



wwPDB EM Model Validation Summary Report ⓘ

May 15, 2020 – 11:28 AM EDT

PDB ID : 6Y9B
EMDB ID : EMD-10735
Title : Cryo-EM structure of trimeric human STEAP1 bound to three Fab120.545 fragments
Authors : Oosterheert, W.; Gros, P.
Deposited on : 2020-03-06
Resolution : 2.97 Å (reported)
Based on initial model : 6HCY

This is a wwPDB EM Model Validation Summary Report for a publicly released PDB/EMDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
buster-report : 1.1.7 (2018)
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.10.1

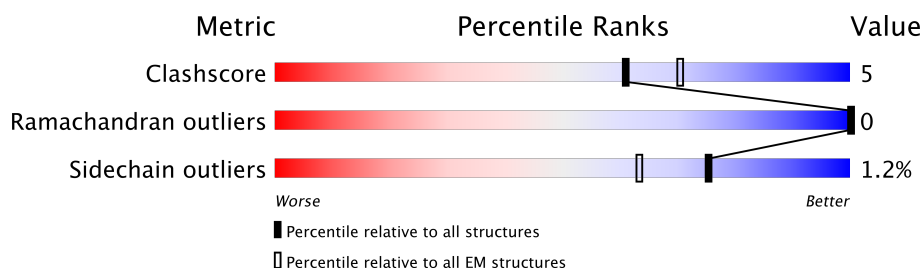
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.97 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)	EM structures (#Entries)
Clashscore	136327	1886
Ramachandran outliers	132723	1663
Sidechain outliers	132532	1531

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments on the 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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	380	58% 6% 36%
1	B	380	57% 7% 36%
1	C	380	57% 7% 36%
2	L	220	44% 8% 49%
2	M	220	44% 8% 49%
2	N	220	42% 9% 49%
3	H	238	42% 8% 49%
3	I	238	42% 8% 49%
3	J	238	42% 8% 49%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 11889 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 Metalloreductase STEAP1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	C	244	Total 2019	C 1373	N 322	O 318	S 6	0	0
1	A	244	Total 2019	C 1373	N 322	O 318	S 6	0	0
1	B	244	Total 2019	C 1373	N 322	O 318	S 6	0	0

There are 126 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-1	MET	-	initiating methionine	UNP Q9UHE8
C	0	GLY	-	expression tag	UNP Q9UHE8
C	1	SER	-	expression tag	UNP Q9UHE8
C	340	ALA	-	expression tag	UNP Q9UHE8
C	341	ALA	-	expression tag	UNP Q9UHE8
C	342	ALA	-	expression tag	UNP Q9UHE8
C	343	GLY	-	expression tag	UNP Q9UHE8
C	344	ALA	-	expression tag	UNP Q9UHE8
C	345	ALA	-	expression tag	UNP Q9UHE8
C	346	TRP	-	expression tag	UNP Q9UHE8
C	347	SER	-	expression tag	UNP Q9UHE8
C	348	HIS	-	expression tag	UNP Q9UHE8
C	349	PRO	-	expression tag	UNP Q9UHE8
C	350	GLN	-	expression tag	UNP Q9UHE8
C	351	PHE	-	expression tag	UNP Q9UHE8
C	352	GLU	-	expression tag	UNP Q9UHE8
C	353	LYS	-	expression tag	UNP Q9UHE8
C	354	GLY	-	expression tag	UNP Q9UHE8
C	355	ALA	-	expression tag	UNP Q9UHE8
C	356	ALA	-	expression tag	UNP Q9UHE8
C	357	TRP	-	expression tag	UNP Q9UHE8
C	358	SER	-	expression tag	UNP Q9UHE8
C	359	HIS	-	expression tag	UNP Q9UHE8
C	360	PRO	-	expression tag	UNP Q9UHE8

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Chain	Residue	Modelled	Actual	Comment	Reference
C	361	GLN	-	expression tag	UNP Q9UHE8
C	362	PHE	-	expression tag	UNP Q9UHE8
C	363	GLU	-	expression tag	UNP Q9UHE8
C	364	LYS	-	expression tag	UNP Q9UHE8
C	365	GLY	-	expression tag	UNP Q9UHE8
C	366	ALA	-	expression tag	UNP Q9UHE8
C	367	ALA	-	expression tag	UNP Q9UHE8
C	368	TRP	-	expression tag	UNP Q9UHE8
C	369	SER	-	expression tag	UNP Q9UHE8
C	370	HIS	-	expression tag	UNP Q9UHE8
C	371	PRO	-	expression tag	UNP Q9UHE8
C	372	GLN	-	expression tag	UNP Q9UHE8
C	373	PHE	-	expression tag	UNP Q9UHE8
C	374	GLU	-	expression tag	UNP Q9UHE8
C	375	LYS	-	expression tag	UNP Q9UHE8
C	376	GLY	-	expression tag	UNP Q9UHE8
C	377	ALA	-	expression tag	UNP Q9UHE8
C	378	ALA	-	expression tag	UNP Q9UHE8
A	-1	MET	-	initiating methionine	UNP Q9UHE8
A	0	GLY	-	expression tag	UNP Q9UHE8
A	1	SER	-	expression tag	UNP Q9UHE8
A	340	ALA	-	expression tag	UNP Q9UHE8
A	341	ALA	-	expression tag	UNP Q9UHE8
A	342	ALA	-	expression tag	UNP Q9UHE8
A	343	GLY	-	expression tag	UNP Q9UHE8
A	344	ALA	-	expression tag	UNP Q9UHE8
A	345	ALA	-	expression tag	UNP Q9UHE8
A	346	TRP	-	expression tag	UNP Q9UHE8
A	347	SER	-	expression tag	UNP Q9UHE8
A	348	HIS	-	expression tag	UNP Q9UHE8
A	349	PRO	-	expression tag	UNP Q9UHE8
A	350	GLN	-	expression tag	UNP Q9UHE8
A	351	PHE	-	expression tag	UNP Q9UHE8
A	352	GLU	-	expression tag	UNP Q9UHE8
A	353	LYS	-	expression tag	UNP Q9UHE8
A	354	GLY	-	expression tag	UNP Q9UHE8
A	355	ALA	-	expression tag	UNP Q9UHE8
A	356	ALA	-	expression tag	UNP Q9UHE8
A	357	TRP	-	expression tag	UNP Q9UHE8
A	358	SER	-	expression tag	UNP Q9UHE8
A	359	HIS	-	expression tag	UNP Q9UHE8
A	360	PRO	-	expression tag	UNP Q9UHE8

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Chain	Residue	Modelled	Actual	Comment	Reference
A	361	GLN	-	expression tag	UNP Q9UHE8
A	362	PHE	-	expression tag	UNP Q9UHE8
A	363	GLU	-	expression tag	UNP Q9UHE8
A	364	LYS	-	expression tag	UNP Q9UHE8
A	365	GLY	-	expression tag	UNP Q9UHE8
A	366	ALA	-	expression tag	UNP Q9UHE8
A	367	ALA	-	expression tag	UNP Q9UHE8
A	368	TRP	-	expression tag	UNP Q9UHE8
A	369	SER	-	expression tag	UNP Q9UHE8
A	370	HIS	-	expression tag	UNP Q9UHE8
A	371	PRO	-	expression tag	UNP Q9UHE8
A	372	GLN	-	expression tag	UNP Q9UHE8
A	373	PHE	-	expression tag	UNP Q9UHE8
A	374	GLU	-	expression tag	UNP Q9UHE8
A	375	LYS	-	expression tag	UNP Q9UHE8
A	376	GLY	-	expression tag	UNP Q9UHE8
A	377	ALA	-	expression tag	UNP Q9UHE8
A	378	ALA	-	expression tag	UNP Q9UHE8
B	-1	MET	-	initiating methionine	UNP Q9UHE8
B	0	GLY	-	expression tag	UNP Q9UHE8
B	1	SER	-	expression tag	UNP Q9UHE8
B	340	ALA	-	expression tag	UNP Q9UHE8
B	341	ALA	-	expression tag	UNP Q9UHE8
B	342	ALA	-	expression tag	UNP Q9UHE8
B	343	GLY	-	expression tag	UNP Q9UHE8
B	344	ALA	-	expression tag	UNP Q9UHE8
B	345	ALA	-	expression tag	UNP Q9UHE8
B	346	TRP	-	expression tag	UNP Q9UHE8
B	347	SER	-	expression tag	UNP Q9UHE8
B	348	HIS	-	expression tag	UNP Q9UHE8
B	349	PRO	-	expression tag	UNP Q9UHE8
B	350	GLN	-	expression tag	UNP Q9UHE8
B	351	PHE	-	expression tag	UNP Q9UHE8
B	352	GLU	-	expression tag	UNP Q9UHE8
B	353	LYS	-	expression tag	UNP Q9UHE8
B	354	GLY	-	expression tag	UNP Q9UHE8
B	355	ALA	-	expression tag	UNP Q9UHE8
B	356	ALA	-	expression tag	UNP Q9UHE8
B	357	TRP	-	expression tag	UNP Q9UHE8
B	358	SER	-	expression tag	UNP Q9UHE8
B	359	HIS	-	expression tag	UNP Q9UHE8
B	360	PRO	-	expression tag	UNP Q9UHE8

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Chain	Residue	Modelled	Actual	Comment	Reference
B	361	GLN	-	expression tag	UNP Q9UHE8
B	362	PHE	-	expression tag	UNP Q9UHE8
B	363	GLU	-	expression tag	UNP Q9UHE8
B	364	LYS	-	expression tag	UNP Q9UHE8
B	365	GLY	-	expression tag	UNP Q9UHE8
B	366	ALA	-	expression tag	UNP Q9UHE8
B	367	ALA	-	expression tag	UNP Q9UHE8
B	368	TRP	-	expression tag	UNP Q9UHE8
B	369	SER	-	expression tag	UNP Q9UHE8
B	370	HIS	-	expression tag	UNP Q9UHE8
B	371	PRO	-	expression tag	UNP Q9UHE8
B	372	GLN	-	expression tag	UNP Q9UHE8
B	373	PHE	-	expression tag	UNP Q9UHE8
B	374	GLU	-	expression tag	UNP Q9UHE8
B	375	LYS	-	expression tag	UNP Q9UHE8
B	376	GLY	-	expression tag	UNP Q9UHE8
B	377	ALA	-	expression tag	UNP Q9UHE8
B	378	ALA	-	expression tag	UNP Q9UHE8

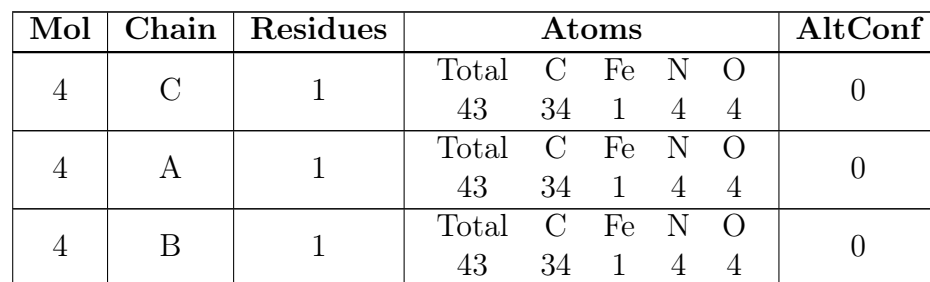
- Molecule 2 is a protein called Fab120.545 light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	L	113	Total	C	N	O	S	0	0
			884	560	146	174	4		
2	M	113	Total	C	N	O	S	0	0
			884	560	146	174	4		
2	N	113	Total	C	N	O	S	0	0
			884	560	146	174	4		

- Molecule 3 is a protein called Fab120.545 heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	H	121	Total	C	N	O	S	0	0
			977	619	157	197	4		
3	I	121	Total	C	N	O	S	0	0
			977	619	157	197	4		
3	J	121	Total	C	N	O	S	0	0
			977	619	157	197	4		

- Molecule 4 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$) (labeled as "Ligand of Interest" by author).

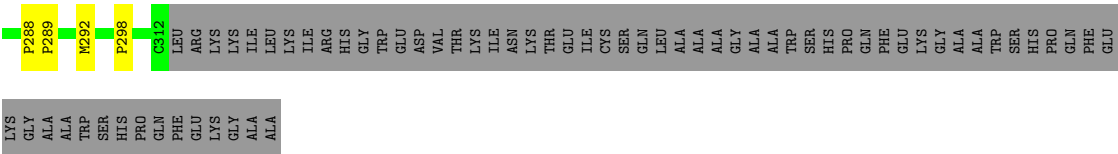


- # XP4

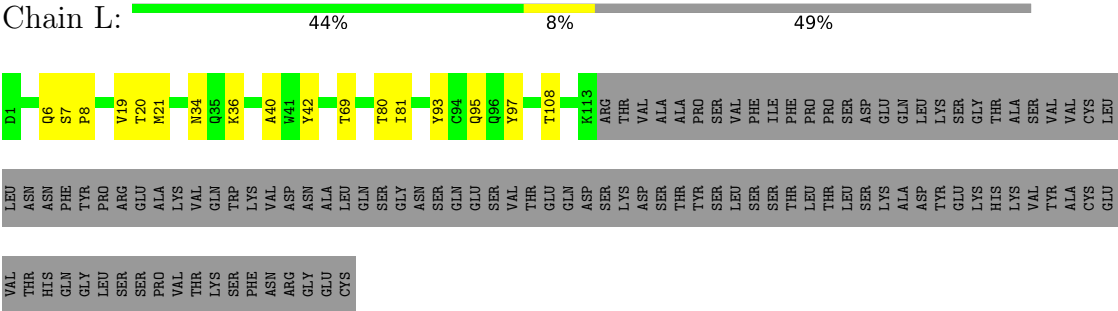
Mol	Chain	Residues	Atoms				AltConf
5	C	1	Total 40	C 31	O 8	P 1	0
5	A	1	Total 40	C 31	O 8	P 1	0
5	B	1	Total 40	C 31	O 8	P 1	0

- Molecule 1: Metalloreductase STEAP1

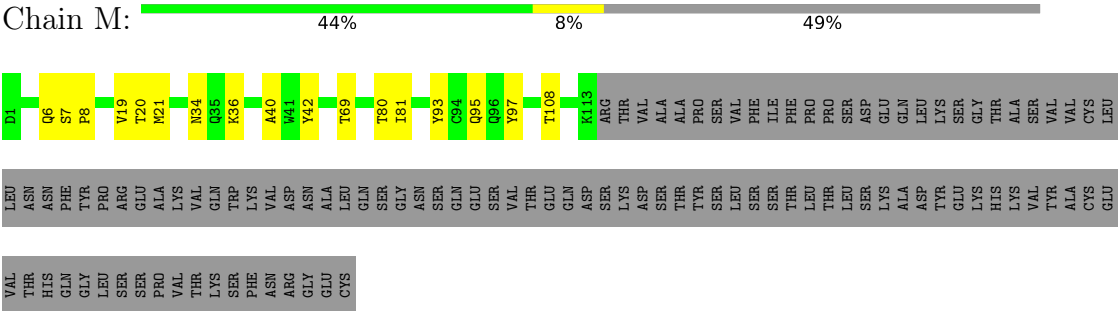




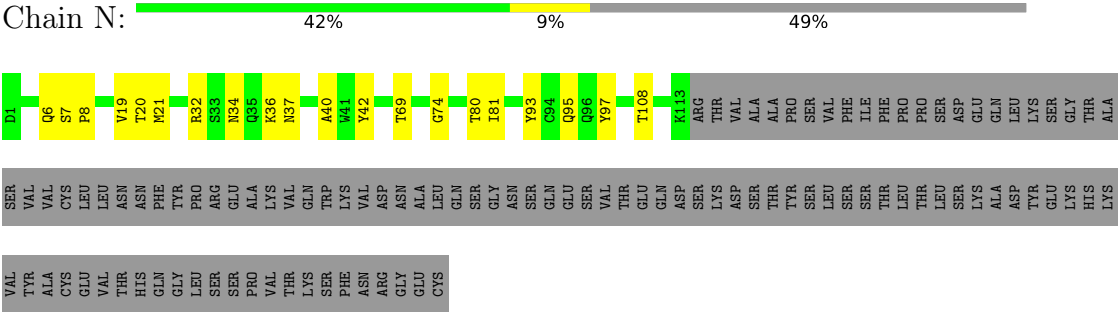
● Molecule 2: Fab120.545 light chain



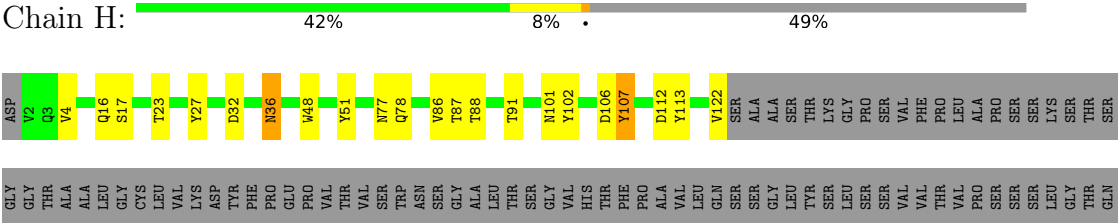
● Molecule 2: Fab120.545 light chain



● Molecule 2: Fab120.545 light chain



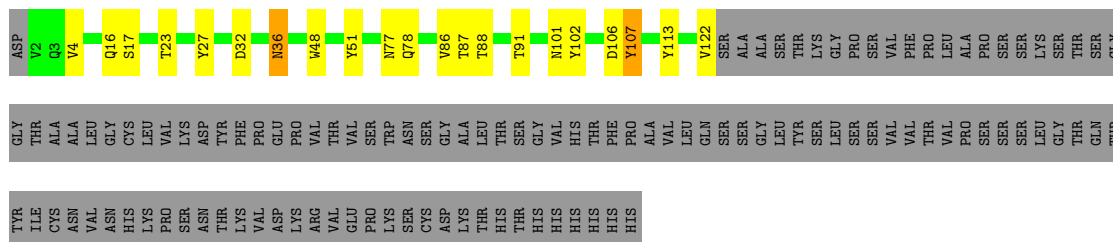
● Molecule 3: Fab120.545 heavy chain



THR	TYR	ILE	CYS	ASN	VAL	ASN	HIS	LYS	PRO	SER	ASN	THR	LYS	VAL	ASP	LYS	ARG	VAL	GLU	PRO	LYS	SER	CYS	ASP	LYS	THR	HIS	THR	HIS	HIS	HIS	HIS	HIS	HIS
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

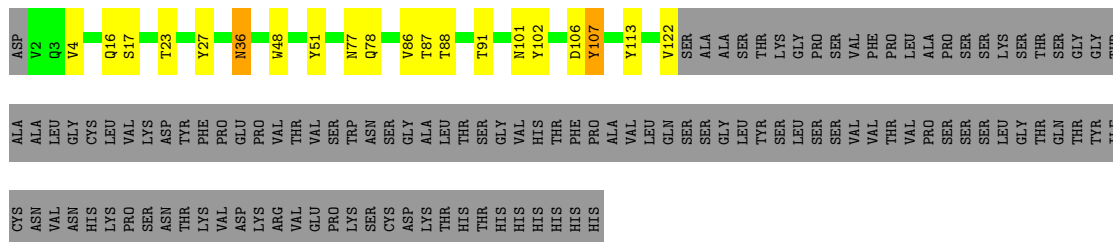
- Molecule 3: Fab120.545 heavy chain

Chain I: 42% 8% • 49%



- Molecule 3: Fab120.545 heavy chain

Chain J:  42% 8% 49%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C3	Depositor
Number of particles used	169426	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	49.5	Depositor
Minimum defocus (nm)	400	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	130000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor

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, XP4

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	0.28	0/2086	0.37	0/2850
1	B	0.28	0/2086	0.37	0/2850
1	C	0.28	0/2086	0.37	0/2850
2	L	0.32	0/904	0.44	0/1223
2	M	0.32	0/904	0.44	0/1223
2	N	0.32	0/904	0.44	0/1223
3	H	0.31	0/1003	0.46	0/1368
3	I	0.31	0/1003	0.46	0/1368
3	J	0.31	0/1003	0.46	0/1368
All	All	0.30	0/11979	0.41	0/16323

There are no bond length outliers.

There are no bond angle outliers.

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	2019	0	2106	18	0
1	B	2019	0	2106	23	0
1	C	2019	0	2106	20	0
2	L	884	0	868	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	M	884	0	868	9	0
2	N	884	0	868	11	0
3	H	977	0	914	14	0
3	I	977	0	914	13	0
3	J	977	0	914	12	0
4	A	43	0	30	1	0
4	B	43	0	30	2	0
4	C	43	0	30	1	0
5	A	40	0	60	0	0
5	B	40	0	60	0	0
5	C	40	0	60	0	0
All	All	11889	0	11934	120	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 5.

The worst 5 of 120 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:92:ARG:NH1	1:A:282:GLN:O	2.28	0.67
1:C:92:ARG:NH1	1:C:282:GLN:O	2.28	0.67
1:B:92:ARG:NH1	1:B:282:GLN:O	2.28	0.66
1:A:174:LEU:HD21	1:B:228:ALA:HB2	1.79	0.63
1:C:174:LEU:HD21	1:A:228:ALA:HB2	1.81	0.62

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 PDB entries followed by that with respect to all EM entries.

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	240/380 (63%)	227 (95%)	13 (5%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	240/380 (63%)	227 (95%)	13 (5%)	0	100	100
1	C	240/380 (63%)	227 (95%)	13 (5%)	0	100	100
2	L	111/220 (50%)	107 (96%)	4 (4%)	0	100	100
2	M	111/220 (50%)	107 (96%)	4 (4%)	0	100	100
2	N	111/220 (50%)	107 (96%)	4 (4%)	0	100	100
3	H	119/238 (50%)	111 (93%)	8 (7%)	0	100	100
3	I	119/238 (50%)	111 (93%)	8 (7%)	0	100	100
3	J	119/238 (50%)	110 (92%)	9 (8%)	0	100	100
All	All	1410/2514 (56%)	1334 (95%)	76 (5%)	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 PDB entries followed by that with respect to all EM entries.

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	220/336 (66%)	219 (100%)	1 (0%)	90	96
1	B	220/336 (66%)	219 (100%)	1 (0%)	90	96
1	C	220/336 (66%)	219 (100%)	1 (0%)	90	96
2	L	99/195 (51%)	99 (100%)	0	100	100
2	M	99/195 (51%)	99 (100%)	0	100	100
2	N	99/195 (51%)	99 (100%)	0	100	100
3	H	109/211 (52%)	105 (96%)	4 (4%)	37	72
3	I	109/211 (52%)	105 (96%)	4 (4%)	37	72
3	J	109/211 (52%)	105 (96%)	4 (4%)	37	72
All	All	1284/2226 (58%)	1269 (99%)	15 (1%)	75	91

5 of 15 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	I	51	TYR
3	I	87	THR
3	J	107	TYR
3	I	36	ASN
3	J	87	THR

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

Mol	Chain	Res	Type
2	N	37	ASN
1	A	96	HIS
1	B	96	HIS
2	M	37	ASN
1	A	254	GLN

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

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
5	XP4	A	402	-	39,39,39	0.30	0	43,44,44	0.40	0
5	XP4	B	402	-	39,39,39	0.30	0	43,44,44	0.40	0
5	XP4	C	402	-	39,39,39	0.30	0	43,44,44	0.40	0
4	HEM	A	401	1	27,50,50	0.99	1 (3%)	17,82,82	1.43	2 (11%)
4	HEM	C	401	1	27,50,50	0.98	1 (3%)	17,82,82	1.43	2 (11%)
4	HEM	B	401	1	27,50,50	0.98	1 (3%)	17,82,82	1.44	2 (11%)

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	XP4	A	402	-	-	9/41/41/41	-
5	XP4	B	402	-	-	9/41/41/41	-
5	XP4	C	402	-	-	9/41/41/41	-
4	HEM	A	401	1	-	0/6/54/54	-
4	HEM	C	401	1	-	0/6/54/54	-
4	HEM	B	401	1	-	0/6/54/54	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	401	HEM	C3B-C2B	-2.99	1.36	1.40
4	B	401	HEM	C3B-C2B	-2.98	1.36	1.40
4	C	401	HEM	C3B-C2B	-2.94	1.36	1.40

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	401	HEM	CBA-CAA-C2A	-3.33	106.35	112.49
4	A	401	HEM	CBA-CAA-C2A	-3.30	106.40	112.49
4	C	401	HEM	CBA-CAA-C2A	-3.29	106.42	112.49
4	C	401	HEM	CAD-CBD-CGD	-2.25	108.90	112.67
4	B	401	HEM	CAD-CBD-CGD	-2.24	108.92	112.67

There are no chirality outliers.

5 of 27 torsion outliers are listed below:

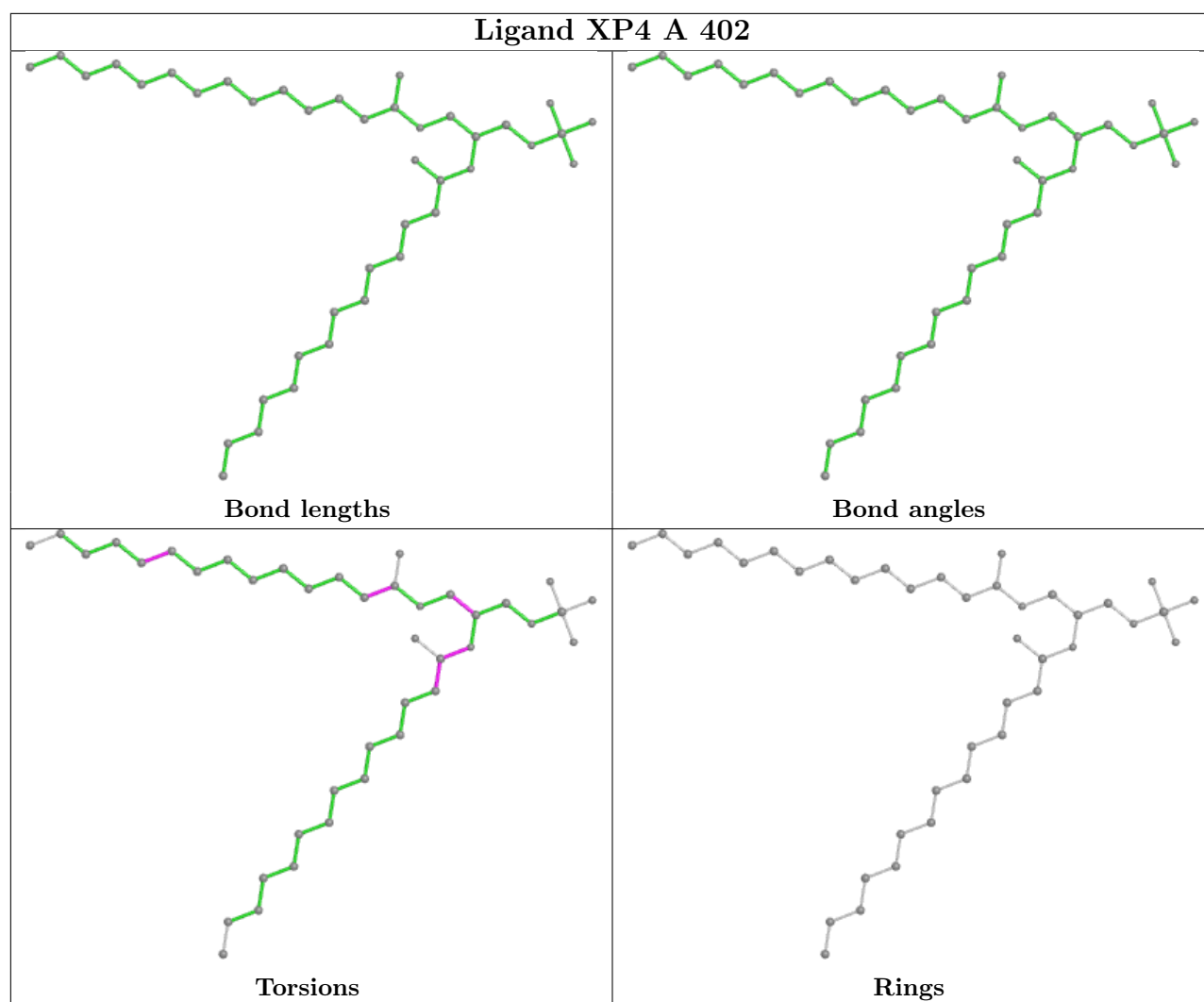
Mol	Chain	Res	Type	Atoms
5	A	402	XP4	C19-C18-O7-C2
5	B	402	XP4	C19-C18-O7-C2
5	C	402	XP4	C19-C18-O7-C2
5	A	402	XP4	O8-C18-O7-C2
5	B	402	XP4	O8-C18-O7-C2

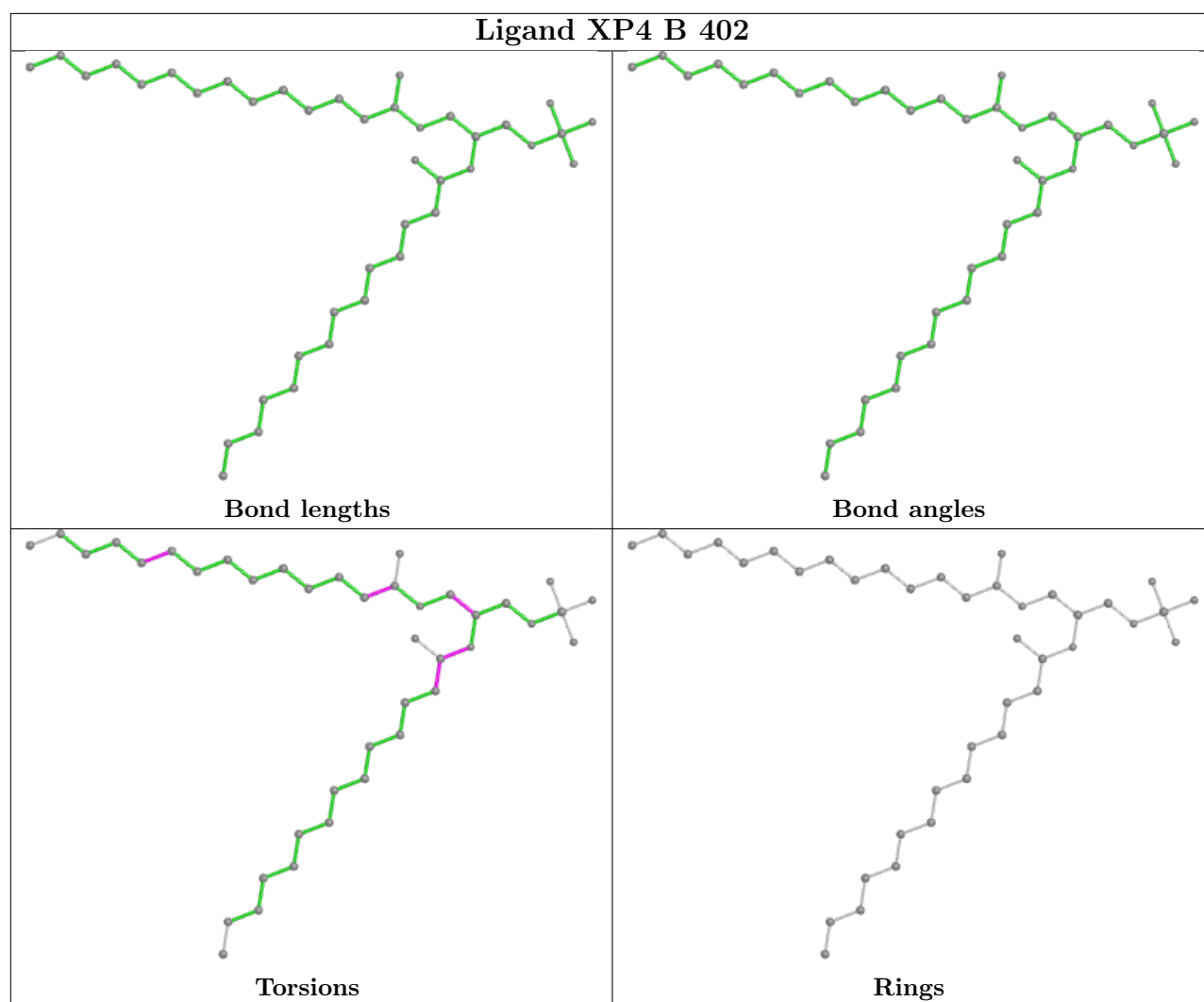
There are no ring outliers.

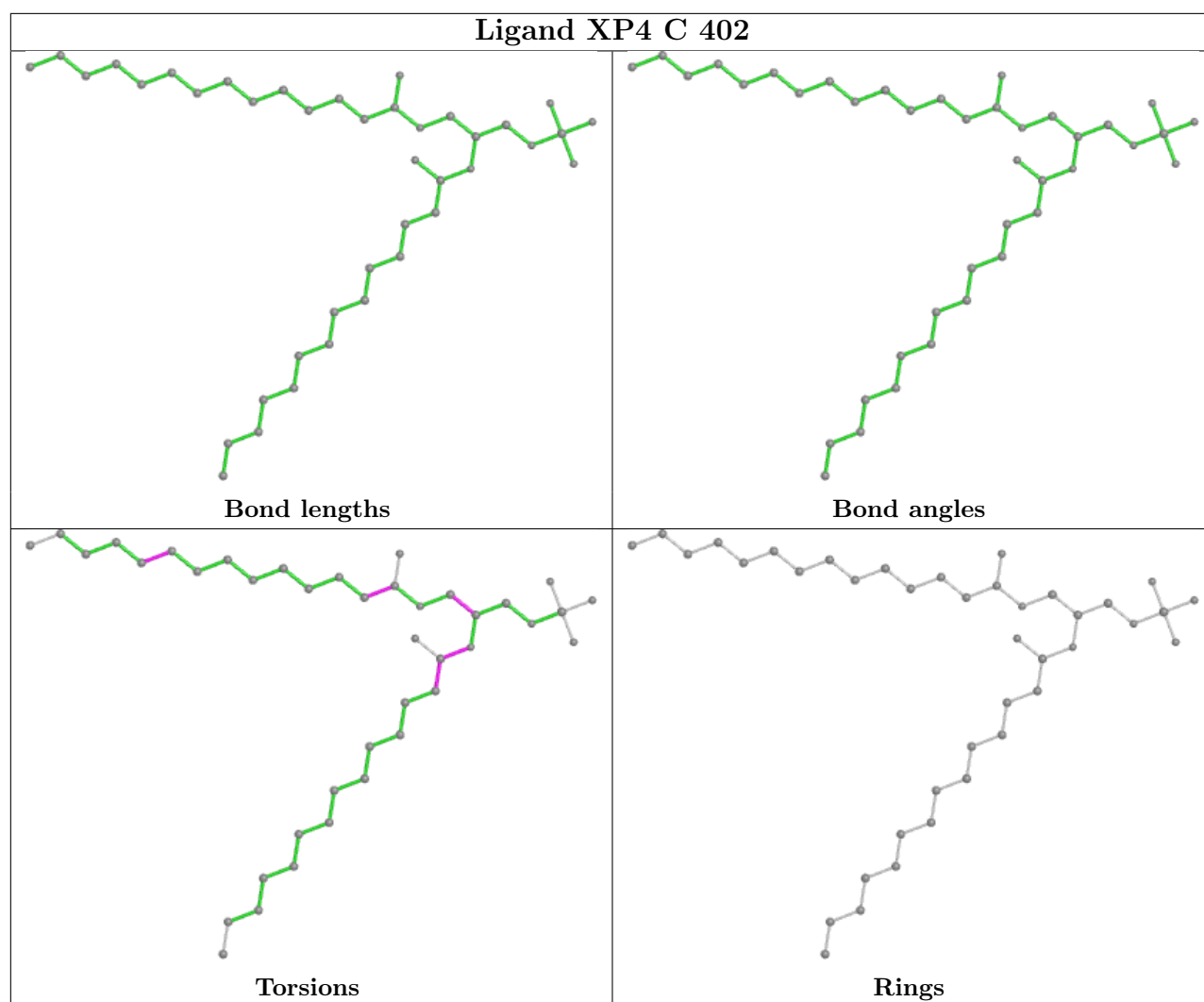
3 monomers are involved in 4 short contacts:

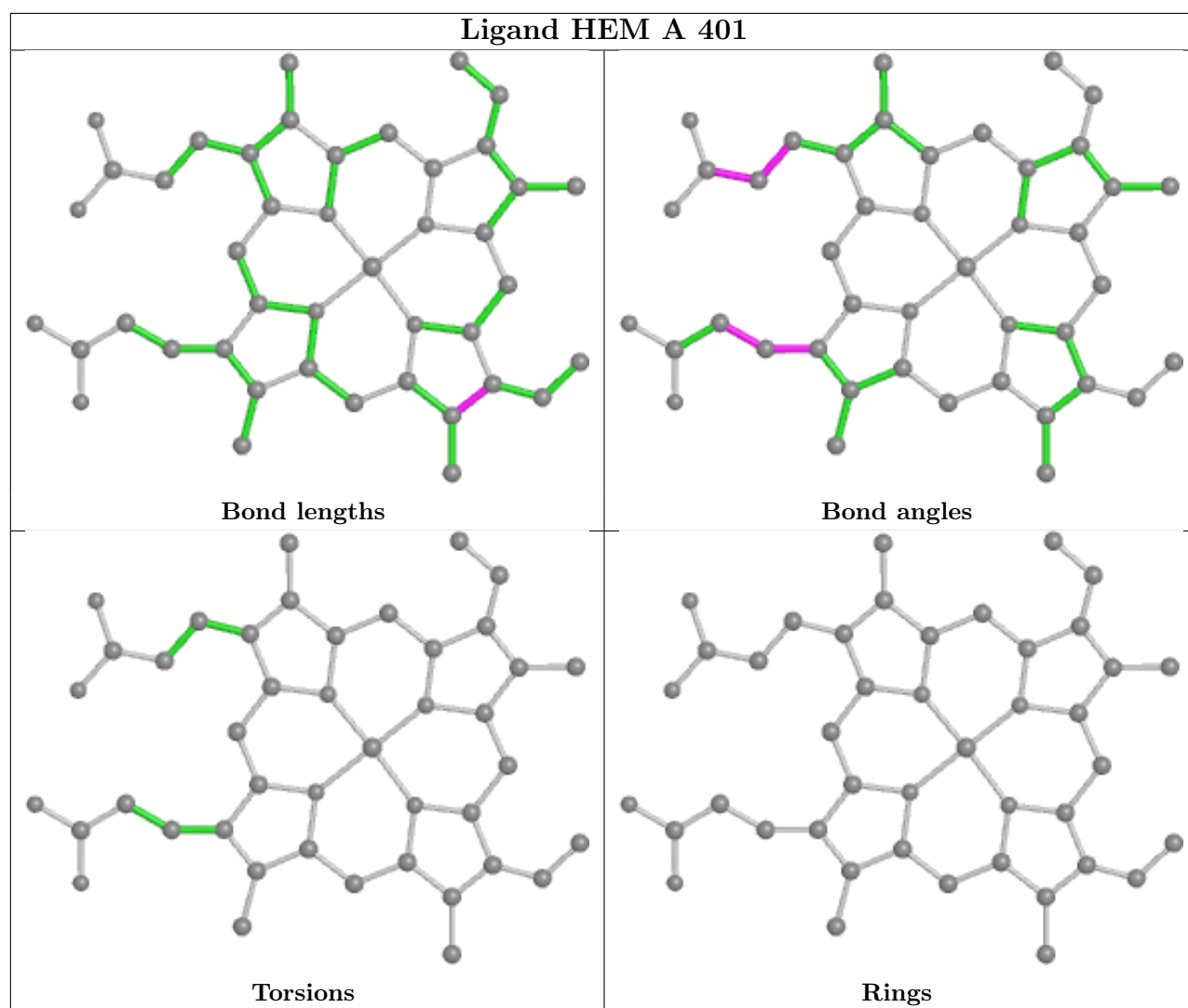
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	401	HEM	1	0
4	C	401	HEM	1	0
4	B	401	HEM	2	0

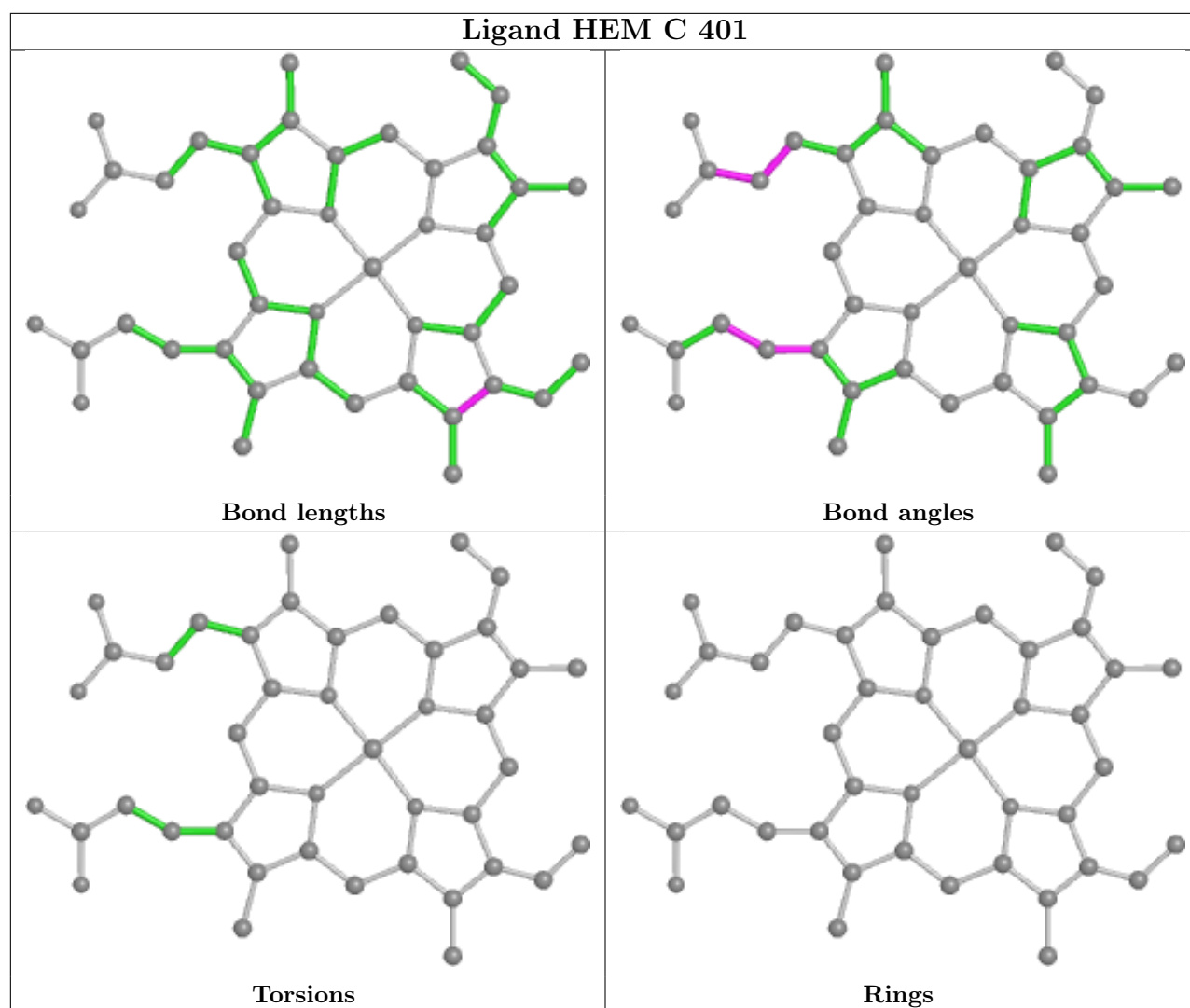
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

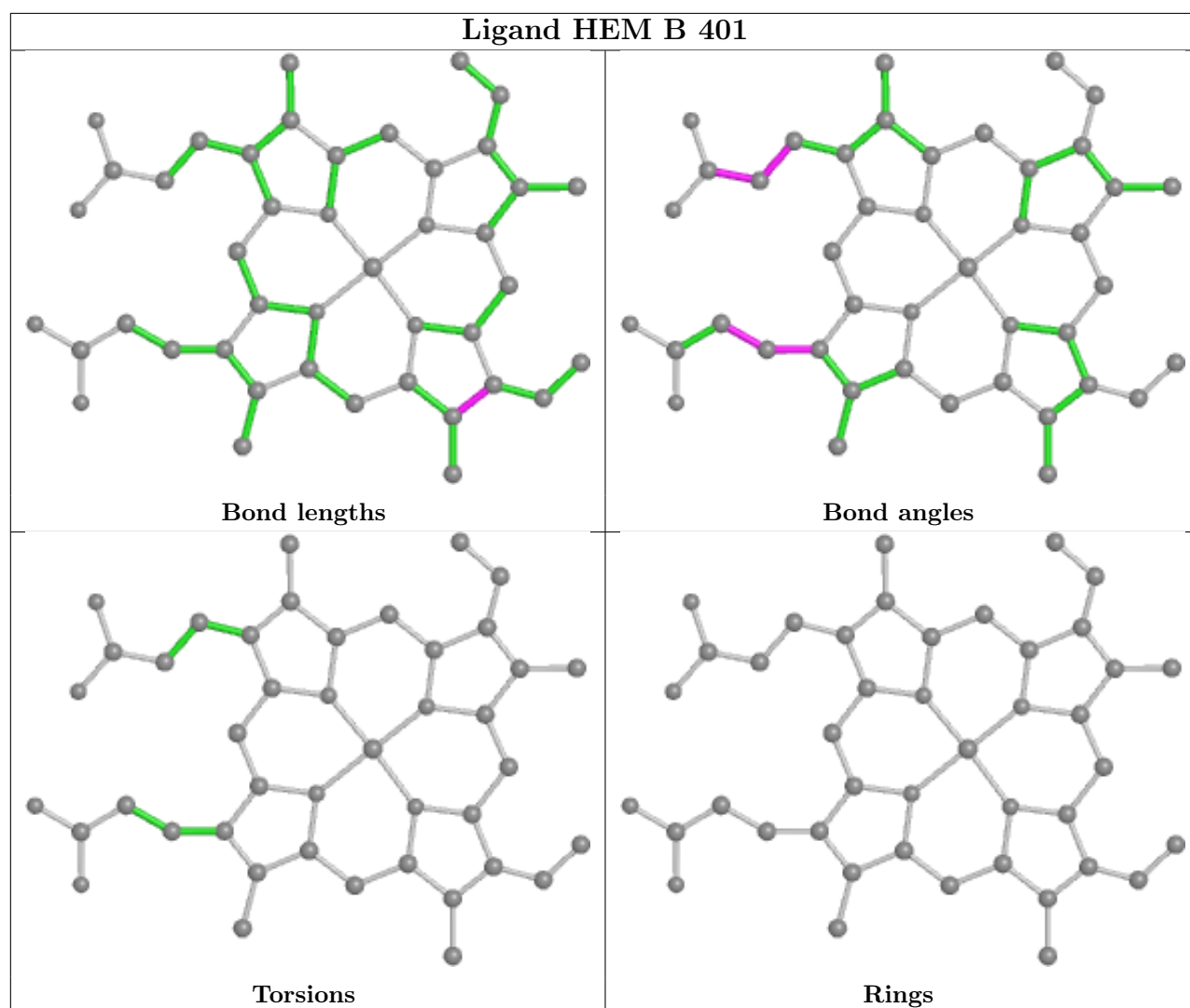












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.