



## Full wwPDB EM Validation Report ⓘ

Apr 2, 2025 – 02:58 am BST

PDB ID : 6HWH / pdb\_00006hwh  
EMDB ID : EMD-0289  
Title : Structure of a functional obligate respiratory supercomplex from *Mycobacterium smegmatis*  
Authors : Wiseman, B.; Nitharwal, R.G.; Fedotovskaya, O.; Schafer, J.; Guo, H.; Kuang, Q.; Benlekbir, S.; Sjostrand, D.; Adelroth, P.; Rubinstein, J.L.; Brzezinski, P.; Hogbom, M.  
Deposited on : 2018-10-12  
Resolution : 3.30 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto: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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

EMDB validation analysis : 0.0.1.dev117  
Mogul : 1.8.4, CSD as541be (2020)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : **FAILED**  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.42

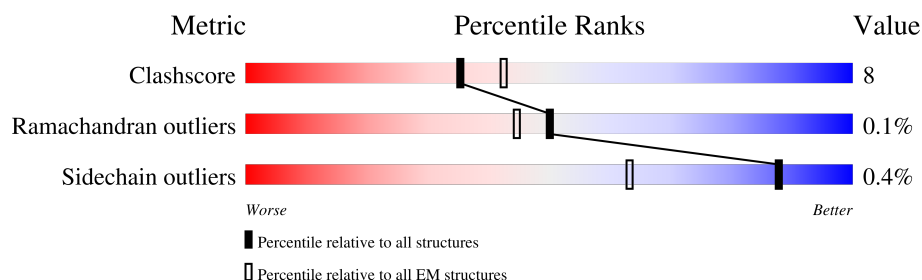
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.30 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.



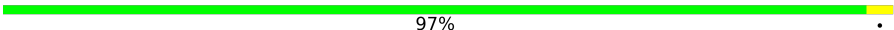










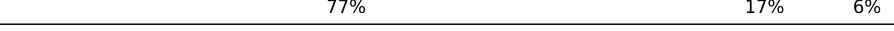






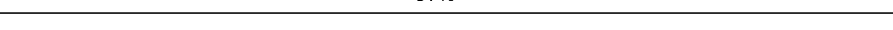
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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 of the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	408	83% 10% 7%
1	B	408	79% 14% 7%
2	C	74	99% .
2	G	74	100%
3	D	65	100%
3	H	65	100%
4	E	20	100%
4	I	20	100%
5	F	35	97% .

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Mol	Chain	Length	Quality of chain
5	J	35	
6	K	268	
6	M	268	
6	i	268	
6	j	268	
7	L	341	
7	P	341	
8	N	79	
8	R	79	
9	O	157	
9	T	157	
10	Q	583	
10	V	583	
11	S	139	
11	X	139	
12	W	203	
12	Z	203	
13	Y	554	
13	b	554	

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
14	FES	B	501	-	-	X	-
18	HAS	Q	801	X	-	-	-
18	HAS	Q	802	X	-	-	-
18	HAS	V	801	X	-	-	-
18	HAS	V	802	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
19	HEC	V	804	-	-	X	-

## 2 Entry composition

There are 20 unique types of molecules in this entry. The entry contains 40632 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 Ubiquinol-cytochrome c reductase iron-sulfur subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	380	Total	C	N	O	S	0	0
			2960	1914	500	535	11		
1	B	380	Total	C	N	O	S	0	0
			2960	1914	500	535	11		

- Molecule 2 is a protein called Co-purified unknown transmembrane helices built as polyALA.

Mol	Chain	Residues	Atoms				AltConf	Trace
2	G	74	Total	C	N	O	0	0
			370	222	74	74		
2	C	74	Total	C	N	O	0	0
			370	222	74	74		

- Molecule 3 is a protein called Co-purified unknown transmembrane helices built as polyALA.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	H	65	Total	C	N	O	0	0
			325	195	65	65		
3	D	65	Total	C	N	O	0	0
			325	195	65	65		

- Molecule 4 is a protein called Co-purified unknown peptide built as polyALA.

Mol	Chain	Residues	Atoms				AltConf	Trace
4	I	20	Total	C	N	O	0	0
			100	60	20	20		
4	E	20	Total	C	N	O	0	0
			100	60	20	20		

- Molecule 5 is a protein called Co-purified unknown peptide built as polyALA.

Mol	Chain	Residues	Atoms				AltConf	Trace
5	J	35	Total	C	N	O	0	0
			175	105	35	35		
5	F	35	Total	C	N	O	0	0
			175	105	35	35		

- Molecule 6 is a protein called Cytochrome bc1 complex cytochrome c subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	M	30	Total	C	N	O	S	0	0
			211	139	35	33	4		
6	K	30	Total	C	N	O	S	0	0
			211	139	35	33	4		
6	i	162	Total	C	N	O		0	0
			648	324	162	162			
6	j	162	Total	C	N	O		0	0
			648	324	162	162			

- Molecule 7 is a protein called Cytochrome c oxidase subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	P	281	Total	C	N	O	S	0	0
			2236	1450	368	409	9		
7	L	281	Total	C	N	O	S	0	0
			2236	1450	368	409	9		

- Molecule 8 is a protein called MSMEG\_4693.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	R	54	Total	C	N	O	S	0	0
			415	276	67	70	2		
8	N	54	Total	C	N	O	S	0	0
			415	276	67	70	2		

- Molecule 9 is a protein called Uncharacterized protein MSMEG\_4692/MSMEI\_4575.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	T	142	Total	C	N	O	S	0	0
			1019	644	173	200	2		
9	O	142	Total	C	N	O	S	0	0
			1019	644	173	200	2		

- Molecule 10 is a protein called Cytochrome c oxidase subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	V	550	Total	C	N	O	S	0	0
			4354	2927	695	709	23		
10	Q	550	Total	C	N	O	S	0	0
			4354	2927	695	709	23		

- Molecule 11 is a protein called Cytochrome c oxidase polypeptide 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	X	139	Total	C	N	O	S	0	0
			1077	719	167	188	3		
11	S	139	Total	C	N	O	S	0	0
			1077	719	167	188	3		

- Molecule 12 is a protein called Cytochrome c oxidase subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	Z	184	Total	C	N	O	S	0	0
			1441	967	229	238	7		
12	W	184	Total	C	N	O	S	0	0
			1441	967	229	238	7		

- Molecule 13 is a protein called Ubiquinol-cytochrome C reductase QcrB.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	b	536	Total	C	N	O	S	0	0
			4190	2757	712	703	18		
13	Y	536	Total	C	N	O	S	0	0
			4190	2757	712	703	18		

There are 16 discrepancies between the modelled and reference sequences:

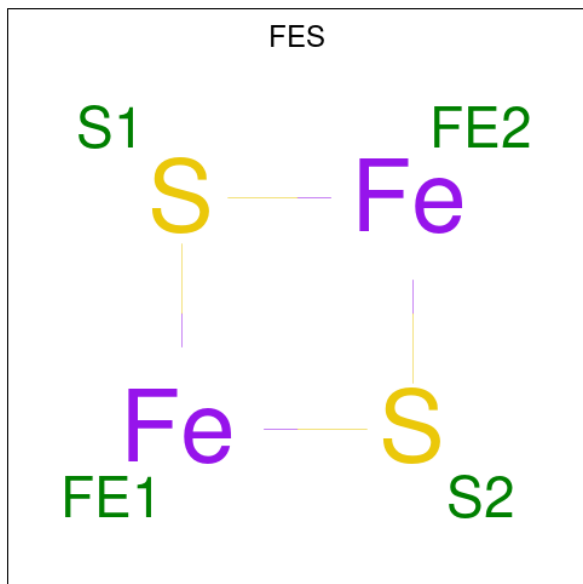
Chain	Residue	Modelled	Actual	Comment	Reference
b	547	ASP	-	expression tag	UNP I7FGS8
b	548	TYR	-	expression tag	UNP I7FGS8
b	549	LYS	-	expression tag	UNP I7FGS8
b	550	ASP	-	expression tag	UNP I7FGS8
b	551	ASP	-	expression tag	UNP I7FGS8
b	552	ASP	-	expression tag	UNP I7FGS8
b	553	ASP	-	expression tag	UNP I7FGS8
b	554	LYS	-	expression tag	UNP I7FGS8
Y	547	ASP	-	expression tag	UNP I7FGS8
Y	548	TYR	-	expression tag	UNP I7FGS8
Y	549	LYS	-	expression tag	UNP I7FGS8

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Chain	Residue	Modelled	Actual	Comment	Reference
Y	550	ASP	-	expression tag	UNP I7FGS8
Y	551	ASP	-	expression tag	UNP I7FGS8
Y	552	ASP	-	expression tag	UNP I7FGS8
Y	553	ASP	-	expression tag	UNP I7FGS8
Y	554	LYS	-	expression tag	UNP I7FGS8

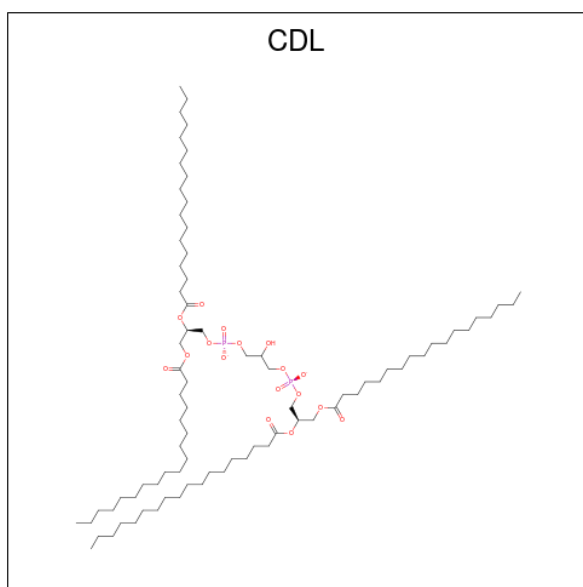
- Molecule 14 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula:  $\text{Fe}_2\text{S}_2$ ).



Mol	Chain	Residues	Atoms			AltConf
14	A	1	Total	Fe	S	0
			4	2	2	
14	B	1	Total	Fe	S	0
			4	2	2	

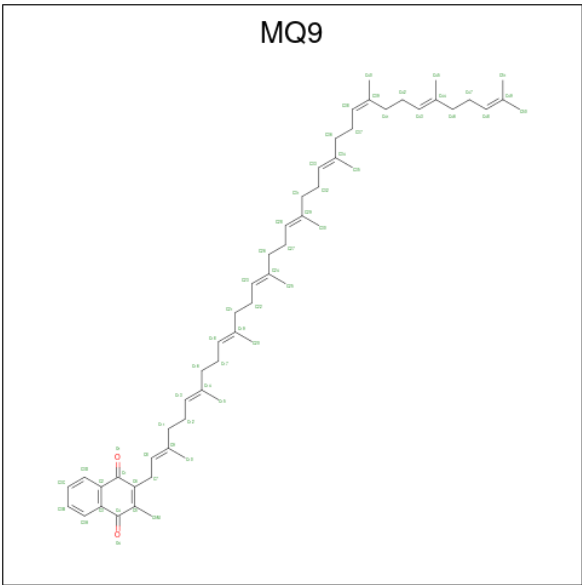
- Molecule 15 is CARDIOLIPIN (CCD ID: CDL) (formula:  $\text{C}_{81}\text{H}_{156}\text{O}_{17}\text{P}_2$ ).





Mol	Chain	Residues	Atoms				AltConf
15	M	1	Total	C	O	P	0
			100	81	17	2	
15	V	1	Total	C	O	P	0
			87	68	17	2	
15	b	1	Total	C	O	P	0
			92	73	17	2	
15	b	1	Total	C	O	P	0
			91	72	17	2	
15	K	1	Total	C	O	P	0
			100	81	17	2	
15	Q	1	Total	C	O	P	0
			87	68	17	2	
15	Y	1	Total	C	O	P	0
			91	72	17	2	
15	Y	1	Total	C	O	P	0
			92	73	17	2	

- Molecule 16 is MENAQUINONE-9 (CCD ID: MQ9) (formula:  $C_{56}H_{80}O_2$ ).

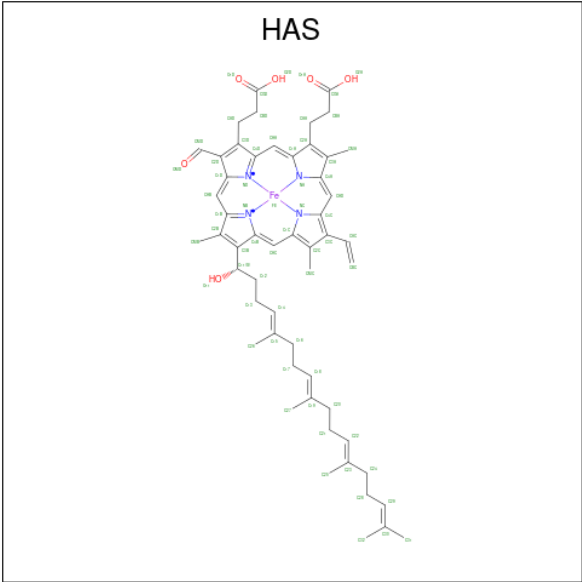


Mol	Chain	Residues	Atoms			AltConf
16	M	1	Total	C	O	0
			58	56	2	
16	b	1	Total	C	O	0
			58	56	2	
16	Y	1	Total	C	O	0
			58	56	2	
16	Y	1	Total	C	O	0
			58	56	2	

- Molecule 17 is COPPER (II) ION (CCD ID: CU) (formula: Cu).

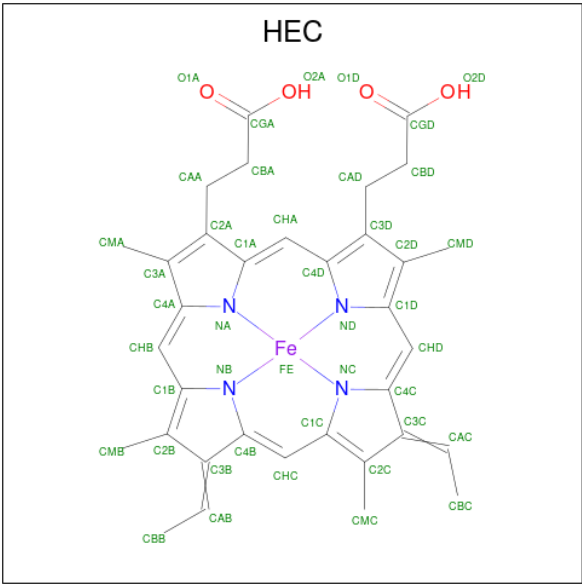
Mol	Chain	Residues	Atoms		AltConf
17	P	2	Total	Cu	0
			2	2	
17	V	1	Total	Cu	0
			1	1	
17	L	2	Total	Cu	0
			2	2	
17	Q	1	Total	Cu	0
			1	1	

- Molecule 18 is HEME-AS (CCD ID: HAS) (formula: C<sub>54</sub>H<sub>64</sub>FeN<sub>4</sub>O<sub>6</sub>).



Mol	Chain	Residues	Atoms					AltConf
18	V	1	Total	C	Fe	N	O	0
			65	54	1	4	6	
18	V	1	Total	C	Fe	N	O	0
			65	54	1	4	6	
18	Q	1	Total	C	Fe	N	O	0
			65	54	1	4	6	
18	Q	1	Total	C	Fe	N	O	0
			65	54	1	4	6	

- Molecule 19 is HEME C (CCD ID: HEC) (formula:  $C_{34}H_{34}FeN_4O_4$ ).

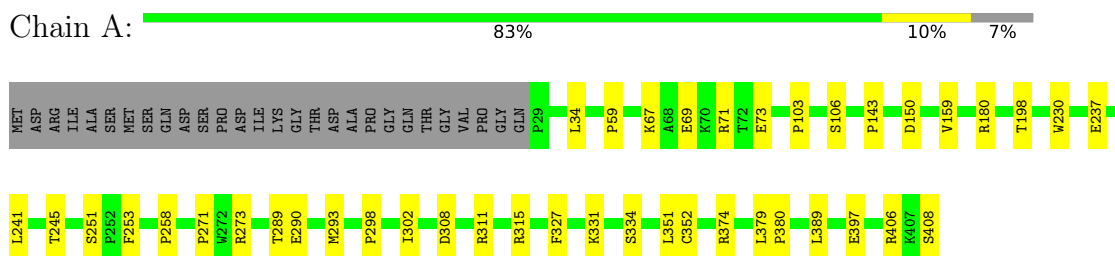




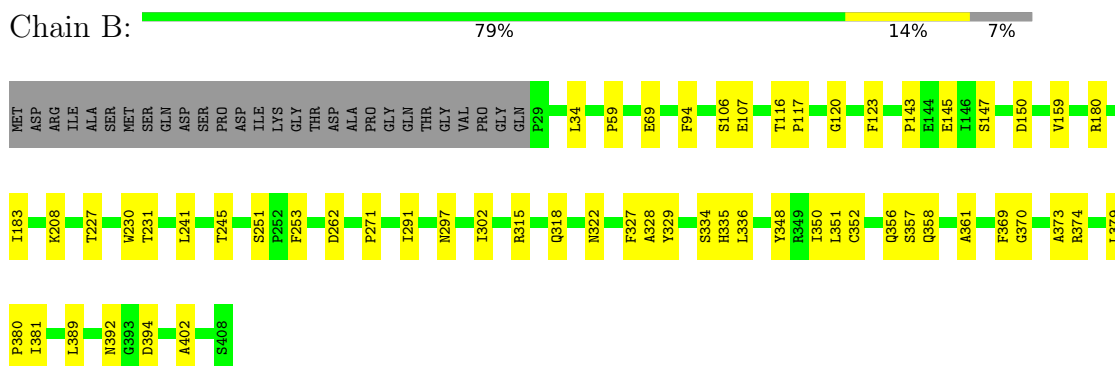
### 3 Residue-property plots

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.

- Molecule 1: Ubiquinol-cytochrome c reductase iron-sulfur subunit



- Molecule 1: Ubiquinol-cytochrome c reductase iron-sulfur subunit



- Molecule 2: Co-purified unknown transmembrane helices built as polyALA



There are no outlier residues recorded for this chain.

- Molecule 2: Co-purified unknown transmembrane helices built as polyALA



- Molecule 3: Co-purified unknown transmembrane helices built as polyALA



There are no outlier residues recorded for this chain.

- Molecule 3: Co-purified unknown transmembrane helices built as polyALA

Chain D:  100%

There are no outlier residues recorded for this chain.

- Molecule 4: Co-purified unknown peptide built as polyALA

Chain I:  100%

There are no outlier residues recorded for this chain.

- Molecule 4: Co-purified unknown peptide built as polyALA

Chain E:  100%

There are no outlier residues recorded for this chain.

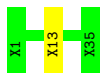
- Molecule 5: Co-purified unknown peptide built as polyALA

Chain J:  97%



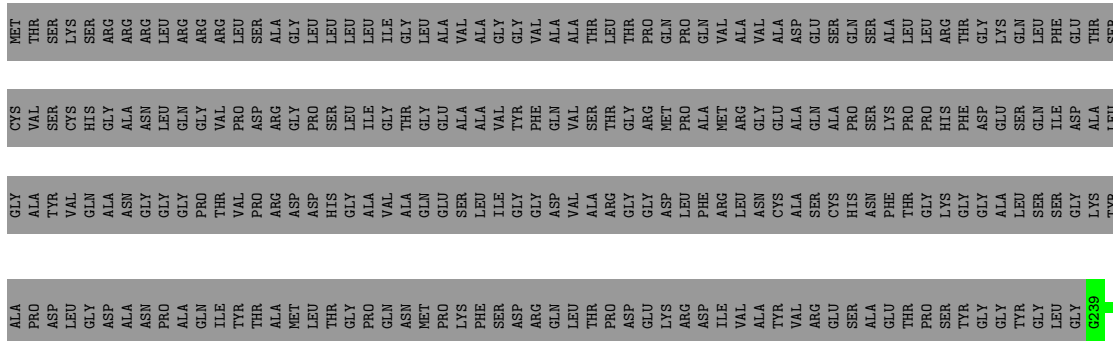
- Molecule 5: Co-purified unknown peptide built as polyALA

Chain F:  97%



- Molecule 6: Cytochrome bc1 complex cytochrome c subunit

Chain M:  11% 89%

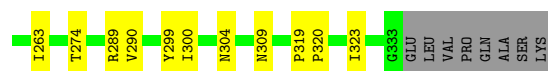
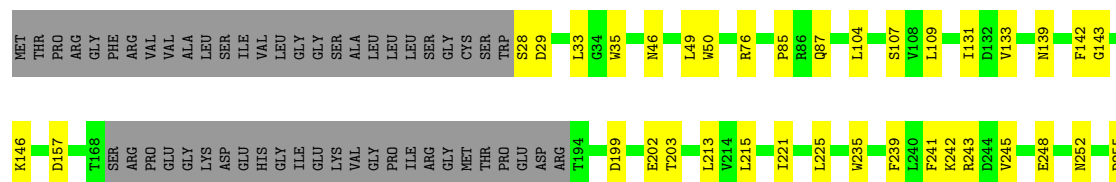






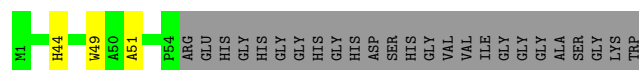
• Molecule 7: Cytochrome c oxidase subunit 2

Chain L: 69% 14% 18%



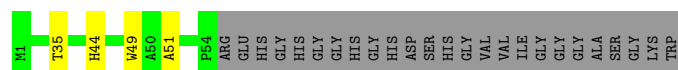
• Molecule 8: MSMEG\_4693

Chain R: 65% 0% 32%



• Molecule 8: MSMEG\_4693

Chain N: 63% 5% 32%



• Molecule 9: Uncharacterized protein MSMEG\_4692/MSMEI\_4575

Chain T: 83% 8% 10%



• Molecule 9: Uncharacterized protein MSMEG\_4692/MSMEI\_4575

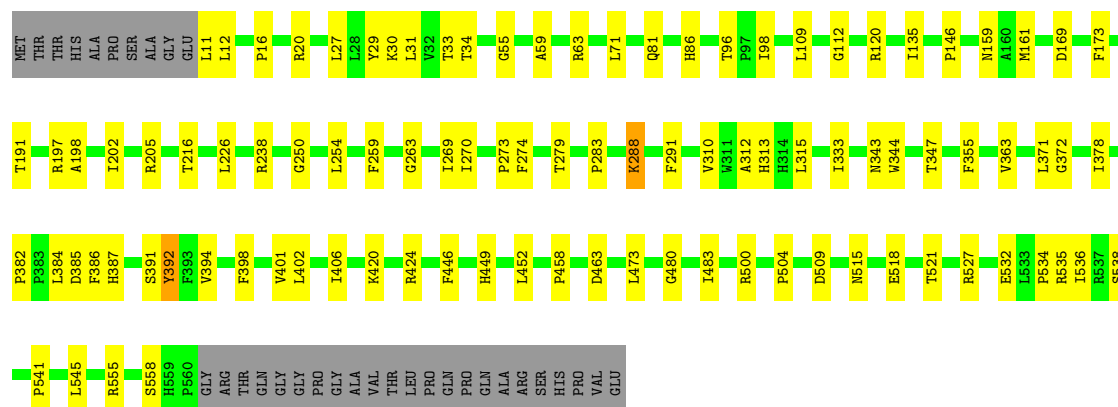
Chain O: 80% 10% 10%



• Molecule 10: Cytochrome c oxidase subunit 1

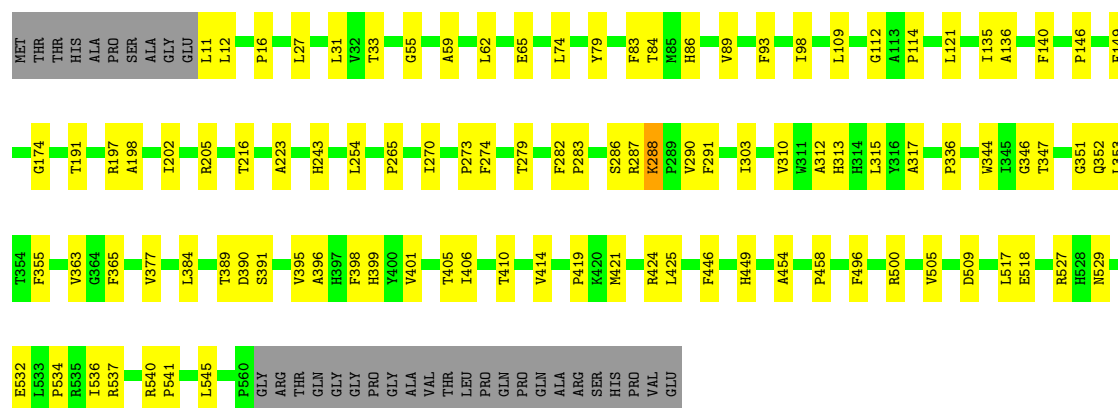
Chain V: 78% 16% 6%





• Molecule 10: Cytochrome c oxidase subunit 1

Chain Q: 77% 17% 6%



• Molecule 11: Cytochrome c oxidase polypeptide 4

Chain X: 90% 10%



• Molecule 11: Cytochrome c oxidase polypeptide 4

Chain S: 86% 14%




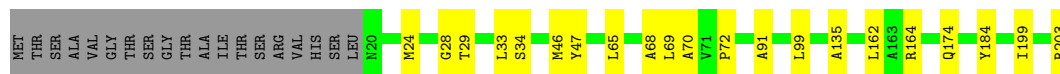
• Molecule 12: Cytochrome c oxidase subunit 3

Chain Z: 82% 9% 9%



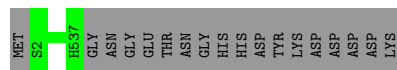
- Molecule 12: Cytochrome c oxidase subunit 3

Chain W:  80% 10% 9%




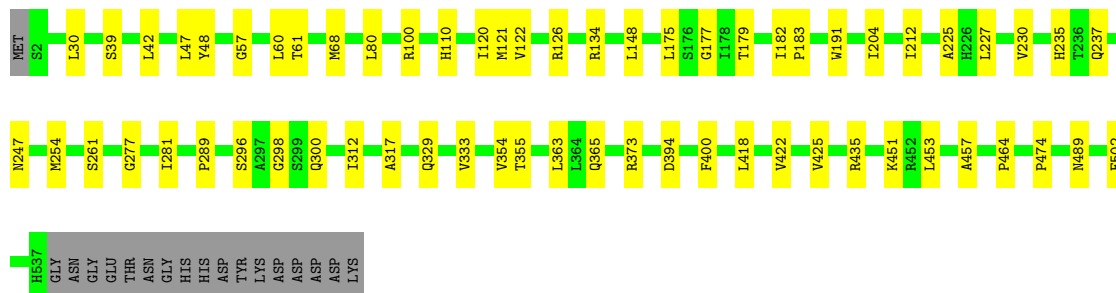
- Molecule 13: Ubiquinol-cytochrome C reductase QcrB

Chain b:  97%



- Molecule 13: Ubiquinol-cytochrome C reductase QcrB

Chain Y:  86% 11%



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	104198	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	43	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: HEC, CDL, HAS, FES, MQ9, HEM, CU

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	0.35	0/3039	0.59	0/4120
1	B	0.40	0/3039	0.61	0/4120
6	K	0.42	0/217	0.56	0/293
6	M	0.41	0/217	0.52	0/293
6	i	0.73	0/646	0.91	0/804
6	j	0.66	0/646	0.97	0/804
7	L	0.44	0/2297	0.63	0/3126
7	P	0.38	0/2297	0.59	0/3126
8	N	0.32	0/430	0.65	0/591
8	R	0.29	0/430	0.63	0/591
9	O	0.38	0/1037	0.57	0/1416
9	T	0.35	0/1037	0.57	0/1416
10	Q	0.51	0/4515	0.68	0/6176
10	V	0.48	0/4515	0.67	0/6176
11	S	0.46	0/1112	0.62	0/1524
11	X	0.42	0/1112	0.59	0/1524
12	W	0.45	0/1488	0.58	0/2032
12	Z	0.40	0/1488	0.56	0/2032
13	Y	0.46	0/4324	0.62	0/5897
13	b	0.41	0/4324	0.61	0/5897
All	All	0.44	0/38210	0.63	0/51958

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 ⓘ

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	2960	0	2963	27	0
1	B	2960	0	2965	45	0
2	C	370	0	80	1	0
2	G	370	0	80	0	0
3	D	325	0	67	0	0
3	H	325	0	67	0	0
4	E	100	0	23	0	0
4	I	100	0	23	0	0
5	F	175	0	38	1	0
5	J	175	0	41	1	0
6	K	211	0	212	2	0
6	M	211	0	212	1	0
6	i	648	0	182	0	0
6	j	648	0	185	0	0
7	L	2236	0	2189	29	0
7	P	2236	0	2189	28	0
8	N	415	0	424	4	0
8	R	415	0	424	3	0
9	O	1019	0	1030	11	0
9	T	1019	0	1030	10	0
10	Q	4354	0	4342	69	0
10	V	4354	0	4341	84	0
11	S	1077	0	1058	20	0
11	X	1077	0	1058	12	0
12	W	1441	0	1439	18	0
12	Z	1441	0	1439	12	0
13	Y	4190	0	4211	45	0
13	b	4190	0	4211	0	0
14	A	4	0	0	0	0
14	B	4	0	0	2	0
15	K	100	0	154	6	0
15	M	100	0	154	4	0
15	Q	87	0	118	3	0
15	V	87	0	118	2	0
15	Y	183	0	266	9	0
15	b	183	0	266	0	0
16	M	58	0	80	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
16	Y	116	0	160	10	0
16	b	58	0	80	0	0
17	L	2	0	0	0	0
17	P	2	0	0	0	0
17	Q	1	0	0	0	0
17	V	1	0	0	0	0
18	Q	130	0	124	6	0
18	V	130	0	124	7	0
19	V	43	0	32	22	0
19	i	43	0	32	0	0
19	j	86	0	63	0	0
20	Y	86	0	60	6	0
20	b	86	0	60	0	0
All	All	40632	0	38414	391	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 8.

All (391) 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)
10:V:161:MET:CG	19:V:804:HEC:HBC2	1.36	1.53
10:V:161:MET:CB	19:V:804:HEC:HBC2	1.58	1.31
10:V:161:MET:CG	19:V:804:HEC:CBC	2.15	1.23
10:V:161:MET:HG2	19:V:804:HEC:CBC	1.73	1.19
10:V:161:MET:O	19:V:804:HEC:HBC1	1.46	1.16
10:V:161:MET:HB2	19:V:804:HEC:HBC2	1.35	1.07
10:V:161:MET:CB	19:V:804:HEC:CBC	2.31	1.06
10:V:161:MET:C	19:V:804:HEC:HBC1	1.78	1.03
11:S:63:LEU:HD23	11:S:64:ASP:O	1.58	1.03
10:Q:62:LEU:HD21	18:Q:802:HAS:HBD2	1.42	1.00
10:V:161:MET:HG3	19:V:804:HEC:HBC2	1.40	1.00
10:V:161:MET:HB2	19:V:804:HEC:CBC	1.89	0.99
11:S:63:LEU:CD2	11:S:64:ASP:O	2.12	0.97
10:V:161:MET:HG3	19:V:804:HEC:HMC1	1.63	0.79
10:Q:84:THR:OG1	10:Q:149:PHE:O	2.01	0.75
10:Q:62:LEU:HD23	10:Q:62:LEU:O	1.88	0.74
1:A:351:LEU:HD23	1:A:352:CYS:N	2.04	0.72
10:V:398:PHE:HA	10:V:401:VAL:HG12	1.73	0.71
10:Q:62:LEU:CD1	10:Q:83:PHE:HB3	2.21	0.70
10:Q:62:LEU:HD11	10:Q:83:PHE:HB3	1.74	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:Q:62:LEU:CD2	18:Q:802:HAS:HBD2	2.22	0.68
10:V:402:LEU:HD13	18:V:802:HAS:HAC	1.74	0.68
10:V:161:MET:HB2	19:V:804:HEC:CAC	2.24	0.68
11:S:63:LEU:HD23	11:S:64:ASP:N	2.09	0.67
7:P:263:ILE:HG21	7:P:290:VAL:HG11	1.76	0.66
11:S:63:LEU:HD23	11:S:63:LEU:C	2.17	0.65
10:V:161:MET:O	19:V:804:HEC:CBC	2.35	0.65
7:P:83:GLU:HG2	7:P:85:PRO:HD3	1.77	0.65
10:Q:391:SER:HA	10:Q:458:PRO:HA	1.79	0.65
9:T:31:VAL:HG23	10:V:509:ASP:HB3	1.79	0.65
7:L:225:LEU:HB3	7:L:245:VAL:HG12	1.78	0.65
9:O:31:VAL:HG23	10:Q:509:ASP:HB3	1.79	0.64
1:B:335:HIS:NE2	13:Y:329:GLN:OE1	2.30	0.63
1:A:351:LEU:HD23	1:A:351:LEU:C	2.20	0.62
7:P:121:MET:SD	7:P:243:ARG:NH2	2.72	0.62
10:V:391:SER:HA	10:V:458:PRO:HA	1.82	0.62
1:A:289:THR:HA	1:A:293:MET:HB2	1.81	0.62
1:B:334:SER:O	1:B:374:ARG:NH2	2.33	0.61
1:B:350:ILE:O	1:B:350:ILE:HG22	2.00	0.61
12:W:68:ALA:O	12:W:69:LEU:HB3	2.00	0.61
9:O:130:ALA:HB2	9:O:146:ALA:HB2	1.83	0.61
11:X:48:LEU:HG	12:Z:34:SER:HB3	1.82	0.61
10:V:197:ARG:NH2	11:X:4:GLU:OE2	2.33	0.61
13:Y:365:GLN:OE1	13:Y:373:ARG:NH1	2.33	0.60
10:Q:197:ARG:NH2	11:S:4:GLU:OE2	2.34	0.60
7:L:263:ILE:HG21	7:L:290:VAL:HG11	1.82	0.60
19:V:804:HEC:CBB	19:V:804:HEC:HMB1	2.32	0.60
10:V:109:LEU:HB3	10:V:518:GLU:HB3	1.84	0.60
7:P:242:LYS:NZ	10:V:387:HIS:O	2.35	0.60
19:V:804:HEC:CBC	19:V:804:HEC:HMC1	2.32	0.60
10:Q:398:PHE:HA	10:Q:401:VAL:HG12	1.83	0.59
7:P:139:ASN:ND2	7:P:205:GLY:O	2.35	0.59
10:V:161:MET:HG2	19:V:804:HEC:HBC1	1.79	0.59
10:V:538:SER:HB3	10:V:555:ARG:HH12	1.68	0.59
7:L:87:GLN:NE2	10:Q:287:ARG:O	2.35	0.59
11:S:48:LEU:HG	12:W:34:SER:HB3	1.84	0.59
11:S:81:GLU:HA	13:Y:451:LYS:HA	1.85	0.58
15:M:301:CDL:HA22	11:X:137:GLU:HG2	1.86	0.58
10:V:310:VAL:O	10:V:313:HIS:ND1	2.29	0.58
1:B:351:LEU:HD23	1:B:358:GLN:HG2	1.84	0.58
10:V:270:ILE:HG23	10:V:406:ILE:HD11	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:P:252:ASN:ND2	10:V:250:GLY:O	2.36	0.58
7:P:225:LEU:HB3	7:P:245:VAL:HG12	1.86	0.57
1:B:335:HIS:ND1	14:B:501:FES:S1	2.78	0.57
1:B:351:LEU:HD13	1:B:352:CYS:N	2.19	0.57
1:B:208:LYS:HB2	13:Y:191:TRP:HB3	1.86	0.57
12:W:69:LEU:HD12	12:W:69:LEU:O	2.04	0.57
10:Q:270:ILE:HG23	10:Q:406:ILE:HD11	1.86	0.57
11:S:42:LEU:HA	11:S:45:THR:HG22	1.86	0.57
13:Y:418:LEU:HD21	15:Y:604:CDL:H621	1.87	0.57
10:V:30:LYS:HG2	10:V:30:LYS:O	2.03	0.57
10:V:112:GLY:HA3	10:V:198:ALA:HB2	1.86	0.57
7:P:289:ARG:HH12	7:P:323:ILE:HG23	1.70	0.56
6:K:242:PRO:HG2	13:Y:300:GLN:HG3	1.87	0.56
9:T:25:SER:OG	10:V:532:GLU:OE2	2.24	0.56
10:V:279:THR:HG22	10:V:344:TRP:HE1	1.70	0.56
7:L:87:GLN:OE1	10:Q:540:ARG:NH2	2.35	0.56
7:L:248:GLU:O	7:L:252:ASN:ND2	2.38	0.56
1:A:241:LEU:HD12	1:A:389:LEU:HB3	1.87	0.56
1:B:241:LEU:HD12	1:B:389:LEU:HB3	1.86	0.56
9:O:25:SER:OG	10:Q:532:GLU:OE2	2.22	0.56
9:T:25:SER:H	10:V:532:GLU:HG2	1.71	0.56
10:Q:291:PHE:H	10:Q:347:THR:HB	1.71	0.56
13:Y:39:SER:HB3	13:Y:126:ARG:HG3	1.87	0.56
12:Z:131:ILE:HG23	12:Z:132:PRO:HD3	1.88	0.55
15:Y:603:CDL:H132	15:Y:603:CDL:H512	1.89	0.55
6:K:256:ALA:HB2	15:K:301:CDL:H432	1.89	0.55
7:L:35:TRP:HZ3	7:L:46:ASN:HB3	1.72	0.55
13:Y:121:MET:HB3	16:Y:606:MQ9:H272	1.86	0.55
10:V:29:TYR:O	10:V:30:LYS:HB3	2.06	0.55
1:B:351:LEU:HD13	1:B:351:LEU:C	2.26	0.55
8:N:51:ALA:HB2	9:O:55:LEU:HB3	1.87	0.55
10:Q:283:PRO:HG2	10:Q:290:VAL:HG22	1.88	0.55
10:Q:312:ALA:HA	10:Q:315:LEU:HD13	1.89	0.55
15:V:805:CDL:H441	12:Z:149:LEU:HD22	1.88	0.55
10:Q:197:ARG:NH1	11:S:68:GLU:O	2.39	0.55
1:B:94:PHE:O	13:Y:100:ARG:NH2	2.38	0.55
13:Y:134:ARG:NH1	13:Y:363:LEU:O	2.40	0.55
8:R:44:HIS:NE2	9:T:40:HIS:O	2.41	0.54
1:B:322:ASN:HD22	1:B:327:PHE:HE1	1.54	0.54
10:Q:496:PHE:O	10:Q:500:ARG:NH1	2.41	0.54
13:Y:212:ILE:HG23	20:Y:601:HEM:HAC	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:180:ARG:NH1	1:B:69:GLU:OE2	2.40	0.54
13:Y:464:PRO:HB3	13:Y:474:PRO:HB3	1.88	0.54
1:B:59:PRO:HA	1:B:143:PRO:HB3	1.89	0.54
15:Q:804:CDL:OA3	12:W:164:ARG:NH2	2.41	0.53
13:Y:225:ALA:HB2	16:Y:605:MQ9:H451	1.91	0.53
1:B:120:GLY:HA3	13:Y:277:GLY:HA3	1.91	0.53
11:S:5:ALA:HB3	11:S:57:ARG:HH21	1.73	0.53
2:C:5:UNK:O	13:Y:435:ARG:NH1	2.42	0.53
10:Q:395:VAL:O	10:Q:399:HIS:ND1	2.32	0.53
10:Q:140:PHE:HA	10:Q:146:PRO:HD3	1.89	0.53
7:P:215:LEU:HD22	7:P:221:ILE:HG21	1.91	0.53
12:W:65:LEU:O	12:W:203:ARG:NH2	2.42	0.52
1:B:357:SER:OG	14:B:501:FES:S1	2.68	0.52
10:Q:317:ALA:HB2	10:Q:389:THR:HG21	1.91	0.52
11:X:42:LEU:HA	11:X:45:THR:HG22	1.90	0.52
10:Q:33:THR:HG22	11:S:90:TRP:HB3	1.90	0.52
10:V:63:ARG:NH2	18:V:802:HAS:OMD	2.42	0.52
10:V:202:ILE:HG12	10:V:205:ARG:HG2	1.92	0.52
10:V:291:PHE:O	10:V:343:ASN:ND2	2.42	0.52
10:Q:279:THR:HG22	10:Q:344:TRP:HE1	1.74	0.52
10:V:534:PRO:HB3	10:V:545:LEU:HD22	1.91	0.52
12:W:162:LEU:HB3	13:Y:502:PHE:HZ	1.75	0.51
7:L:133:VAL:HG21	7:L:225:LEU:HD23	1.92	0.51
1:B:145:GLU:OE1	1:B:147:SER:OG	2.28	0.51
8:N:35:THR:HG22	9:O:44:PRO:HD3	1.91	0.51
1:A:253:PHE:HE2	1:A:290:GLU:HG2	1.75	0.51
10:Q:65:GLU:HG3	10:Q:74:LEU:HD12	1.92	0.51
8:N:44:HIS:NE2	9:O:40:HIS:O	2.43	0.51
7:L:33:LEU:H	7:L:50:TRP:HE1	1.58	0.51
9:O:100:SER:HB2	9:O:105:ALA:HB3	1.91	0.51
10:V:161:MET:C	19:V:804:HEC:CBC	2.64	0.50
10:V:355:PHE:HE1	10:V:363:VAL:HG21	1.76	0.50
12:Z:25:VAL:HG12	12:Z:180:VAL:HG11	1.93	0.50
7:L:131:ILE:HD13	7:L:213:LEU:HD11	1.92	0.50
13:Y:30:LEU:HG	13:Y:254:MET:HB2	1.93	0.50
13:Y:230:VAL:HG21	20:Y:602:HEM:HAD1	1.92	0.50
10:Q:223:ALA:HB2	10:Q:265:PRO:HB2	1.93	0.50
1:A:237:GLU:OE2	1:A:273:ARG:NH1	2.43	0.50
10:Q:114:PRO:O	10:Q:529:ASN:ND2	2.44	0.50
9:T:55:LEU:HD23	9:T:147:VAL:HG11	1.94	0.50
10:V:81:GLN:HB2	10:V:146:PRO:HG2	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:Q:216:THR:HG21	10:Q:273:PRO:HD3	1.93	0.50
7:L:143:GLY:HA2	7:L:202:GLU:HA	1.94	0.50
13:Y:296:SER:OG	13:Y:298:GLY:O	2.29	0.50
1:A:245:THR:HG1	1:A:251:SER:HG	1.54	0.50
10:V:291:PHE:H	10:V:347:THR:HB	1.77	0.50
10:Q:310:VAL:O	10:Q:313:HIS:ND1	2.45	0.50
10:V:535:ARG:HH22	11:X:72:ASP:HB2	1.76	0.49
7:L:199:ASP:OD1	7:L:199:ASP:N	2.45	0.49
1:A:315:ARG:NH1	1:A:397:GLU:OE2	2.38	0.49
10:V:312:ALA:HA	10:V:315:LEU:HD13	1.93	0.49
11:S:52:THR:HG1	12:W:34:SER:HG	1.59	0.49
10:V:536:ILE:HD13	10:V:541:PRO:HG3	1.94	0.49
12:Z:71:VAL:HA	12:Z:74:THR:HG22	1.95	0.49
10:Q:446:PHE:HA	10:Q:449:HIS:HD1	1.77	0.49
7:P:65:TRP:HZ2	10:V:371:LEU:HD11	1.77	0.49
10:V:191:THR:HG22	12:Z:27:VAL:HG12	1.95	0.49
7:L:28:SER:OG	7:L:29:ASP:N	2.46	0.49
15:Y:604:CDL:H512	15:Y:604:CDL:H711	1.94	0.49
10:Q:534:PRO:HB3	10:Q:545:LEU:HD22	1.93	0.49
15:K:301:CDL:H182	15:K:301:CDL:H412	1.93	0.49
13:Y:453:LEU:HB2	13:Y:457:ALA:HB3	1.94	0.49
10:V:27:LEU:O	10:V:31:LEU:HB2	2.13	0.49
10:V:120:ARG:NH2	11:X:128:LEU:O	2.45	0.49
10:V:216:THR:HG21	10:V:273:PRO:HD3	1.95	0.49
1:B:150:ASP:OD1	1:B:150:ASP:N	2.45	0.49
5:F:13:UNK:HA	11:S:84:PHE:HB2	1.93	0.49
7:L:274:THR:HB	10:Q:390:ASP:HB3	1.95	0.49
13:Y:47:LEU:HD11	13:Y:227:LEU:HD21	1.95	0.48
1:B:245:THR:OG1	1:B:251:SER:OG	2.28	0.48
10:Q:287:ARG:HD3	10:Q:352:GLN:HG2	1.94	0.48
10:Q:377:VAL:HG21	18:Q:801:HAS:H241	1.95	0.48
10:V:159:ASN:O	10:V:238:ARG:NH1	2.45	0.48
1:B:328:ALA:HB2	1:B:381:ILE:HD11	1.95	0.48
7:P:220:ARG:NH2	7:P:259:GLN:OE1	2.47	0.48
10:Q:136:ALA:HB2	10:Q:174:GLY:HA3	1.95	0.48
13:Y:148:LEU:HB2	20:Y:602:HEM:HBB1	1.95	0.48
13:Y:312:ILE:HG12	13:Y:333:VAL:HG21	1.94	0.48
10:V:254:LEU:HD21	12:Z:46:MET:HG2	1.95	0.48
10:V:424:ARG:NH1	10:V:500:ARG:O	2.46	0.48
7:L:239:PHE:O	7:L:241:PHE:N	2.47	0.48
1:A:334:SER:O	1:A:374:ARG:NH2	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:59:PRO:HA	1:A:143:PRO:HB3	1.94	0.48
13:Y:126:ARG:HH22	20:Y:602:HEM:HBA1	1.78	0.48
15:Y:603:CDL:H251	15:Y:604:CDL:H272	1.96	0.48
7:P:60:VAL:HG11	18:V:801:HAS:H22	1.96	0.48
8:R:49:TRP:CG	10:V:16:PRO:HG3	2.49	0.48
1:B:379:LEU:HD12	1:B:380:PRO:HD2	1.95	0.48
15:K:301:CDL:H791	15:K:301:CDL:H762	1.63	0.47
15:Y:603:CDL:H712	15:Y:604:CDL:H712	1.96	0.47
10:V:310:VAL:HG11	10:V:333:ILE:HD11	1.96	0.47
7:P:167:MET:O	7:P:194:THR:N	2.47	0.47
10:Q:55:GLY:O	10:Q:86:HIS:ND1	2.43	0.47
7:P:239:PHE:O	7:P:241:PHE:N	2.48	0.47
7:L:215:LEU:HD22	7:L:221:ILE:HD13	1.97	0.47
10:Q:536:ILE:HD13	10:Q:541:PRO:HG3	1.95	0.47
7:P:167:MET:HB3	7:P:194:THR:HG23	1.95	0.47
12:Z:36:GLU:OE1	12:Z:150:HIS:NE2	2.48	0.47
1:B:231:THR:HA	1:B:394:ASP:HB3	1.95	0.47
9:O:85:LEU:HD21	9:O:111:GLY:HA2	1.96	0.47
10:Q:135:ILE:HD11	11:S:100:SER:HB2	1.97	0.47
18:Q:801:HAS:H172	18:Q:801:HAS:H202	1.74	0.47
11:S:52:THR:OG1	12:W:34:SER:OG	2.32	0.47
13:Y:227:LEU:HA	13:Y:230:VAL:HG12	1.97	0.47
15:M:301:CDL:H572	11:X:123:THR:HG21	1.96	0.47
13:Y:57:GLY:O	13:Y:61:THR:OG1	2.25	0.47
1:B:348:TYR:HB3	1:B:361:ALA:HB3	1.97	0.47
10:Q:254:LEU:HD21	12:W:46:MET:HG2	1.97	0.47
10:V:270:ILE:HG22	18:V:801:HAS:HBC2	1.96	0.47
13:Y:68:MET:HG2	13:Y:204:ILE:HD12	1.96	0.47
9:T:43:PHE:HZ	9:T:139:LEU:HD23	1.80	0.46
9:O:55:LEU:HD23	9:O:147:VAL:HG11	1.97	0.46
9:O:114:VAL:HG12	9:O:117:ARG:HH11	1.80	0.46
10:Q:112:GLY:HA3	10:Q:198:ALA:HB2	1.98	0.46
13:Y:120:ILE:HG12	20:Y:602:HEM:HMC1	1.97	0.46
10:Q:424:ARG:NH1	10:Q:500:ARG:O	2.42	0.46
1:A:103:PRO:HG2	1:A:106:SER:HB2	1.96	0.46
10:V:161:MET:HG3	19:V:804:HEC:CMC	2.41	0.46
10:V:535:ARG:NH1	10:V:536:ILE:O	2.48	0.46
16:Y:605:MQ9:H303	16:Y:605:MQ9:H351	1.97	0.46
10:V:382:PRO:HA	10:V:385:ASP:HB3	1.98	0.46
7:L:85:PRO:HG2	10:Q:351:GLY:HA2	1.98	0.46
1:A:379:LEU:HD12	1:A:380:PRO:HD2	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:357:SER:HA	1:B:370:GLY:HA3	1.98	0.46
7:P:250:LYS:HE2	7:P:256:ASN:HD22	1.80	0.46
9:T:38:SER:OG	10:V:504:PRO:O	2.30	0.46
11:S:2:HIS:HE1	11:S:6:ARG:HH21	1.63	0.46
7:L:319:PRO:HA	7:L:320:PRO:HD3	1.79	0.46
7:P:194:THR:OG1	7:P:195:TYR:N	2.44	0.46
1:B:116:THR:HG23	1:B:117:PRO:HD3	1.97	0.46
7:P:85:PRO:HG2	7:P:87:GLN:HG3	1.98	0.46
1:A:308:ASP:HB3	1:A:311:ARG:HH21	1.81	0.45
1:B:230:TRP:CE2	1:B:271:PRO:HG3	2.51	0.45
10:Q:396:ALA:HB2	10:Q:449:HIS:HB2	1.98	0.45
15:M:301:CDL:H751	15:M:301:CDL:H781	1.69	0.45
1:B:351:LEU:C	1:B:351:LEU:CD1	2.85	0.45
7:L:109:LEU:HD12	18:Q:801:HAS:H321	1.99	0.45
15:Q:804:CDL:HB62	15:Q:804:CDL:H712	1.73	0.45
10:Q:288:LYS:NZ	10:Q:346:GLY:O	2.32	0.45
13:Y:237:GLN:NE2	13:Y:247:ASN:O	2.49	0.45
16:M:302:MQ9:H353	16:M:302:MQ9:H371	1.78	0.45
7:L:235:TRP:HB2	7:L:242:LYS:HG3	1.97	0.45
9:T:85:LEU:HD21	9:T:111:GLY:HA2	1.98	0.45
1:B:373:ALA:HB2	13:Y:317:ALA:HB1	1.97	0.45
10:Q:109:LEU:HB3	10:Q:518:GLU:HB3	1.98	0.45
16:Y:605:MQ9:H5M3	16:Y:605:MQ9:H71	1.67	0.45
9:O:122:ALA:O	9:O:126:GLY:N	2.49	0.45
7:L:35:TRP:CD1	10:Q:454:ALA:HB1	2.51	0.45
10:Q:11:LEU:HD13	10:Q:12:LEU:HB2	1.98	0.45
10:V:283:PRO:HB2	10:V:515:ASN:HD21	1.82	0.45
7:L:142:PHE:HB2	7:L:203:THR:HB	1.98	0.45
10:Q:98:ILE:HG23	10:Q:274:PHE:HZ	1.82	0.45
10:Q:365:PHE:HE1	10:Q:405:THR:HG22	1.81	0.44
10:V:259:PHE:O	10:V:263:GLY:N	2.50	0.44
12:Z:192:TRP:O	12:Z:196:PHE:N	2.47	0.44
13:Y:235:HIS:NE2	20:Y:602:HEM:O2D	2.46	0.44
10:Q:355:PHE:HE1	10:Q:363:VAL:HG21	1.82	0.44
10:V:11:LEU:HD13	10:V:12:LEU:HB2	1.99	0.44
10:V:98:ILE:HG23	10:V:274:PHE:HZ	1.82	0.44
10:V:446:PHE:HA	10:V:449:HIS:HD1	1.82	0.44
19:V:804:HEC:HMB1	19:V:804:HEC:HBB3	2.00	0.44
7:L:289:ARG:HH12	7:L:323:ILE:HG23	1.83	0.44
7:L:299:TYR:OH	7:L:309:ASN:OD1	2.33	0.44
11:S:63:LEU:CD2	11:S:63:LEU:C	2.86	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:Y:604:CDL:H351	16:Y:606:MQ9:H202	1.99	0.44
19:V:804:HEC:HMB1	19:V:804:HEC:HBB2	2.00	0.44
11:X:9:GLU:HA	11:X:12:THR:HG22	2.00	0.44
19:V:804:HEC:HBC2	19:V:804:HEC:HMC1	2.00	0.44
11:S:108:LEU:HD13	13:Y:400:PHE:HA	2.00	0.44
10:V:96:THR:HG22	10:V:269:ILE:HD11	1.99	0.44
10:Q:59:ALA:HB2	10:Q:86:HIS:CE1	2.52	0.44
1:A:67:LYS:HG2	1:A:71:ARG:HH21	1.83	0.43
10:V:169:ASP:OD1	10:V:238:ARG:NE	2.40	0.43
1:B:230:TRP:NE1	1:B:297:ASN:O	2.47	0.43
10:Q:282:PHE:O	10:Q:286:SER:OG	2.34	0.43
19:V:804:HEC:HMC1	19:V:804:HEC:HBC3	2.00	0.43
15:V:805:CDL:OA4	12:Z:164:ARG:NH2	2.51	0.43
1:A:230:TRP:CE2	1:A:271:PRO:HG3	2.54	0.43
7:P:46:ASN:ND2	7:P:240:LEU:O	2.50	0.43
13:Y:48:TYR:OH	13:Y:261:SER:OG	2.34	0.43
7:P:88:PHE:HA	10:V:558:SER:HA	2.00	0.43
7:P:215:LEU:HD13	7:P:221:ILE:HD13	2.00	0.43
9:T:88:VAL:HA	9:T:89:PRO:HD3	1.92	0.43
10:V:29:TYR:O	10:V:30:LYS:CB	2.66	0.43
10:Q:202:ILE:HG12	10:Q:205:ARG:HG2	2.01	0.43
16:Y:605:MQ9:H153	16:Y:605:MQ9:H171	1.71	0.43
10:V:372:GLY:HA3	10:V:401:VAL:HB	2.00	0.43
10:Q:121:LEU:HD11	15:Q:804:CDL:H712	2.01	0.43
10:Q:517:LEU:HG	10:Q:541:PRO:HG2	2.00	0.43
10:V:33:THR:HG22	11:X:90:TRP:HB3	2.00	0.43
7:L:300:ILE:O	7:L:304:ASN:N	2.43	0.43
1:A:351:LEU:C	1:A:351:LEU:CD2	2.86	0.43
7:P:131:ILE:HD13	7:P:213:LEU:HD11	2.01	0.43
15:K:301:CDL:H451	15:K:301:CDL:H611	1.76	0.43
10:Q:27:LEU:HG	10:Q:31:LEU:HD13	2.01	0.43
1:A:302:ILE:HG23	1:A:327:PHE:HB2	2.01	0.43
10:V:452:LEU:HD12	10:V:473:LEU:HB3	2.01	0.43
1:B:358:GLN:HB2	1:B:369:PHE:HB3	2.00	0.43
5:J:6:UNK:N	12:Z:21:ARG:O	2.52	0.43
7:P:242:LYS:HE3	7:P:274:THR:HG21	2.00	0.43
12:W:91:ALA:HB2	12:W:99:LEU:HD13	2.00	0.43
13:Y:110:HIS:HB3	13:Y:281:ILE:HG12	2.00	0.43
7:P:114:VAL:HA	7:P:117:GLN:HG2	2.01	0.42
1:B:336:LEU:HG	13:Y:177:GLY:HA3	2.01	0.42
10:V:378:ILE:HG23	10:V:384:LEU:HD23	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:V:394:VAL:HG12	10:V:398:PHE:HE2	1.85	0.42
1:B:315:ARG:HB3	1:B:318:GLN:HB2	1.99	0.42
12:W:24:MET:HB2	12:W:24:MET:HE3	1.84	0.42
13:Y:422:VAL:HA	13:Y:425:VAL:HG12	2.01	0.42
7:P:141:LYS:NZ	7:P:202:GLU:OE1	2.43	0.42
16:Y:605:MQ9:H253	16:Y:605:MQ9:H271	1.64	0.42
1:A:198:THR:HG22	1:B:123:PHE:HE1	1.85	0.42
7:L:146:LYS:HA	7:L:157:ASP:HA	2.02	0.42
10:Q:537:ARG:HE	11:S:72:ASP:HB2	1.84	0.42
10:V:59:ALA:HB2	10:V:86:HIS:CE1	2.53	0.42
1:B:351:LEU:HD23	1:B:358:GLN:CG	2.48	0.42
12:W:70:ALA:N	12:W:72:PRO:HD2	2.34	0.42
7:L:215:LEU:HD22	7:L:221:ILE:HG21	2.00	0.42
12:W:164:ARG:O	12:W:174:GLN:NE2	2.49	0.42
13:Y:42:LEU:HD13	13:Y:122:VAL:HG12	2.01	0.42
10:V:382:PRO:O	10:V:386:PHE:N	2.50	0.42
13:Y:422:VAL:HG13	15:Y:604:CDL:H771	2.02	0.42
16:M:302:MQ9:H221	16:M:302:MQ9:H262	1.83	0.42
10:V:391:SER:OG	10:V:392:TYR:N	2.52	0.42
15:K:301:CDL:H832	11:S:119:ALA:HB2	2.01	0.42
1:A:34:LEU:HD11	1:B:159:VAL:HG12	2.02	0.42
6:M:247:MET:SD	16:M:302:MQ9:H3D	2.60	0.42
13:Y:80:LEU:HD11	13:Y:289:PRO:HD3	2.02	0.42
16:Y:606:MQ9:H203	16:Y:606:MQ9:H221	1.80	0.42
16:M:302:MQ9:H172	16:M:302:MQ9:H211	1.84	0.42
10:Q:62:LEU:HG	10:Q:79:TYR:CZ	2.54	0.42
12:W:47:TYR:CZ	12:W:199:ILE:HG22	2.54	0.42
13:Y:182:ILE:HA	13:Y:183:PRO:HD3	1.92	0.42
10:V:197:ARG:HB2	11:X:68:GLU:HG2	2.02	0.41
12:Z:69:LEU:HD21	12:Z:119:TYR:HD2	1.85	0.41
15:K:301:CDL:H371	15:K:301:CDL:H142	2.01	0.41
1:A:159:VAL:HG12	1:B:34:LEU:HD11	2.02	0.41
18:V:801:HAS:H251	18:V:801:HAS:H281	1.79	0.41
10:Q:89:VAL:HG22	10:Q:93:PHE:HD2	1.85	0.41
7:L:243:ARG:HH12	7:L:255:ASP:HB3	1.85	0.41
10:Q:243:HIS:HB2	12:W:135:ALA:HA	2.02	0.41
10:Q:410:THR:O	10:Q:414:VAL:N	2.49	0.41
1:A:73:GLU:HB2	1:B:183:ILE:HD11	2.02	0.41
15:M:301:CDL:H471	15:M:301:CDL:H861	2.03	0.41
7:P:49:LEU:HD22	7:P:116:VAL:HG21	2.03	0.41
10:V:31:LEU:O	10:V:34:THR:HG22	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:V:420:LYS:NZ	10:V:521:THR:O	2.54	0.41
18:Q:802:HAS:H171	18:Q:802:HAS:H261	1.74	0.41
12:W:29:THR:O	12:W:33:LEU:N	2.48	0.41
12:W:33:LEU:HD21	12:W:184:TYR:HD1	1.86	0.41
15:Y:604:CDL:H181	16:Y:606:MQ9:H18	2.03	0.41
1:A:150:ASP:OD1	1:A:150:ASP:N	2.51	0.41
1:B:227:THR:HA	1:B:231:THR:HG21	2.02	0.41
1:B:374:ARG:CZ	1:B:402:ALA:HB2	2.51	0.41
1:B:380:PRO:HB2	1:B:392:ASN:HB2	2.02	0.41
7:L:49:LEU:HG	10:Q:384:LEU:HD11	2.02	0.41
8:N:49:TRP:CG	10:Q:16:PRO:HG3	2.55	0.41
10:Q:425:LEU:HG	10:Q:505:VAL:HG22	2.03	0.41
13:Y:175:LEU:O	13:Y:179:THR:OG1	2.39	0.41
13:Y:489:ASN:N	13:Y:489:ASN:OD1	2.54	0.41
10:Q:62:LEU:HG	10:Q:79:TYR:CE1	2.55	0.41
10:Q:191:THR:HG21	12:W:28:GLY:HA2	2.03	0.41
1:A:406:ARG:NE	1:A:408:SER:OG	2.53	0.40
10:V:480:GLY:HA2	10:V:483:ILE:HD12	2.03	0.40
1:B:356:GLN:NE2	13:Y:394:ASP:HB3	2.35	0.40
1:B:262:ASP:OD1	1:B:262:ASP:N	2.54	0.40
10:Q:419:PRO:HG3	10:Q:425:LEU:HD23	2.03	0.40
13:Y:354:VAL:HG23	13:Y:355:THR:HG23	2.04	0.40
1:A:69:GLU:OE2	1:B:180:ARG:NH1	2.45	0.40
7:P:87:GLN:HG2	10:V:288:LYS:HA	2.02	0.40
18:V:801:HAS:HMB1	18:V:801:HAS:H11	1.89	0.40
1:B:253:PHE:HZ	1:B:291:ILE:HD11	1.86	0.40
7:L:104:LEU:HA	7:L:107:SER:HB3	2.03	0.40
10:Q:274:PHE:CE1	10:Q:410:THR:HG22	2.57	0.40
1:A:258:PRO:HB3	1:A:389:LEU:HD21	2.03	0.40
10:V:71:LEU:HD12	10:V:463:ASP:HB2	2.03	0.40
10:V:135:ILE:HD11	11:X:100:SER:HB2	2.03	0.40
10:V:313:HIS:HD2	18:V:801:HAS:C2D	2.35	0.40
1:B:106:SER:OG	1:B:107:GLU:N	2.53	0.40
1:B:302:ILE:HD12	1:B:329:TYR:HD2	1.86	0.40
10:Q:303:ILE:HG13	10:Q:336:PRO:HB2	2.03	0.40
1:A:298:PRO:HB2	1:A:331:LYS:HD3	2.04	0.40
7:P:299:TYR:OH	7:P:309:ASN:OD1	2.37	0.40
8:R:51:ALA:HB2	9:T:55:LEU:HB3	2.02	0.40
10:V:55:GLY:O	10:V:86:HIS:ND1	2.40	0.40
10:V:173:PHE:HB3	11:X:103:ALA:HB1	2.04	0.40
13:Y:61:THR:HG23	13:Y:212:ILE:HD13	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:Y:603:CDL:H782	15:Y:604:CDL:H781	2.02	0.40
16:Y:605:MQ9:H303	16:Y:605:MQ9:H322	1.69	0.40

There are no symmetry-related clashes.

## 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 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	378/408 (93%)	335 (89%)	43 (11%)	0	100	100
1	B	378/408 (93%)	335 (89%)	43 (11%)	0	100	100
6	K	28/268 (10%)	27 (96%)	1 (4%)	0	100	100
6	M	28/268 (10%)	26 (93%)	2 (7%)	0	100	100
6	i	158/268 (59%)	143 (90%)	11 (7%)	4 (2%)	4	24
6	j	158/268 (59%)	145 (92%)	13 (8%)	0	100	100
7	L	277/341 (81%)	234 (84%)	43 (16%)	0	100	100
7	P	277/341 (81%)	236 (85%)	41 (15%)	0	100	100
8	N	52/79 (66%)	41 (79%)	11 (21%)	0	100	100
8	R	52/79 (66%)	44 (85%)	8 (15%)	0	100	100
9	O	140/157 (89%)	130 (93%)	10 (7%)	0	100	100
9	T	140/157 (89%)	129 (92%)	11 (8%)	0	100	100
10	Q	548/583 (94%)	504 (92%)	44 (8%)	0	100	100
10	V	548/583 (94%)	504 (92%)	44 (8%)	0	100	100
11	S	137/139 (99%)	131 (96%)	6 (4%)	0	100	100
11	X	137/139 (99%)	131 (96%)	6 (4%)	0	100	100
12	W	182/203 (90%)	166 (91%)	16 (9%)	0	100	100
12	Z	182/203 (90%)	169 (93%)	13 (7%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	Y	534/554 (96%)	489 (92%)	45 (8%)	0	100	100
13	b	534/554 (96%)	486 (91%)	48 (9%)	0	100	100
All	All	4868/6000 (81%)	4405 (90%)	459 (9%)	4 (0%)	50	76

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	i	73	PRO
6	i	77	PRO
6	i	110	PRO
6	i	200	PRO

### 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	310/333 (93%)	310 (100%)	0	100	100
1	B	310/333 (93%)	310 (100%)	0	100	100
6	K	18/197 (9%)	18 (100%)	0	100	100
6	M	18/197 (9%)	18 (100%)	0	100	100
7	L	239/288 (83%)	237 (99%)	2 (1%)	79	87
7	P	239/288 (83%)	236 (99%)	3 (1%)	65	79
8	N	44/59 (75%)	44 (100%)	0	100	100
8	R	44/59 (75%)	44 (100%)	0	100	100
9	O	105/114 (92%)	105 (100%)	0	100	100
9	T	105/114 (92%)	105 (100%)	0	100	100
10	Q	456/481 (95%)	452 (99%)	4 (1%)	75	85
10	V	456/481 (95%)	451 (99%)	5 (1%)	70	82
11	S	106/106 (100%)	106 (100%)	0	100	100
11	X	106/106 (100%)	106 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
12	W	146/161 (91%)	146 (100%)	0	100	100
12	Z	146/161 (91%)	146 (100%)	0	100	100
13	Y	431/446 (97%)	430 (100%)	1 (0%)	92	95
13	b	431/446 (97%)	431 (100%)	0	100	100
All	All	3710/4370 (85%)	3695 (100%)	15 (0%)	88	93

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
7	P	76	ARG
7	P	77	LYS
7	P	86	ARG
10	V	20	ARG
10	V	226	LEU
10	V	288	LYS
10	V	392	TYR
10	V	527	ARG
7	L	76	ARG
7	L	139	ASN
10	Q	288	LYS
10	Q	353	LEU
10	Q	421	MET
10	Q	527	ARG
13	Y	60	LEU

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

Mol	Chain	Res	Type
13	b	365	GLN

### 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 ⓘ

Of 32 ligands modelled in this entry, 6 are monoatomic - leaving 26 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
15	CDL	Q	804	-	86,86,99	1.23	8 (9%)	92,98,111	1.06	4 (4%)
19	HEC	j	301	6	32,50,50	2.26	12 (37%)	24,82,82	1.92	3 (12%)
15	CDL	K	301	-	99,99,99	1.19	8 (8%)	105,111,111	0.97	4 (3%)
18	HAS	Q	801	10	69,72,72	1.23	7 (10%)	73,109,109	1.39	10 (13%)
16	MQ9	M	302	-	59,59,59	1.02	4 (6%)	72,75,75	1.40	11 (15%)
14	FES	A	501	1	0,4,4	-	-	-	-	-
16	MQ9	b	605	-	59,59,59	0.93	1 (1%)	72,75,75	1.52	15 (20%)
18	HAS	Q	802	10	69,72,72	1.29	8 (11%)	73,109,109	1.37	6 (8%)
16	MQ9	Y	606	-	59,59,59	1.24	7 (11%)	72,75,75	1.47	11 (15%)
15	CDL	M	301	-	99,99,99	1.19	8 (8%)	105,111,111	0.97	4 (3%)
19	HEC	V	804	-	32,50,50	2.25	12 (37%)	24,82,82	1.93	3 (12%)
19	HEC	j	302	-	32,50,50	2.24	12 (37%)	24,82,82	1.92	3 (12%)
20	HEM	b	601	13	41,50,50	1.44	7 (17%)	45,82,82	2.49	17 (37%)
20	HEM	Y	602	13	41,50,50	1.47	7 (17%)	45,82,82	2.05	12 (26%)
20	HEM	Y	601	13	41,50,50	1.38	6 (14%)	45,82,82	1.97	12 (26%)
19	HEC	i	301	-	32,50,50	2.25	12 (37%)	24,82,82	1.93	3 (12%)
15	CDL	Y	603	-	90,90,99	1.19	8 (8%)	96,102,111	1.03	5 (5%)
14	FES	B	501	1	0,4,4	-	-	-	-	-
18	HAS	V	802	10	69,72,72	1.23	7 (10%)	73,109,109	1.33	7 (9%)
15	CDL	b	604	-	90,90,99	1.21	8 (8%)	96,102,111	0.97	4 (4%)
18	HAS	V	801	10	69,72,72	1.24	6 (8%)	73,109,109	1.45	13 (17%)
20	HEM	b	602	13	41,50,50	1.45	7 (17%)	45,82,82	2.48	15 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
16	MQ9	Y	605	-	59,59,59	0.88	1 (1%)	72,75,75	1.50	12 (16%)
15	CDL	V	805	-	86,86,99	1.23	9 (10%)	92,98,111	1.01	4 (4%)
15	CDL	Y	604	-	91,91,99	1.18	7 (7%)	97,103,111	1.04	5 (5%)
15	CDL	b	603	-	91,91,99	1.18	6 (6%)	97,103,111	1.08	4 (4%)

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
15	CDL	Q	804	-	-	47/97/97/110	-
19	HEC	j	301	6	-	3/10/54/54	-
15	CDL	K	301	-	-	56/110/110/110	-
18	HAS	Q	801	10	1/1/8/18	7/40/82/82	-
16	MQ9	M	302	-	-	8/53/73/73	0/2/2/2
16	MQ9	b	605	-	-	15/53/73/73	0/2/2/2
14	FES	A	501	1	-	-	0/1/1/1
18	HAS	Q	802	10	1/1/8/18	11/40/82/82	-
16	MQ9	Y	606	-	-	9/53/73/73	0/2/2/2
15	CDL	M	301	-	-	55/110/110/110	-
19	HEC	V	804	-	-	3/10/54/54	-
19	HEC	j	302	-	-	3/10/54/54	-
20	HEM	b	601	13	-	10/12/54/54	-
20	HEM	Y	602	13	-	4/12/54/54	-
20	HEM	Y	601	13	-	5/12/54/54	-
19	HEC	i	301	-	-	3/10/54/54	-
15	CDL	Y	603	-	-	56/101/101/110	-
14	FES	B	501	1	-	-	0/1/1/1
18	HAS	V	802	10	1/1/8/18	11/40/82/82	-
15	CDL	b	604	-	-	55/101/101/110	-
18	HAS	V	801	10	1/1/8/18	11/40/82/82	-
20	HEM	b	602	13	-	5/12/54/54	-
16	MQ9	Y	605	-	-	16/53/73/73	0/2/2/2
15	CDL	V	805	-	-	46/97/97/110	-
15	CDL	Y	604	-	-	61/102/102/110	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	CDL	b	603	-	-	44/102/102/110	-

All (178) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	j	301	HEC	C2B-C3B	6.07	1.47	1.40
19	j	301	HEC	C3C-C2C	6.05	1.47	1.40
19	V	804	HEC	C2B-C3B	6.04	1.47	1.40
19	i	301	HEC	C2B-C3B	6.03	1.47	1.40
19	j	302	HEC	C2B-C3B	6.00	1.47	1.40
19	V	804	HEC	C3C-C2C	6.00	1.47	1.40
19	i	301	HEC	C3C-C2C	5.99	1.47	1.40
19	j	302	HEC	C3C-C2C	5.95	1.47	1.40
18	V	801	HAS	C3C-CAC	-4.71	1.38	1.47
18	Q	801	HAS	C3C-CAC	-4.43	1.38	1.47
18	Q	802	HAS	C3C-CAC	-4.41	1.39	1.47
20	b	602	HEM	CBB-CAB	4.29	1.51	1.30
20	Y	601	HEM	CBB-CAB	4.09	1.50	1.30
20	Y	602	HEM	CBB-CAB	4.09	1.50	1.30
20	b	601	HEM	CBB-CAB	3.91	1.49	1.30
18	V	802	HAS	C3C-CAC	-3.83	1.40	1.47
15	K	301	CDL	OA8-CA7	3.67	1.44	1.33
15	Y	604	CDL	OA8-CA7	3.52	1.43	1.33
15	b	604	CDL	OA8-CA7	3.50	1.43	1.33
15	Y	603	CDL	OA8-CA7	3.49	1.43	1.33
15	M	301	CDL	OA8-CA7	3.48	1.43	1.33
20	b	601	HEM	C4D-ND	-3.47	1.34	1.40
18	Q	801	HAS	C3C-C2C	-3.44	1.35	1.40
16	Y	606	MQ9	C25-C24	-3.44	1.41	1.50
15	b	603	CDL	OA8-CA7	3.44	1.43	1.33
15	Q	804	CDL	OA8-CA7	3.35	1.43	1.33
19	j	301	HEC	C2A-C3A	3.35	1.47	1.37
15	b	604	CDL	OA6-CA4	-3.35	1.38	1.46
19	j	301	HEC	C3D-C2D	3.35	1.47	1.37
19	V	804	HEC	C2A-C3A	3.35	1.47	1.37
19	i	301	HEC	C2A-C3A	3.34	1.47	1.37
19	i	301	HEC	C3D-C2D	3.34	1.47	1.37
15	V	805	CDL	OA8-CA7	3.32	1.43	1.33
19	j	302	HEC	C2A-C3A	3.32	1.47	1.37
15	K	301	CDL	OB8-CB7	3.31	1.43	1.33
19	V	804	HEC	C3D-C2D	3.31	1.47	1.37
20	Y	602	HEM	C4D-ND	-3.31	1.34	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	j	302	HEC	C3D-C2D	3.29	1.47	1.37
15	Y	603	CDL	OA6-CA4	-3.28	1.38	1.46
15	Q	804	CDL	OB8-CB7	3.27	1.42	1.33
20	b	602	HEM	C4D-ND	-3.27	1.34	1.40
15	K	301	CDL	OA6-CA4	-3.25	1.38	1.46
15	Y	604	CDL	OB6-CB5	3.24	1.43	1.34
15	Q	804	CDL	OB6-CB5	3.20	1.43	1.34
15	V	805	CDL	OB8-CB7	3.20	1.42	1.33
15	b	604	CDL	OB6-CB5	3.17	1.43	1.34
15	V	805	CDL	OB6-CB5	3.16	1.43	1.34
18	V	801	HAS	C3C-C2C	-3.16	1.36	1.40
15	b	603	CDL	OB8-CB7	3.15	1.42	1.33
18	Q	802	HAS	C3C-C2C	-3.15	1.36	1.40
20	Y	601	HEM	C4D-ND	-3.15	1.34	1.40
20	b	602	HEM	C1B-NB	-3.14	1.34	1.40
15	b	603	CDL	OB6-CB5	3.14	1.43	1.34
15	b	603	CDL	OA6-CA4	-3.13	1.38	1.46
15	b	604	CDL	OB8-CB7	3.13	1.42	1.33
15	M	301	CDL	OB8-CB7	3.12	1.42	1.33
16	Y	606	MQ9	C46-C44	-3.12	1.44	1.51
15	M	301	CDL	OB6-CB5	3.12	1.43	1.34
15	Q	804	CDL	OA6-CA4	-3.10	1.38	1.46
20	Y	602	HEM	C3C-C2C	-3.10	1.36	1.40
18	V	802	HAS	C14-C15	3.08	1.40	1.33
15	Y	603	CDL	OB8-CB7	3.06	1.42	1.33
20	b	601	HEM	C3C-C2C	-3.05	1.36	1.40
15	V	805	CDL	OA6-CA4	-3.05	1.39	1.46
18	Q	802	HAS	C22-C23	3.05	1.40	1.33
16	Y	606	MQ9	C11-C9	-3.03	1.45	1.51
18	V	802	HAS	C22-C23	3.03	1.40	1.33
15	Y	604	CDL	OA6-CA4	-3.01	1.39	1.46
19	j	302	HEC	C4B-C3B	3.00	1.48	1.43
15	K	301	CDL	OB6-CB5	2.99	1.42	1.34
19	V	804	HEC	C4B-C3B	2.97	1.48	1.43
18	V	801	HAS	C14-C15	2.97	1.40	1.33
19	j	301	HEC	C4B-C3B	2.96	1.48	1.43
15	M	301	CDL	OA6-CA4	-2.96	1.39	1.46
15	Y	603	CDL	OB6-CB5	2.96	1.42	1.34
19	i	301	HEC	C4B-C3B	2.95	1.48	1.43
19	i	301	HEC	C3C-C4C	2.91	1.48	1.43
18	Q	801	HAS	C14-C15	2.91	1.40	1.33
16	b	605	MQ9	C7-C6	2.91	1.56	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	Y	604	CDL	OB8-CB7	2.91	1.41	1.33
19	j	301	HEC	C3C-C4C	2.90	1.48	1.43
19	V	804	HEC	C3C-C4C	2.90	1.48	1.43
19	V	804	HEC	C3A-C4A	2.89	1.49	1.42
19	j	302	HEC	C3A-C4A	2.88	1.49	1.42
19	j	302	HEC	C2A-C1A	2.87	1.49	1.42
19	j	302	HEC	C3C-C4C	2.86	1.48	1.43
19	V	804	HEC	C2A-C1A	2.84	1.49	1.42
19	i	301	HEC	C2A-C1A	2.84	1.49	1.42
19	j	301	HEC	C3A-C4A	2.83	1.49	1.42
19	i	301	HEC	C3A-C4A	2.83	1.49	1.42
19	j	301	HEC	C2A-C1A	2.82	1.48	1.42
18	Q	801	HAS	C18-C19	2.81	1.39	1.33
20	Y	601	HEM	C3C-C2C	-2.79	1.36	1.40
18	V	802	HAS	C3C-C2C	-2.78	1.36	1.40
18	V	802	HAS	C29-C30	2.77	1.40	1.32
15	Y	603	CDL	OB6-CB4	-2.77	1.39	1.46
18	Q	802	HAS	C14-C15	2.77	1.39	1.33
18	Q	802	HAS	C29-C30	2.76	1.40	1.32
18	Q	801	HAS	C22-C23	2.75	1.39	1.33
18	V	801	HAS	C29-C30	2.74	1.40	1.32
18	V	801	HAS	C18-C19	2.72	1.39	1.33
20	b	601	HEM	C4B-NB	-2.70	1.33	1.38
18	V	801	HAS	C22-C23	2.69	1.39	1.33
18	V	802	HAS	C18-C19	2.69	1.39	1.33
20	Y	601	HEM	C1B-NB	-2.69	1.35	1.40
15	K	301	CDL	OB6-CB4	-2.69	1.39	1.46
20	Y	601	HEM	FE-ND	2.67	2.10	1.96
18	Q	802	HAS	C18-C19	2.66	1.39	1.33
20	b	601	HEM	C1B-NB	-2.65	1.35	1.40
18	Q	801	HAS	C29-C30	2.65	1.40	1.32
19	V	804	HEC	C1C-CHC	2.58	1.48	1.41
19	i	301	HEC	C1B-CHB	2.58	1.48	1.41
19	V	804	HEC	C4D-CHA	2.57	1.48	1.41
15	Q	804	CDL	OB6-CB4	-2.57	1.40	1.46
19	j	302	HEC	C4D-CHA	2.57	1.48	1.41
19	j	302	HEC	C1C-CHC	2.57	1.48	1.41
19	j	301	HEC	C1D-CHD	2.57	1.48	1.41
19	j	301	HEC	C1C-CHC	2.56	1.48	1.41
19	j	302	HEC	C1B-CHB	2.56	1.48	1.41
19	i	301	HEC	C1C-CHC	2.55	1.48	1.41
19	i	301	HEC	C1D-CHD	2.55	1.48	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	V	804	HEC	C1B-CHB	2.55	1.48	1.41
19	i	301	HEC	C4D-CHA	2.55	1.48	1.41
15	M	301	CDL	OB6-CB4	-2.55	1.40	1.46
15	V	805	CDL	OB6-CB4	-2.55	1.40	1.46
20	Y	602	HEM	C4B-NB	-2.55	1.33	1.38
19	j	301	HEC	C1B-CHB	2.54	1.48	1.41
15	b	604	CDL	OB6-CB4	-2.54	1.40	1.46
20	b	602	HEM	FE-ND	2.54	2.09	1.96
19	j	301	HEC	C4D-CHA	2.54	1.48	1.41
20	Y	602	HEM	FE-ND	2.53	2.09	1.96
19	V	804	HEC	C1D-CHD	2.52	1.48	1.41
15	b	603	CDL	OB6-CB4	-2.50	1.40	1.46
19	j	302	HEC	C1D-CHD	2.49	1.47	1.41
16	M	302	MQ9	C16-C14	-2.43	1.46	1.51
18	Q	802	HAS	CHD-C4A	2.43	1.38	1.35
20	Y	602	HEM	C1B-NB	-2.41	1.36	1.40
20	b	602	HEM	C3C-C2C	-2.40	1.37	1.40
16	Y	605	MQ9	C36-C34	-2.39	1.46	1.51
15	Y	604	CDL	OB6-CB4	-2.37	1.40	1.46
15	M	301	CDL	OA6-CA5	2.35	1.40	1.34
15	Q	804	CDL	OA6-CA5	2.32	1.40	1.34
15	V	805	CDL	OA6-CA5	2.30	1.40	1.34
20	b	601	HEM	FE-ND	2.29	2.08	1.96
16	M	302	MQ9	C21-C19	-2.27	1.46	1.51
20	b	602	HEM	C4B-NB	-2.25	1.34	1.38
18	Q	802	HAS	O2D-CGD	-2.19	1.23	1.30
16	M	302	MQ9	C41-C39	-2.15	1.46	1.51
16	Y	606	MQ9	C22-C23	-2.15	1.43	1.50
15	V	805	CDL	C51-CB5	2.14	1.57	1.50
15	Q	804	CDL	PA1-OA5	2.13	1.67	1.59
15	b	604	CDL	PA1-OA5	2.13	1.67	1.59
20	Y	602	HEM	O2A-CGA	-2.13	1.23	1.30
15	M	301	CDL	C51-CB5	2.12	1.56	1.50
15	M	301	CDL	PA1-OA5	2.12	1.67	1.59
15	Q	804	CDL	C51-CB5	2.12	1.56	1.50
15	b	603	CDL	OA6-CA5	2.12	1.40	1.34
15	K	301	CDL	OA6-CA5	2.11	1.40	1.34
15	V	805	CDL	PA1-OA5	2.09	1.67	1.59
15	Y	603	CDL	PA1-OA5	2.08	1.67	1.59
18	Q	801	HAS	O2D-CGD	-2.08	1.23	1.30
15	Y	603	CDL	PA1-OA2	2.07	1.67	1.59
15	V	805	CDL	PA1-OA2	2.07	1.67	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	M	302	MQ9	C25-C24	-2.07	1.45	1.50
15	b	604	CDL	C51-CB5	2.07	1.56	1.50
20	Y	601	HEM	C4B-NB	-2.07	1.34	1.38
15	K	301	CDL	PA1-OA5	2.06	1.67	1.59
15	Y	604	CDL	PA1-OA2	2.06	1.67	1.59
15	b	604	CDL	OA6-CA5	2.06	1.40	1.34
15	Y	604	CDL	OA6-CA5	2.06	1.40	1.34
15	Y	603	CDL	OA6-CA5	2.06	1.40	1.34
16	Y	606	MQ9	C30-C29	-2.04	1.45	1.50
15	K	301	CDL	PA1-OA2	2.04	1.67	1.59
20	b	601	HEM	O2A-CGA	-2.04	1.23	1.30
20	b	602	HEM	O2A-CGA	-2.02	1.23	1.30
16	Y	606	MQ9	C36-C34	-2.01	1.47	1.51
18	V	802	HAS	CHD-C4A	2.01	1.38	1.35
16	Y	606	MQ9	C15-C14	-2.00	1.45	1.50

All (187) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	b	602	HEM	CBA-CAA-C2A	8.62	127.33	112.62
20	b	601	HEM	CBA-CAA-C2A	7.56	125.52	112.62
19	V	804	HEC	C1D-C2D-C3D	-6.10	102.75	107.00
19	i	301	HEC	C1D-C2D-C3D	-6.07	102.77	107.00
19	j	302	HEC	C1D-C2D-C3D	-6.06	102.78	107.00
19	j	301	HEC	C1D-C2D-C3D	-6.04	102.79	107.00
20	b	601	HEM	C1B-NB-C4B	5.87	111.14	105.07
20	Y	601	HEM	C1B-NB-C4B	5.73	111.00	105.07
20	Y	602	HEM	C1B-NB-C4B	5.68	110.94	105.07
20	b	601	HEM	C4D-ND-C1D	5.58	110.84	105.07
20	b	602	HEM	C1B-NB-C4B	5.36	110.61	105.07
20	b	601	HEM	CHC-C4B-NB	5.18	130.06	124.43
18	Q	802	HAS	CMC-C2C-C1C	-5.05	120.69	128.46
20	b	602	HEM	C4D-ND-C1D	4.92	110.15	105.07
18	V	802	HAS	CAD-CBD-CGD	-4.86	103.14	113.60
18	Q	802	HAS	CAD-CBD-CGD	-4.79	103.31	113.60
15	b	603	CDL	OB6-CB5-C51	4.66	121.55	111.50
15	Y	604	CDL	OB6-CB5-C51	4.65	121.53	111.50
20	b	602	HEM	CHB-C1B-NB	4.62	130.09	124.38
20	Y	602	HEM	CHC-C4B-NB	4.54	129.36	124.43
20	Y	602	HEM	C4D-ND-C1D	4.43	109.64	105.07
15	M	301	CDL	OA6-CA5-C11	4.29	120.74	111.50
15	Q	804	CDL	OB6-CB5-C51	4.27	120.71	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	V	805	CDL	OB6-CB5-C51	4.27	120.70	111.50
15	Y	603	CDL	OB6-CB5-C51	4.25	120.65	111.50
20	Y	601	HEM	C4D-ND-C1D	4.22	109.43	105.07
15	b	603	CDL	OA6-CA5-C11	4.18	120.51	111.50
20	b	601	HEM	CHD-C1D-ND	4.06	128.84	124.43
15	Q	804	CDL	OA6-CA5-C11	4.06	120.25	111.50
20	Y	601	HEM	CHB-C1B-NB	4.03	129.36	124.38
18	V	801	HAS	CMC-C2C-C1C	-4.02	122.28	128.46
20	b	602	HEM	CMB-C2B-C1B	-4.02	118.92	125.04
15	K	301	CDL	OB6-CB5-C51	4.00	120.12	111.50
18	Q	802	HAS	CMC-C2C-C3C	3.98	132.12	124.68
15	b	604	CDL	OB6-CB5-C51	3.95	120.01	111.50
15	V	805	CDL	OA6-CA5-C11	3.94	119.99	111.50
18	V	802	HAS	CMC-C2C-C1C	-3.88	122.50	128.46
16	b	605	MQ9	C25-C24-C26	3.87	121.77	115.27
15	Y	604	CDL	OA6-CA5-C11	3.85	119.80	111.50
18	Q	801	HAS	CAD-CBD-CGD	-3.78	105.47	113.60
15	K	301	CDL	OA6-CA5-C11	3.77	119.63	111.50
18	V	801	HAS	CMC-C2C-C3C	3.76	131.70	124.68
20	Y	602	HEM	CHD-C1D-ND	3.75	128.50	124.43
16	b	605	MQ9	C30-C29-C31	3.73	121.54	115.27
16	M	302	MQ9	C7-C8-C9	-3.72	120.59	126.79
15	Y	603	CDL	OA6-CA5-C11	3.72	119.53	111.50
16	Y	606	MQ9	C25-C24-C23	-3.72	114.13	123.68
20	b	602	HEM	CHC-C4B-NB	3.72	128.47	124.43
15	M	301	CDL	OB6-CB5-C51	3.70	119.47	111.50
20	Y	601	HEM	C2C-C3C-C4C	3.64	109.44	106.90
18	Q	801	HAS	CMC-C2C-C1C	-3.63	122.89	128.46
20	b	601	HEM	CBB-CAB-C3B	-3.60	109.70	127.62
16	b	605	MQ9	C7-C8-C9	-3.58	120.83	126.79
16	Y	605	MQ9	C15-C14-C16	3.55	121.24	115.27
15	b	604	CDL	OA6-CA5-C11	3.54	119.13	111.50
20	b	601	HEM	CHA-C4D-ND	3.50	128.70	124.38
16	Y	606	MQ9	C7-C8-C9	-3.43	121.09	126.79
20	Y	601	HEM	CHA-C4D-ND	3.38	128.56	124.38
16	Y	605	MQ9	C30-C29-C31	3.33	120.88	115.27
20	b	602	HEM	CHA-C4D-ND	3.28	128.43	124.38
18	V	802	HAS	CMC-C2C-C3C	3.28	130.81	124.68
20	Y	601	HEM	CHD-C1D-ND	3.25	127.97	124.43
19	i	301	HEC	CMB-C2B-C3B	3.25	129.64	125.82
18	Q	801	HAS	CMC-C2C-C3C	3.24	130.74	124.68
20	Y	602	HEM	CHA-C4D-ND	3.23	128.37	124.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	j	301	HEC	CMB-C2B-C3B	3.21	129.60	125.82
20	Y	602	HEM	CAA-CBA-CGA	-3.19	104.80	113.76
18	Q	801	HAS	CMB-C2B-C3B	-3.19	124.27	130.34
15	Q	804	CDL	OB8-CB7-C71	3.18	121.88	111.91
16	Y	605	MQ9	C7-C8-C9	-3.18	121.50	126.79
19	j	302	HEC	CMC-C2C-C3C	3.17	129.55	125.82
19	V	804	HEC	CMB-C2B-C3B	3.17	129.54	125.82
20	Y	602	HEM	CHB-C1B-NB	3.16	128.28	124.38
19	V	804	HEC	CMC-C2C-C3C	3.15	129.53	125.82
19	j	302	HEC	CMB-C2B-C3B	3.13	129.50	125.82
19	i	301	HEC	CMC-C2C-C3C	3.10	129.47	125.82
16	Y	605	MQ9	C40-C39-C41	3.08	120.46	115.27
19	j	301	HEC	CMC-C2C-C3C	3.07	129.44	125.82
15	M	301	CDL	OB8-CB7-C71	3.02	121.39	111.91
16	Y	605	MQ9	C25-C24-C26	3.02	120.34	115.27
20	b	602	HEM	CMC-C2C-C3C	2.98	130.25	124.68
18	V	801	HAS	CMB-C2B-C3B	-2.97	124.68	130.34
15	K	301	CDL	OA8-CA7-C31	2.95	121.17	111.91
18	V	802	HAS	CAD-C3D-C4D	2.93	129.78	124.66
20	b	602	HEM	C2C-C3C-C4C	2.91	108.93	106.90
20	b	601	HEM	CAA-C2A-C3A	-2.91	118.88	127.25
15	b	603	CDL	OB8-CB7-C71	2.87	120.92	111.91
16	b	605	MQ9	C7-C6-C1	2.87	121.57	118.50
15	Y	603	CDL	OB8-CB7-C71	2.85	120.86	111.91
20	b	601	HEM	CAA-CBA-CGA	-2.85	105.78	113.76
15	b	603	CDL	OA8-CA7-C31	2.82	120.74	111.91
20	Y	602	HEM	CBB-CAB-C3B	-2.81	113.64	127.62
16	M	302	MQ9	C25-C24-C26	2.81	120.00	115.27
15	b	604	CDL	OB8-CB7-C71	2.76	120.58	111.91
16	Y	606	MQ9	C25-C24-C26	2.76	119.91	115.27
15	V	805	CDL	OB8-CB7-C71	2.75	120.54	111.91
16	M	302	MQ9	C25-C24-C23	-2.75	116.62	123.68
20	b	602	HEM	CHD-C1D-ND	2.74	127.41	124.43
15	Y	604	CDL	OA8-CA7-C31	2.74	120.52	111.91
20	Y	601	HEM	C3C-C4C-NC	-2.73	105.78	110.94
18	V	801	HAS	CAA-CBA-CGA	-2.72	107.75	113.60
20	Y	601	HEM	CMC-C2C-C3C	2.72	129.76	124.68
16	Y	605	MQ9	C27-C28-C29	-2.72	121.11	127.66
18	V	801	HAS	C13-C14-C15	-2.69	121.17	127.66
15	Y	604	CDL	OB8-CB7-C71	2.69	120.36	111.91
20	Y	602	HEM	C2C-C3C-C4C	2.67	108.76	106.90
20	Y	601	HEM	C4B-CHC-C1C	2.66	126.07	122.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	M	301	CDL	OA8-CA7-C31	2.64	120.18	111.91
18	V	801	HAS	C17-C18-C19	-2.63	121.32	127.66
16	Y	606	MQ9	C47-C46-C44	-2.62	104.37	112.98
16	b	605	MQ9	C25-C24-C23	-2.62	116.97	123.68
18	V	801	HAS	C17-C16-C15	-2.61	104.39	112.98
15	b	604	CDL	OA8-CA7-C31	2.58	120.01	111.91
20	b	601	HEM	C2B-C1B-NB	-2.58	106.78	109.84
15	K	301	CDL	OB8-CB7-C71	2.57	119.98	111.91
20	b	601	HEM	C3D-C4D-ND	-2.57	107.31	110.17
15	Y	603	CDL	OA8-CA7-C31	2.57	119.96	111.91
20	b	602	HEM	C2D-C1D-ND	-2.54	106.84	109.88
16	M	302	MQ9	C35-C34-C36	2.54	119.54	115.27
20	b	602	HEM	C3C-C4C-NC	-2.53	106.17	110.94
16	M	302	MQ9	C12-C13-C14	-2.52	121.60	127.66
20	Y	602	HEM	C3C-C4C-NC	-2.49	106.25	110.94
18	V	801	HAS	C21-C22-C23	-2.47	121.71	127.66
18	V	801	HAS	CAD-CBD-CGD	-2.47	108.29	113.60
20	b	601	HEM	CHB-C1B-NB	2.47	127.43	124.38
18	V	801	HAS	C12-C13-C14	2.47	118.74	112.23
15	Y	603	CDL	CA4-OA6-CA5	-2.45	111.76	117.79
16	b	605	MQ9	C27-C28-C29	-2.45	121.76	127.66
15	Q	804	CDL	OA8-CA7-C31	2.45	119.58	111.91
20	b	601	HEM	C3C-C4C-NC	-2.44	106.33	110.94
16	Y	606	MQ9	C15-C14-C16	2.44	119.38	115.27
18	Q	801	HAS	C21-C22-C23	-2.42	121.82	127.66
16	b	605	MQ9	C30-C29-C28	-2.41	117.50	123.68
16	b	605	MQ9	C40-C39-C41	2.40	119.31	115.27
18	Q	801	HAS	C17-C18-C19	-2.40	121.88	127.66
16	Y	606	MQ9	C20-C19-C21	2.39	119.29	115.27
16	Y	606	MQ9	C51-C49-C50	2.38	119.86	114.60
16	Y	606	MQ9	C26-C24-C23	2.38	125.93	121.12
20	b	601	HEM	C2C-C3C-C4C	2.35	108.54	106.90
20	Y	601	HEM	CHC-C4B-NB	2.34	126.97	124.43
16	b	605	MQ9	O1-C1-C2	-2.32	117.80	121.56
18	Q	801	HAS	CMB-C2B-C1B	2.32	128.57	125.04
18	V	802	HAS	C21-C22-C23	-2.31	122.10	127.66
16	Y	605	MQ9	C10-C9-C11	2.30	119.14	115.27
20	b	601	HEM	C2D-C1D-ND	-2.29	107.14	109.88
15	V	805	CDL	OA8-CA7-C31	2.29	119.10	111.91
16	Y	605	MQ9	C45-C44-C46	2.29	119.12	115.27
16	M	302	MQ9	C37-C38-C39	-2.27	122.19	127.66
18	V	801	HAS	CMA-C3A-C4A	2.24	128.66	124.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	Q	802	HAS	C17-C18-C19	-2.24	122.28	127.66
18	Q	801	HAS	C13-C14-C15	-2.24	122.28	127.66
16	M	302	MQ9	C21-C22-C23	-2.23	104.54	111.88
16	Y	605	MQ9	C51-C49-C50	2.22	119.50	114.60
16	b	605	MQ9	C51-C49-C50	2.21	119.48	114.60
16	Y	606	MQ9	C45-C44-C46	2.21	118.98	115.27
16	b	605	MQ9	C32-C33-C34	-2.21	122.35	127.66
20	Y	601	HEM	C2D-C1D-ND	-2.20	107.24	109.88
18	Q	801	HAS	C3C-C4C-NC	2.20	112.05	109.21
16	b	605	MQ9	C12-C13-C14	-2.19	122.38	127.66
16	M	302	MQ9	C51-C49-C50	2.19	119.44	114.60
20	b	602	HEM	CMB-C2B-C3B	2.19	133.66	128.30
18	V	801	HAS	C25-C23-C24	2.18	118.93	115.27
20	Y	601	HEM	C2B-C1B-NB	-2.17	107.27	109.84
18	Q	801	HAS	CBA-CAA-C2A	2.15	118.61	112.63
16	M	302	MQ9	C42-C43-C44	-2.15	122.47	127.66
18	V	801	HAS	CMB-C2B-C1B	2.15	128.31	125.04
16	b	605	MQ9	C45-C44-C46	2.14	118.87	115.27
16	Y	605	MQ9	C30-C29-C28	-2.13	118.22	123.68
18	Q	802	HAS	C26-C15-C16	2.12	118.83	115.27
16	M	302	MQ9	C45-C44-C46	2.10	118.81	115.27
16	Y	606	MQ9	C12-C11-C9	-2.10	106.08	112.98
20	Y	602	HEM	CBA-CAA-C2A	2.09	116.19	112.62
16	Y	606	MQ9	C15-C14-C13	-2.09	118.32	123.68
18	V	802	HAS	C25-C23-C24	2.08	118.76	115.27
20	b	602	HEM	CAA-CBA-CGA	-2.07	107.96	113.76
16	Y	605	MQ9	C25-C24-C23	-2.06	118.39	123.68
16	Y	605	MQ9	C32-C33-C34	-2.05	122.72	127.66
16	b	605	MQ9	C42-C43-C44	-2.04	122.74	127.66
16	b	605	MQ9	C5M-C5-C6	-2.04	121.07	124.40
20	b	602	HEM	CAA-C2A-C3A	-2.04	121.38	127.25
20	Y	602	HEM	C2B-C1B-NB	-2.04	107.42	109.84
18	V	802	HAS	C3C-C4C-NC	2.04	111.84	109.21
20	b	601	HEM	CMA-C3A-C4A	-2.04	125.33	128.46
15	Y	604	CDL	CA4-OA6-CA5	-2.03	112.79	117.79
18	Q	802	HAS	CHC-C4B-NB	-2.02	121.89	124.38
20	b	601	HEM	CMC-C2C-C3C	2.01	128.44	124.68
16	M	302	MQ9	C32-C33-C34	-2.00	122.83	127.66

All (4) chirality outliers are listed below:

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Mol	Chain	Res	Type	Atom
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Mol	Chain	Res	Type	Atom
18	V	801	HAS	NA
18	V	802	HAS	NA
18	Q	801	HAS	NA
18	Q	802	HAS	NA

All (544) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
15	M	301	CDL	CA2-OA2-PA1-OA3
15	M	301	CDL	CA2-OA2-PA1-OA4
15	M	301	CDL	CA3-OA5-PA1-OA3
15	V	805	CDL	CA2-OA2-PA1-OA3
15	V	805	CDL	CB2-OB2-PB2-OB3
15	b	603	CDL	O1-C1-CA2-OA2
15	b	603	CDL	CB3-OB5-PB2-OB2
15	b	603	CDL	OB7-CB5-OB6-CB4
15	b	604	CDL	CA3-OA5-PA1-OA3
15	b	604	CDL	CA3-OA5-PA1-OA4
15	b	604	CDL	OA6-CA4-CA6-OA8
15	K	301	CDL	CA2-OA2-PA1-OA3
15	K	301	CDL	CA2-OA2-PA1-OA4
15	K	301	CDL	CA2-OA2-PA1-OA5
15	K	301	CDL	CA3-OA5-PA1-OA3
15	K	301	CDL	CA3-OA5-PA1-OA4
15	K	301	CDL	OA7-CA5-OA6-CA4
15	K	301	CDL	C11-CA5-OA6-CA4
15	K	301	CDL	OA9-CA7-OA8-CA6
15	K	301	CDL	C31-CA7-OA8-CA6
15	K	301	CDL	CB3-OB5-PB2-OB2
15	K	301	CDL	CB3-OB5-PB2-OB3
15	K	301	CDL	CB3-OB5-PB2-OB4
15	Q	804	CDL	CA3-OA5-PA1-OA3
15	Q	804	CDL	OB9-CB7-OB8-CB6
15	Q	804	CDL	C71-CB7-OB8-CB6
15	Y	603	CDL	CA2-OA2-PA1-OA3
15	Y	603	CDL	CA2-OA2-PA1-OA4
15	Y	603	CDL	C11-CA5-OA6-CA4
15	Y	603	CDL	CB3-OB5-PB2-OB3
15	Y	603	CDL	CB3-OB5-PB2-OB4
15	Y	604	CDL	O1-C1-CA2-OA2
15	Y	604	CDL	CA2-OA2-PA1-OA3

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Mol	Chain	Res	Type	Atoms
15	Y	604	CDL	CA2-OA2-PA1-OA4
15	Y	604	CDL	CA2-OA2-PA1-OA5
15	Y	604	CDL	CA3-OA5-PA1-OA3
15	Y	604	CDL	C11-CA5-OA6-CA4
15	Y	604	CDL	CB2-OB2-PB2-OB3
15	Y	604	CDL	CB3-OB5-PB2-OB3
15	Y	604	CDL	CB3-OB5-PB2-OB4
15	Y	604	CDL	OB7-CB5-OB6-CB4
15	Y	604	CDL	C51-CB5-OB6-CB4
16	M	302	MQ9	C24-C26-C27-C28
16	b	605	MQ9	C23-C24-C26-C27
16	b	605	MQ9	C25-C24-C26-C27
16	b	605	MQ9	C44-C46-C47-C48
16	Y	605	MQ9	C13-C14-C16-C17
16	Y	605	MQ9	C15-C14-C16-C17
16	Y	605	MQ9	C28-C29-C31-C32
16	Y	605	MQ9	C30-C29-C31-C32
16	Y	605	MQ9	C29-C31-C32-C33
16	Y	605	MQ9	C38-C39-C41-C42
16	Y	605	MQ9	C40-C39-C41-C42
16	Y	606	MQ9	C19-C21-C22-C23
18	V	801	HAS	C1D-C2D-CMD-OMD
18	V	801	HAS	C3D-C2D-CMD-OMD
18	V	801	HAS	C23-C24-C28-C29
18	V	802	HAS	C1D-C2D-CMD-OMD
18	V	802	HAS	C3D-C2D-CMD-OMD
18	Q	802	HAS	C3D-C2D-CMD-OMD
18	Q	802	HAS	C3B-C11-C12-C13
18	Q	802	HAS	O11-C11-C12-C13
18	Q	802	HAS	C26-C15-C16-C17
20	b	601	HEM	C1A-C2A-CAA-CBA
20	b	601	HEM	C3A-C2A-CAA-CBA
20	b	601	HEM	C2B-C3B-CAB-CBB
20	b	601	HEM	C4B-C3B-CAB-CBB
20	b	602	HEM	C1A-C2A-CAA-CBA
20	b	602	HEM	C3A-C2A-CAA-CBA
20	b	602	HEM	C2A-CAA-CBA-CGA
15	b	603	CDL	OB9-CB7-OB8-CB6
15	b	604	CDL	OA9-CA7-OA8-CA6
15	Y	603	CDL	OA7-CA5-OA6-CA4
15	Y	604	CDL	OA7-CA5-OA6-CA4
15	b	604	CDL	C31-CA7-OA8-CA6

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Mol	Chain	Res	Type	Atoms
15	b	603	CDL	C51-CB5-OB6-CB4
15	Y	604	CDL	OB9-CB7-OB8-CB6
16	Y	605	MQ9	C25-C24-C26-C27
18	V	801	HAS	C25-C23-C24-C28
18	V	802	HAS	C25-C23-C24-C28
16	Y	605	MQ9	C23-C24-C26-C27
18	V	802	HAS	C22-C23-C24-C28
18	Q	802	HAS	C14-C15-C16-C17
15	b	603	CDL	C71-CB7-OB8-CB6
15	Y	604	CDL	C71-CB7-OB8-CB6
15	M	301	CDL	O1-C1-CA2-OA2
15	Y	603	CDL	O1-C1-CB2-OB2
15	Y	604	CDL	O1-C1-CB2-OB2
15	M	301	CDL	C75-C76-C77-C78
16	b	605	MQ9	C30-C29-C31-C32
16	b	605	MQ9	C28-C29-C31-C32
18	V	801	HAS	C22-C23-C24-C28
16	M	302	MQ9	C44-C46-C47-C48
16	b	605	MQ9	C9-C11-C12-C13
16	b	605	MQ9	C39-C41-C42-C43
16	Y	605	MQ9	C9-C11-C12-C13
16	Y	605	MQ9	C19-C21-C22-C23
16	Y	605	MQ9	C34-C36-C37-C38
16	Y	606	MQ9	C9-C11-C12-C13
18	V	802	HAS	C19-C20-C21-C22
18	Q	801	HAS	C23-C24-C28-C29
18	Q	802	HAS	C23-C24-C28-C29
15	M	301	CDL	CB2-C1-CA2-OA2
15	Y	603	CDL	CA2-C1-CB2-OB2
15	K	301	CDL	C71-CB7-OB8-CB6
15	Q	804	CDL	C31-CA7-OA8-CA6
15	K	301	CDL	C56-C57-C58-C59
15	K	301	CDL	C76-C77-C78-C79
15	Y	603	CDL	O1-C1-CA2-OA2
15	V	805	CDL	CA5-C11-C12-C13
15	Q	804	CDL	OA9-CA7-OA8-CA6
15	M	301	CDL	C11-CA5-OA6-CA4
15	Y	604	CDL	CB5-C51-C52-C53
19	V	804	HEC	C3D-CAD-CBD-CGD
19	i	301	HEC	C3D-CAD-CBD-CGD
19	j	301	HEC	C3D-CAD-CBD-CGD
19	j	302	HEC	C3D-CAD-CBD-CGD

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Mol	Chain	Res	Type	Atoms
20	b	601	HEM	C2A-CAA-CBA-CGA
15	Y	603	CDL	CA5-C11-C12-C13
15	Y	604	CDL	CA7-C31-C32-C33
15	Q	804	CDL	CA7-C31-C32-C33
15	M	301	CDL	C21-C22-C23-C24
15	V	805	CDL	CB7-C71-C72-C73
15	b	603	CDL	CA5-C11-C12-C13
15	Q	804	CDL	CA5-C11-C12-C13
20	b	601	HEM	C3D-CAD-CBD-CGD
15	K	301	CDL	OB9-CB7-OB8-CB6
16	M	302	MQ9	C19-C21-C22-C23
16	b	605	MQ9	C14-C16-C17-C18
16	b	605	MQ9	C29-C31-C32-C33
16	b	605	MQ9	C34-C36-C37-C38
16	Y	605	MQ9	C44-C46-C47-C48
18	Q	801	HAS	C15-C16-C17-C18
15	b	604	CDL	O1-C1-CB2-OB2
15	M	301	CDL	CA2-OA2-PA1-OA5
15	V	805	CDL	CA2-OA2-PA1-OA5
15	K	301	CDL	CB2-OB2-PB2-OB5
15	Q	804	CDL	CB2-OB2-PB2-OB5
15	Y	603	CDL	CA3-OA5-PA1-OA2
15	Y	604	CDL	CA3-OA5-PA1-OA2
15	Y	604	CDL	CB2-OB2-PB2-OB5
15	V	805	CDL	C71-CB7-OB8-CB6
15	M	301	CDL	C77-C78-C79-C80
15	b	604	CDL	CA2-C1-CB2-OB2
15	Y	603	CDL	CB2-C1-CA2-OA2
15	Y	604	CDL	CB2-C1-CA2-OA2
15	Y	604	CDL	CA2-C1-CB2-OB2
15	M	301	CDL	OA7-CA5-OA6-CA4
15	b	604	CDL	C13-C14-C15-C16
15	b	604	CDL	C51-C52-C53-C54
15	Y	604	CDL	C35-C36-C37-C38
15	b	604	CDL	C11-CA5-OA6-CA4
15	M	301	CDL	C39-C40-C41-C42
15	b	604	CDL	C54-C55-C56-C57
15	Q	804	CDL	C12-C13-C14-C15
15	Q	804	CDL	C57-C58-C59-C60
15	Y	604	CDL	C59-C60-C61-C62
15	b	604	CDL	C37-C38-C39-C40
15	K	301	CDL	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
15	K	301	CDL	C32-C33-C34-C35
15	Y	603	CDL	C13-C14-C15-C16
15	b	604	CDL	OA7-CA5-OA6-CA4
15	b	603	CDL	C14-C15-C16-C17
15	b	603	CDL	C51-C52-C53-C54
15	b	604	CDL	C19-C20-C21-C22
15	Y	604	CDL	C75-C76-C77-C78
15	b	603	CDL	C12-C13-C14-C15
15	M	301	CDL	C13-C14-C15-C16
15	M	301	CDL	C60-C61-C62-C63
15	V	805	CDL	C13-C14-C15-C16
15	b	603	CDL	C38-C39-C40-C41
15	b	604	CDL	C72-C73-C74-C75
15	K	301	CDL	C12-C13-C14-C15
15	Y	604	CDL	C23-C24-C25-C26
15	Y	604	CDL	C54-C55-C56-C57
15	V	805	CDL	OB9-CB7-OB8-CB6
15	V	805	CDL	C39-C40-C41-C42
15	b	603	CDL	C54-C55-C56-C57
15	M	301	CDL	C15-C16-C17-C18
15	M	301	CDL	C17-C18-C19-C20
15	b	603	CDL	C76-C77-C78-C79
15	K	301	CDL	C42-C43-C44-C45
15	K	301	CDL	C58-C59-C60-C61
15	Y	604	CDL	C52-C53-C54-C55
15	Y	604	CDL	C56-C57-C58-C59
15	b	603	CDL	C19-C20-C21-C22
15	b	604	CDL	C12-C13-C14-C15
15	b	604	CDL	C74-C75-C76-C77
15	Y	603	CDL	OB7-CB5-OB6-CB4
15	Y	603	CDL	C51-CB5-OB6-CB4
15	V	805	CDL	C35-C36-C37-C38
15	b	603	CDL	C17-C18-C19-C20
15	b	604	CDL	C23-C24-C25-C26
15	K	301	CDL	C21-C22-C23-C24
15	M	301	CDL	C23-C24-C25-C26
15	M	301	CDL	C62-C63-C64-C65
15	b	603	CDL	C15-C16-C17-C18
15	b	603	CDL	C83-C84-C85-C86
15	b	604	CDL	C15-C16-C17-C18
15	b	604	CDL	C60-C61-C62-C63
15	Y	603	CDL	C60-C61-C62-C63

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Mol	Chain	Res	Type	Atoms
15	Y	603	CDL	C75-C76-C77-C78
15	Y	604	CDL	C15-C16-C17-C18
15	b	604	CDL	C17-C18-C19-C20
15	K	301	CDL	C75-C76-C77-C78
15	Q	804	CDL	C39-C40-C41-C42
15	Y	603	CDL	C41-C42-C43-C44
15	Y	603	CDL	C72-C73-C74-C75
15	Y	604	CDL	C12-C13-C14-C15
15	b	604	CDL	C20-C21-C22-C23
15	Y	603	CDL	C53-C54-C55-C56
15	Y	604	CDL	C19-C20-C21-C22
15	Y	604	CDL	C37-C38-C39-C40
15	b	603	CDL	C34-C35-C36-C37
15	Y	604	CDL	C32-C33-C34-C35
15	M	301	CDL	C38-C39-C40-C41
15	b	604	CDL	C58-C59-C60-C61
15	Y	603	CDL	C56-C57-C58-C59
15	Y	604	CDL	C83-C84-C85-C86
15	b	603	CDL	C35-C36-C37-C38
15	K	301	CDL	C15-C16-C17-C18
15	K	301	CDL	C23-C24-C25-C26
15	Y	603	CDL	C58-C59-C60-C61
15	b	603	CDL	C11-CA5-OA6-CA4
15	K	301	CDL	C52-C53-C54-C55
15	K	301	CDL	C54-C55-C56-C57
15	Y	604	CDL	C51-C52-C53-C54
15	b	603	CDL	CB2-C1-CA2-OA2
15	Y	603	CDL	C11-C12-C13-C14
15	b	603	CDL	OA7-CA5-OA6-CA4
15	K	301	CDL	C17-C18-C19-C20
15	Q	804	CDL	C14-C15-C16-C17
15	V	805	CDL	C11-C12-C13-C14
15	V	805	CDL	C31-CA7-OA8-CA6
20	Y	601	HEM	C3D-CAD-CBD-CGD
15	b	604	CDL	C51-CB5-OB6-CB4
15	Y	603	CDL	C37-C38-C39-C40
15	V	805	CDL	C61-C62-C63-C64
15	Y	604	CDL	C13-C14-C15-C16
15	K	301	CDL	C38-C39-C40-C41
15	b	604	CDL	C71-CB7-OB8-CB6
15	b	604	CDL	C32-C33-C34-C35
15	Y	604	CDL	C60-C61-C62-C63

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Mol	Chain	Res	Type	Atoms
15	M	301	CDL	C42-C43-C44-C45
15	b	603	CDL	C32-C33-C34-C35
15	Y	604	CDL	C74-C75-C76-C77
20	Y	601	HEM	C2B-C3B-CAB-CBB
20	Y	602	HEM	C2B-C3B-CAB-CBB
15	Y	603	CDL	C71-CB7-OB8-CB6
15	V	805	CDL	C53-C54-C55-C56
15	Y	604	CDL	C71-C72-C73-C74
15	K	301	CDL	CA7-C31-C32-C33
20	Y	601	HEM	C4B-C3B-CAB-CBB
15	V	805	CDL	C80-C81-C82-C83
15	Y	603	CDL	C17-C18-C19-C20
15	Y	604	CDL	C38-C39-C40-C41
15	Y	604	CDL	C58-C59-C60-C61
15	M	301	CDL	C51-C52-C53-C54
15	M	301	CDL	C41-C42-C43-C44
15	Y	604	CDL	C20-C21-C22-C23
15	M	301	CDL	C52-C53-C54-C55
15	b	604	CDL	C55-C56-C57-C58
15	b	604	CDL	C57-C58-C59-C60
15	b	604	CDL	C41-C42-C43-C44
15	V	805	CDL	OA9-CA7-OA8-CA6
15	b	604	CDL	OB7-CB5-OB6-CB4
15	K	301	CDL	C51-CB5-OB6-CB4
15	b	603	CDL	C31-C32-C33-C34
15	Y	604	CDL	C21-C22-C23-C24
15	b	603	CDL	CA3-OA5-PA1-OA2
15	b	604	CDL	CA3-OA5-PA1-OA2
15	b	604	CDL	CB3-OB5-PB2-OB2
15	Q	804	CDL	CB3-OB5-PB2-OB2
15	V	805	CDL	OB5-CB3-CB4-CB6
15	K	301	CDL	C19-C20-C21-C22
15	Y	603	CDL	C36-C37-C38-C39
15	M	301	CDL	C37-C38-C39-C40
15	Q	804	CDL	C79-C80-C81-C82
15	M	301	CDL	C53-C54-C55-C56
15	V	805	CDL	C79-C80-C81-C82
15	K	301	CDL	C72-C73-C74-C75
15	M	301	CDL	C24-C25-C26-C27
15	M	301	CDL	C57-C58-C59-C60
15	b	603	CDL	C72-C73-C74-C75
15	b	604	CDL	OB9-CB7-OB8-CB6

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Mol	Chain	Res	Type	Atoms
15	M	301	CDL	CA3-CA4-CA6-OA8
15	b	604	CDL	CA3-CA4-CA6-OA8
15	Y	603	CDL	CB3-CB4-CB6-OB8
15	V	805	CDL	C51-C52-C53-C54
16	b	605	MQ9	C5-C6-C7-C8
15	Y	603	CDL	C15-C16-C17-C18
15	b	603	CDL	C52-C53-C54-C55
15	K	301	CDL	C34-C35-C36-C37
15	Y	603	CDL	OB9-CB7-OB8-CB6
15	M	301	CDL	C40-C41-C42-C43
15	V	805	CDL	C56-C57-C58-C59
15	b	603	CDL	C55-C56-C57-C58
15	Y	604	CDL	CB7-C71-C72-C73
15	M	301	CDL	C31-CA7-OA8-CA6
16	b	605	MQ9	C1-C6-C7-C8
15	M	301	CDL	C76-C77-C78-C79
15	V	805	CDL	C57-C58-C59-C60
15	Y	604	CDL	CA5-C11-C12-C13
15	M	301	CDL	C12-C13-C14-C15
15	b	603	CDL	C20-C21-C22-C23
15	b	604	CDL	C56-C57-C58-C59
15	Y	603	CDL	C35-C36-C37-C38
15	Q	804	CDL	OA6-CA4-CA6-OA8
15	b	603	CDL	C23-C24-C25-C26
15	Y	603	CDL	C23-C24-C25-C26
15	V	805	CDL	C75-C76-C77-C78
15	Q	804	CDL	C11-CA5-OA6-CA4
15	Q	804	CDL	C17-C18-C19-C20
15	b	604	CDL	OB5-CB3-CB4-CB6
16	Y	606	MQ9	C24-C26-C27-C28
15	b	604	CDL	C36-C37-C38-C39
15	M	301	CDL	CA5-C11-C12-C13
15	Y	603	CDL	C76-C77-C78-C79
15	b	604	CDL	C61-C62-C63-C64
15	Y	603	CDL	C40-C41-C42-C43
15	M	301	CDL	OA9-CA7-OA8-CA6
15	K	301	CDL	C11-C12-C13-C14
15	Q	804	CDL	C32-C33-C34-C35
15	M	301	CDL	CB3-CB4-CB6-OB8
15	K	301	CDL	CB3-CB4-CB6-OB8
15	K	301	CDL	OB7-CB5-OB6-CB4
15	b	603	CDL	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
15	K	301	CDL	C39-C40-C41-C42
15	M	301	CDL	C55-C56-C57-C58
15	Q	804	CDL	C55-C56-C57-C58
15	Y	603	CDL	CB3-OB5-PB2-OB2
15	Y	603	CDL	C73-C74-C75-C76
15	b	603	CDL	OB5-CB3-CB4-OB6
15	b	604	CDL	OB5-CB3-CB4-OB6
15	Q	804	CDL	OB5-CB3-CB4-OB6
15	b	604	CDL	C42-C43-C44-C45
15	Q	804	CDL	C62-C63-C64-C65
15	K	301	CDL	C80-C81-C82-C83
15	M	301	CDL	OA6-CA4-CA6-OA8
15	b	603	CDL	OA6-CA4-CA6-OA8
15	Q	804	CDL	C40-C41-C42-C43
15	Q	804	CDL	OA7-CA5-OA6-CA4
15	Q	804	CDL	C41-C42-C43-C44
15	b	604	CDL	C1-CA2-OA2-PA1
15	Y	603	CDL	C39-C40-C41-C42
15	V	805	CDL	C76-C77-C78-C79
15	Q	804	CDL	OB5-CB3-CB4-CB6
15	V	805	CDL	C15-C16-C17-C18
15	Q	804	CDL	C81-C82-C83-C84
15	b	604	CDL	C34-C35-C36-C37
15	Y	603	CDL	C19-C20-C21-C22
15	V	805	CDL	C37-C38-C39-C40
15	b	603	CDL	C57-C58-C59-C60
15	V	805	CDL	C32-C31-CA7-OA8
15	M	301	CDL	C31-C32-C33-C34
15	b	603	CDL	CA3-CA4-CA6-OA8
15	Y	604	CDL	CA3-CA4-CA6-OA8
15	Y	603	CDL	OB5-CB3-CB4-OB6
15	Y	603	CDL	C61-C62-C63-C64
15	Y	604	CDL	C82-C83-C84-C85
20	Y	602	HEM	C4B-C3B-CAB-CBB
15	b	604	CDL	C64-C65-C66-C67
15	Q	804	CDL	C53-C54-C55-C56
15	K	301	CDL	OB6-CB4-CB6-OB8
15	Y	603	CDL	OB6-CB4-CB6-OB8
15	Y	604	CDL	OA6-CA4-CA6-OA8
15	Y	604	CDL	OB6-CB4-CB6-OB8
15	M	301	CDL	C56-C57-C58-C59
15	V	805	CDL	C33-C34-C35-C36

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Mol	Chain	Res	Type	Atoms
15	b	603	CDL	C82-C83-C84-C85
15	Q	804	CDL	C80-C81-C82-C83
15	Y	603	CDL	CA2-OA2-PA1-OA5
15	Y	604	CDL	CB3-OB5-PB2-OB2
15	Y	603	CDL	C18-C19-C20-C21
15	Y	604	CDL	C57-C58-C59-C60
15	Q	804	CDL	C78-C79-C80-C81
16	M	302	MQ9	C45-C44-C46-C47
15	M	301	CDL	CB2-OB2-PB2-OB3
15	V	805	CDL	CA2-OA2-PA1-OA4
15	b	604	CDL	CA2-OA2-PA1-OA3
15	b	604	CDL	CB3-OB5-PB2-OB3
15	b	604	CDL	CB3-OB5-PB2-OB4
15	K	301	CDL	CB2-OB2-PB2-OB4
15	Q	804	CDL	CB2-OB2-PB2-OB4
15	Q	804	CDL	CB3-OB5-PB2-OB4
15	Y	603	CDL	CA3-OA5-PA1-OA3
15	Y	603	CDL	CA3-OA5-PA1-OA4
15	M	301	CDL	OB5-CB3-CB4-CB6
15	Y	603	CDL	OB5-CB3-CB4-CB6
15	K	301	CDL	C63-C64-C65-C66
15	Y	603	CDL	C74-C75-C76-C77
18	Q	801	HAS	O11-C11-C12-C13
15	Y	604	CDL	C80-C81-C82-C83
15	M	301	CDL	OB5-CB3-CB4-OB6
15	V	805	CDL	OB5-CB3-CB4-OB6
15	V	805	CDL	C60-C61-C62-C63
15	M	301	CDL	C32-C31-CA7-OA8
15	Y	603	CDL	C24-C25-C26-C27
15	K	301	CDL	C20-C21-C22-C23
15	b	603	CDL	C18-C19-C20-C21
15	V	805	CDL	C71-C72-C73-C74
15	Q	804	CDL	CA3-CA4-CA6-OA8
18	Q	801	HAS	C1D-C2D-CMD-OMD
18	Q	802	HAS	C1D-C2D-CMD-OMD
15	M	301	CDL	OB6-CB4-CB6-OB8
15	Q	804	CDL	C31-C32-C33-C34
16	M	302	MQ9	C12-C11-C9-C10
15	b	604	CDL	C33-C34-C35-C36
15	Y	603	CDL	C59-C60-C61-C62
15	Q	804	CDL	C52-C51-CB5-OB6
16	Y	605	MQ9	C24-C26-C27-C28

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Mol	Chain	Res	Type	Atoms
15	V	805	CDL	C34-C35-C36-C37
15	K	301	CDL	C53-C54-C55-C56
15	Y	603	CDL	C12-C13-C14-C15
15	M	301	CDL	C72-C71-CB7-OB8
15	V	805	CDL	C17-C18-C19-C20
16	M	302	MQ9	C43-C44-C46-C47
15	b	604	CDL	C11-C12-C13-C14
15	Q	804	CDL	C15-C16-C17-C18
18	V	801	HAS	C11-C12-C13-C14
15	b	604	CDL	C14-C15-C16-C17
15	V	805	CDL	C36-C37-C38-C39
15	Q	804	CDL	C77-C78-C79-C80
15	Q	804	CDL	OA5-CA3-CA4-OA6
15	M	301	CDL	C44-C45-C46-C47
15	b	604	CDL	CB2-OB2-PB2-OB5
15	Q	804	CDL	CA2-OA2-PA1-OA5
15	Y	603	CDL	C63-C64-C65-C66
15	Y	604	CDL	CB3-CB4-CB6-OB8
15	b	604	CDL	C39-C40-C41-C42
15	Y	604	CDL	C76-C77-C78-C79
15	Y	603	CDL	C55-C56-C57-C58
15	b	604	CDL	C31-C32-C33-C34
15	Y	604	CDL	C24-C25-C26-C27
15	K	301	CDL	C74-C75-C76-C77
15	Y	604	CDL	C22-C23-C24-C25
15	V	805	CDL	C40-C41-C42-C43
20	Y	602	HEM	CAD-CBD-CGD-O2D
15	b	604	CDL	C52-C53-C54-C55
15	b	603	CDL	C21-C22-C23-C24
15	Q	804	CDL	C38-C39-C40-C41
18	Q	802	HAS	CAD-CBD-CGD-O1D
20	b	601	HEM	CAD-CBD-CGD-O1D
15	Y	603	CDL	C52-C53-C54-C55
15	M	301	CDL	C71-CB7-OB8-CB6
20	b	602	HEM	CAD-CBD-CGD-O1D
15	Q	804	CDL	C51-C52-C53-C54
15	b	604	CDL	C21-C22-C23-C24
20	Y	602	HEM	CAD-CBD-CGD-O1D
15	b	603	CDL	CB3-CB4-OB6-CB5
15	b	603	CDL	CB6-CB4-OB6-CB5
15	Y	604	CDL	CB3-CB4-OB6-CB5
15	Y	604	CDL	CB6-CB4-OB6-CB5

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Mol	Chain	Res	Type	Atoms
15	K	301	CDL	C78-C79-C80-C81
15	K	301	CDL	CA3-OA5-PA1-OA2
18	Q	801	HAS	C3D-C2D-CMD-OMD
18	V	802	HAS	CAD-CBD-CGD-O2D
15	Q	804	CDL	C54-C55-C56-C57
15	K	301	CDL	C35-C36-C37-C38
15	Y	604	CDL	C84-C85-C86-C87
18	Q	802	HAS	CAD-CBD-CGD-O2D
15	K	301	CDL	O1-C1-CB2-OB2
18	V	802	HAS	CAD-CBD-CGD-O1D
20	b	602	HEM	CAD-CBD-CGD-O2D
15	M	301	CDL	OB9-CB7-OB8-CB6
15	Y	603	CDL	C21-C22-C23-C24
15	Y	603	CDL	C16-C17-C18-C19
16	Y	606	MQ9	C20-C19-C21-C22
18	Q	801	HAS	CAD-CBD-CGD-O2D
20	b	601	HEM	CAD-CBD-CGD-O2D
15	V	805	CDL	C41-C42-C43-C44
18	V	801	HAS	CAA-CBA-CGA-O2A
15	V	805	CDL	C31-C32-C33-C34
15	b	604	CDL	C16-C17-C18-C19
15	Q	804	CDL	C35-C36-C37-C38
16	Y	605	MQ9	C35-C34-C36-C37
16	M	302	MQ9	C12-C11-C9-C8
15	K	301	CDL	C83-C84-C85-C86
19	j	302	HEC	CAD-CBD-CGD-O2D
20	Y	601	HEM	CAA-CBA-CGA-O2A
15	M	301	CDL	C34-C35-C36-C37
18	V	801	HAS	CAD-CBD-CGD-O2D
18	Q	801	HAS	CAD-CBD-CGD-O1D
19	V	804	HEC	CAD-CBD-CGD-O2D
19	j	301	HEC	CAD-CBD-CGD-O2D
15	b	603	CDL	OB5-CB3-CB4-CB6
15	Q	804	CDL	OA5-CA3-CA4-CA6
18	V	802	HAS	C27-C19-C20-C21
16	M	302	MQ9	C39-C41-C42-C43
16	b	605	MQ9	C24-C26-C27-C28
16	Y	605	MQ9	C14-C16-C17-C18
19	i	301	HEC	CAD-CBD-CGD-O2D
15	K	301	CDL	CA2-C1-CB2-OB2
18	V	801	HAS	CAD-CBD-CGD-O1D
16	b	605	MQ9	C40-C39-C41-C42

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Mol	Chain	Res	Type	Atoms
16	Y	606	MQ9	C12-C11-C9-C10
18	V	801	HAS	C27-C19-C20-C21
18	V	802	HAS	C11-C12-C13-C14
15	V	805	CDL	C32-C33-C34-C35
16	Y	606	MQ9	C12-C11-C9-C8
18	V	801	HAS	CAA-CBA-CGA-O1A
19	V	804	HEC	CAD-CBD-CGD-O1D
20	Y	601	HEM	CAA-CBA-CGA-O1A
15	Y	604	CDL	C61-C62-C63-C64
19	j	302	HEC	CAD-CBD-CGD-O1D
15	Q	804	CDL	C42-C43-C44-C45
15	K	301	CDL	C59-C60-C61-C62
15	M	301	CDL	C52-C51-CB5-OB6
15	Q	804	CDL	C72-C71-CB7-OB8
19	i	301	HEC	CAD-CBD-CGD-O1D
19	j	301	HEC	CAD-CBD-CGD-O1D
20	b	601	HEM	CAA-CBA-CGA-O2A
15	M	301	CDL	C18-C19-C20-C21
15	K	301	CDL	C40-C41-C42-C43
18	V	802	HAS	C18-C19-C20-C21
15	b	603	CDL	CB5-C51-C52-C53
16	Y	606	MQ9	C34-C36-C37-C38
15	M	301	CDL	C59-C60-C61-C62
16	b	605	MQ9	C31-C32-C33-C34
15	Y	603	CDL	C71-C72-C73-C74
15	M	301	CDL	C19-C20-C21-C22
15	b	603	CDL	CB3-CB4-CB6-OB8
20	b	601	HEM	CAA-CBA-CGA-O1A
15	K	301	CDL	C77-C78-C79-C80
15	V	805	CDL	CB2-OB2-PB2-OB4
15	V	805	CDL	CB3-OB5-PB2-OB3
15	b	603	CDL	CB3-OB5-PB2-OB3
15	Q	804	CDL	C72-C71-CB7-OB9
15	Y	604	CDL	C32-C31-CA7-OA8
15	V	805	CDL	C14-C15-C16-C17
18	V	802	HAS	C16-C17-C18-C19
15	V	805	CDL	C72-C71-CB7-OB8
15	M	301	CDL	C52-C51-CB5-OB7
15	Q	804	CDL	C12-C11-CA5-OA6
15	K	301	CDL	C33-C34-C35-C36
15	V	805	CDL	C1-CA2-OA2-PA1
16	Y	606	MQ9	C45-C44-C46-C47

*Continued on next page...*

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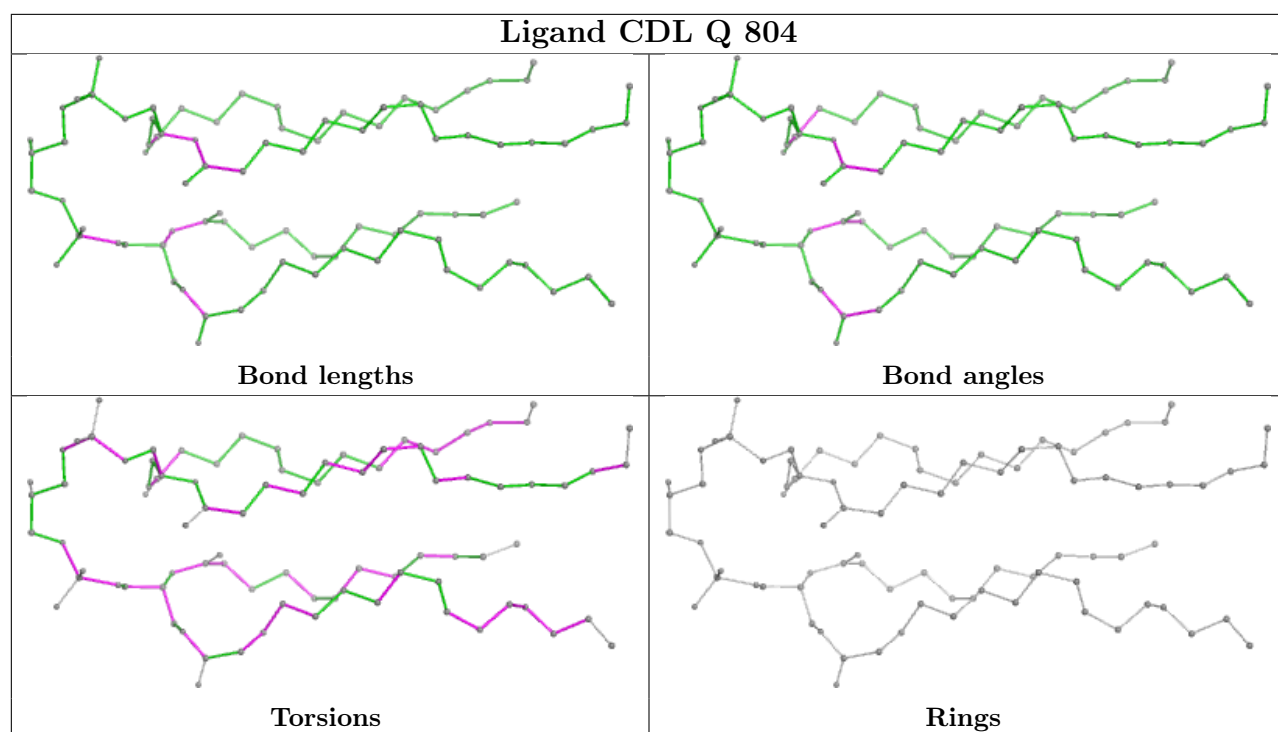
Mol	Chain	Res	Type	Atoms
16	Y	606	MQ9	C18-C19-C21-C22
18	Q	802	HAS	C18-C19-C20-C21
15	V	805	CDL	C32-C31-CA7-OA9
18	Q	802	HAS	C15-C16-C17-C18
15	M	301	CDL	C81-C82-C83-C84
15	V	805	CDL	C72-C71-CB7-OB9
15	V	805	CDL	C52-C51-CB5-OB6

There are no ring outliers.

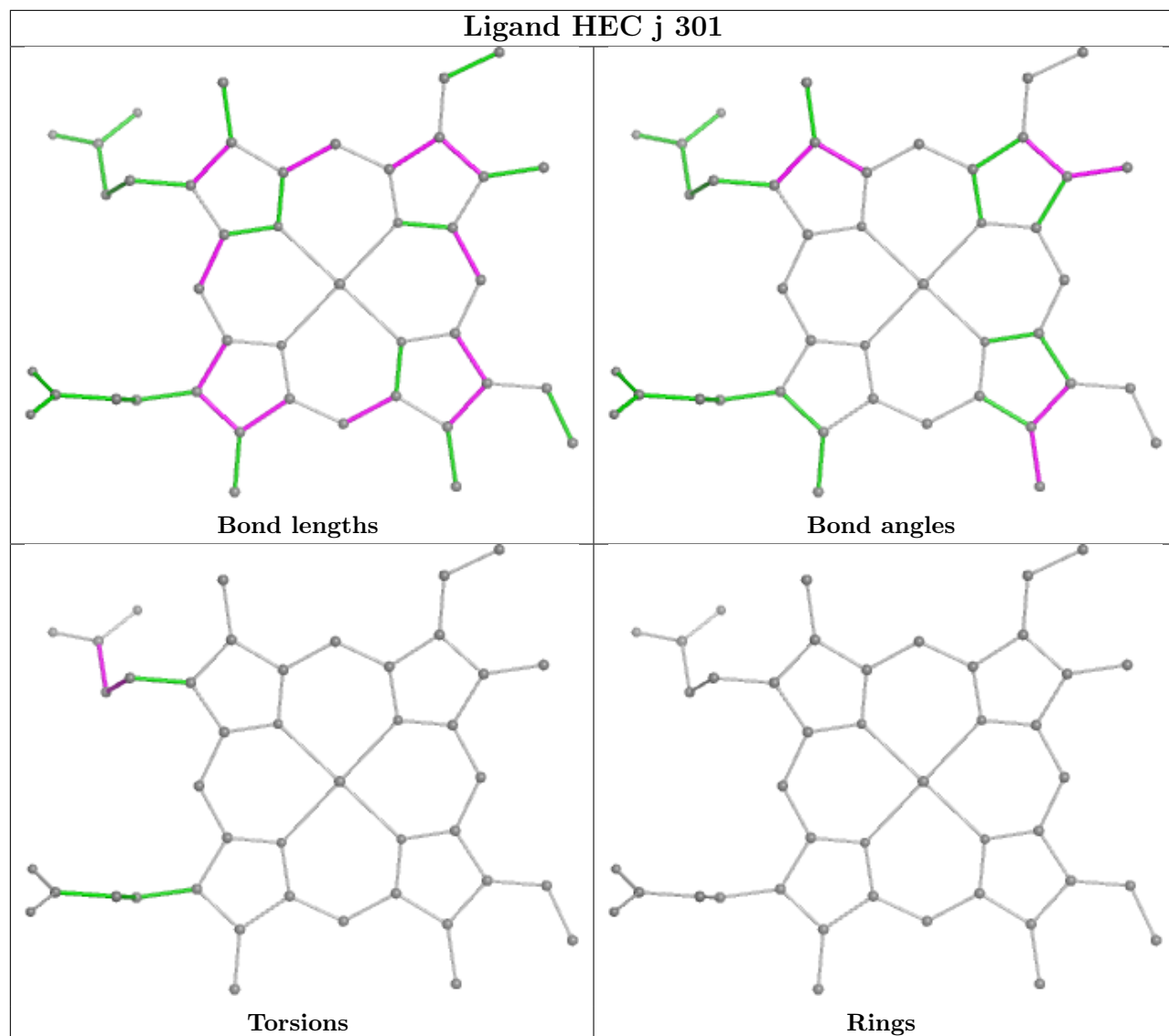
17 monomers are involved in 79 short contacts:

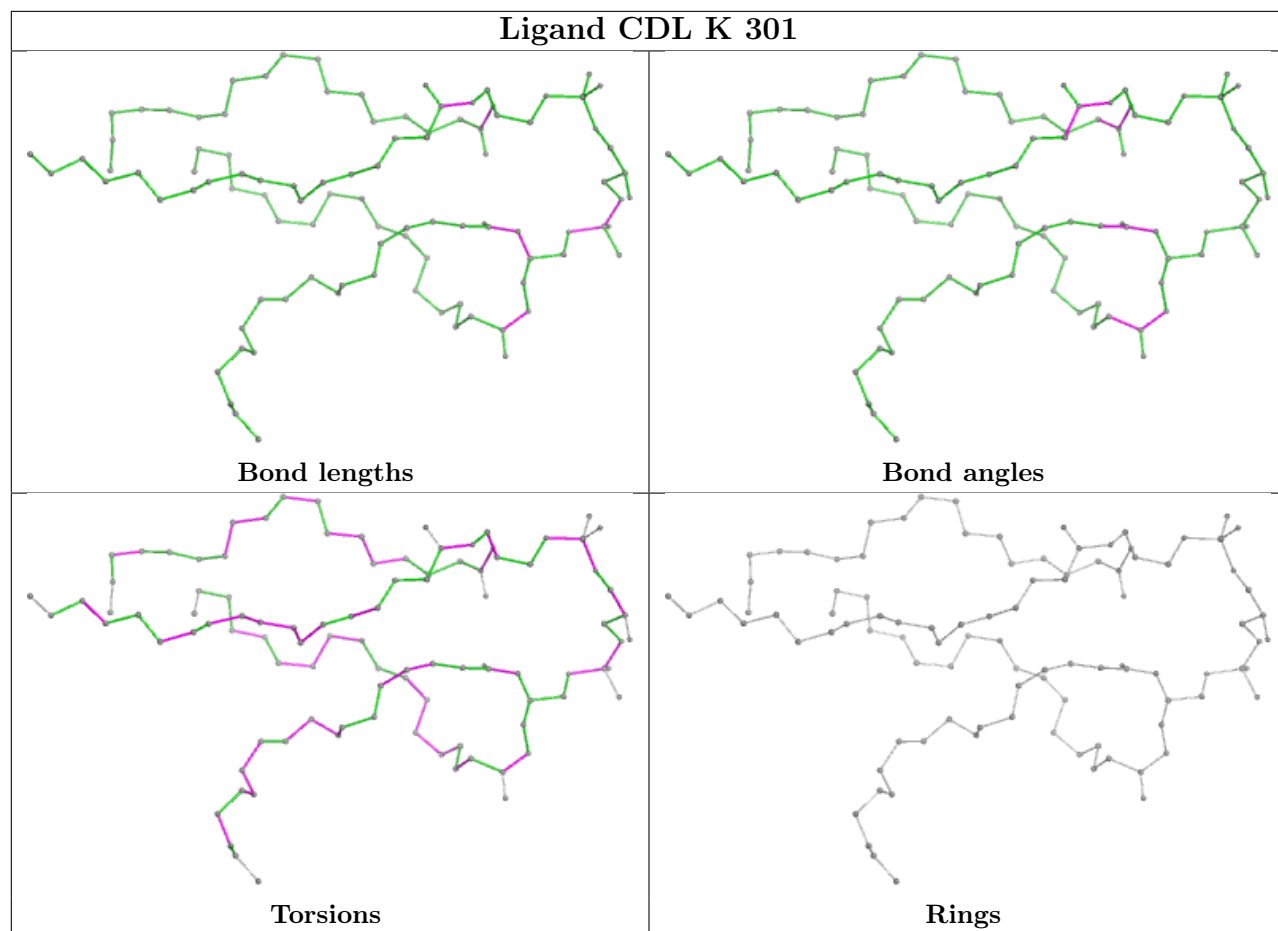
Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	Q	804	CDL	3	0
15	K	301	CDL	6	0
18	Q	801	HAS	3	0
16	M	302	MQ9	4	0
18	Q	802	HAS	3	0
16	Y	606	MQ9	4	0
15	M	301	CDL	4	0
19	V	804	HEC	22	0
20	Y	602	HEM	5	0
20	Y	601	HEM	1	0
15	Y	603	CDL	4	0
14	B	501	FES	2	0
18	V	802	HAS	2	0
18	V	801	HAS	5	0
16	Y	605	MQ9	6	0
15	V	805	CDL	2	0
15	Y	604	CDL	8	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.

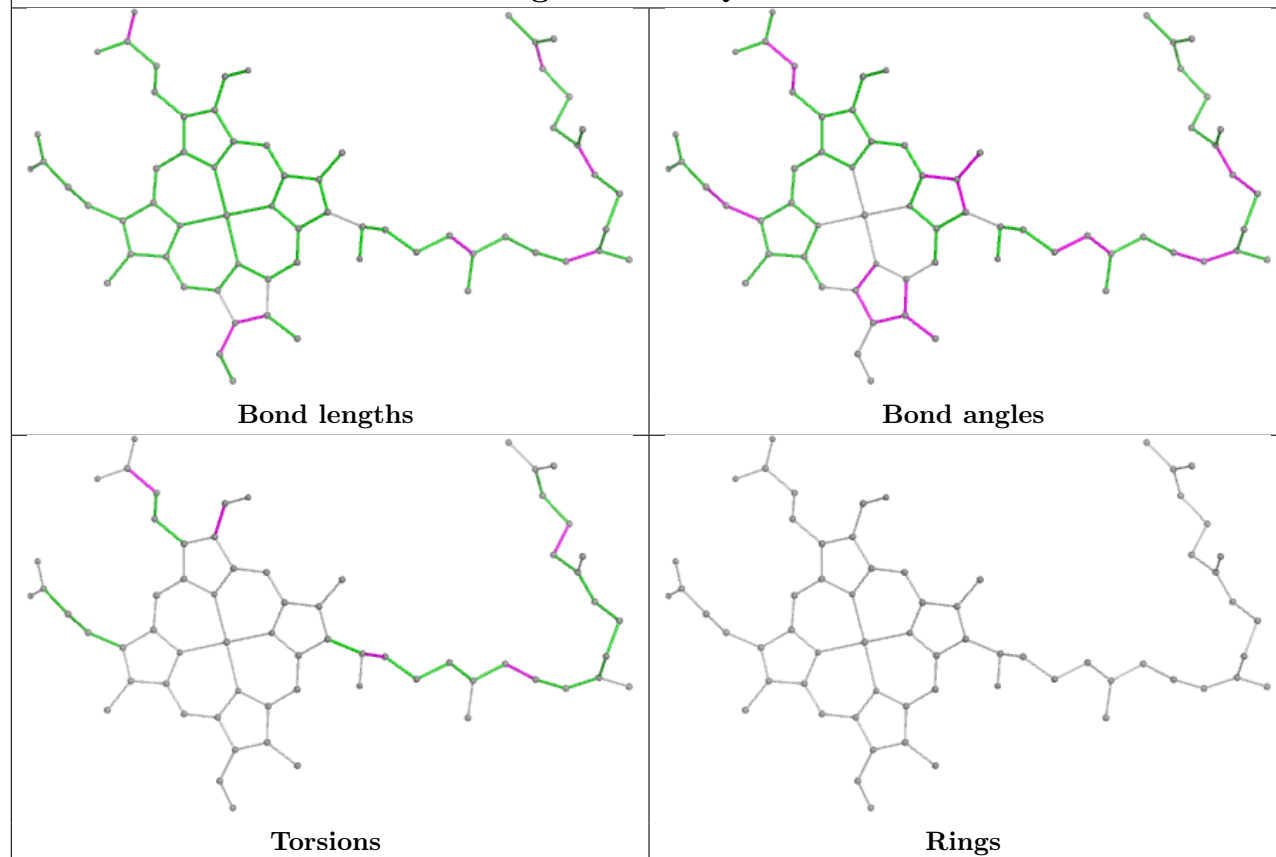


## Ligand HEC j 301

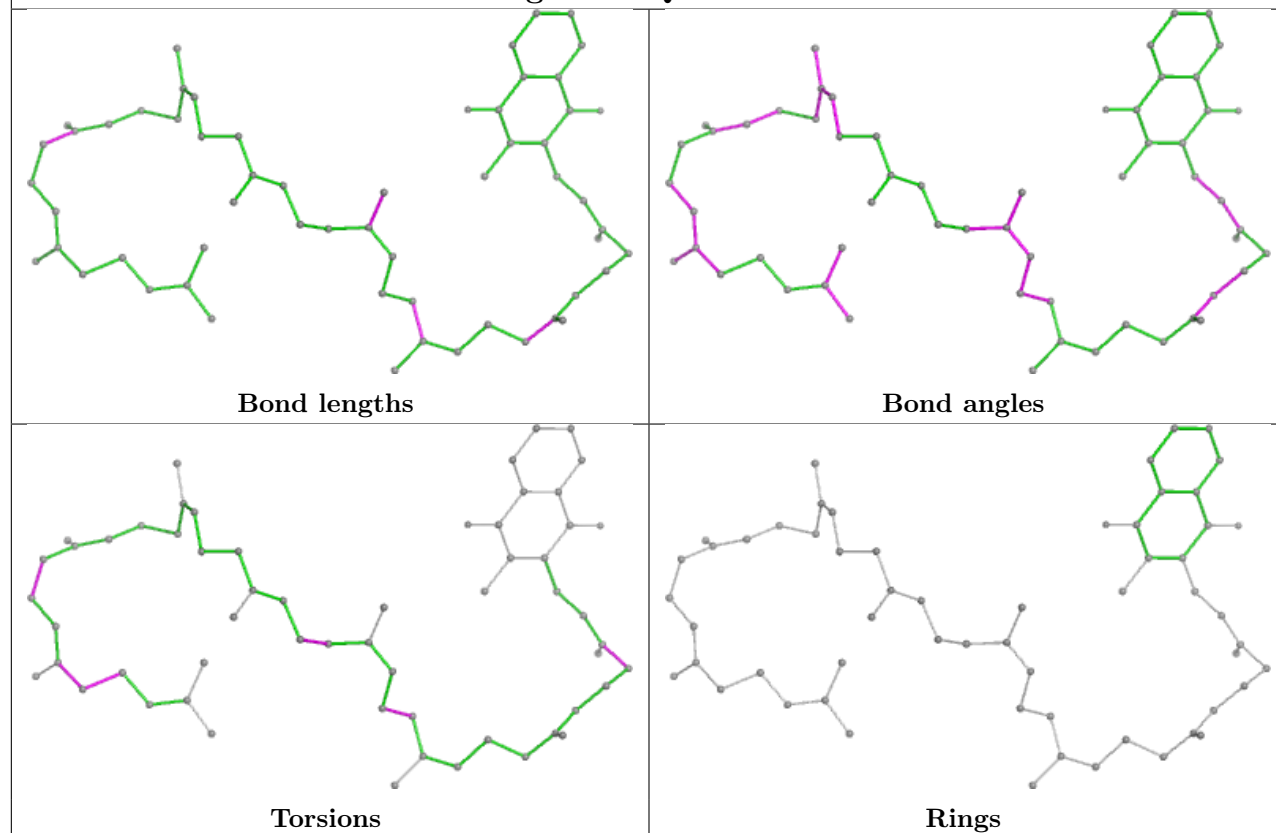




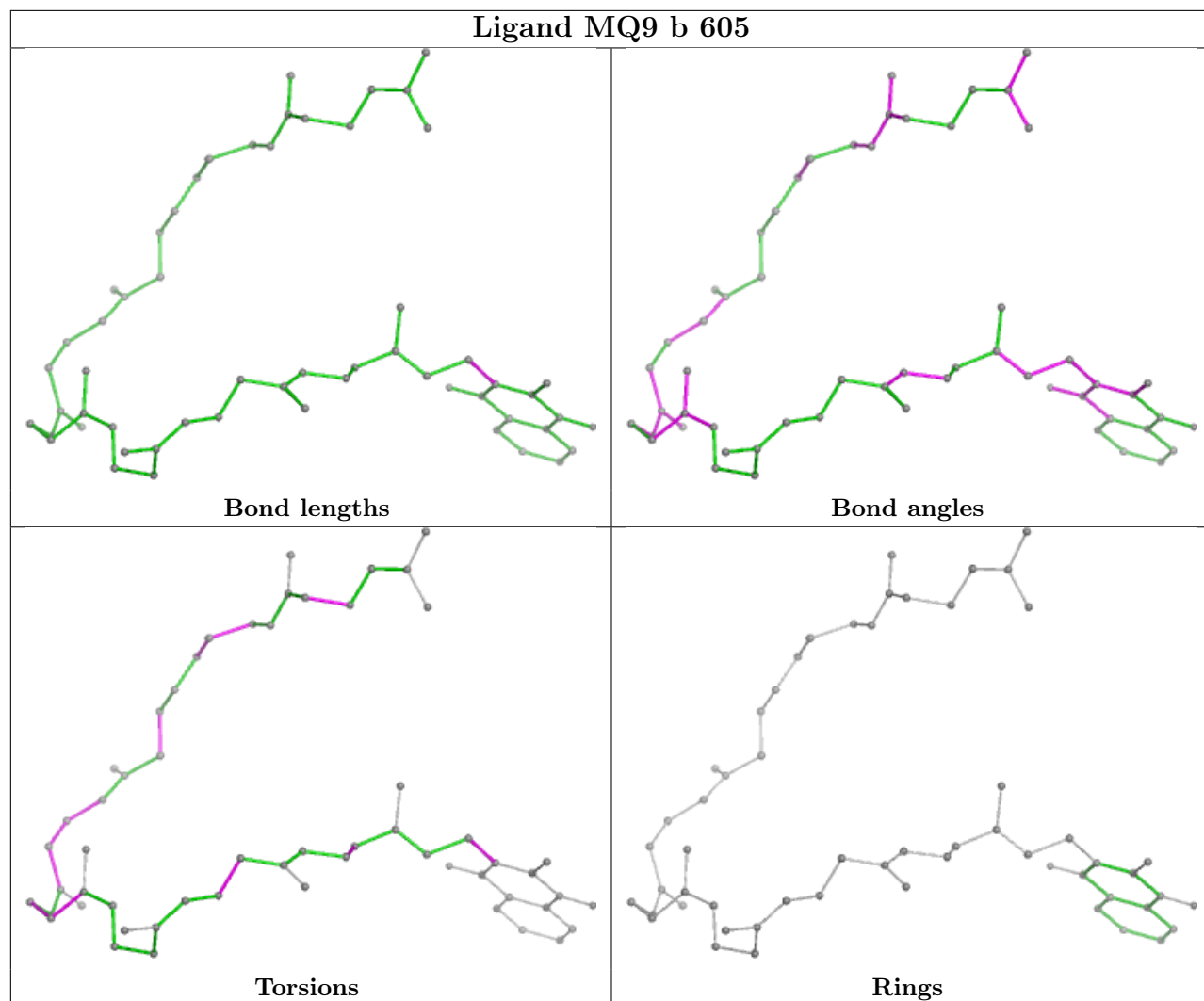
## Ligand HAS Q 801



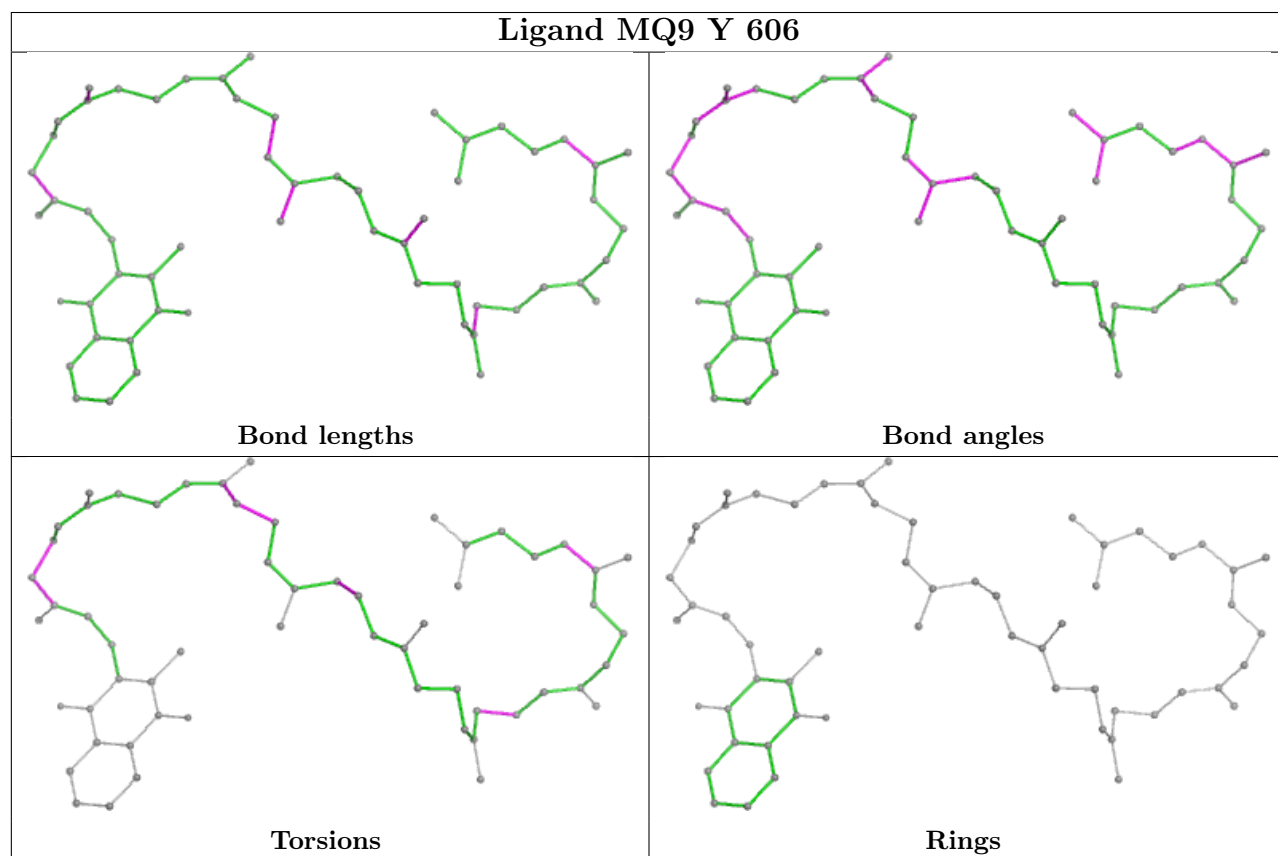
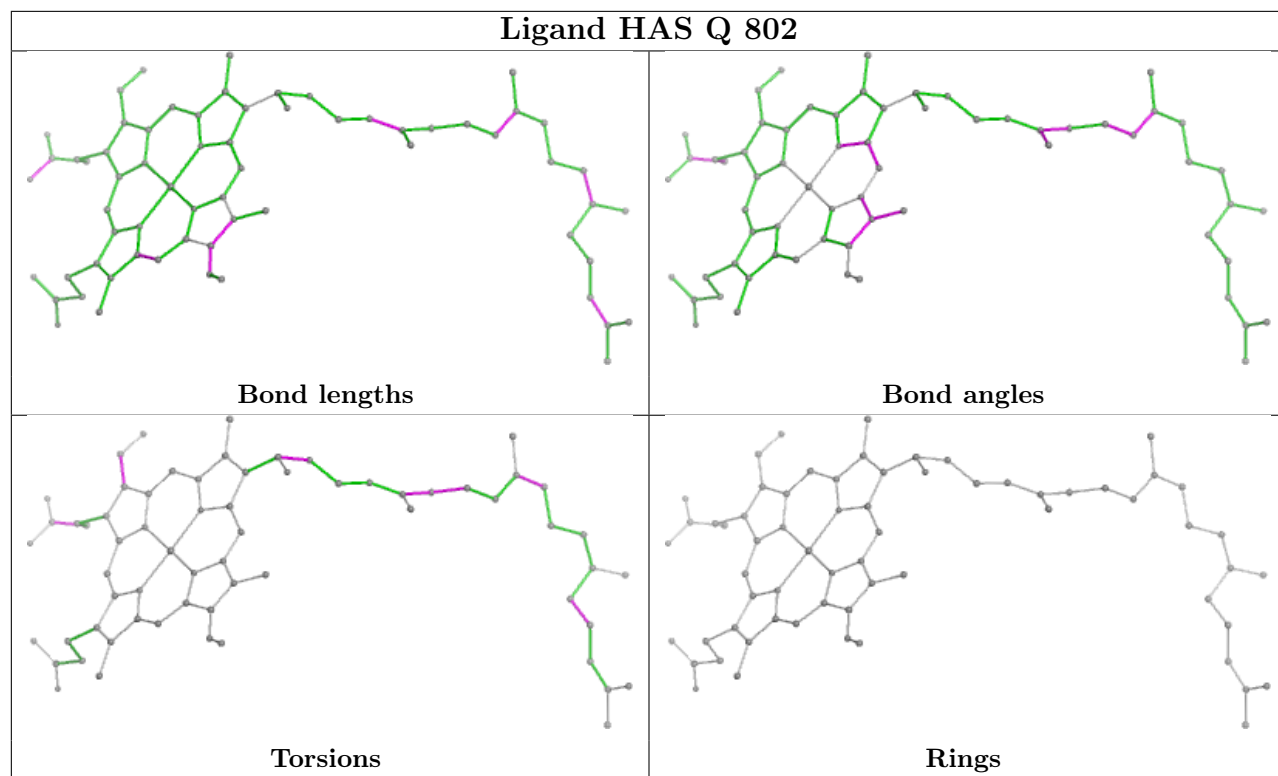
## Ligand MQ9 M 302

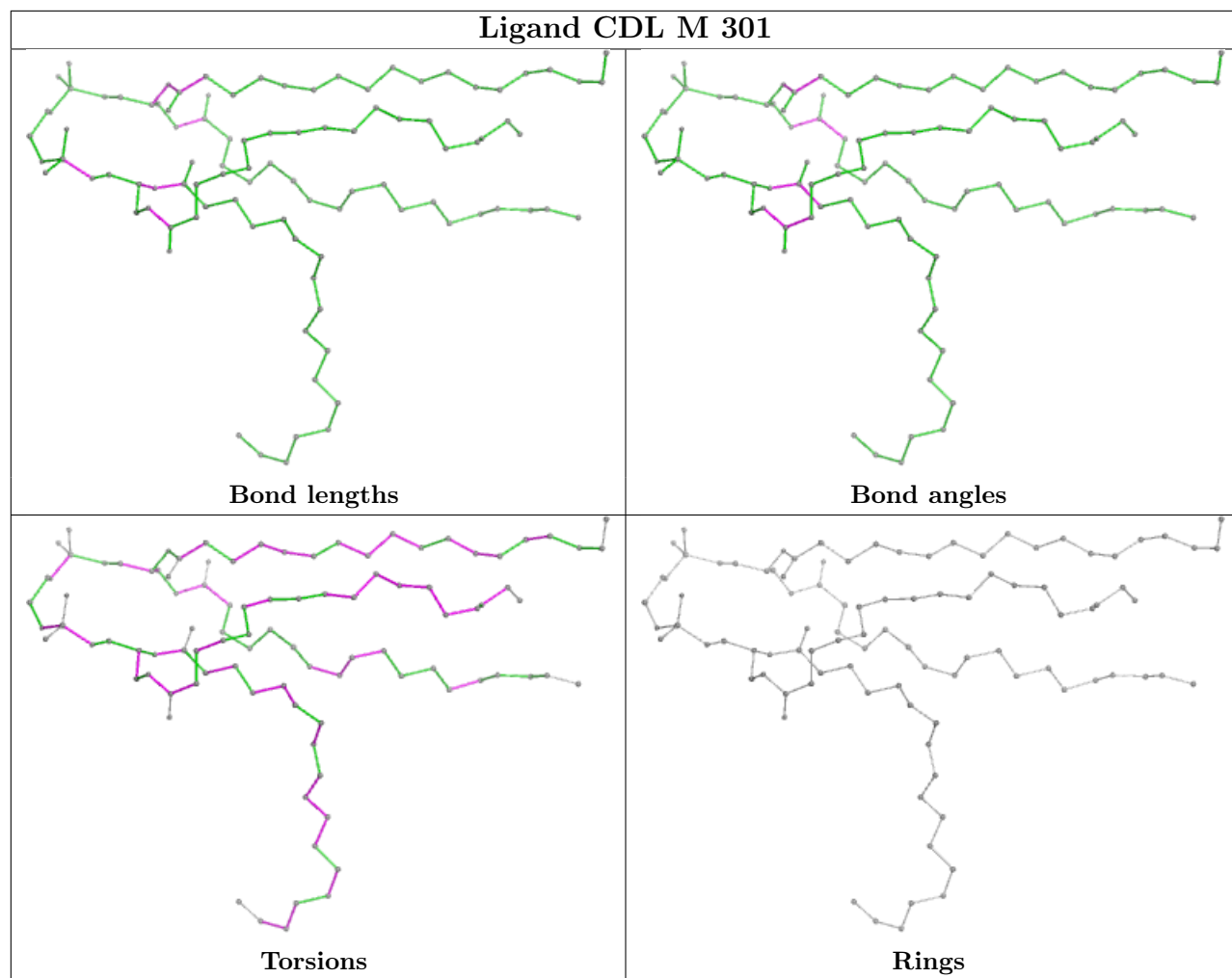


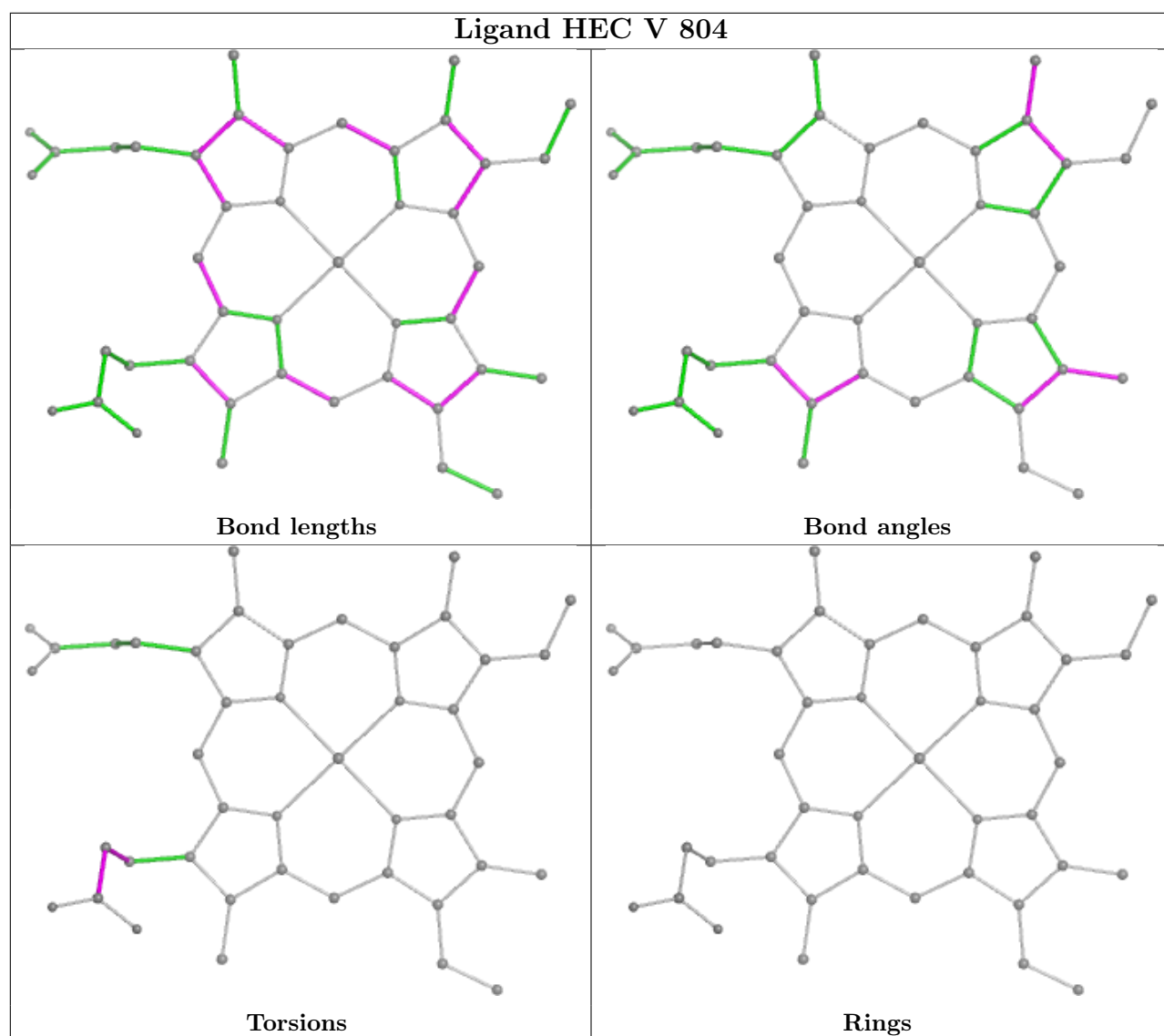
## Ligand MQ9 b 605



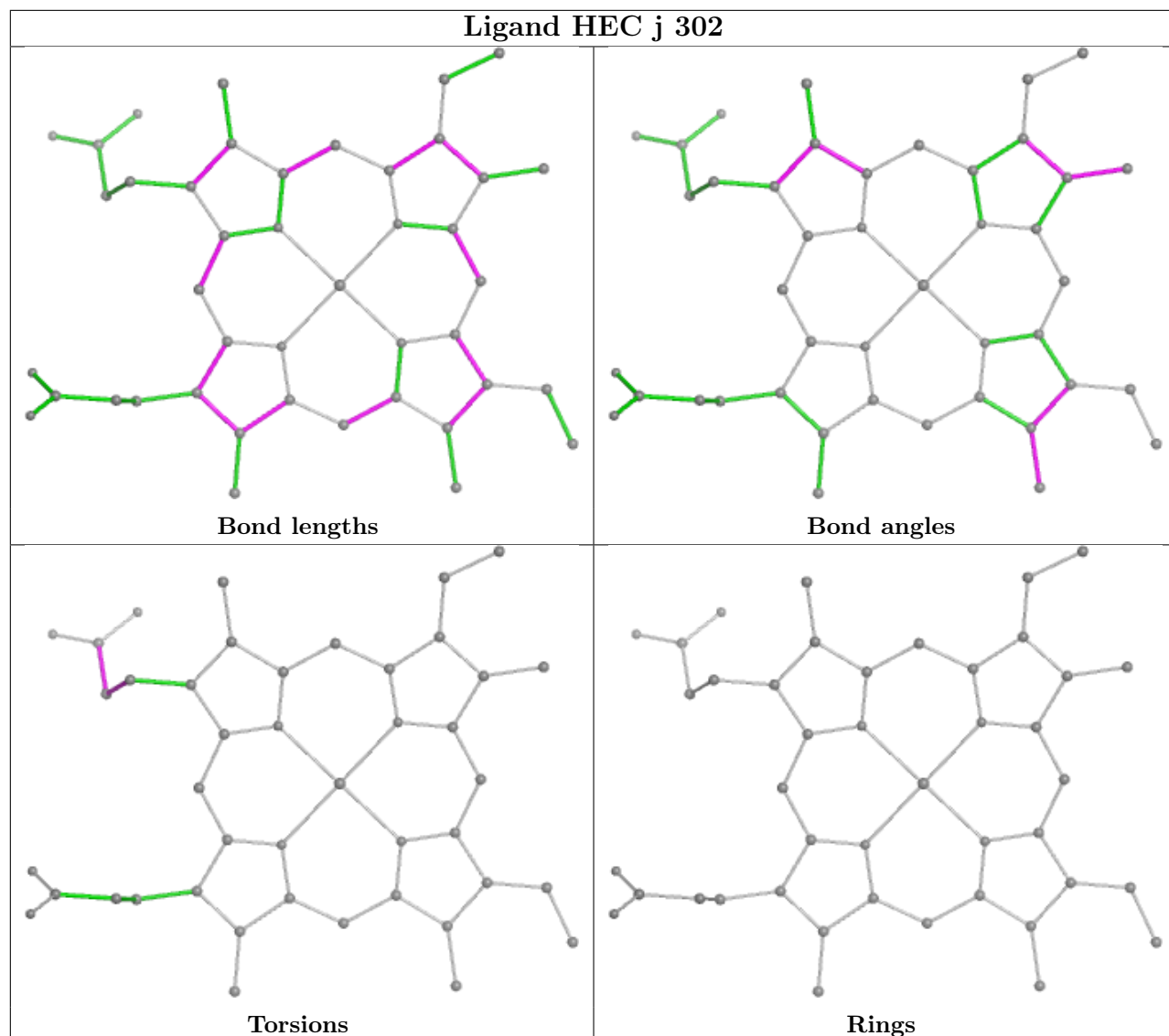


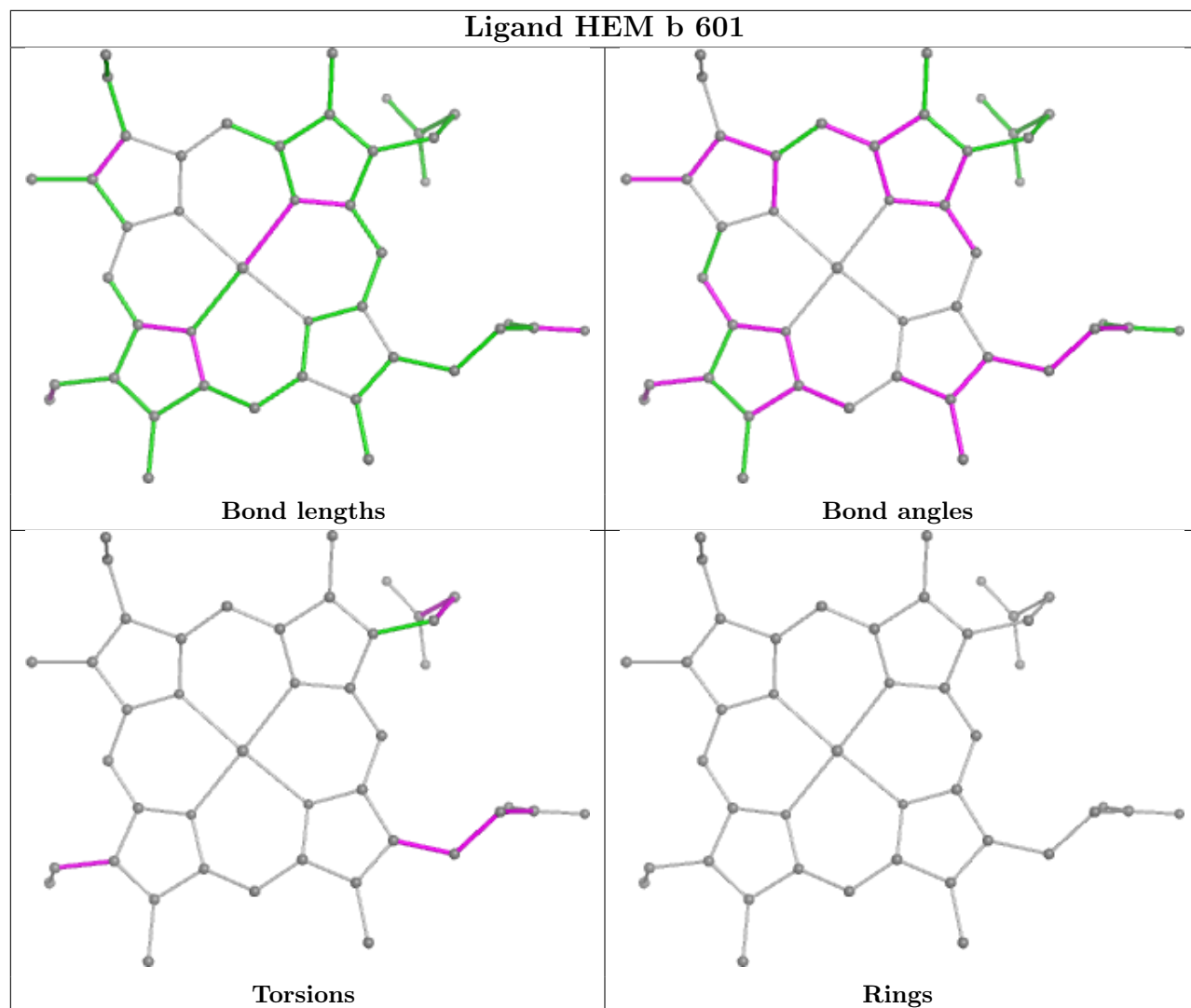


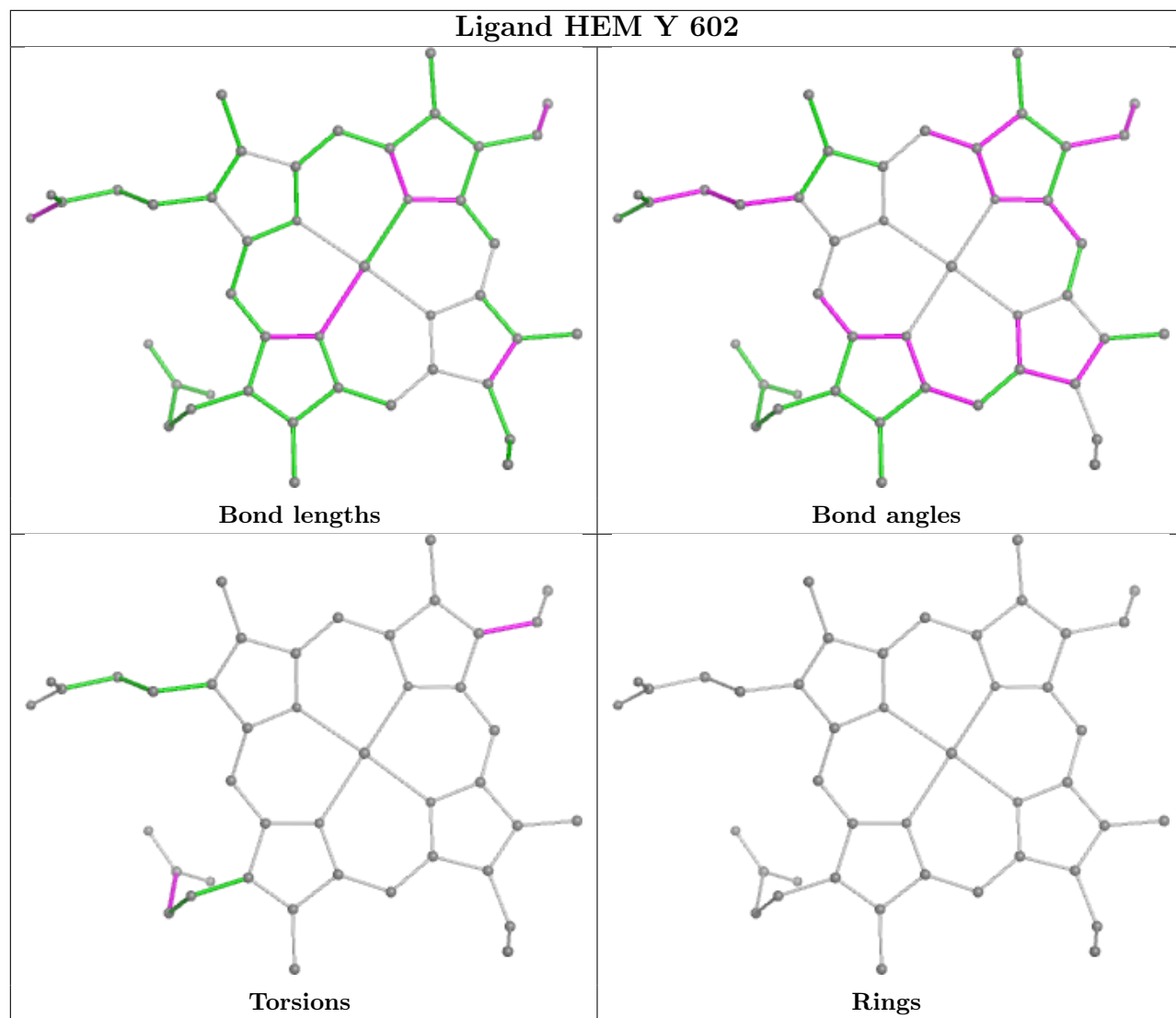


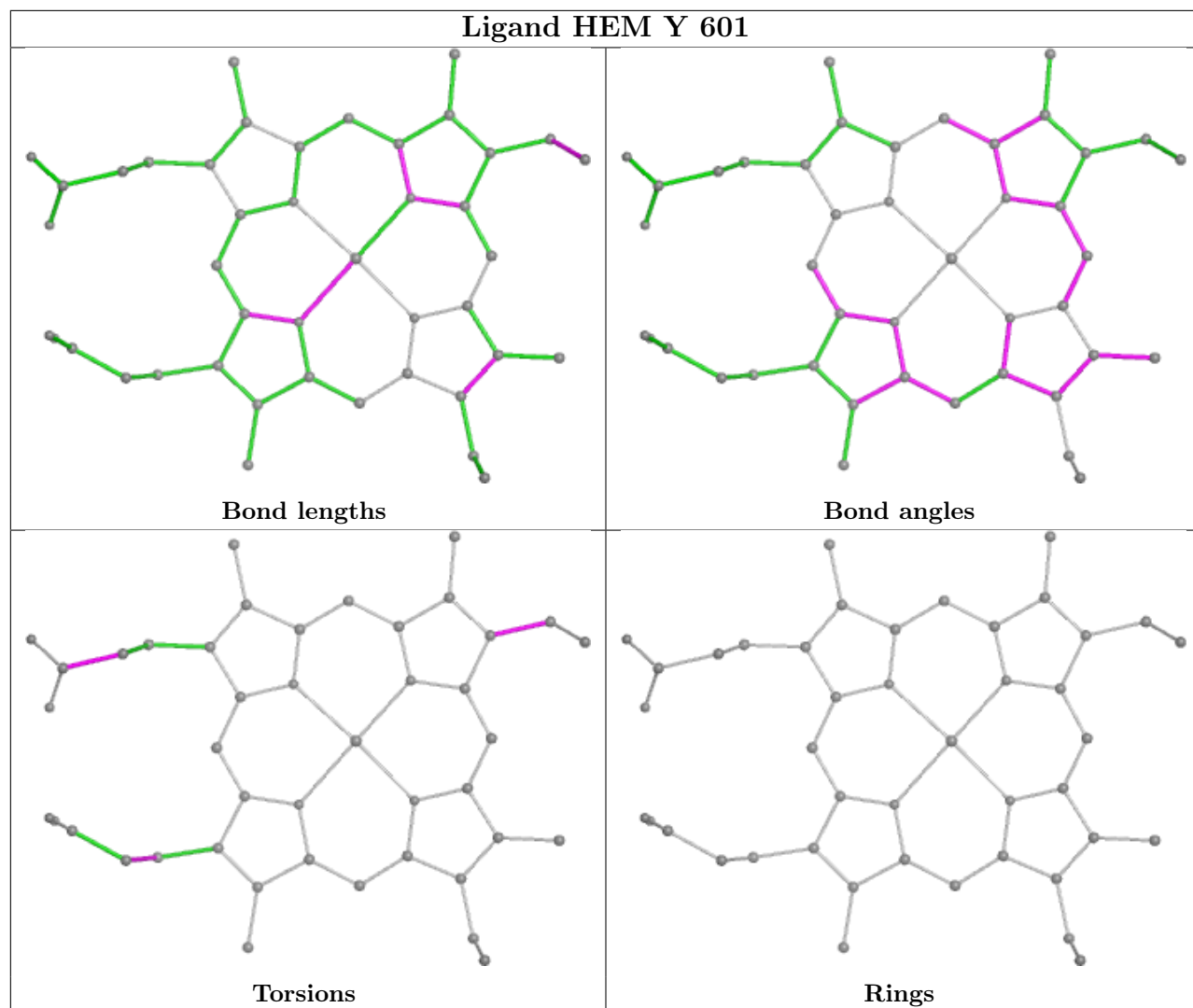


## Ligand HEC j 302

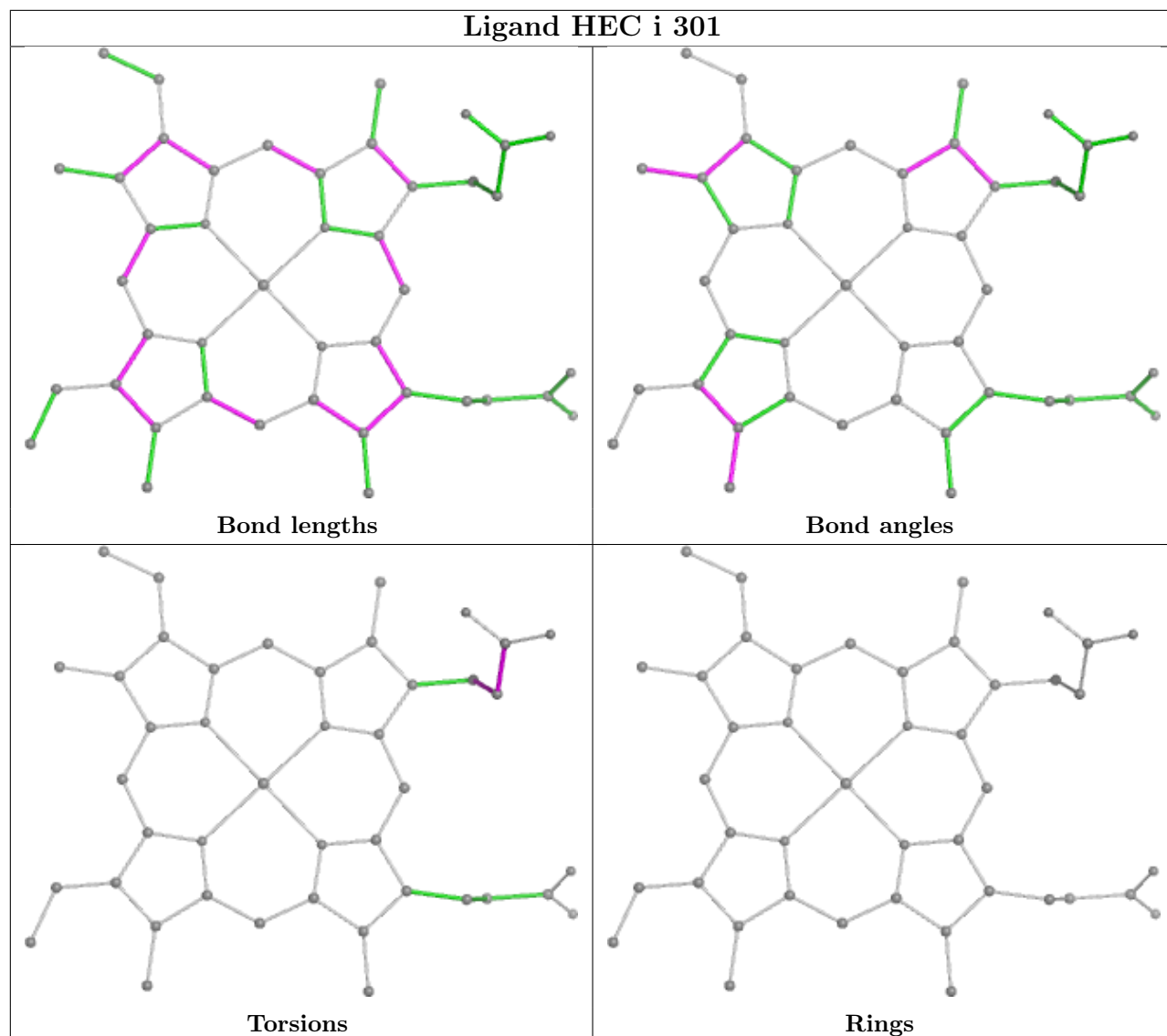




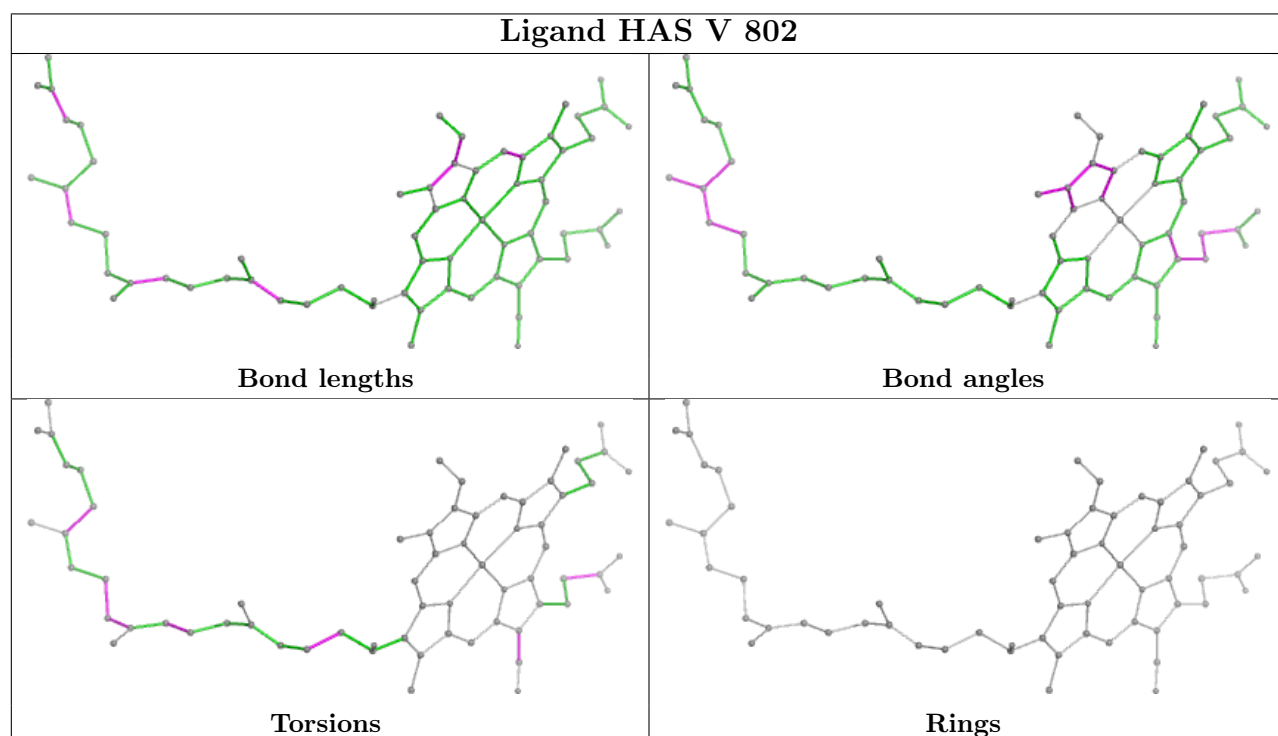
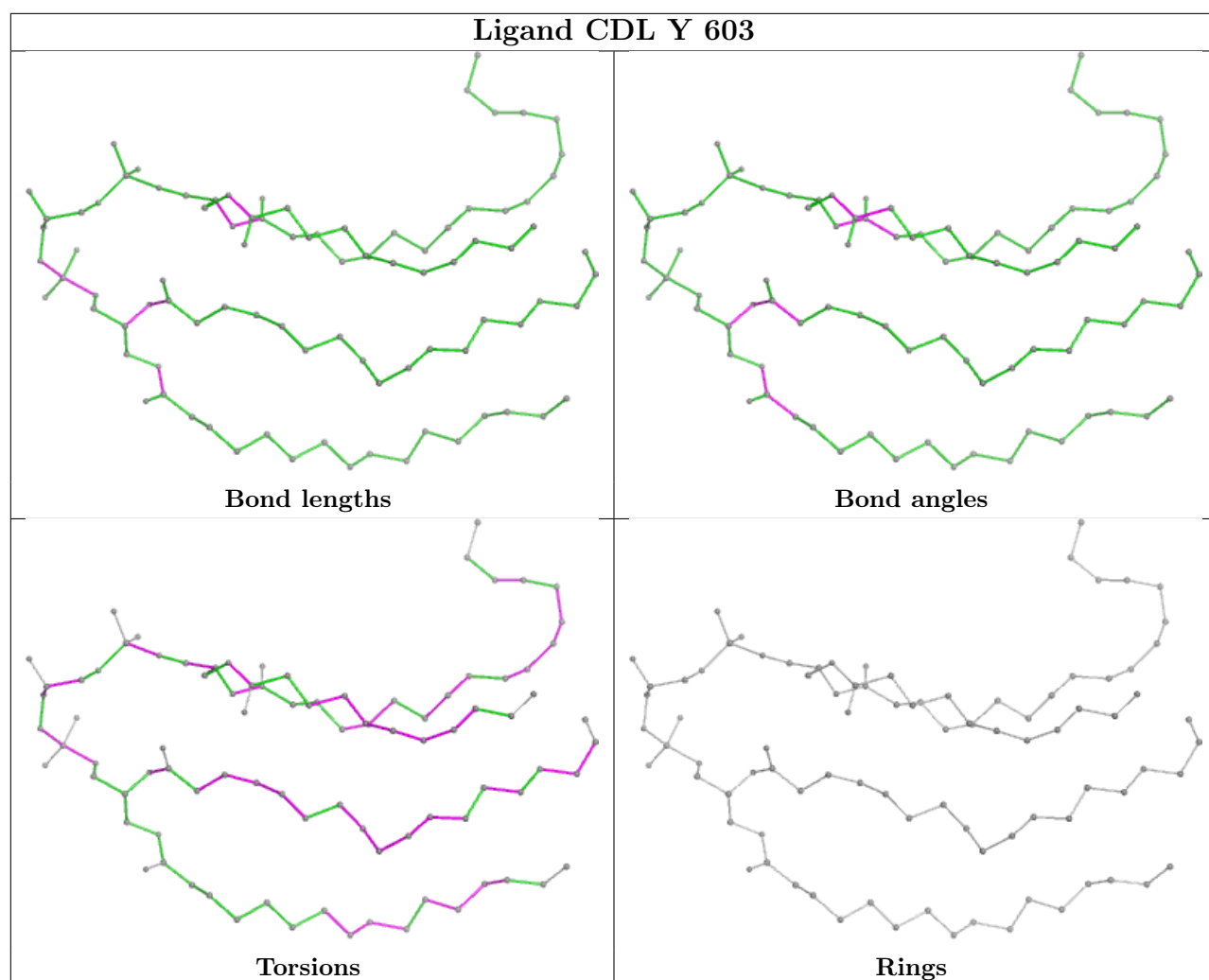


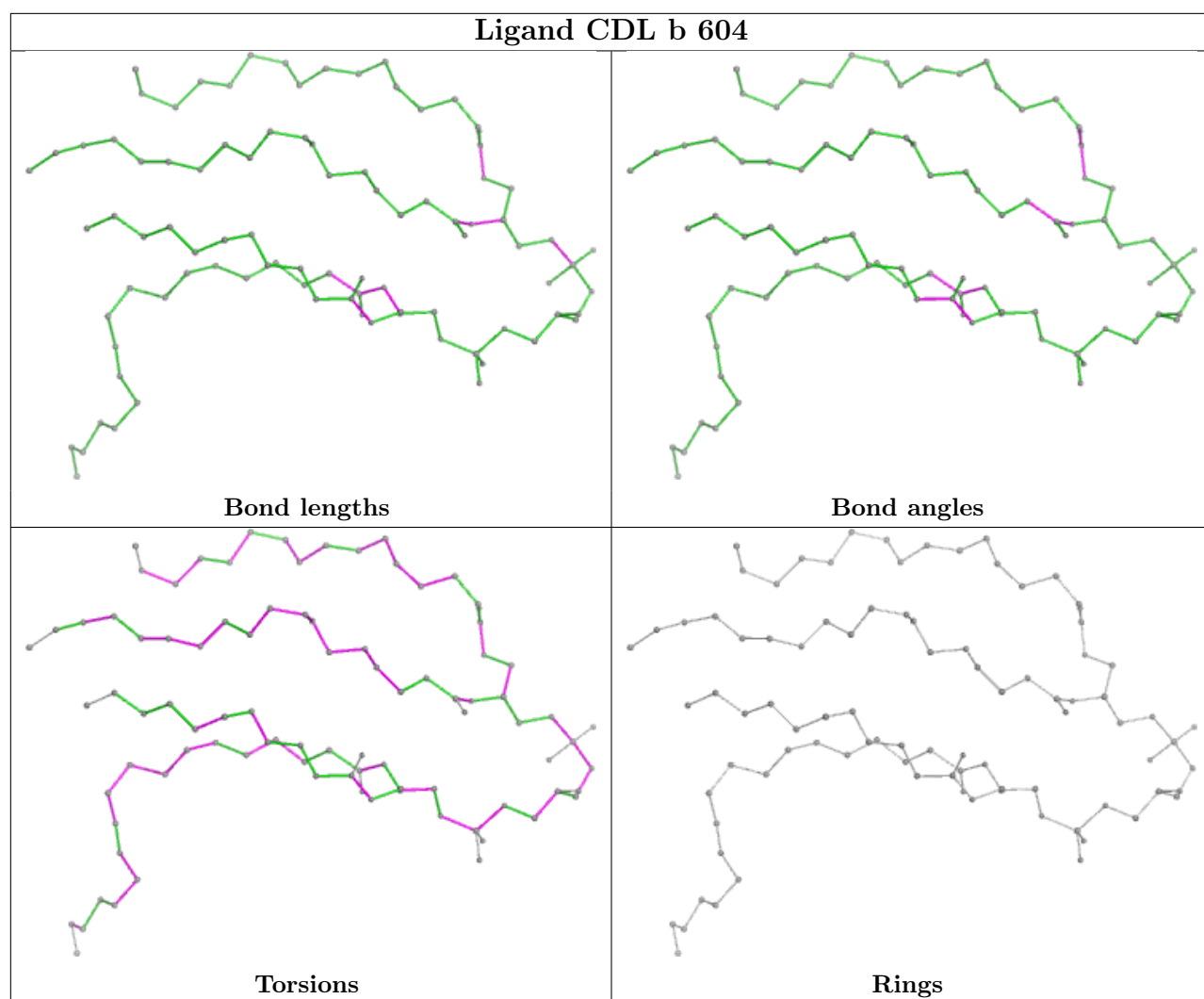


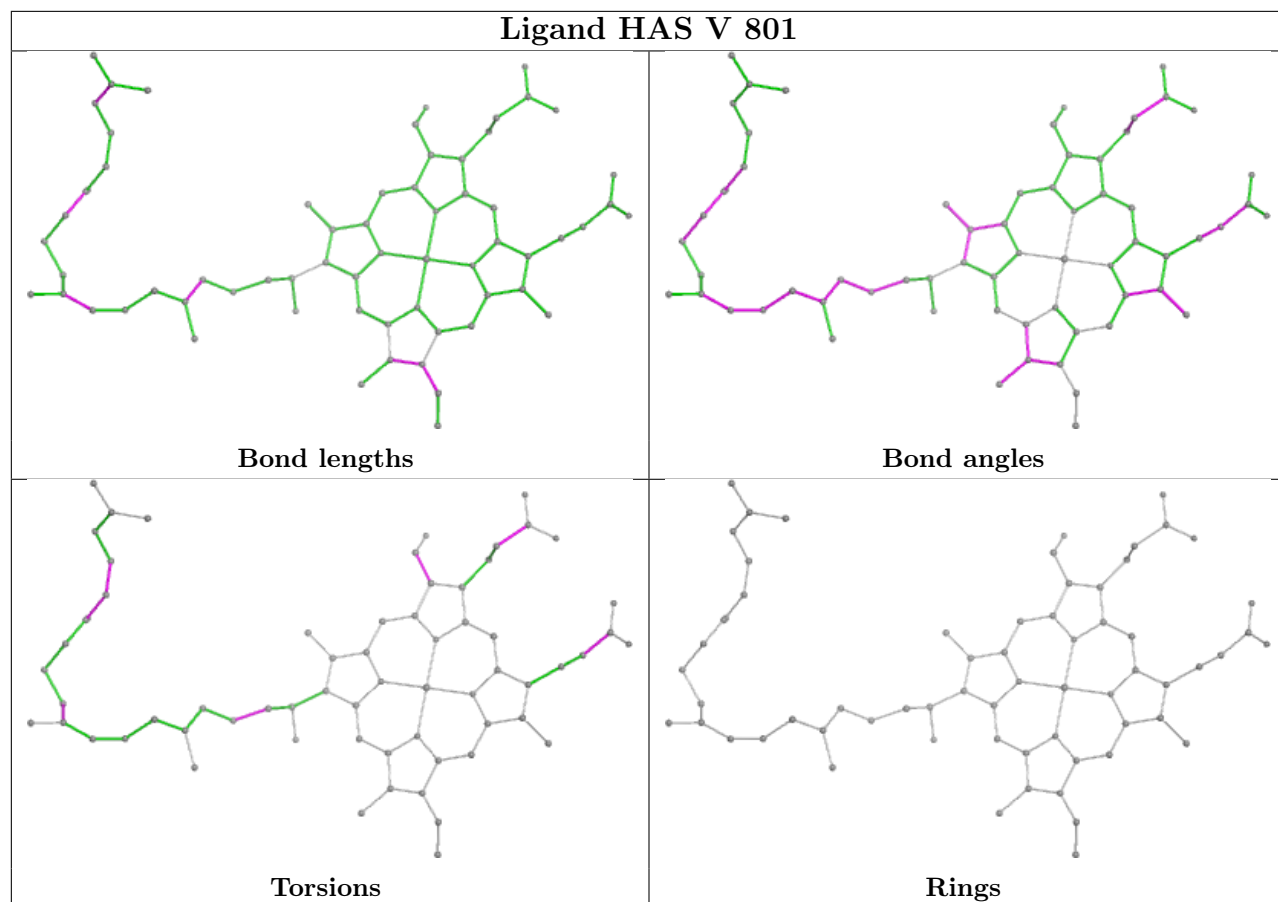
## Ligand HEC i 301

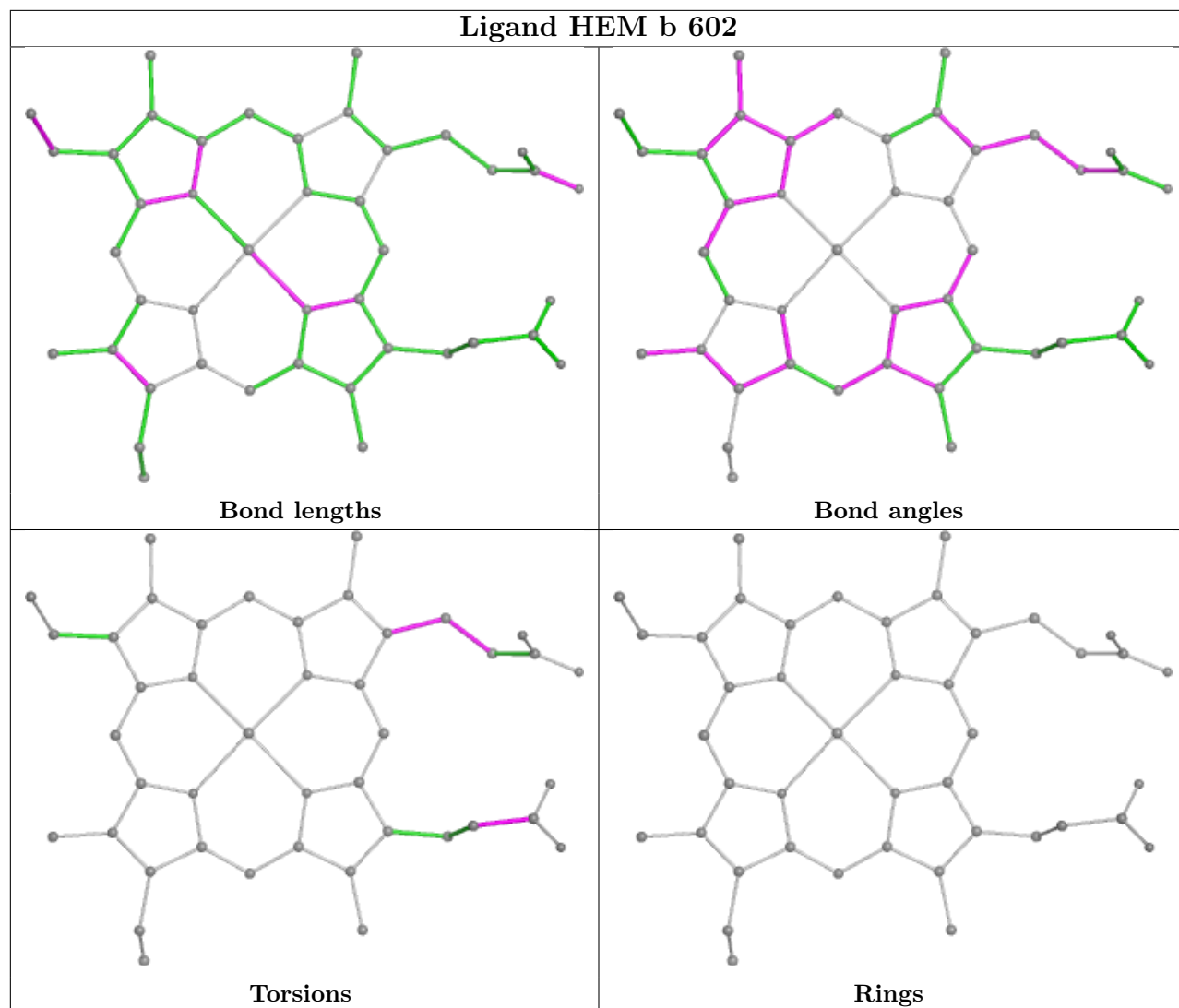


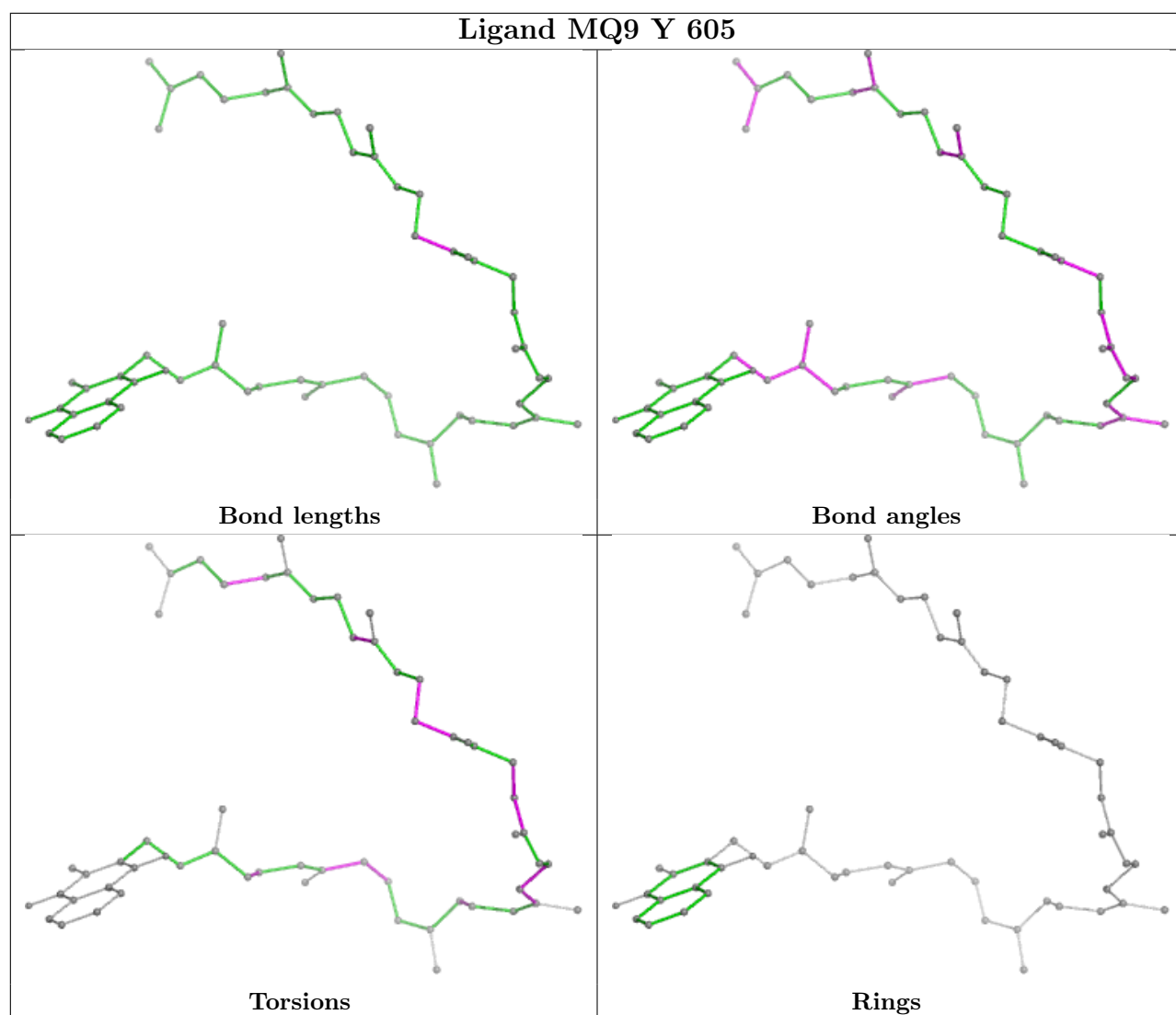


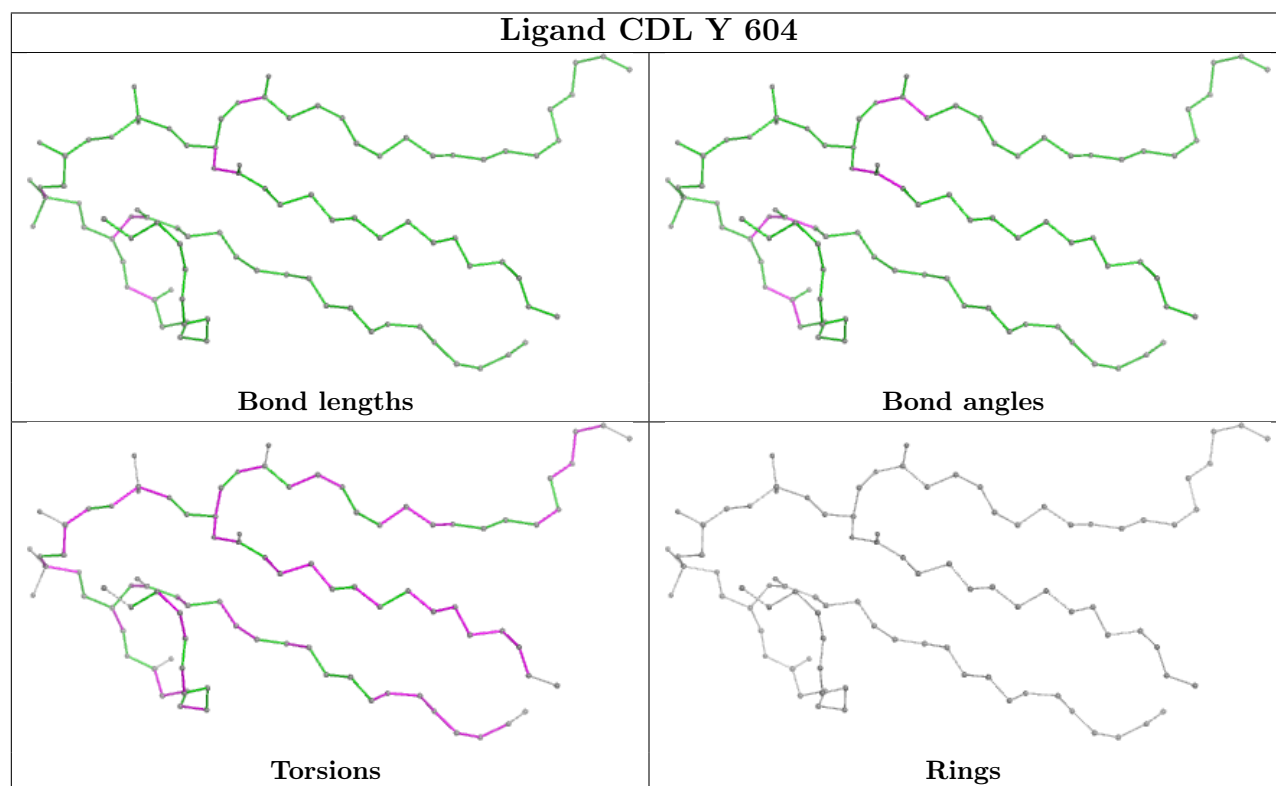
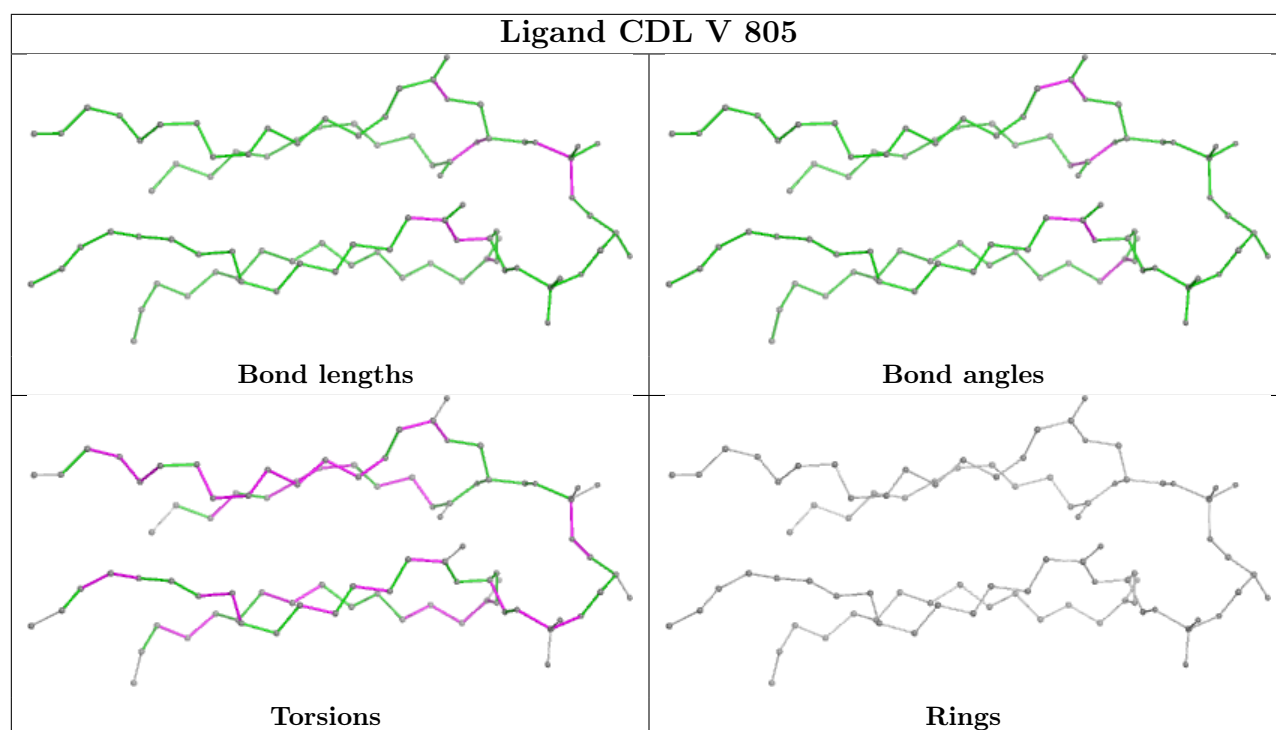


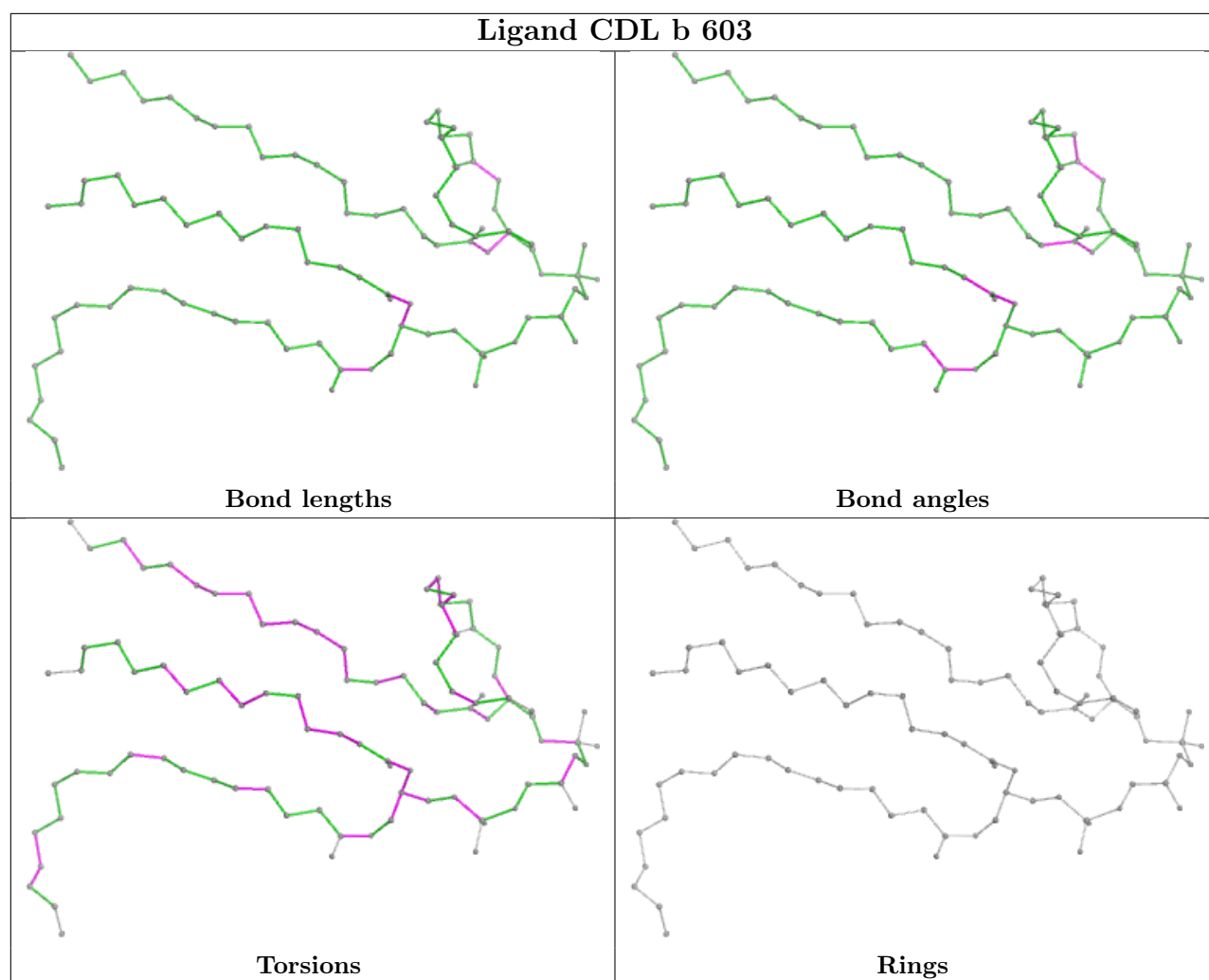












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Map visualisation

This section contains visualisations of the EMDB entry EMD-0289. These allow visual inspection of the internal detail of the map and identification of artifacts.

No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

### 6.1 Orthogonal projections

This section was not generated.

### 6.2 Central slices

This section was not generated.

### 6.3 Largest variance slices

This section was not generated.

### 6.4 Orthogonal standard-deviation projections (False-color)

This section was not generated.

### 6.5 Orthogonal surface views

This section was not generated.

### 6.6 Mask visualisation

This section was not generated. No masks/segmentation were deposited.



## 7 Map analysis ⓘ

This section contains the results of statistical analysis of the map.

### 7.1 Map-value distribution ⓘ

This section was not generated.

### 7.2 Volume estimate versus contour level ⓘ

This section was not generated.

### 7.3 Rotationally averaged power spectrum ⓘ

This section was not generated. The rotationally averaged power spectrum had issues being displayed.

## 8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

## 9 Map-model fit

This section was not generated.