	HEM	CAD-CBD-CGD-O2D
3	C	142	HEM	CAA-CBA-CGA-O2A
5	B	147	COH	CAA-CBA-CGA-O2A
3	A	142	HEM	C4B-C3B-CAB-CBB
5	D	147	COH	C4C-C3C-CAC-CBC
3	C	142	HEM	CAA-CBA-CGA-O1A
5	B	147	COH	CAA-CBA-CGA-O1A
5	B	147	COH	CAD-CBD-CGD-O2D

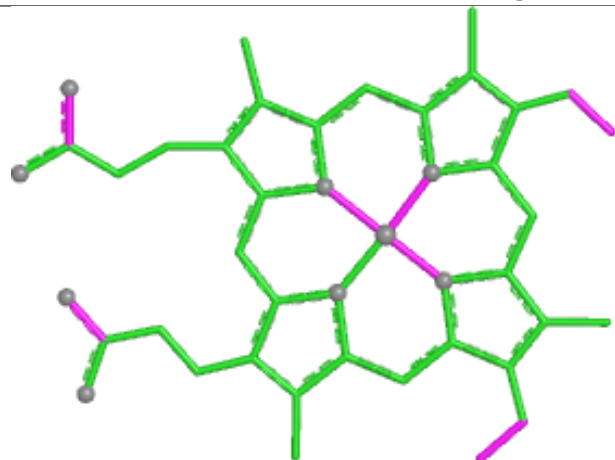
There are no ring outliers.

No monomer is involved in short contacts.

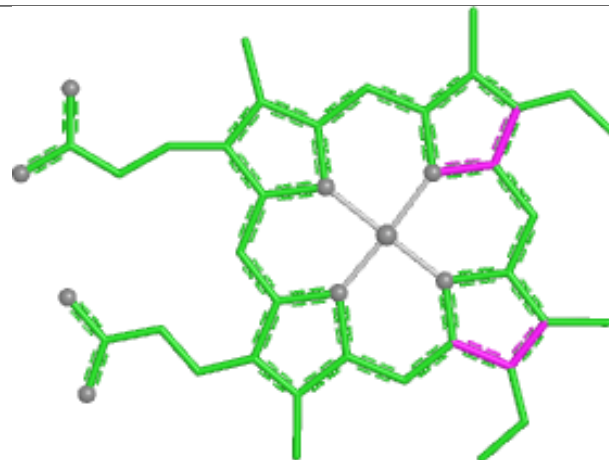
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



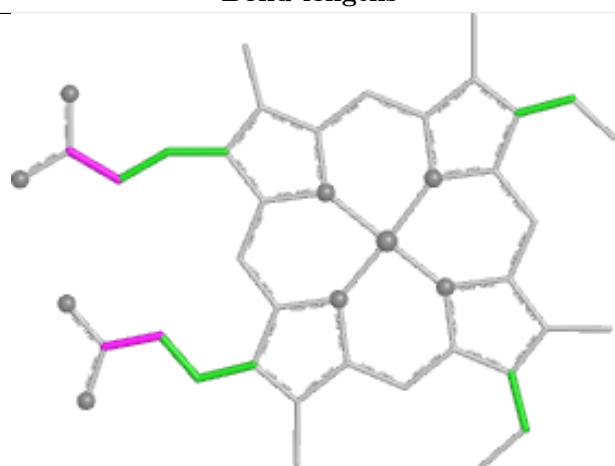
Ligand HEM C 142



Bond lengths



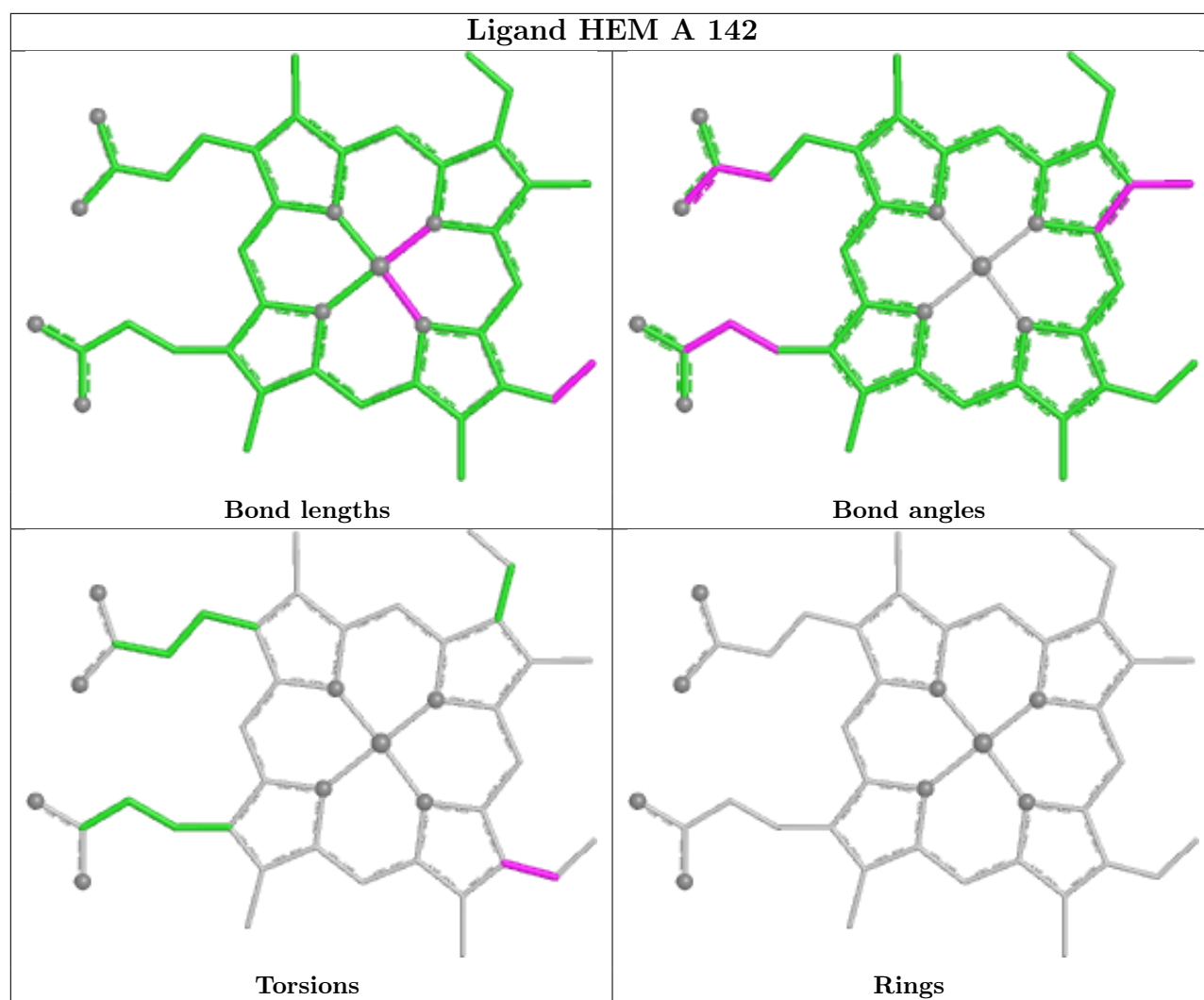
Bond angles

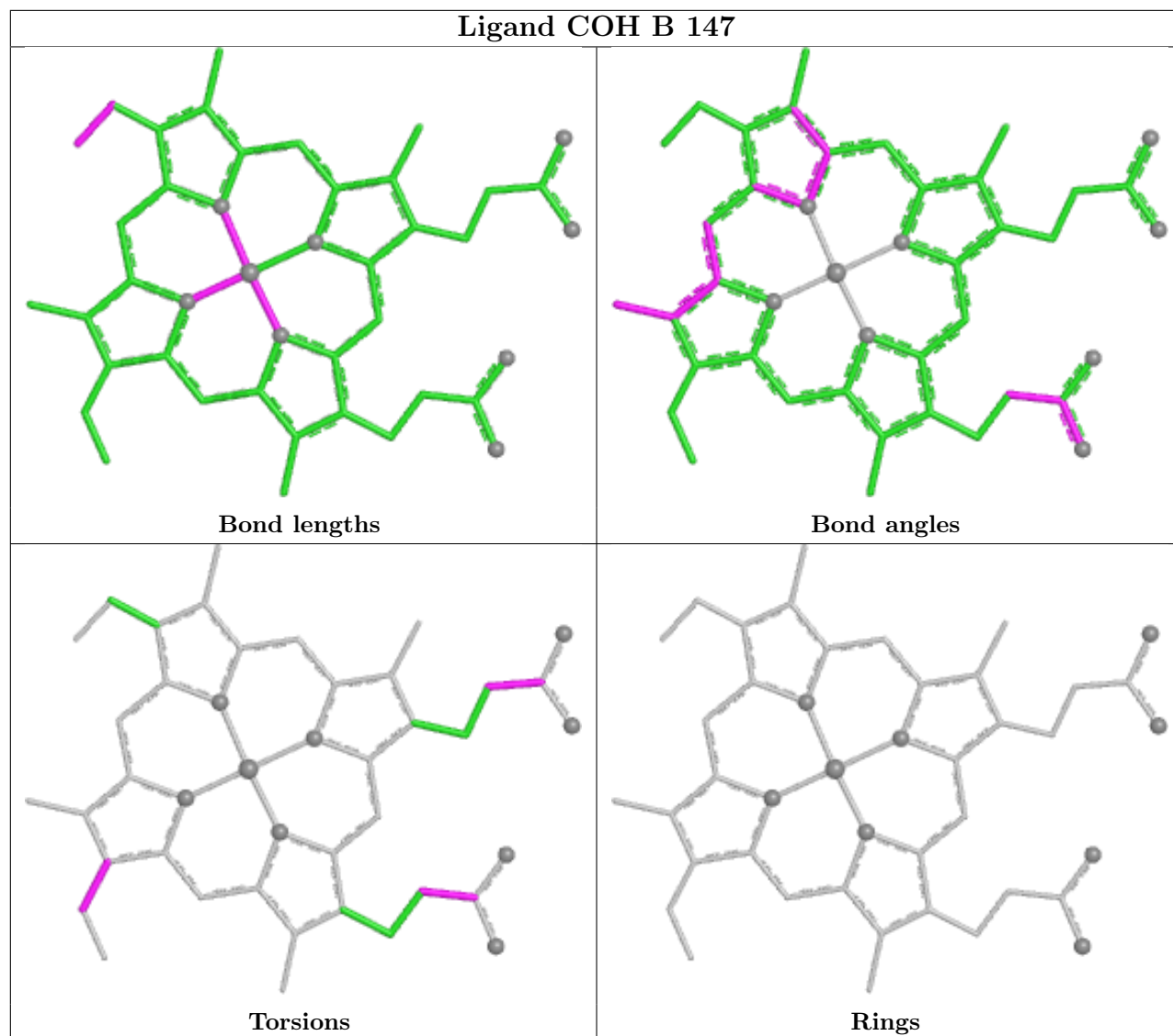


Torsions



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.