



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 08:03 AM UTC

PDB ID : 1J7W / pdb_00001j7w
Title : Crystal structure of deoxy HbbetaYQ, a site directed mutant of HbA
Authors : Miele, A.E.; Draghi, F.; Arcovito, A.; Bellelli, A.; Brunori, M.; Travaglini-All
ocatelli, C.; Vallone, B.
Deposited on : 2001-05-19
Resolution : 2.00 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)	:	2.49

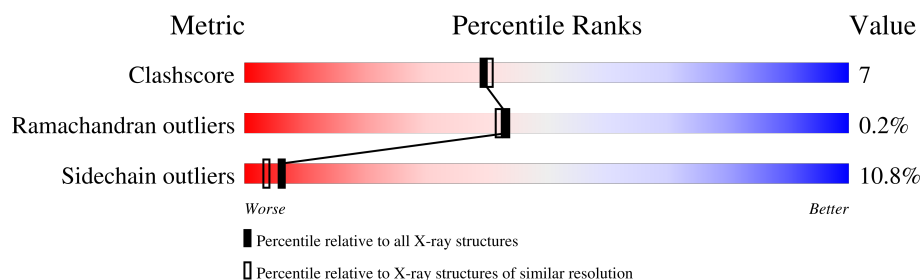
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)

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	 70% 22% 8%
1	C	141	 71% 25% .
2	B	146	 73% 21% 5%
2	D	146	 68% 28% .

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 4809 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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	141	Total	C	N	O	S	3	0	0
			1070	685	187	194	4			
1	C	141	Total	C	N	O	S	3	0	0
			1070	685	187	194	4			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	VAL	engineered mutation	UNP P69905
C	1	MET	VAL	engineered mutation	UNP P69905

- Molecule 2 is a protein called hemoglobin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	146	Total	C	N	O	S	12	0	0
			1127	726	194	203	4			
2	D	146	Total	C	N	O	S	18	0	0
			1124	724	193	203	4			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	1	MET	VAL	engineered mutation	UNP P68871
B	28	TYR	LEU	engineered mutation	UNP P68871
B	63	GLN	HIS	engineered mutation	UNP P68871
D	1	MET	VAL	engineered mutation	UNP P68871
D	28	TYR	LEU	engineered mutation	UNP P68871
D	63	GLN	HIS	engineered mutation	UNP P68871

- Molecule 3 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: C₃₄H₃₂FeN₄O₄).



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

- Molecule 4 is water.

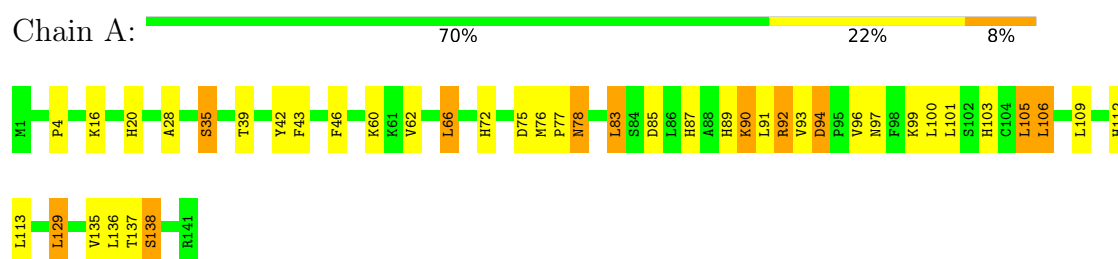
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	74	Total	O	0	0
			74	74		
4	B	57	Total	O	0	0
			57	57		
4	C	55	Total	O	0	0
			55	55		
4	D	60	Total	O	0	0
			60	60		

3 Residue-property plots [i](#)

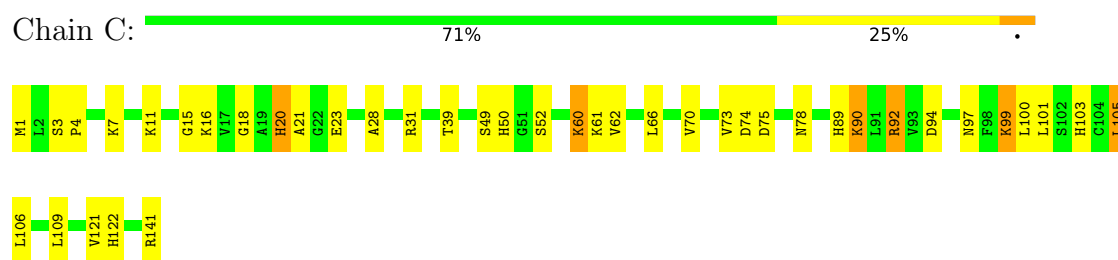
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

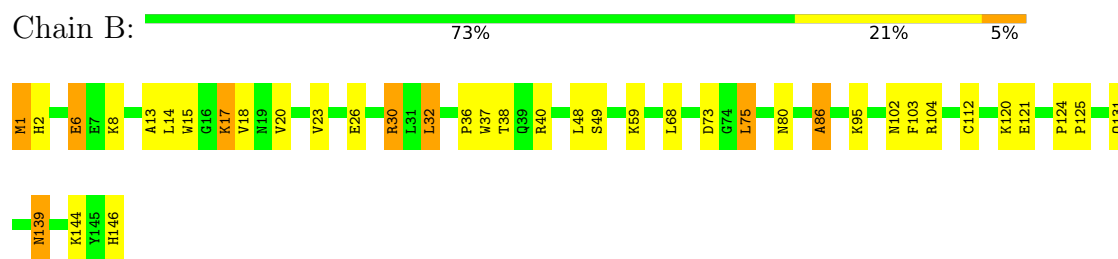
- Molecule 1: hemoglobin



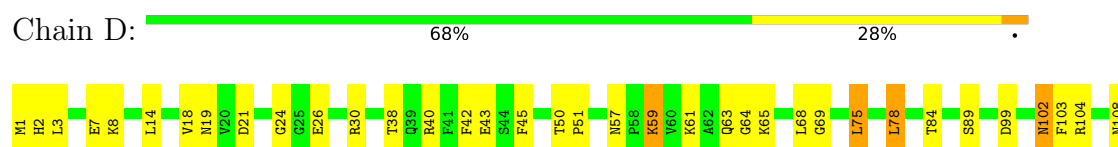
- Molecule 1: hemoglobin

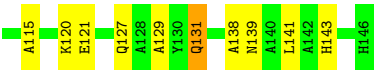


- Molecule 2: hemoglobin



- Molecule 2: hemoglobin





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	63.36 Å 84.32 Å 54.00 Å 90.00° 99.43° 90.00°	Depositor
Resolution (Å)	29.00 – 2.00	Depositor
% Data completeness (in resolution range)	(Not available) (29.00-2.00)	Depositor
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	REFMAC	Depositor
R, R_{free}	0.181 , 0.223	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	4809	wwPDB-VP
Average B, all atoms (Å ²)	27.0	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: HEM

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	1.21	0/1098	1.72	20/1491 (1.3%)
1	C	1.62	1/1098 (0.1%)	1.77	23/1491 (1.5%)
2	B	1.62	3/1157 (0.3%)	1.78	25/1570 (1.6%)
2	D	1.15	0/1154	1.85	24/1567 (1.5%)
All	All	1.42	4/4507 (0.1%)	1.78	92/6119 (1.5%)

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
2	D	0	1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	16	LYS	CG-CD	38.99	2.69	1.52
2	B	6	GLU	CG-CD	38.84	2.49	1.52
2	B	37	TRP	NE1-CE2	9.97	1.48	1.37
2	B	2	HIS	CA-CB	-5.07	1.46	1.53

All (92) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	16	LYS	CB-CG-CD	-17.42	71.23	111.30
2	D	99	ASP	O-C-N	-14.73	109.30	121.38
2	B	6	GLU	CG-CD-OE1	-12.26	90.20	118.40
2	D	102	ASN	CA-CB-CG	11.95	124.55	112.60
2	B	6	GLU	CG-CD-OE2	11.31	144.41	118.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	6	GLU	CB-CG-CD	-9.42	96.58	112.60
1	C	89	HIS	CA-CB-CG	-8.81	104.99	113.80
2	D	102	ASN	OD1-CG-ND2	-8.16	114.44	122.60
2	D	30	ARG	NE-CZ-NH2	8.15	126.54	119.20
1	C	122	HIS	CA-CB-CG	8.02	121.82	113.80
1	C	49	SER	CA-C-O	7.68	130.30	121.47
1	C	50	HIS	CA-CB-CG	-7.60	106.20	113.80
2	B	49	SER	N-CA-C	7.39	119.34	111.28
1	C	20	HIS	CA-CB-CG	-7.30	106.50	113.80
1	A	20	HIS	CA-CB-CG	-7.17	106.63	113.80
1	C	74	ASP	CA-CB-CG	-7.07	105.53	112.60
1	A	43	PHE	O-C-N	-7.04	113.22	121.32
2	D	143	HIS	N-CA-C	6.95	119.70	111.71
2	B	13	ALA	CA-C-O	6.92	127.76	120.42
1	A	46	PHE	CA-CB-CG	6.73	120.53	113.80
1	A	94	ASP	CA-CB-CG	-6.66	105.94	112.60
2	B	146	HIS	CA-CB-CG	-6.55	107.25	113.80
1	A	129	LEU	N-CA-C	6.47	118.33	111.28
2	B	2	HIS	N-CA-CB	6.39	121.08	110.47
1	A	85	ASP	CA-CB-CG	6.22	118.82	112.60
2	B	73	ASP	CA-CB-CG	6.21	118.81	112.60
1	A	78	ASN	CA-CB-CG	-6.16	106.44	112.60
2	B	17	LYS	CA-C-O	6.15	126.50	119.18
2	D	63	GLN	N-CA-C	-6.11	104.54	111.07
2	D	84	THR	CA-C-O	-6.00	114.19	120.55
1	C	70	VAL	CA-C-O	5.97	127.16	120.95
1	A	94	ASP	CA-C-N	5.96	125.64	119.56
1	A	94	ASP	C-N-CA	5.96	125.64	119.56
2	D	103	PHE	CA-CB-CG	5.94	119.74	113.80
2	D	69	GLY	CA-C-O	5.93	126.86	120.75
1	A	113	LEU	CB-CA-C	-5.93	101.50	110.87
2	B	14	LEU	N-CA-C	-5.91	104.75	111.14
1	C	15	GLY	N-CA-C	-5.91	105.64	112.73
2	D	89	SER	CA-CB-OG	-5.89	99.31	111.10
2	D	64	GLY	CA-C-O	5.89	127.11	121.05
1	C	23	GLU	CA-CB-CG	5.80	125.70	114.10
2	D	21	ASP	CA-CB-CG	5.71	118.31	112.60
2	D	99	ASP	CA-C-N	5.71	125.81	119.87
2	D	99	ASP	C-N-CA	5.71	125.81	119.87
2	D	129	ALA	CA-C-O	-5.69	114.84	120.82
1	A	137	THR	CA-C-N	5.67	127.88	120.28
1	A	137	THR	C-N-CA	5.67	127.88	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	70	VAL	O-C-N	-5.66	116.38	121.87
2	D	24	GLY	CA-C-N	5.59	126.14	119.94
2	D	24	GLY	C-N-CA	5.59	126.14	119.94
2	D	115	ALA	O-C-N	-5.54	116.25	122.12
2	B	40	ARG	NE-CZ-NH2	5.49	124.14	119.20
2	B	139	ASN	CA-CB-CG	-5.46	107.14	112.60
1	C	141	ARG	CD-NE-CZ	-5.45	116.78	124.40
2	B	20	VAL	N-CA-C	5.44	116.07	110.36
1	C	92	ARG	CB-CA-C	-5.44	104.17	111.89
2	B	17	LYS	O-C-N	-5.43	114.70	122.41
1	C	18	GLY	CA-C-N	5.42	130.62	121.14
1	C	18	GLY	C-N-CA	5.42	130.62	121.14
2	D	108	ASN	CA-CB-CG	-5.39	107.21	112.60
1	C	121	VAL	CA-C-O	-5.34	115.19	120.85
2	D	131	GLN	OE1-CD-NE2	5.33	127.93	122.60
2	B	112	CYS	CA-C-O	-5.30	115.26	120.82
1	A	113	LEU	CA-C-N	5.29	125.10	119.28
1	A	113	LEU	C-N-CA	5.29	125.10	119.28
1	A	112	HIS	CA-C-N	5.28	130.15	123.34
1	A	112	HIS	C-N-CA	5.28	130.15	123.34
1	A	42	TYR	CA-C-O	5.26	125.84	119.11
2	B	1	MET	CA-CB-CG	5.24	124.58	114.10
1	A	35	SER	CA-C-O	5.23	126.05	120.24
2	B	36	PRO	N-CA-CB	5.21	108.47	103.52
2	B	48	LEU	CA-C-N	5.21	127.27	120.28
2	B	48	LEU	C-N-CA	5.21	127.27	120.28
2	D	40	ARG	CD-NE-CZ	-5.16	117.17	124.40
1	C	121	VAL	O-C-N	5.16	127.14	121.83
1	C	52	SER	O-C-N	-5.16	116.47	122.81
1	A	89	HIS	CA-CB-CG	-5.15	108.65	113.80
1	C	75	ASP	N-CA-CB	-5.12	101.64	111.53
2	D	120	LYS	N-CA-C	5.08	118.58	112.38
2	B	30	ARG	CD-NE-CZ	-5.08	117.29	124.40
2	B	40	ARG	CA-C-O	-5.08	113.34	119.49
2	B	15	TRP	CA-C-O	-5.07	114.37	120.10
1	C	78	ASN	CA-CB-CG	-5.07	107.53	112.60
2	D	102	ASN	CB-CG-ND2	5.06	124.00	116.40
2	D	63	GLN	OE1-CD-NE2	-5.05	117.55	122.60
1	C	62	VAL	O-C-N	5.05	126.86	121.91
1	A	72	HIS	CA-CB-CG	-5.04	108.76	113.80
1	C	92	ARG	CA-CB-CG	-5.02	104.06	114.10
1	C	94	ASP	CA-CB-CG	-5.02	107.58	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	86	ALA	N-CA-C	5.01	116.75	111.28
2	B	14	LEU	CB-CA-C	5.01	118.82	110.90
2	B	103	PHE	N-CA-CB	5.01	117.57	110.16

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	D	141	LEU	Mainchain

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	1070	0	1073	22	0
1	C	1070	0	1073	15	0
2	B	1127	0	1117	10	0
2	D	1124	0	1108	16	0
3	A	43	0	30	0	0
3	B	43	0	30	1	0
3	C	43	0	30	0	0
3	D	43	0	30	0	0
4	A	74	0	0	2	0
4	B	57	0	0	1	0
4	C	55	0	0	1	0
4	D	60	0	0	1	0
All	All	4809	0	4491	60	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 7.

All (60) 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:28:ALA:CB	1:A:105:LEU:HD13	2.02	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:28:ALA:HB1	1:A:105:LEU:HD13	1.72	0.68
1:A:28:ALA:CB	1:A:105:LEU:CD1	2.73	0.67
1:C:7:LYS:HE2	1:C:73:VAL:HG13	1.81	0.62
1:A:28:ALA:HB2	1:A:105:LEU:CD1	2.30	0.61
2:D:75:LEU:O	2:D:78:LEU:HD22	2.01	0.60
3:B:147:HEM:HMC2	3:B:147:HEM:HBC2	1.83	0.59
1:C:103:HIS:HD2	4:C:145:HOH:O	1.86	0.58
2:D:50:THR:HB	2:D:51:PRO:HD2	1.88	0.56
2:D:38:THR:HG22	2:D:102:ASN:HD22	1.71	0.56
1:A:39:THR:HG22	1:A:97:ASN:HD22	1.71	0.56
1:A:103:HIS:HD2	4:A:146:HOH:O	1.89	0.55
2:B:124:PRO:HB2	2:B:125:PRO:HD3	1.88	0.55
1:C:90:LYS:HD2	1:C:90:LYS:C	2.32	0.54
2:B:86:ALA:HB1	2:B:144:LYS:HE3	1.88	0.54
1:C:99:LYS:HE2	1:C:100:LEU:HD21	1.91	0.52
2:B:139:ASN:N	2:B:139:ASN:HD22	2.07	0.52
2:D:38:THR:HG22	2:D:102:ASN:ND2	2.24	0.52
1:A:103:HIS:HE1	2:B:131:GLN:OE1	1.94	0.50
1:A:99:LYS:HG2	1:A:100:LEU:N	2.27	0.49
1:A:93:VAL:O	1:A:94:ASP:C	2.53	0.49
2:D:19:ASN:C	2:D:19:ASN:OD1	2.56	0.49
2:D:75:LEU:HD12	2:D:75:LEU:HA	1.69	0.48
1:C:3:SER:HB2	1:C:4:PRO:CD	2.44	0.48
1:A:87:HIS:O	1:A:92:ARG:N	2.44	0.48
2:D:139:ASN:ND2	4:D:167:HOH:O	2.47	0.47
1:C:39:THR:HG22	1:C:97:ASN:HD22	1.80	0.46
1:C:28:ALA:CB	1:C:105:LEU:HD13	2.45	0.46
2:B:32:LEU:HD12	2:B:38:THR:OG1	2.16	0.46
1:A:62:VAL:O	1:A:66:LEU:HD22	2.16	0.46
1:C:99:LYS:HE2	1:C:100:LEU:CD2	2.45	0.46
1:A:75:ASP:OD1	1:A:78:ASN:OD1	2.33	0.46
2:B:18:VAL:HG13	2:B:23:VAL:HG21	1.98	0.46
1:A:106:LEU:HD13	1:A:129:LEU:HD12	1.97	0.45
1:C:106:LEU:HD12	1:C:106:LEU:HA	1.82	0.45
2:D:104:ARG:NH2	2:D:139:ASN:HD22	2.14	0.45
1:C:31:ARG:HD3	2:D:127:GLN:OE1	2.16	0.45
2:D:57:ASN:O	2:D:61:LYS:HG3	2.16	0.45
2:B:102:ASN:ND2	4:B:163:HOH:O	2.50	0.44
1:C:103:HIS:HE1	2:D:131:GLN:OE1	2.00	0.44
2:D:104:ARG:HE	2:D:138:ALA:HB1	1.82	0.43
1:A:105:LEU:HD12	1:A:105:LEU:HA	1.74	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:28:ALA:HB1	1:C:105:LEU:HD13	2.00	0.43
2:B:30:ARG:HH11	2:B:30:ARG:HD3	1.60	0.42
2:B:75:LEU:HD12	2:B:75:LEU:HA	1.82	0.42
2:D:3:LEU:HB3	2:D:7:GLU:HB2	2.01	0.42
1:A:91:LEU:O	1:A:92:ARG:HB2	2.20	0.42
1:C:20:HIS:O	1:C:21:ALA:C	2.63	0.42
2:D:50:THR:HB	2:D:51:PRO:CD	2.49	0.42
1:A:4:PRO:HD2	4:A:168:HOH:O	2.18	0.42
1:A:76:MET:N	1:A:77:PRO:CD	2.82	0.42
1:A:106:LEU:HA	1:A:106:LEU:HD12	1.82	0.42
1:C:60:LYS:HB2	1:C:60:LYS:HE2	1.61	0.42
2:D:57:ASN:OD1	2:D:59:LYS:N	2.51	0.42
1:A:35:SER:HB3	2:B:131:GLN:HG3	2.02	0.42
1:C:3:SER:HB2	1:C:4:PRO:HD2	2.02	0.42
2:D:42:PHE:O	2:D:45:PHE:HB2	2.20	0.42
1:A:90:LYS:O	1:A:92:ARG:HD2	2.21	0.40
1:A:135:VAL:O	1:A:138:SER:HB2	2.21	0.40
1:A:83:LEU:HD12	1:A:83:LEU:HA	1.79	0.40

There are no symmetry-related clashes.

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%)	133 (96%)	6 (4%)	0	100	100
1	C	139/141 (99%)	133 (96%)	6 (4%)	0	100	100
2	B	144/146 (99%)	143 (99%)	1 (1%)	0	100	100
2	D	144/146 (99%)	141 (98%)	2 (1%)	1 (1%)	18	14
All	All	566/574 (99%)	550 (97%)	15 (3%)	1 (0%)	43	42

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	2	HIS

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%)	100 (88%)	13 (12%)	5	3
1	C	113/113 (100%)	102 (90%)	11 (10%)	8	5
2	B	118/118 (100%)	104 (88%)	14 (12%)	5	3
2	D	117/118 (99%)	105 (90%)	12 (10%)	7	4
All	All	461/462 (100%)	411 (89%)	50 (11%)	6	3

All (50) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	16	LYS
1	A	60	LYS
1	A	66	LEU
1	A	83	LEU
1	A	90	LYS
1	A	92	ARG
1	A	96	VAL
1	A	101	LEU
1	A	105	LEU
1	A	106	LEU
1	A	109	LEU
1	A	136	LEU
1	A	138	SER
2	B	1	MET
2	B	6	GLU
2	B	8	LYS
2	B	17	LYS
2	B	26	GLU
2	B	32	LEU
2	B	59	LYS
2	B	68	LEU

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Mol	Chain	Res	Type
2	B	75	LEU
2	B	80	ASN
2	B	95	LYS
2	B	104	ARG
2	B	120	LYS
2	B	121	GLU
1	C	1	MET
1	C	11	LYS
1	C	60	LYS
1	C	61	LYS
1	C	66	LEU
1	C	90	LYS
1	C	92	ARG
1	C	99	LYS
1	C	101	LEU
1	C	105	LEU
1	C	109	LEU
2	D	1	MET
2	D	8	LYS
2	D	14	LEU
2	D	18	VAL
2	D	26	GLU
2	D	43	GLU
2	D	59	LYS
2	D	65	LYS
2	D	68	LEU
2	D	75	LEU
2	D	78	LEU
2	D	121	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	58	HIS
1	A	72	HIS
1	A	78	ASN
1	A	97	ASN
1	A	103	HIS
2	B	77	HIS
2	B	80	ASN
2	B	102	ASN
2	B	117	HIS

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Mol	Chain	Res	Type
2	B	127	GLN
2	B	131	GLN
2	B	139	ASN
1	C	72	HIS
1	C	78	ASN
1	C	97	ASN
1	C	103	HIS
2	D	80	ASN
2	D	102	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 ⓘ

4 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	142	1	50,50,50	1.58	11 (22%)	67,82,82	1.05	5 (7%)
3	HEM	B	147	2	50,50,50	1.86	15 (30%)	67,82,82	1.12	3 (4%)
3	HEM	C	142	1	50,50,50	1.67	10 (20%)	67,82,82	1.20	6 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	HEM	D	147	2	50,50,50	1.56	8 (16%)	67,82,82	1.26	9 (13%)

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	142	1	-	4/14/54/54	-
3	HEM	B	147	2	-	9/14/54/54	-
3	HEM	C	142	1	-	2/14/54/54	-
3	HEM	D	147	2	-	2/14/54/54	-

All (44) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	147	HEM	FE-NC	4.72	2.10	1.95
3	C	142	HEM	CMA-C3A	4.14	1.59	1.50
3	A	142	HEM	FE-NA	3.91	2.08	1.95
3	D	147	HEM	FE-NB	3.87	2.06	1.94
3	D	147	HEM	CMA-C3A	3.77	1.58	1.50
3	C	142	HEM	FE-NC	3.72	2.07	1.95
3	B	147	HEM	CAC-C3C	3.69	1.57	1.47
3	B	147	HEM	CAB-C3B	3.50	1.56	1.47
3	A	142	HEM	CMA-C3A	3.43	1.57	1.50
3	A	142	HEM	FE-NC	3.40	2.06	1.95
3	C	142	HEM	FE-NA	3.37	2.06	1.95
3	B	147	HEM	C1C-C2C	3.29	1.51	1.45
3	A	142	HEM	CAC-C3C	3.28	1.56	1.47
3	B	147	HEM	FE-ND	3.19	2.04	1.94
3	D	147	HEM	CMB-C2B	3.08	1.57	1.50
3	B	147	HEM	FE-NA	3.05	2.05	1.95
3	C	142	HEM	CAC-C3C	3.04	1.55	1.47
3	C	142	HEM	FE-ND	3.03	2.04	1.94
3	D	147	HEM	CMC-C2C	2.98	1.56	1.50
3	B	147	HEM	CMA-C3A	2.98	1.56	1.50
3	D	147	HEM	CAB-C3B	2.97	1.55	1.47
3	D	147	HEM	CMD-C2D	2.95	1.56	1.50
3	A	142	HEM	CMB-C2B	2.94	1.56	1.50
3	C	142	HEM	FE-NB	2.89	2.03	1.94
3	D	147	HEM	FE-NA	2.89	2.04	1.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	147	HEM	CMB-C2B	2.79	1.56	1.50
3	A	142	HEM	CMD-C2D	2.72	1.56	1.50
3	C	142	HEM	CAB-C3B	2.63	1.54	1.47
3	B	147	HEM	CMC-C2C	2.60	1.56	1.50
3	B	147	HEM	C3C-C4C	2.56	1.50	1.46
3	C	142	HEM	CMD-C2D	2.52	1.55	1.50
3	C	142	HEM	CMB-C2B	2.47	1.55	1.50
3	B	147	HEM	FE-NB	2.44	2.02	1.94
3	B	147	HEM	CMD-C2D	2.42	1.55	1.50
3	C	142	HEM	CMC-C2C	2.36	1.55	1.50
3	D	147	HEM	CAC-C3C	2.34	1.53	1.47
3	A	142	HEM	CAA-C2A	2.29	1.57	1.51
3	B	147	HEM	C3C-C2C	-2.21	1.32	1.37
3	A	142	HEM	CAB-C3B	2.17	1.53	1.47
3	A	142	HEM	C2A-C3A	-2.16	1.33	1.38
3	A	142	HEM	FE-NB	2.16	2.01	1.94
3	B	147	HEM	C4A-C3A	2.04	1.47	1.43
3	A	142	HEM	CMC-C2C	2.04	1.54	1.50
3	B	147	HEM	O1D-CGD	2.01	1.28	1.22

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	147	HEM	O1D-CGD-CBD	-3.13	113.16	123.09
3	D	147	HEM	C4A-CHB-C1B	-3.12	118.90	126.25
3	A	142	HEM	CAD-CBD-CGD	2.84	121.20	113.67
3	C	142	HEM	O1A-CGA-CBA	-2.61	114.81	123.09
3	C	142	HEM	CHA-C4D-ND	2.55	127.53	124.37
3	D	147	HEM	O1A-CGA-CBA	-2.51	115.12	123.09
3	B	147	HEM	CBD-CAD-C3D	-2.46	105.72	112.53
3	C	142	HEM	CHA-C1A-NA	2.46	128.32	123.86
3	D	147	HEM	CHB-C4A-NA	2.43	128.26	123.86
3	C	142	HEM	C1A-CHA-C4D	-2.36	120.70	126.25
3	D	147	HEM	CMA-C3A-C2A	2.36	130.63	125.62
3	C	142	HEM	CHC-C4B-NB	2.32	126.92	124.42
3	A	142	HEM	CHD-C4C-NC	2.31	126.97	124.45
3	A	142	HEM	O1A-CGA-CBA	-2.26	115.92	123.09
3	D	147	HEM	C2A-C1A-NA	-2.18	107.73	110.15
3	D	147	HEM	C3D-C4D-ND	-2.13	107.84	110.17
3	A	142	HEM	C4C-CHD-C1D	-2.11	121.53	126.02
3	D	147	HEM	CAA-C2A-C1A	-2.10	120.83	124.94
3	C	142	HEM	C3B-C4B-NB	-2.09	107.97	109.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	147	HEM	C4C-CHD-C1D	-2.08	121.61	126.02
3	B	147	HEM	CBB-CAB-C3B	-2.07	117.18	127.53
3	D	147	HEM	CBA-CAA-C2A	-2.07	106.81	112.53
3	A	142	HEM	C4A-CHB-C1B	-2.01	121.53	126.25

There are no chirality outliers.

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	147	HEM	C1A-C2A-CAA-CBA
3	B	147	HEM	C2A-CAA-CBA-CGA
3	A	142	HEM	CAD-CBD-CGD-O1D
3	B	147	HEM	CAD-CBD-CGD-O2D
3	C	142	HEM	CAD-CBD-CGD-O1D
3	B	147	HEM	CAD-CBD-CGD-O1D
3	C	142	HEM	CAD-CBD-CGD-O2D
3	B	147	HEM	CAA-CBA-CGA-O1A
3	D	147	HEM	CAA-CBA-CGA-O1A
3	A	142	HEM	CAA-CBA-CGA-O1A
3	A	142	HEM	CAD-CBD-CGD-O2D
3	A	142	HEM	CAA-CBA-CGA-O2A
3	B	147	HEM	CAA-CBA-CGA-O2A
3	D	147	HEM	CAA-CBA-CGA-O2A
3	B	147	HEM	C4B-C3B-CAB-CBB
3	B	147	HEM	C3A-C2A-CAA-CBA
3	B	147	HEM	C2B-C3B-CAB-CBB

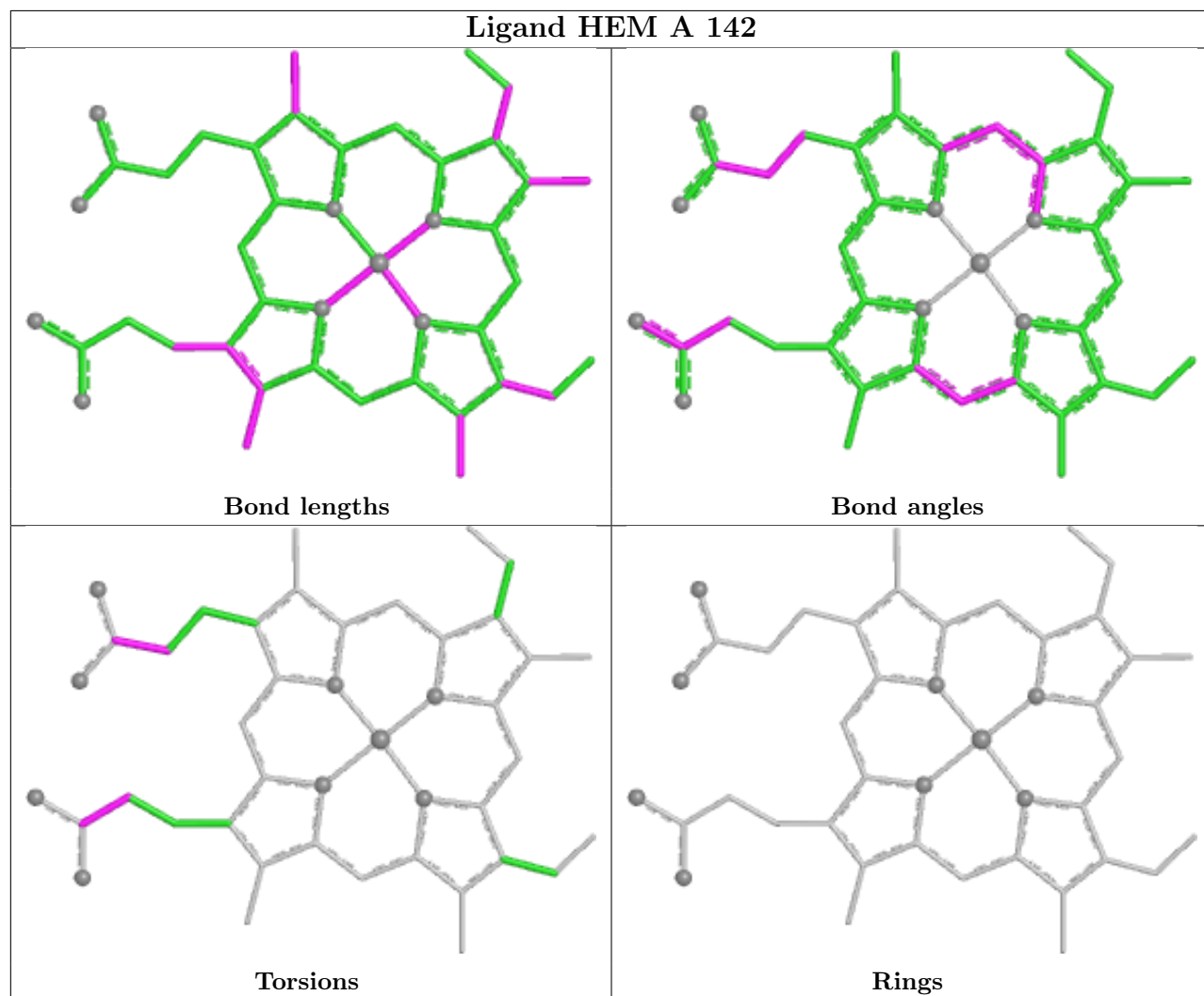
There are no ring outliers.

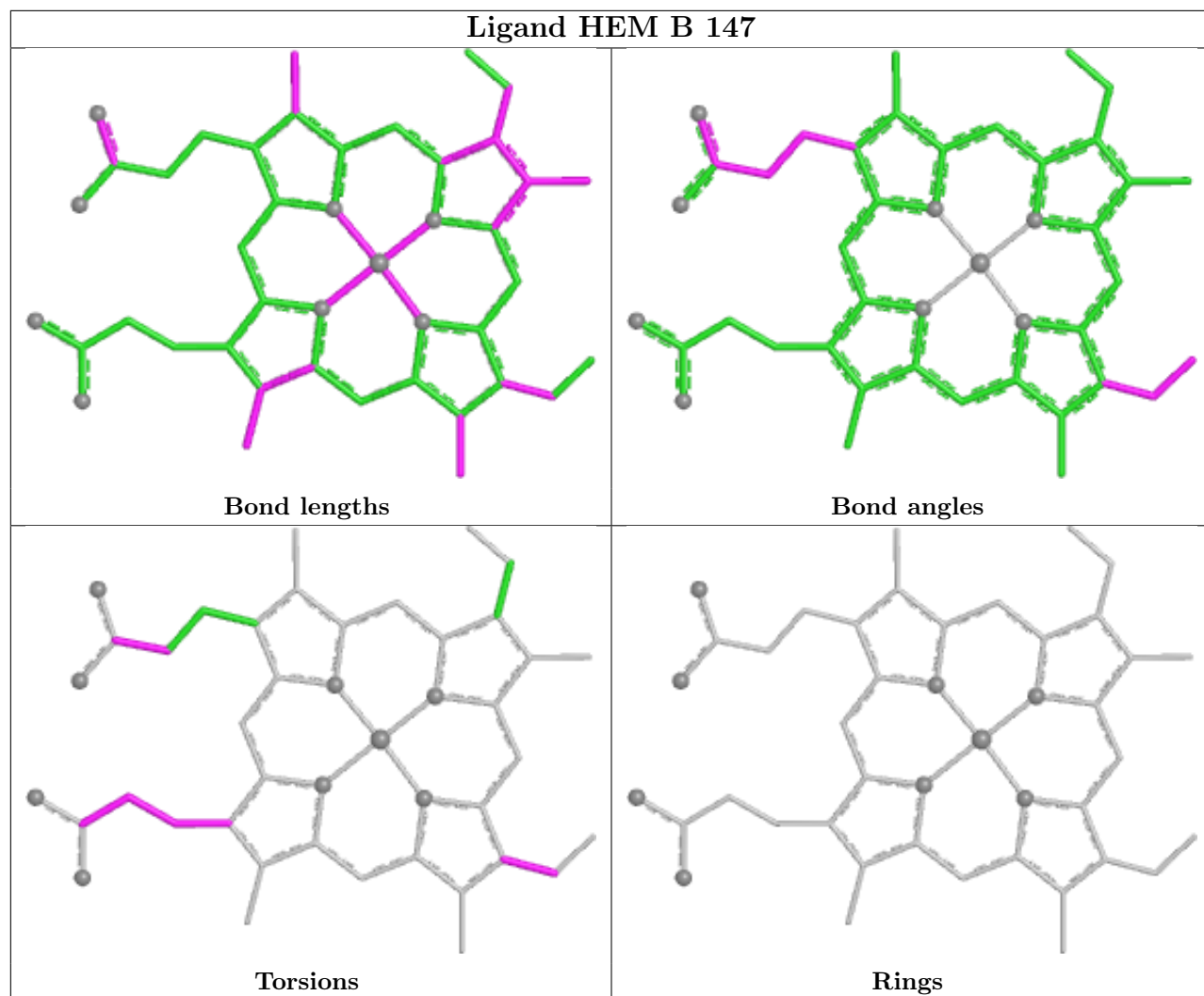
1 monomer is involved in 1 short contact:

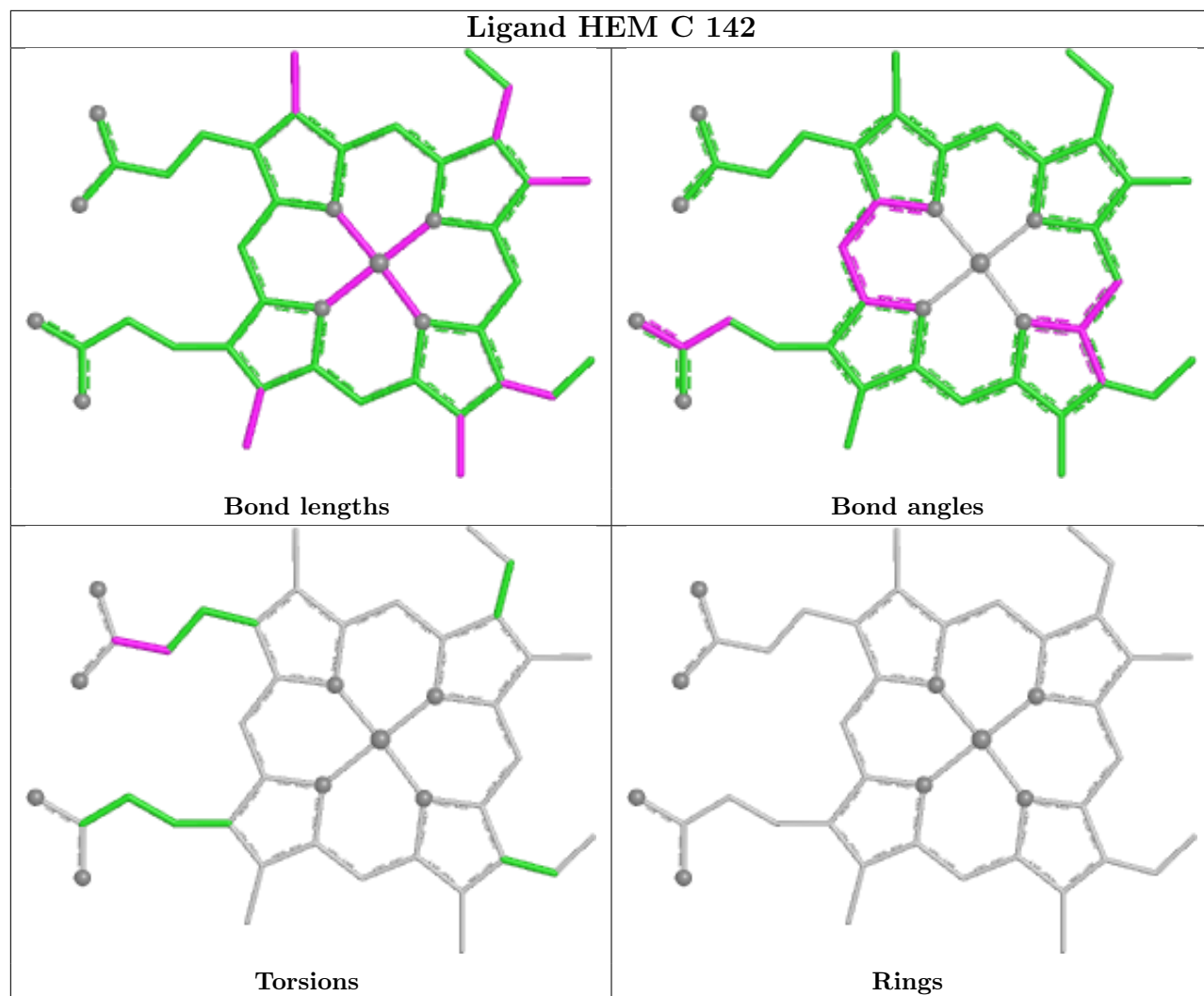
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	147	HEM	1	0

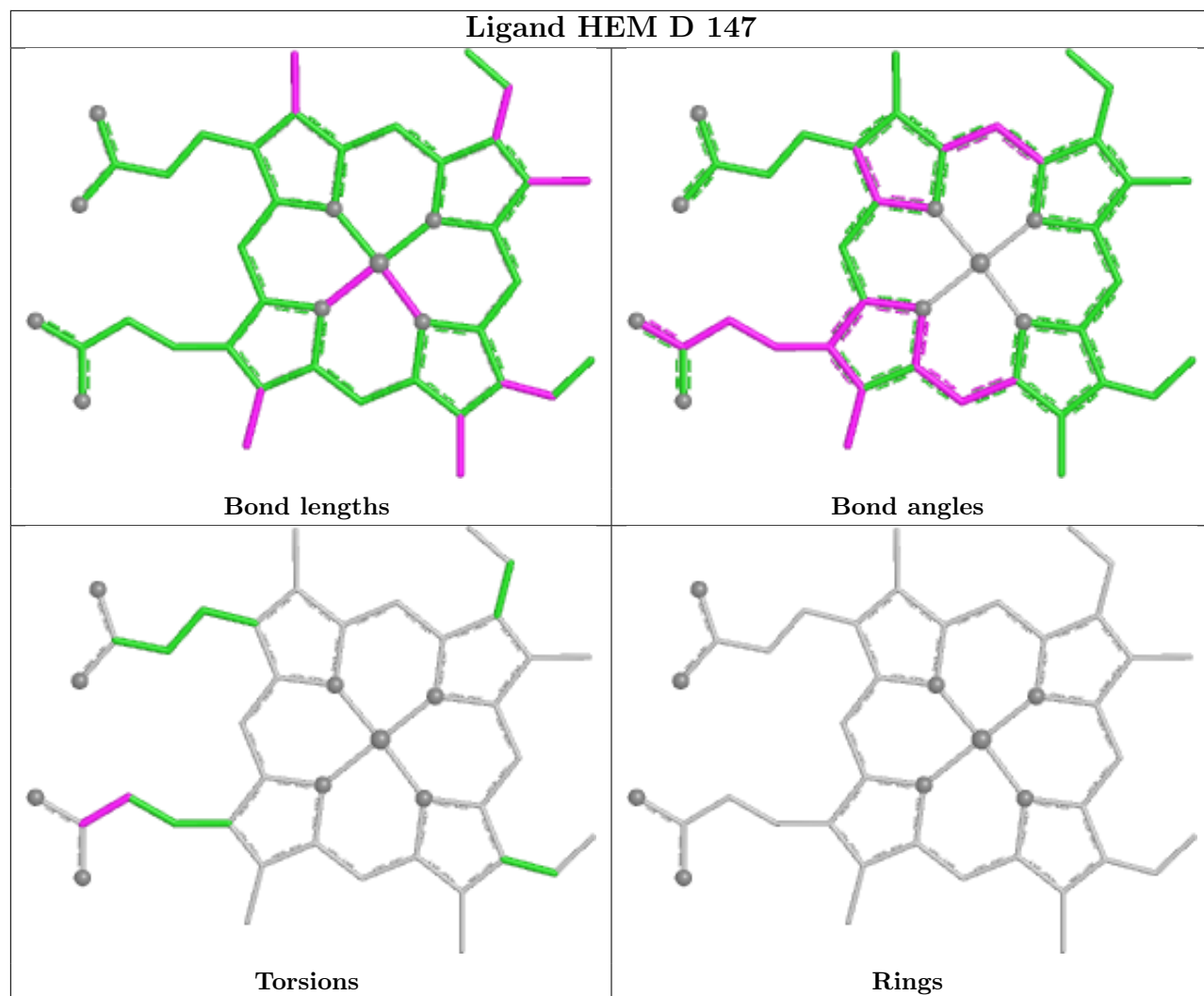
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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









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.