



Full wwPDB EM Validation Report ⓘ

Mar 12, 2026 – 07:54 PM UTC

PDB ID : 8OVD / pdb_00008ovd
EMDB ID : EMD-17211
Title : Respiratory supercomplex (III2-IV2) from Mycobacterium smegmatis
Authors : Kovalova, T.; Krol, S.; Sjostrand, D.; Riepl, D.; Gamiz-Hernandez, A.;
Brzezinski, P.; Kaila, V.; Hogbom, M.
Deposited on : 2023-04-25
Resolution : 2.30 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

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>.

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

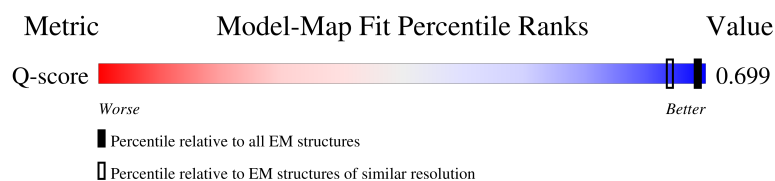
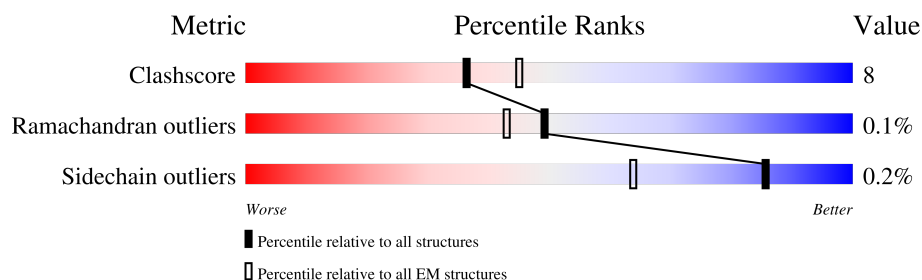
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 2.30 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	4254 (1.80 - 2.80)

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 ≥ 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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	C	278	
1	O	278	
2	G	408	
2	M	408	

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Mol	Chain	Length	Quality of chain
3	H	556	
3	N	556	
4	I	100	
4	P	100	
5	J	203	
5	S	203	
6	K	139	
6	T	139	
7	L	575	
7	R	575	
8	Q	341	
8	X	341	
9	U	79	
9	Z	79	
10	V	157	
10	a	157	
11	W	186	
11	b	186	
12	Y	236	
12	c	236	

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
21	CDL	H	903	-	-	X	-
21	CDL	N	602	-	-	X	-

2 Entry composition

There are 30 unique types of molecules in this entry. The entry contains 47246 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 Cytochrome bc1 complex cytochrome c subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	O	223	Total	C	N	O	S	0	0
			1623	1008	289	314	12		
1	C	223	Total	C	N	O	S	0	0
			1623	1008	289	314	12		

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
O	17	MET	-	initiating methionine	UNP A0R050
O	18	HIS	-	expression tag	UNP A0R050
O	19	HIS	-	expression tag	UNP A0R050
O	20	HIS	-	expression tag	UNP A0R050
O	21	HIS	-	expression tag	UNP A0R050
O	22	HIS	-	expression tag	UNP A0R050
O	23	HIS	-	expression tag	UNP A0R050
O	24	MET	-	expression tag	UNP A0R050
O	25	GLY	-	expression tag	UNP A0R050
O	26	SER	-	expression tag	UNP A0R050
C	17	MET	-	initiating methionine	UNP A0R050
C	18	HIS	-	expression tag	UNP A0R050
C	19	HIS	-	expression tag	UNP A0R050
C	20	HIS	-	expression tag	UNP A0R050
C	21	HIS	-	expression tag	UNP A0R050
C	22	HIS	-	expression tag	UNP A0R050
C	23	HIS	-	expression tag	UNP A0R050
C	24	MET	-	expression tag	UNP A0R050
C	25	GLY	-	expression tag	UNP A0R050
C	26	SER	-	expression tag	UNP A0R050

- Molecule 2 is a protein called Cytochrome bc1 complex cytochrome c subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	M	380	Total	C	N	O	S	0	0
			2967	1919	502	535	11		
2	G	380	Total	C	N	O	S	0	0
			2967	1919	502	535	11		

- Molecule 3 is a protein called Cytochrome bc1 complex cytochrome b subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	N	533	Total	C	N	O	S	0	0
			4167	2743	707	699	18		
3	H	533	Total	C	N	O	S	0	0
			4167	2743	707	699	18		

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
N	547	LYS	-	expression tag	UNP A0R052
N	548	LEU	-	expression tag	UNP A0R052
N	549	ASP	-	expression tag	UNP A0R052
N	550	TYR	-	expression tag	UNP A0R052
N	551	LYS	-	expression tag	UNP A0R052
N	552	ASP	-	expression tag	UNP A0R052
N	553	ASP	-	expression tag	UNP A0R052
N	554	ASP	-	expression tag	UNP A0R052
N	555	ASP	-	expression tag	UNP A0R052
N	556	LYS	-	expression tag	UNP A0R052
H	547	LYS	-	expression tag	UNP A0R052
H	548	LEU	-	expression tag	UNP A0R052
H	549	ASP	-	expression tag	UNP A0R052
H	550	TYR	-	expression tag	UNP A0R052
H	551	LYS	-	expression tag	UNP A0R052
H	552	ASP	-	expression tag	UNP A0R052
H	553	ASP	-	expression tag	UNP A0R052
H	554	ASP	-	expression tag	UNP A0R052
H	555	ASP	-	expression tag	UNP A0R052
H	556	LYS	-	expression tag	UNP A0R052

- Molecule 4 is a protein called Transmembrane protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	P	73	Total	C	N	O	S	0	0
			586	385	107	90	4		

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Mol	Chain	Residues	Atoms					AltConf	Trace
4	I	73	Total	C	N	O	S	0	0
			586	385	107	90	4		

- Molecule 5 is a protein called Probable cytochrome c oxidase subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	S	184	Total	C	N	O	S	0	0
			1441	967	229	238	7		
5	J	184	Total	C	N	O	S	0	0
			1441	967	229	238	7		

- Molecule 6 is a protein called Cytochrome c oxidase polypeptide 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	T	139	Total	C	N	O	S	0	0
			1077	719	167	188	3		
6	K	139	Total	C	N	O	S	0	0
			1077	719	167	188	3		

- Molecule 7 is a protein called Cytochrome c oxidase subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	R	551	Total	C	N	O	S	0	0
			4369	2936	694	713	26		
7	L	551	Total	C	N	O	S	0	0
			4369	2936	694	713	26		

- Molecule 8 is a protein called cytochrome-c oxidase.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	Q	299	Total	C	N	O	S	0	0
			2382	1541	396	435	10		
8	X	300	Total	C	N	O	S	0	0
			2391	1547	398	436	10		

- Molecule 9 is a protein called Cytochrome c oxidase subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	U	66	Total	C	N	O	S	0	0
			499	329	84	85	1		
9	Z	67	Total	C	N	O	S	0	0
			507	334	85	86	2		

- Molecule 10 is a protein called Uncharacterized protein MSMEG_4692/MSMEI_4575.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	V	143	Total	C	N	O	S	0	0
			1024	647	174	201	2		
10	a	143	Total	C	N	O	S	0	0
			1024	647	174	201	2		

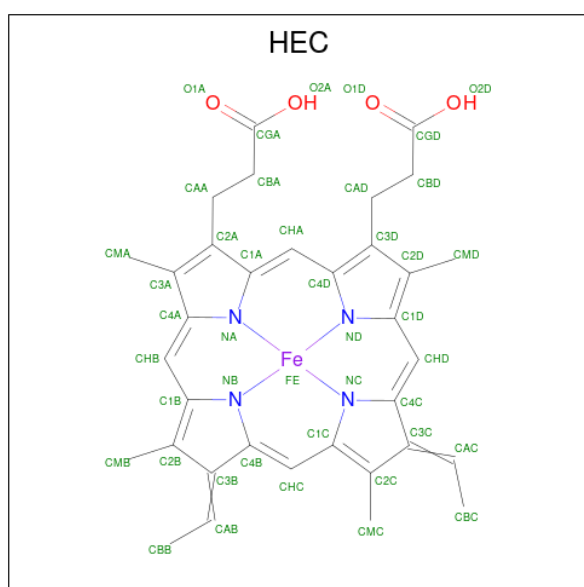
- Molecule 11 is a protein called LpqE protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	W	149	Total	C	N	O	S	0	0
			1083	670	181	231	1		
11	b	149	Total	C	N	O	S	0	0
			1083	670	181	231	1		

- Molecule 12 is a protein called Superoxide dismutase [Cu-Zn].

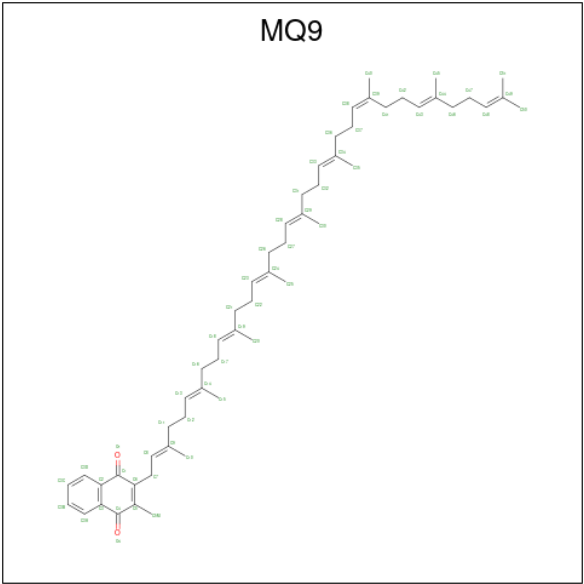
Mol	Chain	Residues	Atoms					AltConf	Trace
12	Y	25	Total	C	N	O	S	0	0
			168	103	26	38	1		
12	c	25	Total	C	N	O	S	0	0
			168	103	26	38	1		

- Molecule 13 is HEME C (CCD ID: HEC) (formula: $C_{34}H_{34}FeN_4O_4$).



Mol	Chain	Residues	Atoms					AltConf
13	O	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
13	O	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
13	C	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
13	C	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

- Molecule 14 is MENAQUINONE-9 (CCD ID: MQ9) (formula: C₅₆H₈₀O₂).



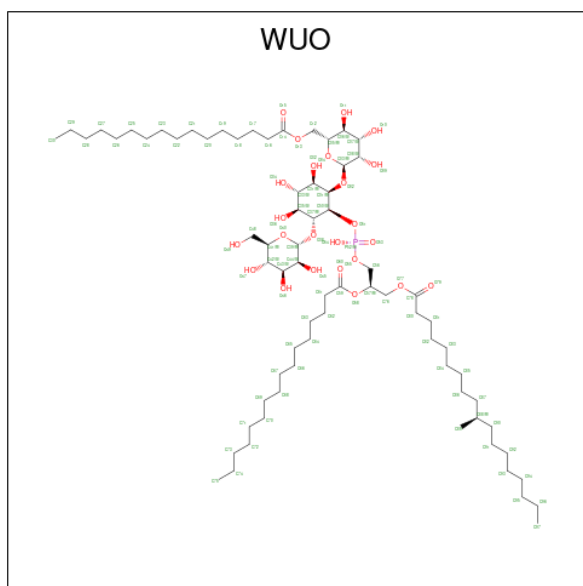
Mol	Chain	Residues	Atoms			AltConf
14	O	1	Total	C	O	0
			58	56	2	
14	M	1	Total	C	O	0
			58	56	2	
14	N	1	Total	C	O	0
			43	41	2	
14	N	1	Total	C	O	0
			58	56	2	
14	N	1	Total	C	O	0
			58	56	2	
14	T	1	Total	C	O	0
			58	56	2	
14	C	1	Total	C	O	0
			58	56	2	
14	G	1	Total	C	O	0
			58	56	2	

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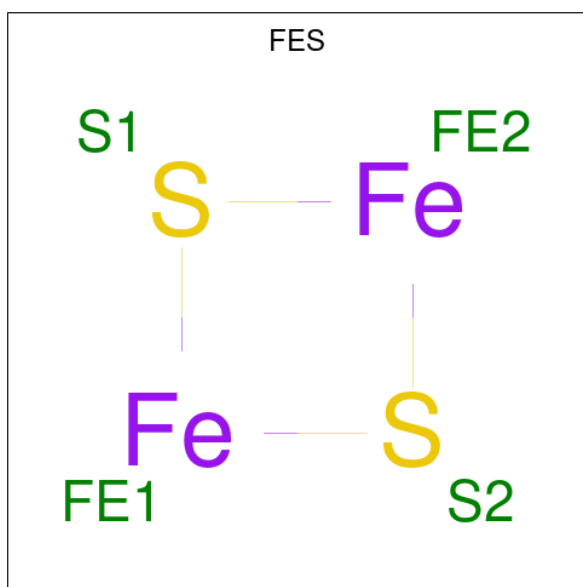
Mol	Chain	Residues	Atoms			AltConf
14	H	1	Total	C	O	0
			43	41	2	
14	H	1	Total	C	O	0
			58	56	2	
14	H	1	Total	C	O	0
			58	56	2	
14	K	1	Total	C	O	0
			58	56	2	

- Molecule 15 is acyl-phosphatidyl-myo-inositol dimannoside (AcPIM2) (CCD ID: WUO) (formula: $C_{72}H_{135}O_{24}P$).



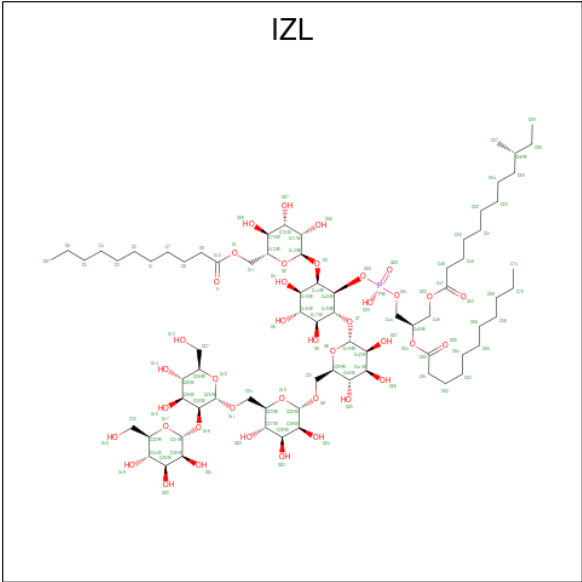
Mol	Chain	Residues	Atoms				AltConf
15	O	1	Total	C	O	P	0
			97	72	24	1	
15	P	1	Total	C	O	P	0
			97	72	24	1	
15	C	1	Total	C	O	P	0
			97	72	24	1	
15	I	1	Total	C	O	P	0
			97	72	24	1	

- Molecule 16 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2).



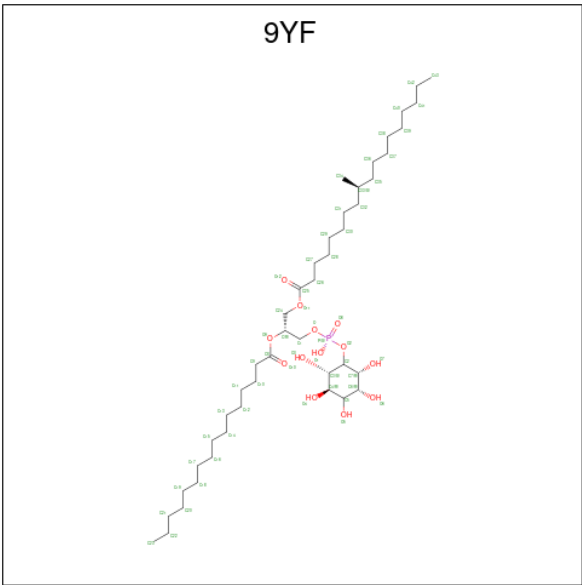
Mol	Chain	Residues	Atoms			AltConf
16	M	1	Total	Fe	S	0
			4	2	2	
16	G	1	Total	Fe	S	0
			4	2	2	

- Molecule 17 is [(2 {R})-3-[(1 {S},2 {R},3 {S},4 {S},5 {R},6 {R})-2-[(2 {R},3 {S},4 {S},5 {S},6 {R})-6-[(2 {S},3 {S},4 {S},5 {S},6 {R})-6-[(2 {S},3 {S},4 {S},5 {S},6 {R})-6-(hydroxymethyl)-3-[(2 {R},3 {S},4 {S},5 {S},6 {R})-6-(hydroxymethyl)-3,4,5-tris(oxidanyl)oxan-2-yl]oxy-4,5-bis(oxidanyl)oxan-2-yl]oxymethyl]-3,4,5-tris(oxidanyl)oxan-2-yl]oxy-3,4,5-tris(oxidanyl)-6-[(2 {R},3 {S},4 {S},5 {S},6 {R})-3,4,5-tris(oxidanyl)-6-(undecanoyloxymethyl)oxan-2-yl]oxy-cyclohexyl]oxy-oxidanyl-phosphoryl]oxy-2-undecanoyloxy-propyl] (10 {R})-10-methyldodecanoate (CCD ID: IZL) (formula: C₇₄H₁₃₃O₃₉P).



Mol	Chain	Residues	Atoms				AltConf
17	M	1	Total	C	O	P	0
			114	74	39	1	
17	G	1	Total	C	O	P	0
			114	74	39	1	

- Molecule 18 is (2R)-2-(hexadecanoyloxy)-3-{[(S)-hydroxy{[(1R,2R,3R,4R,5R,6S)-2,3,4,5,6-pentahydroxycyclohexyl]oxy}phosphoryl]oxy}propyl (9S)-9-methyloctadecanoate (CCD ID: 9YF) (formula: C₄₄H₈₅O₁₃P).



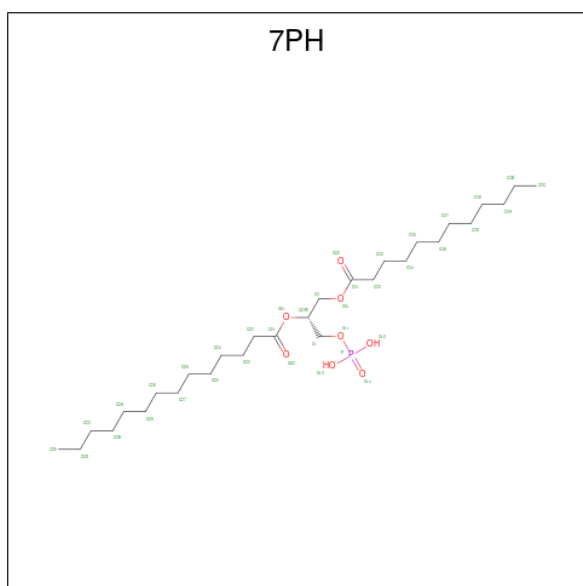
Mol	Chain	Residues	Atoms				AltConf
18	M	1	Total	C	O	P	0
			58	44	13	1	

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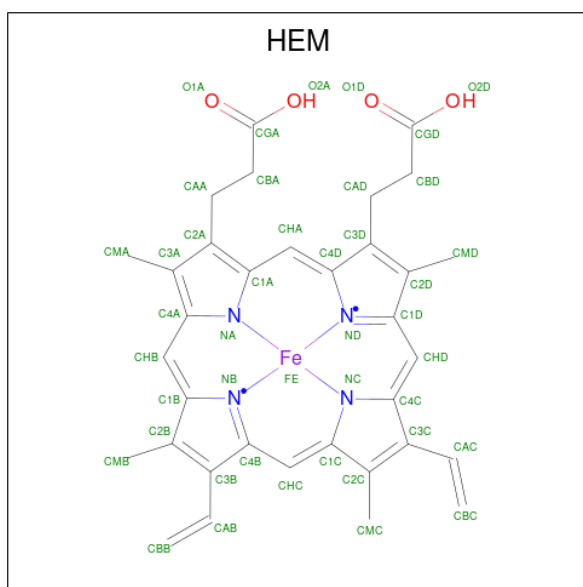
Mol	Chain	Residues	Atoms				AltConf
18	W	1	Total	C	O	P	0
			58	44	13	1	
18	G	1	Total	C	O	P	0
			58	44	13	1	
18	b	1	Total	C	O	P	0
			58	44	13	1	

- Molecule 19 is (1R)-2-(dodecanoyloxy)-1-[(phosphonooxy)methyl]ethyl tetradecanoate (CCD ID: 7PH) (formula: C₂₉H₅₇O₈P).



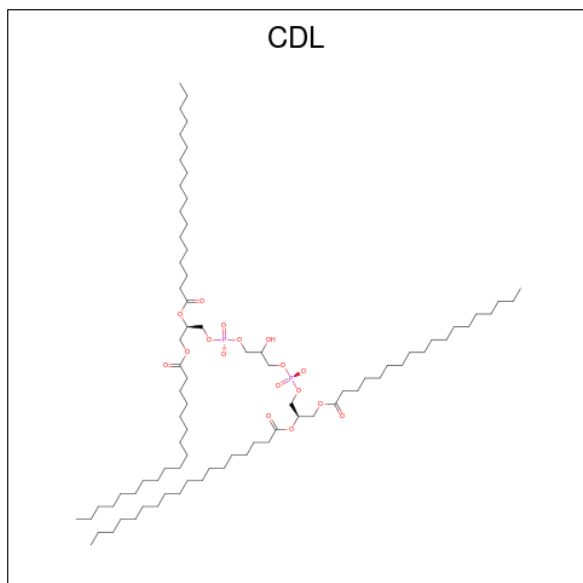
Mol	Chain	Residues	Atoms				AltConf
19	M	1	Total	C	O	P	0
			38	29	8	1	
19	N	1	Total	C	O	P	0
			38	29	8	1	
19	S	1	Total	C	O	P	0
			38	29	8	1	
19	G	1	Total	C	O	P	0
			38	29	8	1	
19	H	1	Total	C	O	P	0
			38	29	8	1	

- Molecule 20 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: C₃₄H₃₂FeN₄O₄).



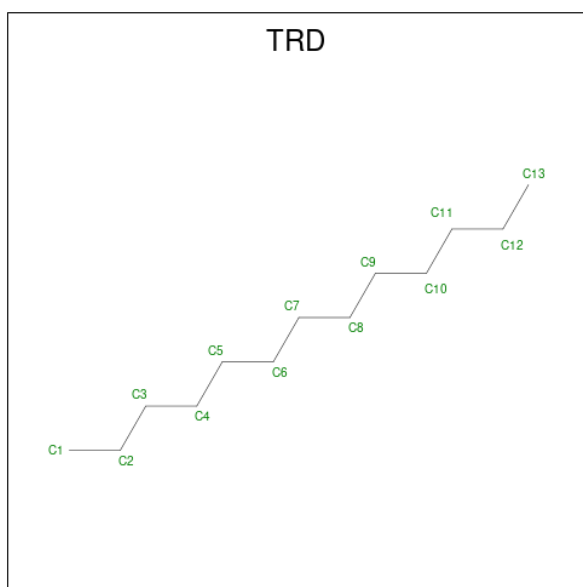
Mol	Chain	Residues	Atoms					AltConf
20	N	1	Total 43	C 34	Fe 1	N 4	O 4	0
20	N	1	Total 43	C 34	Fe 1	N 4	O 4	0
20	H	1	Total 43	C 34	Fe 1	N 4	O 4	0
20	H	1	Total 43	C 34	Fe 1	N 4	O 4	0

- Molecule 21 is CARDIOLIPIN (CCD ID: CDL) (formula: $\text{C}_{81}\text{H}_{156}\text{O}_{17}\text{P}_2$).



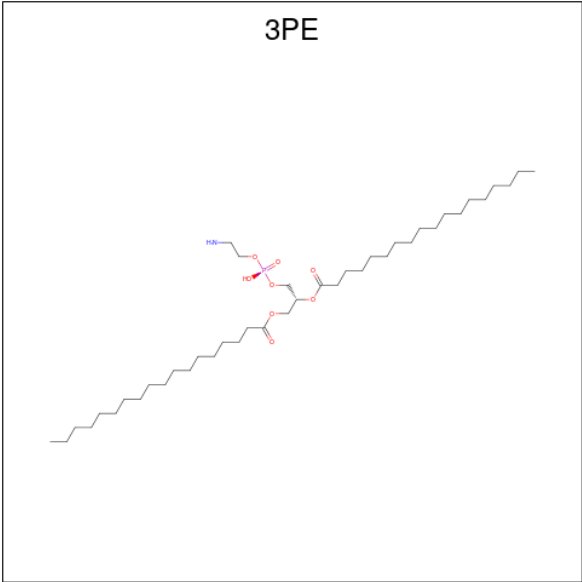
Mol	Chain	Residues	Atoms				AltConf
21	N	1	Total	C	O	P	0
			74	55	17	2	
21	N	1	Total	C	O	P	0
			77	58	17	2	
21	N	1	Total	C	O	P	0
			79	60	17	2	
21	P	1	Total	C	O	P	0
			77	58	17	2	
21	T	1	Total	C	O	P	0
			79	60	17	2	
21	R	1	Total	C	O	P	0
			77	58	17	2	
21	R	1	Total	C	O	P	0
			77	58	17	2	
21	C	1	Total	C	O	P	0
			79	60	17	2	
21	H	1	Total	C	O	P	0
			74	55	17	2	
21	H	1	Total	C	O	P	0
			77	58	17	2	
21	H	1	Total	C	O	P	0
			79	60	17	2	
21	I	1	Total	C	O	P	0
			77	58	17	2	
21	I	1	Total	C	O	P	0
			77	58	17	2	
21	J	1	Total	C	O	P	0
			79	60	17	2	
21	L	1	Total	C	O	P	0
			79	60	17	2	

- Molecule 22 is TRIDECANE (CCD ID: TRD) (formula: C₁₃H₂₈).



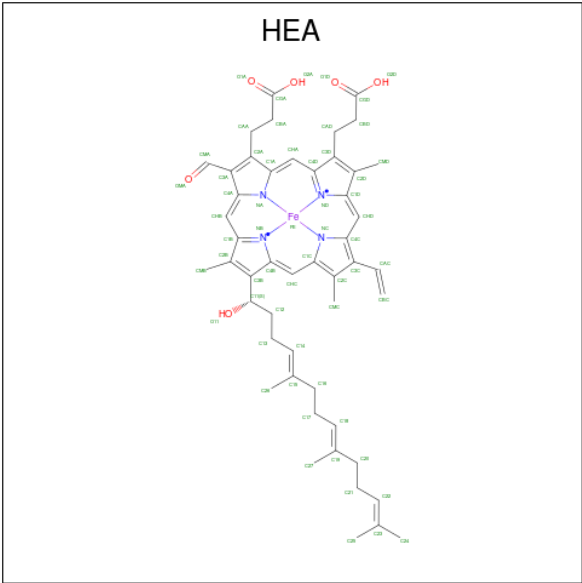
Mol	Chain	Residues	Atoms	AltConf
22	S	1	Total C 13 13	0
22	T	1	Total C 13 13	0
22	R	1	Total C 13 13	0
22	R	1	Total C 13 13	0
22	Q	1	Total C 13 13	0
22	J	1	Total C 13 13	0
22	K	1	Total C 13 13	0
22	L	1	Total C 13 13	0
22	L	1	Total C 13 13	0
22	X	1	Total C 13 13	0

- Molecule 23 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (CCD ID: 3PE) (formula: $C_{41}H_{82}NO_8P$).



Mol	Chain	Residues	Atoms					AltConf
23	S	1	Total	C	N	O	P	0
			32	22	1	8	1	
23	J	1	Total	C	N	O	P	0
			32	22	1	8	1	

- Molecule 24 is HEME-A (CCD ID: HEA) (formula: C₄₉H₅₆FeN₄O₆).



Mol	Chain	Residues	Atoms					AltConf
24	R	1	Total	C	Fe	N	O	0
			60	49	1	4	6	
24	R	1	Total	C	Fe	N	O	0
			60	49	1	4	6	

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Mol	Chain	Residues	Atoms				AltConf	
24	L	1	Total 60	C 49	Fe 1	N 4	O 6	0
24	L	1	Total 60	C 49	Fe 1	N 4	O 6	0

- Molecule 25 is COPPER (II) ION (CCD ID: CU) (formula: Cu).

Mol	Chain	Residues	Atoms		AltConf
25	R	1	Total	Cu	0
			1	1	
25	Q	2	Total	Cu	0
			2	2	
25	L	1	Total	Cu	0
			1	1	
25	X	2	Total	Cu	0
			2	2	

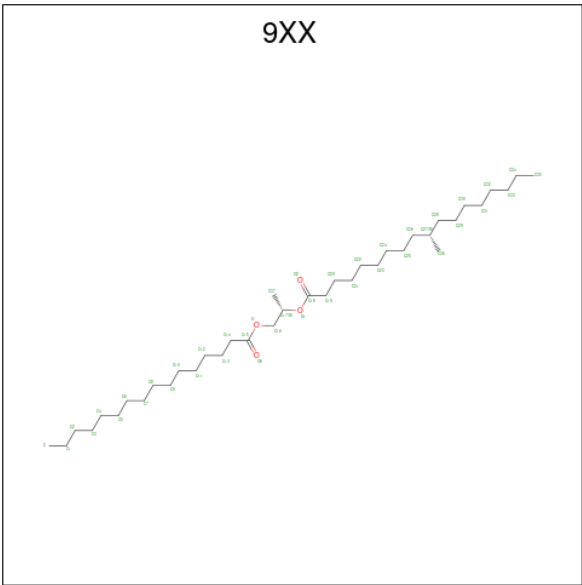
- Molecule 26 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
26	R	1	Total	Mg	0
			1	1	
26	L	1	Total	Mg	0
			1	1	

- Molecule 27 is CALCIUM ION (CCD ID: CA) (formula: Ca).

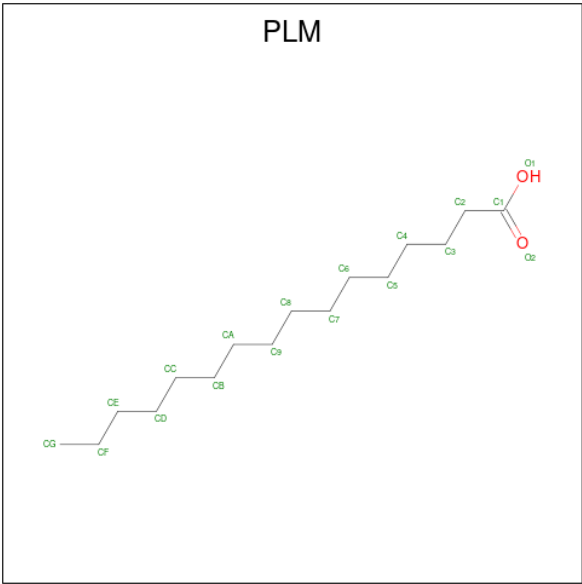
Mol	Chain	Residues	Atoms		AltConf
27	R	1	Total	Ca	0
			1	1	
27	L	1	Total	Ca	0
			1	1	

- Molecule 28 is (2S)-1-(hexadecanoyloxy)propan-2-yl (10S)-10-methyloctadecanoate (CCD ID: 9XX) (formula: C₃₈H₇₄O₄).



Mol	Chain	Residues	Atoms			AltConf
28	W	1	Total	C	O	0
			42	38	4	
28	Y	1	Total	C	O	0
			32	28	4	
28	b	1	Total	C	O	0
			32	28	4	
28	c	1	Total	C	O	0
			32	28	4	

- Molecule 29 is PALMITIC ACID (CCD ID: PLM) (formula: C₁₆H₃₂O₂).



Mol	Chain	Residues	Atoms			AltConf
29	W	1	Total	C	O	0
			11	10	1	
29	Y	1	Total	C	O	0
			11	10	1	
29	b	1	Total	C	O	0
			11	10	1	
29	c	1	Total	C	O	0
			11	10	1	

- Molecule 30 is water.

Mol	Chain	Residues	Atoms		AltConf
30	O	43	Total	O	0
			43	43	
30	M	51	Total	O	0
			51	51	
30	N	67	Total	O	0
			67	67	
30	P	2	Total	O	0
			2	2	
30	S	6	Total	O	0
			6	6	
30	T	11	Total	O	0
			11	11	
30	R	68	Total	O	0
			68	68	
30	Q	30	Total	O	0
			30	30	
30	W	4	Total	O	0
			4	4	
30	C	56	Total	O	0
			56	56	
30	G	60	Total	O	0
			60	60	
30	H	64	Total	O	0
			64	64	
30	I	3	Total	O	0
			3	3	
30	J	8	Total	O	0
			8	8	
30	K	14	Total	O	0
			14	14	
30	L	78	Total	O	0
			78	78	

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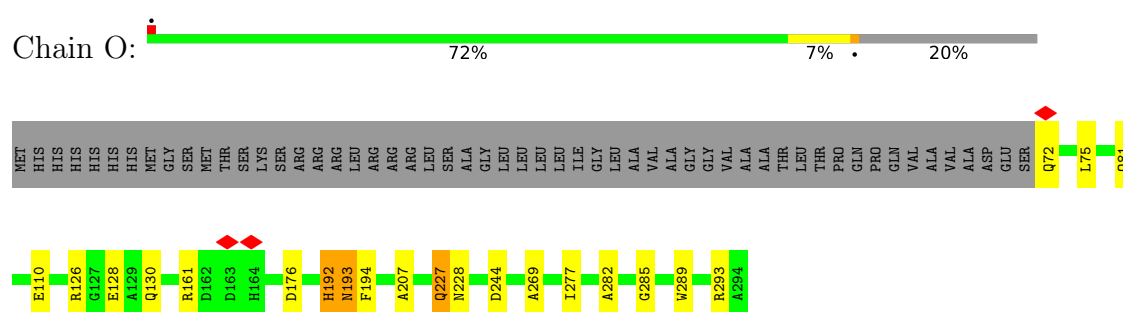
Continued from previous page...

Mol	Chain	Residues	Atoms		AltConf
30	X	35	Total 35	O 35	0
30	Z	2	Total 2	O 2	0
30	a	1	Total 1	O 1	0
30	b	10	Total 10	O 10	0
30	c	1	Total 1	O 1	0

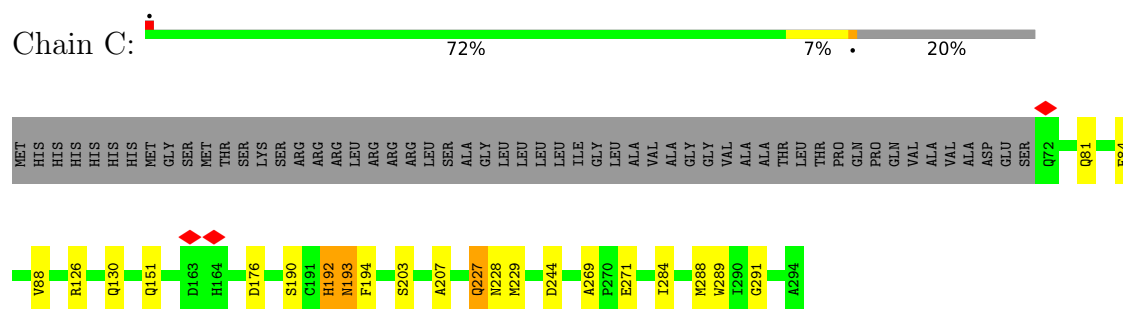
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. 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. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). 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.

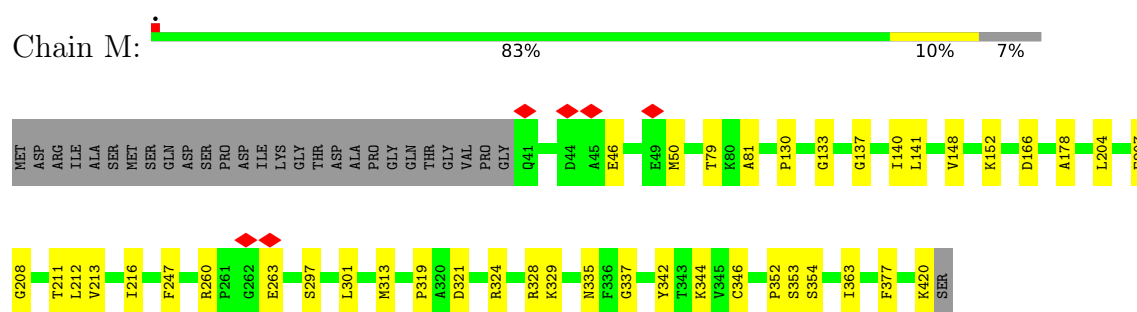
- Molecule 1: Cytochrome bc1 complex cytochrome c subunit



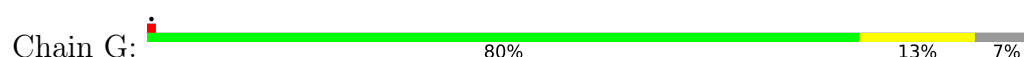
- Molecule 1: Cytochrome bc1 complex cytochrome c subunit

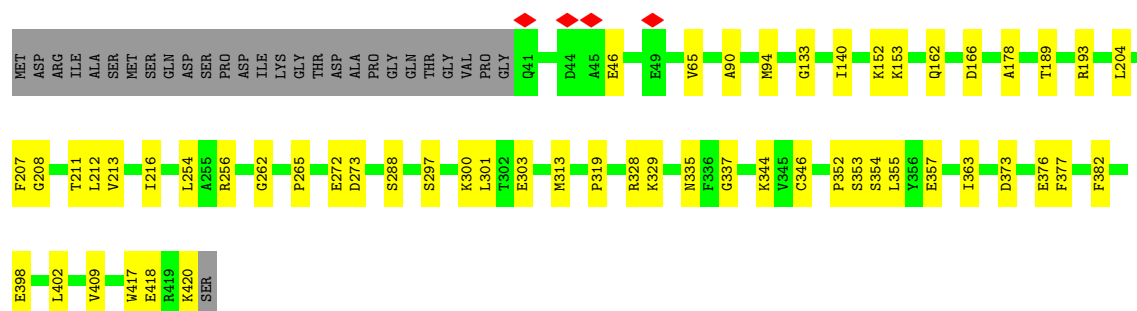


- Molecule 2: Cytochrome bc1 complex cytochrome c subunit

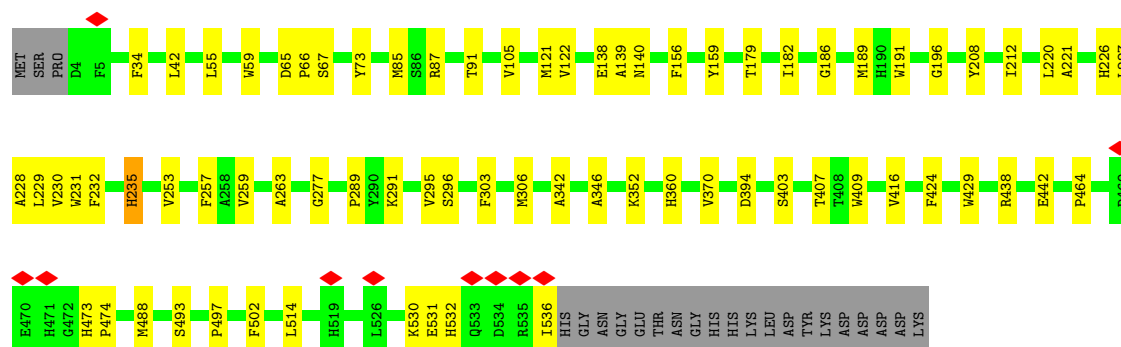
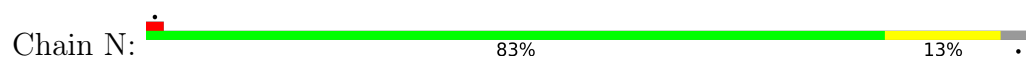


- Molecule 2: Cytochrome bc1 complex cytochrome c subunit

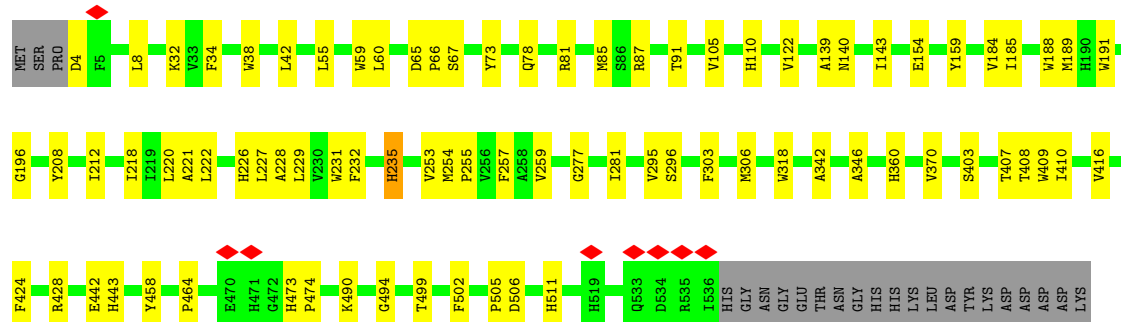
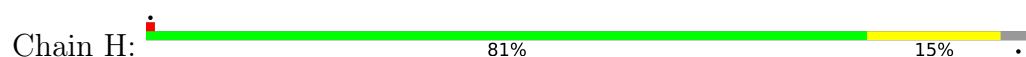




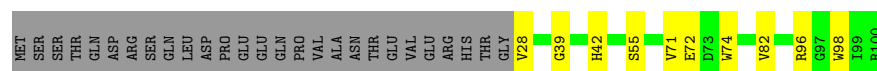
- Molecule 3: Cytochrome bc1 complex cytochrome b subunit



- Molecule 3: Cytochrome bc1 complex cytochrome b subunit

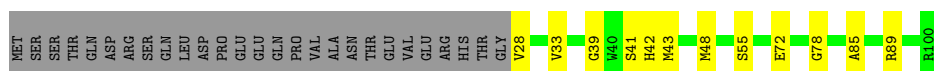


- Molecule 4: Transmembrane protein

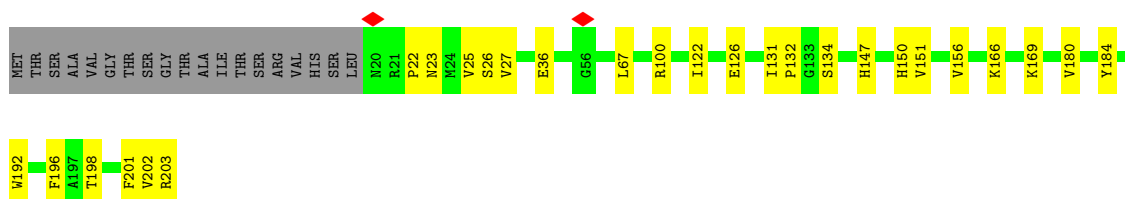
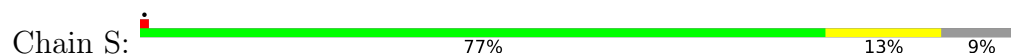


- Molecule 4: Transmembrane protein

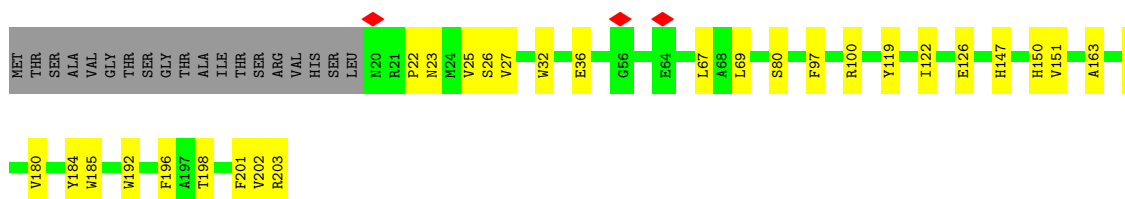




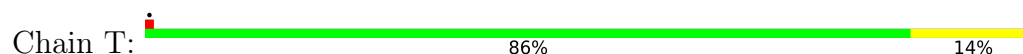
- Molecule 5: Probable cytochrome c oxidase subunit 3



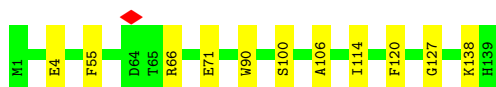
- Molecule 5: Probable cytochrome c oxidase subunit 3



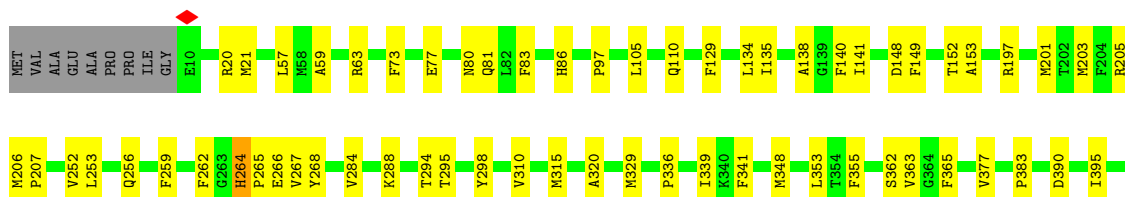
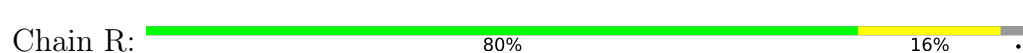
- Molecule 6: Cytochrome c oxidase polypeptide 4

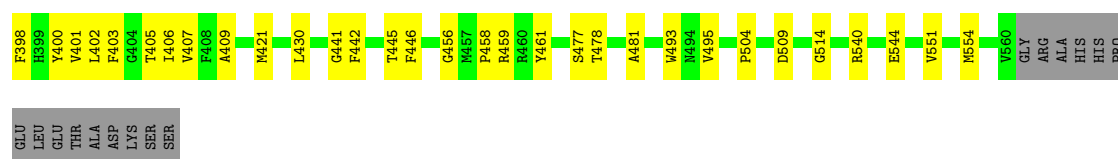


- Molecule 6: Cytochrome c oxidase polypeptide 4



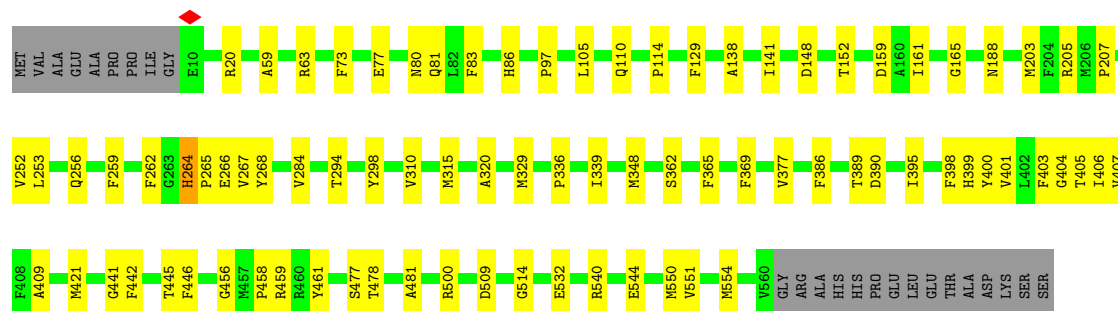
- Molecule 7: Cytochrome c oxidase subunit 1





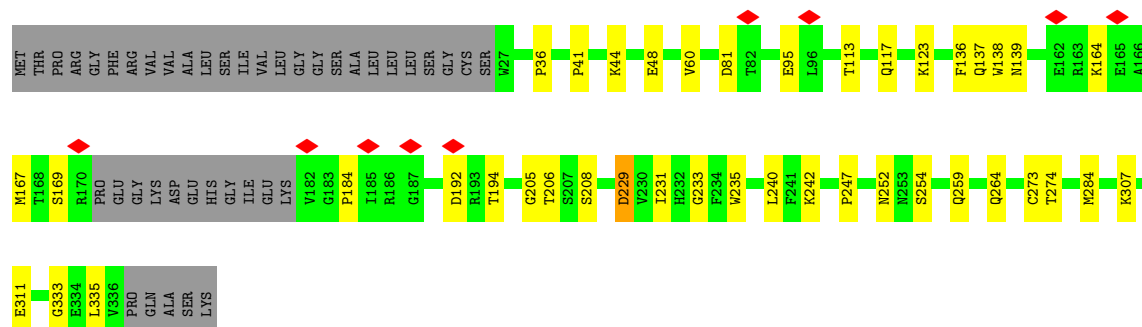
• Molecule 7: Cytochrome c oxidase subunit 1

Chain L: 81% 14% .



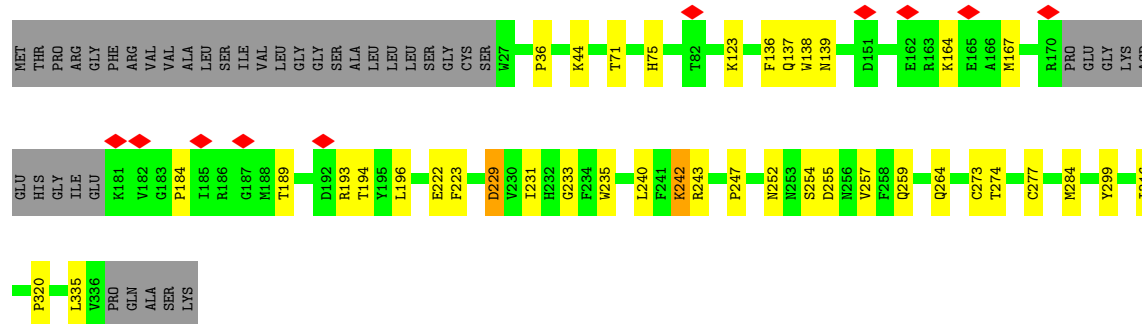
• Molecule 8: cytochrome-c oxidase

Chain Q: 76% 12% 12%

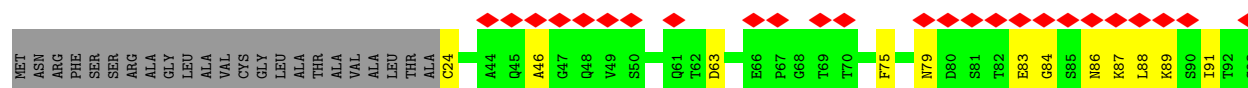
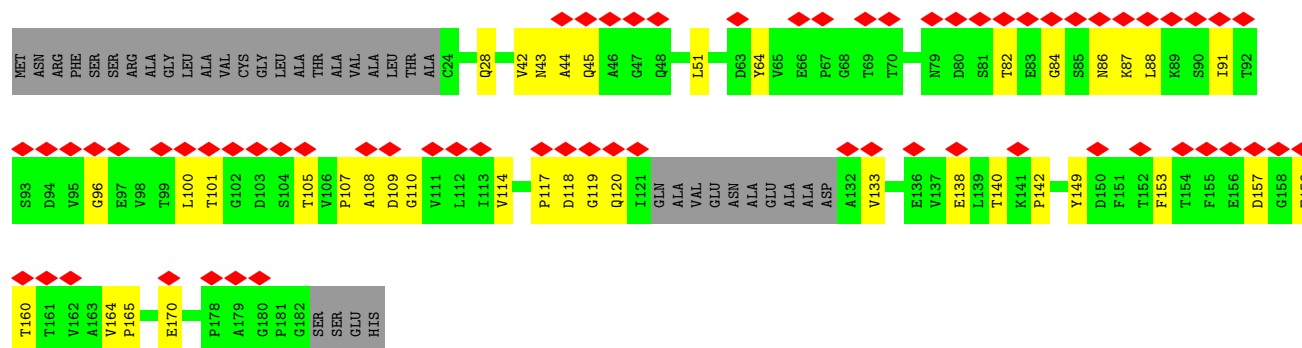
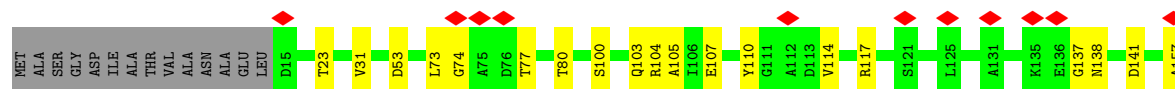
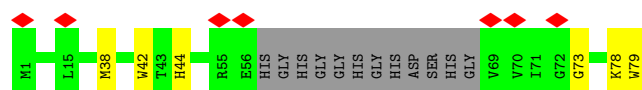
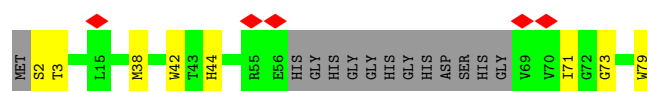


• Molecule 8: cytochrome-c oxidase

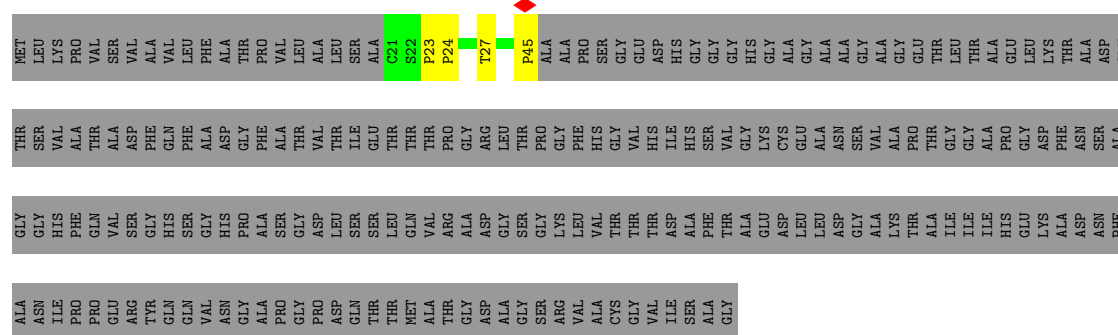
Chain X: 76% 11% 12%



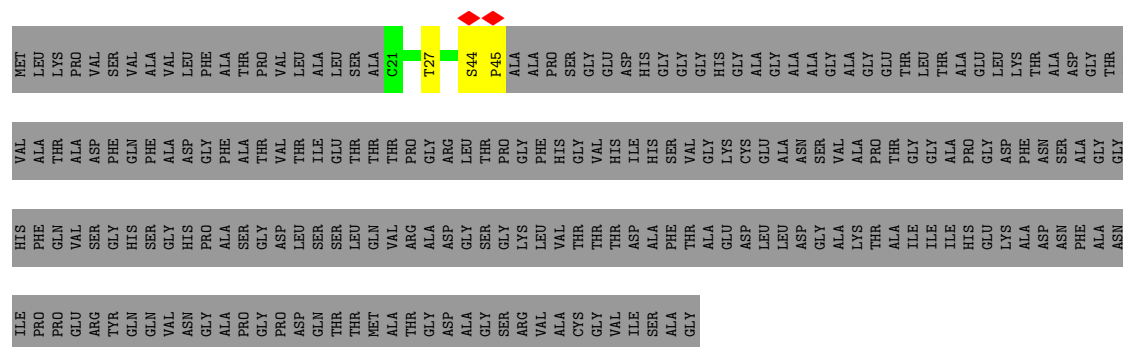
• Molecule 9: Cytochrome c oxidase subunit



- Molecule 12: Superoxide dismutase [Cu-Zn]



- Molecule 12: Superoxide dismutase [Cu-Zn]



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	208243	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	2.515	Depositor
Minimum map value	-1.210	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.061	Depositor
Recommended contour level	0.32	Depositor
Map size (Å)	447.12, 447.12, 447.12	wwPDB
Map dimensions	540, 540, 540	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.828, 0.828, 0.828	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, PLM, HEM, 9XX, CDL, HEC, 3PE, CA, CU, 9YF, IZL, WUO, MQ9, FES, 7PH, TRD, HEA

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	C	0.45	1/1660 (0.1%)	0.61	3/2250 (0.1%)
1	O	0.46	2/1660 (0.1%)	0.61	3/2250 (0.1%)
2	G	0.39	2/3046 (0.1%)	0.48	0/4129
2	M	0.34	0/3046	0.44	0/4129
3	H	0.37	0/4299	0.49	0/5862
3	N	0.37	0/4299	0.51	0/5862
4	I	0.29	0/606	0.38	0/825
4	P	0.28	0/606	0.37	0/825
5	J	0.30	0/1488	0.43	0/2032
5	S	0.30	0/1488	0.42	0/2032
6	K	0.29	0/1112	0.40	0/1524
6	T	0.29	0/1112	0.43	0/1524
7	L	0.45	3/4529 (0.1%)	0.64	7/6187 (0.1%)
7	R	0.45	3/4529 (0.1%)	0.63	7/6187 (0.1%)
8	Q	0.36	0/2447	0.46	0/3330
8	X	0.37	0/2456	0.48	0/3341
9	U	0.24	0/515	0.34	0/704
9	Z	0.25	0/523	0.37	0/714
10	V	0.26	0/1042	0.40	0/1423
10	a	0.27	0/1042	0.45	0/1423
11	W	0.24	0/1100	0.45	0/1508
11	b	0.22	0/1100	0.47	0/1508
12	Y	0.34	0/175	0.47	0/244
12	c	0.30	0/175	0.44	0/244
All	All	0.37	11/44055 (0.0%)	0.51	20/60057 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
7	L	0	1
7	R	0	1
All	All	0	2

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	R	268	TYR	C-N	8.88	1.44	1.34
7	L	268	TYR	C-N	8.54	1.44	1.34
2	G	46	GLU	C-N	-8.36	1.23	1.33
7	R	267	VAL	CA-CB	-6.63	1.45	1.54
7	L	267	VAL	CA-CB	-6.63	1.45	1.54
7	L	262	PHE	C-N	5.86	1.41	1.33
7	R	262	PHE	C-N	5.69	1.40	1.33
2	G	418	GLU	C-N	5.47	1.41	1.33
1	O	228	ASN	C-N	-5.14	1.23	1.33
1	O	192	HIS	CE1-NE2	-5.08	1.27	1.32
1	C	192	HIS	CE1-NE2	-5.01	1.27	1.32

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	L	262	PHE	CA-C-N	11.21	132.33	120.00
7	L	262	PHE	C-N-CA	11.21	132.33	120.00
7	R	262	PHE	CA-C-N	10.66	131.73	120.00
7	R	262	PHE	C-N-CA	10.66	131.73	120.00
1	C	192	HIS	CA-C-O	-7.93	109.68	119.28
1	O	192	HIS	CA-C-O	-7.92	109.69	119.28
7	R	266	GLU	N-CA-C	6.67	119.12	111.11
7	L	266	GLU	N-CA-C	6.67	119.11	111.11
7	R	265	PRO	CA-C-N	5.80	128.38	120.54
7	R	265	PRO	C-N-CA	5.80	128.38	120.54
7	L	265	PRO	CA-C-N	5.80	128.38	120.54
7	L	265	PRO	C-N-CA	5.80	128.38	120.54
7	L	264	HIS	CA-C-N	5.66	126.92	119.84
7	L	264	HIS	C-N-CA	5.66	126.92	119.84
7	R	264	HIS	CA-C-N	5.65	126.90	119.84
7	R	264	HIS	C-N-CA	5.65	126.90	119.84
1	O	192	HIS	CA-CB-CG	-5.62	108.19	113.80
1	C	192	HIS	CA-CB-CG	-5.57	108.23	113.80
1	C	193	ASN	CA-CB-CG	5.37	117.97	112.60
1	O	193	ASN	CA-CB-CG	5.36	117.96	112.60

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
7	L	264	HIS	Sidechain
7	R	264	HIS	Sidechain

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	1623	0	1560	26	0
1	O	1623	0	1560	21	0
2	G	2967	0	2976	51	0
2	M	2967	0	2976	41	0
3	H	4167	0	4192	85	0
3	N	4167	0	4192	72	0
4	I	586	0	578	11	0
4	P	586	0	578	10	0
5	J	1441	0	1439	22	0
5	S	1441	0	1439	24	0
6	K	1077	0	1058	11	0
6	T	1077	0	1058	17	0
7	L	4369	0	4345	63	0
7	R	4369	0	4345	69	0
8	Q	2382	0	2335	33	0
8	X	2391	0	2348	39	0
9	U	499	0	504	9	0
9	Z	507	0	516	6	0
10	V	1024	0	1035	13	0
10	a	1024	0	1035	17	0
11	W	1083	0	1055	27	0
11	b	1083	0	1055	26	0
12	Y	168	0	151	3	0
12	c	168	0	151	2	0
13	C	86	0	60	3	0
13	O	86	0	60	2	0
14	C	58	0	80	1	0
14	G	58	0	77	17	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
14	H	159	0	211	17	0
14	K	58	0	80	9	0
14	M	58	0	77	16	0
14	N	159	0	211	24	0
14	O	58	0	80	3	0
14	T	58	0	80	12	0
15	C	97	0	0	4	0
15	I	97	0	0	2	0
15	O	97	0	0	7	0
15	P	97	0	0	4	0
16	G	4	0	0	0	0
16	M	4	0	0	0	0
17	G	114	0	0	2	0
17	M	114	0	0	0	0
18	G	58	0	0	4	0
18	M	58	0	0	3	0
18	W	58	0	0	1	0
18	b	58	0	0	4	0
19	G	38	0	55	5	0
19	H	38	0	55	10	0
19	M	38	0	55	5	0
19	N	38	0	55	9	0
19	S	38	0	55	2	0
20	H	86	0	60	4	0
20	N	86	0	60	0	0
21	C	79	0	105	10	0
21	H	230	0	295	37	0
21	I	154	0	196	9	0
21	J	79	0	105	7	0
21	L	79	0	105	8	0
21	N	230	0	295	32	0
21	P	77	0	98	6	0
21	R	154	0	196	6	0
21	T	79	0	105	8	0
22	J	13	0	28	4	0
22	K	13	0	28	0	0
22	L	26	0	56	1	0
22	Q	13	0	28	1	0
22	R	26	0	56	1	0
22	S	13	0	28	4	0
22	T	13	0	28	0	0
22	X	13	0	28	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
23	J	32	0	38	1	0
23	S	32	0	38	4	0
24	L	120	0	108	5	0
24	R	120	0	108	12	0
25	L	1	0	0	0	0
25	Q	2	0	0	0	0
25	R	1	0	0	0	0
25	X	2	0	0	0	0
26	L	1	0	0	0	0
26	R	1	0	0	0	0
27	L	1	0	0	0	0
27	R	1	0	0	0	0
28	W	42	0	0	0	0
28	Y	32	0	0	0	0
28	b	32	0	0	0	0
28	c	32	0	0	0	0
29	W	11	0	16	1	0
29	Y	11	0	16	0	0
29	b	11	0	16	0	0
29	c	11	0	16	1	0
30	C	56	0	0	2	0
30	G	60	0	0	0	0
30	H	64	0	0	0	0
30	I	3	0	0	0	0
30	J	8	0	0	0	0
30	K	14	0	0	0	0
30	L	78	0	0	1	0
30	M	51	0	0	0	0
30	N	67	0	0	0	0
30	O	43	0	0	3	0
30	P	2	0	0	0	0
30	Q	30	0	0	0	0
30	R	68	0	0	0	0
30	S	6	0	0	0	0
30	T	11	0	0	1	0
30	W	4	0	0	0	0
30	X	35	0	0	1	0
30	Z	2	0	0	0	0
30	a	1	0	0	0	0
30	b	10	0	0	0	0
30	c	1	0	0	0	0
All	All	47246	0	46028	713	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 (713) 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)
14:M:505:MQ9:H23	3:H:55:LEU:HD23	1.31	1.12
6:K:100:SER:HB3	14:K:1301:MQ9:H252	1.33	1.09
3:N:55:LEU:HD23	14:G:901:MQ9:H23	1.29	1.08
15:O:304:WUO:C95	14:T:1301:MQ9:H202	1.85	1.06
5:J:198:THR:HG22	22:J:502:TRD:H101	1.38	1.05
5:S:198:THR:HG22	22:S:502:TRD:H101	1.38	1.03
21:N:602:CDL:H511	21:H:903:CDL:CA5	1.89	1.03
21:N:602:CDL:CA5	21:H:903:CDL:H511	1.89	1.01
3:H:220:LEU:HD21	14:H:907:MQ9:H451	1.42	1.01
3:N:220:LEU:HD21	14:N:606:MQ9:H451	1.41	0.99
21:N:602:CDL:C11	21:H:903:CDL:H511	1.95	0.97
21:N:602:CDL:H511	21:H:903:CDL:C11	1.95	0.96
7:L:252:VAL:HG13	8:X:231:ILE:HD11	1.53	0.91
15:O:304:WUO:C94	14:T:1301:MQ9:H202	2.01	0.90
7:R:252:VAL:HG13	8:Q:231:ILE:HD11	1.53	0.90
21:L:601:CDL:HA32	21:L:601:CDL:HA22	1.52	0.90
11:b:101:THR:O	11:b:133:VAL:HA	1.73	0.88
8:Q:136:PHE:CZ	8:Q:139:ASN:HB3	2.11	0.86
14:M:505:MQ9:H23	3:H:55:LEU:CD2	2.07	0.85
3:H:220:LEU:HD21	14:H:907:MQ9:C45	2.06	0.85
15:O:304:WUO:C95	14:T:1301:MQ9:C20	2.55	0.84
1:C:194:PHE:CZ	3:H:296:SER:HB3	2.11	0.84
3:N:55:LEU:CD2	14:G:901:MQ9:H23	2.06	0.83
11:W:101:THR:O	11:W:133:VAL:HA	1.78	0.83
8:X:222:GLU:HG2	8:X:259:GLN:HG2	1.60	0.82
3:N:220:LEU:HD21	14:N:606:MQ9:C45	2.08	0.82
2:G:208:GLY:HA3	14:G:901:MQ9:H412	1.63	0.81
2:M:208:GLY:HA2	14:M:505:MQ9:H38	1.62	0.81
2:G:208:GLY:HA2	14:G:901:MQ9:H38	1.63	0.81
7:L:406:ILE:HD11	24:L:603:HEA:HAC	1.62	0.81
5:J:198:THR:CG2	22:J:502:TRD:H101	2.11	0.81
5:S:198:THR:CG2	22:S:502:TRD:H101	2.11	0.80
19:N:609:7PH:H25	19:N:609:7PH:C21	2.12	0.80
19:H:901:7PH:C21	19:H:901:7PH:H25	2.12	0.79
24:R:603:HEA:H202	24:R:603:HEA:H243	1.65	0.79
2:M:208:GLY:HA3	14:M:505:MQ9:H412	1.63	0.78
14:O:303:MQ9:H272	3:N:121:MET:HG2	1.65	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:L:252:VAL:CG1	8:X:231:ILE:HD11	2.16	0.75
7:R:406:ILE:HD11	24:R:603:HEA:HAC	1.67	0.75
7:R:252:VAL:CG1	8:Q:231:ILE:HD11	2.17	0.74
8:X:123:LYS:HG2	8:X:259:GLN:HG3	1.68	0.74
3:N:229:LEU:HD23	21:N:602:CDL:H312	1.68	0.74
6:T:100:SER:HB2	7:R:135:ILE:HD11	1.68	0.74
2:G:133:GLY:HA3	3:H:277:GLY:HA3	1.71	0.73
2:G:344:LYS:HE3	2:G:354:SER:HB3	1.70	0.73
8:X:242:LYS:HE2	8:X:274:THR:HG21	1.69	0.73
2:M:344:LYS:HE3	2:M:354:SER:HB3	1.71	0.73
6:K:100:SER:CB	14:K:1301:MQ9:H252	2.18	0.71
21:N:602:CDL:H511	21:H:903:CDL:H112	1.71	0.71
11:W:88:LEU:HD21	11:W:91:ILE:HD11	1.73	0.71
2:M:204:LEU:HB3	14:M:505:MQ9:H43	1.73	0.70
21:R:601:CDL:H182	21:R:601:CDL:H372	1.73	0.70
21:L:601:CDL:HA32	21:L:601:CDL:CA2	2.19	0.70
3:H:229:LEU:HD23	21:H:903:CDL:H312	1.72	0.70
7:R:398:PHE:HA	7:R:401:VAL:HG12	1.73	0.70
21:N:602:CDL:H112	21:H:903:CDL:H511	1.70	0.70
3:H:346:ALA:HB2	14:H:909:MQ9:H271	1.72	0.70
6:T:137:GLU:HG3	21:T:1302:CDL:HB22	1.74	0.69
1:O:293:ARG:NH1	30:O:401:HOH:O	2.24	0.69
21:P:301:CDL:H112	21:R:605:CDL:HA62	1.73	0.69
3:N:182:ILE:HB	3:N:186:GLY:HA2	1.74	0.69
3:N:34:PHE:CE1	14:N:606:MQ9:O4	2.46	0.69
2:G:254:LEU:HD12	2:G:402:LEU:HB3	1.74	0.68
3:N:346:ALA:HB2	14:N:608:MQ9:H271	1.75	0.68
2:G:204:LEU:HB3	14:G:901:MQ9:H43	1.74	0.68
8:Q:139:ASN:OD1	8:Q:205:GLY:HA3	1.93	0.68
14:N:606:MQ9:H48	3:H:221:ALA:HA	1.74	0.68
3:N:34:PHE:CE1	14:N:606:MQ9:C4	2.78	0.67
3:N:212:ILE:HD11	3:H:212:ILE:HD11	1.76	0.67
2:G:409:VAL:O	17:G:903:IZL:C33	2.42	0.67
21:I:301:CDL:H341	21:I:302:CDL:H111	1.77	0.67
1:C:227:GLN:HG3	13:C:302:HEC:O1D	1.93	0.67
3:N:221:ALA:HA	14:H:907:MQ9:H48	1.75	0.67
7:L:105:LEU:HD22	7:L:421:MET:HG3	1.77	0.67
11:W:117:PRO:HD2	11:W:120:GLN:HG3	1.77	0.66
6:K:4:GLU:HG3	7:L:203:MET:HE2	1.77	0.66
5:S:25:VAL:HG12	5:S:180:VAL:HG11	1.77	0.66
6:T:71:GLU:OE2	7:R:205:ARG:NH1	2.28	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:W:118:ASP:HB2	11:W:170:GLU:HG2	1.76	0.66
3:H:110:HIS:HD2	3:H:281:ILE:CD1	2.08	0.66
10:a:74:GLY:H	10:a:80:THR:HG21	1.57	0.66
4:P:74:TRP:CD1	15:P:302:WUO:O60	2.47	0.66
21:J:501:CDL:H521	21:J:501:CDL:HB61	1.77	0.66
7:L:80:ASN:HA	7:L:83:PHE:CE1	2.31	0.66
7:L:456:GLY:HA2	8:X:235:TRP:CH2	2.31	0.65
7:R:80:ASN:HA	7:R:83:PHE:CE1	2.31	0.65
2:M:130:PRO:HA	3:N:277:GLY:O	1.97	0.65
11:b:117:PRO:HD2	11:b:120:GLN:HG3	1.77	0.65
9:Z:38:MET:HG3	10:a:137:GLY:HA2	1.77	0.65
5:S:166:LYS:HD2	19:S:501:7PH:H1A	1.79	0.65
5:J:25:VAL:HG12	5:J:180:VAL:HG11	1.79	0.65
11:b:97:GLU:O	11:b:137:VAL:HA	1.97	0.65
7:L:398:PHE:HA	7:L:401:VAL:HG12	1.79	0.65
3:H:185:ILE:O	3:H:189:MET:HG3	1.97	0.65
7:L:389:THR:HG22	8:X:242:LYS:HD2	1.79	0.64
7:R:20:ARG:NH1	10:V:53:ASP:OD2	2.30	0.64
8:X:44:LYS:NZ	8:X:264:GLN:OE1	2.30	0.64
11:b:87:LYS:HG3	11:b:105:THR:HG22	1.79	0.64
3:N:34:PHE:HE1	14:N:606:MQ9:O4	1.80	0.64
7:R:105:LEU:HD22	7:R:421:MET:HG3	1.78	0.64
2:G:208:GLY:CA	14:G:901:MQ9:H412	2.28	0.64
2:M:79:THR:HG22	2:M:81:ALA:H	1.62	0.64
1:O:227:GLN:HG3	13:O:302:HEC:O1D	1.98	0.63
7:R:456:GLY:HA2	8:Q:235:TRP:CH2	2.32	0.63
8:Q:44:LYS:NZ	8:Q:264:GLN:OE1	2.30	0.63
3:N:530:LYS:NZ	3:N:531:GLU:OE2	2.31	0.63
2:M:208:GLY:CA	14:M:505:MQ9:H38	2.28	0.63
2:G:208:GLY:HA3	14:G:901:MQ9:C41	2.29	0.63
19:H:901:7PH:H25	19:H:901:7PH:H3	1.80	0.63
5:J:198:THR:HG22	22:J:502:TRD:C10	2.23	0.63
3:N:67:SER:HB3	3:N:87:ARG:HB2	1.81	0.63
11:b:87:LYS:HA	11:b:105:THR:HA	1.80	0.63
21:C:305:CDL:HA22	3:H:490:LYS:NZ	2.13	0.63
2:M:208:GLY:HA3	14:M:505:MQ9:C41	2.29	0.63
21:N:602:CDL:C51	21:H:903:CDL:OA6	2.47	0.63
11:b:88:LEU:HB3	11:b:104:SER:HB3	1.80	0.63
7:L:20:ARG:NH1	10:a:53:ASP:OD2	2.30	0.62
2:M:208:GLY:CA	14:M:505:MQ9:H412	2.28	0.62
19:N:609:7PH:H22	2:G:178:ALA:HB1	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:208:GLY:CA	14:G:901:MQ9:H38	2.29	0.62
21:N:602:CDL:OA6	21:H:903:CDL:C51	2.47	0.62
11:W:96:GLY:HA3	11:W:138:GLU:O	1.99	0.62
3:N:259:VAL:HG22	14:N:605:MQ9:H101	1.79	0.62
21:N:602:CDL:H522	21:H:903:CDL:H112	1.82	0.62
19:N:609:7PH:H25	19:N:609:7PH:H3	1.80	0.62
3:H:67:SER:HB3	3:H:87:ARG:HB2	1.81	0.61
8:X:235:TRP:CD2	8:X:242:LYS:HE3	2.35	0.61
7:R:395:ILE:HD11	7:R:459:ARG:HB2	1.82	0.61
21:N:602:CDL:H112	21:H:903:CDL:H522	1.82	0.61
21:N:602:CDL:OA6	21:H:903:CDL:H511	2.00	0.61
4:I:78:GLY:HA3	15:I:303:WUO:C89	2.31	0.61
21:N:602:CDL:H511	21:H:903:CDL:OA6	2.00	0.61
14:T:1301:MQ9:H28	7:R:134:LEU:CB	2.31	0.61
7:R:253:LEU:HD21	7:R:320:ALA:HB3	1.83	0.60
7:L:395:ILE:HD11	7:L:459:ARG:HB2	1.83	0.60
1:O:130:GLN:HG3	1:O:227:GLN:HE22	1.66	0.60
3:H:259:VAL:HG22	14:H:906:MQ9:H101	1.80	0.60
3:N:303:PHE:HA	3:N:306:MET:SD	2.42	0.60
5:S:198:THR:HG22	22:S:502:TRD:C10	2.24	0.60
8:X:235:TRP:CG	8:X:242:LYS:HE3	2.37	0.60
11:b:114:VAL:HG13	11:b:133:VAL:HG12	1.84	0.60
3:H:416:VAL:HG13	4:I:55:SER:HB2	1.84	0.59
3:H:409:TRP:CE2	4:I:72:GLU:HG3	2.38	0.59
23:J:503:3PE:O31	23:J:503:3PE:H221	2.02	0.59
7:L:386:PHE:O	8:X:242:LYS:HG2	2.02	0.59
7:R:406:ILE:HD11	24:R:603:HEA:CAC	2.33	0.59
11:W:86:ASN:ND2	11:W:157:ASP:OD1	2.35	0.59
3:H:303:PHE:HA	3:H:306:MET:SD	2.42	0.59
7:L:509:ASP:HB3	10:a:31:VAL:HG12	1.83	0.59
21:N:604:CDL:HA61	6:T:90:TRP:HZ2	1.67	0.59
8:Q:206:THR:HG22	8:Q:208:SER:H	1.67	0.59
5:J:147:HIS:CE1	5:J:192:TRP:HB2	2.38	0.59
2:M:178:ALA:HB1	19:H:901:7PH:H22	1.84	0.59
7:L:400:TYR:HA	7:L:442:PHE:HZ	1.67	0.59
21:P:301:CDL:HA4	7:R:21:MET:HE1	1.83	0.59
23:S:503:3PE:H221	23:S:503:3PE:O31	2.02	0.59
21:H:905:CDL:H732	6:K:90:TRP:HB2	1.85	0.59
1:C:130:GLN:HG3	1:C:227:GLN:NE2	2.18	0.58
3:N:182:ILE:HB	3:N:186:GLY:CA	2.33	0.58
19:N:609:7PH:H23	19:G:905:7PH:H1	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:J:122:ILE:O	5:J:126:GLU:HG2	2.04	0.58
11:b:88:LEU:HD21	11:b:91:ILE:HD11	1.85	0.58
5:S:122:ILE:O	5:S:126:GLU:HG2	2.04	0.58
21:C:305:CDL:HA22	3:H:490:LYS:HZ3	1.69	0.58
11:b:86:ASN:O	11:b:106:VAL:N	2.31	0.58
21:N:603:CDL:H371	21:N:603:CDL:H172	1.85	0.58
7:L:256:GLN:HB3	7:L:315:MET:SD	2.44	0.58
19:M:504:7PH:H1	19:H:901:7PH:H23	1.85	0.58
2:M:79:THR:HG21	3:N:514:LEU:HD11	1.86	0.58
3:H:42:LEU:HD13	3:H:122:VAL:HG12	1.85	0.58
21:N:602:CDL:CA5	21:H:903:CDL:C51	2.75	0.57
3:N:42:LEU:HD13	3:N:122:VAL:HG12	1.85	0.57
5:S:147:HIS:CE1	5:S:192:TRP:HB2	2.38	0.57
11:W:114:VAL:HG13	11:W:133:VAL:HG12	1.86	0.57
7:R:57:LEU:HD22	24:R:603:HEA:H242	1.85	0.57
18:G:904:9YF:C34	3:H:185:ILE:HD12	2.34	0.57
9:Z:73:GLY:HA3	10:a:110:TYR:CZ	2.38	0.57
7:R:509:ASP:HB3	10:V:31:VAL:HG12	1.86	0.57
1:O:130:GLN:HG3	1:O:227:GLN:NE2	2.19	0.57
5:S:132:PRO:HD2	23:S:503:3PE:H12	1.86	0.57
5:J:23:ASN:HB3	5:J:26:SER:HB2	1.86	0.57
7:R:253:LEU:HD13	8:Q:252:ASN:HB3	1.86	0.57
7:L:389:THR:CG2	8:X:242:LYS:HD2	2.35	0.57
3:N:229:LEU:CD2	21:N:602:CDL:H312	2.34	0.56
21:C:305:CDL:H172	21:J:501:CDL:H361	1.87	0.56
3:N:409:TRP:CE2	4:P:72:GLU:HG3	2.40	0.56
9:U:71:ILE:HG22	9:U:73:GLY:H	1.69	0.56
21:H:904:CDL:OB9	21:H:905:CDL:H131	2.05	0.56
21:H:905:CDL:H311	21:H:905:CDL:HB4	1.86	0.56
7:L:406:ILE:HD11	24:L:603:HEA:CAC	2.35	0.56
8:X:193:ARG:HB3	8:X:196:LEU:HD12	1.87	0.56
8:Q:113:THR:O	8:Q:117:GLN:HG2	2.05	0.56
3:H:464:PRO:HB3	3:H:474:PRO:HB3	1.87	0.56
21:L:601:CDL:HA61	21:L:601:CDL:CB3	2.35	0.56
5:S:23:ASN:HB3	5:S:26:SER:HB2	1.86	0.56
5:J:22:PRO:HD3	6:K:66:ARG:HD3	1.88	0.56
2:M:133:GLY:HA3	3:N:277:GLY:HA3	1.88	0.56
8:Q:44:LYS:O	8:Q:48:GLU:HG3	2.06	0.56
2:M:335:ASN:ND2	2:M:337:GLY:O	2.36	0.56
3:H:231:TRP:CZ3	14:H:907:MQ9:H112	2.41	0.56
8:Q:307:LYS:HD2	8:Q:311:GLU:HG3	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:b:112:LEU:HD11	11:b:133:VAL:HG21	1.87	0.56
11:W:91:ILE:HD12	11:W:100:LEU:HD21	1.87	0.55
3:H:110:HIS:HD2	3:H:281:ILE:HD11	1.70	0.55
19:H:901:7PH:H3	19:H:901:7PH:O22	2.06	0.55
3:N:464:PRO:HB3	3:N:474:PRO:HB3	1.88	0.55
24:R:603:HEA:H243	24:R:603:HEA:C20	2.34	0.55
11:W:87:LYS:HG3	11:W:105:THR:HG22	1.87	0.55
14:K:1301:MQ9:C8	14:K:1301:MQ9:H5M3	2.36	0.55
19:M:504:7PH:C1	19:H:901:7PH:H23	2.37	0.55
8:X:136:PHE:CE2	8:X:139:ASN:HB2	2.42	0.55
21:N:602:CDL:H112	21:H:903:CDL:C51	2.36	0.55
9:Z:78:LYS:HD3	10:a:105:ALA:HA	1.89	0.55
7:R:197:ARG:NH1	7:R:201:MET:O	2.35	0.55
5:S:22:PRO:HD3	6:T:66:ARG:HD3	1.88	0.55
8:Q:136:PHE:HZ	8:Q:139:ASN:HB3	1.68	0.55
24:R:603:HEA:C20	24:R:603:HEA:C24	2.85	0.55
10:V:138:ASN:HB3	10:V:141:ASP:HB3	1.88	0.55
7:L:63:ARG:HG2	7:L:481:ALA:CB	2.37	0.55
1:C:203:SER:HB2	18:b:201:9YF:O7	2.07	0.55
3:H:231:TRP:HZ3	14:H:907:MQ9:H112	1.71	0.55
5:J:80:SER:HB3	5:J:185:TRP:HE1	1.71	0.55
14:K:1301:MQ9:H5M3	14:K:1301:MQ9:H8	1.89	0.55
7:L:445:THR:HG23	7:L:446:PHE:CD1	2.42	0.55
3:H:32:LYS:HE3	3:H:34:PHE:CZ	2.42	0.55
8:X:138:TRP:O	8:X:284:MET:HB3	2.07	0.55
8:X:243:ARG:NH2	8:X:255:ASP:O	2.40	0.55
3:N:231:TRP:CZ3	14:N:606:MQ9:H112	2.43	0.54
14:T:1301:MQ9:H28	7:R:134:LEU:HB3	1.88	0.54
7:L:362:SER:O	7:L:365:PHE:HB3	2.07	0.54
19:N:609:7PH:H3	19:N:609:7PH:O22	2.06	0.54
6:T:72:ASP:OD1	6:T:72:ASP:N	2.40	0.54
1:O:289:TRP:O	2:M:152:LYS:NZ	2.31	0.54
3:N:235:HIS:CD2	14:N:606:MQ9:C3A	2.91	0.54
4:P:28:VAL:HG13	4:P:42:HIS:HB2	1.90	0.54
7:R:445:THR:HG23	7:R:446:PHE:CD2	2.42	0.54
9:U:38:MET:SD	10:V:139:LEU:HB2	2.48	0.54
7:L:253:LEU:HD21	7:L:320:ALA:HB3	1.89	0.54
19:N:609:7PH:H23	19:G:905:7PH:C1	2.37	0.54
24:R:603:HEA:H202	24:R:603:HEA:C24	2.37	0.54
1:O:128:GLU:HG3	30:O:443:HOH:O	2.08	0.54
3:N:232:PHE:CE1	21:N:602:CDL:HB21	2.43	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:R:110:GLN:HB3	7:R:207:PRO:HG2	1.90	0.54
7:L:389:THR:O	8:X:242:LYS:NZ	2.31	0.54
21:N:602:CDL:C51	21:H:903:CDL:CA5	2.75	0.54
7:R:400:TYR:HA	7:R:442:PHE:HZ	1.74	0.54
9:U:38:MET:HG3	10:V:137:GLY:HA2	1.88	0.54
3:N:289:PRO:HG2	3:N:291:LYS:HE2	1.91	0.53
7:L:441:GLY:O	7:L:445:THR:HG22	2.08	0.53
21:N:602:CDL:C51	21:H:903:CDL:H112	2.36	0.53
7:R:441:GLY:O	7:R:445:THR:HG22	2.08	0.53
15:C:304:WUO:C88	21:C:305:CDL:H862	2.39	0.53
2:G:166:ASP:OD1	3:H:360:HIS:NE2	2.42	0.53
7:R:362:SER:O	7:R:365:PHE:HB3	2.08	0.53
7:R:320:ALA:HB2	8:Q:254:SER:HA	1.90	0.53
2:G:382:PHE:CE2	3:H:408:THR:HG21	2.44	0.53
3:H:409:TRP:CZ2	4:I:72:GLU:HG3	2.44	0.53
5:J:32:TRP:CZ2	21:L:601:CDL:H181	2.43	0.53
2:M:166:ASP:OD1	3:N:360:HIS:NE2	2.41	0.53
3:N:55:LEU:HD23	14:G:901:MQ9:C23	2.20	0.53
6:T:58:PHE:HD2	6:T:62:ARG:HH22	1.57	0.53
7:R:63:ARG:HG2	7:R:481:ALA:CB	2.38	0.53
7:R:284:VAL:HG22	7:R:514:GLY:HA2	1.91	0.53
7:R:310:VAL:HG12	7:R:329:MET:HB3	1.91	0.53
1:C:130:GLN:HG3	1:C:227:GLN:HE22	1.73	0.53
1:C:194:PHE:CE2	3:H:296:SER:HB3	2.43	0.53
19:M:504:7PH:H1	19:H:901:7PH:C23	2.39	0.53
3:N:231:TRP:HZ3	14:N:606:MQ9:H112	1.74	0.53
6:T:126:CYS:HB3	21:T:1302:CDL:H131	1.91	0.53
7:L:253:LEU:HD13	8:X:252:ASN:HB3	1.91	0.53
7:L:284:VAL:HG22	7:L:514:GLY:HA2	1.91	0.53
3:H:4:ASP:O	3:H:8:LEU:HG	2.09	0.52
3:N:140:ASN:OD1	3:N:226:HIS:ND1	2.42	0.52
1:O:192:HIS:CE1	1:O:207:ALA:HB1	2.45	0.52
5:S:202:VAL:HG11	22:S:502:TRD:H62	1.90	0.52
1:C:151:GLN:NE2	11:b:119:GLY:O	2.32	0.52
2:G:319:PRO:HG3	11:b:165:PRO:HG3	1.91	0.52
7:L:59:ALA:HB2	7:L:86:HIS:CE1	2.45	0.52
1:C:176:ASP:HB3	1:C:244:ASP:OD2	2.10	0.52
1:O:289:TRP:CE2	21:T:1302:CDL:H711	2.43	0.52
7:R:405:THR:O	7:R:409:ALA:HB3	2.09	0.52
1:C:81:GLN:NE2	8:X:167:MET:HE3	2.25	0.52
3:H:140:ASN:OD1	3:H:226:HIS:ND1	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:L:403:PHE:CD1	7:L:407:VAL:HG21	2.45	0.52
19:N:609:7PH:C23	19:G:905:7PH:H1	2.39	0.52
3:H:220:LEU:CD2	14:H:907:MQ9:H451	2.26	0.52
3:H:229:LEU:CD2	21:H:903:CDL:H312	2.39	0.52
3:N:409:TRP:CZ2	4:P:72:GLU:HG3	2.45	0.52
21:N:602:CDL:OA6	21:H:903:CDL:H512	2.10	0.52
3:H:232:PHE:CE2	21:H:903:CDL:HB21	2.45	0.52
5:J:202:VAL:HG11	22:J:502:TRD:H62	1.91	0.52
21:N:602:CDL:H512	21:H:903:CDL:OA6	2.10	0.52
3:H:110:HIS:CD2	3:H:281:ILE:HG12	2.45	0.52
19:H:901:7PH:H25	19:H:901:7PH:C3	2.40	0.52
7:L:320:ALA:HB2	8:X:254:SER:HA	1.90	0.52
11:b:79:ASN:ND2	11:b:107:PRO:O	2.37	0.52
3:H:34:PHE:CE2	14:H:907:MQ9:O4	2.63	0.51
4:I:28:VAL:HG13	4:I:42:HIS:HB2	1.92	0.51
5:S:184:TYR:CZ	21:R:601:CDL:H172	2.45	0.51
15:C:304:WUO:C90	15:C:304:WUO:C65	2.88	0.51
7:R:81:GLN:HG3	7:R:148:ASP:HB3	1.93	0.51
11:W:87:LYS:HA	11:W:105:THR:HA	1.92	0.51
11:W:118:ASP:CB	11:W:170:GLU:HG2	2.39	0.51
21:P:301:CDL:H782	21:P:301:CDL:H552	1.92	0.51
6:T:26:THR:O	6:T:30:ALA:HB3	2.10	0.51
21:J:501:CDL:HB61	21:J:501:CDL:H542	1.93	0.51
10:a:73:LEU:HD22	10:a:80:THR:HG23	1.91	0.51
3:N:220:LEU:CD2	14:N:606:MQ9:H451	2.26	0.51
3:H:140:ASN:OD1	3:H:226:HIS:CE1	2.64	0.51
3:H:424:PHE:HD2	21:I:301:CDL:OB7	1.94	0.51
3:N:140:ASN:OD1	3:N:226:HIS:CE1	2.64	0.51
19:N:609:7PH:H25	19:N:609:7PH:C3	2.40	0.51
7:L:405:THR:O	7:L:409:ALA:HB3	2.10	0.51
5:S:196:PHE:CE2	5:S:201:PHE:HE2	2.29	0.51
14:T:1301:MQ9:H28	7:R:134:LEU:HB2	1.93	0.51
1:C:192:HIS:CE1	1:C:207:ALA:HB1	2.46	0.51
3:N:416:VAL:CG1	4:P:55:SER:HB2	2.41	0.51
7:L:386:PHE:O	8:X:242:LYS:CG	2.59	0.51
8:X:136:PHE:CZ	8:X:139:ASN:CB	2.94	0.51
2:G:256:ARG:HH12	2:G:273:ASP:HB3	1.75	0.50
7:L:110:GLN:HB3	7:L:207:PRO:HG2	1.93	0.50
7:L:395:ILE:HA	7:L:398:PHE:CE1	2.45	0.50
2:M:212:LEU:HD13	14:M:505:MQ9:H351	1.92	0.50
7:R:59:ALA:HB2	7:R:86:HIS:CE1	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:C:304:WUO:C23	15:C:304:WUO:C84	2.90	0.50
14:K:1301:MQ9:H262	14:K:1301:MQ9:H302	1.94	0.50
1:C:288:MET:HA	3:H:38:TRP:HB2	1.94	0.50
7:R:138:ALA:O	7:R:141:ILE:HG12	2.12	0.50
2:G:208:GLY:CA	14:G:901:MQ9:C38	2.90	0.50
5:J:196:PHE:CE1	5:J:201:PHE:HE2	2.29	0.50
14:K:1301:MQ9:C25	14:K:1301:MQ9:C28	2.86	0.50
2:M:140:ILE:HB	2:G:207:PHE:CE1	2.46	0.50
9:U:79:TRP:CH2	10:V:104:ARG:HA	2.47	0.50
3:H:159:TYR:HA	20:H:902:HEM:HAA2	1.93	0.50
7:L:310:VAL:HG12	7:L:329:MET:HB3	1.92	0.50
3:N:138:GLU:OE2	3:N:352:LYS:NZ	2.32	0.50
3:H:370:VAL:HG22	4:I:39:GLY:HA3	1.94	0.50
4:I:89:ARG:HB2	21:I:302:CDL:H311	1.94	0.50
2:M:208:GLY:CA	14:M:505:MQ9:C38	2.89	0.50
3:N:230:VAL:HG12	14:N:606:MQ9:H5M1	1.94	0.50
3:N:139:ALA:HB2	14:N:608:MQ9:H452	1.93	0.49
6:T:95:ILE:HG12	6:T:124:SER:HB3	1.93	0.49
1:C:126:ARG:HH22	7:L:165:GLY:HA3	1.77	0.49
7:L:81:GLN:HG3	7:L:148:ASP:HB3	1.93	0.49
2:M:344:LYS:HE3	2:M:354:SER:CB	2.41	0.49
8:Q:164:LYS:NZ	8:Q:194:THR:O	2.43	0.49
8:X:136:PHE:CZ	8:X:139:ASN:HB2	2.47	0.49
10:a:73:LEU:O	10:a:103:GLN:NE2	2.45	0.49
7:L:390:ASP:OD2	8:X:274:THR:O	2.31	0.49
7:R:430:LEU:HD21	7:R:493:TRP:HD1	1.77	0.49
8:Q:123:LYS:HG2	8:Q:259:GLN:HG3	1.95	0.49
19:G:905:7PH:O21	19:G:905:7PH:H24A	2.12	0.49
7:R:97:PRO:HG3	7:R:129:PHE:CE1	2.48	0.49
21:H:905:CDL:H311	21:H:905:CDL:OB9	2.13	0.49
5:J:36:GLU:OE2	5:J:150:HIS:NE2	2.39	0.49
11:b:24:CYS:SG	18:b:201:9YF:O11	2.70	0.49
11:b:96:GLY:HA3	11:b:138:GLU:O	2.13	0.49
1:O:282:ALA:HA	21:T:1302:CDL:H792	1.94	0.49
2:M:207:PHE:CE1	2:G:140:ILE:HB	2.47	0.49
15:P:302:WUO:C30	15:P:302:WUO:C26	2.91	0.49
7:L:138:ALA:O	7:L:141:ILE:HG12	2.13	0.49
11:b:46:ALA:HA	11:b:160:THR:HB	1.94	0.49
21:L:601:CDL:OB4	30:L:701:HOH:O	2.20	0.49
5:S:36:GLU:OE2	5:S:150:HIS:NE2	2.39	0.48
14:T:1301:MQ9:H272	7:R:135:ILE:HG13	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:G:903:IZL:O37	3:H:188:TRP:NE1	2.27	0.48
2:M:260:ARG:NH2	2:M:263:GLU:O	2.46	0.48
19:M:504:7PH:O21	19:M:504:7PH:H24A	2.12	0.48
7:R:63:ARG:HG3	7:R:478:THR:HA	1.94	0.48
1:C:291:GLY:O	30:C:401:HOH:O	2.20	0.48
3:N:532:HIS:O	3:N:536:ILE:HG12	2.13	0.48
3:H:154:GLU:HG2	20:H:902:HEM:CBB	2.43	0.48
7:L:294:THR:HG22	7:L:298:TYR:CE2	2.48	0.48
1:C:194:PHE:CE1	3:H:296:SER:HB3	2.47	0.48
2:G:65:VAL:HG22	2:G:162:GLN:HB2	1.96	0.48
2:G:344:LYS:HE3	2:G:354:SER:CB	2.42	0.48
21:N:604:CDL:H312	6:T:90:TRP:CZ2	2.48	0.48
8:Q:169:SER:HB3	8:Q:192:ASP:HA	1.95	0.48
21:C:305:CDL:H732	21:J:501:CDL:H742	1.94	0.48
14:H:909:MQ9:H103	14:H:909:MQ9:H122	1.50	0.48
8:X:164:LYS:NZ	8:X:194:THR:O	2.34	0.48
8:Q:235:TRP:CD1	8:Q:242:LYS:HB3	2.48	0.48
2:G:300:LYS:O	2:G:303:GLU:HG3	2.14	0.48
21:N:602:CDL:H112	21:H:903:CDL:C52	2.44	0.48
8:Q:136:PHE:CZ	8:Q:139:ASN:CB	2.91	0.48
2:G:328:ARG:HB2	2:G:377:PHE:CG	2.49	0.48
21:I:302:CDL:OA9	21:I:302:CDL:H731	2.13	0.48
7:R:294:THR:HG22	7:R:298:TYR:CE2	2.49	0.48
10:V:114:VAL:HA	10:V:117:ARG:HD3	1.96	0.48
14:M:505:MQ9:H5M1	3:H:227:LEU:HB3	1.95	0.48
21:C:305:CDL:H802	21:C:305:CDL:H771	1.71	0.48
5:J:163:ALA:HA	21:J:501:CDL:H112	1.96	0.48
2:M:247:PHE:CE1	12:Y:45:PRO:HA	2.49	0.47
3:N:253:VAL:HA	3:N:257:PHE:HB3	1.96	0.47
11:W:118:ASP:CG	11:W:170:GLU:HG2	2.39	0.47
2:G:319:PRO:HB3	11:b:148:LEU:HD21	1.96	0.47
14:K:1301:MQ9:H171	18:b:201:9YF:C40	2.44	0.47
7:L:540:ARG:HD3	7:L:554:MET:HE3	1.96	0.47
1:O:289:TRP:CD2	21:T:1302:CDL:H711	2.49	0.47
14:M:505:MQ9:C23	3:H:55:LEU:HD23	2.21	0.47
3:H:139:ALA:HB2	14:H:909:MQ9:H452	1.96	0.47
7:L:544:GLU:HG2	7:L:551:VAL:HG22	1.95	0.47
8:Q:138:TRP:O	8:Q:284:MET:HB3	2.14	0.47
11:W:153:PHE:O	11:W:159:GLU:HA	2.14	0.47
2:G:346:CYS:HB2	2:G:353:SER:HB3	1.96	0.47
2:G:417:TRP:CG	3:H:184:VAL:H	2.33	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:253:VAL:HA	3:H:257:PHE:HB3	1.96	0.47
7:L:97:PRO:HG3	7:L:129:PHE:CE1	2.48	0.47
11:b:118:ASP:OD1	11:b:119:GLY:N	2.43	0.47
6:T:131:GLU:OE2	30:T:1401:HOH:O	2.20	0.47
8:X:139:ASN:ND2	30:X:503:HOH:O	2.46	0.47
19:G:905:7PH:H28A	19:G:905:7PH:H25A	1.69	0.47
2:M:346:CYS:HB2	2:M:353:SER:HB3	1.96	0.47
18:W:201:9YF:C43	18:W:201:9YF:C38	2.92	0.47
22:L:608:TRD:H71	22:X:403:TRD:H81	1.96	0.47
10:a:114:VAL:HA	10:a:117:ARG:HD3	1.95	0.47
18:b:201:9YF:C38	18:b:201:9YF:C43	2.93	0.47
21:P:301:CDL:H401	21:P:301:CDL:H372	1.70	0.47
7:R:355:PHE:HE1	7:R:363:VAL:HG21	1.79	0.47
10:V:77:THR:O	10:V:107:GLU:HG3	2.15	0.47
11:W:96:GLY:HA2	11:W:140:THR:HG23	1.97	0.47
15:C:304:WUO:C84	15:C:304:WUO:C22	2.92	0.47
2:G:212:LEU:HD13	14:G:901:MQ9:H351	1.95	0.47
10:a:138:ASN:HB3	10:a:141:ASP:HB3	1.97	0.47
21:N:602:CDL:C52	21:H:903:CDL:H112	2.44	0.47
21:N:604:CDL:OB9	21:N:604:CDL:H321	2.14	0.47
14:T:1301:MQ9:H122	14:T:1301:MQ9:H103	1.68	0.47
22:R:609:TRD:H71	22:Q:403:TRD:H81	1.97	0.47
3:H:191:TRP:CE3	3:H:196:GLY:HA2	2.50	0.47
14:H:909:MQ9:H371	14:H:909:MQ9:H33	1.64	0.47
1:O:285:GLY:HA3	21:T:1302:CDL:H761	1.97	0.47
2:M:46:GLU:O	2:M:50:MET:HG3	2.15	0.47
7:L:400:TYR:HA	7:L:442:PHE:CZ	2.49	0.47
6:T:126:CYS:CB	21:T:1302:CDL:H131	2.45	0.47
4:I:85:ALA:HA	21:I:302:CDL:H371	1.97	0.47
7:L:458:PRO:HG2	7:L:461:TYR:CE2	2.50	0.47
3:N:228:ALA:HB2	21:N:602:CDL:H751	1.97	0.46
7:R:21:MET:HE2	21:R:605:CDL:HA21	1.97	0.46
3:H:66:PRO:HG3	3:H:208:TYR:CD2	2.49	0.46
3:H:494:GLY:O	5:J:169:LYS:HG2	2.15	0.46
3:N:66:PRO:HG3	3:N:208:TYR:CD2	2.49	0.46
3:N:73:TYR:HB2	3:N:85:MET:HE3	1.96	0.46
5:S:27:VAL:HG12	6:T:55:PHE:HE2	1.80	0.46
2:G:373:ASP:HB3	2:G:376:GLU:HB3	1.97	0.46
5:S:156:VAL:HG22	19:S:501:7PH:H3B	1.97	0.46
7:R:152:THR:HA	7:R:259:PHE:CZ	2.51	0.46
7:R:402:LEU:O	7:R:406:ILE:HG12	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:R:403:PHE:O	7:R:407:VAL:HB	2.15	0.46
2:G:212:LEU:O	2:G:216:ILE:HG12	2.16	0.46
21:I:301:CDL:H512	21:I:301:CDL:H541	1.51	0.46
2:M:328:ARG:HB2	2:M:377:PHE:CG	2.50	0.46
14:N:608:MQ9:H371	14:N:608:MQ9:H33	1.64	0.46
3:N:438:ARG:O	3:N:442:GLU:OE1	2.33	0.46
7:R:256:GLN:HB3	7:R:315:MET:SD	2.55	0.46
11:W:64:TYR:CD1	11:W:142:PRO:HB2	2.51	0.46
21:L:601:CDL:H582	21:L:601:CDL:H782	1.98	0.46
21:R:605:CDL:H782	21:R:605:CDL:H751	1.60	0.46
15:O:304:WUO:C73	15:O:304:WUO:C69	2.94	0.46
21:P:301:CDL:H762	21:P:301:CDL:H541	1.98	0.46
19:H:901:7PH:H24A	19:H:901:7PH:H27	1.56	0.46
9:Z:73:GLY:HA3	10:a:110:TYR:CE1	2.51	0.46
14:N:608:MQ9:H122	14:N:608:MQ9:H103	1.50	0.46
6:T:70:TYR:HB3	6:T:73:ALA:HB2	1.97	0.46
3:H:428:ARG:HH22	21:I:301:CDL:HB21	1.81	0.46
3:N:191:TRP:CE3	3:N:196:GLY:HA2	2.50	0.46
3:N:235:HIS:CD2	14:N:606:MQ9:H3A	2.51	0.46
14:N:608:MQ9:H453	14:N:608:MQ9:H472	1.60	0.46
1:C:289:TRP:CG	21:C:305:CDL:H722	2.51	0.46
7:R:458:PRO:HG2	7:R:461:TYR:CE2	2.51	0.46
11:W:84:GLY:O	11:W:108:ALA:HA	2.15	0.46
18:G:904:9YF:C34	3:H:189:MET:HG2	2.46	0.46
7:R:504:PRO:HB2	10:V:39:VAL:HG21	1.98	0.45
24:R:603:HEA:H271	24:R:603:HEA:H211	1.37	0.45
19:H:901:7PH:H39	19:H:901:7PH:H36A	1.57	0.45
1:O:81:GLN:NE2	8:Q:167:MET:HE3	2.31	0.45
1:O:194:PHE:CZ	3:N:296:SER:HB3	2.50	0.45
3:N:227:LEU:HB3	14:G:901:MQ9:H5M1	1.98	0.45
3:H:159:TYR:HA	20:H:902:HEM:CAA	2.46	0.45
8:X:137:GLN:HA	8:X:138:TRP:HA	1.73	0.45
15:O:304:WUO:C94	14:T:1301:MQ9:C20	2.86	0.45
1:C:84:GLU:HA	1:C:88:VAL:HG13	1.98	0.45
2:G:208:GLY:HA2	14:G:901:MQ9:C38	2.41	0.45
14:H:909:MQ9:H253	14:H:909:MQ9:H272	1.63	0.45
18:M:503:9YF:O7	18:M:503:9YF:O9	2.35	0.45
3:N:424:PHE:HB2	21:P:301:CDL:H522	1.98	0.45
14:N:608:MQ9:H222	14:N:608:MQ9:H203	1.44	0.45
7:R:445:THR:HA	7:R:477:SER:HA	1.99	0.45
9:U:79:TRP:CH2	10:V:101:PRO:HA	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:W:118:ASP:OD1	11:W:119:GLY:N	2.43	0.45
7:R:383:PRO:HG3	8:Q:117:GLN:HB3	1.99	0.45
1:C:126:ARG:HB2	7:L:77:GLU:HG2	1.98	0.45
18:G:904:9YF:O7	18:G:904:9YF:O9	2.35	0.45
4:I:43:MET:HB3	4:I:48:MET:HE3	1.99	0.45
21:L:601:CDL:HA61	21:L:601:CDL:HB32	1.99	0.45
19:N:609:7PH:H39	19:N:609:7PH:H36A	1.56	0.45
1:C:271:GLU:OE2	30:C:402:HOH:O	2.21	0.45
2:G:398:GLU:O	11:b:63:ASP:HB2	2.17	0.45
3:H:228:ALA:HB2	21:H:903:CDL:H751	1.97	0.45
3:H:235:HIS:CD2	14:H:907:MQ9:C3A	3.00	0.45
7:L:152:THR:HA	7:L:259:PHE:CZ	2.52	0.45
2:M:319:PRO:HG3	11:W:165:PRO:HG3	1.99	0.45
3:N:497:PRO:HA	5:S:169:LYS:HA	1.99	0.45
7:R:544:GLU:HG2	7:R:551:VAL:HG22	1.99	0.45
4:I:33:VAL:HG11	4:I:41:SER:HB2	1.98	0.45
7:L:63:ARG:HG3	7:L:478:THR:HA	1.98	0.45
7:L:369:PHE:CE2	7:L:401:VAL:HG23	2.51	0.45
10:a:77:THR:O	10:a:107:GLU:HG3	2.16	0.45
14:O:303:MQ9:H153	14:O:303:MQ9:H172	1.66	0.45
7:R:203:MET:HA	7:R:206:MET:HE2	1.99	0.45
7:R:336:PRO:HA	7:R:339:ILE:HD12	1.98	0.45
7:R:540:ARG:HD3	7:R:554:MET:HE3	1.98	0.45
5:J:67:LEU:HD11	5:J:203:ARG:HH11	1.81	0.45
11:b:89:LYS:HD2	11:b:155:PHE:O	2.16	0.45
2:M:213:VAL:HG13	18:M:503:9YF:C13	2.47	0.45
3:H:73:TYR:HB2	3:H:85:MET:HE3	1.99	0.45
8:X:71:THR:HG23	8:X:75:HIS:ND1	2.32	0.45
14:N:606:MQ9:H371	3:H:218:ILE:HG12	1.99	0.44
11:W:44:ALA:HB3	11:W:51:LEU:HB2	1.99	0.44
1:C:81:GLN:CD	8:X:167:MET:HE3	2.42	0.44
21:C:305:CDL:HA4	21:H:905:CDL:H111	1.98	0.44
5:J:69:LEU:HD21	5:J:119:TYR:HD1	1.81	0.44
8:X:137:GLN:NE2	8:X:277:CYS:O	2.40	0.44
1:C:227:GLN:HE21	13:C:302:HEC:CGD	2.29	0.44
14:C:303:MQ9:H153	14:C:303:MQ9:H172	1.66	0.44
2:G:213:VAL:HG13	18:G:904:9YF:C13	2.48	0.44
2:G:272:GLU:OE2	11:b:174:ARG:NH1	2.47	0.44
2:G:297:SER:O	2:G:301:LEU:HG	2.16	0.44
2:G:319:PRO:HB3	11:b:148:LEU:CD2	2.47	0.44
1:O:176:ASP:HB3	1:O:244:ASP:OD2	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:P:71:VAL:HG22	15:P:302:WUO:C76	2.48	0.44
2:G:313:MET:HE1	2:G:363:ILE:HG21	1.98	0.44
14:H:909:MQ9:H203	14:H:909:MQ9:H222	1.44	0.44
7:L:159:ASP:CG	7:L:161:ILE:HG22	2.42	0.44
1:O:126:ARG:HB2	7:R:77:GLU:HG2	1.99	0.44
3:H:254:MET:HA	3:H:255:PRO:HA	1.70	0.44
11:b:84:GLY:O	11:b:108:ALA:HA	2.18	0.44
15:O:304:WUO:C69	15:O:304:WUO:C65	2.96	0.44
10:a:100:SER:HB3	10:a:103:GLN:HB2	1.98	0.44
14:T:1301:MQ9:H362	7:R:141:ILE:HD11	2.00	0.44
2:G:335:ASN:ND2	2:G:337:GLY:O	2.46	0.44
21:H:905:CDL:H141	21:H:905:CDL:H112	1.50	0.44
11:W:107:PRO:HG2	11:W:110:GLY:HA3	1.99	0.44
21:H:905:CDL:H531	21:H:905:CDL:OB7	2.17	0.44
8:Q:137:GLN:HA	8:Q:138:TRP:HA	1.81	0.44
2:G:352:PRO:HG2	3:H:295:VAL:HB	2.00	0.44
2:M:297:SER:O	2:M:301:LEU:HG	2.18	0.43
3:N:34:PHE:CD1	14:N:606:MQ9:C4	3.01	0.43
3:N:156:PHE:HA	3:N:159:TYR:CE2	2.53	0.43
3:N:502:PHE:CE1	5:S:100:ARG:HD3	2.53	0.43
3:N:473:HIS:CG	3:N:474:PRO:HD2	2.54	0.43
21:N:602:CDL:H511	21:H:903:CDL:C12	2.46	0.43
8:Q:41:PRO:HG3	8:Q:264:GLN:HE21	1.83	0.43
2:G:262:GLY:O	2:G:265:PRO:HD3	2.18	0.43
7:L:336:PRO:HA	7:L:339:ILE:HD12	1.99	0.43
10:a:117:ARG:HG2	10:a:157:ALA:HB3	2.00	0.43
18:M:503:9YF:C34	3:N:189:MET:HG2	2.48	0.43
3:N:370:VAL:HG22	4:P:39:GLY:HA3	2.00	0.43
3:H:65:ASP:HB3	3:H:91:THR:HG21	1.99	0.43
3:H:473:HIS:CG	3:H:474:PRO:HD2	2.53	0.43
2:M:211:THR:HG22	14:M:505:MQ9:H33	2.01	0.43
2:M:329:LYS:HE3	12:Y:27:THR:OG1	2.19	0.43
5:J:27:VAL:HG12	6:K:55:PHE:HE2	1.83	0.43
5:S:134:SER:HA	8:Q:184:PRO:HA	1.99	0.43
21:C:305:CDL:H112	6:K:127:GLY:HA2	2.00	0.43
21:H:905:CDL:H252	6:K:120:PHE:CD2	2.53	0.43
7:L:445:THR:HA	7:L:477:SER:HA	2.00	0.43
7:L:532:GLU:HG3	10:a:23:THR:HB	2.00	0.43
1:O:227:GLN:HE21	13:O:302:HEC:CGD	2.30	0.43
14:M:505:MQ9:C3C	3:H:257:PHE:HZ	2.32	0.43
21:N:602:CDL:C12	21:H:903:CDL:H511	2.46	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:R:403:PHE:CZ	7:R:407:VAL:HG11	2.54	0.43
3:H:110:HIS:CD2	3:H:281:ILE:HD11	2.50	0.43
3:H:342:ALA:HB2	14:H:909:MQ9:H211	2.01	0.43
7:L:73:PHE:HA	8:X:335:LEU:HD11	2.01	0.43
7:R:377:VAL:HG23	24:R:602:HEA:H263	1.99	0.43
3:H:110:HIS:HD2	3:H:281:ILE:CG1	2.31	0.43
3:H:458:TYR:CG	7:L:114:PRO:HB3	2.53	0.43
21:J:501:CDL:H771	21:J:501:CDL:H741	1.55	0.43
24:R:602:HEA:H212	8:Q:60:VAL:HG11	1.99	0.43
7:L:377:VAL:HG23	24:L:602:HEA:H263	2.00	0.43
7:L:399:HIS:O	7:L:403:PHE:HD2	2.02	0.43
8:X:299:TYR:HB2	8:X:316:ILE:HD13	1.99	0.43
1:O:269:ALA:HA	3:N:306:MET:HE1	2.00	0.43
3:N:179:THR:O	3:N:182:ILE:HG12	2.19	0.43
3:H:34:PHE:CE2	14:H:907:MQ9:C4	3.01	0.43
1:O:110:GLU:OE2	1:O:161:ARG:NH1	2.51	0.43
5:S:131:ILE:HD12	23:S:503:3PE:H242	2.01	0.43
10:V:117:ARG:HG2	10:V:157:ALA:HB3	2.00	0.43
3:H:110:HIS:HD2	3:H:281:ILE:HG12	1.83	0.43
7:L:458:PRO:HG2	7:L:461:TYR:CZ	2.53	0.43
2:M:148:VAL:HG23	3:N:263:ALA:HB1	2.01	0.42
19:M:504:7PH:H28A	19:M:504:7PH:H25A	1.69	0.42
8:Q:233:GLY:O	8:Q:273:CYS:HA	2.18	0.42
8:Q:229:ASP:O	8:Q:247:PRO:HG3	2.19	0.42
12:Y:23:PRO:HA	12:Y:24:PRO:HD3	1.93	0.42
3:H:318:TRP:CD1	29:c:301:PLM:H21	2.52	0.42
3:H:410:ILE:CG2	14:K:1301:MQ9:H48	2.49	0.42
3:H:502:PHE:CE1	5:J:100:ARG:HD3	2.54	0.42
2:M:208:GLY:HA3	14:M:505:MQ9:C38	2.49	0.42
2:M:319:PRO:HG2	11:W:42:VAL:HG22	2.00	0.42
3:N:342:ALA:HB2	14:N:608:MQ9:H211	2.01	0.42
3:N:394:ASP:OD1	3:N:394:ASP:N	2.52	0.42
1:C:269:ALA:HA	3:H:306:MET:HE1	2.00	0.42
2:G:329:LYS:HE3	12:c:27:THR:OG1	2.19	0.42
8:X:223:PHE:O	8:X:257:VAL:HA	2.19	0.42
2:M:342:TYR:OH	2:M:377:PHE:HA	2.19	0.42
3:N:416:VAL:HG13	4:P:55:SER:HB2	2.01	0.42
3:N:488:MET:HE3	3:N:493:SER:OG	2.18	0.42
6:T:106:ALA:HA	6:T:114:ILE:HD11	2.01	0.42
9:U:79:TRP:O	10:V:104:ARG:NH1	2.53	0.42
3:H:505:PRO:HB3	5:J:97:PHE:CE2	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:R:390:ASP:OD2	8:Q:274:THR:O	2.37	0.42
7:R:458:PRO:HG2	7:R:461:TYR:CZ	2.54	0.42
9:U:2:SER:OG	9:U:3:THR:N	2.47	0.42
21:H:904:CDL:H532	21:H:904:CDL:OA7	2.20	0.42
8:X:229:ASP:O	8:X:247:PRO:HG3	2.20	0.42
1:C:284:ILE:HG21	21:H:904:CDL:H731	2.01	0.42
14:T:1301:MQ9:H361	7:R:138:ALA:HB1	2.01	0.42
11:W:117:PRO:CD	11:W:120:GLN:HG3	2.48	0.42
2:G:90:ALA:HB1	2:G:94:MET:HE3	2.02	0.42
3:N:59:TRP:CE3	3:N:105:VAL:HG11	2.55	0.42
5:S:147:HIS:O	5:S:151:VAL:HG23	2.19	0.42
7:R:73:PHE:HA	8:Q:335:LEU:HD11	2.00	0.42
9:U:42:TRP:CZ2	9:U:44:HIS:HB3	2.55	0.42
11:W:45:GLN:O	11:W:160:THR:HG21	2.19	0.42
12:c:44:SER:HB3	12:c:45:PRO:HD3	2.01	0.42
2:M:212:LEU:O	2:M:216:ILE:HG12	2.20	0.42
2:M:321:ASP:OD1	2:M:324:ARG:NH1	2.47	0.42
5:S:132:PRO:CD	23:S:503:3PE:H12	2.49	0.42
1:O:72:GLN:HG3	1:O:75:LEU:H	1.85	0.42
2:M:313:MET:HE1	2:M:363:ILE:HG21	2.02	0.42
3:N:257:PHE:HZ	14:G:901:MQ9:C3C	2.32	0.42
14:K:1301:MQ9:H271	14:K:1301:MQ9:H253	1.55	0.42
1:O:277:ILE:HG12	15:O:304:WUO:C89	2.50	0.41
7:R:403:PHE:CD1	7:R:407:VAL:HG21	2.55	0.41
5:J:147:HIS:O	5:J:151:VAL:HG23	2.20	0.41
21:J:501:CDL:O1	6:K:138:LYS:NZ	2.25	0.41
7:L:348:MET:HB3	8:X:71:THR:HG21	2.02	0.41
7:L:401:VAL:HG21	24:L:602:HEA:C2C	2.49	0.41
2:G:288:SER:O	11:b:182:GLY:HA3	2.19	0.41
3:H:59:TRP:CE3	3:H:105:VAL:HG11	2.55	0.41
3:H:499:THR:HG22	3:H:511:HIS:HB2	2.01	0.41
4:I:89:ARG:HD2	21:I:301:CDL:H342	2.02	0.41
3:N:429:TRP:CG	21:N:603:CDL:H322	2.55	0.41
7:R:149:PHE:HD2	7:R:153:ALA:HA	1.84	0.41
3:H:78:GLN:HA	3:H:81:ARG:CG	2.51	0.41
6:K:106:ALA:HA	6:K:114:ILE:HD11	2.01	0.41
8:X:184:PRO:HD2	8:X:189:THR:HA	2.01	0.41
9:Z:42:TRP:CZ2	9:Z:44:HIS:HB3	2.55	0.41
11:W:82:THR:HG22	11:W:109:ASP:HB3	2.01	0.41
1:C:271:GLU:CD	3:H:281:ILE:HG13	2.45	0.41
21:C:305:CDL:H111	21:C:305:CDL:HA62	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:313:MET:HE2	2:G:344:LYS:HA	2.02	0.41
3:H:442:GLU:HG2	3:H:443:HIS:CE1	2.55	0.41
10:a:100:SER:CB	10:a:103:GLN:HB2	2.50	0.41
3:N:403:SER:O	3:N:407:THR:HG23	2.21	0.41
1:C:190:SER:O	2:G:355:LEU:HD11	2.20	0.41
2:G:189:THR:O	2:G:193:ARG:HG2	2.20	0.41
3:H:499:THR:HG23	3:H:506:ASP:OD1	2.20	0.41
7:L:365:PHE:HD1	7:L:404:GLY:O	2.03	0.41
1:O:128:GLU:CG	30:O:443:HOH:O	2.66	0.41
14:O:303:MQ9:H71	14:O:303:MQ9:H5M3	1.87	0.41
14:T:1301:MQ9:H72	14:T:1301:MQ9:H5M3	1.80	0.41
2:G:153:LYS:HA	2:G:153:LYS:HD3	1.98	0.41
2:G:208:GLY:HA3	14:G:901:MQ9:C38	2.50	0.41
3:H:403:SER:O	3:H:407:THR:HG23	2.20	0.41
7:L:20:ARG:HG3	7:L:500:ARG:O	2.21	0.41
7:L:550:MET:HE3	7:L:550:MET:HB3	1.87	0.41
8:X:233:GLY:O	8:X:273:CYS:HA	2.21	0.41
8:X:320:PRO:HB2	11:b:83:GLU:OE2	2.21	0.41
9:Z:79:TRP:CH2	10:a:104:ARG:HA	2.56	0.41
2:M:208:GLY:HA3	14:M:505:MQ9:C39	2.50	0.41
5:S:147:HIS:NE2	5:S:192:TRP:HB2	2.36	0.41
8:Q:81:ASP:OD1	8:Q:81:ASP:N	2.54	0.41
2:G:211:THR:HG22	14:G:901:MQ9:H33	2.02	0.41
2:M:137:GLY:O	2:M:141:LEU:HB2	2.20	0.41
2:M:352:PRO:HG2	3:N:295:VAL:HB	2.02	0.41
3:N:65:ASP:HB3	3:N:91:THR:HG21	2.03	0.41
21:N:604:CDL:H242	21:N:604:CDL:H211	1.62	0.41
14:N:606:MQ9:H502	21:H:903:CDL:H191	2.03	0.41
7:R:57:LEU:HB2	24:R:603:HEA:H242	2.02	0.41
7:R:288:LYS:HB3	7:R:288:LYS:HE2	1.81	0.41
7:R:295:THR:HG21	8:Q:95:GLU:OE1	2.20	0.41
8:Q:333:GLY:HA3	11:W:28:GLN:CD	2.46	0.41
1:C:228:ASN:OD1	2:G:357:GLU:HB3	2.21	0.41
2:G:152:LYS:HB3	2:G:152:LYS:HE2	1.86	0.41
15:I:303:WUO:C23	15:I:303:WUO:C19	2.98	0.41
5:S:67:LEU:HD11	5:S:203:ARG:HH11	1.86	0.41
8:Q:36:PRO:HD2	8:Q:240:LEU:HD21	2.03	0.41
7:L:401:VAL:CG2	24:L:602:HEA:HMC2	2.51	0.41
8:X:36:PRO:HD2	8:X:240:LEU:HD21	2.02	0.41
7:R:348:MET:HG2	7:R:353:LEU:HD21	2.03	0.40
11:W:149:TYR:O	11:W:164:VAL:N	2.47	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:229:MET:HB2	13:C:302:HEC:C1D	2.51	0.40
6:K:71:GLU:OE1	7:L:205:ARG:NH1	2.54	0.40
3:N:346:ALA:CB	14:N:608:MQ9:H271	2.49	0.40
9:U:79:TRP:HH2	10:V:101:PRO:HA	1.86	0.40
2:G:313:MET:HG3	2:G:344:LYS:HG3	2.02	0.40
3:H:143:ILE:HG23	3:H:222:LEU:HD22	2.02	0.40
21:I:302:CDL:H191	21:I:302:CDL:H161	1.77	0.40
5:J:184:TYR:CZ	21:L:601:CDL:H572	2.55	0.40
4:P:82:VAL:HG21	15:P:302:WUO:C92	2.52	0.40
6:T:95:ILE:CG1	6:T:124:SER:HB3	2.51	0.40
21:T:1302:CDL:H521	21:T:1302:CDL:H141	2.02	0.40
7:R:140:PHE:CE1	29:W:203:PLM:H41	2.57	0.40
7:R:495:VAL:HG11	21:R:605:CDL:H402	2.03	0.40
2:M:313:MET:HG3	2:M:344:LYS:HG3	2.03	0.40
4:P:96:ARG:NE	4:P:98:TRP:HE1	2.20	0.40
11:W:43:ASN:HA	11:W:51:LEU:O	2.22	0.40
3:H:60:LEU:HD13	20:H:902:HEM:HBD1	2.03	0.40
11:b:75:PHE:CZ	11:b:114:VAL:HG21	2.56	0.40
24:R:603:HEA:H261	24:R:603:HEA:H172	1.65	0.40
2:G:208:GLY:HA3	14:G:901:MQ9:C39	2.51	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	C	221/278 (80%)	211 (96%)	9 (4%)	1 (0%)	24	31
1	O	221/278 (80%)	208 (94%)	12 (5%)	1 (0%)	24	31
2	G	378/408 (93%)	364 (96%)	14 (4%)	0	100	100
2	M	378/408 (93%)	364 (96%)	14 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	H	531/556 (96%)	518 (98%)	12 (2%)	1 (0%)	43	55
3	N	531/556 (96%)	518 (98%)	12 (2%)	1 (0%)	43	55
4	I	71/100 (71%)	68 (96%)	3 (4%)	0	100	100
4	P	71/100 (71%)	70 (99%)	1 (1%)	0	100	100
5	J	182/203 (90%)	179 (98%)	3 (2%)	0	100	100
5	S	182/203 (90%)	180 (99%)	2 (1%)	0	100	100
6	K	137/139 (99%)	136 (99%)	1 (1%)	0	100	100
6	T	137/139 (99%)	134 (98%)	3 (2%)	0	100	100
7	L	549/575 (96%)	543 (99%)	6 (1%)	0	100	100
7	R	549/575 (96%)	542 (99%)	7 (1%)	0	100	100
8	Q	295/341 (86%)	287 (97%)	8 (3%)	0	100	100
8	X	296/341 (87%)	286 (97%)	10 (3%)	0	100	100
9	U	62/79 (78%)	61 (98%)	1 (2%)	0	100	100
9	Z	63/79 (80%)	62 (98%)	1 (2%)	0	100	100
10	V	141/157 (90%)	138 (98%)	3 (2%)	0	100	100
10	a	141/157 (90%)	134 (95%)	7 (5%)	0	100	100
11	W	145/186 (78%)	129 (89%)	16 (11%)	0	100	100
11	b	145/186 (78%)	129 (89%)	16 (11%)	0	100	100
12	Y	23/236 (10%)	20 (87%)	3 (13%)	0	100	100
12	c	23/236 (10%)	20 (87%)	3 (13%)	0	100	100
All	All	5472/6516 (84%)	5301 (97%)	167 (3%)	4 (0%)	49	60

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	N	235	HIS
1	O	227	GLN
1	C	227	GLN
3	H	235	HIS

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	C	163/206 (79%)	162 (99%)	1 (1%)	78	89
1	O	163/206 (79%)	162 (99%)	1 (1%)	78	89
2	G	311/333 (93%)	310 (100%)	1 (0%)	86	93
2	M	311/333 (93%)	310 (100%)	1 (0%)	86	93
3	H	428/448 (96%)	428 (100%)	0	100	100
3	N	428/448 (96%)	428 (100%)	0	100	100
4	I	58/83 (70%)	58 (100%)	0	100	100
4	P	58/83 (70%)	58 (100%)	0	100	100
5	J	146/161 (91%)	146 (100%)	0	100	100
5	S	146/161 (91%)	146 (100%)	0	100	100
6	K	106/106 (100%)	106 (100%)	0	100	100
6	T	106/106 (100%)	106 (100%)	0	100	100
7	L	453/471 (96%)	452 (100%)	1 (0%)	87	94
7	R	453/471 (96%)	452 (100%)	1 (0%)	87	94
8	Q	255/288 (88%)	254 (100%)	1 (0%)	84	92
8	X	256/288 (89%)	254 (99%)	2 (1%)	73	86
9	U	51/59 (86%)	51 (100%)	0	100	100
9	Z	52/59 (88%)	52 (100%)	0	100	100
10	V	105/114 (92%)	105 (100%)	0	100	100
10	a	105/114 (92%)	105 (100%)	0	100	100
11	W	121/146 (83%)	121 (100%)	0	100	100
11	b	121/146 (83%)	121 (100%)	0	100	100
12	Y	20/167 (12%)	20 (100%)	0	100	100
12	c	20/167 (12%)	20 (100%)	0	100	100
All	All	4436/5164 (86%)	4427 (100%)	9 (0%)	85	94

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	O	193	ASN
2	M	420	LYS
7	R	341	PHE

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Mol	Chain	Res	Type
8	Q	229	ASP
1	C	193	ASN
2	G	420	LYS
7	L	188	ASN
8	X	229	ASP
8	X	242	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (39) such sidechains are listed below:

Mol	Chain	Res	Type
1	O	94	ASN
1	O	227	GLN
2	M	115	GLN
2	M	371	GLN
3	N	70	HIS
3	N	300	GLN
3	N	462	HIS
5	S	20	ASN
7	R	26	ASN
7	R	239	HIS
7	R	528	HIS
8	Q	117	GLN
8	Q	126	ASN
8	Q	226	ASN
8	Q	265	GLN
8	Q	302	GLN
10	V	87	ASN
11	W	61	GLN
1	C	94	ASN
1	C	116	GLN
1	C	227	GLN
2	G	358	GLN
3	H	70	HIS
3	H	300	GLN
3	H	462	HIS
3	H	463	GLN
3	H	519	HIS
4	I	67	HIS
5	J	20	ASN
5	J	174	GLN
7	L	26	ASN
7	L	239	HIS

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Mol	Chain	Res	Type
7	L	249	ASN
7	L	528	HIS
8	X	139	ASN
8	X	226	ASN
8	X	265	GLN
8	X	302	GLN
8	X	318	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 86 ligands modelled in this entry, 10 are monoatomic - leaving 76 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	$\# Z > 2$
29	PLM	W	203	-	9,10,17	0.93	0	8,9,17	0.50	0
18	9YF	G	904	-	58,58,58	1.38	4 (6%)	68,71,71	1.10	2 (2%)
19	7PH	H	901	-	37,37,37	0.31	0	40,42,42	0.33	0
22	TRD	R	608	-	12,12,12	0.10	0	11,11,11	0.05	0
29	PLM	c	301	-	9,10,17	0.81	0	8,9,17	0.54	0
21	CDL	C	305	-	78,78,99	0.29	0	84,90,111	0.34	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
13	HEC	C	301	1	46,50,50	1.98	6 (13%)	58,82,82	1.61	5 (8%)
22	TRD	L	607	-	12,12,12	0.10	0	11,11,11	0.05	0
16	FES	G	902	2	0,4,4	-	-	-		
21	CDL	P	301	-	76,76,99	0.30	0	82,88,111	0.36	0
22	TRD	L	608	-	12,12,12	0.26	0	11,11,11	0.53	0
15	WUO	O	304	-	99,99,99	1.36	6 (6%)	122,125,125	1.25	15 (12%)
17	IZL	G	903	-	119,119,119	1.77	22 (18%)	160,163,163	1.17	14 (8%)
18	9YF	W	201	-	58,58,58	1.38	5 (8%)	68,71,71	1.11	2 (2%)
14	MQ9	H	907	14	59,59,59	0.36	0	73,75,75	0.42	1 (1%)
19	7PH	M	504	-	37,37,37	0.30	0	40,42,42	0.33	0
14	MQ9	T	1301	-	59,59,59	0.68	0	73,75,75	0.72	1 (1%)
21	CDL	R	605	-	76,76,99	0.29	0	82,88,111	0.35	0
17	IZL	M	502	-	119,119,119	1.73	29 (24%)	160,163,163	1.30	19 (11%)
14	MQ9	M	505	14	59,59,59	0.35	0	73,75,75	0.41	1 (1%)
21	CDL	N	602	-	73,73,99	0.30	0	79,85,111	0.36	0
20	HEM	H	908	3	50,50,50	2.64	19 (38%)	67,82,82	2.10	19 (28%)
22	TRD	J	502	-	12,12,12	0.26	0	11,11,11	0.27	0
21	CDL	H	904	-	76,76,99	0.30	0	82,88,111	0.35	0
14	MQ9	N	608	-	59,59,59	0.35	0	73,75,75	0.41	1 (1%)
18	9YF	M	503	-	58,58,58	1.38	4 (6%)	68,71,71	1.10	2 (2%)
29	PLM	Y	301	-	9,10,17	0.70	0	8,9,17	0.51	0
19	7PH	S	501	-	37,37,37	0.30	0	40,42,42	0.35	0
14	MQ9	H	906	-	44,44,59	0.40	0	55,57,75	0.49	1 (1%)
22	TRD	T	1303	-	12,12,12	0.43	0	11,11,11	0.38	0
24	HEA	L	602	7	67,67,67	2.40	25 (37%)	81,103,103	2.38	29 (35%)
21	CDL	T	1302	-	78,78,99	0.29	0	84,90,111	0.34	0
20	HEM	N	601	3	50,50,50	2.50	19 (38%)	67,82,82	2.11	17 (25%)
21	CDL	N	603	-	76,76,99	0.29	0	82,88,111	0.35	0
28	9XX	c	302	-	31,31,41	1.11	4 (12%)	34,34,44	1.35	2 (5%)
13	HEC	C	302	1	46,50,50	2.03	8 (17%)	58,82,82	1.76	9 (15%)
13	HEC	O	302	1	46,50,50	2.04	9 (19%)	58,82,82	1.74	7 (12%)
14	MQ9	O	303	-	59,59,59	0.37	0	73,75,75	0.43	1 (1%)
15	WUO	C	304	-	99,99,99	1.35	6 (6%)	122,125,125	1.26	15 (12%)
24	HEA	L	603	7	67,67,67	2.82	29 (43%)	81,103,103	2.09	29 (35%)
24	HEA	R	603	7	67,67,67	2.89	29 (43%)	81,103,103	2.37	34 (41%)
18	9YF	b	201	-	58,58,58	1.39	5 (8%)	68,71,71	1.11	3 (4%)
21	CDL	N	604	-	78,78,99	0.29	0	84,90,111	0.34	0
19	7PH	G	905	-	37,37,37	0.30	0	40,42,42	0.34	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
21	CDL	H	903	-	73,73,99	0.30	0	79,85,111	0.36	0
21	CDL	I	302	-	76,76,99	0.30	0	82,88,111	0.40	0
22	TRD	S	502	-	12,12,12	0.26	0	11,11,11	0.27	0
15	WUO	P	302	-	99,99,99	1.37	6 (6%)	122,125,125	1.25	15 (12%)
14	MQ9	N	605	-	44,44,59	0.40	0	55,57,75	0.49	1 (1%)
20	HEM	N	607	3	50,50,50	2.65	19 (38%)	67,82,82	2.10	20 (29%)
22	TRD	R	609	-	12,12,12	0.26	0	11,11,11	0.53	0
14	MQ9	G	901	14	59,59,59	0.36	0	73,75,75	0.41	1 (1%)
14	MQ9	N	606	14	59,59,59	0.36	0	73,75,75	0.42	1 (1%)
23	3PE	S	503	-	31,31,50	0.33	0	34,36,55	0.38	0
21	CDL	H	905	-	78,78,99	0.29	0	84,90,111	0.35	0
23	3PE	J	503	-	31,31,50	0.33	0	34,36,55	0.38	0
28	9XX	W	202	-	41,41,41	0.97	4 (9%)	44,44,44	1.40	4 (9%)
24	HEA	R	602	7	67,67,67	2.40	26 (38%)	81,103,103	2.34	29 (35%)
21	CDL	R	601	-	76,76,99	0.30	0	82,88,111	0.35	0
21	CDL	J	501	-	78,78,99	1.00	7 (8%)	84,90,111	1.14	5 (5%)
19	7PH	N	609	-	37,37,37	0.31	0	40,42,42	0.33	0
16	FES	M	501	2	0,4,4	-	-	-	-	-
14	MQ9	K	1301	-	59,59,59	0.65	0	73,75,75	0.81	2 (2%)
22	TRD	K	1302	-	12,12,12	0.43	0	11,11,11	0.38	0
22	TRD	X	403	-	12,12,12	0.10	0	11,11,11	0.05	0
14	MQ9	C	303	-	59,59,59	0.37	0	73,75,75	0.43	1 (1%)
28	9XX	Y	302	-	31,31,41	1.11	4 (12%)	34,34,44	1.33	2 (5%)
13	HEC	O	301	1	46,50,50	1.97	6 (13%)	58,82,82	1.61	5 (8%)
21	CDL	I	301	-	76,76,99	0.29	0	82,88,111	0.35	0
21	CDL	L	601	-	78,78,99	0.29	0	84,90,111	0.34	0
28	9XX	b	203	-	31,31,41	1.08	4 (12%)	34,34,44	1.33	3 (8%)
29	PLM	b	202	-	9,10,17	0.77	0	8,9,17	0.44	0
15	WUO	I	303	-	99,99,99	1.80	22 (22%)	122,125,125	1.39	17 (13%)
20	HEM	H	902	3	50,50,50	2.47	16 (32%)	67,82,82	2.96	30 (44%)
22	TRD	Q	403	-	12,12,12	0.10	0	11,11,11	0.05	0
14	MQ9	H	909	-	59,59,59	0.36	0	73,75,75	0.41	1 (1%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	PLM	W	203	-	-	5/8/8/15	-
18	9YF	G	904	-	-	29/54/78/78	0/1/1/1
19	7PH	H	901	-	-	21/39/39/39	-
22	TRD	R	608	-	-	5/10/10/10	-
29	PLM	c	301	-	-	3/8/8/15	-
21	CDL	C	305	-	-	45/89/89/110	-
13	HEC	C	301	1	-	9/14/54/54	-
22	TRD	L	607	-	-	5/10/10/10	-
21	CDL	P	301	-	-	45/87/87/110	-
16	FES	G	902	2	-	-	0/1/1/1
22	TRD	L	608	-	-	1/10/10/10	-
15	WUO	O	304	-	-	39/84/148/148	0/3/3/3
17	IZL	G	903	-	-	36/84/208/208	0/6/6/6
18	9YF	W	201	-	-	31/54/78/78	0/1/1/1
14	MQ9	H	907	14	-	28/53/73/73	0/2/2/2
19	7PH	M	504	-	-	21/39/39/39	-
14	MQ9	T	1301	-	-	20/53/73/73	0/2/2/2
21	CDL	R	605	-	-	48/87/87/110	-
16	FES	M	501	2	-	-	0/1/1/1
17	IZL	M	502	-	-	37/84/208/208	0/6/6/6
14	MQ9	M	505	14	-	26/53/73/73	0/2/2/2
21	CDL	N	602	-	-	43/84/84/110	-
20	HEM	H	908	3	-	3/14/54/54	-
22	TRD	J	502	-	-	5/10/10/10	-
21	CDL	H	904	-	-	40/87/87/110	-
14	MQ9	N	608	-	-	31/53/73/73	0/2/2/2
18	9YF	M	503	-	-	29/54/78/78	0/1/1/1
29	PLM	Y	301	-	-	2/8/8/15	-
19	7PH	S	501	-	-	15/39/39/39	-
14	MQ9	H	906	-	-	14/35/55/73	0/2/2/2
22	TRD	T	1303	-	-	6/10/10/10	-
24	HEA	L	602	7	-	10/36/76/76	-
21	CDL	T	1302	-	-	53/89/89/110	-
20	HEM	N	601	3	-	5/14/54/54	-
21	CDL	N	603	-	-	35/87/87/110	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	9XX	c	302	-	-	20/33/33/43	-
13	HEC	C	302	1	-	7/14/54/54	-
13	HEC	O	302	1	-	7/14/54/54	-
14	MQ9	O	303	-	-	6/53/73/73	0/2/2/2
15	WUO	C	304	-	-	38/84/148/148	0/3/3/3
24	HEA	L	603	7	-	6/36/76/76	-
24	HEA	R	603	7	-	14/36/76/76	-
18	9YF	b	201	-	-	31/54/78/78	0/1/1/1
21	CDL	N	604	-	-	50/89/89/110	-
19	7PH	G	905	-	-	21/39/39/39	-
21	CDL	H	903	-	-	43/84/84/110	-
21	CDL	I	302	-	-	48/87/87/110	-
22	TRD	S	502	-	-	5/10/10/10	-
15	WUO	P	302	-	-	37/84/148/148	0/3/3/3
14	MQ9	N	605	-	-	14/35/55/73	0/2/2/2
20	HEM	N	607	3	-	3/14/54/54	-
22	TRD	R	609	-	-	1/10/10/10	-
14	MQ9	G	901	14	-	26/53/73/73	0/2/2/2
14	MQ9	N	606	14	-	28/53/73/73	0/2/2/2
23	3PE	S	503	-	-	16/35/35/54	-
21	CDL	H	905	-	-	41/89/89/110	-
23	3PE	J	503	-	-	16/35/35/54	-
28	9XX	W	202	-	-	28/43/43/43	-
24	HEA	R	602	7	-	9/36/76/76	-
21	CDL	R	601	-	-	38/87/87/110	-
21	CDL	J	501	-	-	50/89/89/110	-
19	7PH	N	609	-	-	21/39/39/39	-
22	TRD	K	1302	-	-	6/10/10/10	-
14	MQ9	K	1301	-	-	18/53/73/73	0/2/2/2
28	9XX	Y	302	-	-	16/33/33/43	-
22	TRD	X	403	-	-	6/10/10/10	-
14	MQ9	C	303	-	-	6/53/73/73	0/2/2/2
29	PLM	b	202	-	-	4/8/8/15	-
13	HEC	O	301	1	-	9/14/54/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	CDL	I	301	-	-	58/87/87/110	-
21	CDL	L	601	-	-	50/89/89/110	-
28	9XX	b	203	-	-	21/33/33/43	-
15	WUO	I	303	-	-	36/84/148/148	0/3/3/3
20	HEM	H	902	3	-	4/14/54/54	-
22	TRD	Q	403	-	-	6/10/10/10	-
14	MQ9	H	909	-	-	31/53/73/73	0/2/2/2

All (343) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	C	302	HEC	CAC-C3C	7.65	1.59	1.35
13	O	302	HEC	CAC-C3C	7.61	1.59	1.35
13	C	301	HEC	CAC-C3C	7.56	1.59	1.35
13	O	301	HEC	CAC-C3C	7.53	1.59	1.35
24	R	603	HEA	FE-NC	7.51	2.19	1.95
24	L	603	HEA	FE-ND	7.33	2.17	1.94
20	H	902	HEM	FE-NB	7.23	2.17	1.94
24	R	603	HEA	FE-ND	7.22	2.17	1.94
24	L	603	HEA	FE-NC	7.07	2.18	1.95
13	C	302	HEC	CAB-C3B	6.82	1.57	1.35
20	N	601	HEM	FE-NB	6.81	2.15	1.94
13	O	301	HEC	CAB-C3B	6.79	1.57	1.35
13	C	301	HEC	CAB-C3B	6.79	1.57	1.35
13	O	302	HEC	CAB-C3B	6.77	1.57	1.35
24	R	603	HEA	FE-NB	6.68	2.15	1.94
17	G	903	IZL	P-O28	6.52	1.79	1.59
24	L	603	HEA	FE-NB	6.52	2.15	1.94
20	N	607	HEM	FE-NB	6.43	2.14	1.94
20	H	908	HEM	FE-NB	6.43	2.14	1.94
24	R	603	HEA	C4B-NB	-6.42	1.29	1.40
24	L	603	HEA	C4B-NB	-6.22	1.29	1.40
20	H	908	HEM	C4D-ND	-6.05	1.29	1.40
20	N	607	HEM	C4D-ND	-6.03	1.29	1.40
15	I	303	WUO	O58-C57	-6.02	1.32	1.46
15	C	304	WUO	P52-O51	5.91	1.77	1.59
15	O	304	WUO	P52-O51	5.89	1.77	1.59
15	P	302	WUO	P52-O51	5.88	1.77	1.59
20	N	601	HEM	C3C-C4C	-5.72	1.36	1.46
20	N	607	HEM	C1B-NB	-5.67	1.30	1.40
20	H	908	HEM	C1B-NB	-5.66	1.30	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	L	602	HEA	FE-NC	5.60	2.13	1.95
20	N	601	HEM	FE-NC	5.58	2.13	1.95
24	R	602	HEA	FE-NC	5.57	2.13	1.95
24	L	602	HEA	FE-NB	5.50	2.11	1.94
24	R	602	HEA	FE-NB	5.50	2.11	1.94
20	H	902	HEM	C3C-C4C	-5.39	1.36	1.46
15	I	303	WUO	O36-C35	-5.37	1.29	1.43
24	L	602	HEA	FE-ND	5.37	2.11	1.94
24	R	602	HEA	FE-ND	5.36	2.11	1.94
20	N	601	HEM	O2D-CGD	-5.31	1.13	1.30
18	G	904	9YF	P-O2	5.21	1.75	1.59
18	b	201	9YF	P-O2	5.21	1.75	1.59
18	W	201	9YF	P-O2	5.20	1.75	1.59
18	M	503	9YF	P-O2	5.19	1.75	1.59
20	N	607	HEM	C1A-C2A	-5.16	1.34	1.44
15	P	302	WUO	C50-C37	5.16	1.62	1.52
20	H	908	HEM	C1A-C2A	-5.12	1.34	1.44
24	L	603	HEA	C1D-ND	-5.10	1.31	1.40
24	R	603	HEA	C1D-ND	-5.09	1.31	1.40
20	H	902	HEM	FE-NC	4.98	2.11	1.95
20	H	902	HEM	C1C-C2C	-4.98	1.35	1.45
15	O	304	WUO	C50-C37	4.93	1.62	1.52
20	N	601	HEM	C1B-NB	-4.93	1.31	1.40
24	R	603	HEA	C1C-NC	-4.92	1.30	1.39
17	G	903	IZL	C43-C14	4.86	1.62	1.52
17	G	903	IZL	C44-C45	4.84	1.66	1.50
24	R	603	HEA	C1B-NB	-4.83	1.29	1.38
24	R	603	HEA	CHD-C1D	4.77	1.48	1.38
20	N	607	HEM	C1C-C2C	-4.76	1.35	1.45
15	C	304	WUO	C50-C37	4.73	1.62	1.52
17	M	502	IZL	P-O28	4.72	1.73	1.59
24	L	603	HEA	C1B-NB	-4.72	1.29	1.38
20	H	908	HEM	C1C-C2C	-4.71	1.36	1.45
24	L	603	HEA	C1C-NC	-4.71	1.30	1.39
20	H	902	HEM	O2D-CGD	-4.69	1.15	1.30
15	I	303	WUO	O10-C07	-4.66	1.31	1.43
24	L	603	HEA	CHD-C1D	4.62	1.47	1.38
24	L	602	HEA	C3D-C2D	4.57	1.46	1.36
17	M	502	IZL	C44-C45	4.55	1.65	1.50
17	G	903	IZL	P-O31	4.55	1.77	1.59
24	R	602	HEA	C3D-C2D	4.52	1.46	1.36
20	H	902	HEM	C1B-NB	-4.46	1.32	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	I	303	WUO	O32-C31	-4.45	1.31	1.43
20	N	601	HEM	O2A-CGA	-4.44	1.16	1.30
15	O	304	WUO	P52-O55	4.42	1.76	1.59
18	M	503	9YF	P-O	4.41	1.76	1.59
15	P	302	WUO	P52-O55	4.41	1.76	1.59
18	b	201	9YF	P-O	4.41	1.76	1.59
18	W	201	9YF	P-O	4.40	1.76	1.59
17	M	502	IZL	C43-C14	4.40	1.61	1.52
20	N	607	HEM	FE-NC	4.39	2.09	1.95
20	H	908	HEM	FE-NC	4.39	2.09	1.95
18	G	904	9YF	P-O	4.39	1.76	1.59
15	C	304	WUO	P52-O55	4.39	1.76	1.59
20	H	908	HEM	C1C-NC	-4.36	1.31	1.39
20	N	607	HEM	C1C-NC	-4.35	1.31	1.39
24	R	603	HEA	O2D-CGD	-4.35	1.16	1.30
24	L	603	HEA	O2D-CGD	-4.35	1.16	1.30
24	L	603	HEA	C3B-C2B	4.33	1.44	1.34
24	R	603	HEA	C4C-NC	-4.32	1.31	1.39
20	H	908	HEM	C3C-C4C	-4.30	1.38	1.46
20	N	607	HEM	C3C-C4C	-4.30	1.38	1.46
24	L	603	HEA	C4C-NC	-4.27	1.31	1.39
24	R	603	HEA	C3B-C2B	4.25	1.44	1.34
24	L	602	HEA	CHC-C4B	4.23	1.47	1.38
24	L	602	HEA	C1D-ND	-4.23	1.32	1.40
24	R	602	HEA	CHC-C4B	4.19	1.46	1.38
24	R	602	HEA	C1D-ND	-4.19	1.33	1.40
15	I	303	WUO	O11-C06	-4.13	1.32	1.43
24	R	602	HEA	C4B-NB	-4.07	1.33	1.40
24	L	602	HEA	C4B-NB	-4.07	1.33	1.40
24	L	602	HEA	C3B-C2B	4.06	1.44	1.34
24	R	602	HEA	C3B-C2B	4.06	1.44	1.34
24	L	602	HEA	C4D-ND	-4.06	1.30	1.38
17	M	502	IZL	P-O31	4.06	1.75	1.59
24	R	602	HEA	C4D-ND	-4.01	1.31	1.38
20	H	902	HEM	C1A-NA	-4.01	1.32	1.39
20	N	607	HEM	C4B-NB	-3.93	1.31	1.38
24	R	603	HEA	C1A-NA	3.93	1.47	1.39
24	R	602	HEA	C4C-NC	-3.92	1.32	1.39
28	W	202	9XX	O1-C17	-3.91	1.40	1.47
20	H	908	HEM	C4B-NB	-3.91	1.31	1.38
24	L	603	HEA	C4D-ND	-3.90	1.31	1.38
20	H	908	HEM	O2D-CGD	-3.90	1.17	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	N	607	HEM	O2D-CGD	-3.88	1.18	1.30
24	L	602	HEA	C4C-NC	-3.88	1.32	1.39
24	R	603	HEA	CHD-C4C	3.88	1.48	1.39
20	H	902	HEM	CAC-C3C	-3.85	1.37	1.47
20	N	601	HEM	C1C-C2C	-3.84	1.37	1.45
24	R	603	HEA	C4D-ND	-3.82	1.31	1.38
28	c	302	9XX	O1-C17	-3.79	1.40	1.47
13	C	302	HEC	CBC-CAC	-3.78	1.35	1.49
24	L	603	HEA	CHD-C4C	3.77	1.47	1.39
24	L	603	HEA	C1A-NA	3.76	1.46	1.39
13	O	302	HEC	CBC-CAC	-3.75	1.35	1.49
24	R	602	HEA	C3A-C2A	3.73	1.45	1.37
24	L	602	HEA	C3A-C2A	3.72	1.45	1.37
24	L	602	HEA	CHD-C1D	3.71	1.45	1.38
24	R	602	HEA	CHD-C1D	3.71	1.45	1.38
28	b	203	9XX	O1-C17	-3.70	1.40	1.47
24	L	603	HEA	C3D-C2D	3.68	1.44	1.36
24	R	603	HEA	C3D-C2D	3.64	1.44	1.36
24	L	602	HEA	C1C-NC	-3.62	1.32	1.39
20	N	601	HEM	C4D-ND	-3.61	1.34	1.40
24	R	602	HEA	C1C-NC	-3.59	1.32	1.39
24	L	602	HEA	C11-C3B	-3.59	1.47	1.51
24	R	602	HEA	C11-C3B	-3.55	1.47	1.51
28	Y	302	9XX	O1-C17	-3.53	1.41	1.47
20	H	902	HEM	C3D-C2D	-3.50	1.29	1.36
20	H	908	HEM	C1B-C2B	-3.47	1.37	1.44
15	I	303	WUO	O13-C12	-3.47	1.37	1.45
20	H	902	HEM	C4D-ND	-3.47	1.34	1.40
20	N	607	HEM	C1B-C2B	-3.47	1.37	1.44
15	I	303	WUO	C44-C43	3.46	1.61	1.52
13	O	301	HEC	CBC-CAC	-3.46	1.36	1.49
13	C	301	HEC	CBC-CAC	-3.46	1.36	1.49
24	L	603	HEA	FE-NA	3.45	2.06	1.95
20	N	601	HEM	C4B-NB	-3.45	1.32	1.38
15	I	303	WUO	O38-C37	-3.43	1.35	1.43
24	L	602	HEA	CHA-C1A	3.41	1.45	1.38
24	R	603	HEA	CHC-C4B	3.40	1.45	1.38
20	N	601	HEM	C1A-NA	-3.39	1.33	1.39
15	I	303	WUO	C50-C37	3.37	1.59	1.52
24	R	602	HEA	CHA-C1A	3.36	1.45	1.38
17	G	903	IZL	C43-C18	3.35	1.59	1.52
24	L	603	HEA	CHC-C4B	3.31	1.45	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	R	602	HEA	O2D-CGD	-3.28	1.20	1.30
24	R	603	HEA	FE-NA	3.28	2.06	1.95
24	L	602	HEA	O2D-CGD	-3.28	1.20	1.30
20	N	601	HEM	C1A-C2A	-3.28	1.38	1.44
24	L	603	HEA	CHA-C4D	3.26	1.46	1.39
24	L	602	HEA	CHA-C4D	3.24	1.46	1.39
24	R	603	HEA	CHA-C4D	3.23	1.46	1.39
24	R	602	HEA	CHA-C4D	3.21	1.46	1.39
20	H	902	HEM	O2A-CGA	-3.19	1.20	1.30
15	I	303	WUO	O77-C76	-3.16	1.38	1.45
20	N	607	HEM	C1D-ND	-3.15	1.32	1.38
20	H	908	HEM	C1D-ND	-3.15	1.32	1.38
17	G	903	IZL	C11-C12	3.10	1.60	1.51
24	L	603	HEA	CHB-C4A	3.08	1.44	1.38
24	R	603	HEA	O2A-CGA	-3.08	1.20	1.30
24	L	603	HEA	O2A-CGA	-3.08	1.20	1.30
17	G	903	IZL	C24-C23	3.06	1.60	1.51
24	L	603	HEA	OMA-CMA	-3.06	1.15	1.22
24	R	603	HEA	CHC-C1C	3.05	1.46	1.39
20	N	601	HEM	C4C-NC	-3.05	1.33	1.39
24	R	603	HEA	CHB-C4A	3.05	1.44	1.38
20	H	902	HEM	C1A-C2A	-3.04	1.38	1.44
17	G	903	IZL	O1-C10	3.04	1.42	1.33
15	I	303	WUO	C17-C16	3.03	1.63	1.52
20	N	607	HEM	C4C-NC	-3.03	1.33	1.39
20	H	908	HEM	C4C-NC	-3.03	1.33	1.39
24	R	603	HEA	OMA-CMA	-3.01	1.15	1.22
20	N	601	HEM	FE-NA	3.01	2.05	1.95
17	M	502	IZL	C25-C30	2.99	1.59	1.52
20	H	908	HEM	O2A-CGA	-2.99	1.20	1.30
20	N	607	HEM	O2A-CGA	-2.97	1.21	1.30
15	I	303	WUO	O45-C44	-2.97	1.35	1.43
17	M	502	IZL	C31-C36	2.96	1.61	1.52
24	L	602	HEA	O2A-CGA	-2.96	1.21	1.30
24	R	602	HEA	O2A-CGA	-2.96	1.21	1.30
24	R	602	HEA	C4A-NA	2.94	1.45	1.39
24	L	603	HEA	CHC-C1C	2.94	1.46	1.39
17	G	903	IZL	C25-C30	2.93	1.59	1.52
24	L	602	HEA	C4A-NA	2.93	1.45	1.39
15	I	303	WUO	P52-O51	2.90	1.68	1.59
15	I	303	WUO	O46-C43	-2.89	1.35	1.43
20	H	902	HEM	C4B-NB	-2.88	1.33	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	R	602	HEA	CHD-C4C	2.85	1.45	1.39
24	L	602	HEA	CHD-C4C	2.84	1.45	1.39
24	L	603	HEA	CHB-C1B	2.84	1.45	1.39
24	R	603	HEA	C4D-C3D	-2.83	1.40	1.45
21	J	501	CDL	OA6-CA4	-2.82	1.40	1.46
24	R	602	HEA	C1B-NB	-2.81	1.33	1.38
24	L	602	HEA	C1B-NB	-2.81	1.33	1.38
17	M	502	IZL	O28-C43	-2.81	1.34	1.44
15	P	302	WUO	C50-C01	2.79	1.58	1.52
24	R	603	HEA	CHB-C1B	2.78	1.45	1.39
24	L	603	HEA	CHA-C1A	2.77	1.43	1.38
20	N	601	HEM	C1C-NC	-2.77	1.34	1.39
24	L	603	HEA	C4D-C3D	-2.76	1.40	1.45
17	M	502	IZL	C43-C18	2.75	1.57	1.52
24	R	603	HEA	C11-C3B	-2.72	1.48	1.51
24	R	603	HEA	O11-C11	-2.72	1.37	1.42
24	L	603	HEA	O11-C11	-2.71	1.37	1.42
15	I	303	WUO	O34-C33	-2.71	1.36	1.43
24	R	603	HEA	CHA-C1A	2.68	1.43	1.38
24	R	602	HEA	CHB-C1B	2.68	1.45	1.39
24	L	602	HEA	CHB-C1B	2.68	1.45	1.39
24	L	603	HEA	C3A-C2A	2.65	1.43	1.37
17	M	502	IZL	C61-C60	2.64	1.58	1.50
15	I	303	WUO	O04-C05	-2.62	1.38	1.44
17	G	903	IZL	C21-C20	2.60	1.59	1.51
20	H	908	HEM	CHA-C1A	-2.60	1.33	1.39
21	J	501	CDL	OB8-CB7	2.60	1.40	1.33
24	R	603	HEA	C3A-C2A	2.59	1.43	1.37
17	M	502	IZL	C29-C28	2.57	1.59	1.52
17	G	903	IZL	C48-C47	2.56	1.58	1.50
17	M	502	IZL	O38-C73	-2.55	1.36	1.43
15	I	303	WUO	O09-C08	-2.55	1.36	1.43
21	J	501	CDL	OB6-CB4	-2.54	1.40	1.46
20	H	908	HEM	O1D-CGD	-2.54	1.13	1.22
17	M	502	IZL	C13-C71	2.54	1.60	1.52
28	c	302	9XX	O-C15	2.54	1.40	1.33
20	N	607	HEM	CHA-C1A	-2.54	1.33	1.39
20	N	601	HEM	C1D-ND	-2.54	1.33	1.38
20	N	607	HEM	C4A-C3A	-2.53	1.37	1.43
20	N	607	HEM	O1D-CGD	-2.52	1.13	1.22
20	H	908	HEM	C4A-C3A	-2.50	1.37	1.43
28	Y	302	9XX	O-C15	2.49	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	J	501	CDL	OB6-CB5	2.49	1.41	1.34
15	I	303	WUO	O04-C03	-2.48	1.35	1.41
13	O	302	HEC	C3D-C2D	-2.48	1.32	1.38
17	G	903	IZL	C61-C60	2.46	1.57	1.50
18	G	904	9YF	C1-C	2.46	1.58	1.50
17	G	903	IZL	C46-C45	2.45	1.58	1.50
15	O	304	WUO	C50-C01	2.45	1.57	1.52
18	M	503	9YF	C1-C	2.45	1.58	1.50
18	b	201	9YF	C1-C	2.45	1.58	1.50
15	I	303	WUO	O40-C39	-2.44	1.35	1.41
17	G	903	IZL	O34-C60	2.44	1.41	1.34
18	W	201	9YF	C1-C	2.44	1.58	1.50
17	M	502	IZL	C48-C47	2.44	1.57	1.50
13	O	301	HEC	CMD-C2D	2.43	1.55	1.50
13	C	301	HEC	CMD-C2D	2.43	1.55	1.50
28	Y	302	9XX	O1-C18	2.43	1.41	1.34
17	M	502	IZL	C24-C23	2.42	1.58	1.51
17	M	502	IZL	O1-C10	2.42	1.40	1.33
17	M	502	IZL	O34-C60	2.40	1.41	1.34
20	N	601	HEM	C4A-C3A	-2.39	1.37	1.43
24	R	603	HEA	C4A-NA	2.38	1.44	1.39
28	c	302	9XX	O1-C18	2.38	1.41	1.34
17	G	903	IZL	O32-C47	2.38	1.40	1.33
13	O	301	HEC	CBB-CAB	-2.37	1.40	1.49
13	C	301	HEC	CBB-CAB	-2.37	1.40	1.49
20	N	601	HEM	C1B-C2B	-2.37	1.39	1.44
17	M	502	IZL	O24-C39	-2.37	1.37	1.43
20	N	607	HEM	C1A-NA	-2.36	1.35	1.39
13	C	302	HEC	C3D-C2D	-2.36	1.32	1.38
15	I	303	WUO	O51-C50	-2.36	1.36	1.44
13	O	302	HEC	CBB-CAB	-2.35	1.40	1.49
28	W	202	9XX	O1-C18	2.35	1.40	1.34
13	O	302	HEC	C3C-C4C	-2.34	1.41	1.46
13	C	302	HEC	CBB-CAB	-2.33	1.40	1.49
20	H	908	HEM	C1A-NA	-2.31	1.35	1.39
20	H	902	HEM	C4A-C3A	-2.31	1.37	1.43
17	M	502	IZL	O37-C72	-2.31	1.37	1.43
24	L	603	HEA	C4A-NA	2.30	1.43	1.39
17	G	903	IZL	C13-C71	2.30	1.59	1.52
24	R	602	HEA	CHB-C4A	2.30	1.42	1.38
28	b	203	9XX	O1-C18	2.29	1.40	1.34
28	b	203	9XX	O-C16	-2.28	1.40	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	J	501	CDL	OA8-CA7	2.28	1.40	1.33
24	L	602	HEA	CHB-C4A	2.26	1.42	1.38
13	C	302	HEC	C3C-C4C	-2.26	1.42	1.46
15	O	304	WUO	C56-C57	2.26	1.57	1.50
15	P	302	WUO	C56-C57	2.25	1.57	1.50
18	M	503	9YF	C24-C	2.24	1.57	1.50
18	b	201	9YF	C24-C	2.23	1.57	1.50
20	H	902	HEM	C4A-NA	-2.23	1.35	1.39
15	C	304	WUO	C56-C57	2.22	1.57	1.50
18	W	201	9YF	C24-C	2.22	1.57	1.50
17	M	502	IZL	C35-C34	2.21	1.58	1.52
17	M	502	IZL	O23-C38	-2.21	1.37	1.43
18	G	904	9YF	C24-C	2.21	1.57	1.50
17	G	903	IZL	C9-C10	2.20	1.57	1.50
24	L	603	HEA	C11-C3B	-2.20	1.48	1.51
28	W	202	9XX	O-C15	2.20	1.39	1.33
17	M	502	IZL	C36-C35	2.18	1.58	1.52
28	Y	302	9XX	O-C16	-2.18	1.40	1.45
17	M	502	IZL	O6-C17	-2.18	1.37	1.43
13	O	301	HEC	C3D-C2D	-2.18	1.33	1.38
13	C	301	HEC	C3D-C2D	-2.18	1.33	1.38
28	W	202	9XX	O-C16	-2.17	1.40	1.45
17	M	502	IZL	O26-C41	-2.17	1.37	1.43
15	I	303	WUO	O40-C41	-2.16	1.39	1.44
24	L	602	HEA	OMA-CMA	-2.16	1.17	1.22
17	M	502	IZL	P-O30	-2.15	1.45	1.55
17	M	502	IZL	O1-C11	-2.15	1.40	1.45
13	C	302	HEC	C3B-C2B	-2.15	1.33	1.41
17	G	903	IZL	C19-C42	2.15	1.58	1.52
24	R	602	HEA	C1A-NA	2.15	1.43	1.39
17	G	903	IZL	O28-C43	-2.13	1.36	1.44
13	O	302	HEC	C3B-C4B	-2.13	1.42	1.46
17	M	502	IZL	O9-C21	-2.13	1.40	1.43
24	L	602	HEA	C1A-NA	2.13	1.43	1.39
13	O	302	HEC	C3B-C2B	-2.12	1.34	1.41
21	J	501	CDL	OA8-CA6	-2.11	1.40	1.45
15	C	304	WUO	C50-C01	2.11	1.56	1.52
20	N	601	HEM	C4A-NA	-2.11	1.35	1.39
24	R	602	HEA	OMA-CMA	-2.09	1.17	1.22
20	N	607	HEM	C2A-C3A	-2.09	1.33	1.38
20	H	908	HEM	C2A-C3A	-2.09	1.33	1.38
18	b	201	9YF	C4-C3	2.09	1.57	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	M	502	IZL	O12-C26	-2.08	1.39	1.44
17	M	502	IZL	C33-C32	2.08	1.58	1.51
20	N	601	HEM	O1A-CGA	-2.08	1.15	1.22
15	I	303	WUO	P52-O55	2.07	1.67	1.59
18	W	201	9YF	C4-C3	2.07	1.57	1.52
28	c	302	9XX	O-C16	-2.06	1.40	1.45
20	H	902	HEM	C1B-C2B	-2.05	1.40	1.44
21	J	501	CDL	OA6-CA5	2.05	1.40	1.34
15	O	304	WUO	O51-C50	-2.04	1.37	1.44
17	G	903	IZL	C31-C36	2.04	1.58	1.52
28	b	203	9XX	O-C15	2.03	1.39	1.33
13	C	302	HEC	C3C-C2C	-2.03	1.34	1.41
24	R	602	HEA	CHC-C1C	2.02	1.44	1.39
15	P	302	WUO	O51-C50	-2.02	1.37	1.44
13	O	302	HEC	C3C-C2C	-2.02	1.34	1.41
17	G	903	IZL	C15-C14	2.02	1.57	1.52
17	M	502	IZL	C42-C41	2.01	1.57	1.52
17	G	903	IZL	C22-C39	2.01	1.58	1.52
15	C	304	WUO	O51-C50	-2.01	1.37	1.44

All (366) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	H	902	HEM	CBC-CAC-C3C	10.38	179.40	127.53
13	C	302	HEC	CBB-CAB-C3B	-9.03	109.38	127.43
13	O	302	HEC	CBB-CAB-C3B	-8.75	109.95	127.43
13	O	301	HEC	CBB-CAB-C3B	-8.36	110.72	127.43
13	C	301	HEC	CBB-CAB-C3B	-8.36	110.72	127.43
20	H	902	HEM	C4C-C3C-C2C	7.33	113.17	106.81
20	H	902	HEM	O2A-CGA-O1A	-6.32	107.08	123.33
20	N	601	HEM	O2A-CGA-O1A	-6.30	107.12	123.33
24	R	602	HEA	C3C-C2C-C1C	-6.02	100.07	107.17
24	L	602	HEA	C3C-C2C-C1C	-5.98	100.12	107.17
28	W	202	9XX	O1-C18-C19	5.92	124.29	111.48
24	L	602	HEA	C1D-C2D-C3D	-5.83	100.85	106.98
24	R	602	HEA	C1D-C2D-C3D	-5.81	100.87	106.98
20	N	607	HEM	O2D-CGD-O1D	-5.80	108.40	123.33
20	H	908	HEM	O2D-CGD-O1D	-5.75	108.53	123.33
24	R	603	HEA	C12-C13-C14	-5.67	97.27	112.16
20	H	902	HEM	O2D-CGD-O1D	-5.61	108.89	123.33
20	N	601	HEM	CHC-C4B-NB	5.58	130.43	124.42
17	M	502	IZL	O10-C23-C24	5.46	117.53	106.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	R	603	HEA	C3C-C2C-C1C	-5.40	100.80	107.17
24	L	602	HEA	C2B-C1B-NB	5.39	116.14	109.90
24	R	602	HEA	C2B-C1B-NB	5.34	116.08	109.90
20	H	908	HEM	C1B-NB-C4B	5.29	111.47	105.21
20	N	607	HEM	O2D-CGD-CBD	5.27	130.66	114.00
20	H	908	HEM	O2D-CGD-CBD	5.26	130.63	114.00
24	L	603	HEA	C3C-C2C-C1C	-5.25	100.98	107.17
20	N	607	HEM	C1B-NB-C4B	5.25	111.42	105.21
20	H	902	HEM	CHD-C1D-ND	5.23	130.05	124.42
24	L	602	HEA	C2D-C1D-ND	4.80	115.36	109.84
24	R	602	HEA	C2D-C1D-ND	4.76	115.31	109.84
20	H	902	HEM	CBA-CAA-C2A	-4.73	99.44	112.53
20	H	908	HEM	O2A-CGA-CBA	4.72	128.91	114.00
20	N	607	HEM	O2A-CGA-CBA	4.71	128.88	114.00
24	R	602	HEA	C2C-C1C-NC	4.71	117.69	110.14
24	L	602	HEA	C2C-C1C-NC	4.70	117.67	110.14
24	R	603	HEA	O11-C11-C12	-4.67	96.75	109.14
17	G	903	IZL	O10-C23-C24	4.62	115.86	106.69
20	H	902	HEM	CHD-C4C-NC	4.61	129.48	124.45
15	I	303	WUO	C03-O04-C05	4.56	122.63	113.72
24	L	603	HEA	C2B-C1B-NB	4.54	115.15	109.90
24	L	602	HEA	CAD-CBD-CGD	-4.53	101.65	113.67
24	R	602	HEA	CAD-CBD-CGD	-4.50	101.72	113.67
24	R	603	HEA	C2B-C1B-NB	4.48	115.09	109.90
20	N	601	HEM	C4C-C3C-C2C	4.47	110.69	106.81
20	N	601	HEM	C4C-NC-C1C	4.40	112.99	105.82
24	R	603	HEA	CMD-C2D-C1D	4.40	131.91	125.03
13	C	301	HEC	CBC-CAC-C3C	-4.39	118.66	127.43
13	O	301	HEC	CBC-CAC-C3C	-4.39	118.67	127.43
20	H	902	HEM	CMD-C2D-C1D	4.37	131.86	125.03
24	L	603	HEA	CMD-C2D-C1D	4.32	131.79	125.03
20	N	601	HEM	C1B-NB-C4B	4.30	110.30	105.21
15	C	304	WUO	O54-P52-O53	4.28	132.36	112.44
15	O	304	WUO	O54-P52-O53	4.27	132.32	112.44
24	R	603	HEA	C3D-C4D-ND	4.27	114.48	110.35
15	P	302	WUO	O54-P52-O53	4.26	132.25	112.44
18	W	201	9YF	C7-C2-C3	-4.25	104.97	110.86
18	b	201	9YF	C7-C2-C3	-4.24	104.97	110.86
20	N	601	HEM	O2D-CGD-O1D	-4.22	112.47	123.33
20	H	902	HEM	CHC-C1C-NC	4.22	129.05	124.45
24	L	603	HEA	O11-C11-C12	-4.21	97.97	109.14
20	H	902	HEM	CAC-C3C-C2C	-4.20	114.77	128.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	H	908	HEM	O2A-CGA-O1A	-4.20	112.53	123.33
20	N	607	HEM	O2A-CGA-O1A	-4.20	112.54	123.33
18	M	503	9YF	O1-P-O8	4.17	131.85	112.44
28	Y	302	9XX	O1-C18-C19	4.17	120.49	111.48
18	G	904	9YF	O1-P-O8	4.16	131.81	112.44
18	b	201	9YF	O1-P-O8	4.15	131.76	112.44
24	R	602	HEA	C3C-C4C-NC	4.15	113.30	109.80
18	W	201	9YF	O1-P-O8	4.15	131.75	112.44
24	L	603	HEA	C3B-C4B-NB	4.14	114.60	109.84
24	L	602	HEA	C3C-C4C-NC	4.11	113.26	109.80
18	M	503	9YF	C7-C2-C3	-4.04	105.26	110.86
28	c	302	9XX	O1-C18-C19	4.03	120.20	111.48
18	G	904	9YF	C7-C2-C3	-4.03	105.27	110.86
24	R	602	HEA	C3B-C4B-NB	4.02	114.46	109.84
24	L	602	HEA	C3B-C4B-NB	4.02	114.46	109.84
20	H	902	HEM	O2D-CGD-CBD	4.00	126.64	114.00
21	J	501	CDL	OB6-CB5-C51	3.98	120.10	111.48
17	M	502	IZL	O34-C60-C61	3.95	120.02	111.48
24	L	602	HEA	CMB-C2B-C1B	3.94	131.19	125.03
24	R	603	HEA	C26-C15-C16	3.94	122.06	115.23
24	L	603	HEA	C4B-C3B-C2B	-3.93	100.83	107.44
20	H	902	HEM	C2A-C1A-NA	-3.91	105.81	110.15
24	R	602	HEA	CMB-C2B-C1B	3.91	131.14	125.03
15	I	303	WUO	O54-P52-O53	3.90	130.59	112.44
24	R	602	HEA	C1B-C2B-C3B	-3.90	102.28	106.80
24	L	602	HEA	C1B-C2B-C3B	-3.90	102.28	106.80
24	R	603	HEA	C26-C15-C14	-3.90	113.61	123.63
21	J	501	CDL	OA6-CA5-C11	3.88	119.88	111.48
24	R	603	HEA	C4A-C3A-C2A	3.87	110.17	106.81
24	L	603	HEA	C3D-C4D-ND	3.85	114.08	110.35
24	L	603	HEA	C4A-C3A-C2A	3.81	110.12	106.81
24	L	602	HEA	C3D-C4D-ND	3.77	113.99	110.35
15	I	303	WUO	O77-C76-C57	3.76	119.23	108.40
15	I	303	WUO	O09-C08-C03	-3.75	101.13	110.08
20	N	601	HEM	C2A-C1A-NA	-3.72	106.02	110.15
24	R	602	HEA	C3D-C4D-ND	3.71	113.94	110.35
24	R	603	HEA	C12-C11-C3B	-3.68	106.36	112.12
20	N	601	HEM	O2A-CGA-CBA	3.66	125.57	114.00
20	N	601	HEM	CHD-C4C-NC	3.65	128.42	124.45
15	P	302	WUO	O77-C76-C57	3.63	118.86	108.40
24	R	602	HEA	O2A-CGA-CBA	3.60	125.38	114.00
28	b	203	9XX	O1-C18-C19	3.60	119.27	111.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	R	603	HEA	C4B-C3B-C2B	-3.59	101.40	107.44
20	H	902	HEM	C4C-CHD-C1D	-3.59	118.39	126.02
15	O	304	WUO	O77-C76-C57	3.58	118.72	108.40
24	L	602	HEA	O2A-CGA-CBA	3.57	125.29	114.00
15	C	304	WUO	O77-C76-C57	3.57	118.70	108.40
24	L	602	HEA	C21-C20-C19	3.54	124.92	113.19
20	H	902	HEM	CAD-C3D-C2D	-3.54	121.24	127.87
24	R	602	HEA	O2A-CGA-O1A	-3.53	114.25	123.33
24	R	603	HEA	C3B-C4B-NB	3.53	113.90	109.84
24	L	602	HEA	O2A-CGA-O1A	-3.52	114.27	123.33
17	M	502	IZL	O11-C25-C30	3.50	114.94	108.31
20	H	902	HEM	C4B-C3B-C2B	-3.50	104.07	107.28
17	M	502	IZL	C21-O9-C22	3.39	121.06	113.80
21	J	501	CDL	OA8-CA7-C31	3.39	122.16	111.83
20	H	908	HEM	C3B-C2B-C1B	3.37	108.94	106.41
15	C	304	WUO	C03-O02-C01	3.36	125.95	117.98
24	L	603	HEA	CMC-C2C-C1C	3.35	130.52	125.42
24	R	603	HEA	O2D-CGD-CBD	3.34	124.56	114.00
24	L	603	HEA	O2D-CGD-CBD	3.31	124.45	114.00
20	N	607	HEM	C3B-C2B-C1B	3.30	108.89	106.41
20	H	908	HEM	C3B-C4B-NB	-3.29	107.10	109.47
17	G	903	IZL	O34-C60-C61	3.29	118.61	111.48
24	R	603	HEA	CHB-C1B-C2B	-3.29	119.83	125.03
20	H	902	HEM	C4C-NC-C1C	3.28	111.17	105.82
24	R	603	HEA	CMC-C2C-C1C	3.27	130.40	125.42
20	N	607	HEM	CHA-C4D-ND	3.26	128.40	124.37
13	O	302	HEC	O1D-CGD-CBD	-3.26	112.76	123.09
17	G	903	IZL	O1-C11-C12	3.26	115.29	108.41
24	L	603	HEA	C2C-C1C-NC	3.26	115.36	110.14
20	N	607	HEM	C3B-C4B-NB	-3.24	107.14	109.47
20	H	908	HEM	CHA-C4D-ND	3.23	128.36	124.37
13	C	302	HEC	O1D-CGD-CBD	-3.23	112.86	123.09
20	H	902	HEM	CHD-C1D-C2D	-3.22	119.94	125.03
17	G	903	IZL	C24-O11-C25	3.21	120.68	113.80
24	R	603	HEA	C13-C14-C15	3.21	134.96	127.62
24	L	603	HEA	CHA-C1A-NA	-3.20	120.96	124.45
24	L	603	HEA	C1D-C2D-C3D	-3.20	103.61	106.98
24	R	602	HEA	CBA-CAA-C2A	-3.19	103.73	112.53
24	L	602	HEA	CMD-C2D-C1D	3.18	130.01	125.03
24	R	602	HEA	CMD-C2D-C1D	3.18	130.00	125.03
15	O	304	WUO	C03-O02-C01	3.18	125.50	117.98
24	L	602	HEA	O11-C11-C3B	-3.16	105.46	111.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	L	602	HEA	CBA-CAA-C2A	-3.16	103.80	112.53
24	R	602	HEA	O11-C11-C3B	-3.16	105.47	111.26
13	O	302	HEC	CBC-CAC-C3C	-3.16	121.13	127.43
24	R	603	HEA	C2C-C1C-NC	3.15	115.19	110.14
15	P	302	WUO	C03-O02-C01	3.15	125.44	117.98
15	O	304	WUO	O04-C05-C12	3.13	112.91	106.69
15	P	302	WUO	O04-C05-C12	3.12	112.88	106.69
24	R	603	HEA	C1C-CHC-C4B	3.11	133.57	126.25
24	L	603	HEA	CHB-C1B-C2B	-3.11	120.12	125.03
24	R	603	HEA	CHA-C1A-NA	-3.11	121.07	124.45
20	N	607	HEM	C4C-NC-C1C	3.11	110.89	105.82
15	C	304	WUO	O04-C05-C12	3.10	112.85	106.69
20	H	908	HEM	C4C-NC-C1C	3.10	110.88	105.82
13	C	302	HEC	CBC-CAC-C3C	-3.09	121.26	127.43
24	R	603	HEA	C1D-C2D-C3D	-3.06	103.76	106.98
28	c	302	9XX	O-C15-C14	3.05	121.13	111.83
20	N	601	HEM	C3B-C4B-NB	-3.05	107.28	109.47
24	L	602	HEA	CHA-C1A-NA	-3.03	121.15	124.45
20	H	902	HEM	CAC-C3C-C4C	3.03	132.06	124.82
24	R	602	HEA	CHA-C1A-NA	-3.03	121.16	124.45
17	M	502	IZL	O28-P-O29	-3.01	100.18	109.81
24	R	603	HEA	CHA-C4D-C3D	-2.99	120.41	124.77
15	I	303	WUO	C39-O40-C41	2.96	119.50	113.72
17	M	502	IZL	O11-C24-C23	2.96	116.08	109.42
15	I	303	WUO	O45-C44-C39	-2.95	103.04	110.08
15	I	303	WUO	C03-O02-C01	2.94	124.95	117.98
24	L	603	HEA	C1C-CHC-C4B	2.93	133.14	126.25
24	R	603	HEA	C1B-C2B-C3B	-2.93	103.40	106.80
24	L	603	HEA	CHC-C4B-NB	-2.90	120.78	124.37
15	P	302	WUO	C03-O04-C05	2.89	119.36	113.72
15	P	302	WUO	O40-C41-C42	2.88	114.89	109.70
28	Y	302	9XX	O-C15-C14	2.88	120.61	111.83
28	b	203	9XX	O-C15-C14	2.86	120.55	111.83
17	M	502	IZL	O1-C11-C12	2.85	114.43	108.41
20	H	902	HEM	CAA-C2A-C1A	-2.85	119.37	124.94
15	C	304	WUO	C03-O04-C05	2.83	119.25	113.72
24	R	603	HEA	C3A-C2A-C1A	-2.83	104.37	107.05
20	H	902	HEM	C4A-NA-C1A	2.83	110.43	105.82
15	O	304	WUO	O55-P52-O53	-2.82	97.74	108.94
24	R	603	HEA	C13-C12-C11	2.82	118.91	114.39
20	N	601	HEM	CBA-CAA-C2A	-2.81	104.76	112.53
24	R	603	HEA	O2D-CGD-O1D	-2.81	116.11	123.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	P	302	WUO	O55-P52-O53	-2.80	97.83	108.94
24	R	603	HEA	C17-C18-C19	-2.80	121.21	127.62
15	O	304	WUO	O40-C41-C42	2.80	114.74	109.70
15	C	304	WUO	O55-P52-O53	-2.80	97.85	108.94
24	L	603	HEA	C3A-C2A-C1A	-2.78	104.41	107.05
15	C	304	WUO	O40-C41-C42	2.78	114.70	109.70
14	T	1301	MQ9	C7-C6-C5	-2.77	120.14	124.89
20	H	908	HEM	C3A-C4A-NA	-2.77	105.70	110.14
20	N	607	HEM	C3A-C4A-NA	-2.76	105.71	110.14
24	L	603	HEA	O2D-CGD-O1D	-2.76	116.23	123.33
20	N	607	HEM	C1D-C2D-C3D	-2.75	104.09	106.98
24	L	603	HEA	C26-C15-C16	2.74	119.98	115.23
20	H	902	HEM	CAD-CBD-CGD	-2.74	106.40	113.67
15	O	304	WUO	C03-O04-C05	2.73	119.06	113.72
24	R	602	HEA	CMC-C2C-C3C	2.72	132.96	126.55
24	L	602	HEA	CMC-C2C-C3C	2.72	132.96	126.55
20	H	908	HEM	C1D-C2D-C3D	-2.72	104.11	106.98
15	I	303	WUO	O40-C41-C48	2.72	113.17	106.44
24	R	603	HEA	CHC-C4B-NB	-2.71	121.01	124.37
24	L	603	HEA	CHA-C4D-C3D	-2.71	120.82	124.77
20	N	607	HEM	C4B-C3B-C2B	-2.71	104.79	107.28
20	H	908	HEM	C4B-C3B-C2B	-2.71	104.79	107.28
20	H	902	HEM	CAD-C3D-C4D	2.70	129.41	124.70
13	C	302	HEC	CBA-CAA-C2A	-2.69	105.09	112.53
20	N	601	HEM	CMD-C2D-C1D	2.69	129.24	125.03
24	L	602	HEA	C13-C12-C11	-2.69	110.10	114.39
13	O	302	HEC	CBA-CAA-C2A	-2.69	105.10	112.53
20	N	601	HEM	CAD-C3D-C4D	2.68	129.37	124.70
24	R	602	HEA	CHC-C1C-C2C	-2.66	119.70	127.43
24	L	602	HEA	CHC-C1C-C2C	-2.66	119.71	127.43
20	N	607	HEM	CHB-C1B-NB	2.66	127.66	124.37
24	R	602	HEA	C13-C12-C11	-2.65	110.15	114.39
20	N	607	HEM	CHD-C1D-ND	2.65	127.28	124.42
20	H	908	HEM	CHD-C1D-ND	2.65	127.28	124.42
24	R	603	HEA	C27-C19-C20	2.65	119.83	115.23
20	H	908	HEM	CHB-C1B-NB	2.64	127.64	124.37
24	R	602	HEA	C26-C15-C16	2.64	119.81	115.23
15	C	304	WUO	O58-C57-C76	2.64	117.81	108.34
24	R	603	HEA	CAA-C2A-C1A	2.63	130.20	124.85
20	H	902	HEM	CHA-C1A-NA	2.62	128.62	123.86
15	O	304	WUO	O58-C57-C76	2.62	117.74	108.34
15	P	302	WUO	O58-C57-C76	2.62	117.73	108.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	C	303	MQ9	C7-C6-C5	-2.61	120.42	124.89
17	G	903	IZL	O32-C47-C48	2.60	119.76	111.83
17	G	903	IZL	C21-O9-C22	2.60	119.36	113.80
24	L	603	HEA	C1B-C2B-C3B	-2.59	103.79	106.80
14	O	303	MQ9	C7-C6-C5	-2.59	120.45	124.89
24	R	602	HEA	CHB-C4A-NA	-2.58	121.65	124.45
24	L	602	HEA	C25-C23-C24	2.57	120.50	114.59
24	L	602	HEA	CHB-C4A-NA	-2.57	121.66	124.45
24	R	603	HEA	C4D-C3D-C2D	-2.56	103.17	106.89
13	C	302	HEC	O1A-CGA-CBA	-2.56	114.98	123.09
14	N	605	MQ9	C7-C6-C5	-2.55	120.51	124.89
17	M	502	IZL	O30-P-O29	2.54	124.28	112.44
17	G	903	IZL	O11-C24-C23	2.54	115.14	109.42
15	C	304	WUO	O38-C37-C50	2.53	113.86	107.42
24	L	603	HEA	CAA-C2A-C1A	2.53	130.00	124.85
14	H	906	MQ9	C7-C6-C5	-2.53	120.55	124.89
15	O	304	WUO	O38-C37-C50	2.53	113.83	107.42
28	W	202	9XX	O1-C18-O2	-2.52	117.80	123.70
15	I	303	WUO	C48-C41-C42	-2.52	106.84	113.02
17	M	502	IZL	O32-C47-C48	2.52	119.50	111.83
17	G	903	IZL	O28-P-O29	-2.51	101.79	109.81
13	O	302	HEC	O1A-CGA-CBA	-2.50	115.15	123.09
17	M	502	IZL	C31-O17-C32	2.49	118.59	113.72
28	W	202	9XX	O-C15-C14	2.49	119.44	111.83
14	H	907	MQ9	C7-C6-C5	-2.49	120.62	124.89
17	G	903	IZL	O1-C10-C9	2.49	119.43	111.83
14	N	606	MQ9	C7-C6-C5	-2.49	120.62	124.89
20	H	902	HEM	CHD-C4C-C3C	2.48	129.39	125.21
14	N	608	MQ9	C7-C6-C5	-2.48	120.64	124.89
14	H	909	MQ9	C7-C6-C5	-2.48	120.64	124.89
15	I	303	WUO	O51-C50-C01	2.48	114.03	108.76
24	R	603	HEA	CHB-C4A-NA	-2.47	121.76	124.45
17	M	502	IZL	O1-C10-C9	2.47	119.36	111.83
15	C	304	WUO	O51-C50-C01	2.47	114.01	108.76
13	C	301	HEC	O1D-CGD-CBD	-2.47	115.27	123.09
14	M	505	MQ9	C7-C6-C5	-2.46	120.67	124.89
13	O	301	HEC	O1D-CGD-CBD	-2.46	115.30	123.09
14	G	901	MQ9	C7-C6-C5	-2.45	120.69	124.89
15	P	302	WUO	O38-C37-C50	2.45	113.63	107.42
24	L	603	HEA	C27-C19-C20	2.44	119.47	115.23
20	N	601	HEM	C4A-NA-C1A	2.43	109.78	105.82
24	L	602	HEA	C26-C15-C16	2.41	119.42	115.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	L	603	HEA	C4D-C3D-C2D	-2.41	103.39	106.89
13	C	301	HEC	CBD-CAD-C3D	2.38	119.11	112.53
13	O	301	HEC	CBD-CAD-C3D	2.37	119.10	112.53
24	L	602	HEA	C4B-C3B-C2B	-2.37	103.45	107.44
21	J	501	CDL	OB8-CB7-C71	2.37	119.05	111.83
15	I	303	WUO	O36-C35-C37	-2.37	103.87	109.94
24	R	602	HEA	C4B-C3B-C2B	-2.36	103.47	107.44
13	C	302	HEC	CAD-CBD-CGD	2.36	119.93	113.67
13	O	302	HEC	CHC-C4B-NB	2.35	127.02	124.45
14	K	1301	MQ9	C7-C6-C5	-2.35	120.87	124.89
13	O	302	HEC	CAD-CBD-CGD	2.35	119.89	113.67
24	L	603	HEA	CHB-C4A-NA	-2.34	121.90	124.45
20	H	902	HEM	CMA-C3A-C2A	2.34	130.58	125.62
20	H	902	HEM	CHB-C1B-NB	2.34	127.26	124.37
24	R	603	HEA	C4C-CHD-C1D	2.33	131.72	126.25
17	G	903	IZL	O30-P-O29	2.33	123.26	112.44
24	R	602	HEA	C25-C23-C24	2.32	119.94	114.59
20	N	601	HEM	CMC-C2C-C1C	2.32	128.81	124.73
17	M	502	IZL	C24-O11-C25	2.31	118.76	113.80
20	N	607	HEM	CHD-C1D-C2D	-2.31	121.38	125.03
20	H	908	HEM	CHD-C1D-C2D	-2.31	121.38	125.03
17	M	502	IZL	O1-C10-O	-2.31	117.85	123.63
28	b	203	9XX	O1-C17-C16	2.31	111.52	106.21
20	H	908	HEM	CHC-C4B-NB	2.28	126.88	124.42
20	H	908	HEM	C2A-C1A-NA	-2.28	107.62	110.15
17	G	903	IZL	O1-C10-O	-2.28	117.93	123.63
15	I	303	WUO	O55-P52-O53	-2.28	99.91	108.94
24	L	602	HEA	CHB-C1B-C2B	-2.27	121.44	125.03
20	N	607	HEM	C2A-C1A-NA	-2.26	107.64	110.15
28	W	202	9XX	C37-C17-C16	-2.26	106.33	112.69
15	O	304	WUO	O51-C50-C01	2.26	113.57	108.76
24	R	602	HEA	CHB-C1B-C2B	-2.26	121.46	125.03
24	R	603	HEA	O2A-CGA-CBA	2.24	121.08	114.00
20	N	607	HEM	CHC-C4B-NB	2.24	126.83	124.42
15	O	304	WUO	O13-C12-C05	2.23	113.11	108.41
20	N	607	HEM	CHA-C1A-NA	2.23	127.90	123.86
20	H	908	HEM	CHA-C1A-NA	2.23	127.89	123.86
17	G	903	IZL	O2-C12-C11	2.22	111.10	106.69
15	C	304	WUO	O13-C12-C05	2.22	113.10	108.41
24	L	603	HEA	O2A-CGA-CBA	2.21	120.99	114.00
15	P	302	WUO	O13-C12-C05	2.21	113.07	108.41
14	K	1301	MQ9	C17-C16-C14	2.21	120.49	113.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	O	304	WUO	O40-C41-C48	2.20	111.89	106.44
17	M	502	IZL	O25-C40-C20	-2.20	103.91	109.32
24	L	603	HEA	C4C-CHD-C1D	2.20	131.41	126.25
15	P	302	WUO	O40-C41-C48	2.20	111.88	106.44
15	C	304	WUO	O40-C41-C48	2.19	111.87	106.44
24	L	602	HEA	C20-C19-C18	2.18	126.06	121.17
13	O	301	HEC	O1A-CGA-CBA	-2.18	116.18	123.09
13	C	301	HEC	O1A-CGA-CBA	-2.17	116.19	123.09
15	O	304	WUO	C39-O40-C41	2.17	117.96	113.72
17	M	502	IZL	O17-C32-C33	2.17	111.82	106.44
13	C	302	HEC	CHC-C4B-NB	2.17	126.81	124.45
15	P	302	WUO	C39-O40-C41	2.17	117.95	113.72
13	C	302	HEC	C1D-C2D-C3D	2.16	109.30	106.82
20	H	902	HEM	CHC-C4B-NB	2.14	126.73	124.42
24	R	602	HEA	C25-C23-C22	-2.14	116.23	122.66
17	M	502	IZL	O34-C60-O35	-2.14	118.70	123.70
20	H	902	HEM	CMB-C2B-C1B	2.14	128.37	125.03
20	N	607	HEM	CHA-C4D-C3D	-2.13	121.29	125.23
15	C	304	WUO	C39-O40-C41	2.12	117.87	113.72
20	H	908	HEM	CHA-C4D-C3D	-2.12	121.32	125.23
17	M	502	IZL	O16-C31-O17	-2.11	105.13	110.69
17	G	903	IZL	O11-C25-C30	2.11	112.31	108.31
24	R	602	HEA	C4A-NA-C1A	-2.11	102.38	105.82
17	M	502	IZL	O16-C31-C36	2.11	113.28	108.09
20	N	601	HEM	CMA-C3A-C4A	2.10	128.62	125.42
15	P	302	WUO	O45-C44-C39	-2.10	105.06	110.08
24	L	602	HEA	C4A-NA-C1A	-2.10	102.40	105.82
15	I	303	WUO	O38-C37-C50	2.10	112.75	107.42
15	I	303	WUO	O77-C78-C80	2.10	118.22	111.83
15	P	302	WUO	O51-C50-C01	2.09	113.21	108.76
21	J	501	CDL	C32-C31-CA7	-2.08	106.07	113.69
24	L	603	HEA	C17-C18-C19	-2.08	122.87	127.62
15	O	304	WUO	O45-C44-C39	-2.08	105.13	110.08
15	C	304	WUO	O45-C44-C39	-2.06	105.16	110.08
20	H	902	HEM	C1A-C2A-C3A	2.06	110.06	106.87
15	P	302	WUO	O58-C59-C61	2.06	115.93	111.48
20	H	902	HEM	CHB-C1B-C2B	-2.05	121.11	126.95
24	L	603	HEA	CHB-C4A-C3A	2.05	128.66	125.21
17	M	502	IZL	O32-C46-C45	2.04	114.28	108.40
24	R	602	HEA	C27-C19-C20	2.04	118.77	115.23
15	I	303	WUO	O51-P52-O53	-2.04	103.30	109.81
15	O	304	WUO	O58-C59-C61	2.03	115.88	111.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	N	601	HEM	CHA-C1A-NA	2.03	127.55	123.86
24	L	602	HEA	CHD-C1D-C2D	-2.03	121.17	126.95
15	I	303	WUO	O40-C41-C42	2.03	113.36	109.70
17	G	903	IZL	O8-C20-C21	2.03	110.71	106.69
15	C	304	WUO	O58-C59-C61	2.02	115.86	111.48
24	R	603	HEA	CHB-C4A-C3A	2.02	128.61	125.21
18	b	201	9YF	O6-C6-C7	-2.01	105.63	110.38
20	N	607	HEM	CMA-C3A-C4A	2.01	128.47	125.42
13	C	302	HEC	C2D-C1D-ND	-2.00	106.93	110.14
15	I	303	WUO	O13-C14-O15	-2.00	118.62	123.63
24	R	602	HEA	CHD-C1D-C2D	-2.00	121.26	126.95

There are no chirality outliers.

All (1640) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
13	O	301	HEC	C2B-C3B-CAB-CBB
13	O	301	HEC	C4B-C3B-CAB-CBB
13	O	301	HEC	C2C-C3C-CAC-CBC
13	O	301	HEC	C4C-C3C-CAC-CBC
13	O	302	HEC	C2C-C3C-CAC-CBC
13	O	302	HEC	C4C-C3C-CAC-CBC
13	C	301	HEC	C2B-C3B-CAB-CBB
13	C	301	HEC	C4B-C3B-CAB-CBB
13	C	301	HEC	C2C-C3C-CAC-CBC
13	C	301	HEC	C4C-C3C-CAC-CBC
13	C	302	HEC	C2C-C3C-CAC-CBC
13	C	302	HEC	C4C-C3C-CAC-CBC
14	M	505	MQ9	C12-C13-C14-C15
14	M	505	MQ9	C32-C33-C34-C35
14	M	505	MQ9	C32-C33-C34-C36
14	M	505	MQ9	C35-C34-C36-C37
14	N	605	MQ9	C7-C8-C9-C10
14	N	605	MQ9	C7-C8-C9-C11
14	N	605	MQ9	C18-C19-C21-C22
14	N	605	MQ9	C20-C19-C21-C22
14	N	606	MQ9	C7-C8-C9-C11
14	N	606	MQ9	C17-C18-C19-C20
14	N	606	MQ9	C17-C18-C19-C21
14	N	606	MQ9	C32-C33-C34-C35
14	N	606	MQ9	C32-C33-C34-C36
14	N	608	MQ9	C7-C8-C9-C10

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Mol	Chain	Res	Type	Atoms
14	N	608	MQ9	C7-C8-C9-C11
14	N	608	MQ9	C12-C13-C14-C16
14	N	608	MQ9	C17-C18-C19-C20
14	N	608	MQ9	C22-C23-C24-C25
14	N	608	MQ9	C22-C23-C24-C26
14	N	608	MQ9	C27-C28-C29-C30
14	N	608	MQ9	C27-C28-C29-C31
14	N	608	MQ9	C37-C38-C39-C40
14	N	608	MQ9	C37-C38-C39-C41
14	T	1301	MQ9	C17-C18-C19-C20
14	T	1301	MQ9	C17-C18-C19-C21
14	T	1301	MQ9	C22-C23-C24-C25
14	T	1301	MQ9	C22-C23-C24-C26
14	T	1301	MQ9	C27-C28-C29-C30
14	T	1301	MQ9	C27-C28-C29-C31
14	G	901	MQ9	C12-C13-C14-C15
14	G	901	MQ9	C12-C13-C14-C16
14	G	901	MQ9	C32-C33-C34-C35
14	G	901	MQ9	C32-C33-C34-C36
14	G	901	MQ9	C35-C34-C36-C37
14	H	906	MQ9	C7-C8-C9-C10
14	H	906	MQ9	C7-C8-C9-C11
14	H	906	MQ9	C18-C19-C21-C22
14	H	906	MQ9	C20-C19-C21-C22
14	H	907	MQ9	C7-C8-C9-C11
14	H	907	MQ9	C17-C18-C19-C20
14	H	907	MQ9	C17-C18-C19-C21
14	H	907	MQ9	C32-C33-C34-C35
14	H	907	MQ9	C32-C33-C34-C36
14	H	909	MQ9	C7-C8-C9-C10
14	H	909	MQ9	C7-C8-C9-C11
14	H	909	MQ9	C12-C13-C14-C16
14	H	909	MQ9	C17-C18-C19-C20
14	H	909	MQ9	C22-C23-C24-C25
14	H	909	MQ9	C22-C23-C24-C26
14	H	909	MQ9	C27-C28-C29-C30
14	H	909	MQ9	C27-C28-C29-C31
14	H	909	MQ9	C37-C38-C39-C40
14	H	909	MQ9	C37-C38-C39-C41
14	K	1301	MQ9	C7-C8-C9-C10
14	K	1301	MQ9	C7-C8-C9-C11
14	K	1301	MQ9	C17-C18-C19-C20

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Mol	Chain	Res	Type	Atoms
14	K	1301	MQ9	C17-C18-C19-C21
14	K	1301	MQ9	C25-C24-C26-C27
15	O	304	WUO	C61-C59-O58-C57
15	C	304	WUO	C61-C59-O58-C57
15	C	304	WUO	O60-C59-O58-C57
15	C	304	WUO	C86-C87-C88-C89
15	I	303	WUO	C16-C14-O13-C12
17	M	502	IZL	O31-C44-C45-O34
17	M	502	IZL	C48-C47-O32-C46
17	M	502	IZL	C43-O28-P-O30
17	G	903	IZL	O-C10-O1-C11
17	G	903	IZL	C9-C10-O1-C11
17	G	903	IZL	C18-C43-O28-P
17	G	903	IZL	C48-C47-O32-C46
17	G	903	IZL	O33-C47-O32-C46
17	G	903	IZL	C43-O28-P-O31
18	M	503	9YF	C1-O-P-O1
18	M	503	9YF	C26-C25-O11-C24
18	M	503	9YF	O12-C25-O11-C24
18	W	201	9YF	C2-O2-P-O
18	W	201	9YF	C1-O-P-O1
18	W	201	9YF	C9-C8-O9-C
18	W	201	9YF	O10-C8-O9-C
18	G	904	9YF	C1-O-P-O1
18	G	904	9YF	C26-C25-O11-C24
18	b	201	9YF	C2-O2-P-O
18	b	201	9YF	C1-O-P-O1
18	b	201	9YF	C9-C8-O9-C
18	b	201	9YF	O10-C8-O9-C
19	M	504	7PH	C1-O11-P-O12
19	M	504	7PH	C1-O11-P-O13
19	N	609	7PH	C1-O11-P-O12
19	N	609	7PH	C1-O11-P-O13
19	N	609	7PH	C1-O11-P-O14
19	G	905	7PH	C1-O11-P-O12
19	G	905	7PH	C1-O11-P-O13
19	H	901	7PH	C1-O11-P-O12
19	H	901	7PH	C1-O11-P-O13
19	H	901	7PH	C1-O11-P-O14
21	N	602	CDL	CA2-C1-CB2-OB2
21	N	602	CDL	C11-CA5-OA6-CA4
21	N	602	CDL	CB2-OB2-PB2-OB3

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Mol	Chain	Res	Type	Atoms
21	N	602	CDL	CB2-OB2-PB2-OB4
21	N	602	CDL	CB2-OB2-PB2-OB5
21	N	603	CDL	CA3-OA5-PA1-OA2
21	N	603	CDL	CA3-OA5-PA1-OA3
21	N	603	CDL	CA3-OA5-PA1-OA4
21	N	603	CDL	CB3-OB5-PB2-OB2
21	N	603	CDL	CB3-OB5-PB2-OB4
21	N	604	CDL	CB2-C1-CA2-OA2
21	N	604	CDL	CA2-OA2-PA1-OA3
21	N	604	CDL	CA2-OA2-PA1-OA4
21	N	604	CDL	CA2-OA2-PA1-OA5
21	N	604	CDL	CA4-CA3-OA5-PA1
21	N	604	CDL	CB2-OB2-PB2-OB3
21	N	604	CDL	CB2-OB2-PB2-OB4
21	N	604	CDL	CB2-OB2-PB2-OB5
21	N	604	CDL	C51-CB5-OB6-CB4
21	P	301	CDL	CA2-OA2-PA1-OA3
21	P	301	CDL	CA2-OA2-PA1-OA5
21	P	301	CDL	CA3-OA5-PA1-OA4
21	P	301	CDL	C51-CB5-OB6-CB4
21	T	1302	CDL	CA2-OA2-PA1-OA3
21	T	1302	CDL	CA2-OA2-PA1-OA4
21	T	1302	CDL	CA3-OA5-PA1-OA2
21	T	1302	CDL	CA3-OA5-PA1-OA4
21	T	1302	CDL	C11-CA5-OA6-CA4
21	T	1302	CDL	CB2-OB2-PB2-OB3
21	T	1302	CDL	CB2-OB2-PB2-OB5
21	T	1302	CDL	CB3-OB5-PB2-OB2
21	T	1302	CDL	CB3-OB5-PB2-OB3
21	T	1302	CDL	CB3-OB5-PB2-OB4
21	R	601	CDL	CA2-OA2-PA1-OA4
21	R	601	CDL	CA2-OA2-PA1-OA5
21	R	601	CDL	CB2-OB2-PB2-OB3
21	R	605	CDL	CA2-C1-CB2-OB2
21	R	605	CDL	CA3-OA5-PA1-OA3
21	R	605	CDL	CB2-OB2-PB2-OB3
21	R	605	CDL	CB2-OB2-PB2-OB4
21	R	605	CDL	CB2-OB2-PB2-OB5
21	R	605	CDL	CB3-OB5-PB2-OB2
21	R	605	CDL	CB3-OB5-PB2-OB3
21	C	305	CDL	CA2-OA2-PA1-OA4
21	C	305	CDL	C11-CA5-OA6-CA4

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Mol	Chain	Res	Type	Atoms
21	C	305	CDL	CB2-OB2-PB2-OB4
21	C	305	CDL	CB2-OB2-PB2-OB5
21	C	305	CDL	CB3-OB5-PB2-OB2
21	C	305	CDL	CB3-OB5-PB2-OB3
21	C	305	CDL	CB3-OB5-PB2-OB4
21	C	305	CDL	C51-CB5-OB6-CB4
21	H	903	CDL	CA2-C1-CB2-OB2
21	H	903	CDL	C11-CA5-OA6-CA4
21	H	903	CDL	CB2-OB2-PB2-OB3
21	H	903	CDL	CB2-OB2-PB2-OB4
21	H	903	CDL	CB2-OB2-PB2-OB5
21	H	904	CDL	CA3-OA5-PA1-OA2
21	H	904	CDL	CA3-OA5-PA1-OA3
21	H	904	CDL	CA3-OA5-PA1-OA4
21	H	904	CDL	CB2-OB2-PB2-OB3
21	H	905	CDL	CA2-OA2-PA1-OA3
21	H	905	CDL	CA2-OA2-PA1-OA5
21	H	905	CDL	CB2-OB2-PB2-OB3
21	H	905	CDL	CB2-OB2-PB2-OB4
21	H	905	CDL	CB2-OB2-PB2-OB5
21	H	905	CDL	OB7-CB5-OB6-CB4
21	H	905	CDL	C51-CB5-OB6-CB4
21	I	301	CDL	CA2-OA2-PA1-OA3
21	I	301	CDL	CA2-OA2-PA1-OA4
21	I	301	CDL	CB3-OB5-PB2-OB2
21	I	301	CDL	CB3-OB5-PB2-OB4
21	I	301	CDL	C51-CB5-OB6-CB4
21	I	302	CDL	CA2-C1-CB2-OB2
21	I	302	CDL	CA2-OA2-PA1-OA3
21	I	302	CDL	CA2-OA2-PA1-OA5
21	I	302	CDL	CA3-OA5-PA1-OA2
21	I	302	CDL	CA3-OA5-PA1-OA3
21	I	302	CDL	CA3-OA5-PA1-OA4
21	I	302	CDL	OA6-CA4-CA6-OA8
21	J	501	CDL	CA2-OA2-PA1-OA4
21	J	501	CDL	CA2-OA2-PA1-OA5
21	J	501	CDL	OA5-CA3-CA4-OA6
21	J	501	CDL	OA7-CA5-OA6-CA4
21	J	501	CDL	C11-CA5-OA6-CA4
21	J	501	CDL	CB2-OB2-PB2-OB4
21	J	501	CDL	CB3-OB5-PB2-OB2
21	J	501	CDL	CB3-OB5-PB2-OB4

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Mol	Chain	Res	Type	Atoms
21	J	501	CDL	C51-CB5-OB6-CB4
21	L	601	CDL	CA3-OA5-PA1-OA3
21	L	601	CDL	C11-CA5-OA6-CA4
23	S	503	3PE	C1-O11-P-O13
23	S	503	3PE	C1-O11-P-O14
23	S	503	3PE	C22-C21-O21-C2
23	J	503	3PE	C1-O11-P-O13
23	J	503	3PE	C1-O11-P-O14
23	J	503	3PE	C22-C21-O21-C2
24	R	602	HEA	C2A-C3A-CMA-OMA
24	R	602	HEA	C4A-C3A-CMA-OMA
24	R	603	HEA	C11-C12-C13-C14
24	R	603	HEA	C20-C21-C22-C23
24	L	602	HEA	C2A-C3A-CMA-OMA
24	L	602	HEA	C4A-C3A-CMA-OMA
28	W	202	9XX	O-C16-C17-O1
28	W	202	9XX	C19-C18-O1-C17
28	W	202	9XX	O2-C18-O1-C17
28	Y	302	9XX	C19-C18-O1-C17
28	b	203	9XX	O-C16-C17-C37
28	b	203	9XX	O-C16-C17-O1
28	b	203	9XX	C16-C17-O1-C18
28	c	302	9XX	C14-C15-O-C16
28	c	302	9XX	O6-C15-O-C16
28	c	302	9XX	C19-C18-O1-C17
29	W	203	PLM	O2-C1-C2-C3
29	Y	301	PLM	C1-C2-C3-C4
29	b	202	PLM	O2-C1-C2-C3
15	I	303	WUO	O15-C14-O13-C12
17	M	502	IZL	O33-C47-O32-C46
18	G	904	9YF	O12-C25-O11-C24
21	N	604	CDL	OA9-CA7-OA8-CA6
21	I	301	CDL	OA9-CA7-OA8-CA6
17	M	502	IZL	O10-C23-C24-O11
14	M	505	MQ9	C47-C48-C49-C51
14	G	901	MQ9	C47-C48-C49-C51
21	N	604	CDL	C31-CA7-OA8-CA6
21	I	301	CDL	C71-CB7-OB8-CB6
21	I	302	CDL	C71-CB7-OB8-CB6
15	P	302	WUO	O15-C14-O13-C12
15	P	302	WUO	O79-C78-O77-C76
21	I	301	CDL	OB9-CB7-OB8-CB6

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Mol	Chain	Res	Type	Atoms
21	I	302	CDL	OB9-CB7-OB8-CB6
15	O	304	WUO	O60-C59-O58-C57
21	N	602	CDL	OA7-CA5-OA6-CA4
21	N	604	CDL	OB7-CB5-OB6-CB4
21	P	301	CDL	OB7-CB5-OB6-CB4
21	T	1302	CDL	OA7-CA5-OA6-CA4
21	C	305	CDL	OA7-CA5-OA6-CA4
21	C	305	CDL	OB7-CB5-OB6-CB4
21	H	903	CDL	OA7-CA5-OA6-CA4
21	I	301	CDL	OB7-CB5-OB6-CB4
21	J	501	CDL	OB7-CB5-OB6-CB4
21	L	601	CDL	OA7-CA5-OA6-CA4
23	S	503	3PE	O22-C21-O21-C2
23	J	503	3PE	O22-C21-O21-C2
28	Y	302	9XX	O2-C18-O1-C17
28	c	302	9XX	O2-C18-O1-C17
14	N	606	MQ9	C47-C48-C49-C50
14	N	606	MQ9	C47-C48-C49-C51
14	H	907	MQ9	C47-C48-C49-C50
14	H	907	MQ9	C47-C48-C49-C51
15	P	302	WUO	C16-C14-O13-C12
15	P	302	WUO	C80-C78-O77-C76
21	I	301	CDL	C31-CA7-OA8-CA6
17	M	502	IZL	C61-C60-O34-C45
14	M	505	MQ9	C12-C11-C9-C10
14	M	505	MQ9	C15-C14-C16-C17
14	M	505	MQ9	C20-C19-C21-C22
14	M	505	MQ9	C45-C44-C46-C47
14	N	605	MQ9	C30-C29-C31-C32
14	N	606	MQ9	C12-C11-C9-C10
14	N	606	MQ9	C15-C14-C16-C17
14	N	606	MQ9	C20-C19-C21-C22
14	N	608	MQ9	C20-C19-C21-C22
14	N	608	MQ9	C25-C24-C26-C27
14	N	608	MQ9	C45-C44-C46-C47
14	T	1301	MQ9	C12-C11-C9-C10
14	T	1301	MQ9	C20-C19-C21-C22
14	G	901	MQ9	C12-C11-C9-C10
14	G	901	MQ9	C15-C14-C16-C17
14	G	901	MQ9	C20-C19-C21-C22
14	G	901	MQ9	C45-C44-C46-C47
14	H	906	MQ9	C30-C29-C31-C32

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Mol	Chain	Res	Type	Atoms
14	H	907	MQ9	C12-C11-C9-C10
14	H	907	MQ9	C15-C14-C16-C17
14	H	907	MQ9	C20-C19-C21-C22
14	H	909	MQ9	C20-C19-C21-C22
14	H	909	MQ9	C25-C24-C26-C27
14	H	909	MQ9	C45-C44-C46-C47
24	R	603	HEA	C26-C15-C16-C17
24	R	603	HEA	C27-C19-C20-C21
14	M	505	MQ9	C13-C14-C16-C17
14	M	505	MQ9	C18-C19-C21-C22
14	M	505	MQ9	C33-C34-C36-C37
14	N	605	MQ9	C28-C29-C31-C32
14	N	606	MQ9	C12-C11-C9-C8
14	N	606	MQ9	C13-C14-C16-C17
14	N	606	MQ9	C18-C19-C21-C22
14	N	608	MQ9	C18-C19-C21-C22
14	N	608	MQ9	C23-C24-C26-C27
14	T	1301	MQ9	C12-C11-C9-C8
14	G	901	MQ9	C13-C14-C16-C17
14	G	901	MQ9	C18-C19-C21-C22
14	G	901	MQ9	C33-C34-C36-C37
14	H	906	MQ9	C28-C29-C31-C32
14	H	907	MQ9	C12-C11-C9-C8
14	H	907	MQ9	C13-C14-C16-C17
14	H	907	MQ9	C18-C19-C21-C22
14	H	909	MQ9	C18-C19-C21-C22
14	H	909	MQ9	C23-C24-C26-C27
14	K	1301	MQ9	C23-C24-C26-C27
24	R	603	HEA	C18-C19-C20-C21
28	W	202	9XX	O6-C15-O-C16
21	R	601	CDL	C31-CA7-OA8-CA6
21	L	601	CDL	C31-CA7-OA8-CA6
28	b	203	9XX	C14-C15-O-C16
14	N	606	MQ9	C7-C8-C9-C10
14	N	606	MQ9	C22-C23-C24-C25
14	N	608	MQ9	C12-C13-C14-C15
14	H	907	MQ9	C7-C8-C9-C10
14	H	907	MQ9	C22-C23-C24-C25
14	H	909	MQ9	C12-C13-C14-C15
14	K	1301	MQ9	C12-C13-C14-C15
14	K	1301	MQ9	C22-C23-C24-C25
14	M	505	MQ9	C12-C13-C14-C16

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Mol	Chain	Res	Type	Atoms
14	N	606	MQ9	C22-C23-C24-C26
14	N	608	MQ9	C17-C18-C19-C21
14	H	907	MQ9	C22-C23-C24-C26
14	H	909	MQ9	C17-C18-C19-C21
14	K	1301	MQ9	C12-C13-C14-C16
14	K	1301	MQ9	C22-C23-C24-C26
15	O	304	WUO	O40-C41-C48-O49
21	R	601	CDL	OA9-CA7-OA8-CA6
21	R	605	CDL	OB9-CB7-OB8-CB6
21	L	601	CDL	OA9-CA7-OA8-CA6
17	M	502	IZL	O35-C60-O34-C45
19	M	504	7PH	C25-C26-C27-C28
19	G	905	7PH	C25-C26-C27-C28
17	G	903	IZL	O17-C32-C33-O18
17	M	502	IZL	C36-C31-O16-C30
21	N	602	CDL	O1-C1-CB2-OB2
21	N	604	CDL	O1-C1-CA2-OA2
21	R	601	CDL	O1-C1-CA2-OA2
21	R	605	CDL	O1-C1-CB2-OB2
21	H	903	CDL	O1-C1-CB2-OB2
21	H	904	CDL	O1-C1-CB2-OB2
21	I	302	CDL	O1-C1-CB2-OB2
21	J	501	CDL	O1-C1-CA2-OA2
28	W	202	9XX	C14-C15-O-C16
17	M	502	IZL	O12-C26-C27-O13
17	G	903	IZL	C34-C32-C33-O18
17	G	903	IZL	C61-C60-O34-C45
19	S	501	7PH	C22-C21-O21-C2
21	P	301	CDL	C11-CA5-OA6-CA4
21	R	605	CDL	C51-CB5-OB6-CB4
21	R	605	CDL	C71-CB7-OB8-CB6
15	P	302	WUO	C24-C25-C26-C27
15	I	303	WUO	C90-C91-C92-C93
17	M	502	IZL	O17-C31-O16-C30
14	N	606	MQ9	C25-C24-C26-C27
14	N	608	MQ9	C12-C11-C9-C10
14	N	608	MQ9	C15-C14-C16-C17
14	H	907	MQ9	C25-C24-C26-C27
14	H	909	MQ9	C12-C11-C9-C10
14	H	909	MQ9	C15-C14-C16-C17
14	M	505	MQ9	C12-C11-C9-C8
14	M	505	MQ9	C43-C44-C46-C47

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Mol	Chain	Res	Type	Atoms
14	N	606	MQ9	C23-C24-C26-C27
14	N	606	MQ9	C33-C34-C36-C37
14	N	608	MQ9	C12-C11-C9-C8
14	N	608	MQ9	C13-C14-C16-C17
14	N	608	MQ9	C43-C44-C46-C47
14	T	1301	MQ9	C18-C19-C21-C22
14	G	901	MQ9	C12-C11-C9-C8
14	G	901	MQ9	C43-C44-C46-C47
14	H	907	MQ9	C23-C24-C26-C27
14	H	907	MQ9	C33-C34-C36-C37
14	H	909	MQ9	C12-C11-C9-C8
14	H	909	MQ9	C13-C14-C16-C17
14	H	909	MQ9	C43-C44-C46-C47
24	R	603	HEA	C14-C15-C16-C17
28	b	203	9XX	O6-C15-O-C16
21	P	301	CDL	OA7-CA5-OA6-CA4
14	M	505	MQ9	C24-C26-C27-C28
14	M	505	MQ9	C39-C41-C42-C43
14	N	605	MQ9	C9-C11-C12-C13
14	N	605	MQ9	C29-C31-C32-C33
14	N	606	MQ9	C44-C46-C47-C48
14	N	608	MQ9	C19-C21-C22-C23
14	N	608	MQ9	C24-C26-C27-C28
14	N	608	MQ9	C34-C36-C37-C38
14	G	901	MQ9	C24-C26-C27-C28
14	G	901	MQ9	C39-C41-C42-C43
14	H	906	MQ9	C9-C11-C12-C13
14	H	906	MQ9	C29-C31-C32-C33
14	H	907	MQ9	C44-C46-C47-C48
14	H	909	MQ9	C19-C21-C22-C23
14	H	909	MQ9	C24-C26-C27-C28
14	H	909	MQ9	C34-C36-C37-C38
14	K	1301	MQ9	C19-C21-C22-C23
24	R	602	HEA	C19-C20-C21-C22
24	R	603	HEA	C19-C20-C21-C22
24	L	603	HEA	C19-C20-C21-C22
19	N	609	7PH	C36-C37-C38-C39
19	H	901	7PH	C36-C37-C38-C39
17	G	903	IZL	O12-C26-C27-O13
15	O	304	WUO	C42-C41-C48-O49
14	M	505	MQ9	C47-C48-C49-C50
14	G	901	MQ9	C47-C48-C49-C50

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Mol	Chain	Res	Type	Atoms
17	M	502	IZL	O12-C25-O11-C24
15	O	304	WUO	C16-C17-C18-C19
15	C	304	WUO	C80-C78-O77-C76
15	P	302	WUO	C92-C93-C94-C95
14	T	1301	MQ9	C7-C8-C9-C10
15	O	304	WUO	C61-C62-C63-C64
17	M	502	IZL	O17-C32-C33-O18
21	C	305	CDL	C77-C78-C79-C80
18	W	201	9YF	C38-C39-C40-C41
18	b	201	9YF	C38-C39-C40-C41
19	S	501	7PH	C36-C37-C38-C39
21	I	301	CDL	C51-C52-C53-C54
21	N	603	CDL	CA2-C1-CB2-OB2
21	H	904	CDL	CA2-C1-CB2-OB2
21	J	501	CDL	CB2-C1-CA2-OA2
18	W	201	9YF	C26-C25-O11-C24
18	b	201	9YF	C26-C25-O11-C24
19	N	609	7PH	C32-C31-O31-C3
19	H	901	7PH	C32-C31-O31-C3
21	H	904	CDL	C71-CB7-OB8-CB6
23	S	503	3PE	C32-C31-O31-C3
23	J	503	3PE	C32-C31-O31-C3
15	C	304	WUO	C16-C17-C18-C19
17	M	502	IZL	C37-C23-C24-O11
15	O	304	WUO	C65-C66-C67-C68
17	M	502	IZL	C34-C32-C33-O18
14	M	505	MQ9	C40-C39-C41-C42
14	N	606	MQ9	C35-C34-C36-C37
14	G	901	MQ9	C40-C39-C41-C42
14	H	907	MQ9	C35-C34-C36-C37
15	O	304	WUO	C89-C88-C90-C91
15	I	303	WUO	C86-C87-C88-C89
17	M	502	IZL	C54-C55-C56-C57
18	W	201	9YF	C34-C33-C35-C36
18	b	201	9YF	C34-C33-C35-C36
15	C	304	WUO	C59-C61-C62-C63
21	N	604	CDL	CB5-C51-C52-C53
21	N	603	CDL	O1-C1-CB2-OB2
23	S	503	3PE	O32-C31-O31-C3
23	J	503	3PE	O32-C31-O31-C3
15	O	304	WUO	C70-C71-C72-C73
21	P	301	CDL	C32-C33-C34-C35

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Mol	Chain	Res	Type	Atoms
21	I	301	CDL	CB5-C51-C52-C53
21	H	904	CDL	OB9-CB7-OB8-CB6
21	T	1302	CDL	C51-CB5-OB6-CB4
21	I	301	CDL	C11-CA5-OA6-CA4
15	P	302	WUO	O58-C57-C76-O77
21	H	905	CDL	C71-CB7-OB8-CB6
21	R	605	CDL	C75-C76-C77-C78
14	M	505	MQ9	C27-C28-C29-C30
14	G	901	MQ9	C27-C28-C29-C30
21	C	305	CDL	C15-C16-C17-C18
21	C	305	CDL	C79-C80-C81-C82
21	H	905	CDL	C11-C12-C13-C14
21	N	602	CDL	CA7-C31-C32-C33
21	H	903	CDL	CA7-C31-C32-C33
21	L	601	CDL	CA5-C11-C12-C13
21	L	601	CDL	CB5-C51-C52-C53
21	N	604	CDL	C21-C22-C23-C24
15	C	304	WUO	C78-C80-C81-C82
21	N	602	CDL	CB7-C71-C72-C73
21	H	903	CDL	CB7-C71-C72-C73
23	S	503	3PE	C21-C22-C23-C24
23	J	503	3PE	C21-C22-C23-C24
17	G	903	IZL	O35-C60-O34-C45
19	S	501	7PH	O22-C21-O21-C2
21	R	605	CDL	OB7-CB5-OB6-CB4
14	M	505	MQ9	C44-C46-C47-C48
14	N	606	MQ9	C39-C41-C42-C43
14	G	901	MQ9	C44-C46-C47-C48
14	H	907	MQ9	C39-C41-C42-C43
21	N	604	CDL	CA7-C31-C32-C33
21	P	301	CDL	CB5-C51-C52-C53
21	R	601	CDL	CB7-C71-C72-C73
21	C	305	CDL	CA5-C11-C12-C13
21	H	904	CDL	CA7-C31-C32-C33
18	W	201	9YF	O12-C25-O11-C24
18	b	201	9YF	O12-C25-O11-C24
28	b	203	9XX	C19-C18-O1-C17
28	b	203	9XX	C24-C25-C26-C27
20	H	902	HEM	C3D-CAD-CBD-CGD
15	C	304	WUO	C85-C86-C87-C88
21	R	601	CDL	CB5-C51-C52-C53
21	R	605	CDL	CB5-C51-C52-C53

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Mol	Chain	Res	Type	Atoms
19	N	609	7PH	O32-C31-O31-C3
19	H	901	7PH	O32-C31-O31-C3
19	N	609	7PH	C24-C25-C26-C27
19	H	901	7PH	C24-C25-C26-C27
21	P	301	CDL	C71-C72-C73-C74
21	I	302	CDL	C16-C17-C18-C19
15	P	302	WUO	C85-C86-C87-C88
15	I	303	WUO	C19-C20-C21-C22
21	T	1302	CDL	O1-C1-CA2-OA2
21	I	301	CDL	O1-C1-CA2-OA2
21	H	904	CDL	C57-C58-C59-C60
15	C	304	WUO	O79-C78-O77-C76
21	R	601	CDL	CA5-C11-C12-C13
21	I	301	CDL	CA7-C31-C32-C33
28	Y	302	9XX	C18-C19-C20-C21
21	T	1302	CDL	OB7-CB5-OB6-CB4
15	C	304	WUO	C92-C93-C94-C95
15	I	303	WUO	C67-C68-C69-C70
21	R	605	CDL	C73-C74-C75-C76
17	M	502	IZL	C28-C26-C27-O13
17	M	502	IZL	C53-C54-C55-C56
21	H	905	CDL	OB9-CB7-OB8-CB6
15	P	302	WUO	C59-C61-C62-C63
21	H	905	CDL	CA7-C31-C32-C33
21	L	601	CDL	C51-CB5-OB6-CB4
21	H	905	CDL	CA5-C11-C12-C13
15	P	302	WUO	C35-C37-O38-C39
21	R	605	CDL	C11-C12-C13-C14
21	I	302	CDL	CA7-C31-C32-C33
28	c	302	9XX	C18-C19-C20-C21
21	I	301	CDL	OA7-CA5-OA6-CA4
21	L	601	CDL	OB7-CB5-OB6-CB4
28	b	203	9XX	O2-C18-O1-C17
21	T	1302	CDL	CB2-C1-CA2-OA2
21	R	601	CDL	CB2-C1-CA2-OA2
21	H	904	CDL	C71-C72-C73-C74
18	M	503	9YF	C30-C31-C32-C33
18	G	904	9YF	C30-C31-C32-C33
18	M	503	9YF	C13-C14-C15-C16
18	G	904	9YF	C13-C14-C15-C16
21	I	302	CDL	CA5-C11-C12-C13
14	O	303	MQ9	C15-C14-C16-C17

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Mol	Chain	Res	Type	Atoms
14	C	303	MQ9	C15-C14-C16-C17
15	I	303	WUO	C88-C90-C91-C92
14	O	303	MQ9	C14-C16-C17-C18
14	C	303	MQ9	C14-C16-C17-C18
21	N	604	CDL	O1-C1-CB2-OB2
15	P	302	WUO	C50-C37-O38-C39
28	W	202	9XX	C9-C10-C11-C12
28	W	202	9XX	C24-C25-C26-C27
15	O	304	WUO	C76-C57-O58-C59
17	G	903	IZL	C46-C45-O34-C60
21	H	904	CDL	C51-CB5-OB6-CB4
24	R	603	HEA	O11-C11-C12-C13
18	W	201	9YF	C30-C31-C32-C33
18	b	201	9YF	C30-C31-C32-C33
14	M	505	MQ9	C38-C39-C41-C42
14	G	901	MQ9	C38-C39-C41-C42
21	L	601	CDL	CB7-C71-C72-C73
15	I	303	WUO	C24-C25-C26-C27
18	M	503	9YF	C9-C10-C11-C12
18	G	904	9YF	C9-C10-C11-C12
19	N	609	7PH	C28-C29-C2A-C2B
19	H	901	7PH	C28-C29-C2A-C2B
21	J	501	CDL	C74-C75-C76-C77
28	Y	302	9XX	C9-C10-C11-C12
17	G	903	IZL	C28-C26-C27-O13
15	P	302	WUO	C67-C68-C69-C70
19	S	501	7PH	C34-C35-C36-C37
19	H	901	7PH	C25-C26-C27-C28
21	N	603	CDL	C53-C54-C55-C56
21	N	603	CDL	C71-C72-C73-C74
21	N	604	CDL	C31-C32-C33-C34
21	I	301	CDL	C75-C76-C77-C78
21	I	302	CDL	C14-C15-C16-C17
21	J	501	CDL	C82-C83-C84-C85
28	c	302	9XX	C12-C13-C14-C15
15	O	304	WUO	C20-C21-C22-C23
18	M	503	9YF	C15-C16-C17-C18
18	G	904	9YF	C15-C16-C17-C18
19	N	609	7PH	C25-C26-C27-C28
21	R	605	CDL	C32-C33-C34-C35
21	I	301	CDL	C15-C16-C17-C18
21	J	501	CDL	C77-C78-C79-C80

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Mol	Chain	Res	Type	Atoms
21	L	601	CDL	C81-C82-C83-C84
29	W	203	PLM	C2-C3-C4-C5
17	G	903	IZL	C43-C18-O7-C19
15	O	304	WUO	C90-C91-C92-C93
15	P	302	WUO	C26-C27-C28-C29
15	I	303	WUO	C21-C22-C23-C24
15	I	303	WUO	C84-C85-C86-C87
19	S	501	7PH	C29-C2A-C2B-C2C
21	N	602	CDL	C78-C79-C80-C81
21	N	603	CDL	C34-C35-C36-C37
21	C	305	CDL	C12-C13-C14-C15
21	H	903	CDL	C78-C79-C80-C81
21	I	302	CDL	C13-C14-C15-C16
21	I	302	CDL	C73-C74-C75-C76
21	J	501	CDL	C16-C17-C18-C19
28	c	302	9XX	C19-C20-C21-C22
18	b	201	9YF	C12-C13-C14-C15
21	J	501	CDL	C14-C15-C16-C17
15	I	303	WUO	C85-C86-C87-C88
15	I	303	WUO	C59-C61-C62-C63
18	W	201	9YF	C11-C10-C9-C8
18	b	201	9YF	C11-C10-C9-C8
21	P	301	CDL	CA5-C11-C12-C13
15	O	304	WUO	C19-C20-C21-C22
18	W	201	9YF	C12-C13-C14-C15
21	P	301	CDL	C37-C38-C39-C40
21	R	601	CDL	C12-C13-C14-C15
21	N	602	CDL	C51-C52-C53-C54
21	N	604	CDL	C20-C21-C22-C23
21	R	605	CDL	C53-C54-C55-C56
21	H	903	CDL	C51-C52-C53-C54
28	b	203	9XX	C23-C24-C25-C26
15	P	302	WUO	C71-C72-C73-C74
19	M	504	7PH	C29-C2A-C2B-C2C
21	C	305	CDL	C57-C58-C59-C60
28	W	202	9XX	C22-C23-C24-C25
15	I	303	WUO	C14-C16-C17-C18
15	O	304	WUO	C81-C82-C83-C84
19	N	609	7PH	C29-C2A-C2B-C2C
19	G	905	7PH	C29-C2A-C2B-C2C
19	H	901	7PH	C29-C2A-C2B-C2C
21	I	302	CDL	C75-C76-C77-C78

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Mol	Chain	Res	Type	Atoms
22	T	1303	TRD	C6-C7-C8-C9
22	Q	403	TRD	C7-C8-C9-C10
22	K	1302	TRD	C6-C7-C8-C9
22	X	403	TRD	C7-C8-C9-C10
18	M	503	9YF	C26-C27-C28-C29
18	G	904	9YF	C26-C27-C28-C29
21	P	301	CDL	C34-C35-C36-C37
28	b	203	9XX	C6-C7-C8-C9
21	I	301	CDL	C52-C53-C54-C55
17	G	903	IZL	C47-C48-C49-C50
15	I	303	WUO	C61-C62-C63-C64
19	M	504	7PH	C36-C37-C38-C39
19	G	905	7PH	C36-C37-C38-C39
21	C	305	CDL	C71-C72-C73-C74
21	J	501	CDL	C51-C52-C53-C54
15	I	303	WUO	C64-C65-C66-C67
17	M	502	IZL	C2-C1-C7-C8
18	M	503	9YF	C12-C13-C14-C15
18	W	201	9YF	C17-C18-C19-C20
18	G	904	9YF	C12-C13-C14-C15
18	b	201	9YF	C17-C18-C19-C20
19	N	609	7PH	C33-C34-C35-C36
28	Y	302	9XX	C23-C24-C25-C26
21	I	301	CDL	CB2-C1-CA2-OA2
21	L	601	CDL	C71-CB7-OB8-CB6
21	C	305	CDL	CB3-CB4-CB6-OB8
15	O	304	WUO	C18-C19-C20-C21
18	W	201	9YF	C28-C29-C30-C31
18	b	201	9YF	C28-C29-C30-C31
19	H	901	7PH	C33-C34-C35-C36
21	N	604	CDL	C22-C23-C24-C25
21	N	604	CDL	C73-C74-C75-C76
21	P	301	CDL	C38-C39-C40-C41
21	P	301	CDL	C52-C53-C54-C55
21	T	1302	CDL	C12-C13-C14-C15
21	I	301	CDL	C59-C60-C61-C62
28	b	203	9XX	C11-C12-C13-C14
19	M	504	7PH	C31-C32-C33-C34
19	G	905	7PH	C31-C32-C33-C34
21	N	603	CDL	CA7-C31-C32-C33
21	I	301	CDL	CA5-C11-C12-C13
15	C	304	WUO	C26-C27-C28-C29

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Mol	Chain	Res	Type	Atoms
15	C	304	WUO	C83-C84-C85-C86
17	M	502	IZL	C51-C52-C53-C54
17	G	903	IZL	C2-C1-C7-C8
21	N	602	CDL	C14-C15-C16-C17
21	N	604	CDL	C57-C58-C59-C60
21	R	601	CDL	C73-C74-C75-C76
21	C	305	CDL	C53-C54-C55-C56
21	C	305	CDL	C76-C77-C78-C79
21	H	903	CDL	C14-C15-C16-C17
21	I	302	CDL	C52-C53-C54-C55
22	Q	403	TRD	C5-C6-C7-C8
22	X	403	TRD	C5-C6-C7-C8
18	b	201	9YF	C29-C30-C31-C32
21	R	601	CDL	C16-C17-C18-C19
22	T	1303	TRD	C3-C4-C5-C6
22	K	1302	TRD	C3-C4-C5-C6
28	c	302	9XX	C9-C10-C11-C12
18	W	201	9YF	C29-C30-C31-C32
19	G	905	7PH	C34-C35-C36-C37
21	P	301	CDL	C17-C18-C19-C20
17	G	903	IZL	C17-C18-O7-C19
19	M	504	7PH	C34-C35-C36-C37
21	R	605	CDL	C34-C35-C36-C37
21	H	904	CDL	C38-C39-C40-C41
21	H	905	CDL	C21-C22-C23-C24
21	I	302	CDL	C55-C56-C57-C58
28	c	302	9XX	C6-C7-C8-C9
18	b	201	9YF	C10-C11-C12-C13
21	N	602	CDL	C54-C55-C56-C57
21	N	602	CDL	C72-C73-C74-C75
21	H	903	CDL	C54-C55-C56-C57
21	H	903	CDL	C72-C73-C74-C75
29	b	202	PLM	C5-C6-C7-C8
15	I	303	WUO	C65-C66-C67-C68
18	W	201	9YF	C10-C11-C12-C13
28	W	202	9XX	C31-C32-C33-C34
28	Y	302	9XX	C6-C7-C8-C9
17	G	903	IZL	C60-C61-C62-C63
28	b	203	9XX	C12-C13-C14-C15
15	P	302	WUO	C69-C70-C71-C72
17	G	903	IZL	C49-C50-C51-C52
21	R	605	CDL	C33-C34-C35-C36

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Mol	Chain	Res	Type	Atoms
21	H	905	CDL	C73-C74-C75-C76
21	I	301	CDL	C72-C73-C74-C75
28	Y	302	9XX	C22-C23-C24-C25
15	O	304	WUO	C63-C64-C65-C66
17	G	903	IZL	C50-C51-C52-C53
21	T	1302	CDL	C75-C76-C77-C78
21	H	905	CDL	C31-C32-C33-C34
21	H	904	CDL	OB7-CB5-OB6-CB4
21	R	601	CDL	C75-C76-C77-C78
21	L	601	CDL	C51-C52-C53-C54
22	Q	403	TRD	C9-C10-C11-C12
28	b	203	9XX	C22-C23-C24-C25
14	O	303	MQ9	C13-C14-C16-C17
14	C	303	MQ9	C13-C14-C16-C17
14	N	608	MQ9	C47-C48-C49-C50
14	H	909	MQ9	C47-C48-C49-C50
18	W	201	9YF	C16-C17-C18-C19
18	b	201	9YF	C16-C17-C18-C19
21	N	602	CDL	C11-C12-C13-C14
21	N	602	CDL	C15-C16-C17-C18
21	N	604	CDL	C11-C12-C13-C14
21	H	903	CDL	C11-C12-C13-C14
21	H	903	CDL	C15-C16-C17-C18
21	H	905	CDL	C12-C13-C14-C15
21	H	905	CDL	C20-C21-C22-C23
21	I	301	CDL	C57-C58-C59-C60
22	X	403	TRD	C9-C10-C11-C12
21	R	605	CDL	CA7-C31-C32-C33
21	I	302	CDL	C31-CA7-OA8-CA6
21	N	602	CDL	C73-C74-C75-C76
21	R	605	CDL	C55-C56-C57-C58
21	H	903	CDL	C73-C74-C75-C76
21	H	904	CDL	C59-C60-C61-C62
21	N	602	CDL	C75-C76-C77-C78
21	N	603	CDL	C36-C37-C38-C39
21	P	301	CDL	C55-C56-C57-C58
21	C	305	CDL	C83-C84-C85-C86
21	H	903	CDL	C75-C76-C77-C78
21	H	905	CDL	C77-C78-C79-C80
18	M	503	9YF	C17-C18-C19-C20
18	G	904	9YF	C17-C18-C19-C20
21	H	905	CDL	C14-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
21	L	601	CDL	C56-C57-C58-C59
21	L	601	CDL	C77-C78-C79-C80
22	R	609	TRD	C3-C4-C5-C6
21	N	602	CDL	C56-C57-C58-C59
21	H	903	CDL	C56-C57-C58-C59
22	L	608	TRD	C3-C4-C5-C6
15	I	303	WUO	C91-C92-C93-C94
18	M	503	9YF	C28-C29-C30-C31
19	N	609	7PH	C38-C39-C3A-C3B
19	H	901	7PH	C38-C39-C3A-C3B
21	R	601	CDL	C71-C72-C73-C74
21	C	305	CDL	C11-C12-C13-C14
21	L	601	CDL	C13-C14-C15-C16
21	N	604	CDL	C71-CB7-OB8-CB6
19	N	609	7PH	C2B-C2C-C2D-C2E
19	H	901	7PH	C2B-C2C-C2D-C2E
18	M	503	9YF	C9-C8-O9-C
18	G	904	9YF	C9-C8-O9-C
21	N	602	CDL	C51-CB5-OB6-CB4
21	H	903	CDL	C51-CB5-OB6-CB4
18	G	904	9YF	C28-C29-C30-C31
21	J	501	CDL	C56-C57-C58-C59
18	M	503	9YF	O10-C8-O9-C
18	G	904	9YF	O10-C8-O9-C
21	N	602	CDL	OB7-CB5-OB6-CB4
21	H	903	CDL	OB7-CB5-OB6-CB4
21	J	501	CDL	C55-C56-C57-C58
21	C	305	CDL	C58-C59-C60-C61
21	R	601	CDL	C32-C33-C34-C35
21	R	605	CDL	C37-C38-C39-C40
21	P	301	CDL	C59-C60-C61-C62
21	T	1302	CDL	CA7-C31-C32-C33
15	P	302	WUO	C63-C64-C65-C66
21	N	602	CDL	C77-C78-C79-C80
21	H	903	CDL	C77-C78-C79-C80
15	I	303	WUO	C83-C84-C85-C86
21	I	302	CDL	C33-C34-C35-C36
21	L	601	CDL	C33-C34-C35-C36
15	C	304	WUO	C64-C65-C66-C67
21	N	603	CDL	C73-C74-C75-C76
19	H	901	7PH	C32-C33-C34-C35
21	N	603	CDL	C52-C53-C54-C55

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Mol	Chain	Res	Type	Atoms
17	G	903	IZL	C3-C4-C5-C6
21	H	905	CDL	C78-C79-C80-C81
28	Y	302	9XX	C21-C22-C23-C24
21	L	601	CDL	OB9-CB7-OB8-CB6
19	N	609	7PH	C32-C33-C34-C35
29	c	301	PLM	C6-C7-C8-C9
21	I	302	CDL	CB5-C51-C52-C53
21	H	904	CDL	C74-C75-C76-C77
18	W	201	9YF	O9-C-C1-O
18	b	201	9YF	O9-C-C1-O
21	H	904	CDL	C17-C18-C19-C20
21	I	301	CDL	C34-C35-C36-C37
20	H	902	HEM	C4C-C3C-CAC-CBC
21	N	603	CDL	C55-C56-C57-C58
21	N	603	CDL	C17-C18-C19-C20
21	N	604	CDL	C13-C14-C15-C16
21	L	601	CDL	C72-C73-C74-C75
15	P	302	WUO	C90-C91-C92-C93
21	H	905	CDL	C17-C18-C19-C20
28	W	202	9XX	C5-C6-C7-C8
19	S	501	7PH	C27-C28-C29-C2A
15	P	302	WUO	C66-C67-C68-C69
18	M	503	9YF	C10-C11-C12-C13
21	H	905	CDL	C76-C77-C78-C79
23	S	503	3PE	C27-C28-C29-C2A
21	H	905	CDL	C75-C76-C77-C78
21	I	301	CDL	C56-C57-C58-C59
23	J	503	3PE	C27-C28-C29-C2A
15	C	304	WUO	C81-C82-C83-C84
18	G	904	9YF	C10-C11-C12-C13
15	C	304	WUO	C24-C25-C26-C27
15	C	304	WUO	C67-C68-C69-C70
21	R	601	CDL	C13-C14-C15-C16
21	N	604	CDL	CA2-C1-CB2-OB2
21	P	301	CDL	C73-C74-C75-C76
19	G	905	7PH	C32-C31-O31-C3
19	M	504	7PH	C22-C23-C24-C25
19	G	905	7PH	C22-C23-C24-C25
21	L	601	CDL	C78-C79-C80-C81
18	W	201	9YF	C13-C14-C15-C16
18	b	201	9YF	C13-C14-C15-C16
19	N	609	7PH	C34-C35-C36-C37

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Mol	Chain	Res	Type	Atoms
19	N	609	7PH	C23-C24-C25-C26
19	H	901	7PH	C34-C35-C36-C37
21	N	603	CDL	C33-C34-C35-C36
28	W	202	9XX	C10-C11-C12-C13
21	T	1302	CDL	C58-C59-C60-C61
21	H	905	CDL	C18-C19-C20-C21
18	M	503	9YF	C37-C38-C39-C40
19	H	901	7PH	C23-C24-C25-C26
28	c	302	9XX	C20-C21-C22-C23
18	G	904	9YF	C37-C38-C39-C40
28	W	202	9XX	C20-C21-C22-C23
19	M	504	7PH	C32-C31-O31-C3
15	C	304	WUO	C93-C94-C95-C96
21	I	301	CDL	C14-C15-C16-C17
21	T	1302	CDL	C76-C77-C78-C79
21	H	905	CDL	C57-C58-C59-C60
21	I	302	CDL	C34-C35-C36-C37
21	L	601	CDL	C15-C16-C17-C18
17	M	502	IZL	O31-C44-C45-C46
19	S	501	7PH	O11-C1-C2-C3
21	N	602	CDL	OA5-CA3-CA4-CA6
21	H	903	CDL	OA5-CA3-CA4-CA6
21	J	501	CDL	OA5-CA3-CA4-CA6
21	N	604	CDL	C32-C33-C34-C35
21	I	302	CDL	C71-C72-C73-C74
21	N	603	CDL	C38-C39-C40-C41
21	I	302	CDL	OA9-CA7-OA8-CA6
15	P	302	WUO	C78-C80-C81-C82
21	N	602	CDL	CB5-C51-C52-C53
21	T	1302	CDL	CB5-C51-C52-C53
21	H	903	CDL	CB5-C51-C52-C53
21	J	501	CDL	CA5-C11-C12-C13
15	I	303	WUO	C82-C83-C84-C85
28	b	203	9XX	C11-C10-C9-C8
21	R	605	CDL	C51-C52-C53-C54
21	L	601	CDL	C80-C81-C82-C83
21	R	605	CDL	C17-C18-C19-C20
22	S	502	TRD	C3-C4-C5-C6
22	J	502	TRD	C3-C4-C5-C6
17	G	903	IZL	C48-C49-C50-C51
21	N	604	CDL	C71-C72-C73-C74
21	L	601	CDL	C83-C84-C85-C86

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Mol	Chain	Res	Type	Atoms
28	b	203	9XX	C10-C11-C12-C13
21	P	301	CDL	C31-CA7-OA8-CA6
21	T	1302	CDL	C31-CA7-OA8-CA6
21	N	604	CDL	C19-C20-C21-C22
28	W	202	9XX	C28-C29-C30-C31
21	T	1302	CDL	C84-C85-C86-C87
14	T	1301	MQ9	C14-C16-C17-C18
15	P	302	WUO	C56-C57-C76-O77
17	G	903	IZL	C44-C45-C46-O32
18	M	503	9YF	C1-C-C24-O11
18	G	904	9YF	C1-C-C24-O11
21	N	603	CDL	CB3-CB4-CB6-OB8
21	T	1302	CDL	CA3-CA4-CA6-OA8
21	T	1302	CDL	CB3-CB4-CB6-OB8
21	R	605	CDL	CA3-CA4-CA6-OA8
21	I	301	CDL	CA3-CA4-CA6-OA8
21	I	301	CDL	CB3-CB4-CB6-OB8
21	L	601	CDL	CB3-CB4-CB6-OB8
24	R	603	HEA	C15-C16-C17-C18
21	N	602	CDL	C18-C19-C20-C21
21	H	903	CDL	C18-C19-C20-C21
21	N	604	CDL	OB9-CB7-OB8-CB6
21	I	302	CDL	C51-C52-C53-C54
17	G	903	IZL	C51-C52-C53-C54
19	M	504	7PH	C35-C36-C37-C38
19	G	905	7PH	C35-C36-C37-C38
15	O	304	WUO	C22-C23-C24-C25
21	I	302	CDL	C53-C54-C55-C56
15	P	302	WUO	C22-C23-C24-C25
17	M	502	IZL	C62-C63-C64-C65
23	S	503	3PE	C26-C27-C28-C29
21	I	302	CDL	C18-C19-C20-C21
21	P	301	CDL	C36-C37-C38-C39
21	I	301	CDL	C53-C54-C55-C56
21	T	1302	CDL	C35-C36-C37-C38
21	I	301	CDL	C32-C33-C34-C35
29	Y	301	PLM	C6-C7-C8-C9
14	T	1301	MQ9	C15-C14-C16-C17
14	T	1301	MQ9	C13-C14-C16-C17
21	N	604	CDL	C16-C17-C18-C19
21	T	1302	CDL	C72-C73-C74-C75
23	J	503	3PE	C26-C27-C28-C29

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Mol	Chain	Res	Type	Atoms
13	O	301	HEC	C3D-CAD-CBD-CGD
13	C	301	HEC	C3D-CAD-CBD-CGD
19	G	905	7PH	O32-C31-O31-C3
19	M	504	7PH	C1-O11-P-O14
19	G	905	7PH	C1-O11-P-O14
15	I	303	WUO	C25-C26-C27-C28
17	M	502	IZL	C1-C7-C8-C9
21	N	604	CDL	C55-C56-C57-C58
17	G	903	IZL	C65-C66-C68-C69
19	S	501	7PH	C38-C39-C3A-C3B
21	N	604	CDL	C78-C79-C80-C81
21	T	1302	CDL	C74-C75-C76-C77
19	M	504	7PH	O32-C31-O31-C3
15	P	302	WUO	C70-C71-C72-C73
21	N	602	CDL	C74-C75-C76-C77
21	H	903	CDL	C74-C75-C76-C77
21	C	305	CDL	CA6-CA4-OA6-CA5
21	L	601	CDL	CA6-CA4-OA6-CA5
21	L	601	CDL	C73-C74-C75-C76
22	Q	403	TRD	C11-C10-C9-C8
22	X	403	TRD	C11-C10-C9-C8
21	R	601	CDL	C33-C34-C35-C36
21	P	301	CDL	C72-C73-C74-C75
21	I	302	CDL	C17-C18-C19-C20
21	R	605	CDL	OB5-CB3-CB4-OB6
19	G	905	7PH	C24-C25-C26-C27
15	I	303	WUO	C50-C37-O38-C39
19	M	504	7PH	C24-C25-C26-C27
21	L	601	CDL	C14-C15-C16-C17
21	N	604	CDL	C24-C25-C26-C27
21	J	501	CDL	C34-C35-C36-C37
21	L	601	CDL	C53-C54-C55-C56
15	C	304	WUO	C94-C95-C96-C97
21	H	905	CDL	C58-C59-C60-C61
15	C	304	WUO	C25-C26-C27-C28
21	P	301	CDL	C15-C16-C17-C18
21	R	601	CDL	C11-C12-C13-C14
28	W	202	9XX	C19-C20-C21-C22
21	R	601	CDL	C14-C15-C16-C17
21	H	904	CDL	C54-C55-C56-C57
28	W	202	9XX	C29-C30-C31-C32
28	Y	302	9XX	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
29	W	203	PLM	C5-C6-C7-C8
21	N	603	CDL	C76-C77-C78-C79
21	N	604	CDL	C58-C59-C60-C61
15	C	304	WUO	C16-C14-O13-C12
21	R	605	CDL	C31-CA7-OA8-CA6
15	C	304	WUO	C72-C73-C74-C75
15	I	303	WUO	C94-C95-C96-C97
21	N	602	CDL	C59-C60-C61-C62
21	I	301	CDL	C39-C40-C41-C42
21	J	501	CDL	C33-C34-C35-C36
17	M	502	IZL	C4-C5-C6-C67
21	H	903	CDL	C59-C60-C61-C62
22	J	502	TRD	C1-C2-C3-C4
21	H	904	CDL	C39-C40-C41-C42
22	S	502	TRD	C1-C2-C3-C4
24	R	602	HEA	C3B-C11-C12-C13
24	R	603	HEA	C3B-C11-C12-C13
24	L	602	HEA	C3B-C11-C12-C13
24	L	603	HEA	C3B-C11-C12-C13
21	J	501	CDL	C54-C55-C56-C57
14	N	608	MQ9	C47-C48-C49-C51
14	H	909	MQ9	C47-C48-C49-C51
15	P	302	WUO	C94-C95-C96-C97
18	b	201	9YF	C40-C41-C42-C43
21	R	605	CDL	C76-C77-C78-C79
21	L	601	CDL	C84-C85-C86-C87
14	N	606	MQ9	C37-C38-C39-C40
14	H	907	MQ9	C37-C38-C39-C40
21	N	604	CDL	C15-C16-C17-C18
21	R	601	CDL	C53-C54-C55-C56
21	H	904	CDL	C13-C14-C15-C16
21	T	1302	CDL	OA9-CA7-OA8-CA6
17	M	502	IZL	C1-C2-C3-C4
15	I	303	WUO	C27-C28-C29-C30
18	W	201	9YF	C40-C41-C42-C43
17	M	502	IZL	C7-C8-C9-C10
21	N	602	CDL	CA5-C11-C12-C13
21	H	903	CDL	CA5-C11-C12-C13
21	I	301	CDL	C12-C11-CA5-OA6
21	H	905	CDL	C13-C14-C15-C16
15	C	304	WUO	C65-C66-C67-C68
19	H	901	7PH	C37-C38-C39-C3A

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Mol	Chain	Res	Type	Atoms
21	N	603	CDL	C13-C14-C15-C16
21	T	1302	CDL	C33-C34-C35-C36
21	I	301	CDL	C13-C14-C15-C16
19	N	609	7PH	C37-C38-C39-C3A
21	N	602	CDL	C53-C54-C55-C56
21	H	903	CDL	C53-C54-C55-C56
15	O	304	WUO	C88-C90-C91-C92
22	J	502	TRD	C5-C6-C7-C8
28	W	202	9XX	C1-C2-C3-C4
22	S	502	TRD	C5-C6-C7-C8
21	R	601	CDL	C74-C75-C76-C77
22	T	1303	TRD	C9-C10-C11-C12
22	K	1302	TRD	C9-C10-C11-C12
15	O	304	WUO	O55-C56-C57-C76
21	P	301	CDL	OA5-CA3-CA4-CA6
21	P	301	CDL	OB5-CB3-CB4-CB6
21	T	1302	CDL	OA5-CA3-CA4-CA6
21	R	601	CDL	OB5-CB3-CB4-CB6
23	J	503	3PE	O11-C1-C2-C3
21	C	305	CDL	C75-C76-C77-C78
15	O	304	WUO	C94-C95-C96-C97
21	H	904	CDL	C76-C77-C78-C79
21	I	302	CDL	C76-C77-C78-C79
22	T	1303	TRD	C1-C2-C3-C4
15	C	304	WUO	C86-C87-C88-C90
22	K	1302	TRD	C1-C2-C3-C4
21	L	601	CDL	O1-C1-CA2-OA2
22	R	608	TRD	C1-C2-C3-C4
22	L	607	TRD	C1-C2-C3-C4
21	J	501	CDL	C52-C53-C54-C55
14	N	606	MQ9	C40-C39-C41-C42
14	H	907	MQ9	C40-C39-C41-C42
28	W	202	9XX	O-C16-C17-C37
28	Y	302	9XX	O-C16-C17-C37
28	c	302	9XX	O-C16-C17-C37
21	P	301	CDL	OA9-CA7-OA8-CA6
28	Y	302	9XX	C14-C15-O-C16
19	M	504	7PH	C38-C39-C3A-C3B
19	G	905	7PH	C38-C39-C3A-C3B
21	N	602	CDL	C17-C18-C19-C20
21	C	305	CDL	C73-C74-C75-C76
21	H	903	CDL	C17-C18-C19-C20

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Mol	Chain	Res	Type	Atoms
21	L	601	CDL	C32-C33-C34-C35
21	N	602	CDL	CB3-CB4-CB6-OB8
21	C	305	CDL	CA3-CA4-CA6-OA8
21	H	903	CDL	CB3-CB4-CB6-OB8
21	I	302	CDL	CA3-CA4-CA6-OA8
15	I	303	WUO	C16-C17-C18-C19
15	O	304	WUO	C62-C63-C64-C65
19	S	501	7PH	C33-C34-C35-C36
21	H	904	CDL	C52-C53-C54-C55
17	M	502	IZL	C66-C68-C69-C70
24	L	602	HEA	C27-C19-C20-C21
29	c	301	PLM	C2-C3-C4-C5
14	N	606	MQ9	C38-C39-C41-C42
14	H	907	MQ9	C38-C39-C41-C42
22	R	608	TRD	C9-C10-C11-C12
22	L	607	TRD	C9-C10-C11-C12
28	Y	302	9XX	O-C16-C17-O1
28	c	302	9XX	O-C16-C17-O1
15	C	304	WUO	C69-C70-C71-C72
21	N	602	CDL	C57-C58-C59-C60
15	O	304	WUO	C14-C16-C17-C18
19	S	501	7PH	O11-C1-C2-O21
21	P	301	CDL	OA5-CA3-CA4-OA6
21	R	601	CDL	OB5-CB3-CB4-OB6
21	H	903	CDL	C57-C58-C59-C60
21	R	605	CDL	C11-CA5-OA6-CA4
18	W	201	9YF	C9-C10-C11-C12
18	b	201	9YF	C9-C10-C11-C12
15	I	303	WUO	C35-C37-O38-C39
21	H	905	CDL	C53-C54-C55-C56
17	G	903	IZL	O34-C45-C46-O32
18	M	503	9YF	O9-C-C24-O11
18	G	904	9YF	O9-C-C24-O11
21	J	501	CDL	OB6-CB4-CB6-OB8
21	L	601	CDL	OB6-CB4-CB6-OB8
21	N	604	CDL	C77-C78-C79-C80
21	I	302	CDL	C36-C37-C38-C39
21	N	603	CDL	C54-C55-C56-C57
24	L	602	HEA	C18-C19-C20-C21
21	N	602	CDL	C16-C17-C18-C19
21	H	903	CDL	C16-C17-C18-C19
21	J	501	CDL	CB5-C51-C52-C53

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Mol	Chain	Res	Type	Atoms
17	G	903	IZL	C7-C1-C2-C3
22	X	403	TRD	C4-C5-C6-C7
22	Q	403	TRD	C4-C5-C6-C7
28	c	302	9XX	C10-C11-C12-C13
18	M	503	9YF	C14-C15-C16-C17
18	G	904	9YF	C14-C15-C16-C17
21	C	305	CDL	C31-C32-C33-C34
21	I	302	CDL	C59-C60-C61-C62
21	T	1302	CDL	C79-C80-C81-C82
21	H	904	CDL	C51-C52-C53-C54
14	N	608	MQ9	C9-C11-C12-C13
14	H	909	MQ9	C9-C11-C12-C13
15	O	304	WUO	C16-C14-O13-C12
21	R	601	CDL	C39-C40-C41-C42
21	P	301	CDL	C58-C59-C60-C61
18	M	503	9YF	C33-C35-C36-C37
18	G	904	9YF	C33-C35-C36-C37
21	H	903	CDL	C12-C13-C14-C15
21	R	601	CDL	CA2-C1-CB2-OB2
21	C	305	CDL	CA2-C1-CB2-OB2
21	I	302	CDL	CB2-C1-CA2-OA2
21	J	501	CDL	CA2-C1-CB2-OB2
15	C	304	WUO	C66-C67-C68-C69
21	N	602	CDL	C12-C13-C14-C15
15	C	304	WUO	O15-C14-O13-C12
21	R	605	CDL	OA9-CA7-OA8-CA6
15	O	304	WUO	C23-C24-C25-C26
21	C	305	CDL	OA5-CA3-CA4-CA6
21	I	301	CDL	OA5-CA3-CA4-CA6
15	O	304	WUO	C64-C65-C66-C67
21	H	904	CDL	C37-C38-C39-C40
15	O	304	WUO	C87-C88-C90-C91
15	I	303	WUO	C86-C87-C88-C90
21	J	501	CDL	C72-C73-C74-C75
23	S	503	3PE	C28-C29-C2A-C2B
15	C	304	WUO	C70-C71-C72-C73
21	H	904	CDL	C33-C34-C35-C36
21	L	601	CDL	C16-C17-C18-C19
23	J	503	3PE	C28-C29-C2A-C2B
20	N	601	HEM	C3D-CAD-CBD-CGD
17	M	502	IZL	C23-C24-O11-C25
21	L	601	CDL	C76-C77-C78-C79

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Mol	Chain	Res	Type	Atoms
21	R	601	CDL	C55-C56-C57-C58
21	J	501	CDL	C12-C13-C14-C15
15	C	304	WUO	C80-C81-C82-C83
20	N	601	HEM	C2C-C3C-CAC-CBC
15	O	304	WUO	C72-C73-C74-C75
28	W	202	9XX	C32-C33-C34-C35
21	L	601	CDL	C54-C55-C56-C57
28	c	302	9XX	C22-C23-C24-C25
15	C	304	WUO	C56-C57-O58-C59
19	N	609	7PH	C3-C2-O21-C21
19	H	901	7PH	C3-C2-O21-C21
15	O	304	WUO	C93-C94-C95-C96
15	I	303	WUO	C81-C82-C83-C84
15	O	304	WUO	C26-C27-C28-C29
15	I	303	WUO	C69-C70-C71-C72
21	J	501	CDL	C76-C77-C78-C79
21	T	1302	CDL	OA5-CA3-CA4-OA6
21	I	301	CDL	OB5-CB3-CB4-OB6
21	I	302	CDL	OA5-CA3-CA4-OA6
21	L	601	CDL	OB5-CB3-CB4-OB6
23	S	503	3PE	O11-C1-C2-O21
23	J	503	3PE	O11-C1-C2-O21
21	I	301	CDL	C31-C32-C33-C34
21	I	301	CDL	C71-C72-C73-C74
15	C	304	WUO	C56-C57-C76-O77
19	M	504	7PH	C1-C2-C3-O31
19	G	905	7PH	C1-C2-C3-O31
21	I	302	CDL	CB3-CB4-CB6-OB8
28	Y	302	9XX	O6-C15-O-C16
14	O	303	MQ9	C47-C48-C49-C50
14	C	303	MQ9	C47-C48-C49-C50
21	C	305	CDL	C72-C73-C74-C75
21	P	301	CDL	C18-C19-C20-C21
15	C	304	WUO	C23-C24-C25-C26
21	N	604	CDL	C53-C54-C55-C56
21	H	904	CDL	C56-C57-C58-C59
18	W	201	9YF	O9-C-C24-O11
18	b	201	9YF	O9-C-C24-O11
21	N	602	CDL	OB6-CB4-CB6-OB8
21	N	603	CDL	OB6-CB4-CB6-OB8
21	T	1302	CDL	OA6-CA4-CA6-OA8
21	R	605	CDL	OA6-CA4-CA6-OA8

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Mol	Chain	Res	Type	Atoms
21	R	605	CDL	OB6-CB4-CB6-OB8
21	C	305	CDL	OA6-CA4-CA6-OA8
21	H	903	CDL	OB6-CB4-CB6-OB8
19	S	501	7PH	C37-C38-C39-C3A
21	I	301	CDL	C36-C37-C38-C39
15	P	302	WUO	C16-C17-C18-C19
15	I	303	WUO	C71-C72-C73-C74
21	H	904	CDL	C16-C17-C18-C19
15	O	304	WUO	O15-C14-O13-C12
21	R	601	CDL	C52-C53-C54-C55
21	I	301	CDL	C18-C19-C20-C21
21	I	302	CDL	C54-C55-C56-C57
21	R	605	CDL	C36-C37-C38-C39
15	O	304	WUO	C17-C18-C19-C20
18	M	503	9YF	C16-C17-C18-C19
18	G	904	9YF	C16-C17-C18-C19
21	L	601	CDL	C79-C80-C81-C82
21	N	602	CDL	C1-CB2-OB2-PB2
21	N	604	CDL	C1-CB2-OB2-PB2
21	H	903	CDL	C1-CB2-OB2-PB2
17	G	903	IZL	C52-C53-C54-C55
18	M	503	9YF	C2-O2-P-O1
18	G	904	9YF	C2-O2-P-O1
21	I	302	CDL	C35-C36-C37-C38
28	b	203	9XX	C20-C21-C22-C23
21	I	301	CDL	O1-C1-CB2-OB2
19	G	905	7PH	C32-C33-C34-C35
19	M	504	7PH	C32-C33-C34-C35
21	N	603	CDL	C16-C17-C18-C19
21	P	301	CDL	C60-C61-C62-C63
21	R	601	CDL	C17-C18-C19-C20
21	I	301	CDL	C37-C38-C39-C40
21	L	601	CDL	C74-C75-C76-C77
21	N	604	CDL	C17-C18-C19-C20
21	R	605	CDL	OA7-CA5-OA6-CA4
21	P	301	CDL	C71-CB7-OB8-CB6
19	S	501	7PH	C28-C29-C2A-C2B
18	M	503	9YF	C20-C21-C22-C23
18	G	904	9YF	C20-C21-C22-C23
21	T	1302	CDL	C36-C37-C38-C39
14	M	505	MQ9	C27-C28-C29-C31
14	G	901	MQ9	C27-C28-C29-C31

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Mol	Chain	Res	Type	Atoms
21	H	905	CDL	C55-C56-C57-C58
21	H	905	CDL	C19-C20-C21-C22
21	P	301	CDL	C57-C58-C59-C60
21	I	301	CDL	C74-C75-C76-C77
21	I	301	CDL	OB5-CB3-CB4-CB6
21	L	601	CDL	OB5-CB3-CB4-CB6
23	S	503	3PE	O11-C1-C2-C3
21	N	604	CDL	C23-C24-C25-C26
17	G	903	IZL	C66-C68-C69-C70
21	T	1302	CDL	C81-C82-C83-C84
18	W	201	9YF	C32-C33-C35-C36
18	b	201	9YF	C32-C33-C35-C36
28	W	202	9XX	C25-C26-C27-C28
18	M	503	9YF	C29-C30-C31-C32
18	G	904	9YF	C29-C30-C31-C32
21	P	301	CDL	C14-C15-C16-C17
21	I	302	CDL	C38-C39-C40-C41
15	O	304	WUO	C21-C22-C23-C24
21	I	301	CDL	C1-CB2-OB2-PB2
13	O	302	HEC	C4B-C3B-CAB-CBB
15	O	304	WUO	O55-C56-C57-O58
21	P	301	CDL	OB5-CB3-CB4-OB6
21	C	305	CDL	OA5-CA3-CA4-OA6
21	H	904	CDL	OB5-CB3-CB4-OB6
21	N	603	CDL	C51-C52-C53-C54
21	P	301	CDL	C56-C57-C58-C59
29	b	202	PLM	C4-C5-C6-C7
15	C	304	WUO	O58-C57-C76-O77
19	M	504	7PH	O21-C2-C3-O31
19	G	905	7PH	O21-C2-C3-O31
21	N	604	CDL	OA6-CA4-CA6-OA8
21	P	301	CDL	OA6-CA4-CA6-OA8
21	T	1302	CDL	OB6-CB4-CB6-OB8
21	C	305	CDL	OB6-CB4-CB6-OB8
21	H	904	CDL	OB6-CB4-CB6-OB8
21	I	301	CDL	OB6-CB4-CB6-OB8
21	I	302	CDL	OB6-CB4-CB6-OB8
21	N	602	CDL	C76-C77-C78-C79
21	H	903	CDL	C76-C77-C78-C79
21	H	904	CDL	C34-C35-C36-C37
18	W	201	9YF	C1-C-C24-O11
18	b	201	9YF	C1-C-C24-O11

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Mol	Chain	Res	Type	Atoms
21	N	604	CDL	CA3-CA4-CA6-OA8
21	H	904	CDL	CB3-CB4-CB6-OB8
21	H	905	CDL	CB3-CB4-CB6-OB8
14	T	1301	MQ9	C25-C24-C26-C27
24	R	603	HEA	O11-C11-C3B-C4B
24	L	603	HEA	O11-C11-C3B-C4B
21	P	301	CDL	OB9-CB7-OB8-CB6
21	T	1302	CDL	CB7-C71-C72-C73
21	T	1302	CDL	C11-C12-C13-C14
21	N	602	CDL	C58-C59-C60-C61
21	H	903	CDL	C58-C59-C60-C61
13	O	302	HEC	C2B-C3B-CAB-CBB
13	C	302	HEC	C2B-C3B-CAB-CBB
15	C	304	WUO	C56-O55-P52-O51
15	C	304	WUO	C56-O55-P52-O53
18	W	201	9YF	C1-O-P-O2
18	W	201	9YF	C1-O-P-O8
18	b	201	9YF	C1-O-P-O2
18	b	201	9YF	C1-O-P-O8
21	N	602	CDL	CB3-OB5-PB2-OB2
21	N	603	CDL	CB2-OB2-PB2-OB4
21	N	603	CDL	CB3-OB5-PB2-OB3
21	N	604	CDL	CB3-OB5-PB2-OB2
21	P	301	CDL	CA2-OA2-PA1-OA4
21	T	1302	CDL	CA2-OA2-PA1-OA5
21	T	1302	CDL	CA3-OA5-PA1-OA3
21	R	601	CDL	CB2-OB2-PB2-OB4
21	R	601	CDL	CB2-OB2-PB2-OB5
21	R	605	CDL	CA2-OA2-PA1-OA3
21	R	605	CDL	CA2-OA2-PA1-OA4
21	R	605	CDL	CA2-OA2-PA1-OA5
21	R	605	CDL	CB3-OB5-PB2-OB4
21	C	305	CDL	CA2-OA2-PA1-OA5
21	C	305	CDL	CB2-OB2-PB2-OB3
21	H	903	CDL	CB3-OB5-PB2-OB2
21	H	904	CDL	CB2-OB2-PB2-OB5
21	H	904	CDL	CB3-OB5-PB2-OB3
21	H	905	CDL	CA2-OA2-PA1-OA4
21	I	301	CDL	CA2-OA2-PA1-OA5
21	I	302	CDL	CB2-OB2-PB2-OB3
21	I	302	CDL	CB2-OB2-PB2-OB4
21	I	302	CDL	CB2-OB2-PB2-OB5

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Mol	Chain	Res	Type	Atoms
21	J	501	CDL	CA3-OA5-PA1-OA3
21	J	501	CDL	CB2-OB2-PB2-OB3
21	J	501	CDL	CB2-OB2-PB2-OB5
21	J	501	CDL	CB3-OB5-PB2-OB3
21	L	601	CDL	CA3-OA5-PA1-OA2
21	L	601	CDL	CA3-OA5-PA1-OA4
21	L	601	CDL	CB2-OB2-PB2-OB3
23	S	503	3PE	C1-O11-P-O12
23	S	503	3PE	C11-O13-P-O14
23	J	503	3PE	C1-O11-P-O12
23	J	503	3PE	C11-O13-P-O14
24	R	603	HEA	O11-C11-C3B-C2B
28	c	302	9XX	C16-C17-O1-C18
14	T	1301	MQ9	C23-C24-C26-C27
14	K	1301	MQ9	C13-C14-C16-C17
21	P	301	CDL	C1-CB2-OB2-PB2
21	H	905	CDL	C1-CB2-OB2-PB2
21	J	501	CDL	CB4-CB3-OB5-PB2
18	M	503	9YF	C38-C39-C40-C41
18	G	904	9YF	C38-C39-C40-C41
21	H	905	CDL	C12-C11-CA5-OA6
21	N	603	CDL	C37-C38-C39-C40
21	P	301	CDL	C11-C12-C13-C14
21	T	1302	CDL	C80-C81-C82-C83
21	C	305	CDL	C51-C52-C53-C54
15	P	302	WUO	C82-C83-C84-C85
21	L	601	CDL	C52-C53-C54-C55
21	L	601	CDL	C11-C12-C13-C14
19	H	901	7PH	C35-C36-C37-C38
21	R	601	CDL	C59-C60-C61-C62
15	P	302	WUO	C56-C57-O58-C59
21	N	604	CDL	CA6-CA4-OA6-CA5
21	T	1302	CDL	CA3-CA4-OA6-CA5
23	S	503	3PE	C3-C2-O21-C21
23	J	503	3PE	C3-C2-O21-C21
19	N	609	7PH	C35-C36-C37-C38
29	c	301	PLM	C7-C8-C9-CA
21	P	301	CDL	C12-C11-CA5-OA6
21	R	601	CDL	C51-C52-C53-C54
21	I	301	CDL	C58-C59-C60-C61
22	Q	403	TRD	C6-C7-C8-C9
22	X	403	TRD	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
15	O	304	WUO	C31-C01-O02-C03
21	R	601	CDL	C35-C36-C37-C38
18	W	201	9YF	C24-C-C1-O
18	b	201	9YF	C24-C-C1-O
21	R	605	CDL	OB5-CB3-CB4-CB6
15	O	304	WUO	C71-C72-C73-C74
28	W	202	9XX	C25-C26-C27-C36
21	N	602	CDL	CB2-C1-CA2-OA2
21	H	903	CDL	CB2-C1-CA2-OA2
21	N	602	CDL	OA5-CA3-CA4-OA6
21	H	903	CDL	OA5-CA3-CA4-OA6
21	I	301	CDL	OA5-CA3-CA4-OA6
21	T	1302	CDL	C53-C54-C55-C56
21	H	904	CDL	C58-C59-C60-C61
15	C	304	WUO	C20-C21-C22-C23
21	I	301	CDL	OA6-CA4-CA6-OA8
19	G	905	7PH	C23-C24-C25-C26
19	M	504	7PH	C23-C24-C25-C26
21	J	501	CDL	C52-C51-CB5-OB6
21	J	501	CDL	C53-C54-C55-C56
21	J	501	CDL	CA3-CA4-CA6-OA8
21	J	501	CDL	CB3-CB4-CB6-OB8
15	I	303	WUO	O40-C41-C48-O49
21	I	302	CDL	C37-C38-C39-C40
21	C	305	CDL	C55-C56-C57-C58
29	b	202	PLM	C3-C4-C5-C6
15	I	303	WUO	C17-C18-C19-C20
14	O	303	MQ9	C47-C48-C49-C51
14	T	1301	MQ9	C31-C32-C33-C34
13	O	301	HEC	CAD-CBD-CGD-O2D
13	C	301	HEC	CAD-CBD-CGD-O2D
21	H	905	CDL	C23-C24-C25-C26
17	G	903	IZL	C68-C69-C70-C74
14	N	606	MQ9	C27-C28-C29-C30
14	H	907	MQ9	C27-C28-C29-C30
21	L	601	CDL	C71-C72-C73-C74
15	C	304	WUO	C31-C01-O02-C03
13	O	302	HEC	CAA-CBA-CGA-O2A
21	R	605	CDL	C13-C14-C15-C16
21	T	1302	CDL	OB5-CB3-CB4-OB6
14	C	303	MQ9	C47-C48-C49-C51
21	H	905	CDL	C24-C25-C26-C27

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Mol	Chain	Res	Type	Atoms
21	I	301	CDL	C54-C55-C56-C57
18	M	503	9YF	C31-C32-C33-C35
18	G	904	9YF	C31-C32-C33-C35
28	b	203	9XX	C25-C26-C27-C28
21	T	1302	CDL	O1-C1-CB2-OB2
21	R	605	CDL	C52-C53-C54-C55
21	I	301	CDL	C55-C56-C57-C58
28	W	202	9XX	C11-C10-C9-C8
21	J	501	CDL	OA6-CA4-CA6-OA8
14	N	605	MQ9	C12-C11-C9-C10
14	K	1301	MQ9	C20-C19-C21-C22
18	W	201	9YF	C26-C27-C28-C29
18	b	201	9YF	C26-C27-C28-C29
18	M	503	9YF	C18-C19-C20-C21
18	G	904	9YF	C18-C19-C20-C21
21	N	603	CDL	C12-C13-C14-C15
21	H	904	CDL	CA4-CA3-OA5-PA1
21	J	501	CDL	C1-CB2-OB2-PB2
21	R	601	CDL	C34-C35-C36-C37
24	R	602	HEA	CAA-CBA-CGA-O2A
24	L	602	HEA	CAA-CBA-CGA-O2A
14	H	906	MQ9	C12-C11-C9-C10
21	C	305	CDL	C71-CB7-OB8-CB6
21	R	605	CDL	CB3-CB4-CB6-OB8
28	Y	302	9XX	C7-C8-C9-C10
15	P	302	WUO	C61-C62-C63-C64
15	P	302	WUO	C84-C85-C86-C87
20	H	902	HEM	CAA-CBA-CGA-O1A
28	c	302	9XX	C25-C26-C27-C36
21	N	603	CDL	C72-C73-C74-C75
29	W	203	PLM	C6-C7-C8-C9
15	P	302	WUO	C21-C22-C23-C24
28	c	302	9XX	C23-C24-C25-C26
24	R	602	HEA	CAA-CBA-CGA-O1A
17	M	502	IZL	C46-C45-O34-C60
21	T	1302	CDL	CA6-CA4-OA6-CA5
21	H	905	CDL	CB3-CB4-OB6-CB5
21	H	905	CDL	CB6-CB4-OB6-CB5
21	N	604	CDL	OA7-CA5-OA6-CA4
15	P	302	WUO	C20-C21-C22-C23
21	T	1302	CDL	C34-C35-C36-C37
13	C	302	HEC	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
24	L	602	HEA	CAA-CBA-CGA-O1A
21	N	603	CDL	C32-C31-CA7-OA8
21	R	601	CDL	C52-C51-CB5-OB6
15	O	304	WUO	C50-C01-O02-C03
20	N	607	HEM	CAA-CBA-CGA-O1A
21	I	301	CDL	C12-C11-CA5-OA7
13	O	301	HEC	CAD-CBD-CGD-O1D
13	C	301	HEC	CAD-CBD-CGD-O1D
19	N	609	7PH	O11-C1-C2-O21
19	H	901	7PH	O11-C1-C2-O21
21	R	601	CDL	O1-C1-CB2-OB2
20	N	607	HEM	CAA-CBA-CGA-O2A
20	H	908	HEM	CAA-CBA-CGA-O2A
28	b	203	9XX	C19-C20-C21-C22
24	R	602	HEA	O11-C11-C12-C13
24	L	602	HEA	O11-C11-C12-C13
24	L	603	HEA	O11-C11-C12-C13
21	L	601	CDL	C55-C56-C57-C58
20	H	908	HEM	CAA-CBA-CGA-O1A
14	K	1301	MQ9	C15-C14-C16-C17
18	G	904	9YF	C24-C-C1-O
21	L	601	CDL	OA5-CA3-CA4-CA6
21	C	305	CDL	OB9-CB7-OB8-CB6
14	K	1301	MQ9	C18-C19-C21-C22
17	G	903	IZL	C14-C43-O28-P
15	O	304	WUO	C50-C37-O38-C39
15	O	304	WUO	C68-C69-C70-C71
20	H	902	HEM	CAA-CBA-CGA-O2A
21	H	904	CDL	C72-C73-C74-C75
14	O	303	MQ9	C29-C31-C32-C33
14	C	303	MQ9	C29-C31-C32-C33
21	H	904	CDL	C12-C13-C14-C15
18	M	503	9YF	C35-C36-C37-C38
18	G	904	9YF	C35-C36-C37-C38
21	I	301	CDL	C33-C34-C35-C36
20	N	601	HEM	CAA-CBA-CGA-O2A
21	N	604	CDL	C11-CA5-OA6-CA4
21	C	305	CDL	C14-C15-C16-C17
21	R	605	CDL	CB4-CB6-OB8-CB7
21	C	305	CDL	C74-C75-C76-C77
28	b	203	9XX	C18-C19-C20-C21
14	N	605	MQ9	C27-C28-C29-C30

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Mol	Chain	Res	Type	Atoms
14	H	906	MQ9	C27-C28-C29-C30
21	N	603	CDL	CA4-CA3-OA5-PA1
21	I	302	CDL	C1-CA2-OA2-PA1
24	R	603	HEA	CAD-CBD-CGD-O2D
15	P	302	WUO	C31-C01-O02-C03
28	b	203	9XX	C5-C6-C7-C8
14	N	608	MQ9	C41-C42-C43-C44
14	H	909	MQ9	C41-C42-C43-C44
24	L	603	HEA	CAD-CBD-CGD-O2D
21	N	603	CDL	OB9-CB7-OB8-CB6
18	W	201	9YF	C36-C37-C38-C39
19	M	504	7PH	O11-C1-C2-O21
19	G	905	7PH	O11-C1-C2-O21
21	N	603	CDL	C71-CB7-OB8-CB6
18	b	201	9YF	C36-C37-C38-C39
22	K	1302	TRD	C11-C10-C9-C8
13	C	302	HEC	CAA-CBA-CGA-O1A
22	T	1303	TRD	C11-C10-C9-C8
22	R	608	TRD	C10-C11-C12-C13
22	L	607	TRD	C10-C11-C12-C13
17	G	903	IZL	C61-C62-C63-C64
15	P	302	WUO	C91-C92-C93-C94
17	M	502	IZL	C3-C4-C5-C6
28	W	202	9XX	C3-C4-C5-C6
14	T	1301	MQ9	C7-C8-C9-C11
21	R	605	CDL	C52-C51-CB5-OB6
21	R	605	CDL	C56-C57-C58-C59
13	O	302	HEC	CAA-CBA-CGA-O1A
21	T	1302	CDL	OB5-CB3-CB4-CB6
28	W	202	9XX	C12-C13-C14-C15
20	N	601	HEM	CAA-CBA-CGA-O1A
24	L	602	HEA	CAD-CBD-CGD-O1D
19	H	901	7PH	O31-C31-C32-C33
14	K	1301	MQ9	C26-C27-C28-C29
17	M	502	IZL	C15-C14-O3-C13
24	R	602	HEA	CAD-CBD-CGD-O1D
21	H	905	CDL	C79-C80-C81-C82
21	L	601	CDL	C36-C37-C38-C39
19	N	609	7PH	O31-C31-C32-C33
21	I	302	CDL	C12-C13-C14-C15
21	J	501	CDL	O1-C1-CB2-OB2
28	W	202	9XX	C7-C8-C9-C10

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Mol	Chain	Res	Type	Atoms
21	J	501	CDL	CB7-C71-C72-C73
28	b	203	9XX	C25-C26-C27-C36
22	T	1303	TRD	C4-C5-C6-C7
22	K	1302	TRD	C4-C5-C6-C7
24	R	603	HEA	CAD-CBD-CGD-O1D
21	T	1302	CDL	C78-C79-C80-C81
21	I	301	CDL	C73-C74-C75-C76
18	M	503	9YF	C36-C37-C38-C39
18	G	904	9YF	C36-C37-C38-C39
24	L	603	HEA	CAD-CBD-CGD-O1D
21	H	905	CDL	C54-C55-C56-C57
24	R	602	HEA	CAD-CBD-CGD-O2D
21	J	501	CDL	C80-C81-C82-C83
24	L	602	HEA	CAD-CBD-CGD-O2D
19	S	501	7PH	C24-C25-C26-C27
14	T	1301	MQ9	C34-C36-C37-C38
20	N	601	HEM	C4C-C3C-CAC-CBC
14	N	606	MQ9	C42-C43-C44-C45
14	H	907	MQ9	C42-C43-C44-C45
13	O	301	HEC	CAA-CBA-CGA-O1A
13	C	301	HEC	CAA-CBA-CGA-O1A
21	H	903	CDL	C13-C14-C15-C16
15	O	304	WUO	C35-C37-O38-C39
21	N	604	CDL	C54-C55-C56-C57
21	N	604	CDL	C74-C75-C76-C77
21	J	501	CDL	C13-C14-C15-C16
21	P	301	CDL	C33-C34-C35-C36
21	H	904	CDL	C73-C74-C75-C76
21	N	602	CDL	C13-C14-C15-C16
21	I	302	CDL	C39-C40-C41-C42
17	M	502	IZL	C43-C14-O3-C13
29	W	203	PLM	C7-C8-C9-CA
21	J	501	CDL	C72-C71-CB7-OB8
21	N	602	CDL	C55-C56-C57-C58
18	W	201	9YF	C11-C12-C13-C14
21	H	903	CDL	C55-C56-C57-C58
21	R	601	CDL	C56-C57-C58-C59
15	I	303	WUO	O58-C59-C61-C62
28	W	202	9XX	C13-C14-C15-O
18	M	503	9YF	C24-C-C1-O
21	H	904	CDL	OB5-CB3-CB4-CB6
21	I	302	CDL	OA5-CA3-CA4-CA6

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Mol	Chain	Res	Type	Atoms
18	b	201	9YF	C11-C12-C13-C14
21	T	1302	CDL	C52-C53-C54-C55
15	P	302	WUO	C50-C01-O02-C03
21	H	905	CDL	C71-C72-C73-C74
18	W	201	9YF	C18-C19-C20-C21
18	b	201	9YF	C18-C19-C20-C21
14	N	605	MQ9	C24-C26-C27-C28
14	H	906	MQ9	C24-C26-C27-C28
21	P	301	CDL	C35-C36-C37-C38
23	S	503	3PE	C22-C23-C24-C25
15	P	302	WUO	C50-O51-P52-O53
17	M	502	IZL	C43-O28-P-O29
17	G	903	IZL	C43-O28-P-O29
17	G	903	IZL	C43-O28-P-O30
18	W	201	9YF	C2-O2-P-O8
18	b	201	9YF	C2-O2-P-O8
22	J	502	TRD	C9-C10-C11-C12
22	S	502	TRD	C9-C10-C11-C12
17	M	502	IZL	O1-C10-C9-C8
21	C	305	CDL	C72-C71-CB7-OB8
17	G	903	IZL	C55-C56-C58-C59
14	N	605	MQ9	C12-C11-C9-C8
14	H	906	MQ9	C12-C11-C9-C8
15	C	304	WUO	C50-C01-O02-C03
15	P	302	WUO	C57-C56-O55-P52
21	I	301	CDL	C11-C12-C13-C14
17	M	502	IZL	C44-C45-C46-O32
21	P	301	CDL	CA3-CA4-CA6-OA8
15	C	304	WUO	C19-C20-C21-C22
28	c	302	9XX	C7-C8-C9-C10
28	W	202	9XX	C2-C3-C4-C5
14	M	505	MQ9	C25-C24-C26-C27
14	G	901	MQ9	C25-C24-C26-C27
28	W	202	9XX	C-C1-C2-C3
15	P	302	WUO	O13-C14-C16-C17
21	P	301	CDL	OB6-CB4-CB6-OB8
14	M	505	MQ9	C11-C12-C13-C14
14	G	901	MQ9	C11-C12-C13-C14
14	K	1301	MQ9	C31-C32-C33-C34
22	S	502	TRD	C7-C8-C9-C10
28	Y	302	9XX	O1-C18-C19-C20
19	S	501	7PH	C32-C33-C34-C35

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Mol	Chain	Res	Type	Atoms
22	J	502	TRD	C7-C8-C9-C10
21	N	603	CDL	C59-C60-C61-C62
13	C	301	HEC	CAA-CBA-CGA-O2A
17	G	903	IZL	C1-C2-C3-C4
19	M	504	7PH	C33-C34-C35-C36
23	J	503	3PE	C22-C23-C24-C25
28	c	302	9XX	C13-C14-C15-O
19	G	905	7PH	C33-C34-C35-C36
19	M	504	7PH	C27-C28-C29-C2A
19	G	905	7PH	C27-C28-C29-C2A
14	M	505	MQ9	C31-C32-C33-C34
14	N	605	MQ9	C11-C12-C13-C14
14	G	901	MQ9	C31-C32-C33-C34
14	H	906	MQ9	C11-C12-C13-C14
15	I	303	WUO	O13-C14-C16-C17
22	R	608	TRD	C5-C6-C7-C8
13	O	301	HEC	CAA-CBA-CGA-O2A
17	M	502	IZL	C44-C45-O34-C60
22	L	607	TRD	C5-C6-C7-C8
21	C	305	CDL	O1-C1-CB2-OB2
17	M	502	IZL	C49-C50-C51-C52
21	T	1302	CDL	C31-C32-C33-C34
21	N	604	CDL	C75-C76-C77-C78
14	K	1301	MQ9	C34-C36-C37-C38
21	L	601	CDL	CA4-CA3-OA5-PA1
13	C	302	HEC	C4B-C3B-CAB-CBB
21	R	605	CDL	C18-C19-C20-C21
21	J	501	CDL	C83-C84-C85-C86
14	N	608	MQ9	C33-C34-C36-C37
14	H	909	MQ9	C33-C34-C36-C37
15	P	302	WUO	O15-C14-C16-C17
22	R	608	TRD	C4-C5-C6-C7
22	L	607	TRD	C4-C5-C6-C7
21	L	601	CDL	C17-C18-C19-C20
15	I	303	WUO	O60-C59-C61-C62
21	C	305	CDL	C72-C71-CB7-OB9
14	N	608	MQ9	C35-C34-C36-C37
14	H	909	MQ9	C35-C34-C36-C37
15	I	303	WUO	O15-C14-C16-C17
28	c	302	9XX	C13-C14-C15-O6
13	O	302	HEC	CAD-CBD-CGD-O2D
14	T	1301	MQ9	C37-C38-C39-C40

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Mol	Chain	Res	Type	Atoms
28	W	202	9XX	C13-C14-C15-O6
19	S	501	7PH	C26-C27-C28-C29
28	Y	302	9XX	O2-C18-C19-C20
21	J	501	CDL	C72-C71-CB7-OB9
14	N	606	MQ9	C36-C37-C38-C39
14	H	907	MQ9	C36-C37-C38-C39
21	T	1302	CDL	CB4-CB3-OB5-PB2
21	I	301	CDL	CA4-CA3-OA5-PA1
20	N	607	HEM	C2C-C3C-CAC-CBC
20	H	908	HEM	C2C-C3C-CAC-CBC
17	M	502	IZL	O-C10-C9-C8
21	H	904	CDL	CA5-C11-C12-C13
21	R	605	CDL	C32-C31-CA7-OA8
21	I	301	CDL	C72-C71-CB7-OB8
15	I	303	WUO	C26-C27-C28-C29
13	C	302	HEC	CAD-CBD-CGD-O2D
14	N	605	MQ9	C27-C28-C29-C31
14	H	906	MQ9	C27-C28-C29-C31

There are no ring outliers.

58 monomers are involved in 288 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
29	W	203	PLM	1	0
18	G	904	9YF	4	0
19	H	901	7PH	10	0
29	c	301	PLM	1	0
21	C	305	CDL	10	0
21	P	301	CDL	6	0
22	L	608	TRD	1	0
15	O	304	WUO	7	0
17	G	903	IZL	2	0
18	W	201	9YF	1	0
14	H	907	MQ9	9	0
19	M	504	7PH	5	0
14	T	1301	MQ9	12	0
21	R	605	CDL	4	0
14	M	505	MQ9	16	0
21	N	602	CDL	26	0
22	J	502	TRD	4	0
21	H	904	CDL	3	0
14	N	608	MQ9	8	0

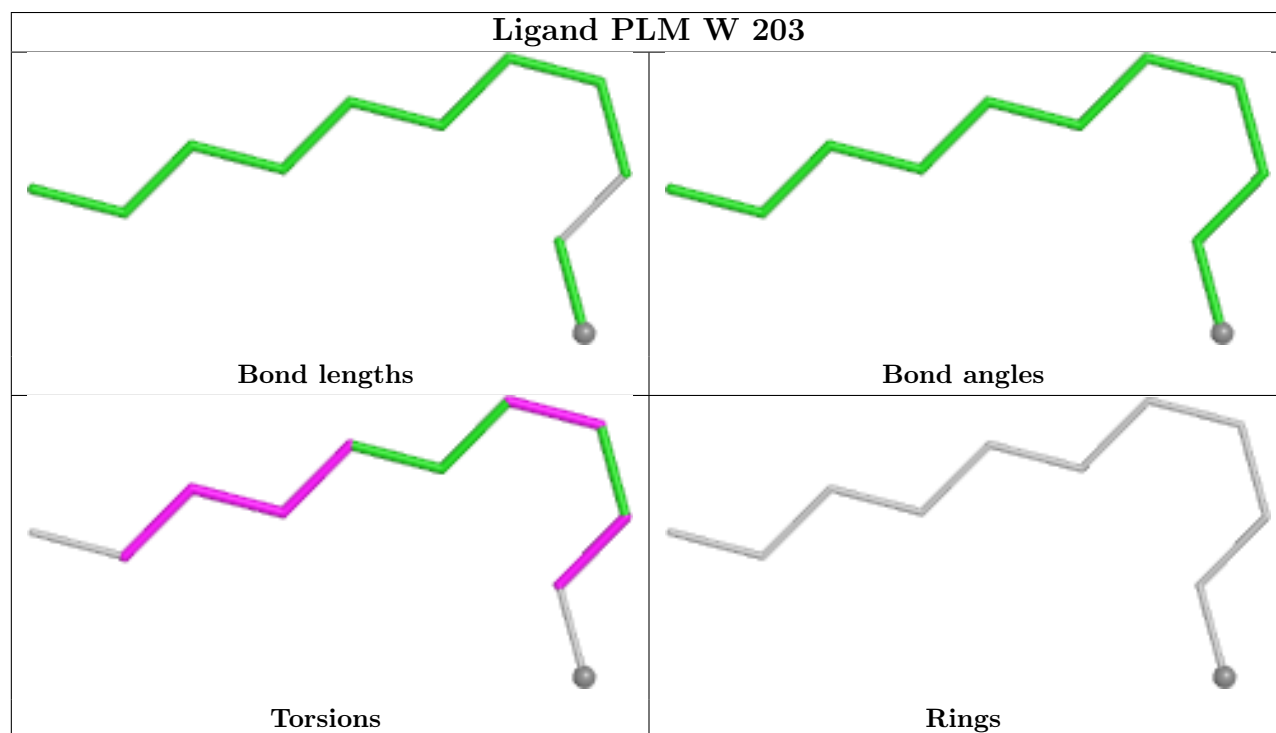
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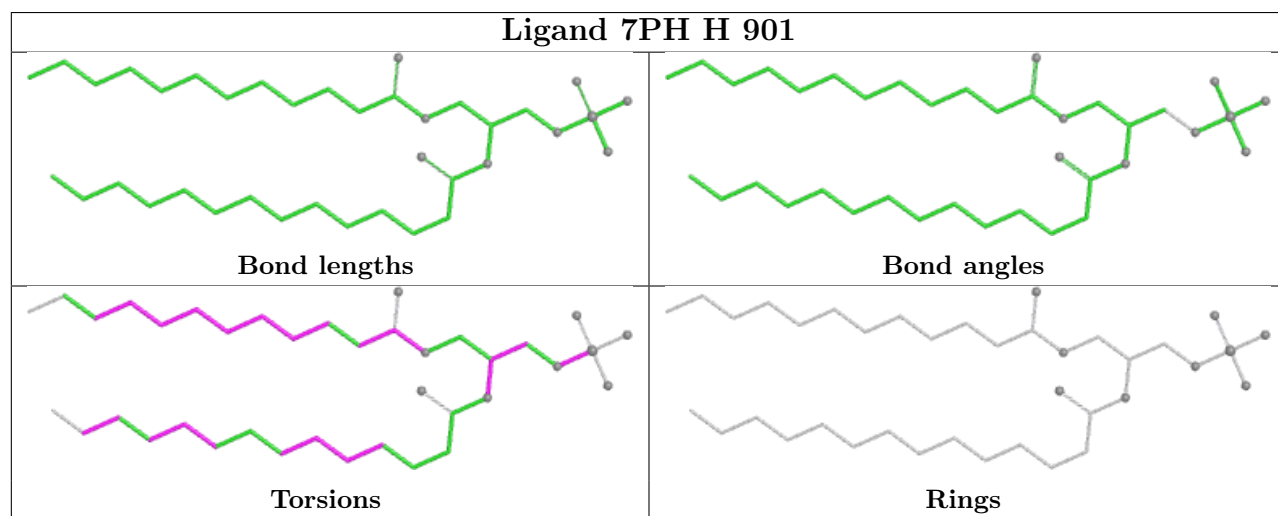
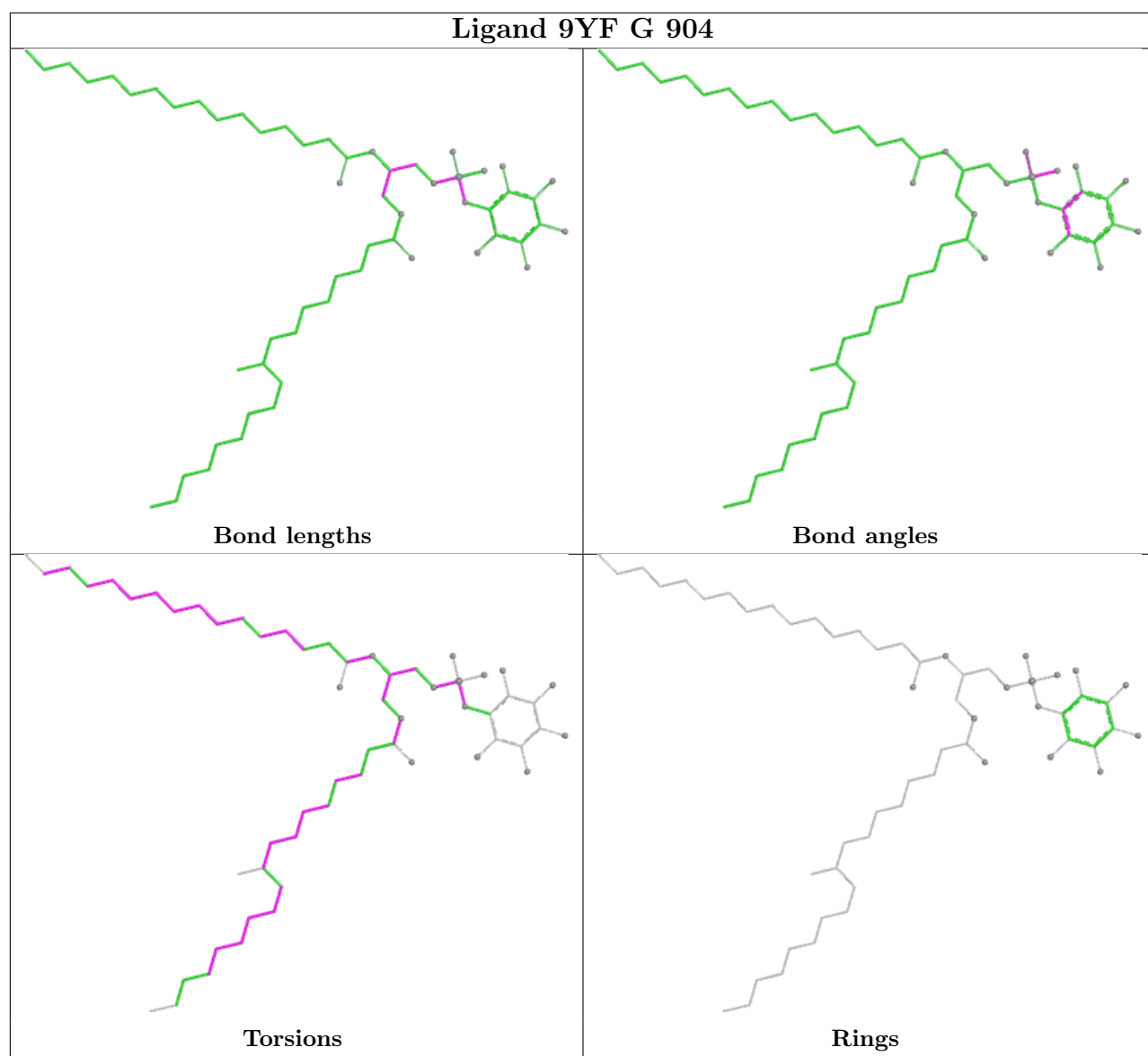
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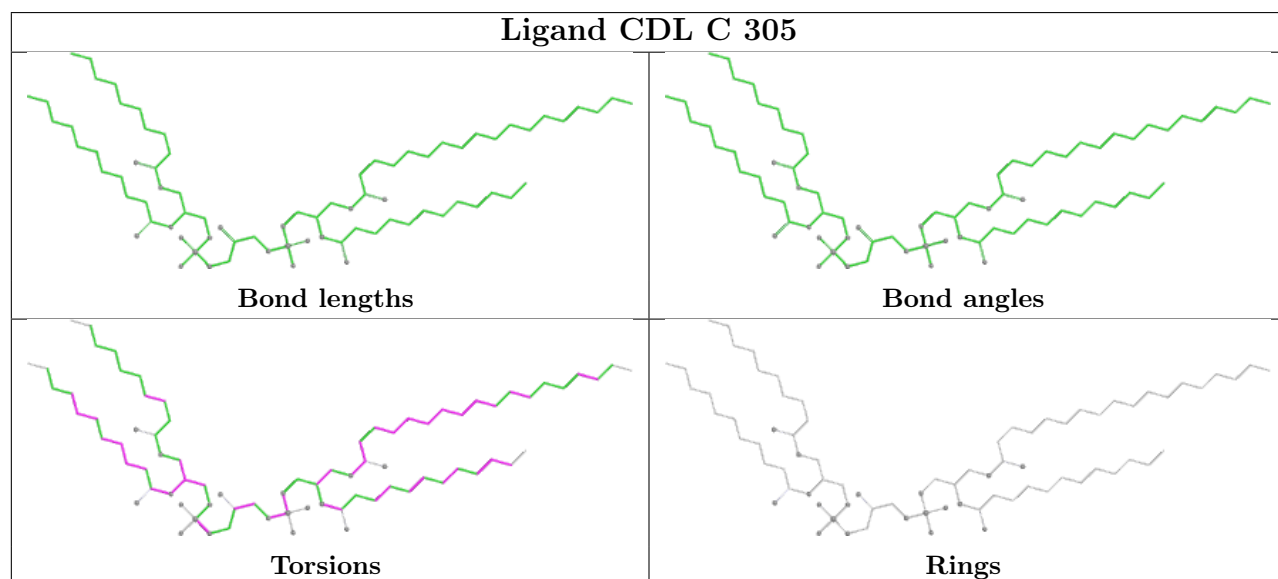
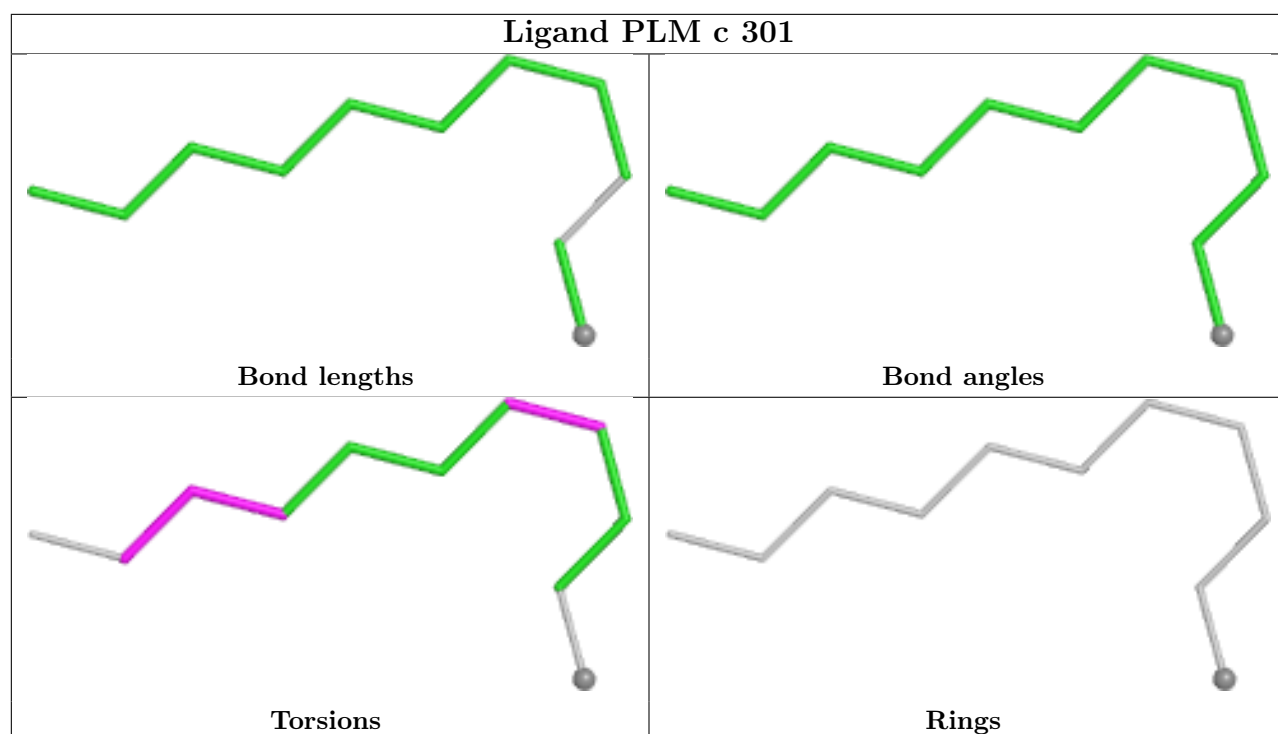
Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	M	503	9YF	3	0
19	S	501	7PH	2	0
14	H	906	MQ9	1	0
24	L	602	HEA	3	0
21	T	1302	CDL	8	0
21	N	603	CDL	2	0
13	C	302	HEC	3	0
13	O	302	HEC	2	0
14	O	303	MQ9	3	0
15	C	304	WUO	4	0
24	L	603	HEA	2	0
24	R	603	HEA	10	0
18	b	201	9YF	4	0
21	N	604	CDL	4	0
19	G	905	7PH	5	0
21	H	903	CDL	27	0
21	I	302	CDL	5	0
22	S	502	TRD	4	0
15	P	302	WUO	4	0
14	N	605	MQ9	1	0
22	R	609	TRD	1	0
14	G	901	MQ9	17	0
14	N	606	MQ9	15	0
23	S	503	3PE	4	0
21	H	905	CDL	8	0
23	J	503	3PE	1	0
24	R	602	HEA	2	0
21	R	601	CDL	2	0
21	J	501	CDL	7	0
19	N	609	7PH	9	0
14	K	1301	MQ9	9	0
22	X	403	TRD	1	0
14	C	303	MQ9	1	0
21	I	301	CDL	5	0
21	L	601	CDL	8	0
15	I	303	WUO	2	0
20	H	902	HEM	4	0
22	Q	403	TRD	1	0
14	H	909	MQ9	7	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

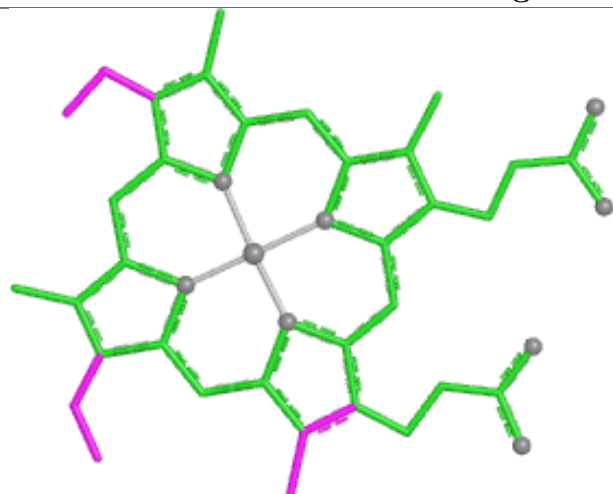
also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted 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.



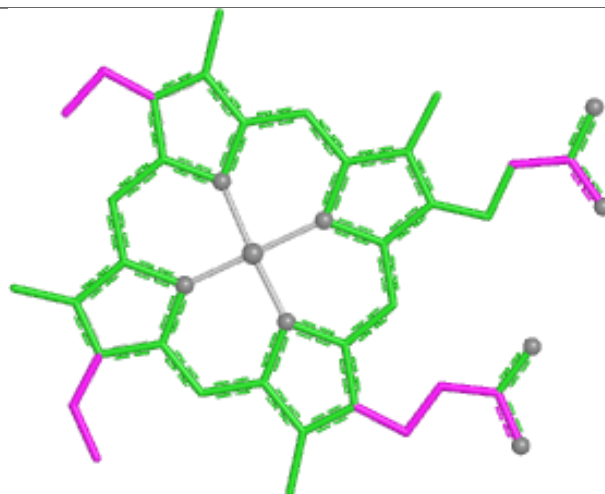




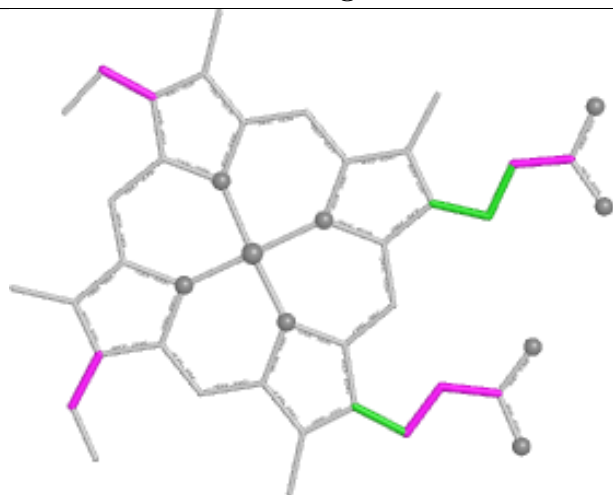
Ligand HEC C 301



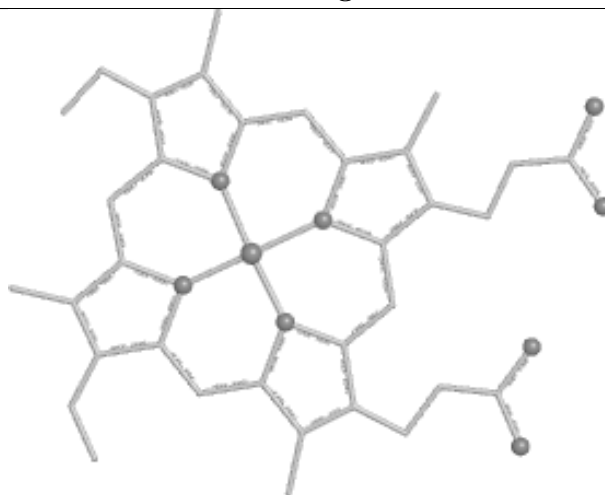
Bond lengths



Bond angles

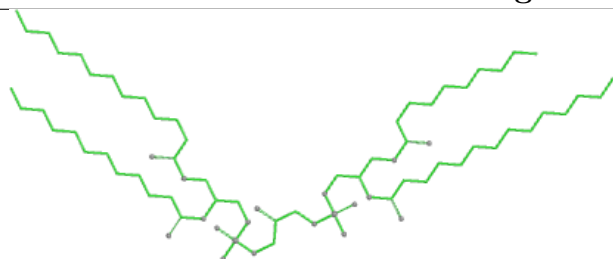


Torsions

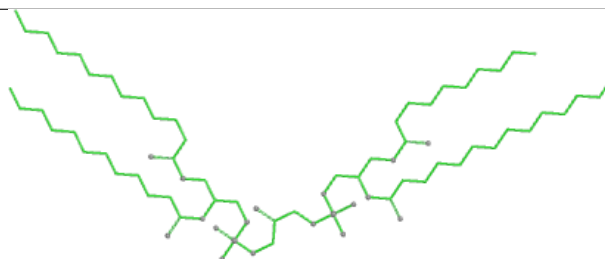


Rings

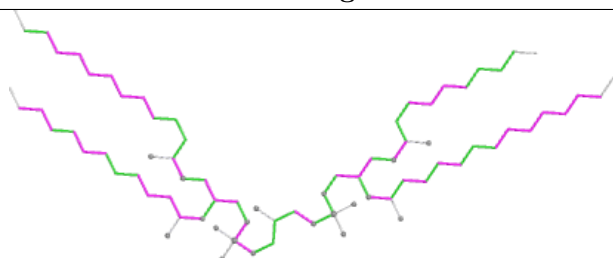
Ligand CDL P 301



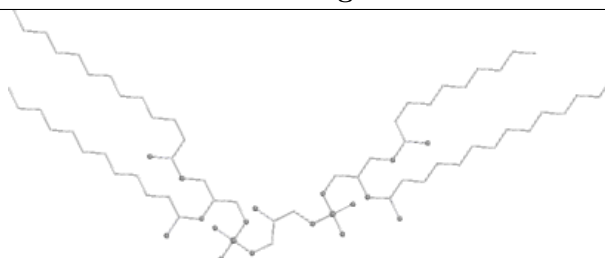
Bond lengths



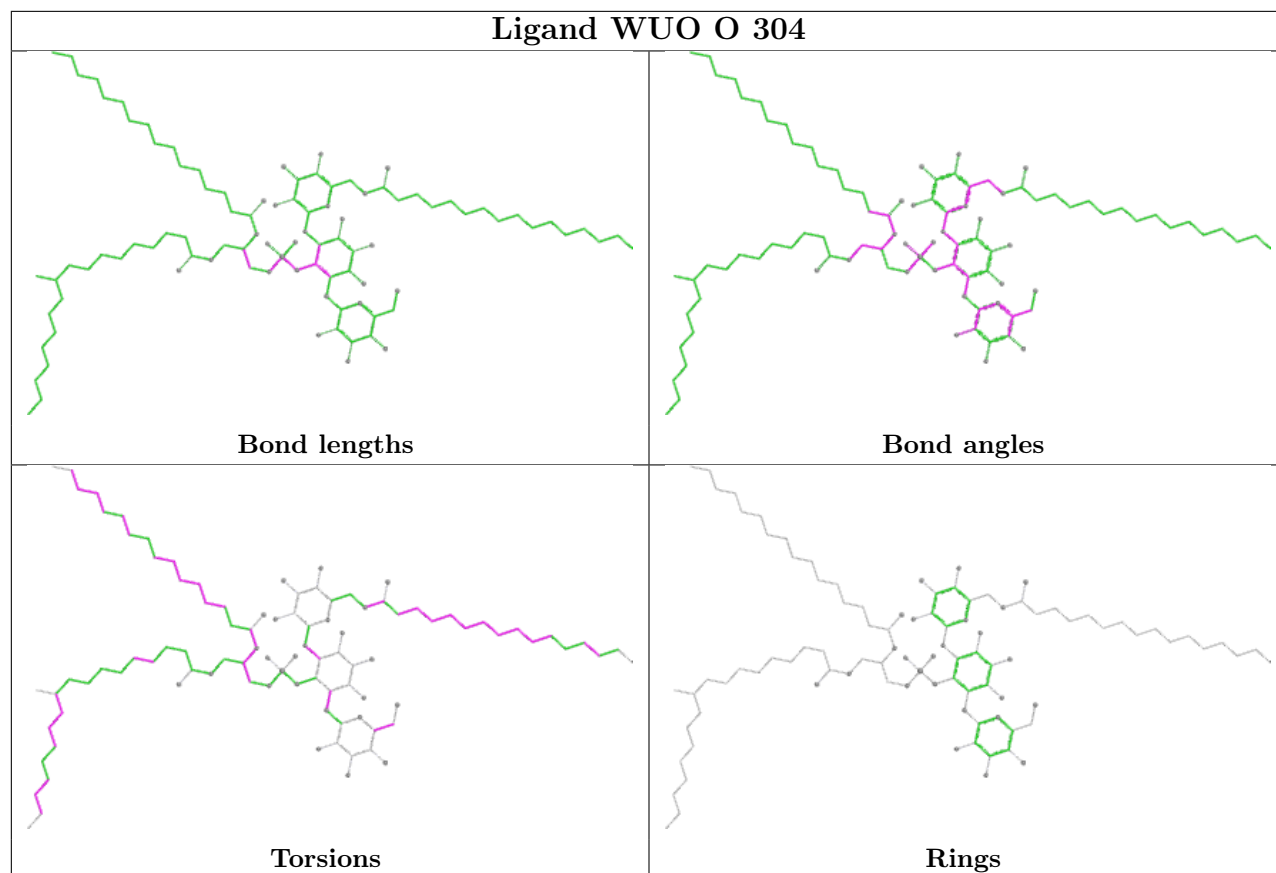
Bond angles

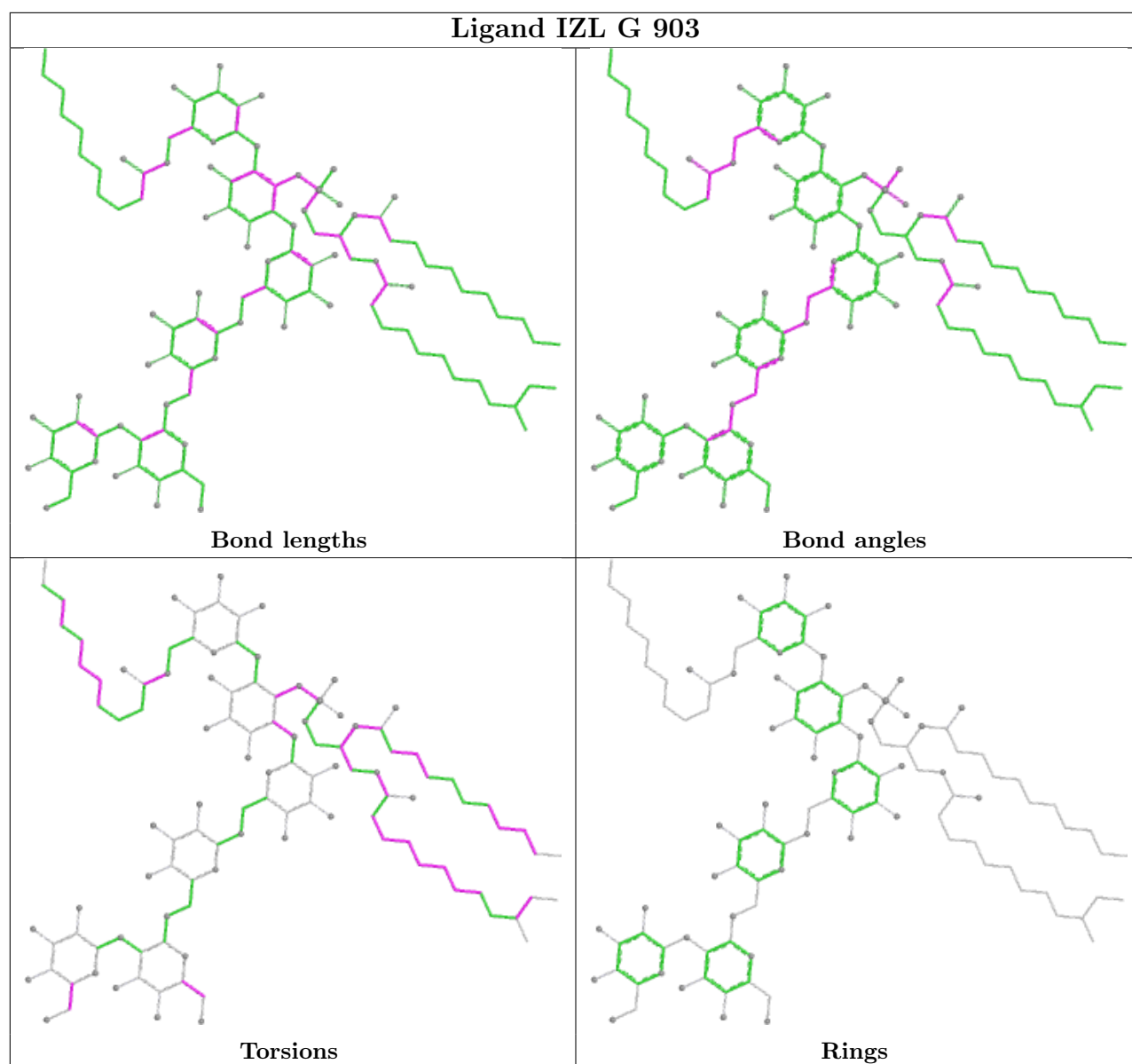


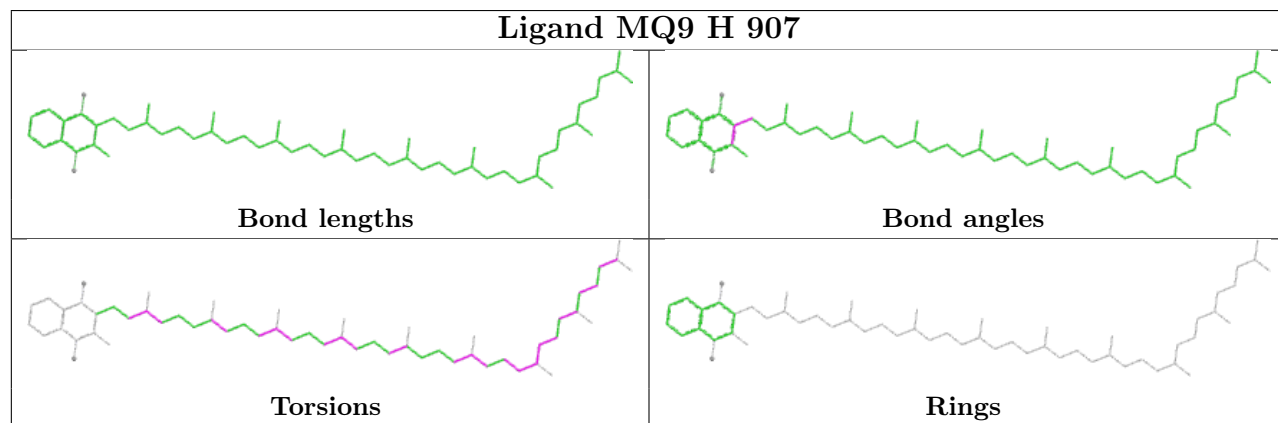
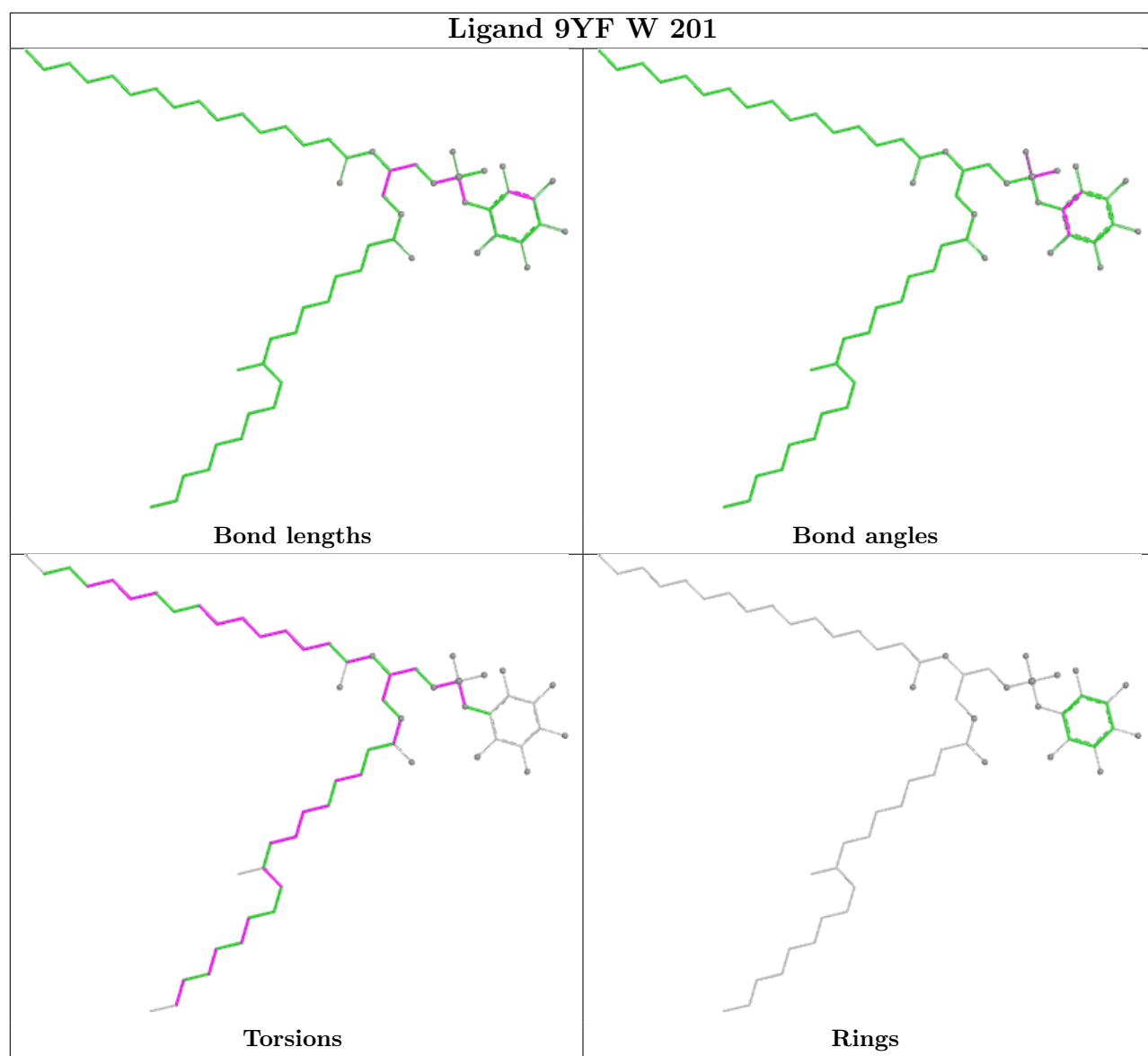
Torsions

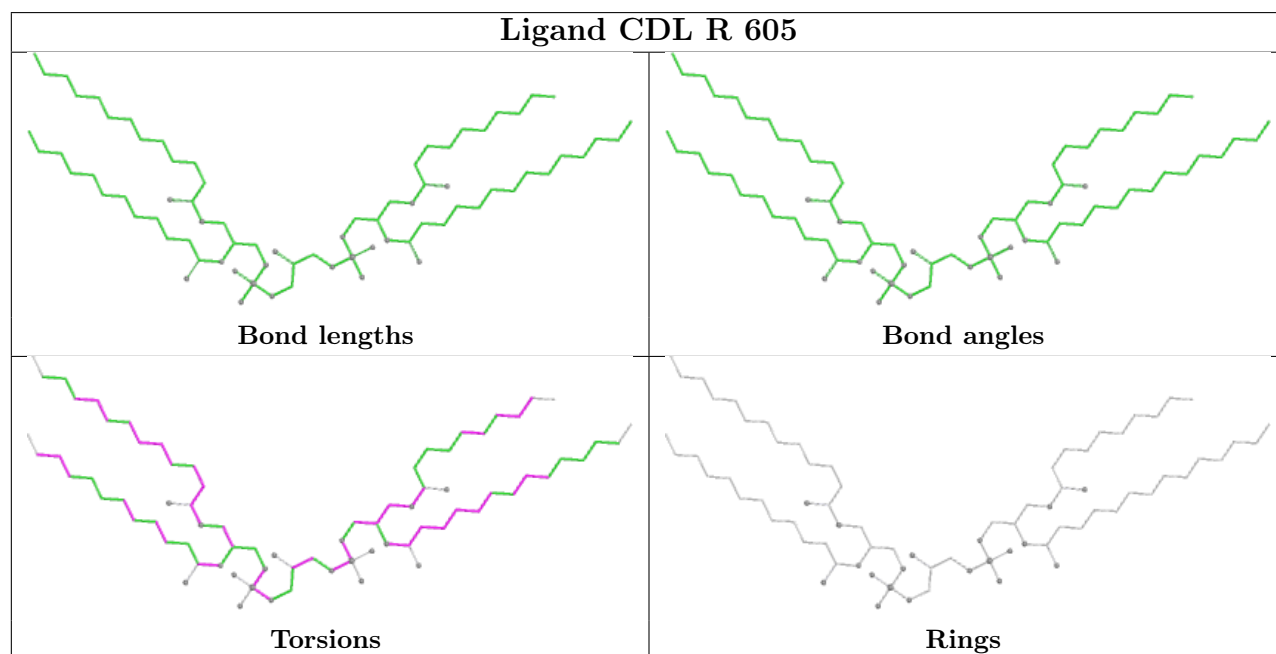
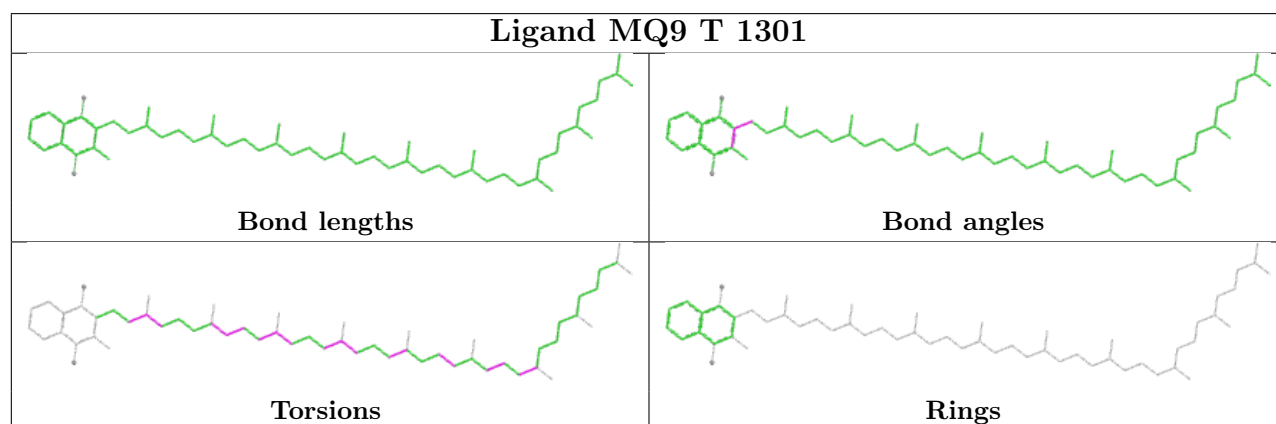
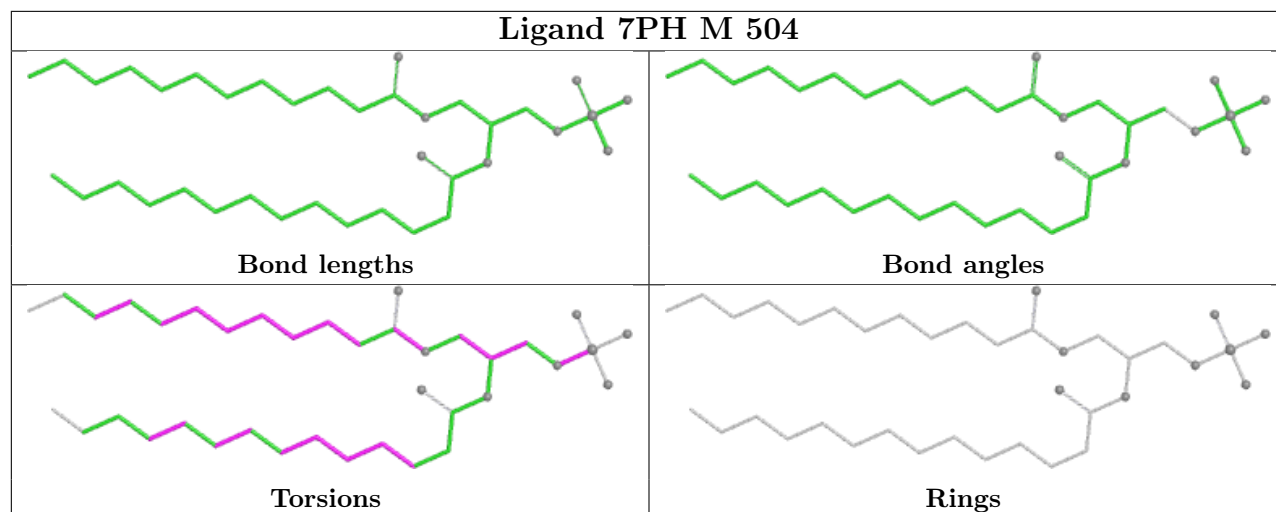


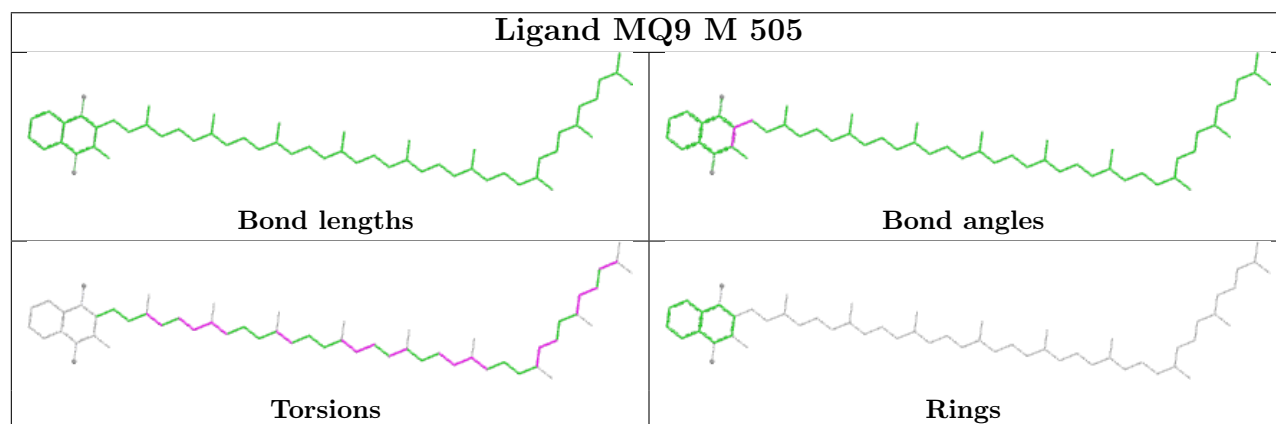
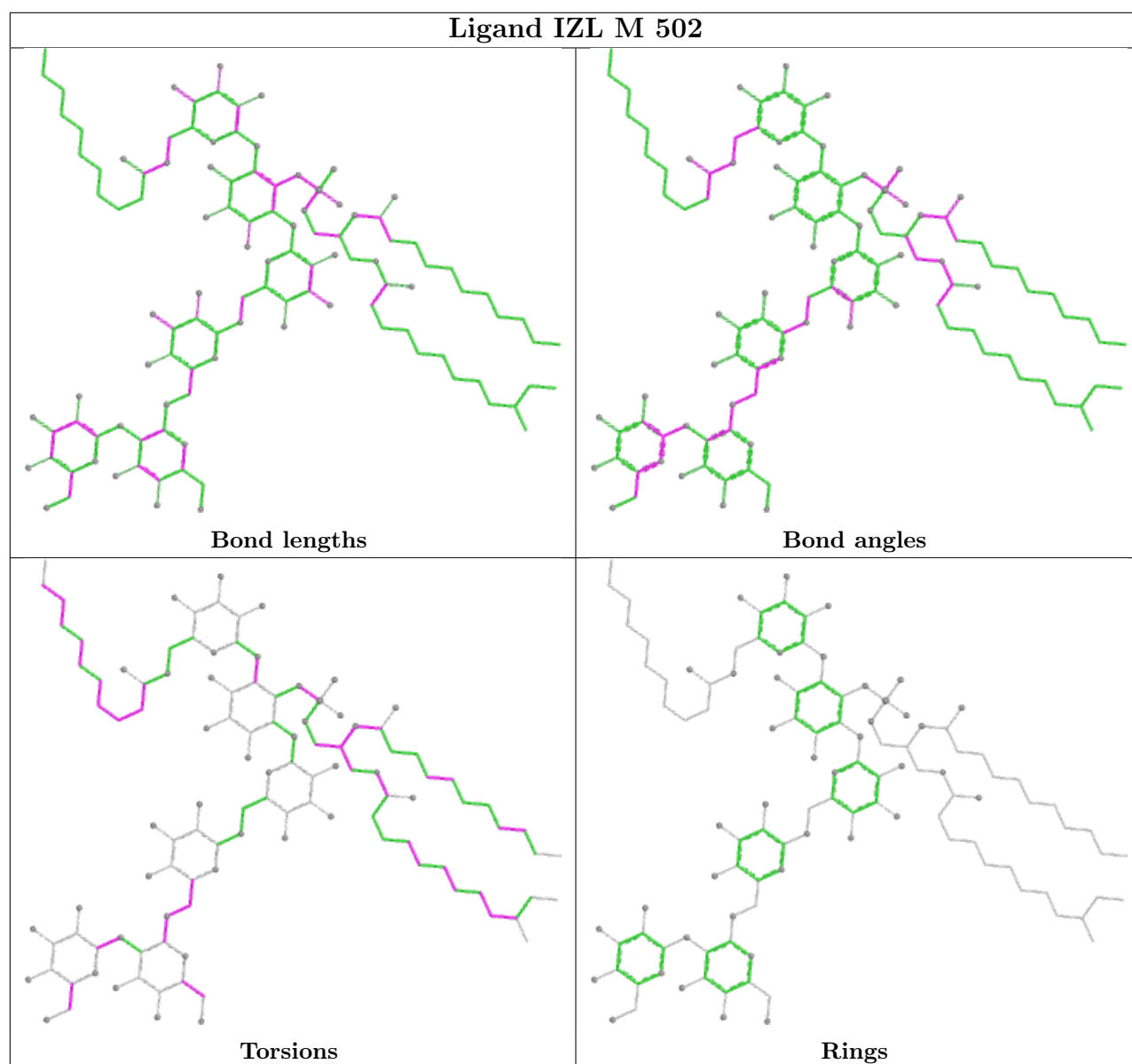
Rings

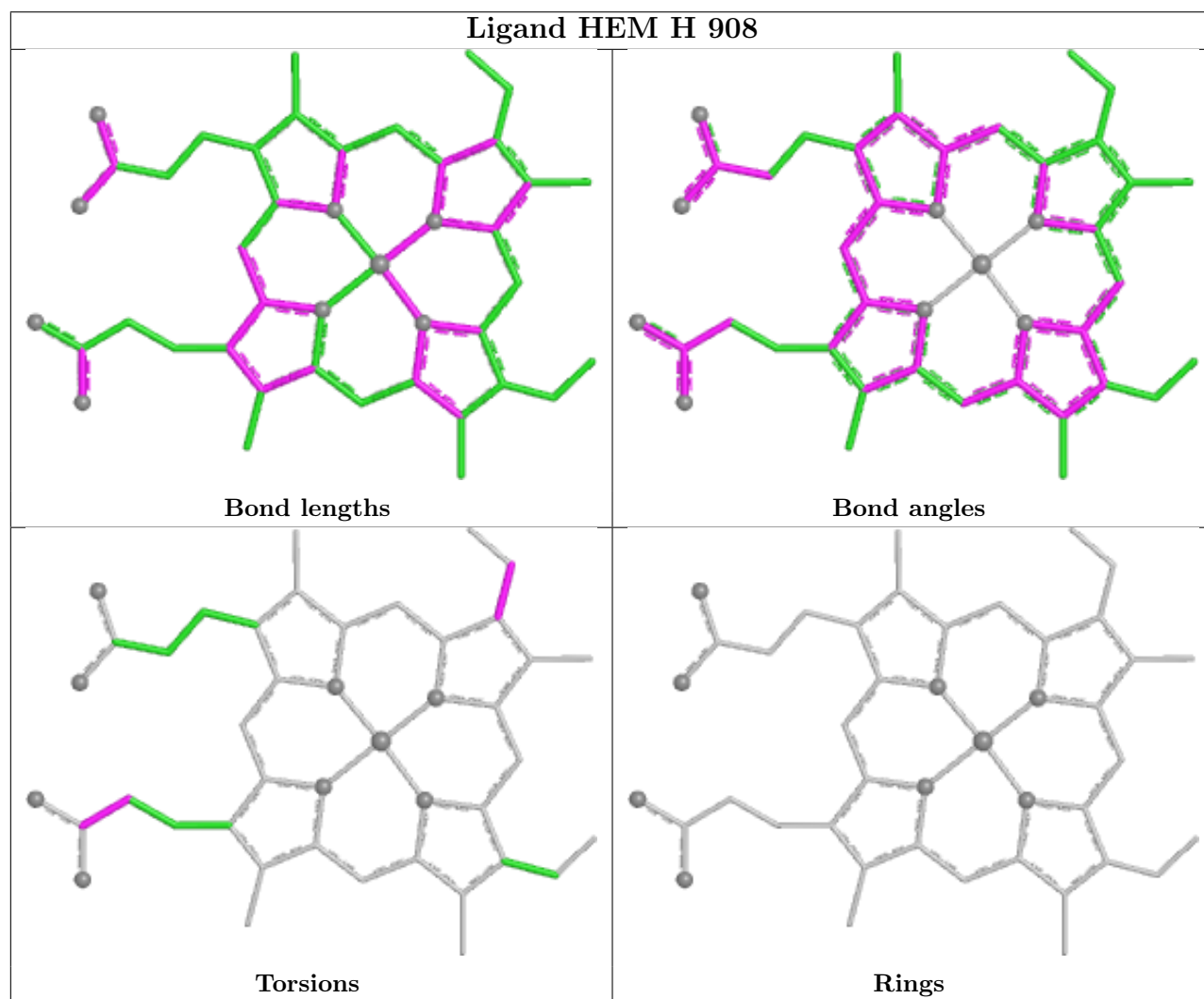
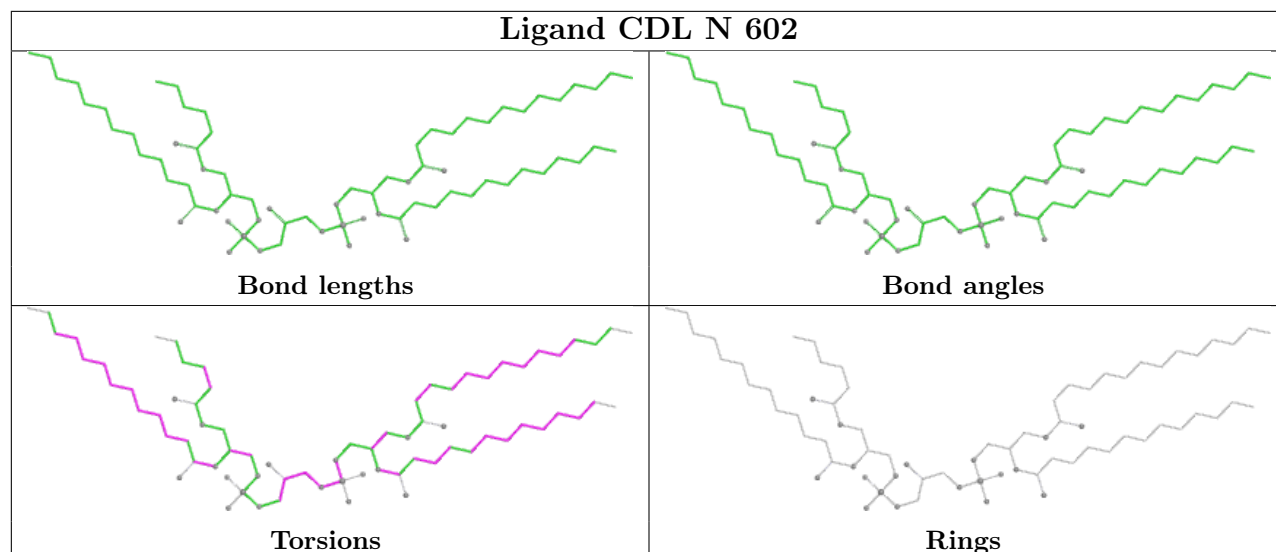


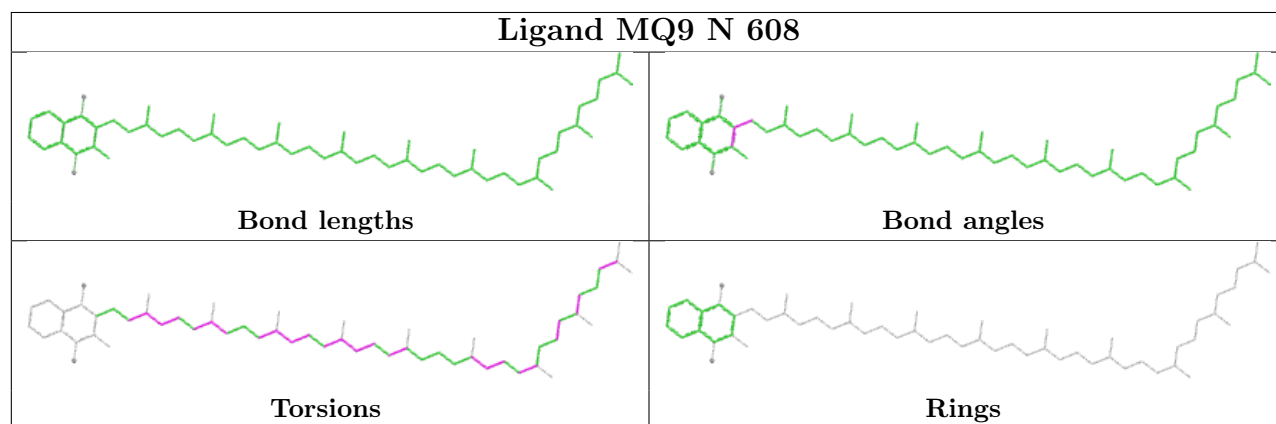
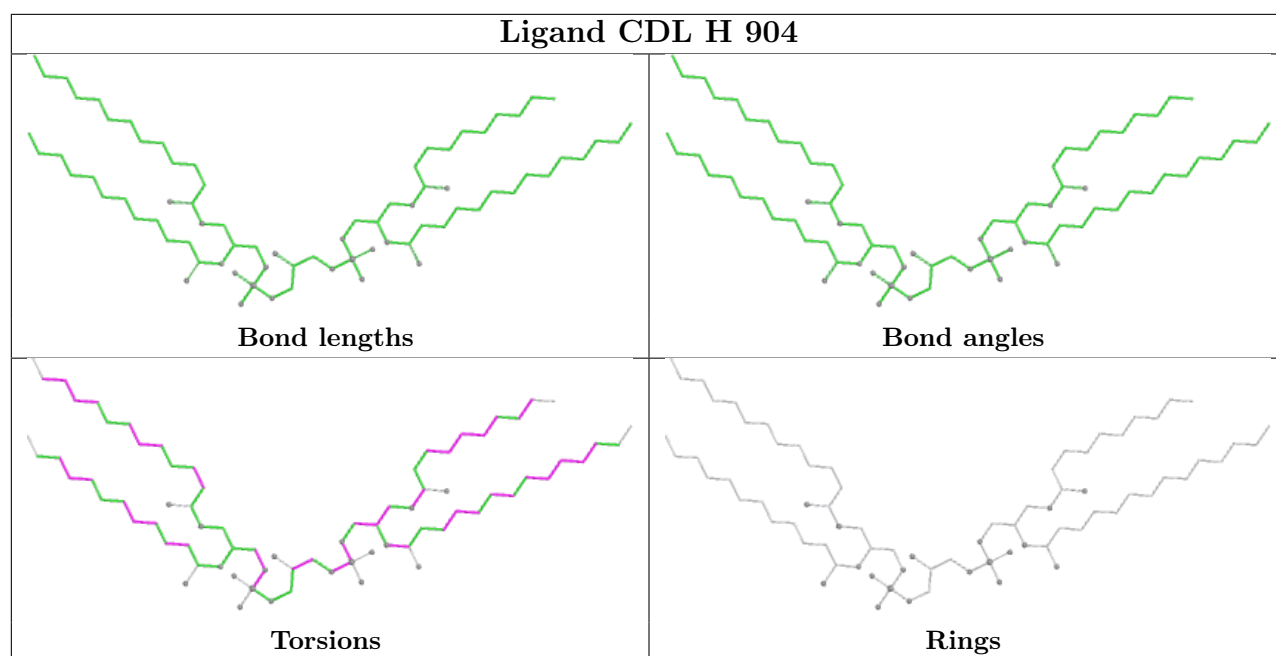


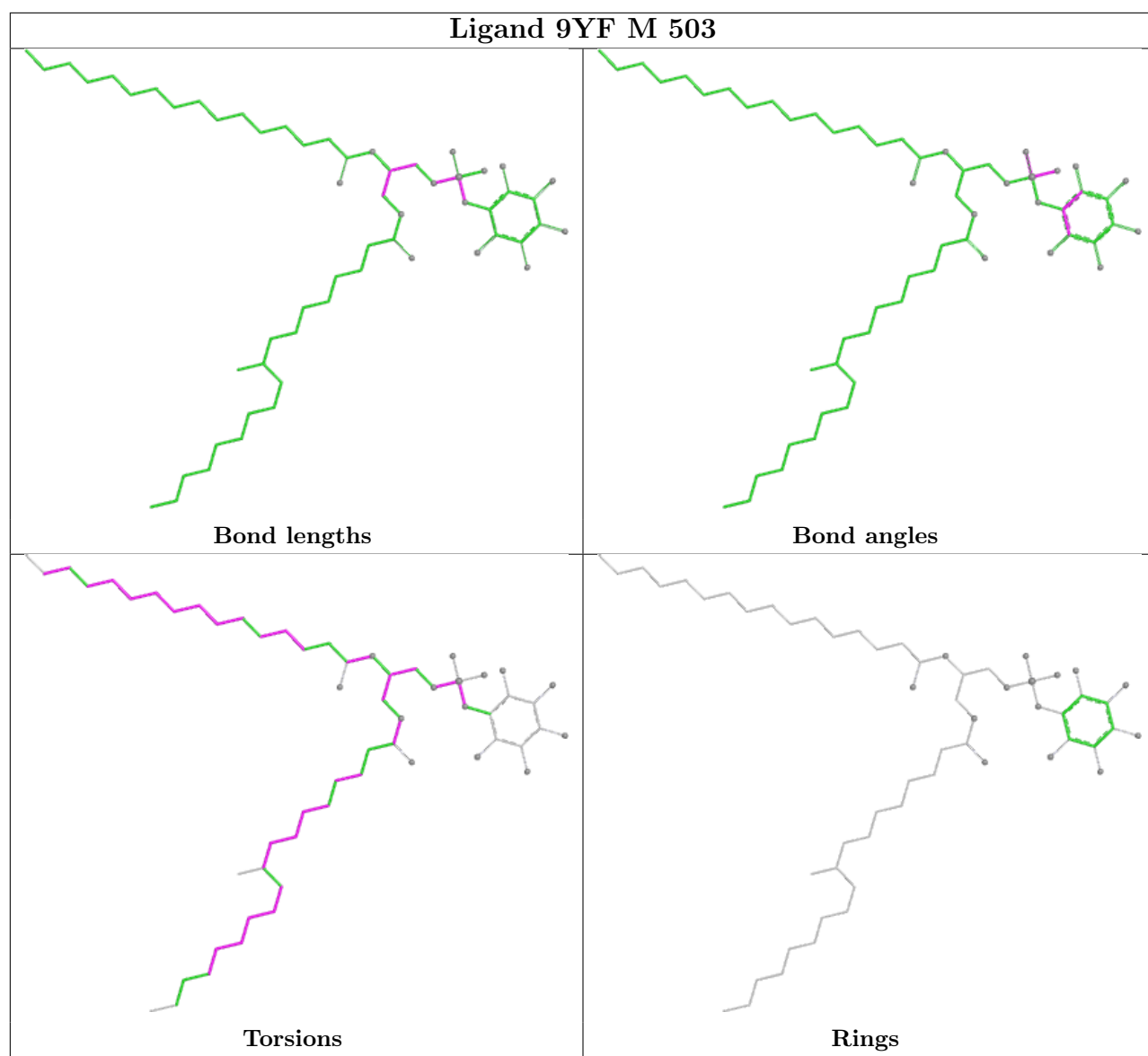


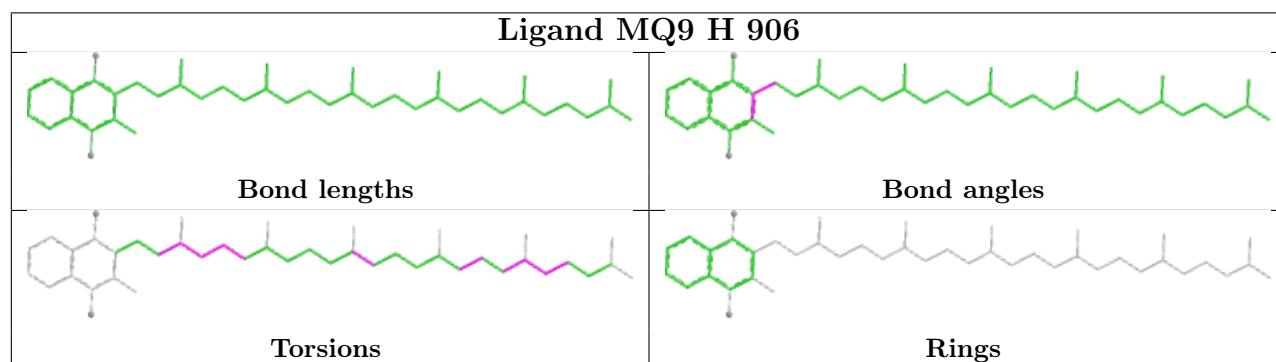
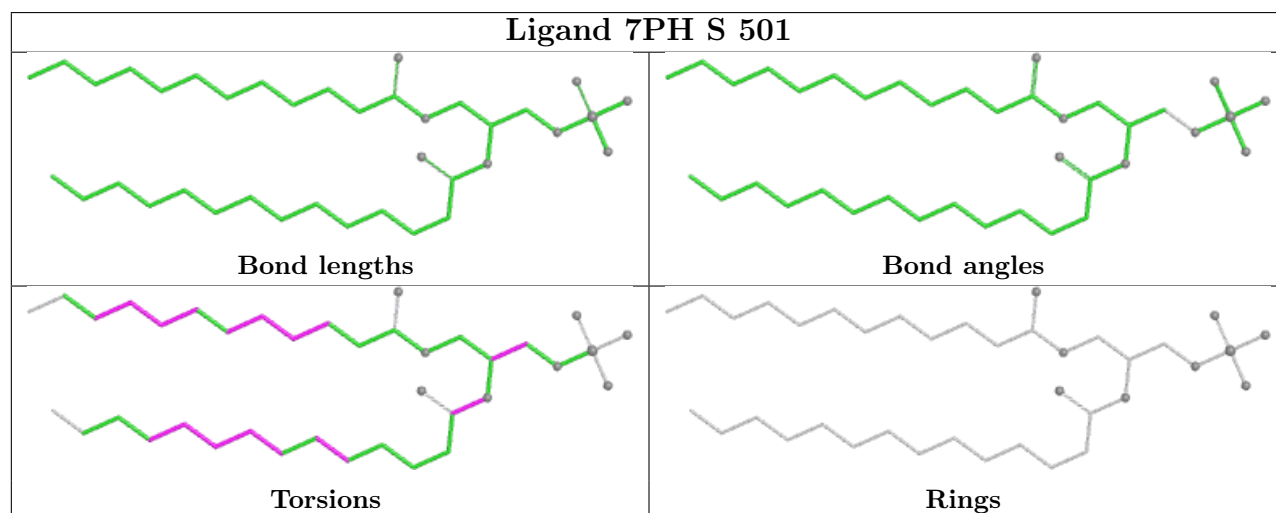
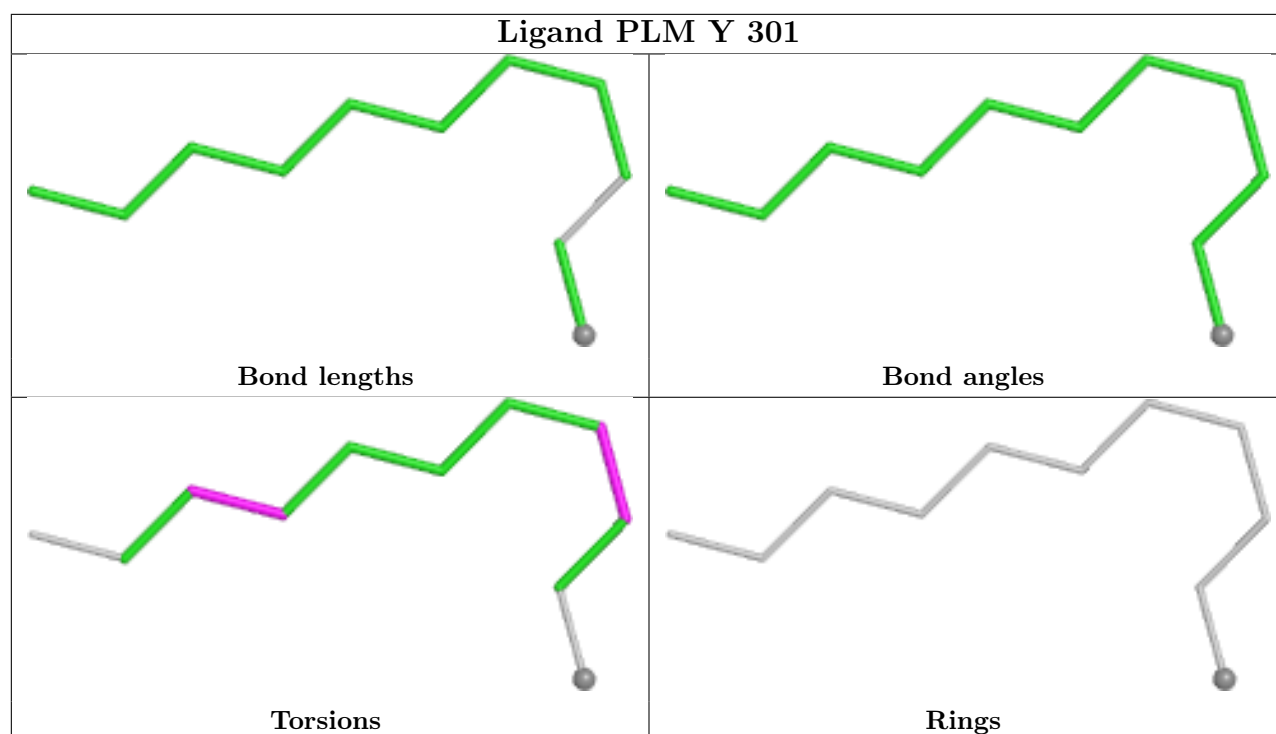


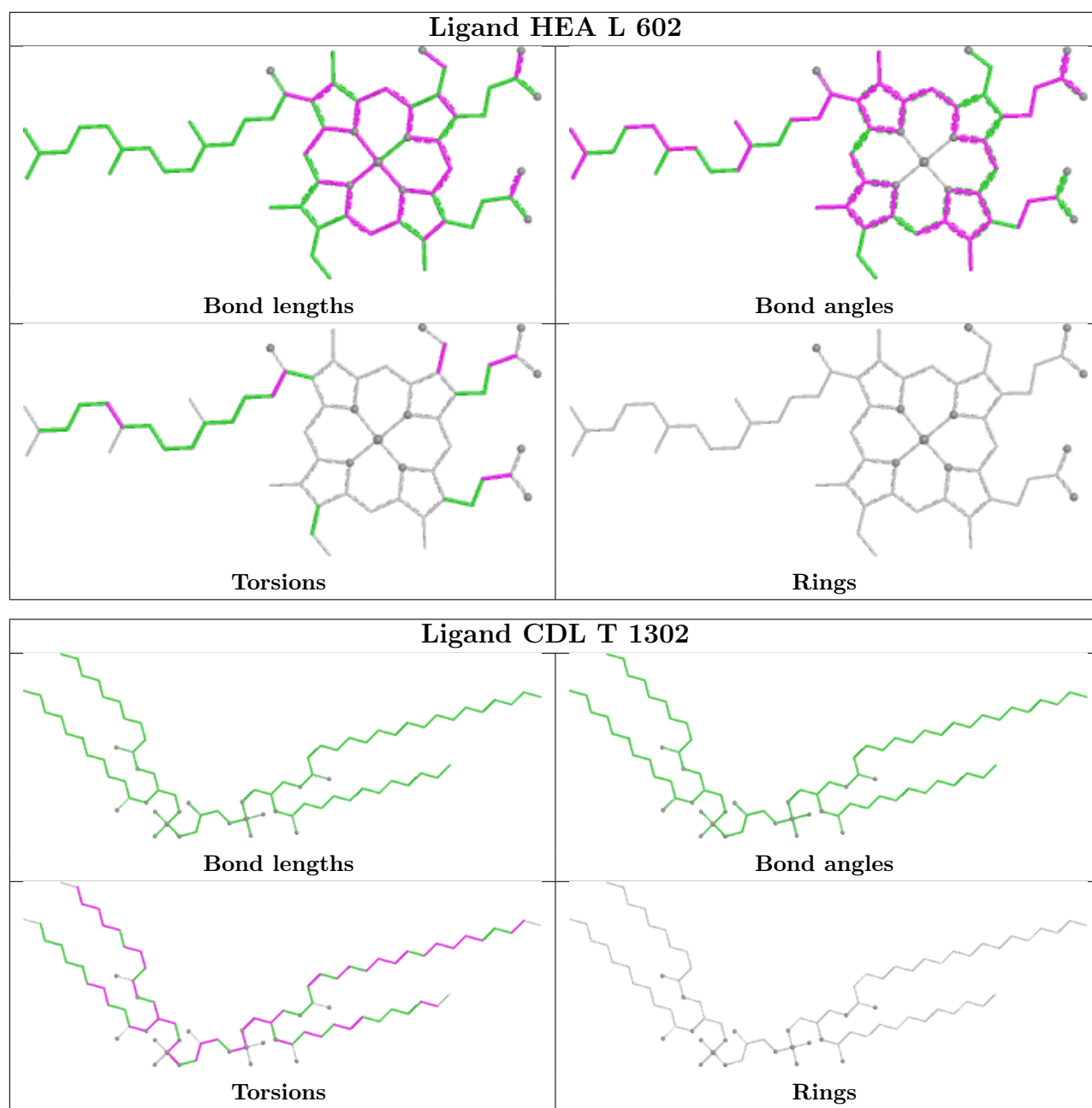


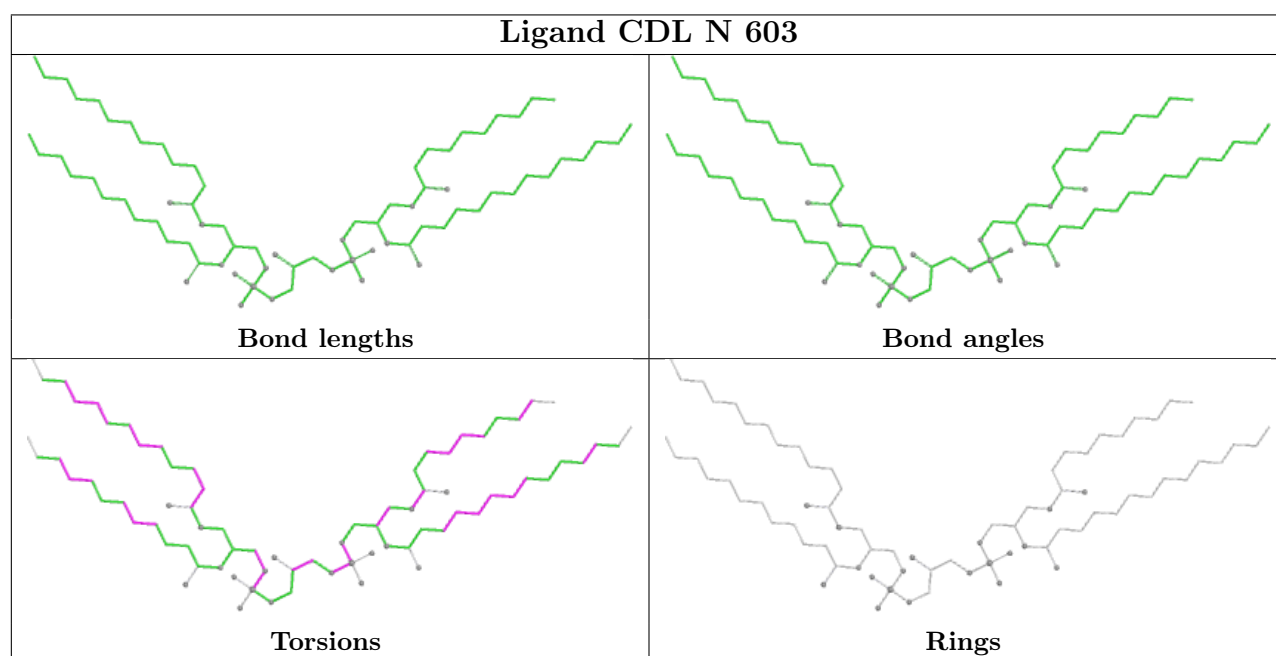
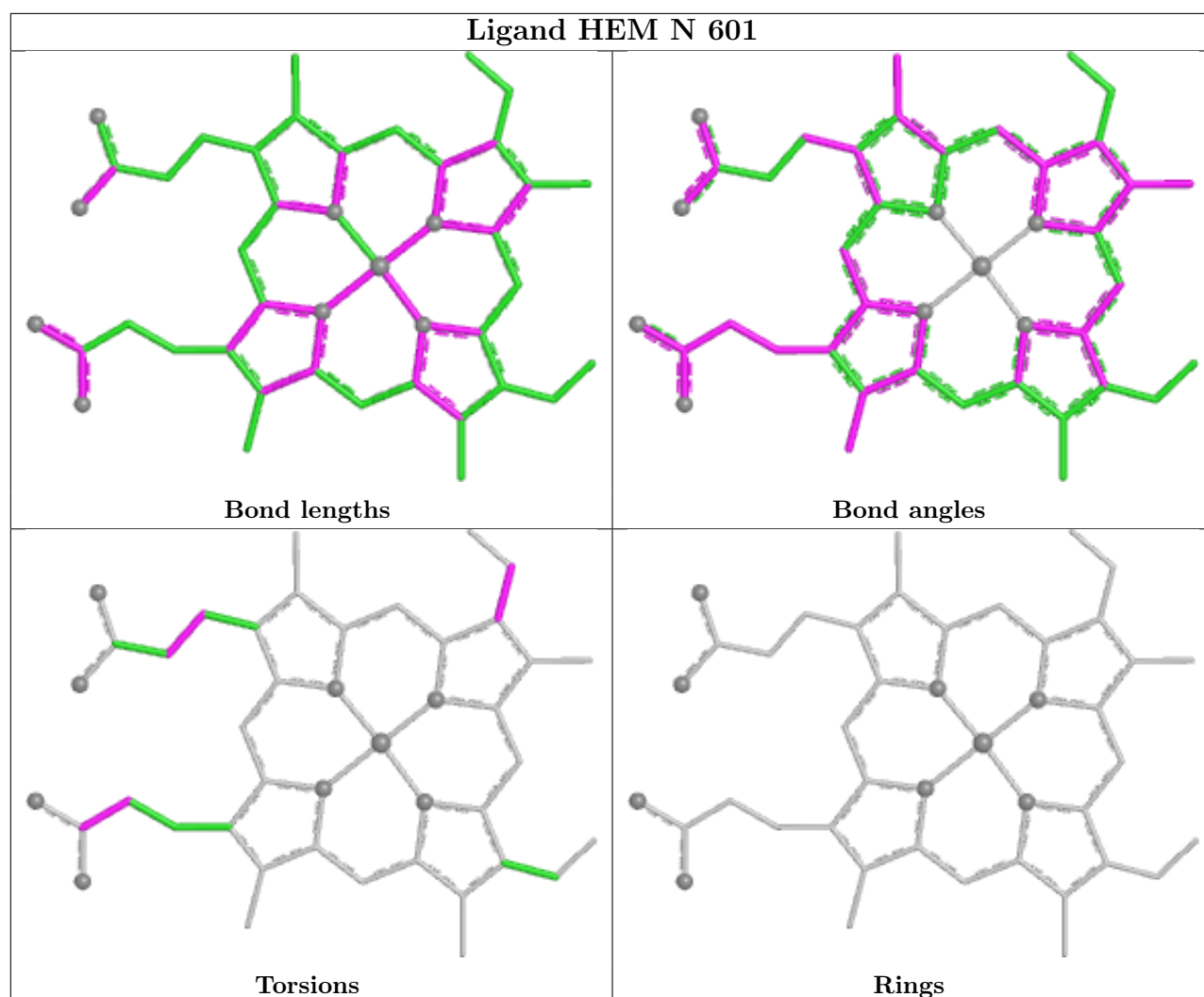


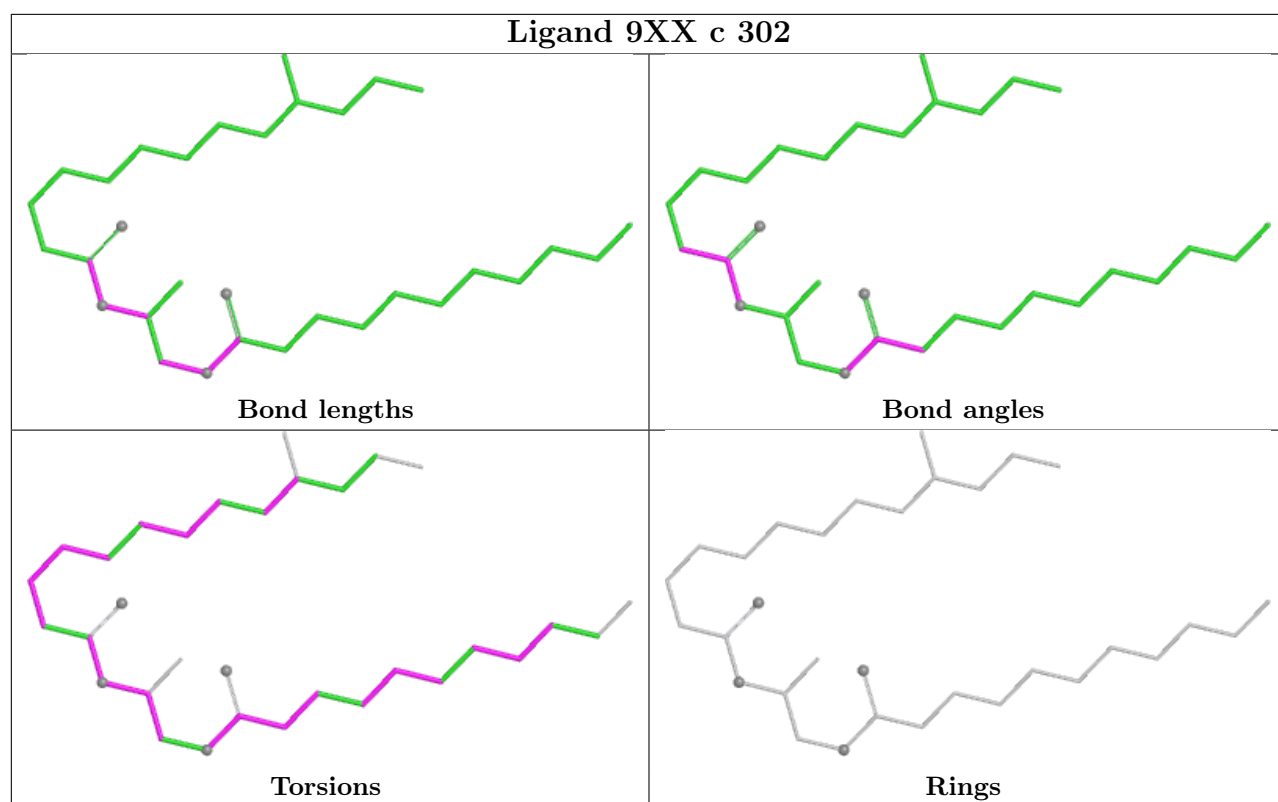




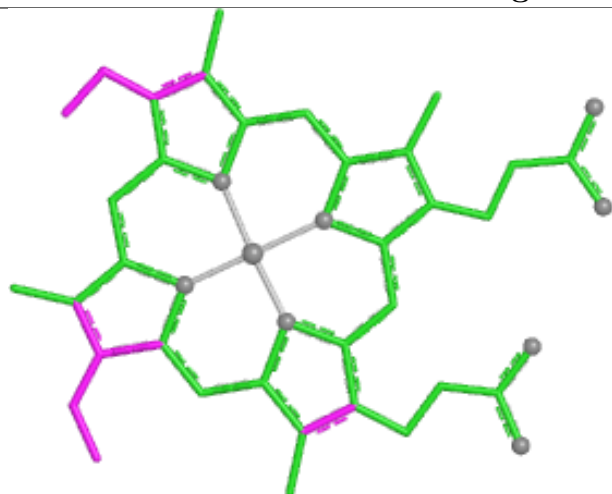




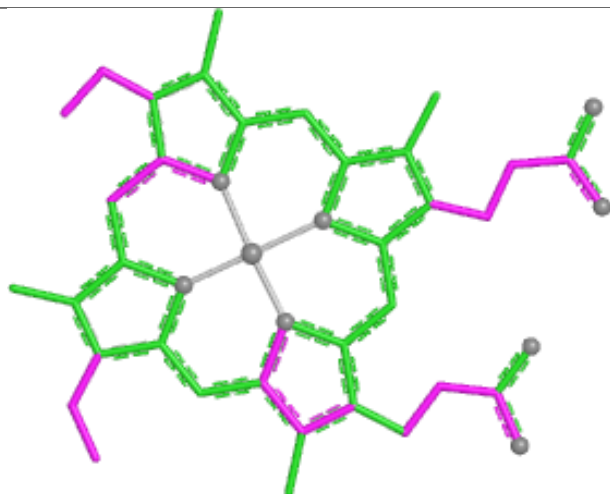




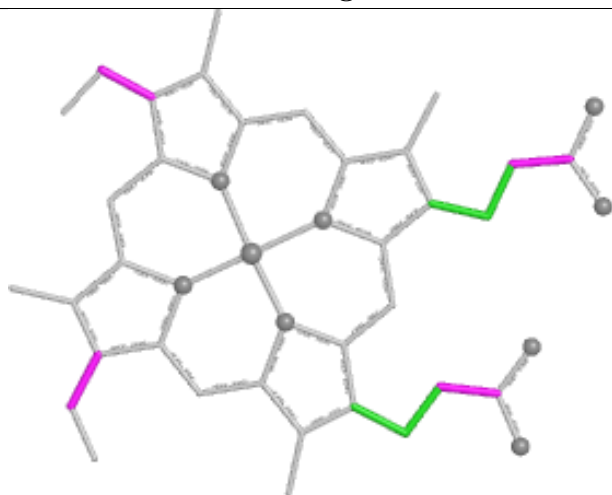
Ligand HEC C 302



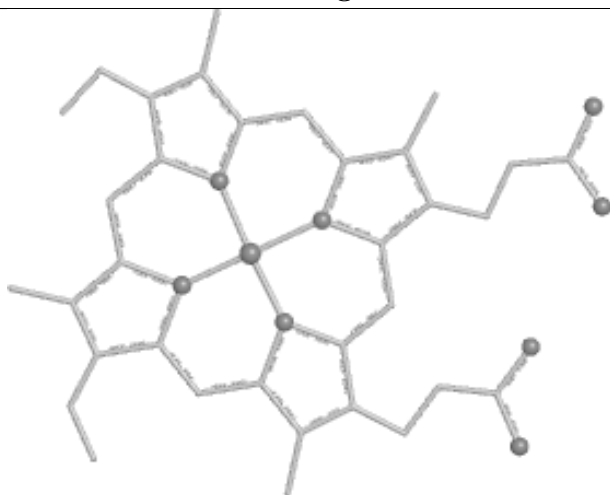
Bond lengths



Bond angles

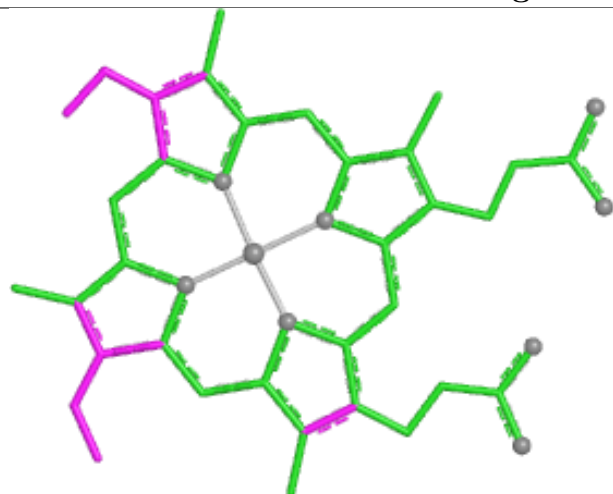


Torsions

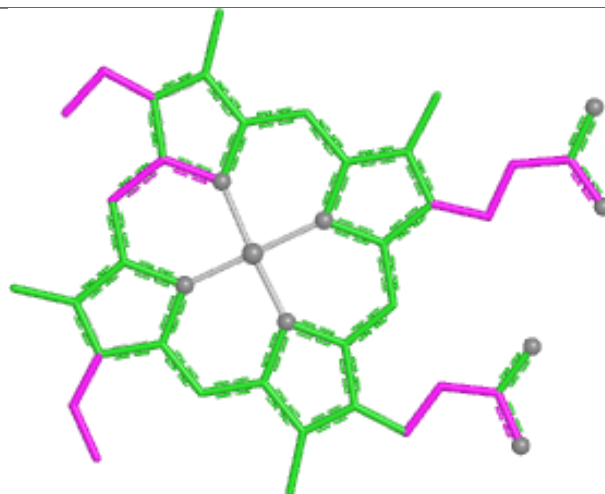


Rings

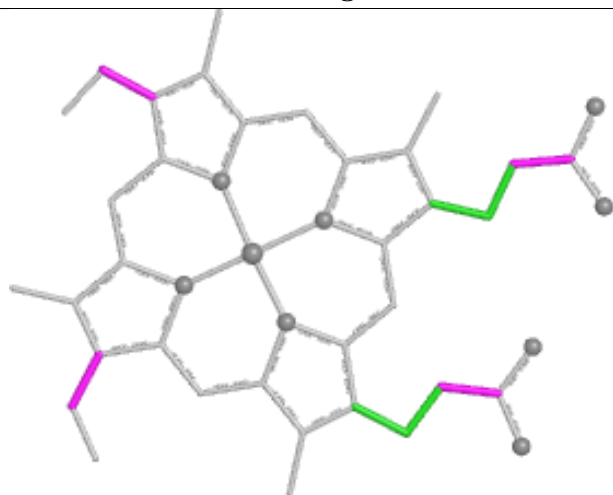
Ligand HEC O 302



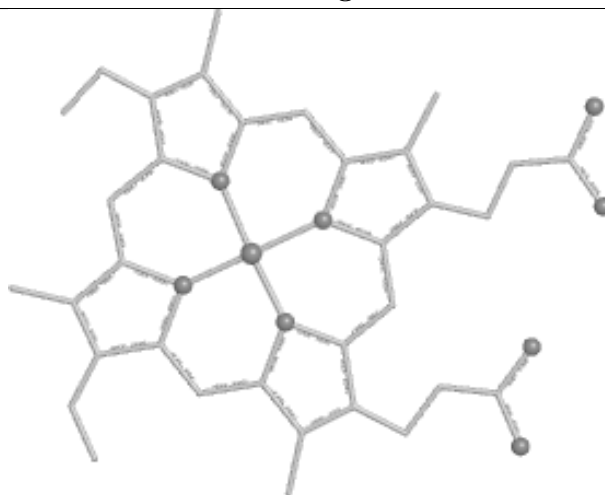
Bond lengths



Bond angles

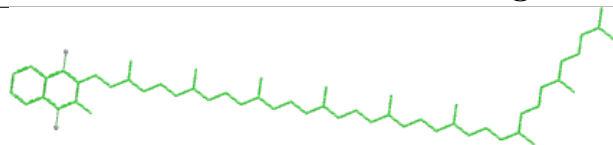


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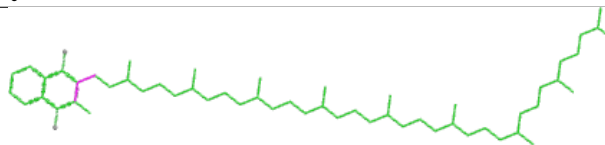


Rings

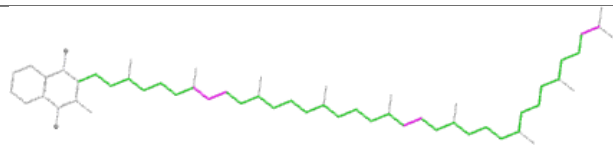
Ligand MQ9 O 303



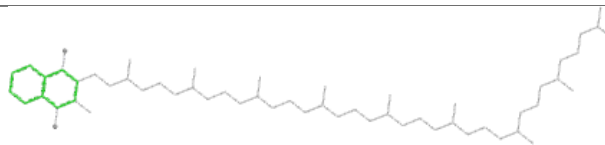
Bond lengths



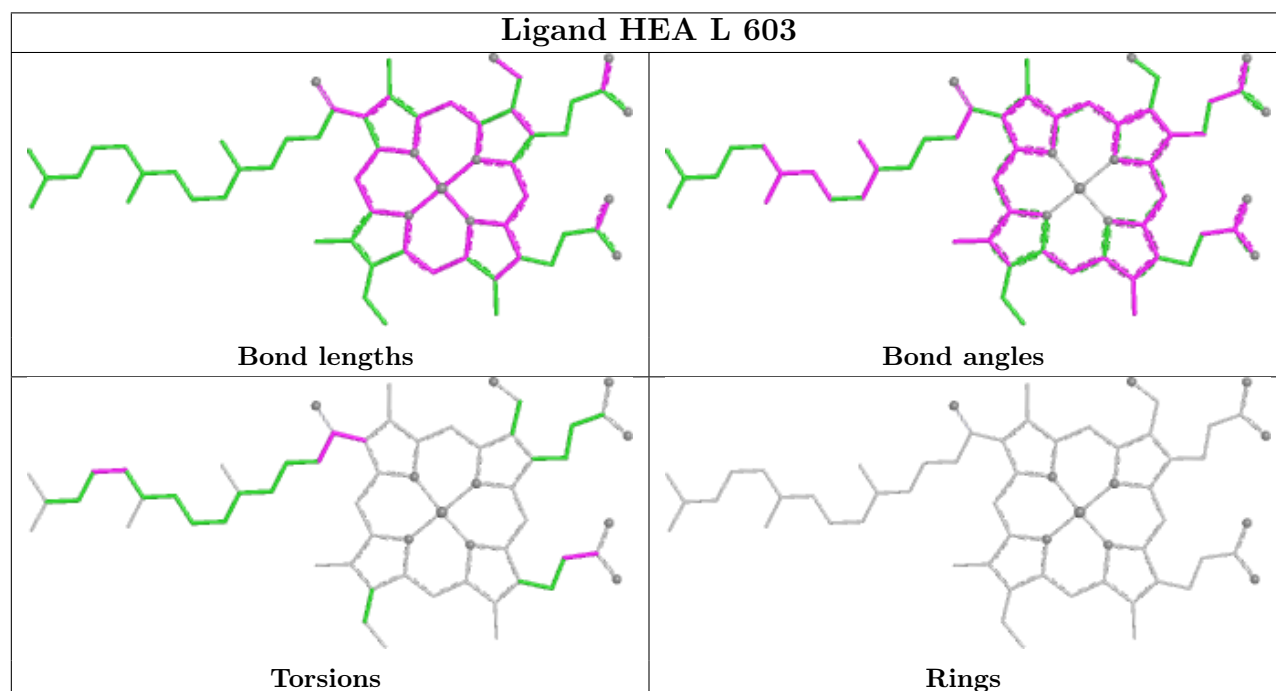
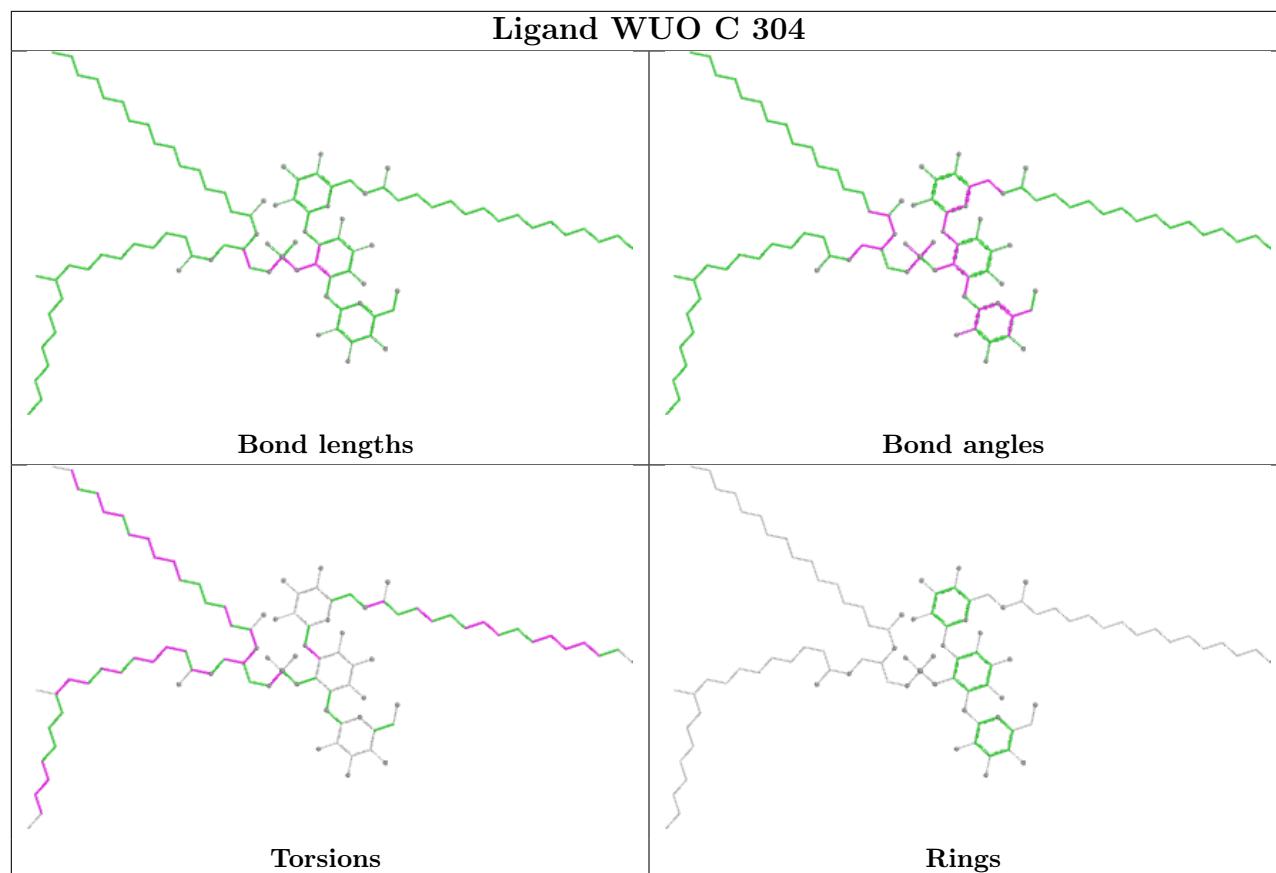
Bond angles

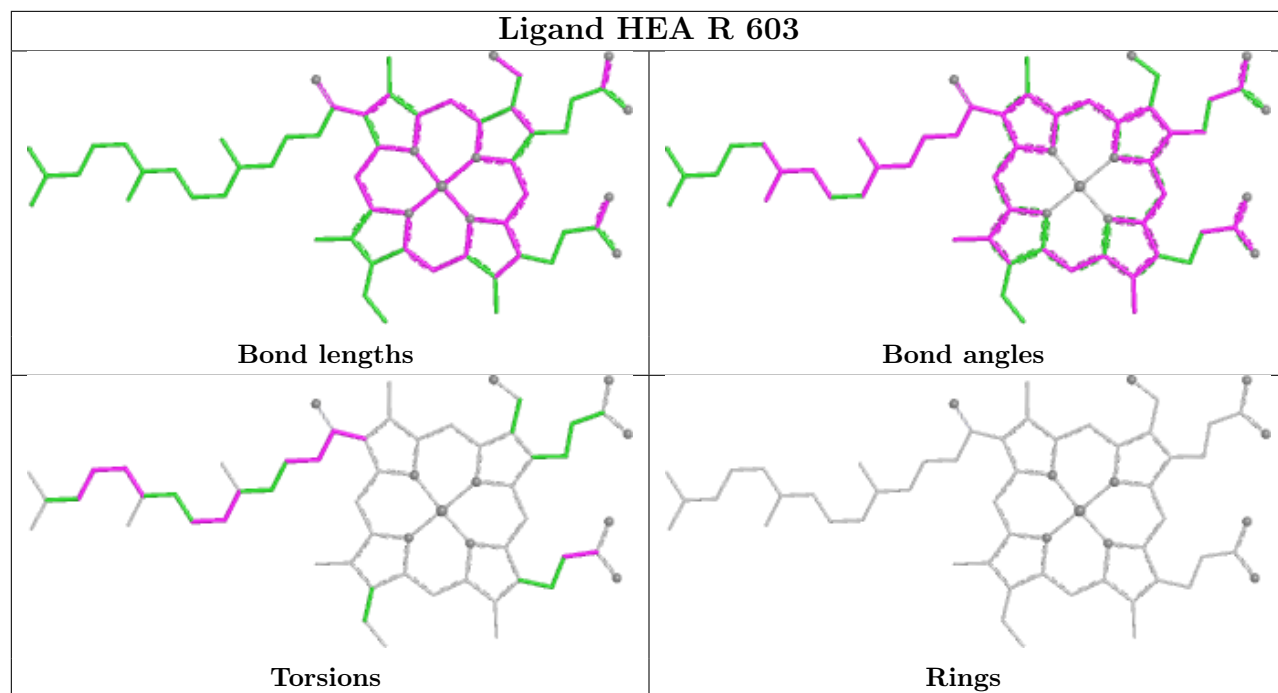


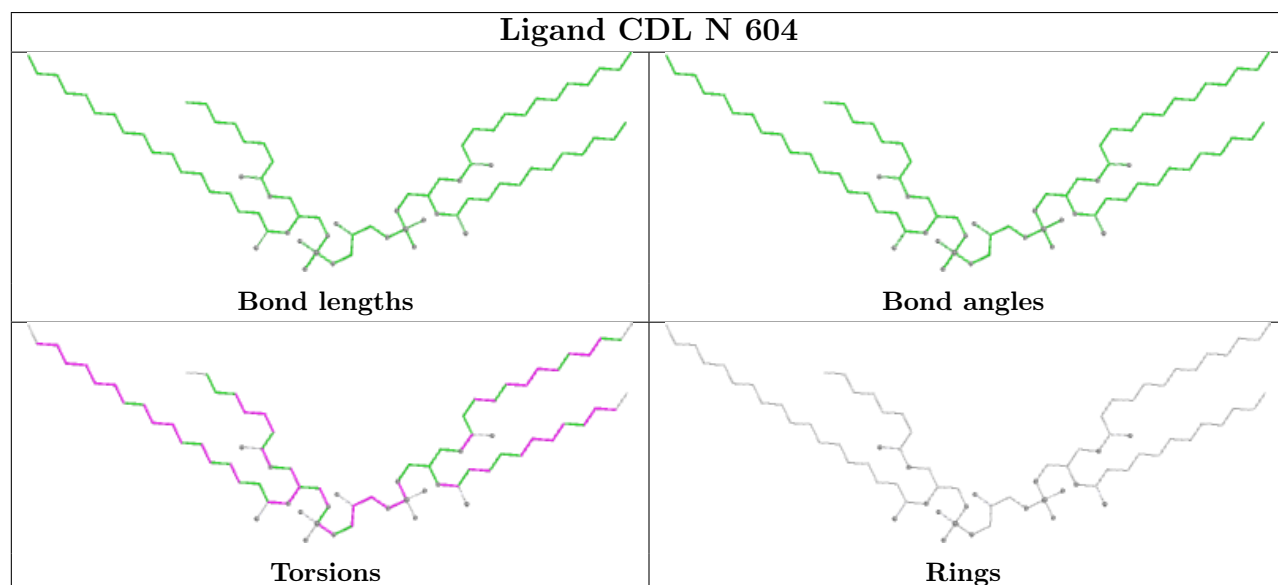
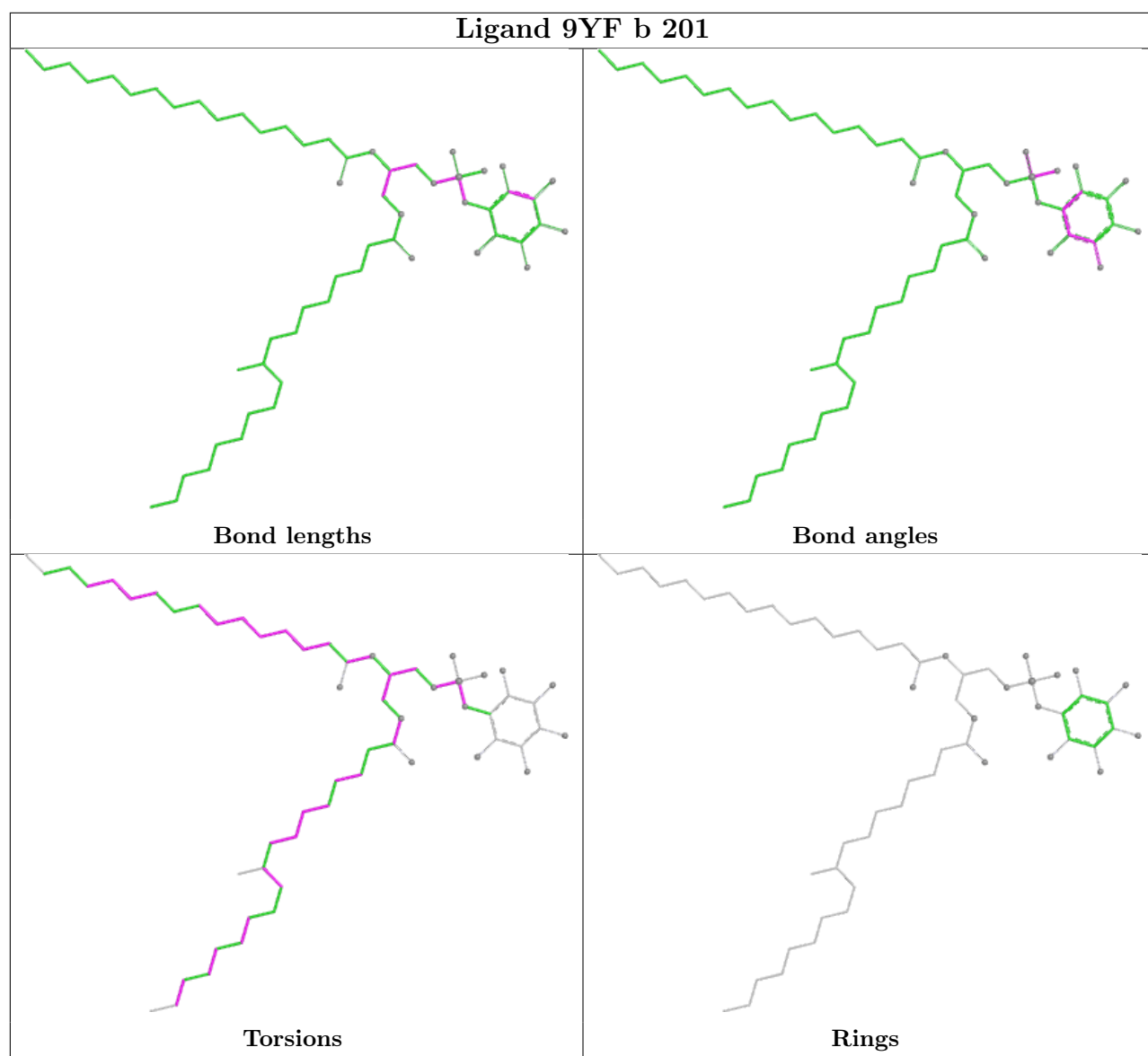
Torsions

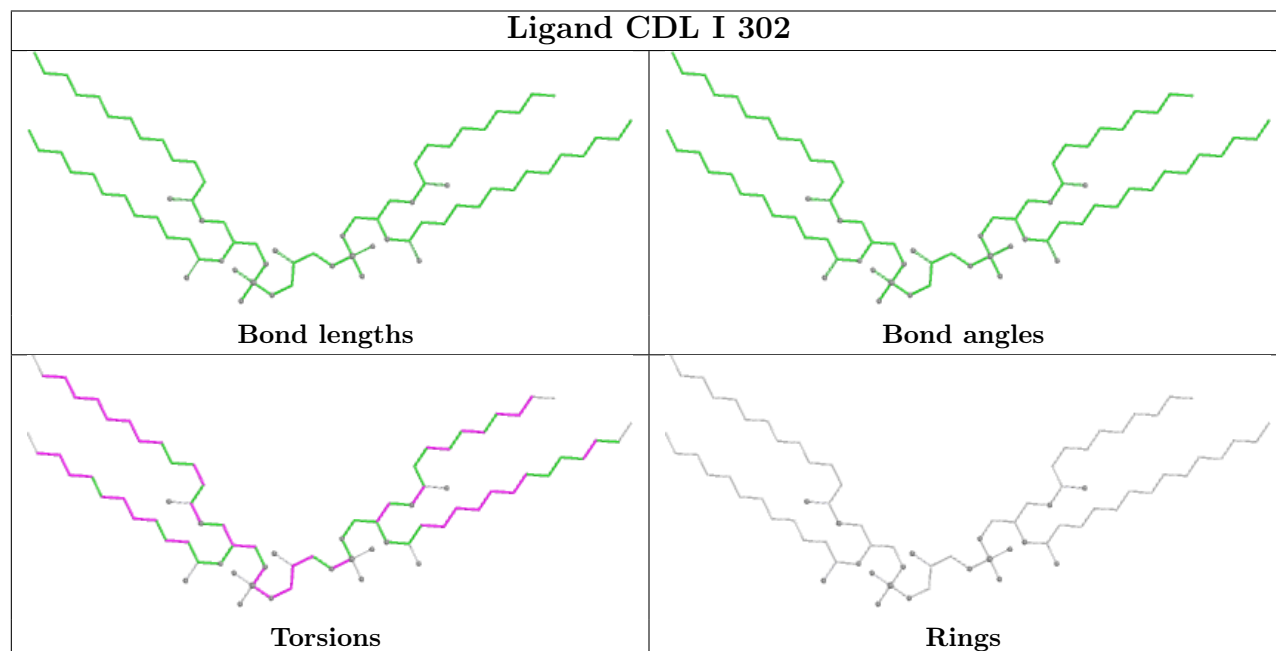
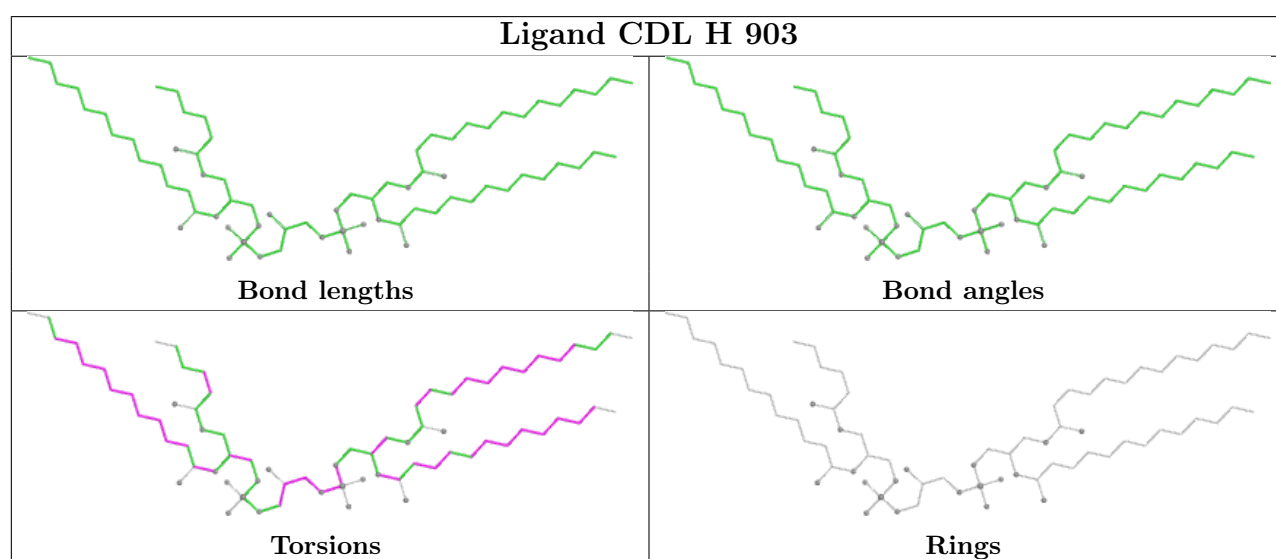
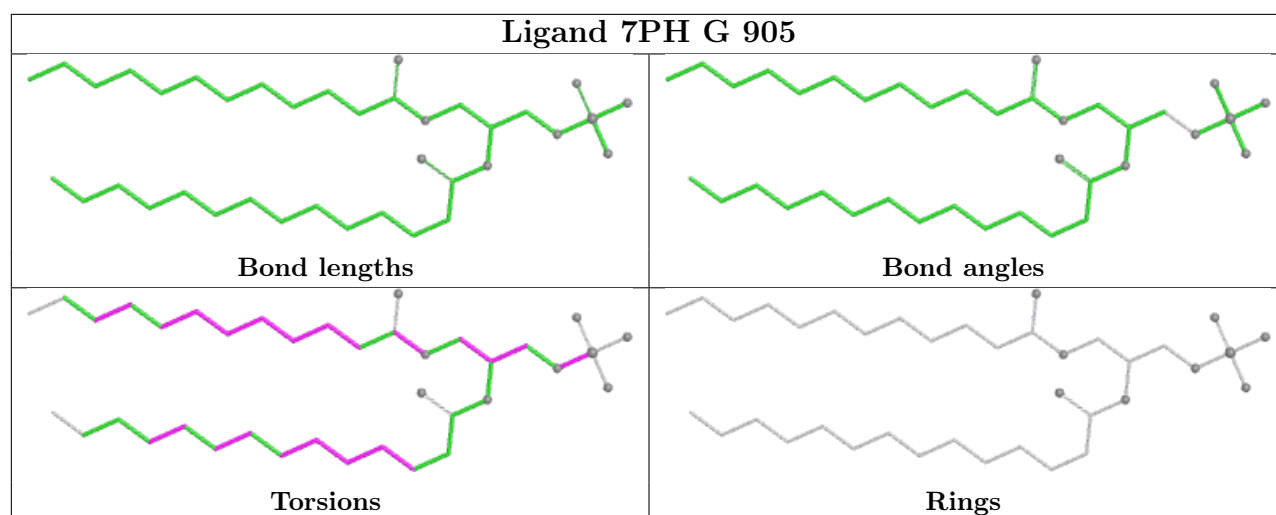


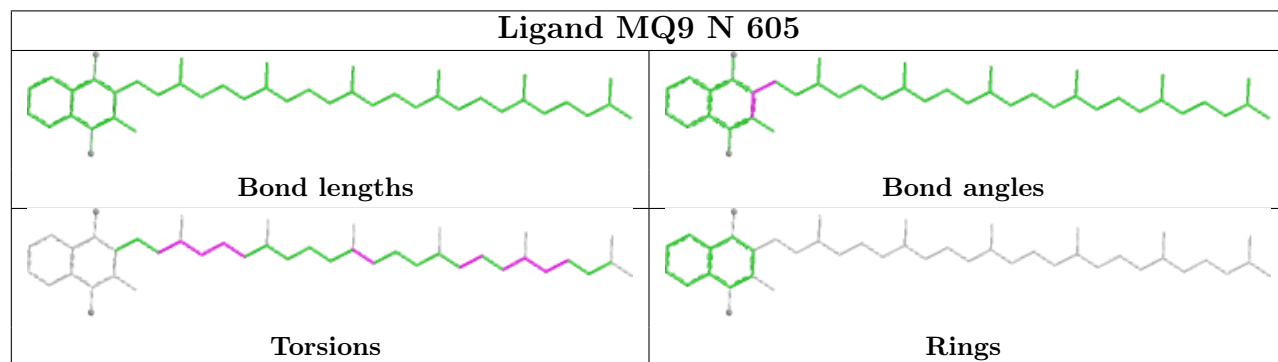
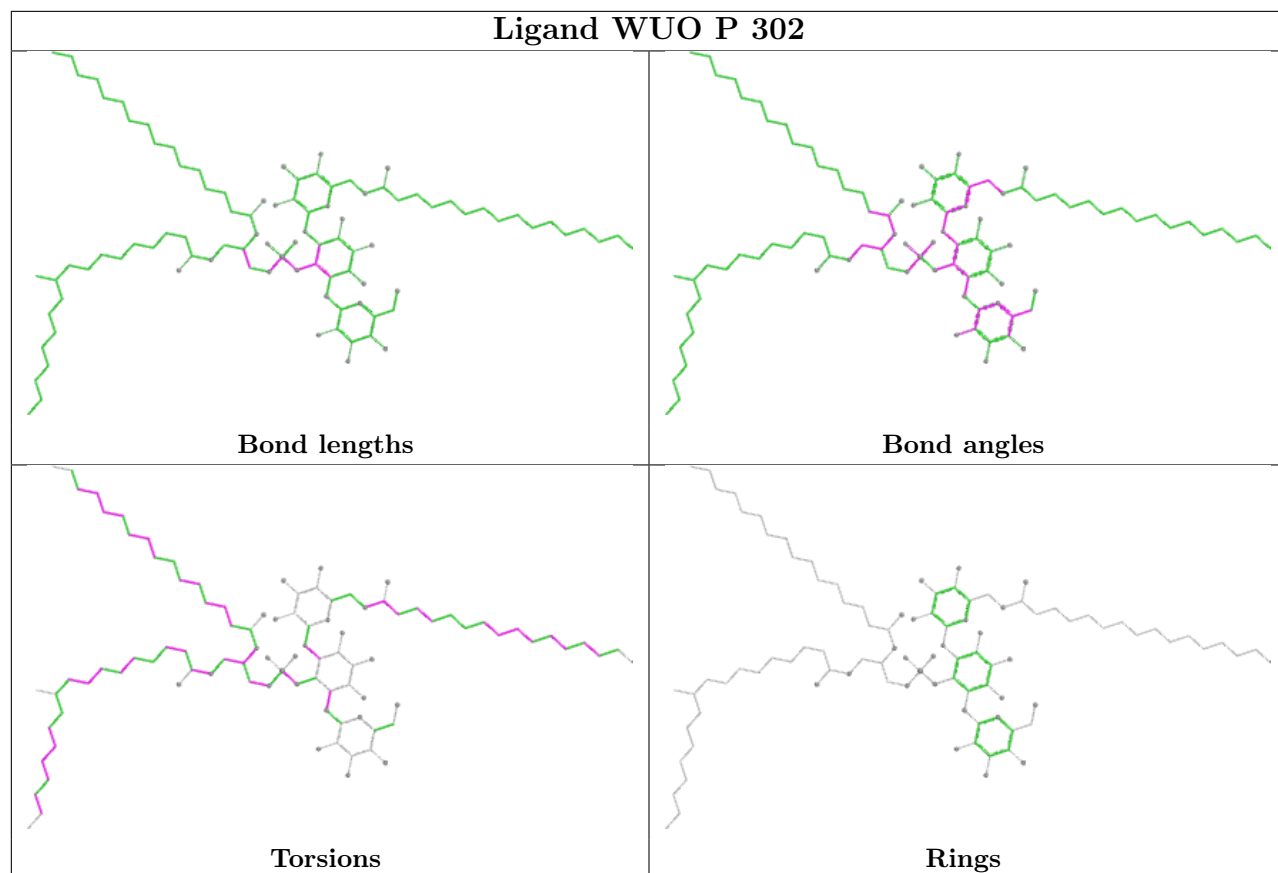
Rings

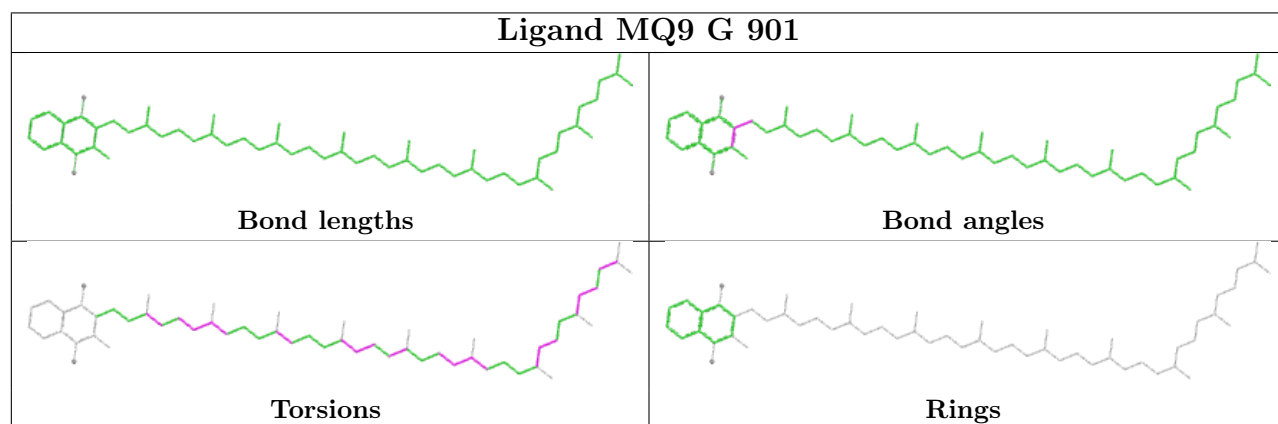
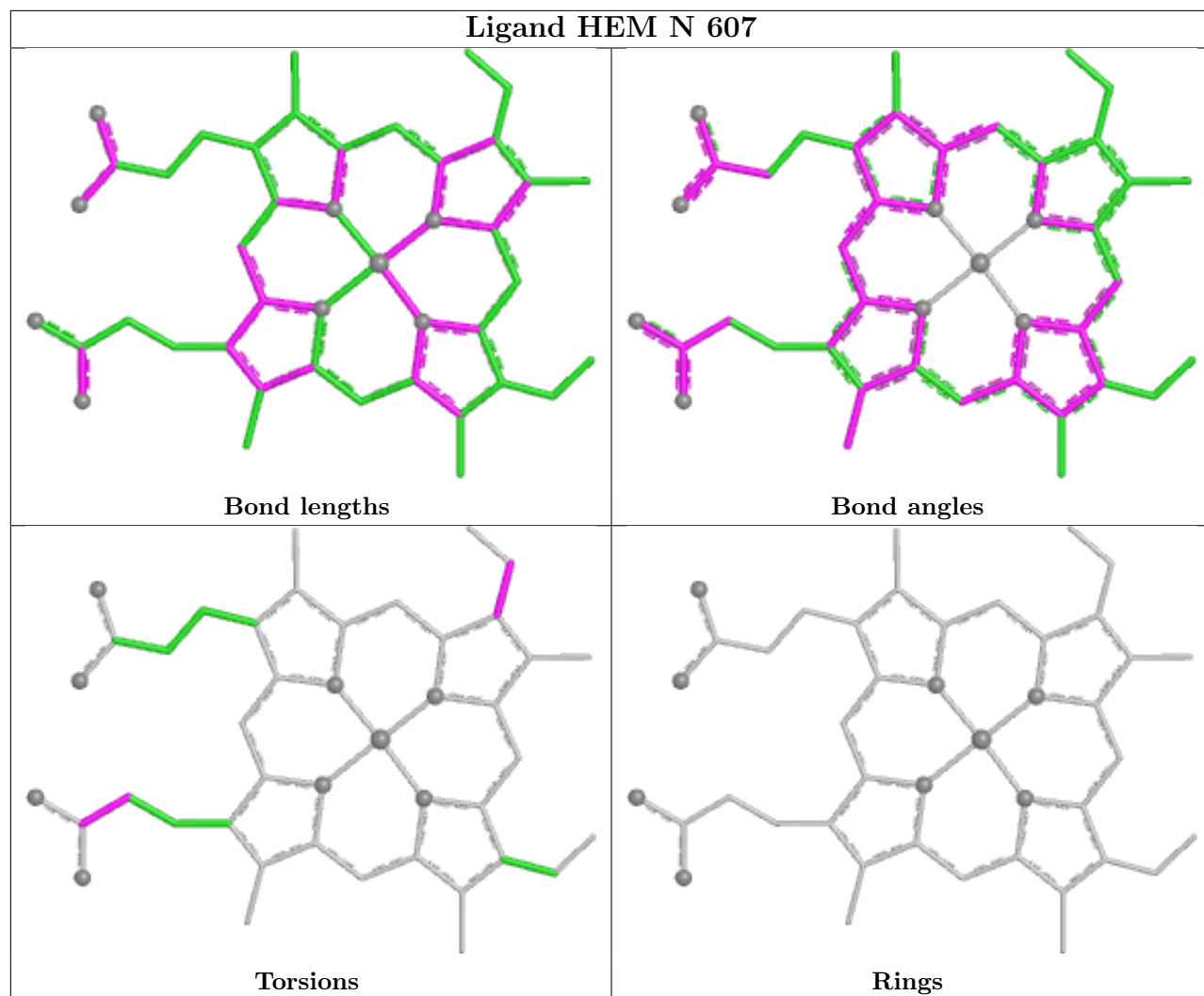


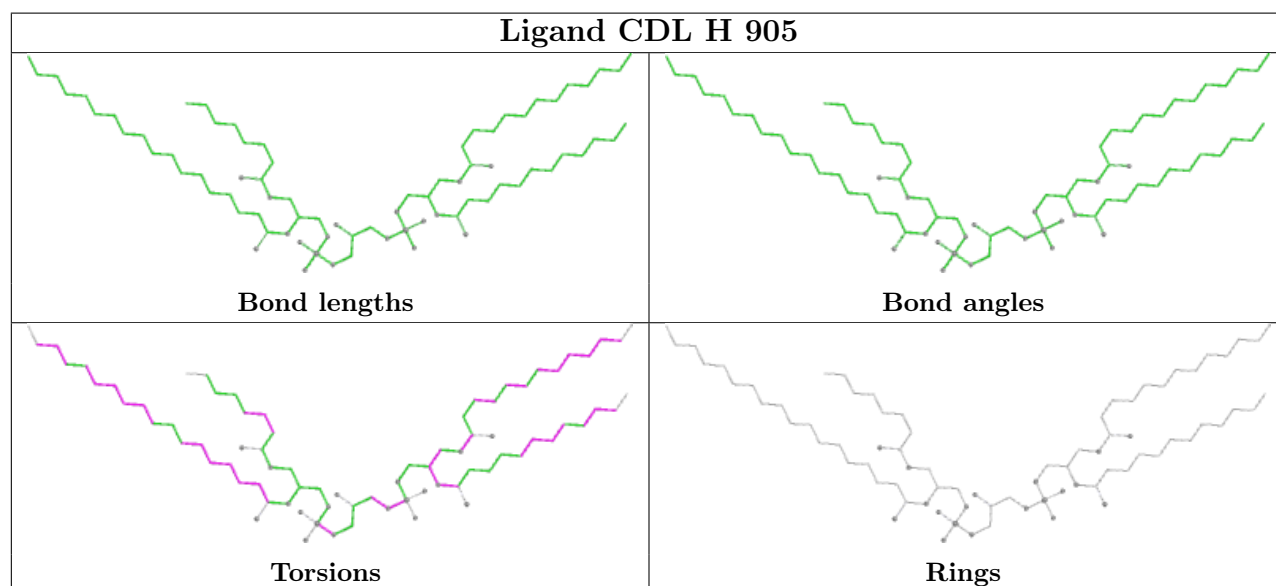
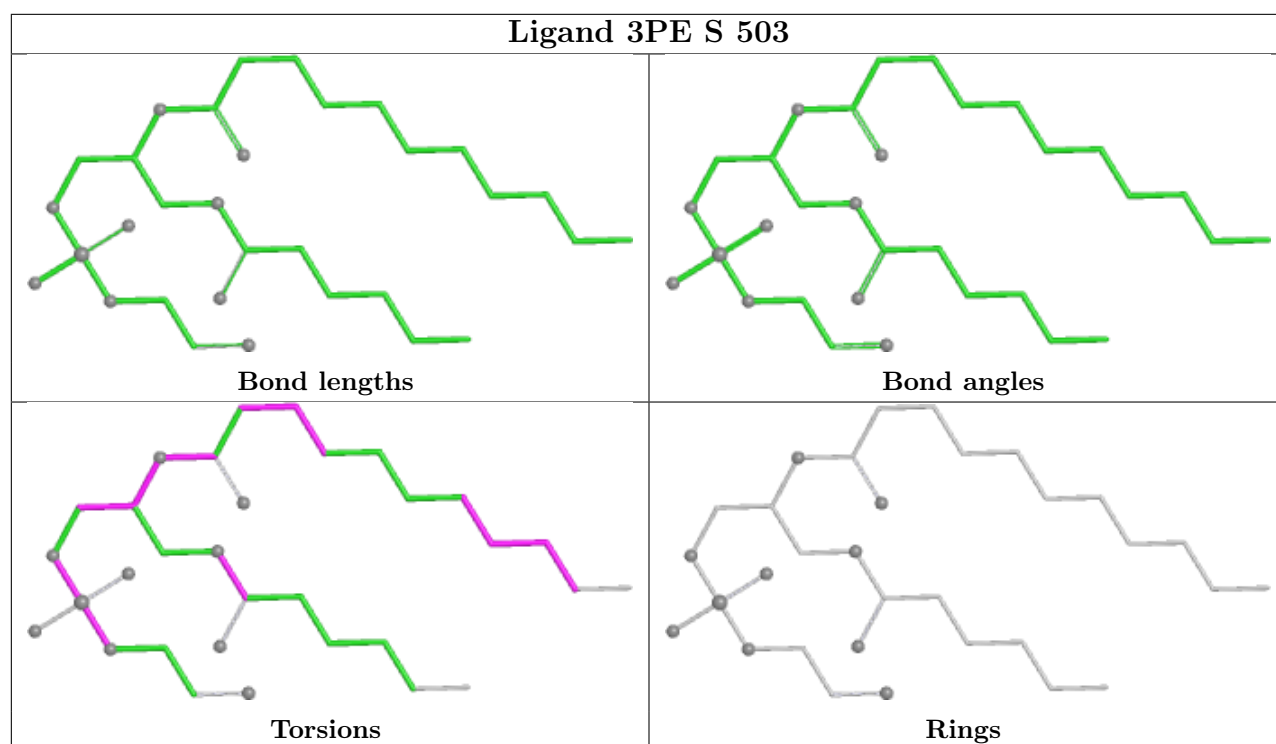
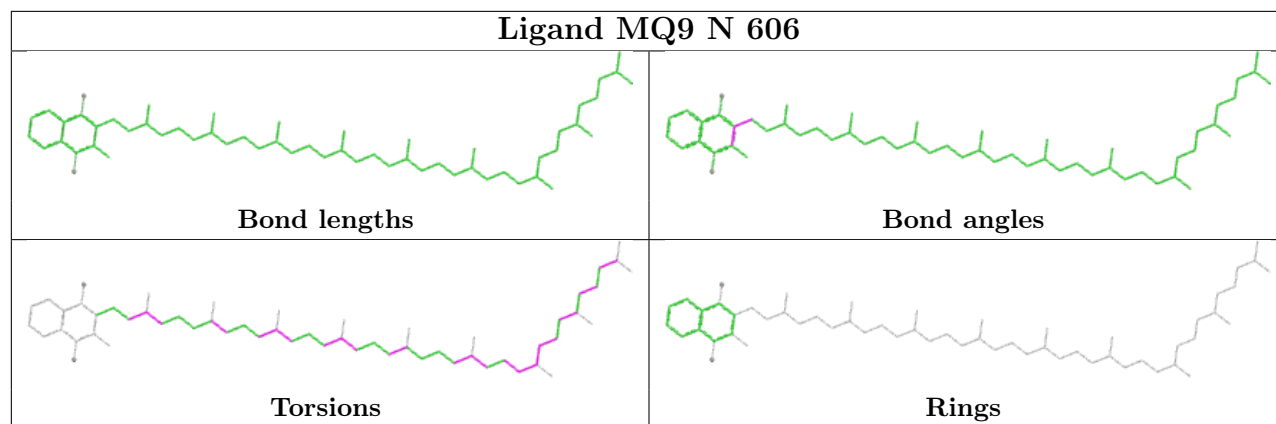


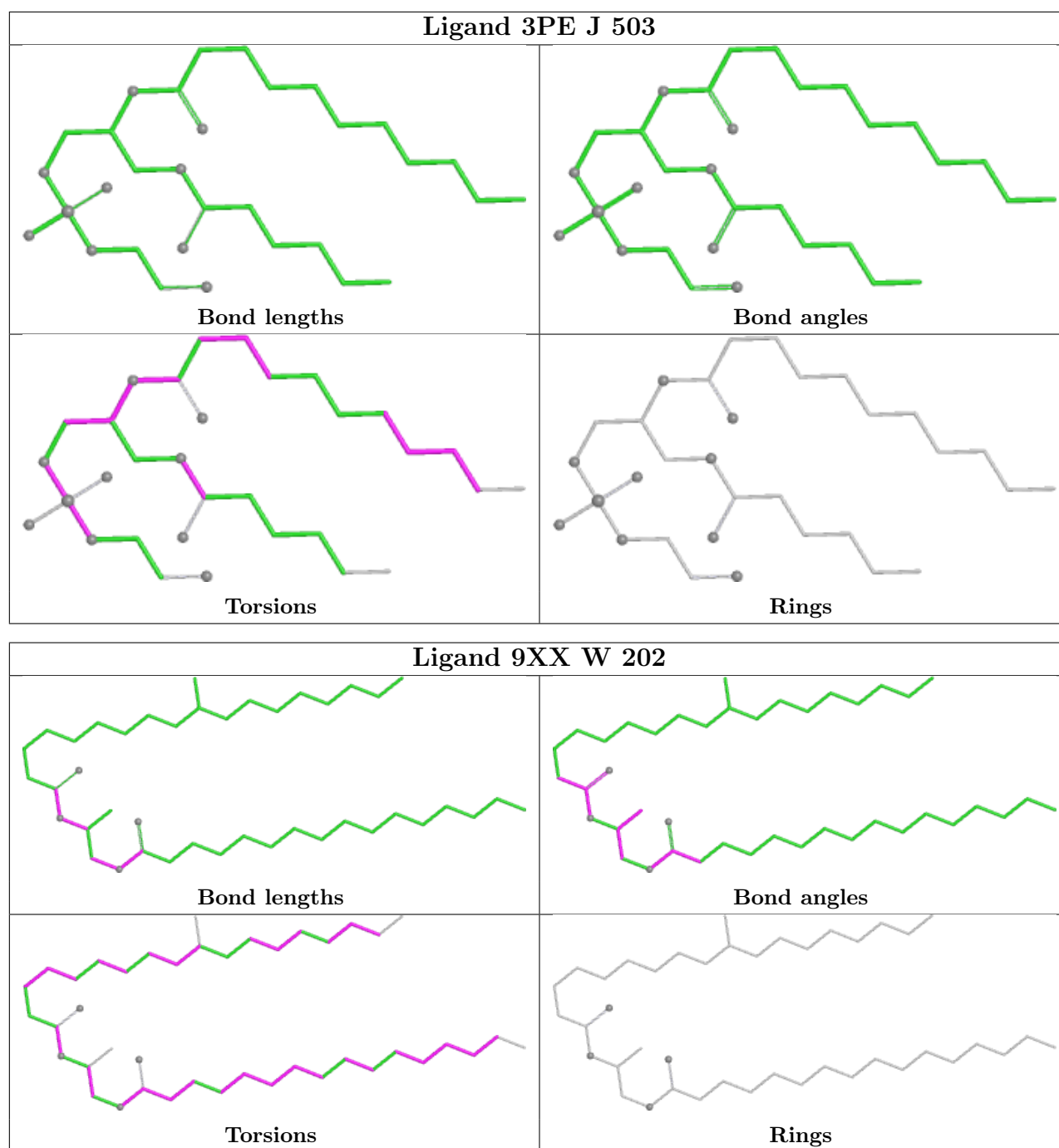


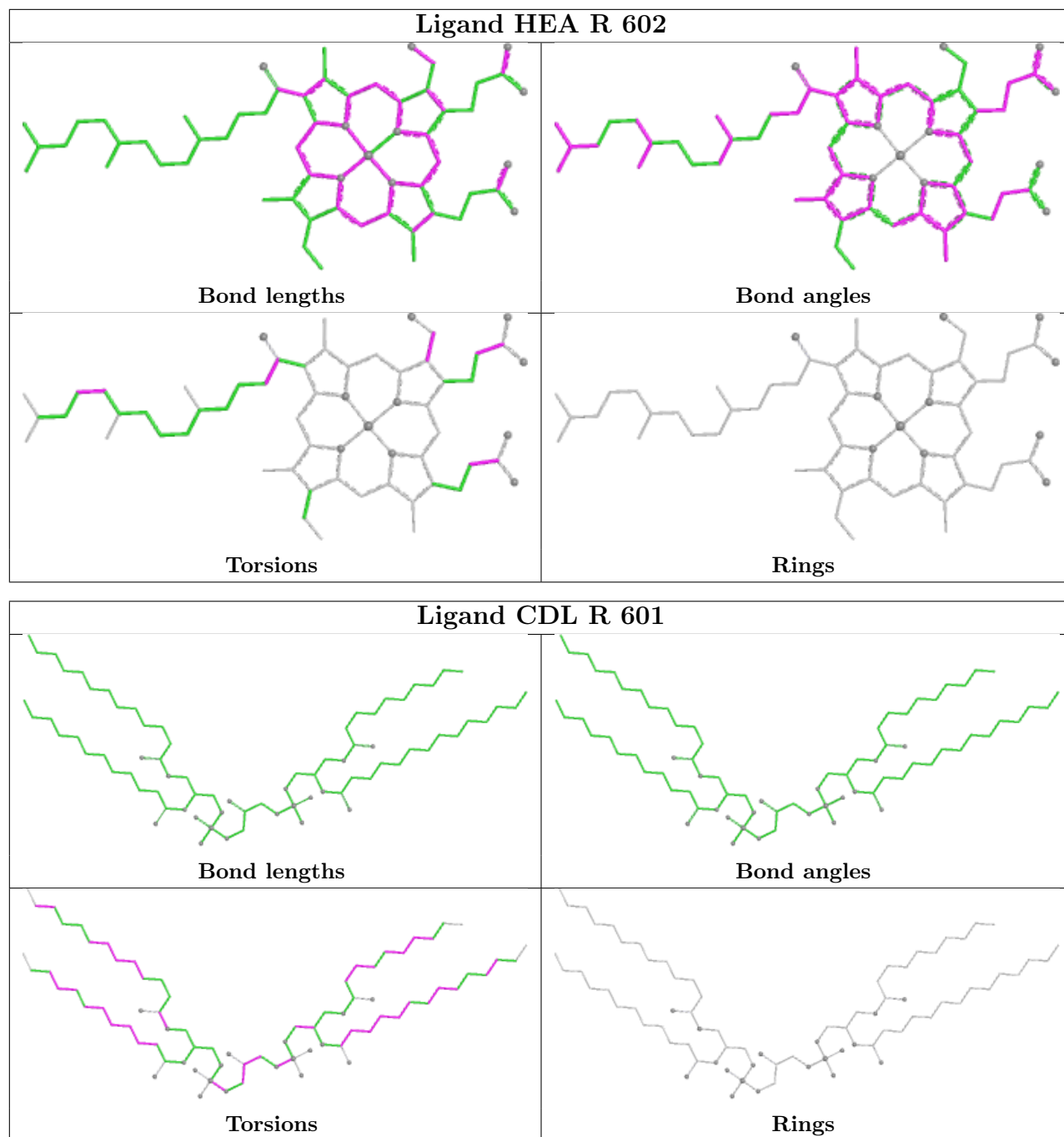


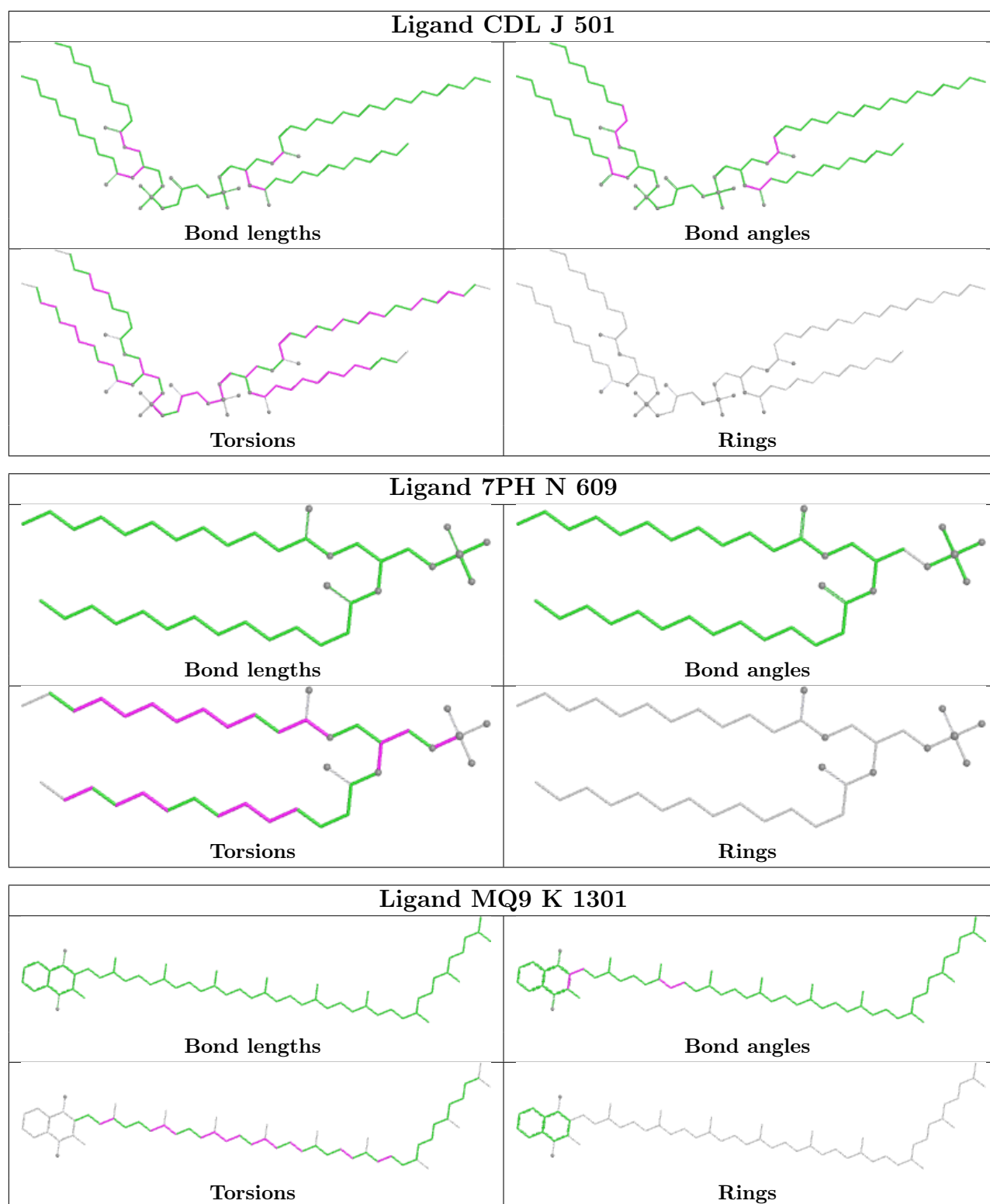


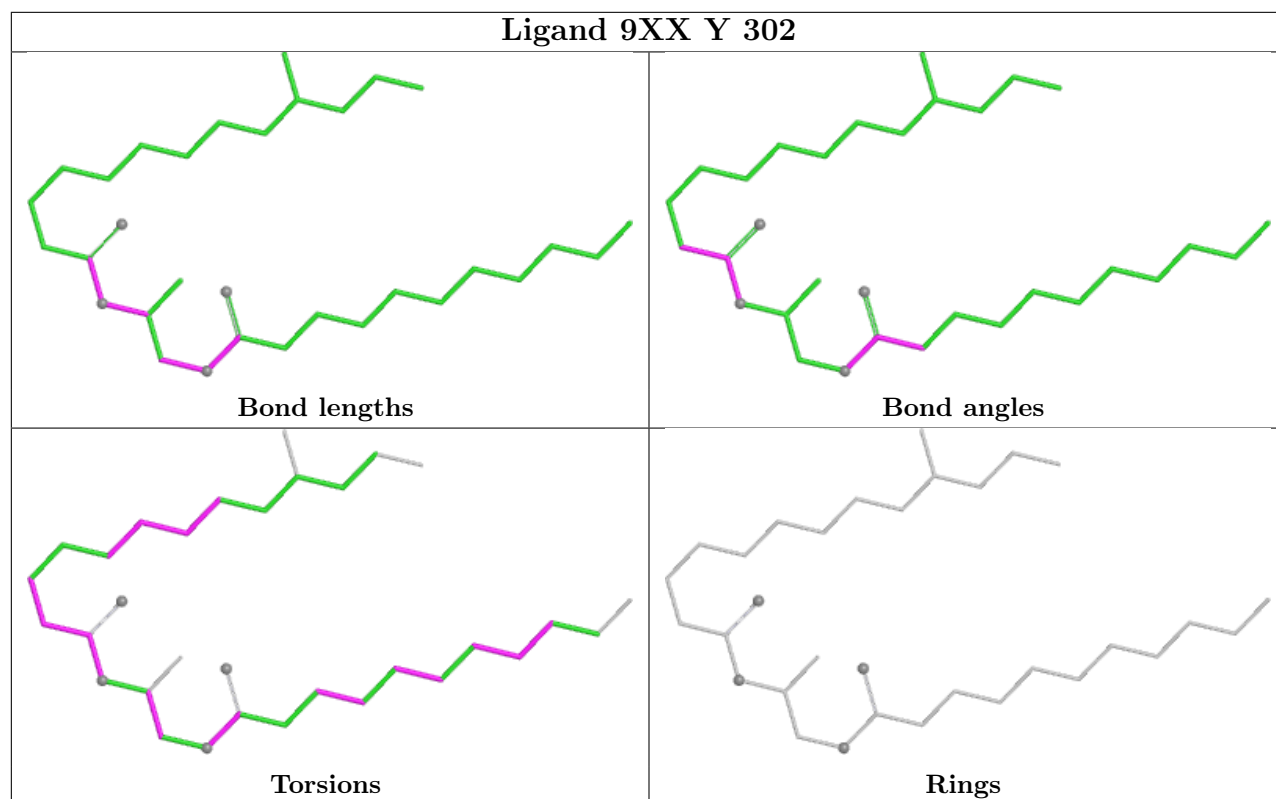
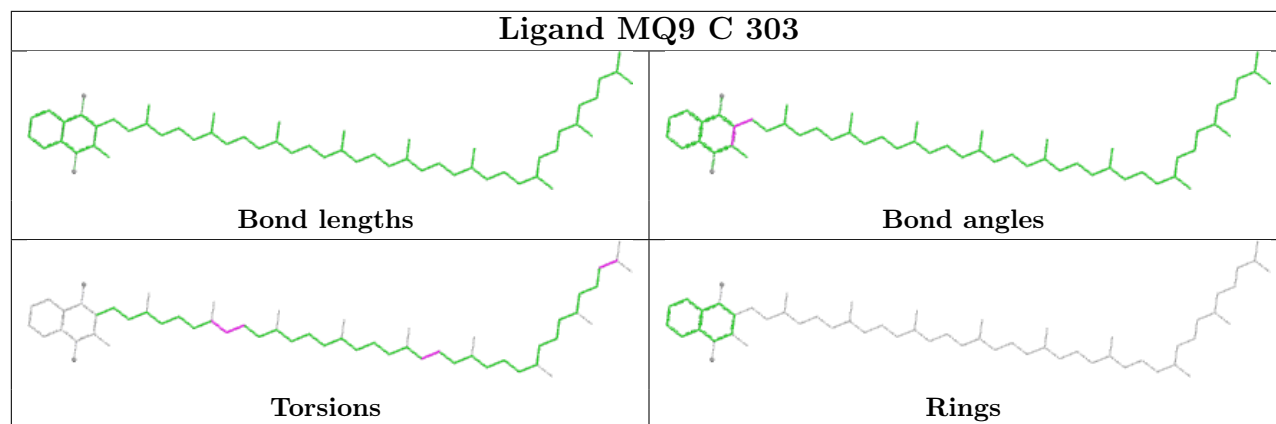


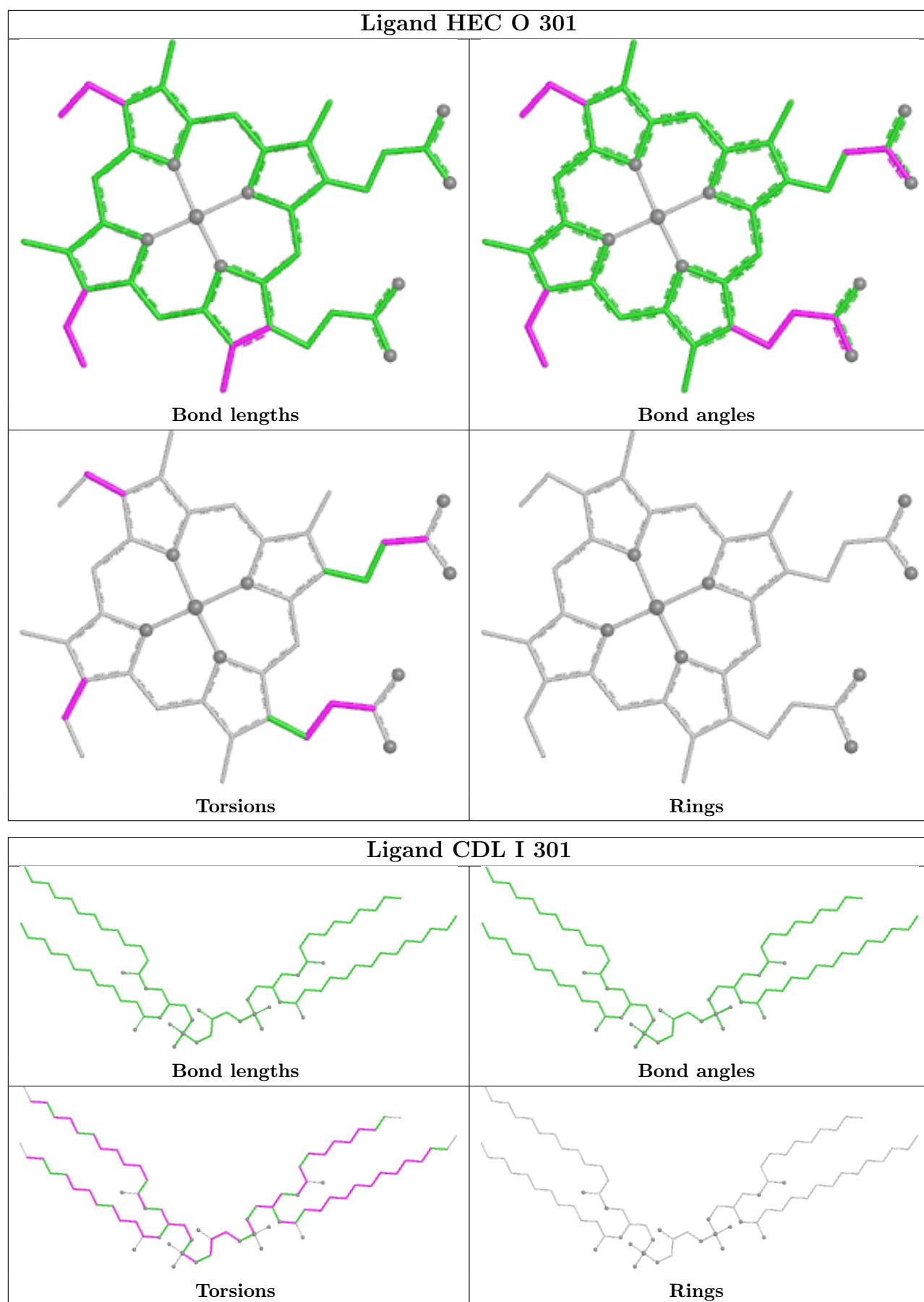


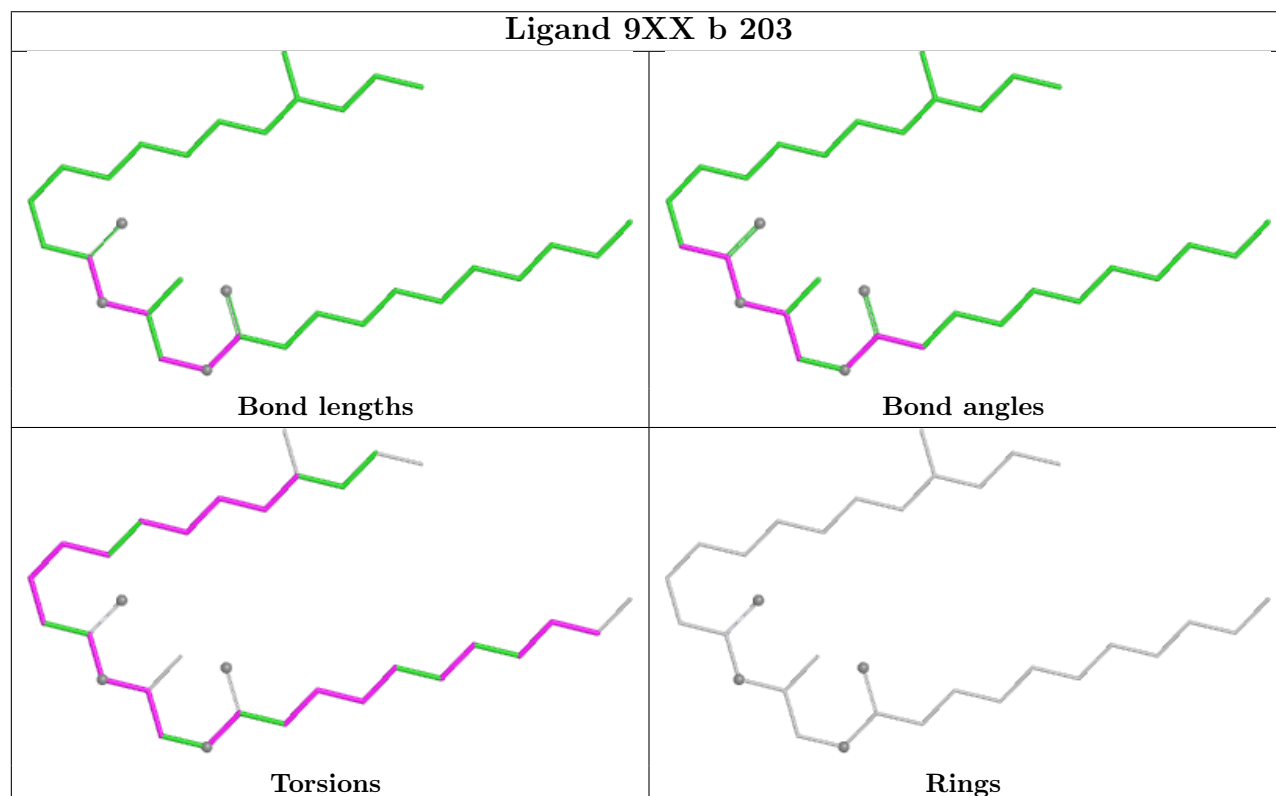
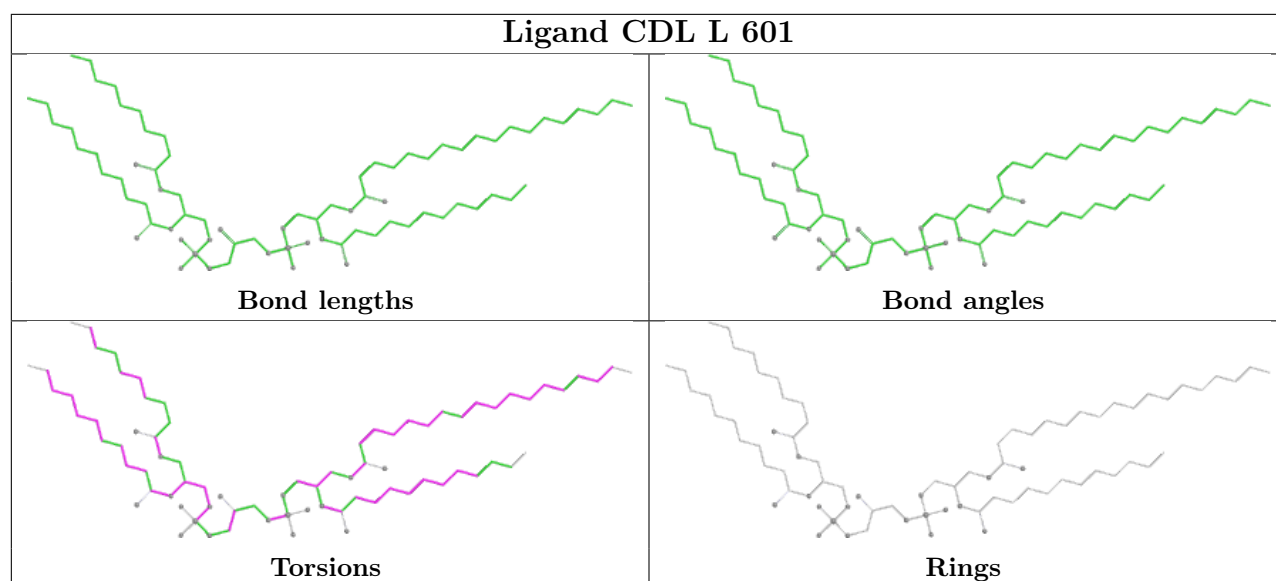


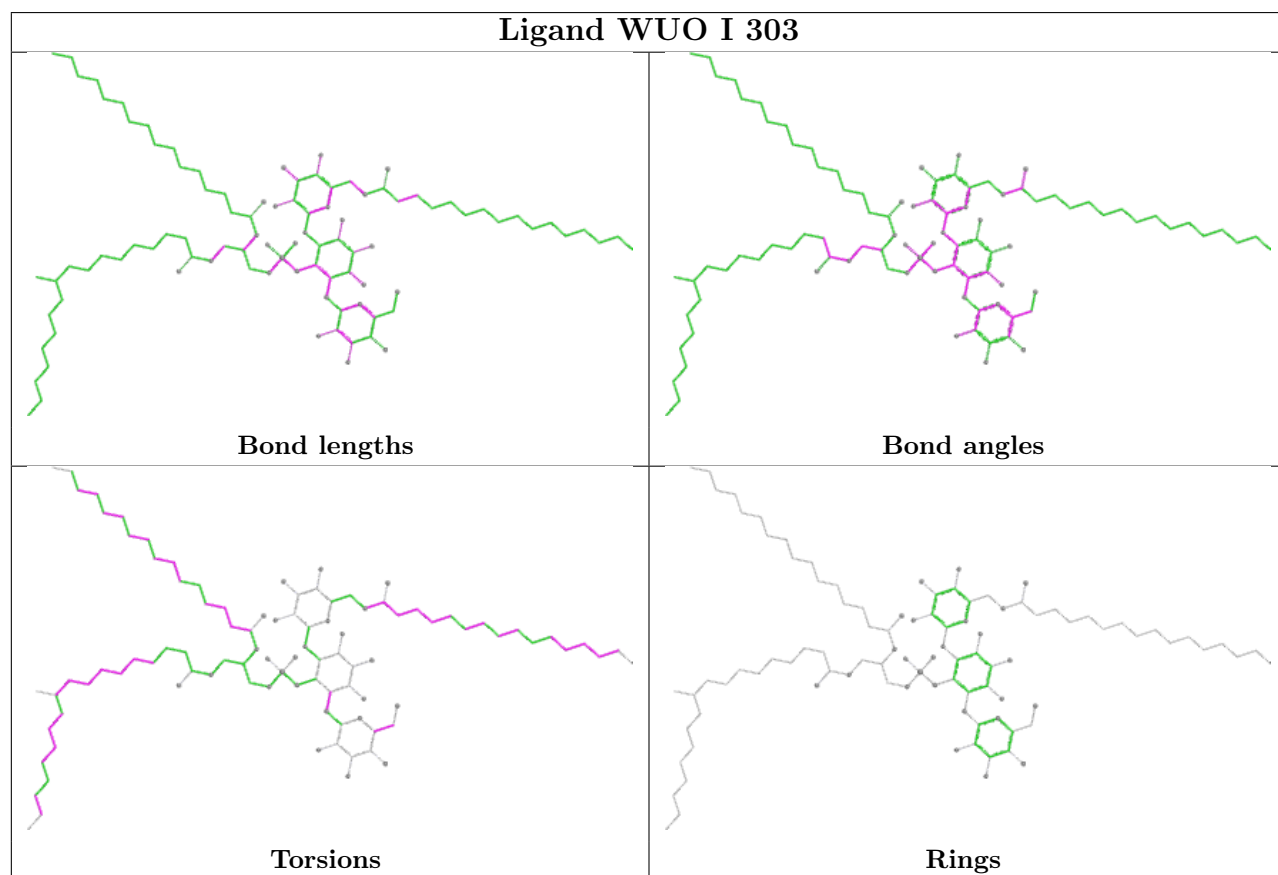
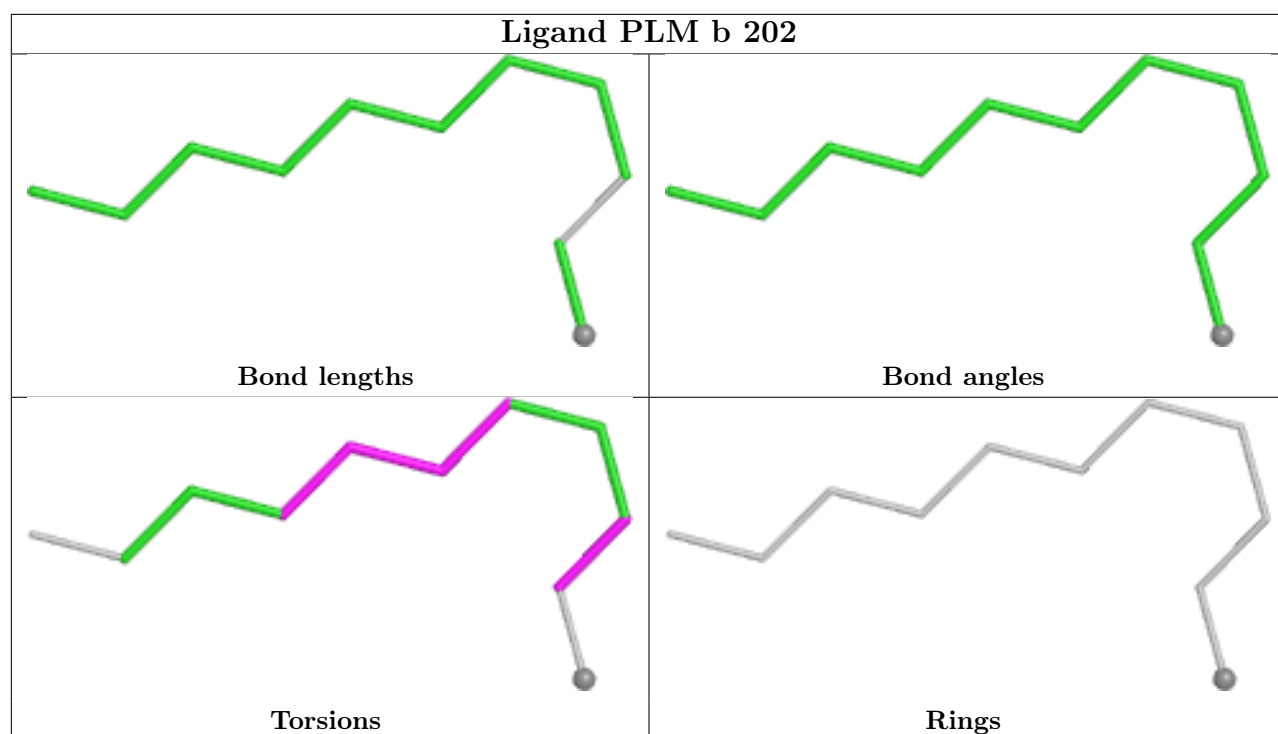


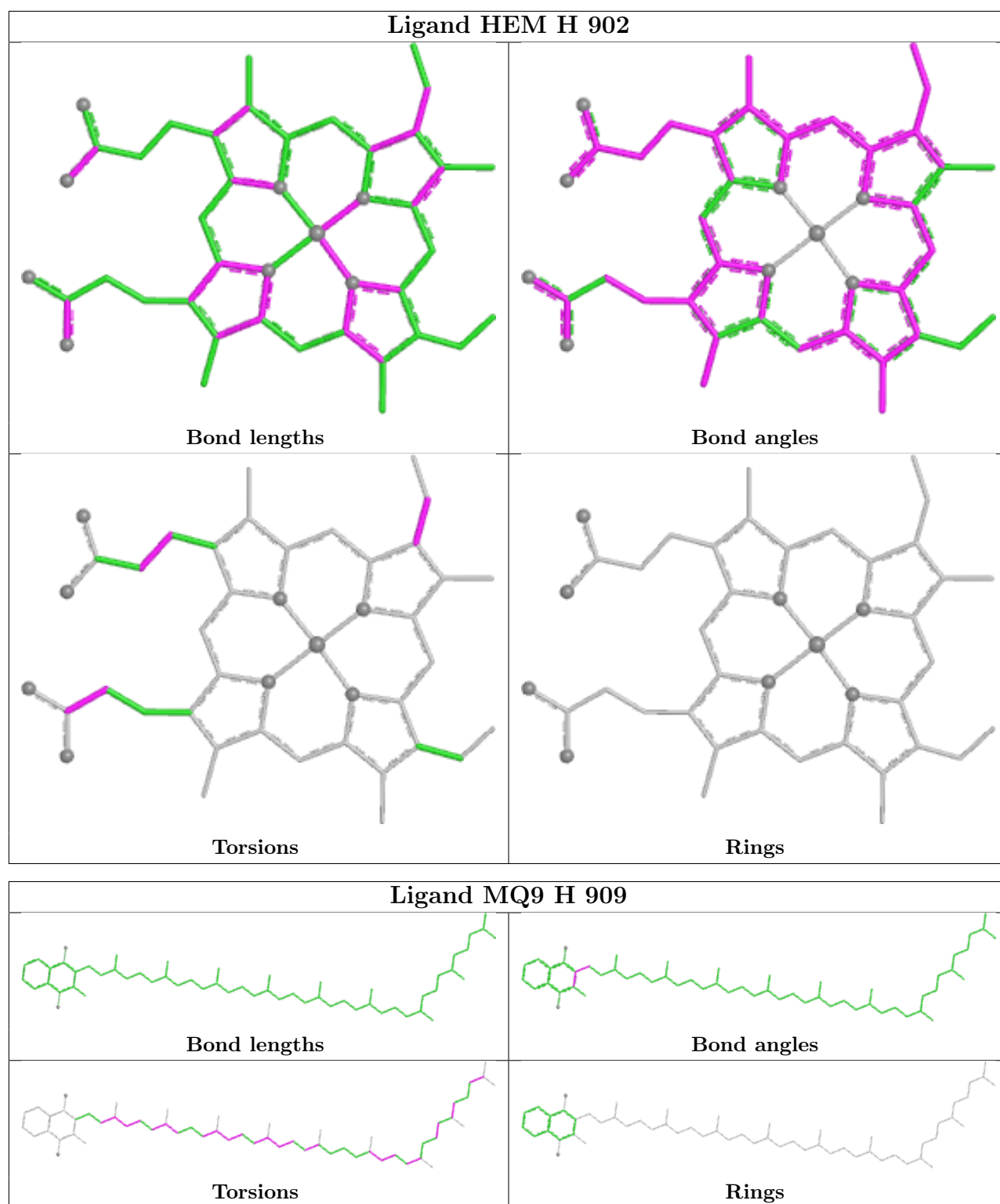












5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

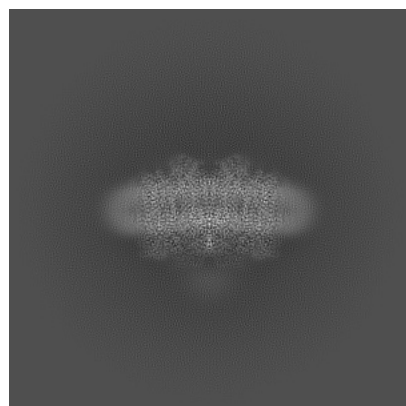
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-17211. These allow visual inspection of the internal detail of the map and identification of artifacts.

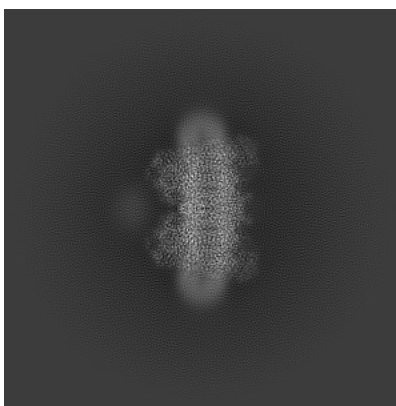
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

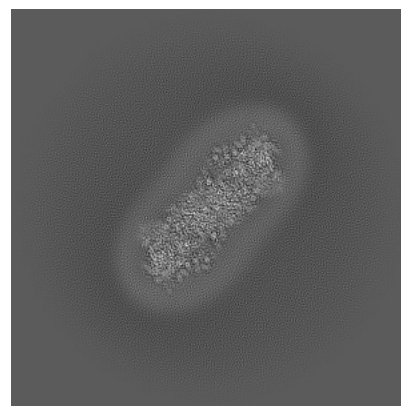
6.1.1 Primary map



X

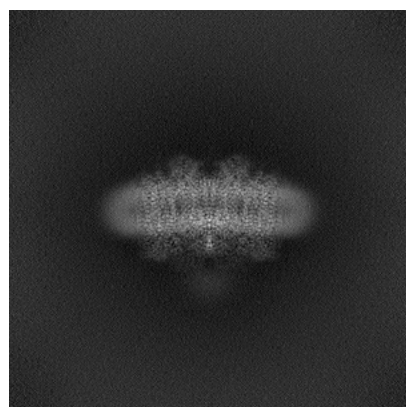


Y

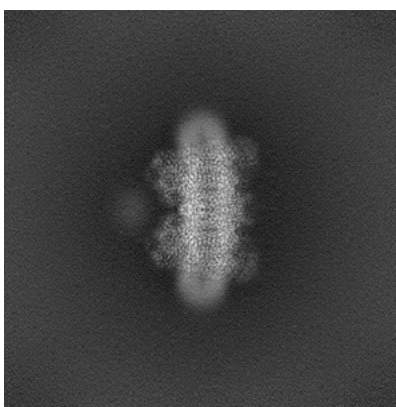


Z

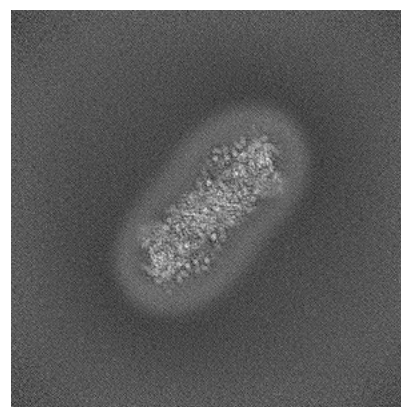
6.1.2 Raw map



X



Y

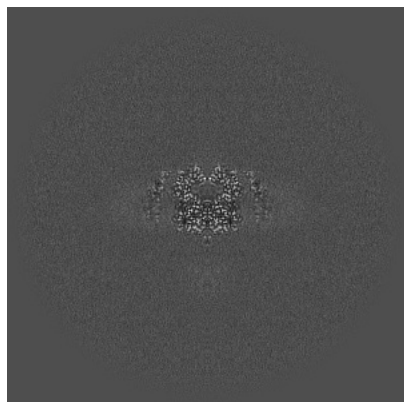


Z

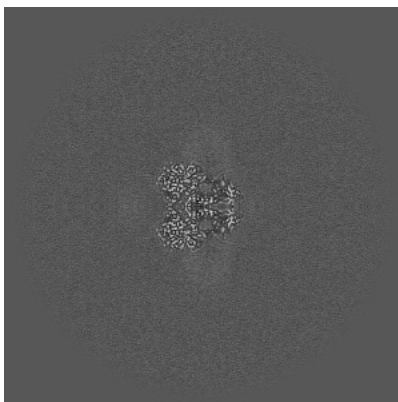
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

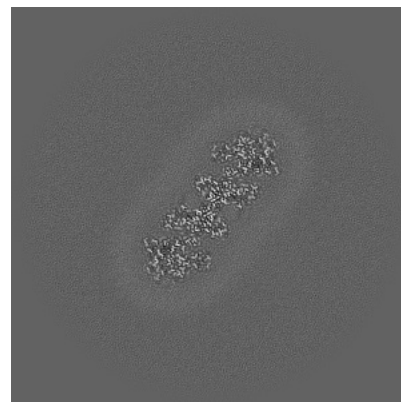
6.2.1 Primary map



X Index: 270

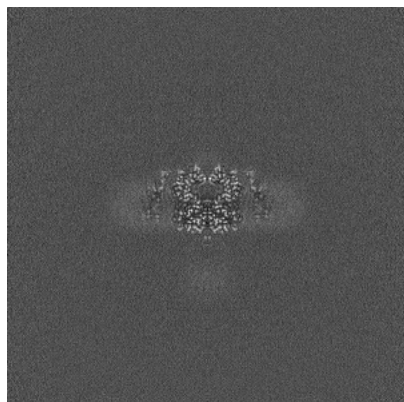


Y Index: 270

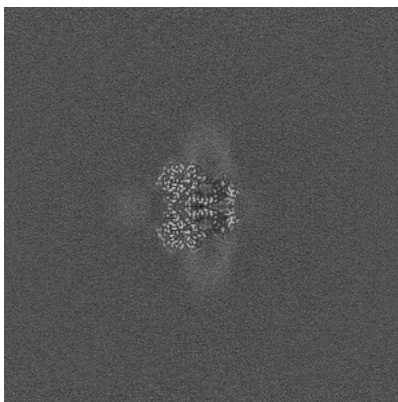


Z Index: 270

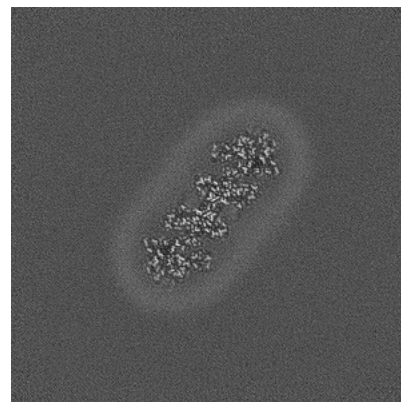
6.2.2 Raw map



X Index: 270



Y Index: 270

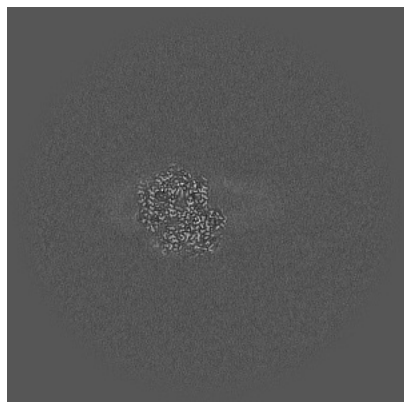


Z Index: 270

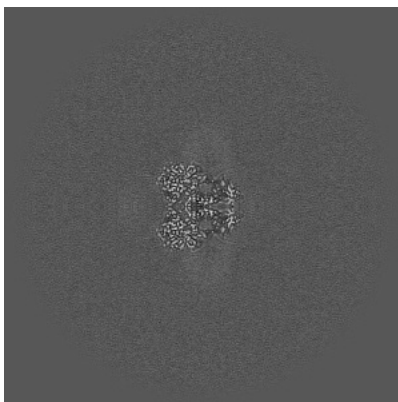
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

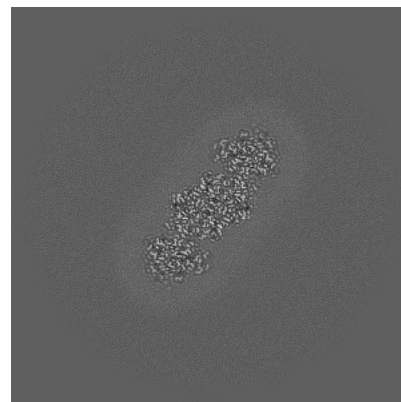
6.3.1 Primary map



X Index: 236

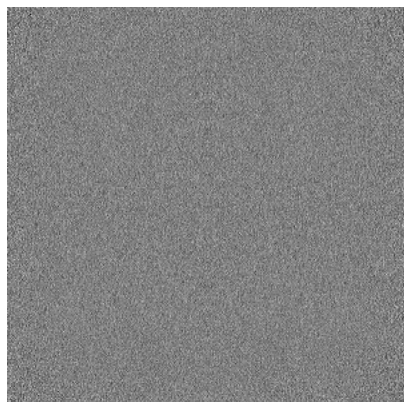


Y Index: 270

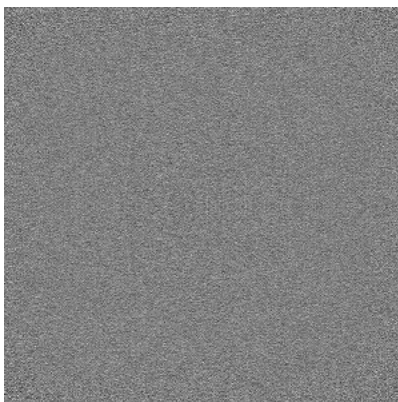


Z Index: 254

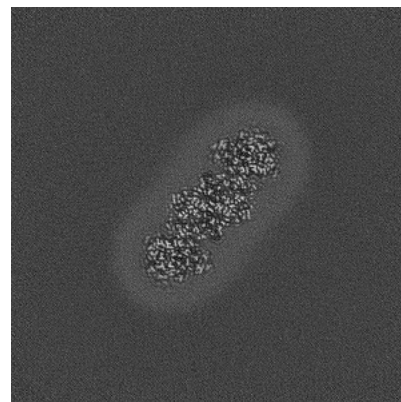
6.3.2 Raw map



X Index: 0



Y Index: 0

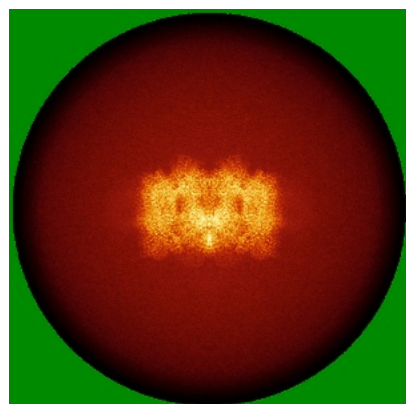


Z Index: 255

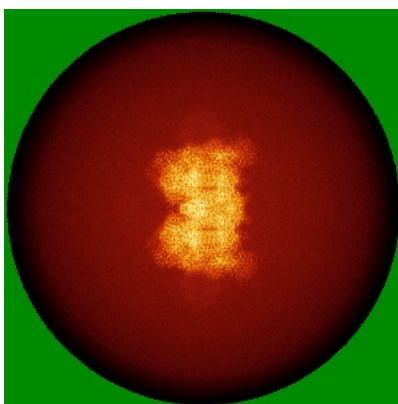
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

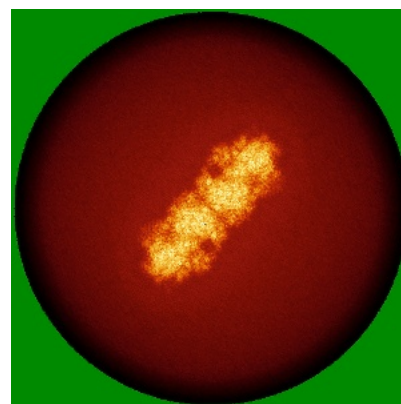
6.4.1 Primary map



X

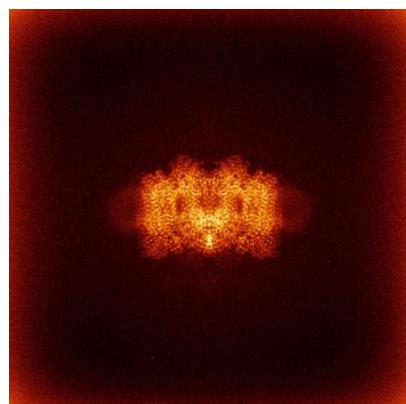


Y

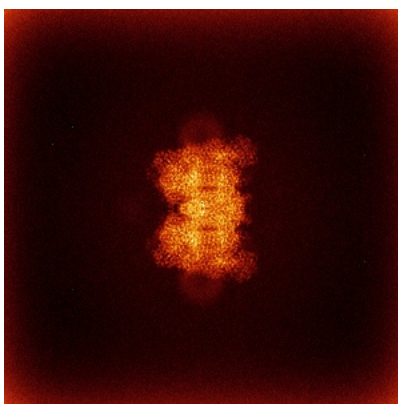


Z

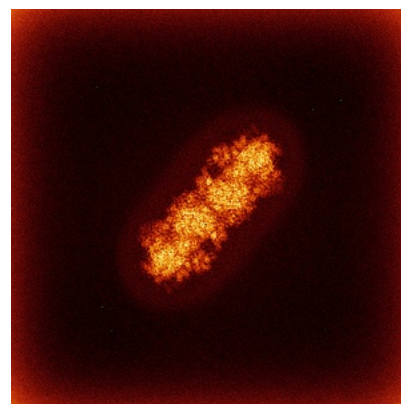
6.4.2 Raw map



X



Y

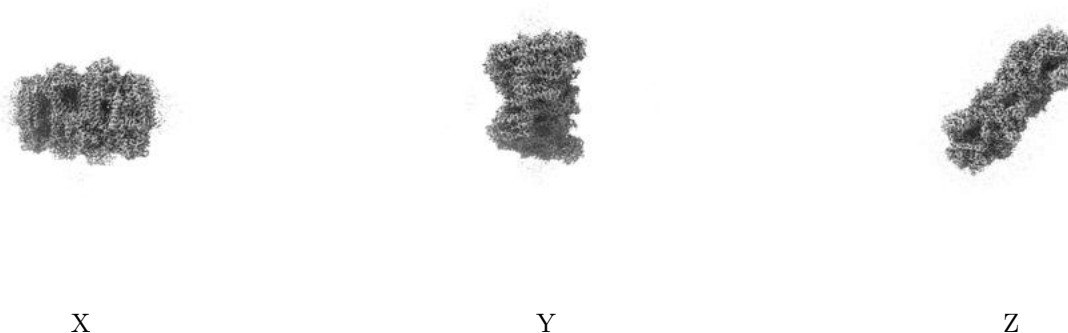


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

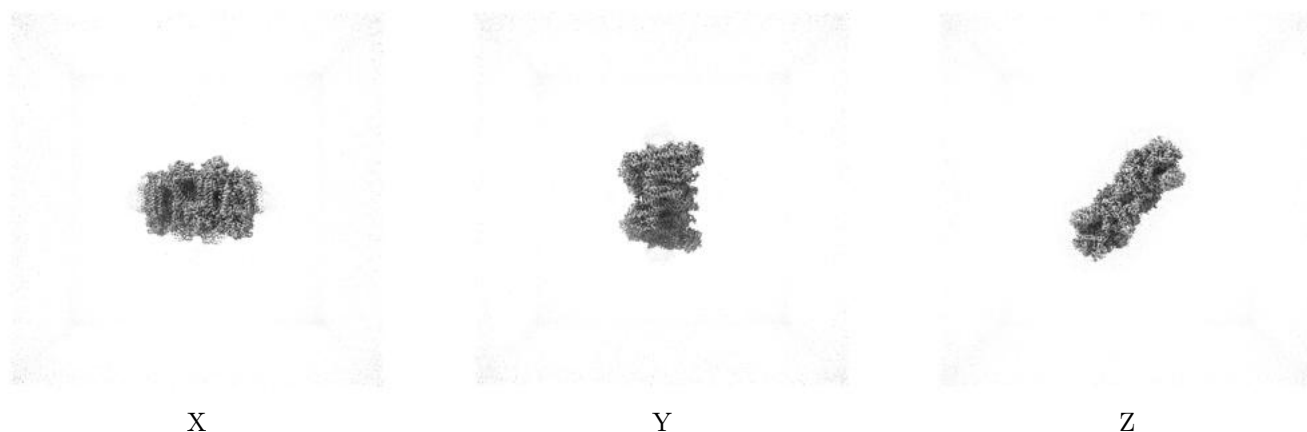
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.32. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

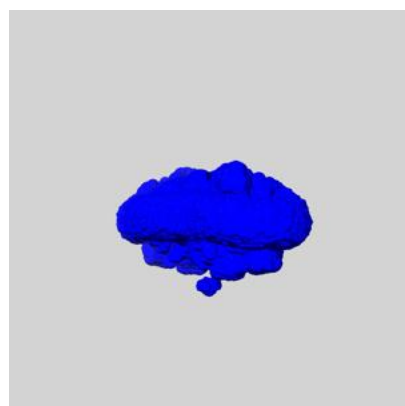
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

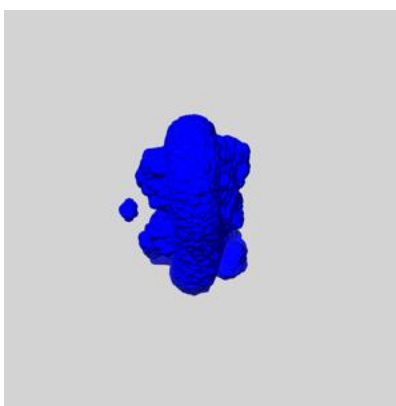
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

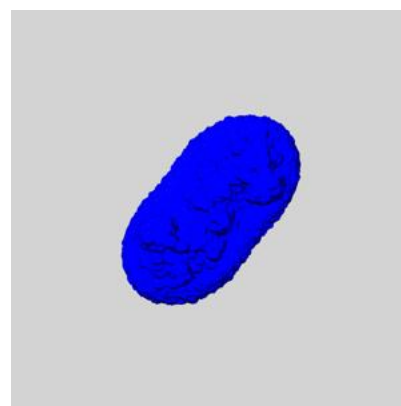
6.6.1 emd_17211_msk_1.map [i](#)



X



Y

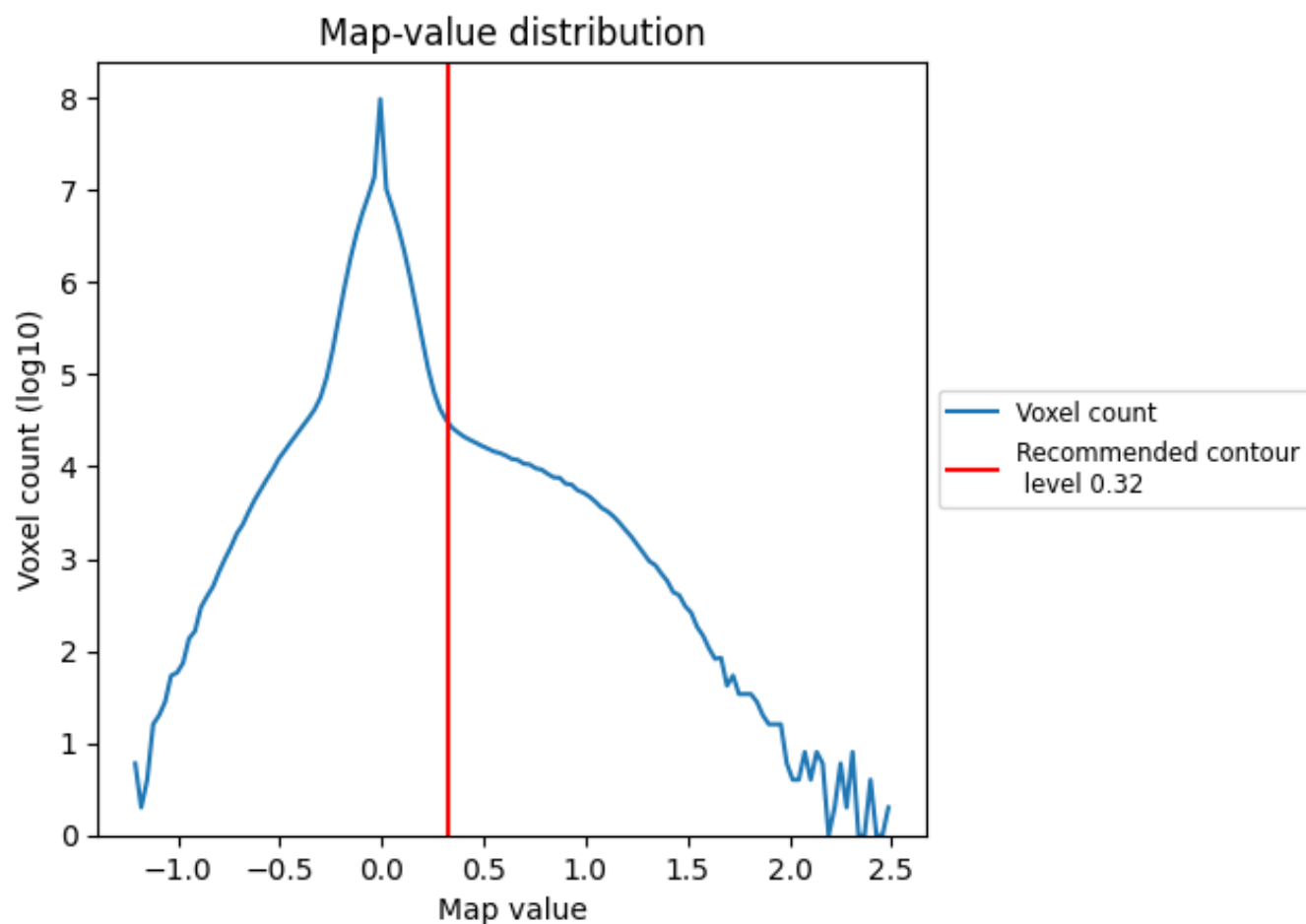


Z

7 Map analysis [i](#)

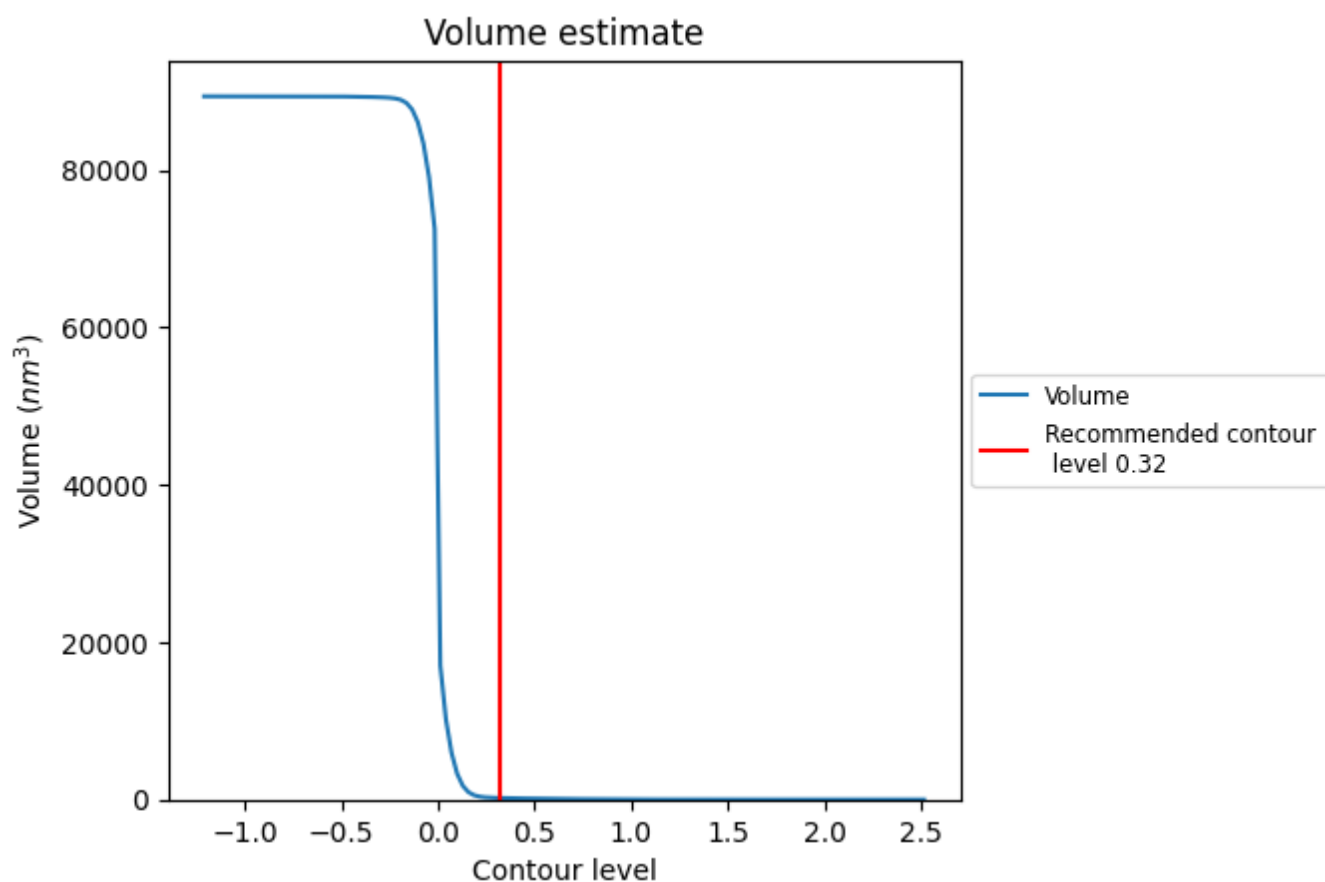
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

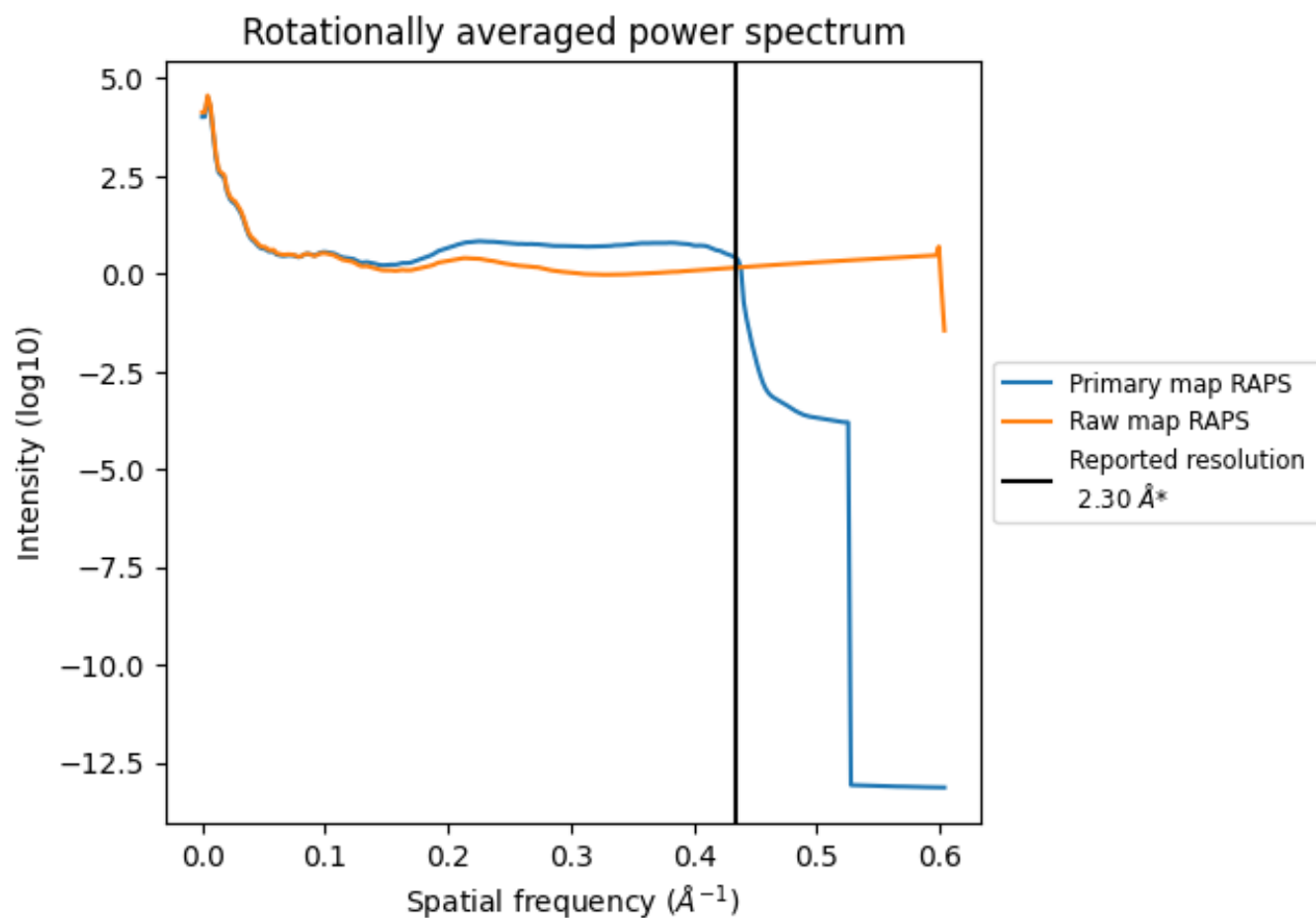
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 201 nm³; this corresponds to an approximate mass of 182 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ

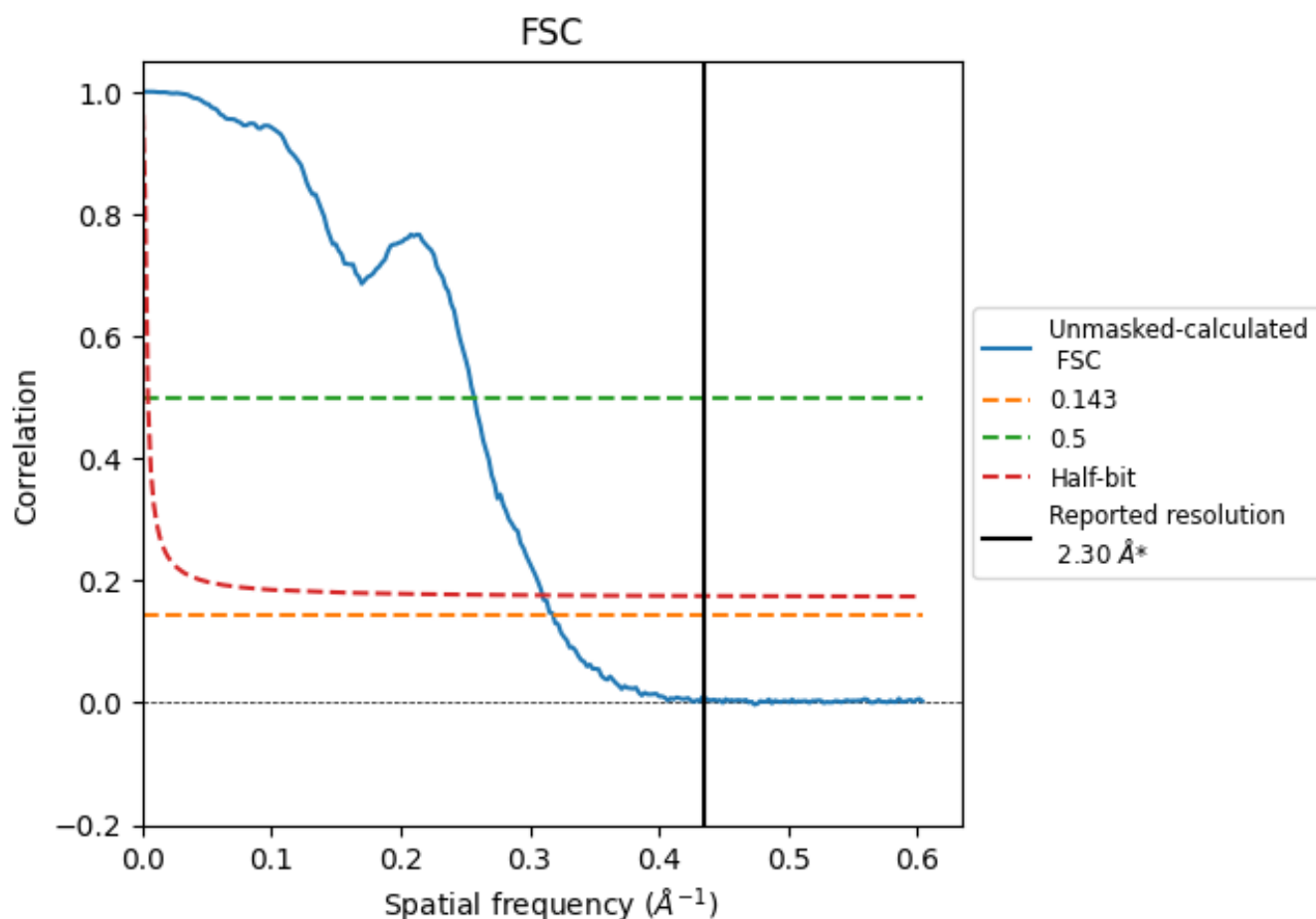


*Reported resolution corresponds to spatial frequency of 0.435 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.435 Å⁻¹

8.2 Resolution estimates [i](#)

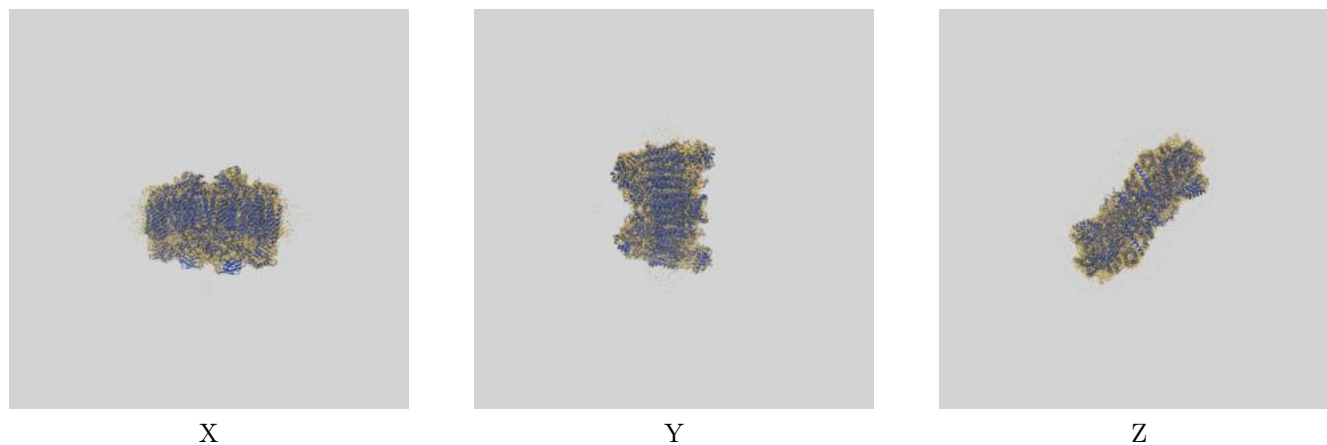
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.30	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.14	3.89	3.23

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.14 differs from the reported value 2.3 by more than 10 %

9 Map-model fit [i](#)

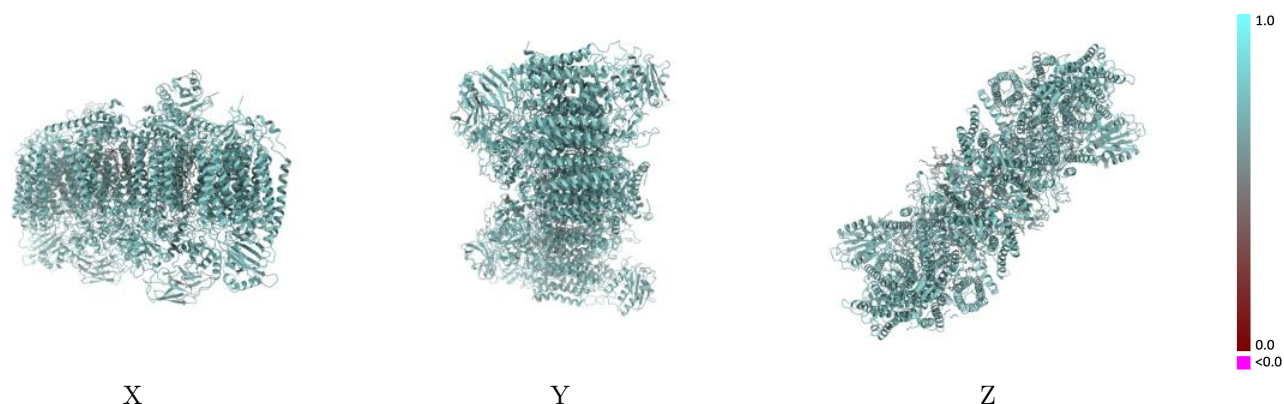
This section contains information regarding the fit between EMDB map EMD-17211 and PDB model 8OVD. Per-residue inclusion information can be found in section [3](#) on page [21](#).

9.1 Map-model overlay [i](#)



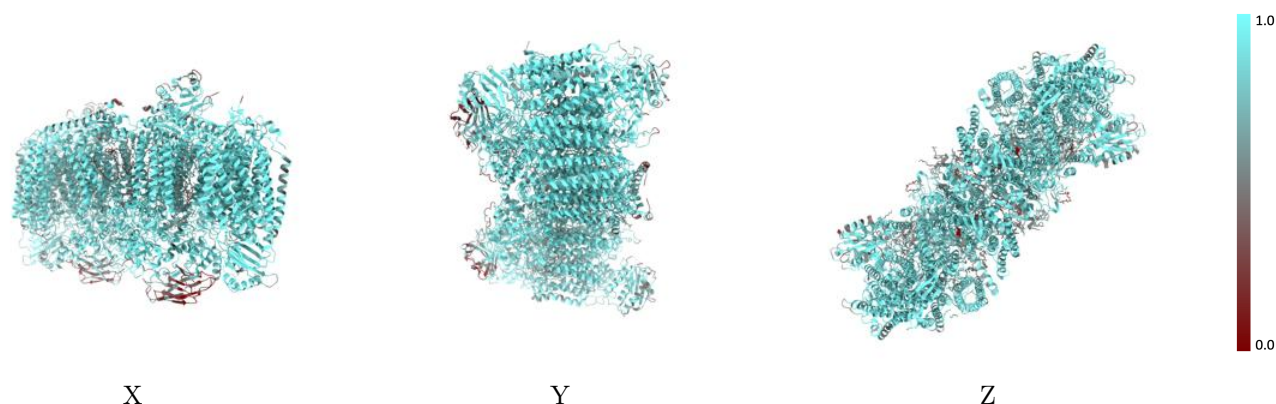
The images above show the 3D surface view of the map at the recommended contour level 0.32 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



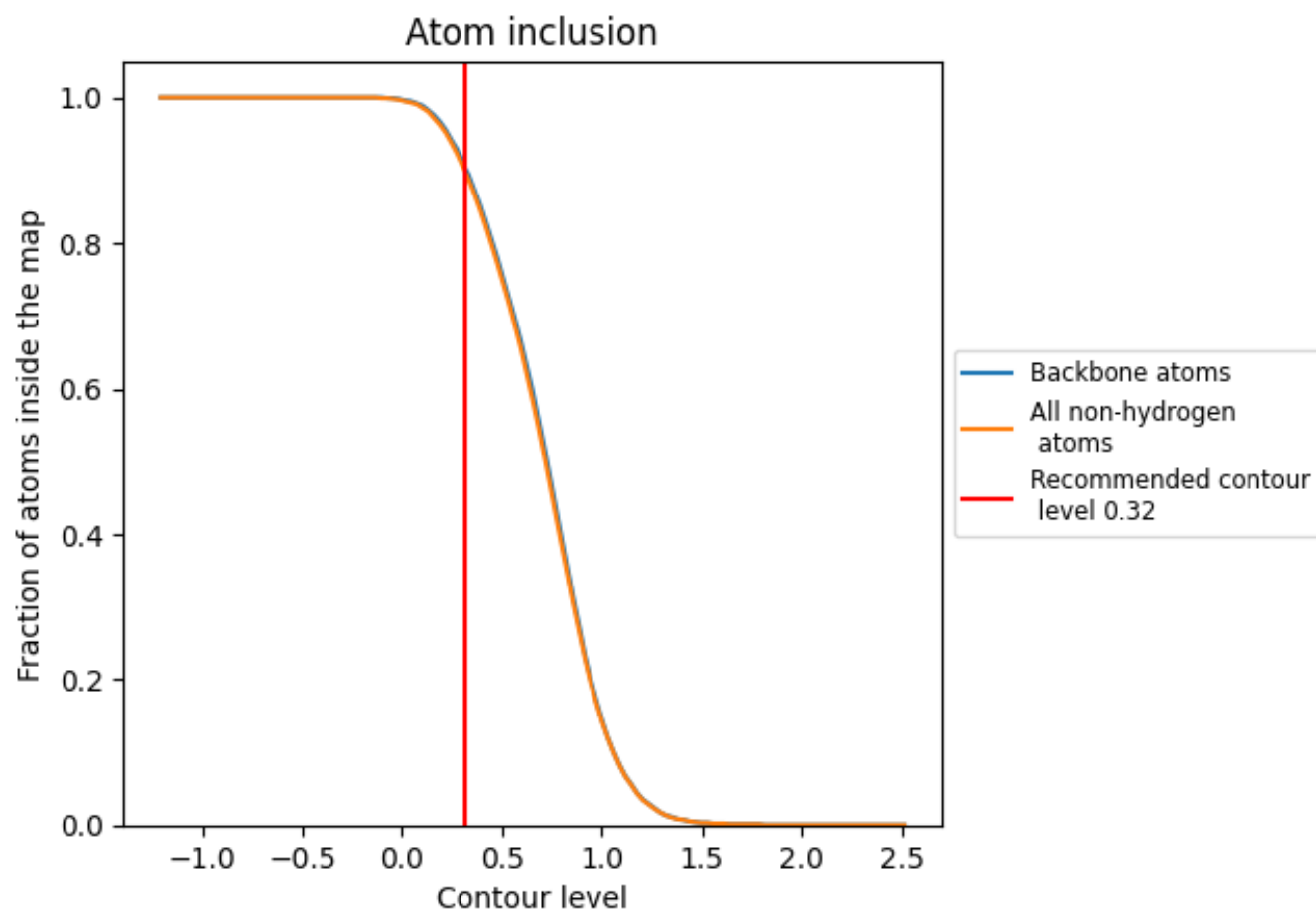
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.32).

9.4 Atom inclusion [i](#)



At the recommended contour level, 90% of all backbone atoms, 90% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.32) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8950	 0.6990
C	 0.9310	 0.7130
G	 0.9050	 0.6920
H	 0.9230	 0.7080
I	 0.8360	 0.6890
J	 0.9110	 0.6960
K	 0.9470	 0.7120
L	 0.9800	 0.7200
M	 0.9090	 0.6990
N	 0.9240	 0.7060
O	 0.9430	 0.7140
P	 0.8570	 0.6910
Q	 0.8700	 0.6910
R	 0.9760	 0.7190
S	 0.9320	 0.6990
T	 0.9290	 0.7000
U	 0.8090	 0.6680
V	 0.8310	 0.6700
W	 0.5000	 0.6370
X	 0.8670	 0.6900
Y	 0.7760	 0.6620
Z	 0.7840	 0.6570
a	 0.8150	 0.6630
b	 0.5080	 0.6300
c	 0.7710	 0.6560

