



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 9, 2026 – 06:36 PM UTC

PDB ID : 1CMY / pdb_00001cmY
Title : THE MUTATION BETA99 ASP-TYR STABILIZES Y-A NEW, COMPOSITE QUATERNARY STATE OF HUMAN HEMOGLOBIN
Authors : Smith, F.R.; Lattman, E.E.; Carter Junior, C.W.
Deposited on : 1992-09-18
Resolution : 3.00 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 ⓘ 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

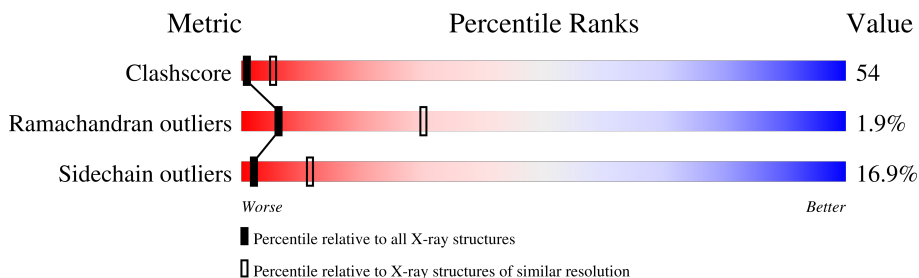
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)

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	
1	C	141	
2	B	146	
2	D	146	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4564 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 YPSILANTI (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			

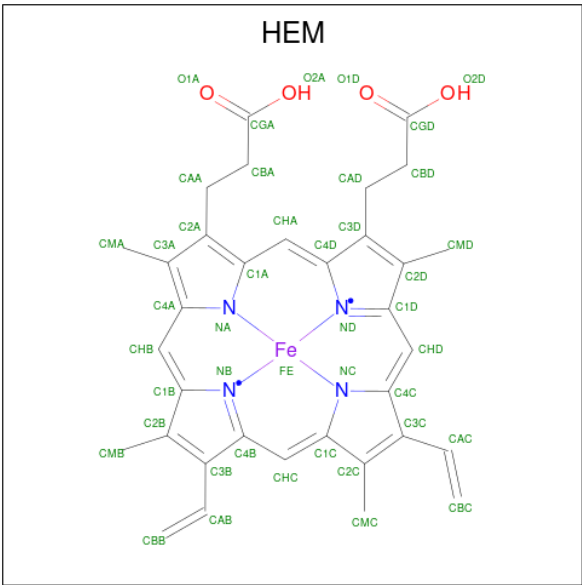
- Molecule 2 is a protein called HEMOGLOBIN YPSILANTI (CARBONMONOXY) (BETA CHAIN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	146	Total	C	N	O	S	0	0	0
			1127	729	195	200	3			
2	D	146	Total	C	N	O	S	0	0	0
			1127	729	195	200	3			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	99	TYR	ASP	conflict	UNP P68871
D	99	TYR	ASP	conflict	UNP P68871

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



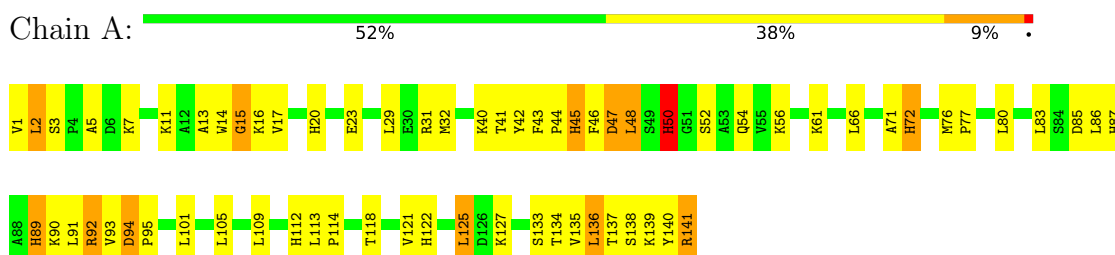
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	B	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	C	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	D	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

3 Residue-property plots

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.

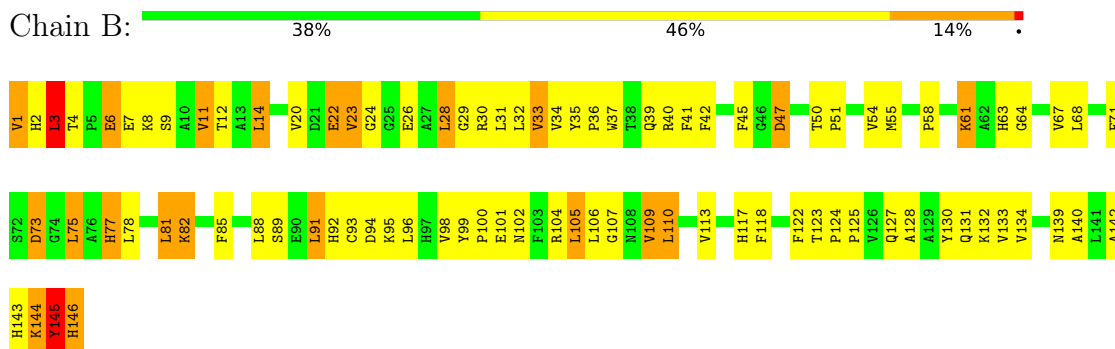
• Molecule 1: HEMOGLOBIN YPSILANTI (CARBONMONOXY) (ALPHA CHAIN)



• Molecule 1: HEMOGLOBIN YPSILANTI (CARBONMONOXY) (ALPHA CHAIN)



• Molecule 2: HEMOGLOBIN YPSILANTI (CARBONMONOXY) (BETA CHAIN)



• Molecule 2: HEMOGLOBIN YPSILANTI (CARBONMONOXY) (BETA CHAIN)



V1	H2	L3	T4	E7	K8	S9	A10	V11	L14	W15	V18	N19	V20	D21	E22	V23	G24	G25	E26	A27	L28	G29	R30	L31	L32	V33	V34	Y35	P36	W37	T38	Q39	R40	S44	S49	T50	V54	M55	G56	N57	P58	K59	A62	H63	G64	V67	L68	F71	S72	D73		
G74	L75	A76	H77	L78	D79	W80	L81	K82	G83	T84	F85	L88	S89	E90	L91	H92	C93	D94	K95	L96	Y99	P100	E101	N102	F103	R104	L105	L106	G107	N108	V109	L110	V111	G112	V113	H116	F122	T123	P124	P125	V126	Q127	Q131	K132	V133	V134	N139	A142	H143	K144	Y145	H146

4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	93.10Å 93.10Å 144.60Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	(Not available) – 3.00	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-3.00)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROLSQ	Depositor
R, R_{free}	0.269 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	4564	wwPDB-VP
Average B, all atoms (Å ²)	15.0	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

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	0.83	0/1097	1.67	10/1491 (0.7%)
1	C	0.84	0/1097	1.65	16/1491 (1.1%)
2	B	0.83	0/1158	1.62	10/1573 (0.6%)
2	D	0.84	0/1158	1.68	10/1573 (0.6%)
All	All	0.84	0/4510	1.66	46/6128 (0.8%)

There are no bond length outliers.

The worst 5 of 46 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	77	HIS	CA-CB-CG	13.66	127.46	113.80
1	A	50	HIS	CA-CB-CG	-9.64	104.16	113.80
1	C	6	ASP	CA-CB-CG	8.81	121.42	112.60
1	A	45	HIS	CA-CB-CG	-7.83	105.97	113.80
2	B	101	GLU	CB-CG-CD	7.60	125.52	112.60

There are no chirality outliers.

There are no planarity outliers.

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	74	11
1	C	1069	0	1073	92	11

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	1127	0	1123	89	3
2	D	1127	0	1123	79	21
3	A	43	0	30	7	1
3	B	43	0	30	5	0
3	C	43	0	30	4	0
3	D	43	0	30	4	0
All	All	4564	0	4512	306	24

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 54.

The worst 5 of 306 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:145:TYR:CE1	2:D:146:HIS:CE1	1.87	1.60
2:D:145:TYR:CD1	2:D:146:HIS:ND1	2.01	1.28
2:B:145:TYR:CE1	2:B:146:HIS:CE1	2.33	1.16
1:C:1:VAL:CG1	1:C:2:LEU:H	1.57	1.14
2:D:145:TYR:HE1	2:D:146:HIS:CE1	1.46	1.09

The worst 5 of 24 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:16:LYS:CA	2:D:90:GLU:OE2[4_567]	0.76	1.44
1:C:90:LYS:CE	2:D:44:SER:CA[2_664]	1.03	1.17
1:C:90:LYS:CE	2:D:44:SER:C[2_664]	1.19	1.01
1:C:90:LYS:NZ	2:D:44:SER:CB[2_664]	1.25	0.95
1:A:15:GLY:O	2:D:90:GLU:OE1[4_567]	1.29	0.91

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%)	131 (94%)	5 (4%)	3 (2%)	5	26
1	C	139/141 (99%)	131 (94%)	5 (4%)	3 (2%)	5	26
2	B	144/146 (99%)	133 (92%)	8 (6%)	3 (2%)	5	27
2	D	144/146 (99%)	133 (92%)	9 (6%)	2 (1%)	9	36
All	All	566/574 (99%)	528 (93%)	27 (5%)	11 (2%)	6	30

5 of 11 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	72	HIS
2	B	3	LEU
2	B	77	HIS
1	C	72	HIS
2	D	3	LEU

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%)	102 (90%)	11 (10%)	8	30
1	C	113/113 (100%)	96 (85%)	17 (15%)	3	14
2	B	118/118 (100%)	92 (78%)	26 (22%)	1	5
2	D	118/118 (100%)	94 (80%)	24 (20%)	1	7
All	All	462/462 (100%)	384 (83%)	78 (17%)	2	11

5 of 78 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	D	14	LEU
2	D	109	VAL
2	D	23	VAL
2	D	81	LEU
2	D	144	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 22 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	97	ASN
2	D	77	HIS
2	D	39	GLN
2	D	97	HIS
2	B	97	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	1.24	4 (8%)	67,82,82	0.89	1 (1%)
3	HEM	C	142	1	50,50,50	1.22	4 (8%)	67,82,82	0.91	2 (2%)
3	HEM	D	147	2	50,50,50	1.19	3 (6%)	67,82,82	0.90	1 (1%)
3	HEM	B	147	2	50,50,50	1.21	5 (10%)	67,82,82	1.02	5 (7%)

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	-	8/14/54/54	-
3	HEM	C	142	1	-	8/14/54/54	-
3	HEM	D	147	2	-	6/14/54/54	-
3	HEM	B	147	2	-	7/14/54/54	-

The worst 5 of 16 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	142	HEM	CAC-C3C	2.83	1.54	1.47
3	B	147	HEM	CAB-C3B	2.80	1.54	1.47
3	A	142	HEM	CAB-C3B	2.78	1.54	1.47
3	D	147	HEM	CAC-C3C	2.74	1.54	1.47
3	D	147	HEM	CAB-C3B	2.70	1.54	1.47

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	147	HEM	CBA-CAA-C2A	3.46	122.09	112.53
3	B	147	HEM	CAA-CBA-CGA	3.05	121.75	113.67
3	B	147	HEM	CBD-CAD-C3D	2.26	118.79	112.53
3	B	147	HEM	O2A-CGA-CBA	2.13	120.73	114.00
3	C	142	HEM	CMA-C3A-C2A	2.12	130.12	125.62

There are no chirality outliers.

5 of 29 torsion outliers are listed below:

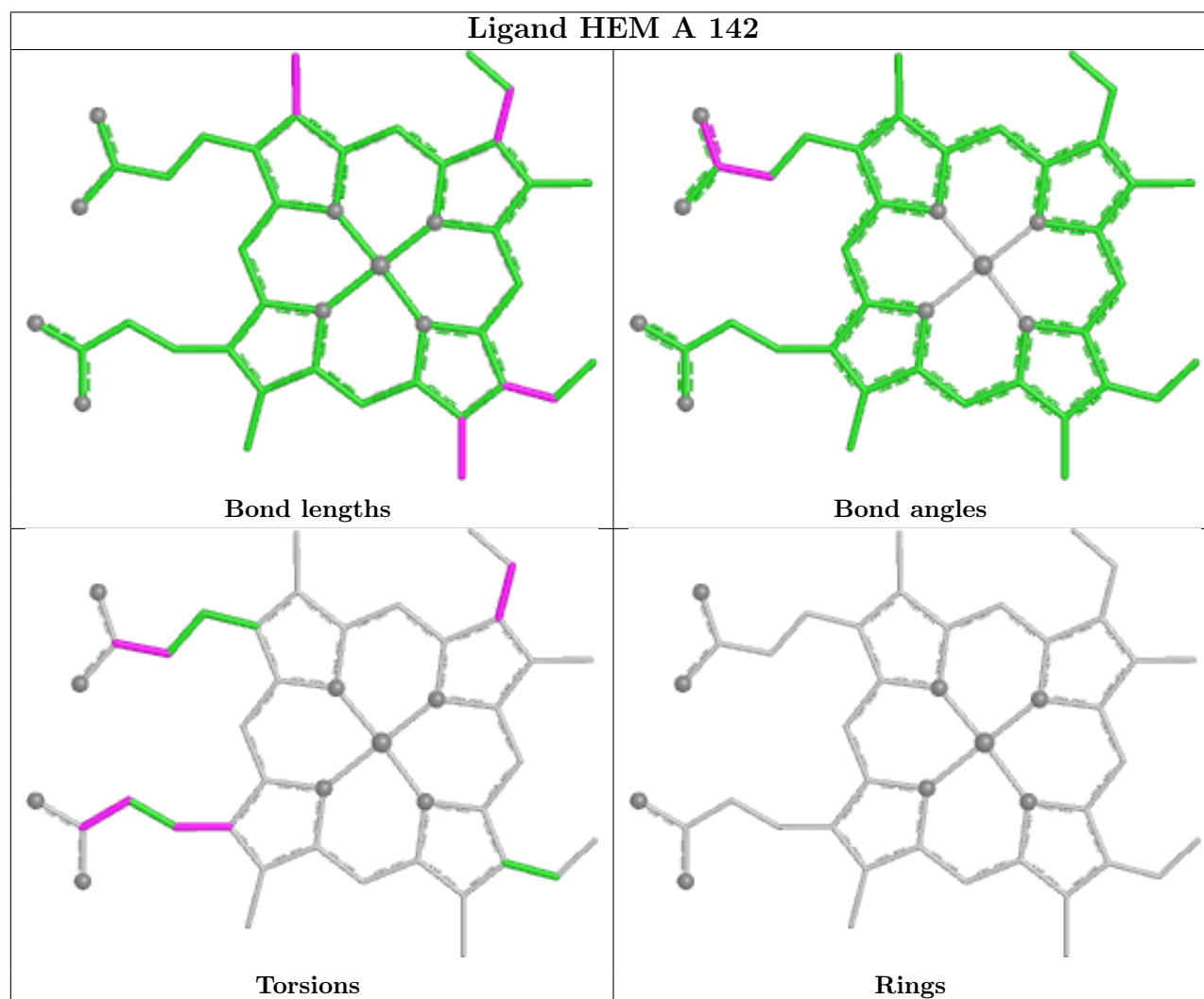
Mol	Chain	Res	Type	Atoms
3	B	147	HEM	C2C-C3C-CAC-CBC
3	C	142	HEM	C2B-C3B-CAB-CBB
3	C	142	HEM	C2C-C3C-CAC-CBC
3	C	142	HEM	C4C-C3C-CAC-CBC
3	D	147	HEM	C1A-C2A-CAA-CBA

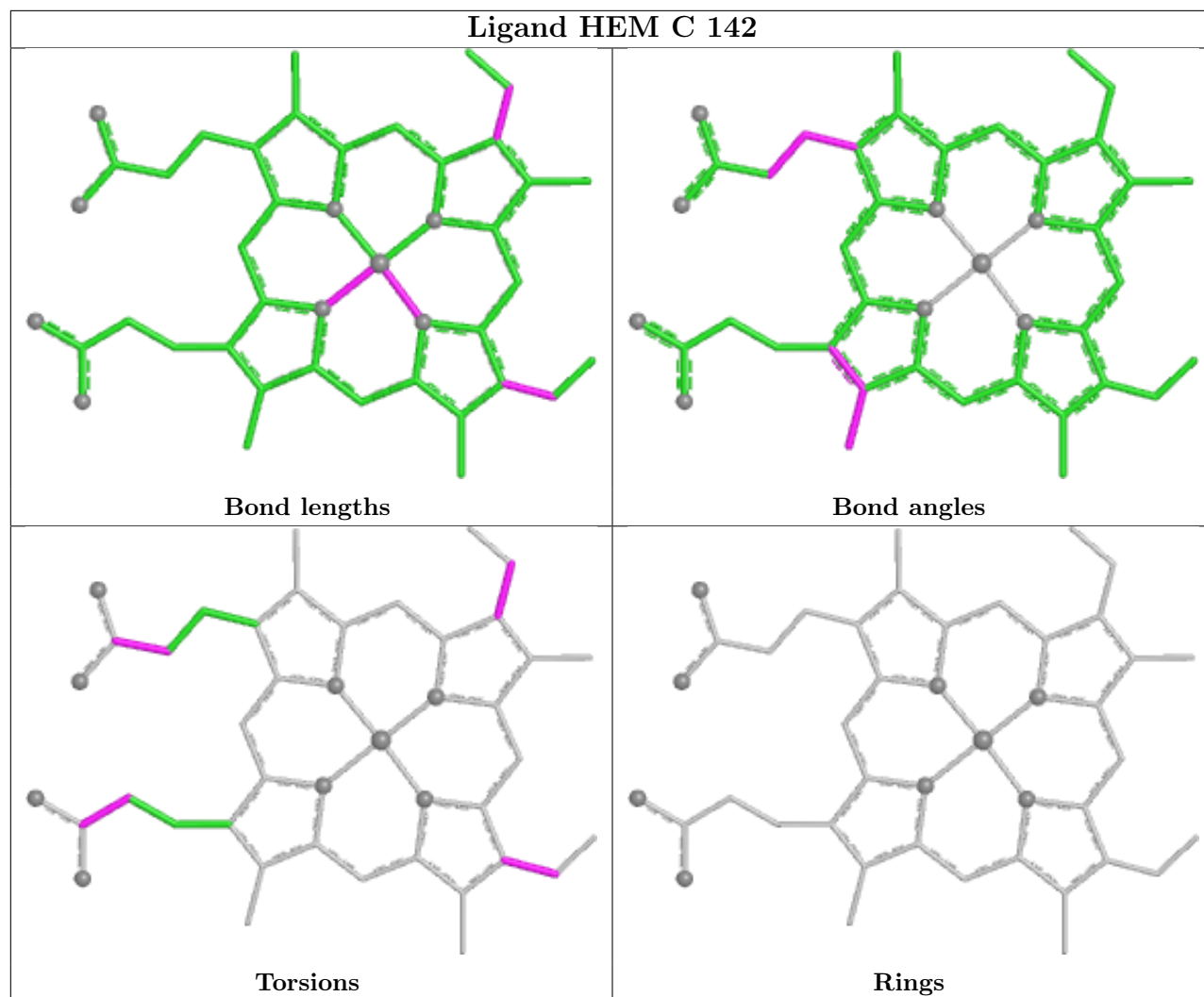
There are no ring outliers.

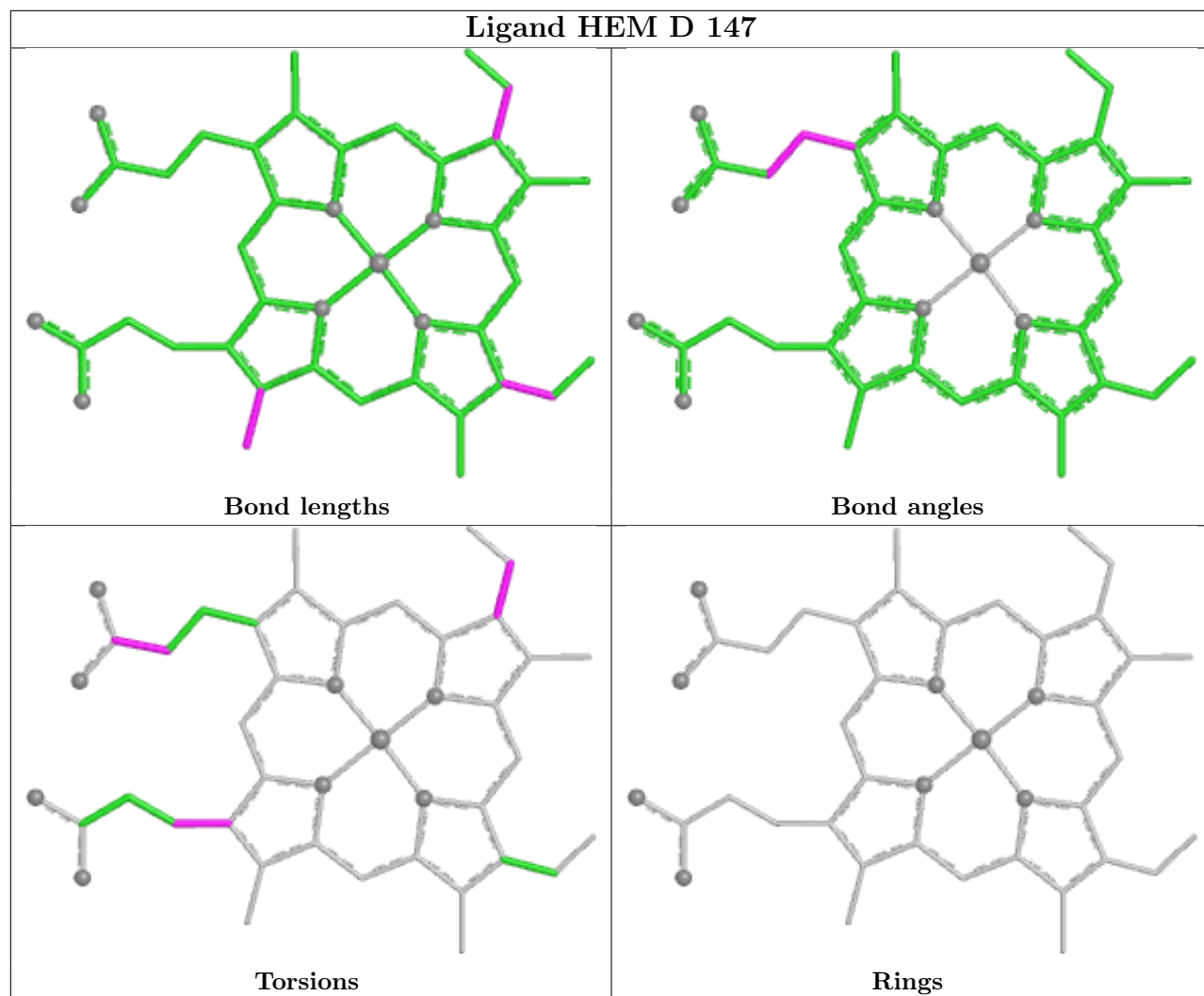
4 monomers are involved in 21 short contacts:

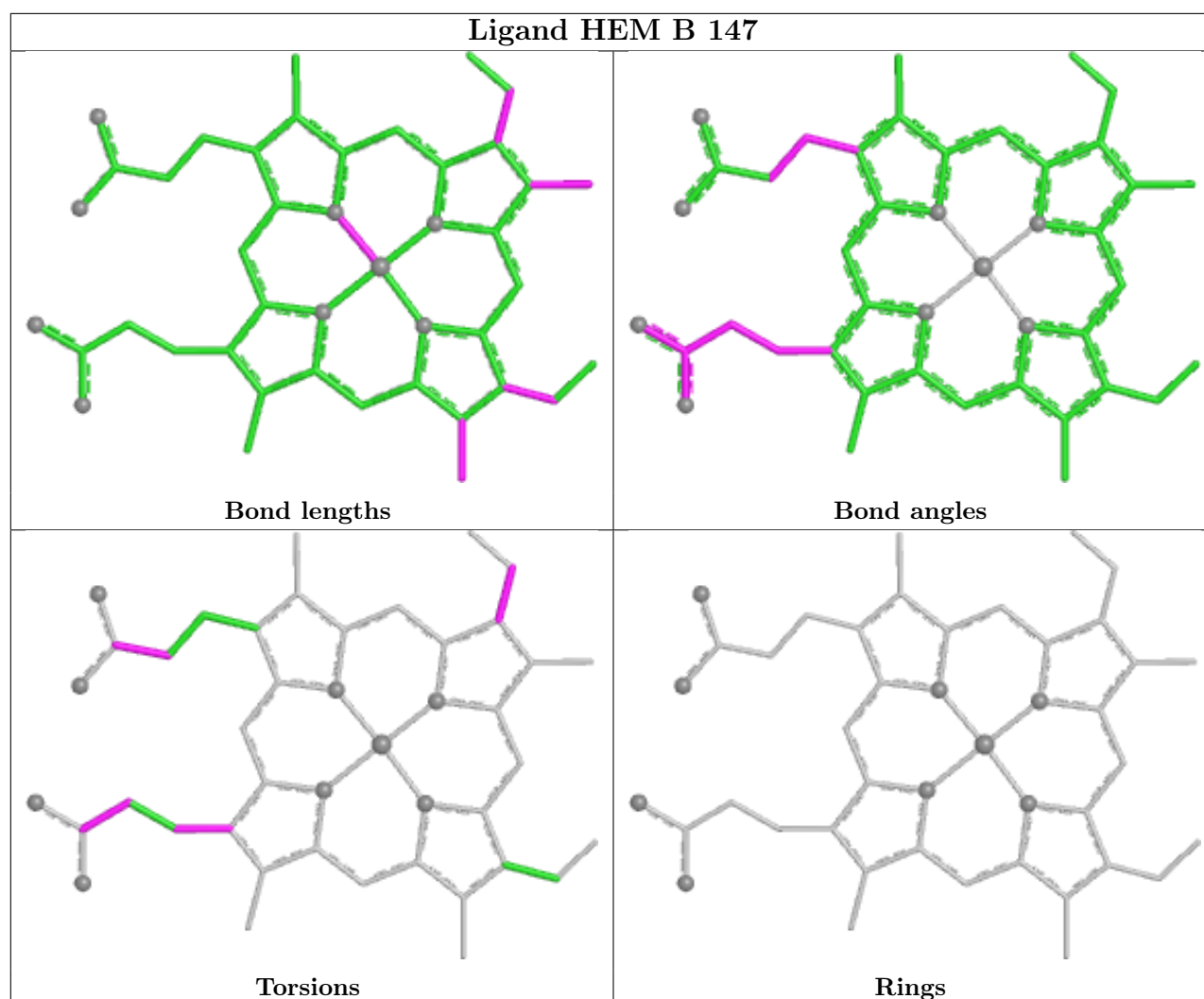
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	142	HEM	7	1
3	C	142	HEM	4	0
3	D	147	HEM	4	0
3	B	147	HEM	5	0

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.









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.