



Full wwPDB EM Validation Report ⓘ

Mar 26, 2026 – 10:49 PM UTC

PDB ID : 8OVC / pdb_00008ovc
EMDB ID : EMD-17210
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 : 2.80 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:

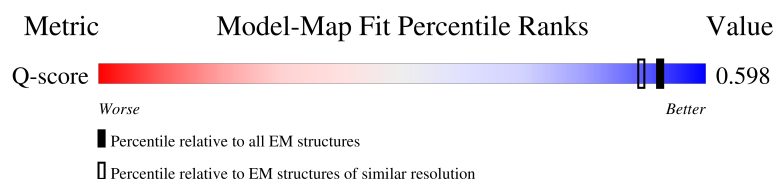
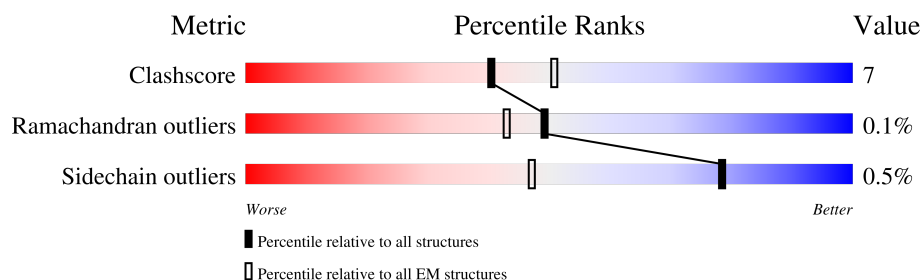
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 2.80 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.



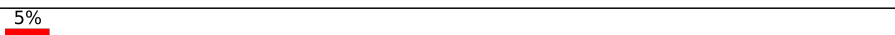
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	11806 (2.30 - 3.30)

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	71% 9% 20%
1	O	278	69% 11% 20%
2	G	408	85% 8% 7%
2	M	408	84% 9% 7%

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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	
13	E	10	
13	f	10	
14	F	25	
14	e	25	

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
16	MQ9	H	607	-	-	X	-

2 Entry composition

There are 29 unique types of molecules in this entry. The entry contains 46771 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	381	Total	C	N	O	S	0	0
			2973	1922	503	537	11		
2	G	380	Total	C	N	O	S	0	0
			2964	1917	501	535	11		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	N	535	Total	C	N	O	S	0	0
			4181	2751	711	701	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	86	Total	C	N	O	S	0	0
			688	443	125	115	5		

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Mol	Chain	Residues	Atoms					AltConf	Trace
4	I	86	Total	C	N	O	S	0	0
			688	443	125	115	5		

- 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	186	Total	C	N	O	S	0	0
			1455	976	231	241	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	552	Total	C	N	O	S	0	0
			4373	2938	695	714	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	286	Total	C	N	O	S	0	0
			2287	1483	377	419	8		
8	X	301	Total	C	N	O	S	0	0
			2398	1552	399	437	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	68	Total	C	N	O	S	0	0
			511	336	86	87	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	V	144	Total	C	N	O	S	0	0
			1032	653	175	202	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	146	Total	C	N	O	S	0	0
			1051	652	176	222	1		
11	b	148	Total	C	N	O	S	0	0
			1074	666	179	228	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
12	Y	26	Total	C	N	O	S	0	0
			173	106	27	39	1		
12	c	25	Total	C	N	O	S	0	0
			168	103	26	38	1		

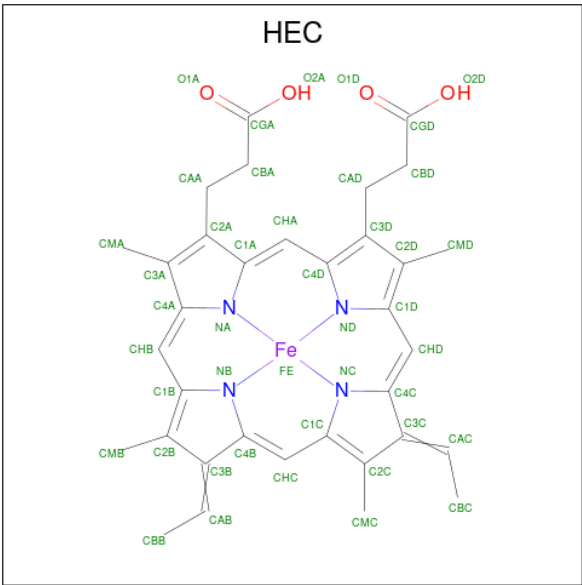
- Molecule 13 is a protein called Co-purified unknown peptide.

Mol	Chain	Residues	Atoms				AltConf	Trace
13	E	7	Total	C	N	O	0	0
			35	21	7	7		
13	f	7	Total	C	N	O	0	0
			35	21	7	7		

- Molecule 14 is a protein called Co-purified unknown peptide.

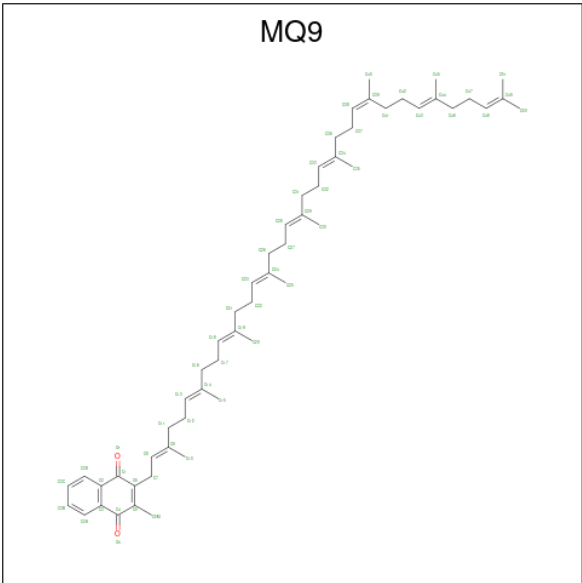
Mol	Chain	Residues	Atoms				AltConf	Trace
14	F	23	Total	C	N	O	0	0
			115	69	23	23		
14	e	23	Total	C	N	O	0	0
			115	69	23	23		

- Molecule 15 is HEME C (CCD ID: HEC) (formula: C₃₄H₃₄FeN₄O₄).



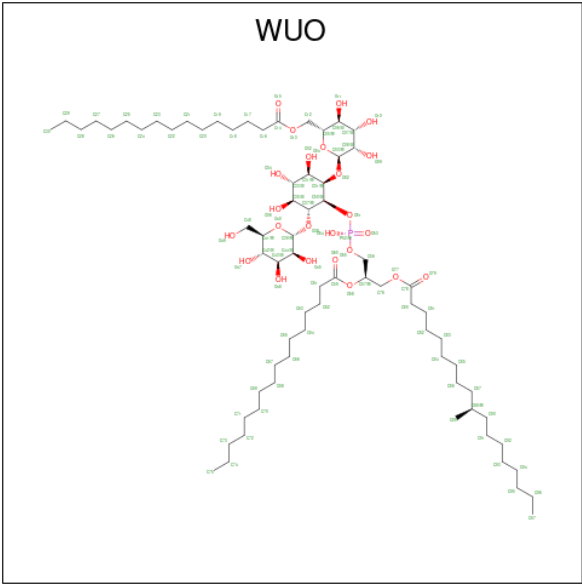
Mol	Chain	Residues	Atoms					AltConf
15	O	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
15	O	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
15	C	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
15	C	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

- Molecule 16 is MENAQUINONE-9 (CCD ID: MQ9) (formula: C₅₆H₈₀O₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
16	O	1	Total	C	O	0
			58	56	2	
16	N	1	Total	C	O	0
			58	56	2	
16	N	1	Total	C	O	0
			58	56	2	
16	N	1	Total	C	O	0
			58	56	2	
16	C	1	Total	C	O	0
			58	56	2	
16	G	1	Total	C	O	0
			43	41	2	
16	H	1	Total	C	O	0
			58	56	2	
16	H	1	Total	C	O	0
			43	41	2	
16	H	1	Total	C	O	0
			58	56	2	
16	H	1	Total	C	O	0
			58	56	2	

- Molecule 17 is acyl-phosphatidyl-myo-inositol dimannoside (AcPIM2) (CCD ID: WUO) (formula: C₇₂H₁₃₅O₂₄P).



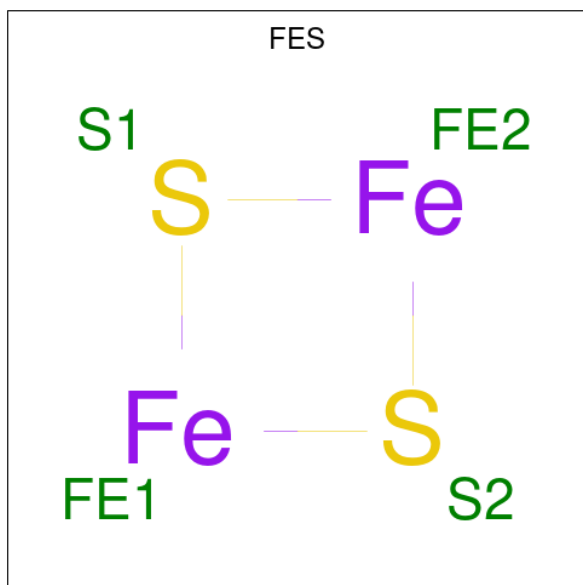
Mol	Chain	Residues	Atoms				AltConf
17	O	1	Total	C	O	P	0
			97	72	24	1	

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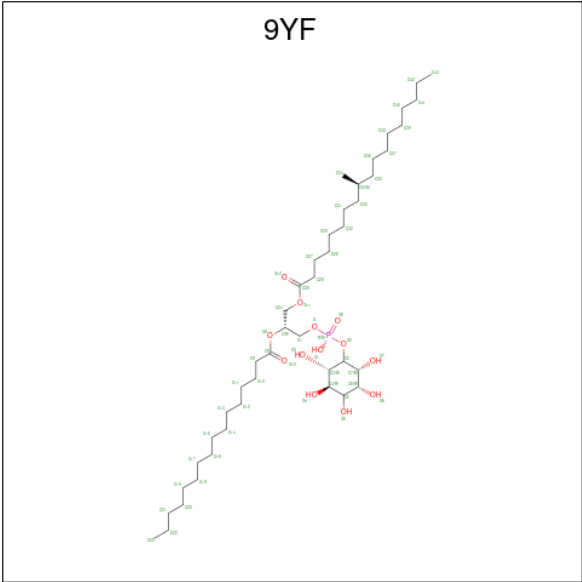
Mol	Chain	Residues	Atoms				AltConf
17	W	1	Total	C	O	P	0
			97	72	24	1	
17	C	1	Total	C	O	P	0
			97	72	24	1	
17	I	1	Total	C	O	P	0
			97	72	24	1	

- Molecule 18 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2).



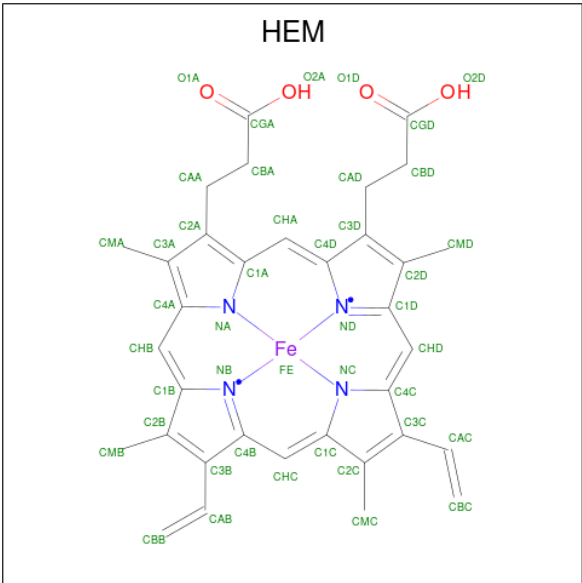
Mol	Chain	Residues	Atoms			AltConf
18	M	1	Total	Fe	S	0
			4	2	2	
18	G	1	Total	Fe	S	0
			4	2	2	

- Molecule 19 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: $\text{C}_{44}\text{H}_{85}\text{O}_{13}\text{P}$).



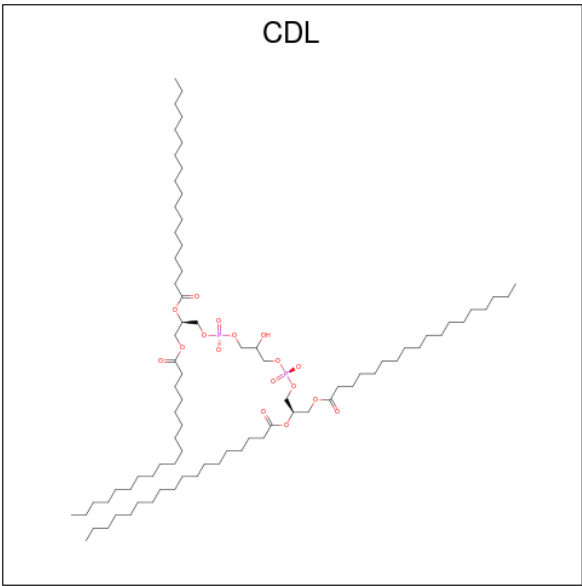
Mol	Chain	Residues	Atoms				AltConf
19	M	1	Total	C	O	P	0
			58	44	13	1	
19	W	1	Total	C	O	P	0
			58	44	13	1	
19	G	1	Total	C	O	P	0
			58	44	13	1	
19	b	1	Total	C	O	P	0
			58	44	13	1	

- Molecule 20 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



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

- Molecule 21 is CARDIOLIPIN (CCD ID: CDL) (formula: C₈₁H₁₅₆O₁₇P₂).



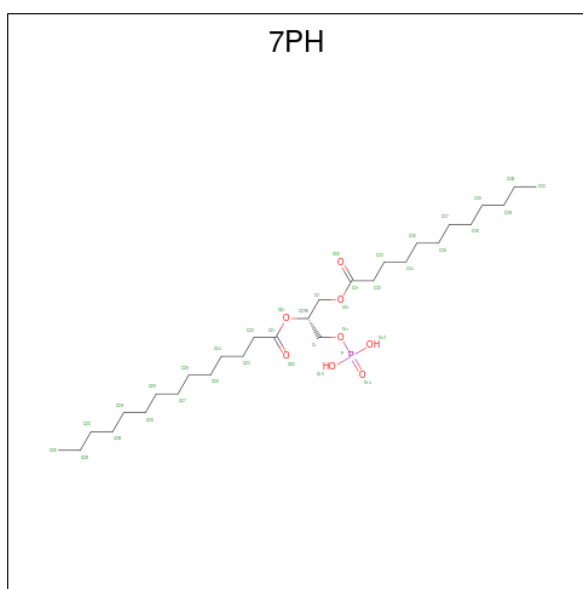
Mol	Chain	Residues	Atoms				AltConf
21	N	1	Total	C	O	P	0
			77	58	17	2	
21	N	1	Total	C	O	P	0
			79	60	17	2	
21	P	1	Total	C	O	P	0
			77	58	17	2	
21	T	1	Total	C	O	P	0
			79	60	17	2	
21	R	1	Total	C	O	P	0
			77	58	17	2	
21	R	1	Total	C	O	P	0
			77	58	17	2	
21	G	1	Total	C	O	P	0
			79	60	17	2	
21	H	1	Total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

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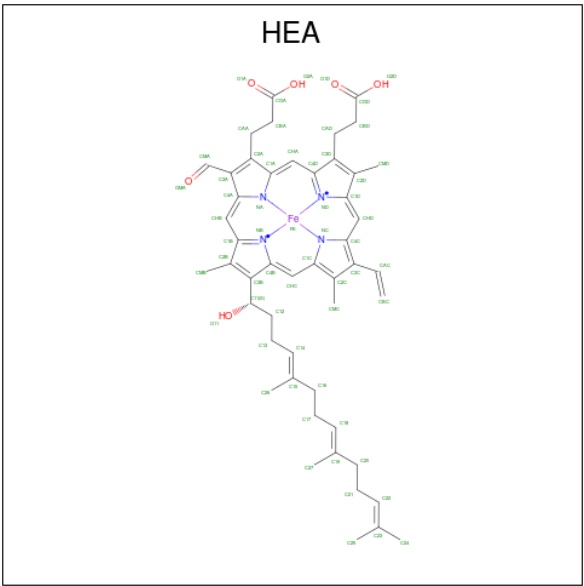
Mol	Chain	Residues	Atoms				AltConf
21	H	1	Total	C	O	P	0
			74	55	17	2	
21	H	1	Total	C	O	P	0
			77	58	17	2	
21	H	1	Total	C	O	P	0
			79	60	17	2	
21	H	1	Total	C	O	P	0
			79	60	17	2	
21	I	1	Total	C	O	P	0
			77	58	17	2	
21	I	1	Total	C	O	P	0
			77	58	17	2	
21	L	1	Total	C	O	P	0
			79	60	17	2	
21	L	1	Total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

- Molecule 22 is (1R)-2-(dodecanoyloxy)-1-[(phosphonoxy)methyl]ethyl tetradecanoate (CCD ID: 7PH) (formula: C₂₉H₅₇O₈P).



Mol	Chain	Residues	Atoms				AltConf
22	S	1	Total	C	O	P	0
			38	29	8	1	
22	S	1	Total	C	O	P	0
			38	29	8	1	
22	J	1	Total	C	O	P	0
			38	29	8	1	

- Molecule 23 is HEME-A (CCD ID: HEA) (formula: $C_{49}H_{56}FeN_4O_6$).



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

- Molecule 24 is COPPER (II) ION (CCD ID: CU) (formula: Cu).

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

- Molecule 25 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
25	R	1	Total	Mg	0
			1	1	

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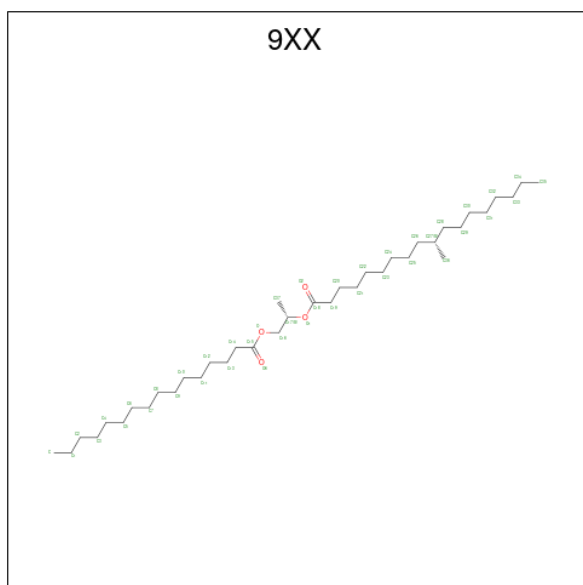
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Mol	Chain	Residues	Atoms		AltConf
25	L	1	Total	Mg	0
			1	1	

- Molecule 26 is CALCIUM ION (CCD ID: CA) (formula: Ca).

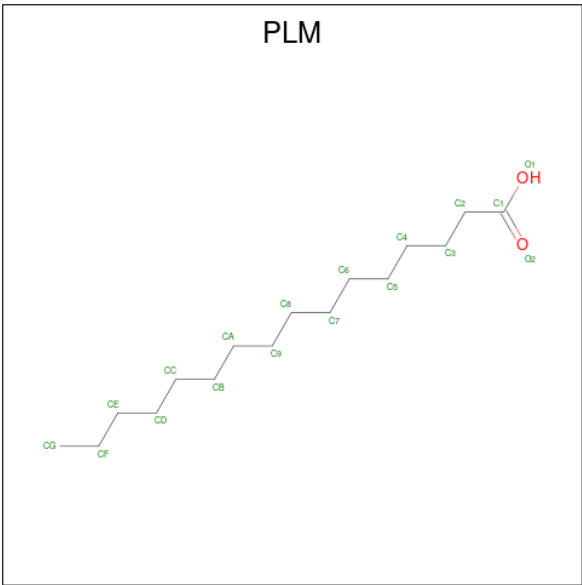
Mol	Chain	Residues	Atoms		AltConf
26	R	1	Total	Ca	0
			1	1	
26	L	1	Total	Ca	0
			1	1	

- Molecule 27 is (2S)-1-(hexadecanoyloxy)propan-2-yl (10S)-10-methyloctadecanoate (CCD ID: 9XX) (formula: C₃₈H₇₄O₄).



Mol	Chain	Residues	Atoms			AltConf
27	R	1	Total	C	O	0
			42	38	4	
27	Y	1	Total	C	O	0
			32	28	4	
27	H	1	Total	C	O	0
			32	28	4	
27	b	1	Total	C	O	0
			32	28	4	

- Molecule 28 is PALMITIC ACID (CCD ID: PLM) (formula: C₁₆H₃₂O₂).



Mol	Chain	Residues	Atoms			AltConf
28	W	1	Total	C	O	0
			11	10	1	
28	Y	1	Total	C	O	0
			11	10	1	
28	L	1	Total	C	O	0
			11	10	1	
28	c	1	Total	C	O	0
			11	10	1	

- Molecule 29 is water.

Mol	Chain	Residues	Atoms		AltConf
29	O	25	Total	O	0
			25	25	
29	M	15	Total	O	0
			15	15	
29	N	22	Total	O	0
			22	22	
29	P	3	Total	O	0
			3	3	
29	S	1	Total	O	0
			1	1	
29	T	3	Total	O	0
			3	3	
29	R	14	Total	O	0
			14	14	
29	Q	5	Total	O	0
			5	5	

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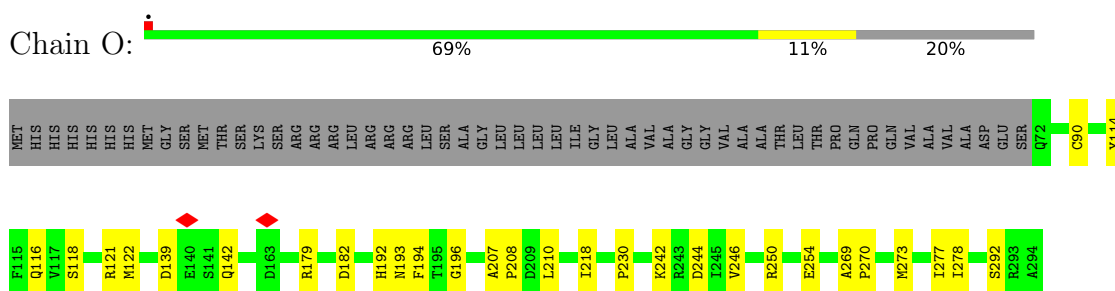
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Mol	Chain	Residues	Atoms		AltConf
29	V	1	Total 1	O 1	0
29	W	5	Total 5	O 5	0
29	Y	2	Total 2	O 2	0
29	C	30	Total 30	O 30	0
29	G	24	Total 24	O 24	0
29	H	39	Total 39	O 39	0
29	I	5	Total 5	O 5	0
29	K	6	Total 6	O 6	0
29	L	25	Total 25	O 25	0
29	X	9	Total 9	O 9	0
29	Z	1	Total 1	O 1	0
29	b	12	Total 12	O 12	0
29	c	2	Total 2	O 2	0

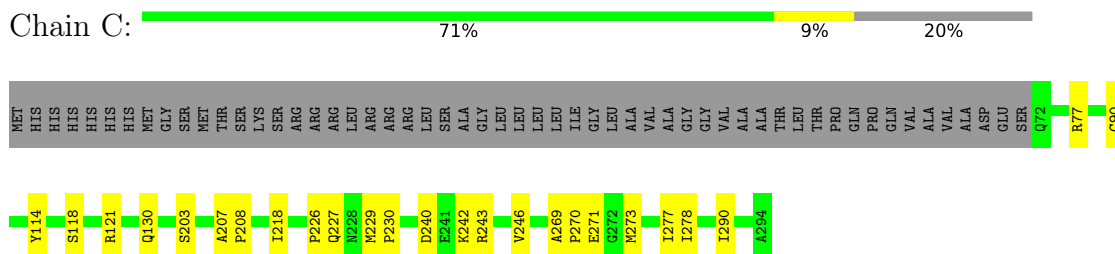
3 Residue-property plots

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

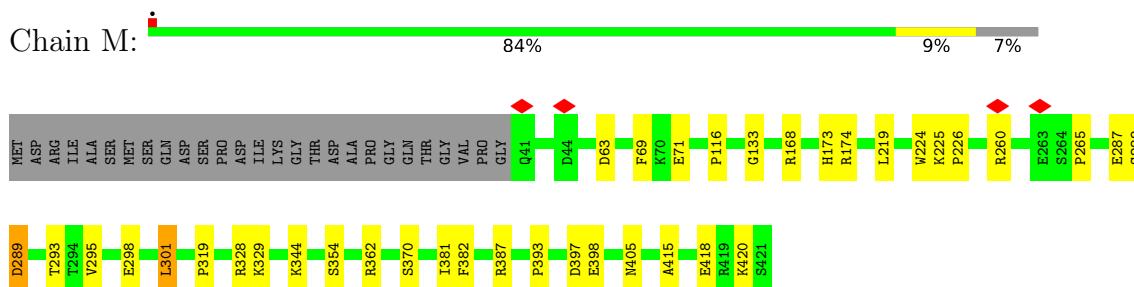
- Molecule 1: Cytochrome bc1 complex cytochrome c subunit



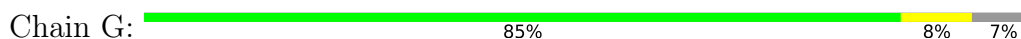
- Molecule 1: Cytochrome bc1 complex cytochrome c subunit

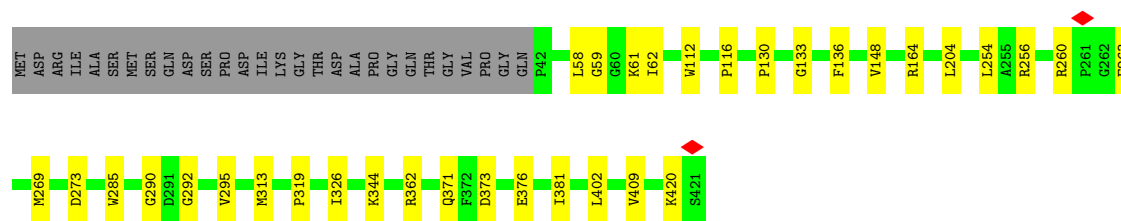


- Molecule 2: Cytochrome bc1 complex cytochrome c subunit

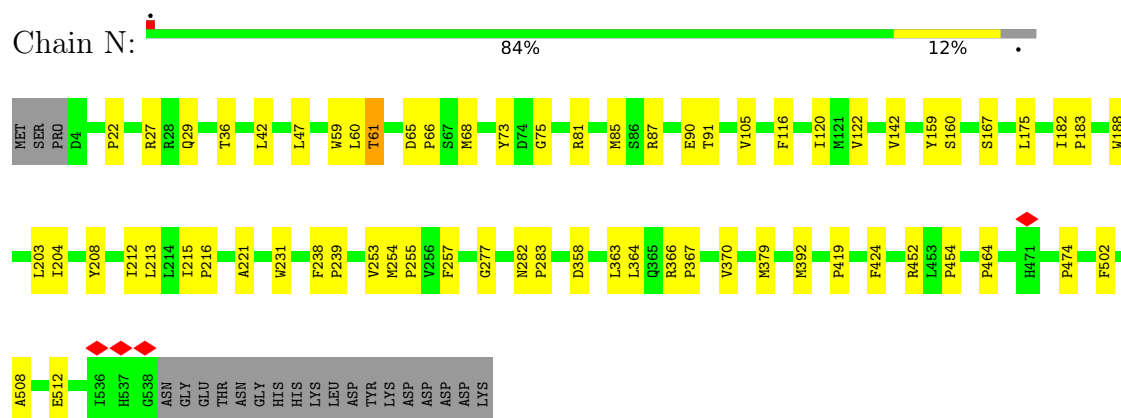


- Molecule 2: Cytochrome bc1 complex cytochrome c subunit

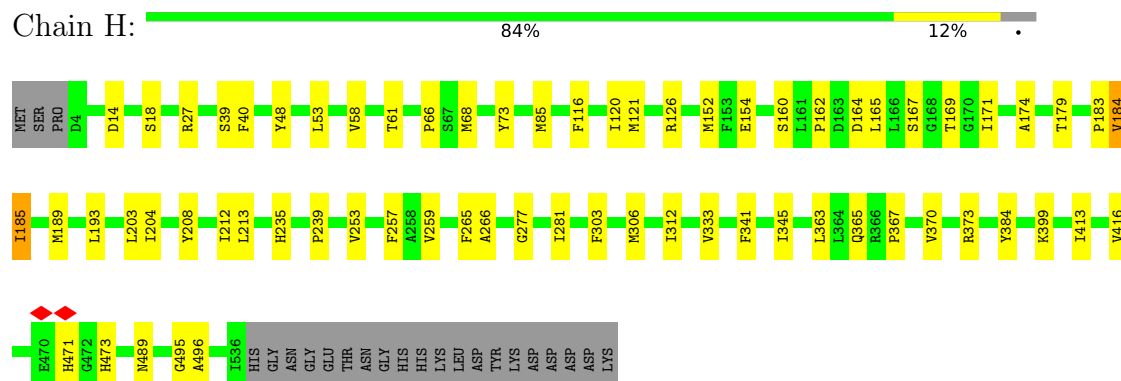




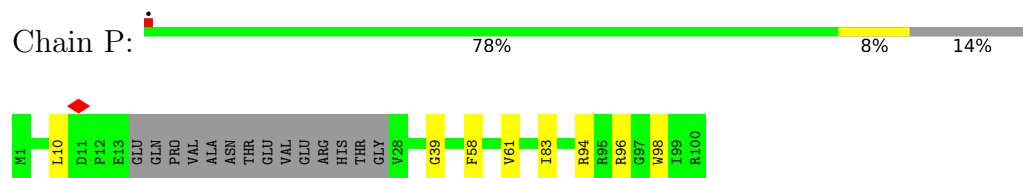
- Molecule 3: Cytochrome bc1 complex cytochrome b subunit



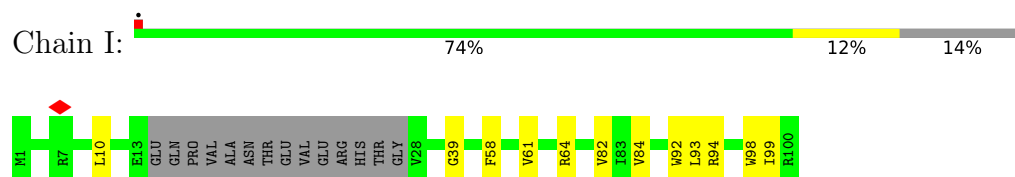
- Molecule 3: Cytochrome bc1 complex cytochrome b subunit



- Molecule 4: Transmembrane protein

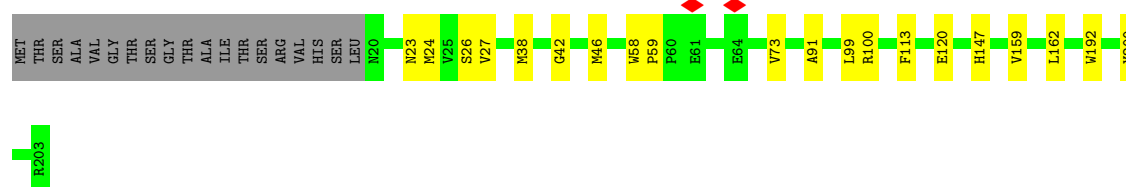


- Molecule 4: Transmembrane protein



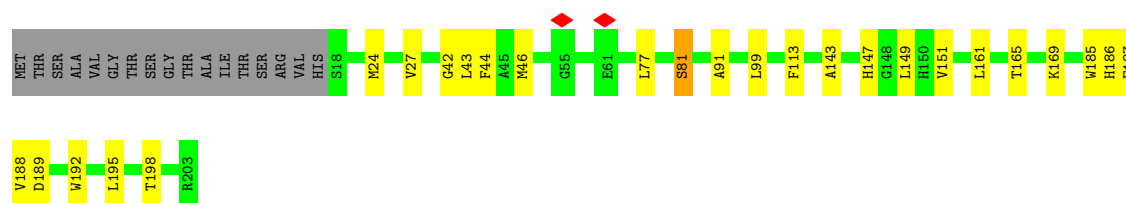
- Molecule 5: Probable cytochrome c oxidase subunit 3

Chain S: 

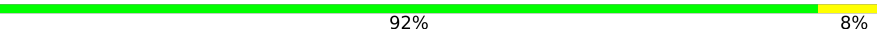


- Molecule 5: Probable cytochrome c oxidase subunit 3

Chain J: 



- Molecule 6: Cytochrome c oxidase polypeptide 4

Chain T: 



- Molecule 6: Cytochrome c oxidase polypeptide 4

Chain K: 

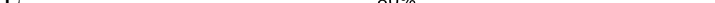


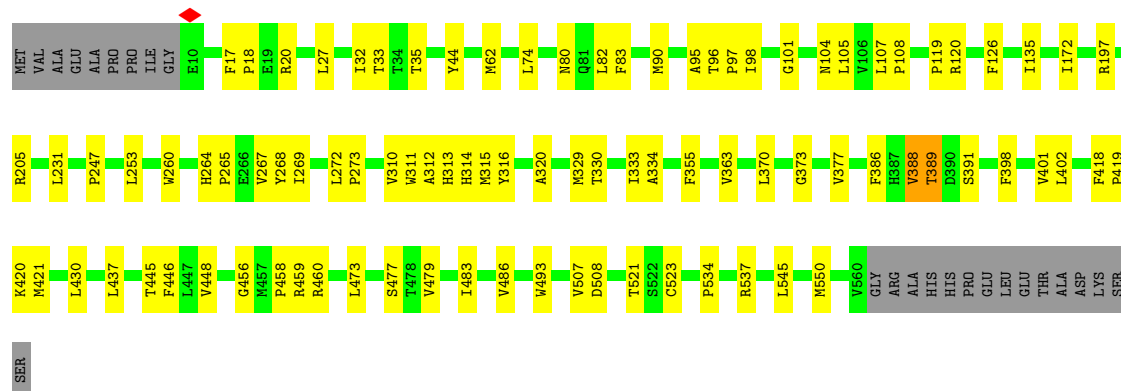
- Molecule 7: Cytochrome c oxidase subunit 1

Chain R: 



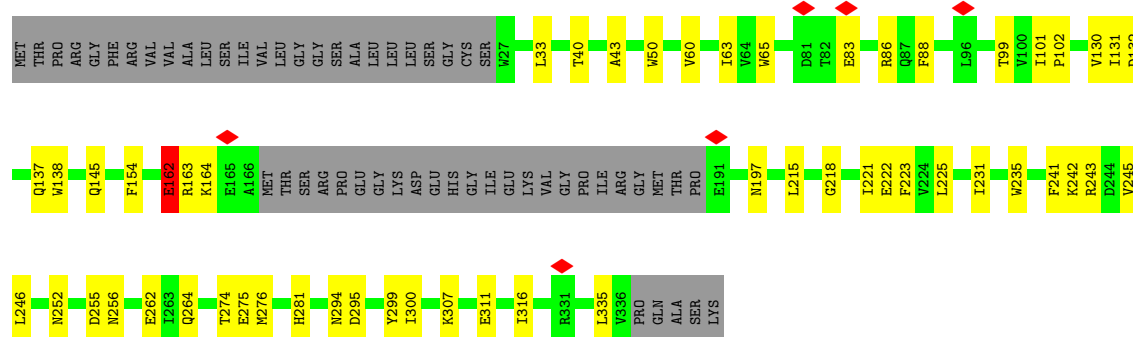
- Molecule 7: Cytochrome c oxidase subunit 1

Chain L:  80% 16% .



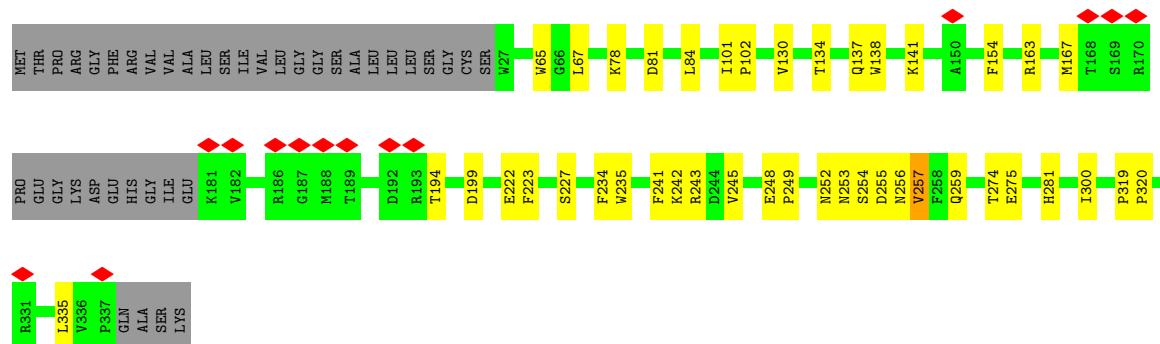
- Molecule 8: cytochrome-c oxidase

Chain Q:  68% 16% 16%

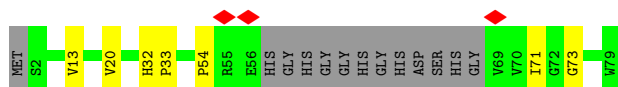
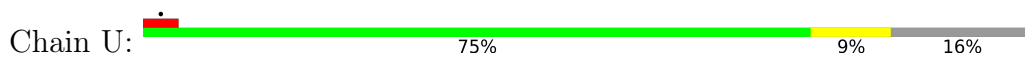


- Molecule 8: cytochrome-c oxidase

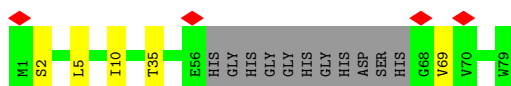
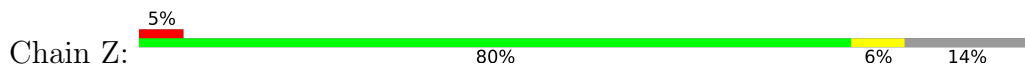
Chain X: 76% 12% 12%



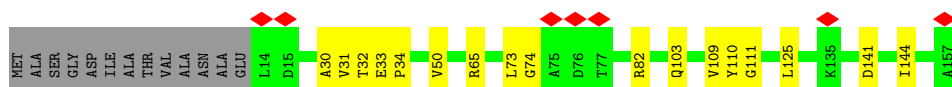
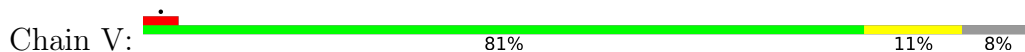
- Molecule 9: Cytochrome c oxidase subunit



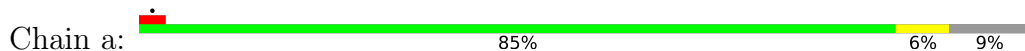
- Molecule 9: Cytochrome c oxidase subunit



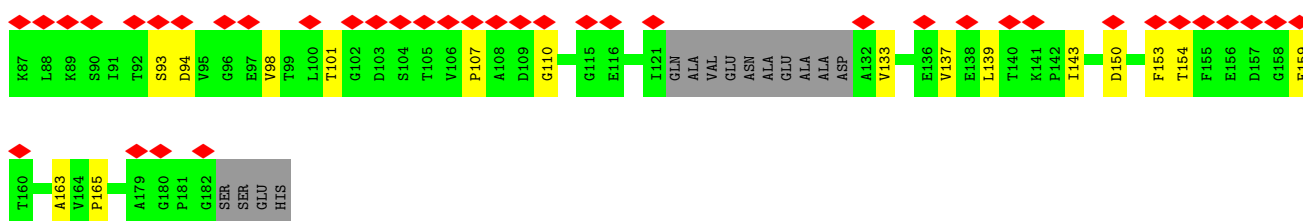
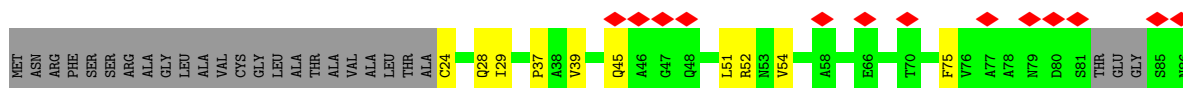
- Molecule 10: Uncharacterized protein MSMEG_4692/MSMEI_4575



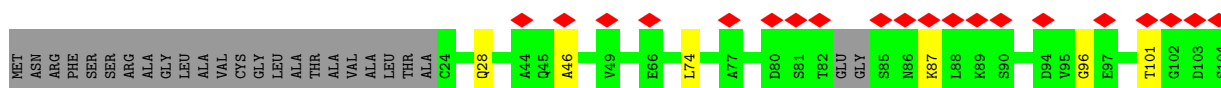
- Molecule 10: Uncharacterized protein MSMEG_4692/MSMEI_4575

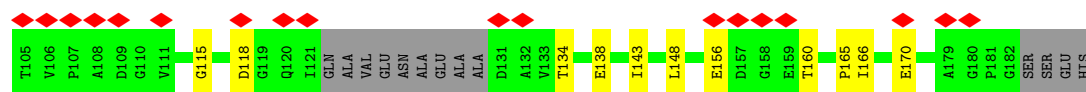


- Molecule 11: LpqE protein

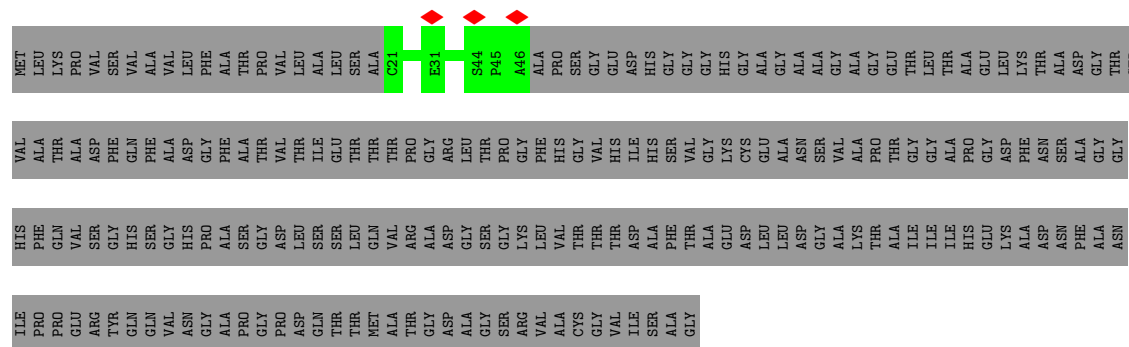


- Molecule 11: LpqE protein

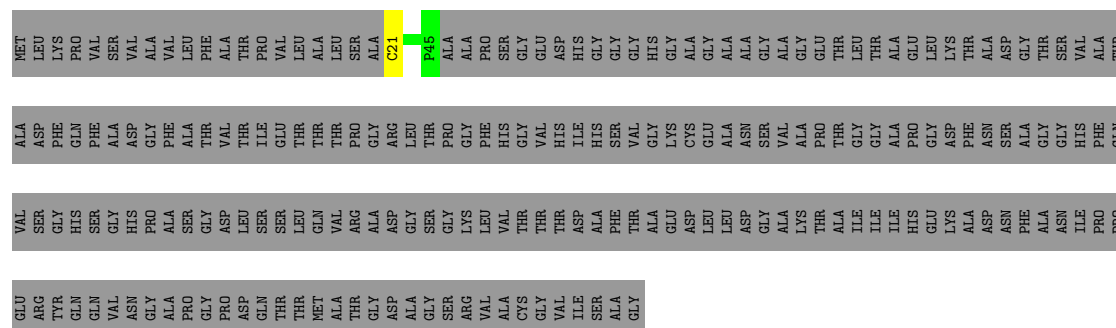




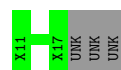
• Molecule 12: Superoxide dismutase [Cu-Zn]



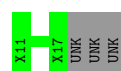
• Molecule 12: Superoxide dismutase [Cu-Zn]



• Molecule 13: Co-purified unknown peptide

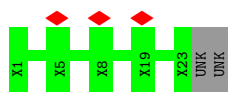


• Molecule 13: Co-purified unknown peptide



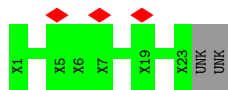
• Molecule 14: Co-purified unknown peptide





- Molecule 14: Co-purified unknown peptide

Chain e: 12% 92% 8%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	90918	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	48.2	Depositor
Minimum defocus (nm)	400	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	105000	Depositor
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	1.509	Depositor
Minimum map value	-0.830	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.037	Depositor
Recommended contour level	0.194	Depositor
Map size (Å)	457.056, 457.056, 457.056	wwPDB
Map dimensions	540, 540, 540	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.8464, 0.8464, 0.8464	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	C	0.51	0/1660	0.78	0/2250
1	O	0.50	0/1660	0.80	0/2250
2	G	0.45	0/3043	0.77	0/4124
2	M	0.49	0/3052	0.80	0/4137
3	H	0.52	0/4299	0.80	1/5862 (0.0%)
3	N	0.49	0/4314	0.77	0/5882
4	I	0.57	0/708	0.85	0/961
4	P	0.44	0/708	0.75	0/961
5	J	0.54	0/1502	0.83	0/2051
5	S	0.46	0/1488	0.77	0/2032
6	K	0.45	0/1112	0.80	0/1524
6	T	0.44	0/1112	0.80	0/1524
7	L	0.50	0/4529	0.79	1/6187 (0.0%)
7	R	0.51	0/4533	0.81	2/6192 (0.0%)
8	Q	0.44	0/2350	0.76	0/3199
8	X	0.49	0/2464	0.78	0/3353
9	U	0.50	0/515	0.80	1/704 (0.1%)
9	Z	0.48	0/527	0.81	0/719
10	V	0.50	0/1050	0.80	0/1434
10	a	0.52	0/1042	0.80	0/1423
11	W	0.48	0/1067	0.77	0/1464
11	b	0.47	0/1090	0.77	0/1494
12	Y	0.58	0/180	0.81	0/251
12	c	0.60	0/175	0.79	0/244
All	All	0.49	0/44180	0.79	5/60222 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	U	20	VAL	N-CA-C	-5.89	107.07	112.96
7	L	389	THR	CB-CA-C	-5.41	99.50	109.46
3	H	416	VAL	N-CA-C	-5.06	108.90	113.71
7	R	526	PRO	CA-C-N	5.03	127.27	120.38
7	R	526	PRO	C-N-CA	5.03	127.27	120.38

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	1623	0	1560	18	0
1	O	1623	0	1560	24	0
2	G	2964	0	2974	24	0
2	M	2973	0	2981	26	0
3	H	4167	0	4192	60	0
3	N	4181	0	4201	58	0
4	I	688	0	672	11	0
4	P	688	0	672	9	0
5	J	1455	0	1455	18	0
5	S	1441	0	1439	14	0
6	K	1077	0	1058	17	0
6	T	1077	0	1058	12	0
7	L	4369	0	4346	84	0
7	R	4373	0	4349	94	0
8	Q	2287	0	2232	40	0
8	X	2398	0	2355	32	0
9	U	499	0	504	6	0
9	Z	511	0	519	4	0
10	V	1032	0	1046	15	0
10	a	1024	0	1035	6	0
11	W	1051	0	1008	17	0
11	b	1074	0	1042	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
12	Y	173	0	156	0	0
12	c	168	0	151	2	0
13	E	35	0	9	0	0
13	f	35	0	9	0	0
14	F	115	0	26	0	0
14	e	115	0	26	0	0
15	C	86	0	60	4	0
15	O	86	0	60	6	0
16	C	58	0	80	16	0
16	G	43	0	53	6	0
16	H	217	0	293	39	0
16	N	174	0	240	25	0
16	O	58	0	80	5	0
17	C	97	0	0	0	0
17	I	97	0	0	2	0
17	O	97	0	0	1	0
17	W	97	0	0	1	0
18	G	4	0	0	0	0
18	M	4	0	0	0	0
19	G	58	0	0	2	0
19	M	58	0	0	7	0
19	W	58	0	0	3	0
19	b	58	0	0	3	0
20	H	86	0	60	15	0
20	N	86	0	60	10	0
21	G	79	0	105	2	0
21	H	383	0	492	21	0
21	I	154	0	196	9	0
21	L	156	0	203	3	0
21	N	156	0	203	9	0
21	P	77	0	98	3	0
21	R	154	0	196	6	0
21	T	79	0	105	4	0
22	J	38	0	55	0	0
22	S	76	0	110	3	0
23	L	120	0	108	13	0
23	R	120	0	108	22	0
24	L	1	0	0	0	0
24	Q	2	0	0	0	0
24	R	1	0	0	0	0
24	X	2	0	0	0	0
25	L	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
25	R	1	0	0	0	0
26	L	1	0	0	0	0
26	R	1	0	0	0	0
27	H	32	0	0	0	0
27	R	42	0	0	1	0
27	Y	32	0	0	0	0
27	b	32	0	0	0	0
28	L	11	0	16	0	0
28	W	11	0	16	2	0
28	Y	11	0	16	0	0
28	c	11	0	16	1	0
29	C	30	0	0	0	0
29	G	24	0	0	0	0
29	H	39	0	0	0	0
29	I	5	0	0	0	0
29	K	6	0	0	0	0
29	L	25	0	0	0	0
29	M	15	0	0	0	0
29	N	22	0	0	0	0
29	O	25	0	0	1	0
29	P	3	0	0	0	0
29	Q	5	0	0	0	0
29	R	14	0	0	0	0
29	S	1	0	0	0	0
29	T	3	0	0	0	0
29	V	1	0	0	0	0
29	W	5	0	0	0	0
29	X	9	0	0	0	0
29	Y	2	0	0	0	0
29	Z	1	0	0	0	0
29	b	12	0	0	0	0
29	c	2	0	0	0	0
All	All	46771	0	45664	643	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

All (643) 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)
7:L:264:HIS:NE2	7:L:268:TYR:HE2	1.35	1.22

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:L:264:HIS:NE2	7:L:268:TYR:CE2	2.12	1.16
7:R:406:ILE:HD11	23:R:603:HEA:CBC	1.77	1.12
1:O:192:HIS:CE1	1:O:210:LEU:HD21	1.84	1.10
23:R:602:HEA:HBC1	23:R:602:HEA:HHD	1.34	1.09
23:L:602:HEA:HHD	23:L:602:HEA:HBC1	1.34	1.09
7:L:264:HIS:CD2	7:L:268:TYR:HE2	1.71	1.07
21:H:601:CDL:H112	21:H:604:CDL:H512	1.12	1.06
3:N:47:LEU:HD21	16:N:605:MQ9:H8	1.40	1.03
16:H:607:MQ9:H3B	16:H:608:MQ9:H5M1	1.38	1.03
7:L:264:HIS:CD2	7:L:268:TYR:CE2	2.49	1.00
16:C:303:MQ9:H251	6:K:100:SER:HB3	1.42	0.99
16:H:607:MQ9:C3B	16:H:608:MQ9:H5M1	1.91	0.99
16:H:607:MQ9:H3A	16:H:608:MQ9:C5M	1.93	0.98
16:C:303:MQ9:C25	6:K:100:SER:CB	2.43	0.95
16:C:303:MQ9:C25	6:K:100:SER:HB3	1.96	0.95
16:C:303:MQ9:H252	6:K:100:SER:HB2	1.50	0.94
11:W:24:CYS:N	28:W:403:PLM:C1	2.32	0.92
21:H:601:CDL:H112	21:H:604:CDL:C51	1.99	0.92
16:N:605:MQ9:H401	16:N:606:MQ9:C50	1.99	0.92
20:N:602:HEM:HBD2	20:N:602:HEM:HHA	1.52	0.89
3:N:452:ARG:HH12	7:R:199:PRO:HD3	1.36	0.88
21:H:601:CDL:C11	21:H:604:CDL:H512	2.03	0.87
20:H:603:HEM:CHA	20:H:603:HEM:HBD2	2.03	0.87
20:H:603:HEM:HBD2	20:H:603:HEM:HHA	1.57	0.87
21:I:301:CDL:C79	17:I:303:WUO:C95	2.54	0.85
3:N:452:ARG:NH1	7:R:199:PRO:HD3	1.91	0.85
7:R:40:ILE:HG12	7:R:43:MET:HE2	1.59	0.85
7:R:406:ILE:CD1	23:R:603:HEA:CBC	2.55	0.84
21:N:604:CDL:H111	21:T:201:CDL:HA32	1.60	0.84
16:H:607:MQ9:C3A	16:H:608:MQ9:C5M	2.55	0.83
7:L:310:VAL:HG12	7:L:313:HIS:CE1	2.14	0.82
16:G:501:MQ9:H5M3	16:G:501:MQ9:C8	2.09	0.82
3:N:142:VAL:HG11	16:N:606:MQ9:H453	1.60	0.82
16:N:601:MQ9:H452	19:W:402:9YF:C34	2.10	0.82
8:X:235:TRP:HD1	8:X:241:PHE:O	1.63	0.82
7:R:406:ILE:CD1	23:R:603:HEA:HBC2	2.10	0.81
3:H:265:PHE:CE2	16:H:607:MQ9:H251	2.15	0.81
3:N:142:VAL:HG11	16:N:606:MQ9:C45	2.10	0.81
20:H:610:HEM:HHA	20:H:610:HEM:HBA1	1.62	0.81
21:H:606:CDL:HB62	21:H:606:CDL:H522	1.62	0.80
16:O:303:MQ9:H102	16:O:303:MQ9:O1	1.82	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:C:303:MQ9:C25	6:K:100:SER:HB2	2.09	0.79
23:L:602:HEA:HBC1	23:L:602:HEA:CHD	2.12	0.78
6:K:90:TRP:HB3	7:L:33:THR:HG22	1.64	0.78
7:R:406:ILE:HD11	23:R:603:HEA:HBC2	1.62	0.78
23:R:602:HEA:HBC1	23:R:602:HEA:CHD	2.12	0.78
10:a:68:VAL:HG11	10:a:143:LEU:HD21	1.63	0.78
3:H:53:LEU:HD13	20:H:603:HEM:HAB	1.65	0.77
16:H:607:MQ9:C3A	16:H:608:MQ9:H5M1	2.15	0.77
3:N:47:LEU:CD2	16:N:605:MQ9:H8	2.15	0.76
5:J:81:SER:OG	5:J:186:HIS:CD2	2.38	0.76
3:H:265:PHE:CE2	16:H:607:MQ9:C25	2.68	0.76
16:H:607:MQ9:H3B	16:H:608:MQ9:C5M	2.15	0.76
3:H:265:PHE:HE2	16:H:607:MQ9:C25	1.99	0.76
1:O:192:HIS:HE1	1:O:210:LEU:HD21	1.52	0.75
7:R:65:GLU:HG2	7:R:74:LEU:HB2	1.67	0.75
16:H:607:MQ9:C3B	16:H:608:MQ9:C5M	2.65	0.75
3:H:174:ALA:HB1	16:H:609:MQ9:C3B	2.18	0.74
21:N:604:CDL:HA62	6:T:90:TRP:HZ2	1.53	0.73
21:R:605:CDL:H201	21:R:605:CDL:H592	1.70	0.73
8:X:130:VAL:HA	8:X:222:GLU:HB2	1.71	0.73
16:N:605:MQ9:H401	16:N:606:MQ9:H503	1.70	0.72
7:L:398:PHE:HA	7:L:401:VAL:HG12	1.70	0.72
7:R:406:ILE:HD11	23:R:603:HEA:HBC1	1.67	0.72
1:O:273:MET:SD	16:O:303:MQ9:H3D	2.30	0.72
7:R:339:ILE:HD11	8:Q:99:THR:HG22	1.71	0.72
3:H:495:GLY:HA2	5:J:169:LYS:H	1.54	0.72
3:H:303:PHE:HA	3:H:306:MET:HE2	1.70	0.72
27:R:608:9XX:C37	11:W:24:CYS:SG	2.77	0.72
19:M:502:9YF:O7	19:M:502:9YF:O	2.08	0.72
2:M:397:ASP:OD1	2:M:398:GLU:N	2.23	0.71
2:G:260:ARG:HB3	2:G:263:GLU:HG2	1.72	0.71
8:X:235:TRP:CD1	8:X:241:PHE:O	2.43	0.71
11:W:139:LEU:HD11	11:W:143:ILE:HG12	1.73	0.70
3:N:47:LEU:HD21	16:N:605:MQ9:C8	2.19	0.70
2:M:287:GLU:CD	2:M:287:GLU:H	1.99	0.70
2:M:298:GLU:HG3	2:G:295:VAL:HG11	1.73	0.70
2:M:219:LEU:HD11	19:M:502:9YF:C40	2.22	0.69
3:H:53:LEU:HD13	20:H:603:HEM:CAB	2.22	0.69
7:R:458:PRO:HB3	8:Q:274:THR:HG22	1.74	0.69
7:L:264:HIS:CE1	7:L:268:TYR:HE2	2.09	0.69
5:J:151:VAL:HG22	5:J:188:VAL:HG11	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:L:44:TYR:HD2	7:L:101:GLY:HA2	1.57	0.69
5:J:91:ALA:HB2	5:J:99:LEU:HD12	1.74	0.69
6:T:90:TRP:HB3	7:R:33:THR:HG22	1.75	0.68
3:N:175:LEU:HD12	16:N:606:MQ9:H5M2	1.74	0.68
16:N:605:MQ9:H401	16:N:606:MQ9:H502	1.75	0.68
5:J:77:LEU:HD22	5:J:113:PHE:CE1	2.29	0.68
1:C:203:SER:HB2	19:b:201:9YF:O8	1.94	0.68
2:M:219:LEU:CD1	19:M:502:9YF:C40	2.72	0.67
7:R:507:VAL:HG12	10:V:30:ALA:HB3	1.76	0.67
3:H:266:ALA:HB2	16:H:607:MQ9:H201	1.74	0.67
16:C:303:MQ9:H251	6:K:100:SER:CB	2.13	0.67
3:H:265:PHE:HE2	16:H:607:MQ9:H252	1.59	0.67
1:O:116:GLN:HB3	1:O:122:MET:HG2	1.78	0.66
20:N:602:HEM:HMC1	20:N:602:HEM:HBC2	1.76	0.66
7:R:152:THR:O	7:R:255:TRP:HH2	1.77	0.66
3:H:259:VAL:HA	16:H:607:MQ9:H111	1.78	0.66
7:R:396:ALA:HB2	7:R:449:GLN:HB2	1.76	0.66
3:N:142:VAL:CG1	16:N:606:MQ9:H453	2.25	0.66
1:O:122:MET:HG3	15:O:301:HEC:CHB	2.25	0.66
21:N:603:CDL:HB62	21:N:604:CDL:H322	1.78	0.65
8:Q:235:TRP:CD1	8:Q:242:LYS:HB3	2.32	0.65
11:W:101:THR:O	11:W:133:VAL:HA	1.96	0.65
2:G:130:PRO:HA	3:H:277:GLY:O	1.95	0.65
3:H:160:SER:HB3	3:H:171:ILE:HD11	1.79	0.65
21:N:604:CDL:H312	21:N:604:CDL:HB4	1.79	0.65
7:L:507:VAL:HG21	10:a:32:THR:HG23	1.77	0.64
1:O:122:MET:HG3	15:O:301:HEC:C4A	2.27	0.64
8:X:227:SER:HB2	8:X:245:VAL:HG12	1.77	0.64
1:O:192:HIS:ND1	1:O:210:LEU:HD21	2.11	0.64
2:M:289:ASP:N	2:M:289:ASP:OD1	2.29	0.64
7:R:56:GLY:O	23:R:603:HEA:H263	1.97	0.64
2:M:265:PRO:HG2	2:M:301:LEU:HD13	1.79	0.64
3:N:363:LEU:HD13	4:P:10:LEU:HD11	1.79	0.64
7:R:402:LEU:HD13	23:R:602:HEA:HBC2	1.79	0.63
1:C:273:MET:CE	16:C:303:MQ9:H111	2.28	0.63
21:I:301:CDL:C79	17:I:303:WUO:C94	2.77	0.63
7:R:253:LEU:HD13	8:Q:252:ASN:HB3	1.80	0.63
5:J:42:GLY:O	5:J:46:MET:HG3	1.99	0.62
7:L:334:ALA:HB1	23:L:602:HEA:H262	1.81	0.62
7:R:288:LYS:HG2	7:R:289:PRO:HD2	1.80	0.62
5:J:151:VAL:HG22	5:J:188:VAL:CG1	2.30	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:L:320:ALA:HB2	8:X:254:SER:HB2	1.80	0.62
11:b:118:ASP:HB2	11:b:170:GLU:HG2	1.81	0.61
2:M:168:ARG:HE	3:H:18:SER:HB3	1.65	0.61
7:R:535:ARG:NH2	7:R:536:ILE:O	2.33	0.61
3:H:73:TYR:HB2	3:H:85:MET:HE3	1.81	0.61
20:N:607:HEM:HBD1	20:N:607:HEM:HHA	1.83	0.61
21:G:504:CDL:H742	21:H:611:CDL:H721	1.83	0.61
8:X:154:PHE:HZ	8:X:300:ILE:HG21	1.65	0.61
7:R:395:ILE:HD13	23:R:603:HEA:CAA	2.31	0.61
19:G:502:9YF:O7	19:G:502:9YF:O9	2.19	0.61
5:S:24:MET:HA	5:S:27:VAL:HG22	1.83	0.61
5:S:27:VAL:HG12	6:T:55:PHE:HE2	1.65	0.61
7:R:509:ASP:OD1	7:R:512:GLY:N	2.33	0.61
23:R:602:HEA:HHC	23:R:602:HEA:O11	2.01	0.61
3:N:221:ALA:HB2	16:N:605:MQ9:H262	1.82	0.60
5:S:91:ALA:HB2	5:S:99:LEU:HD13	1.82	0.60
8:X:134:THR:HG21	8:X:141:LYS:HE2	1.82	0.60
21:I:302:CDL:H521	21:I:302:CDL:OA9	2.01	0.60
23:L:602:HEA:O11	23:L:602:HEA:HHC	2.01	0.60
10:a:138:ASN:HB3	10:a:141:ASP:HB3	1.83	0.60
10:V:33:GLU:HG3	10:V:34:PRO:HD2	1.83	0.60
16:C:303:MQ9:H23	16:C:303:MQ9:H203	1.82	0.60
3:H:384:TYR:HA	16:H:602:MQ9:H352	1.83	0.60
16:H:607:MQ9:H3A	16:H:608:MQ9:H5M2	1.83	0.60
16:N:601:MQ9:O1	16:N:601:MQ9:H8	2.00	0.60
9:U:71:ILE:HG22	10:V:111:GLY:HA2	1.84	0.60
7:L:534:PRO:HB3	7:L:545:LEU:HD12	1.83	0.60
7:R:159:ASP:O	7:R:162:HIS:O	2.20	0.59
2:G:256:ARG:NH1	2:G:273:ASP:OD2	2.35	0.59
7:L:310:VAL:HG12	7:L:313:HIS:HE1	1.66	0.59
6:T:4:GLU:HG2	7:R:194:VAL:HG23	1.83	0.59
8:X:78:LYS:HB2	8:X:81:ASP:HB2	1.83	0.59
3:N:238:PHE:CD2	3:N:364:LEU:HB2	2.37	0.59
16:C:303:MQ9:H28	7:L:135:ILE:HG22	1.83	0.59
7:L:172:ILE:HG23	7:L:231:LEU:HD22	1.85	0.59
7:R:156:PRO:HD3	7:R:252:VAL:HG22	1.84	0.59
21:H:606:CDL:HA31	21:H:606:CDL:HB22	1.84	0.59
3:N:87:ARG:NH2	3:N:90:GLU:OE1	2.36	0.59
7:R:512:GLY:HA2	10:V:31:VAL:HG13	1.84	0.59
1:O:250:ARG:NH2	1:O:254:GLU:OE2	2.36	0.59
5:J:24:MET:HA	5:J:27:VAL:HG22	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:387:ARG:HH12	2:M:415:ALA:HB2	1.68	0.58
3:N:73:TYR:HB2	3:N:85:MET:HE3	1.85	0.58
7:R:395:ILE:HD13	23:R:603:HEA:HAA1	1.85	0.58
5:S:42:GLY:O	5:S:46:MET:HG3	2.04	0.58
1:C:121:ARG:NE	15:C:302:HEC:O2D	2.37	0.58
11:b:74:LEU:HD13	11:b:115:GLY:HA3	1.84	0.58
1:O:121:ARG:NE	15:O:302:HEC:O2D	2.37	0.58
1:C:240:ASP:OD2	1:C:243:ARG:NH2	2.37	0.58
2:G:326:ILE:HB	2:G:376:GLU:HG2	1.85	0.58
7:R:337:THR:HG22	23:R:602:HEA:H172	1.85	0.58
16:H:607:MQ9:H3A	16:H:608:MQ9:H5M3	1.84	0.58
20:H:610:HEM:HBC2	20:H:610:HEM:CMC	2.34	0.57
22:S:401:7PH:H22A	22:S:401:7PH:H33A	1.87	0.57
8:Q:162:GLU:O	8:Q:164:LYS:HE3	2.03	0.57
20:H:603:HEM:HHA	20:H:603:HEM:CBD	2.32	0.57
4:I:82:VAL:HA	21:I:301:CDL:H392	1.86	0.57
7:L:27:LEU:HD21	21:L:607:CDL:H112	1.86	0.57
3:N:68:MET:HE1	3:N:203:LEU:HB3	1.87	0.57
7:R:203:MET:HA	7:R:206:MET:HE3	1.87	0.57
3:H:363:LEU:HD13	4:I:10:LEU:HD11	1.86	0.57
4:P:96:ARG:NE	4:P:98:TRP:HE1	2.02	0.57
1:C:230:PRO:HD3	15:C:302:HEC:HBC3	1.87	0.57
3:N:508:ALA:O	3:N:512:GLU:HG3	2.05	0.57
8:Q:307:LYS:HB3	8:Q:311:GLU:HG2	1.87	0.57
1:C:269:ALA:HB3	1:C:270:PRO:HD3	1.87	0.57
16:N:601:MQ9:C45	19:W:402:9YF:C34	2.81	0.56
7:L:80:ASN:HA	7:L:83:PHE:CE1	2.40	0.56
7:R:496:PHE:O	7:R:500:ARG:NH1	2.38	0.56
19:b:201:9YF:O1	19:b:201:9YF:O3	2.23	0.56
7:R:56:GLY:C	23:R:603:HEA:H263	2.30	0.56
4:I:84:VAL:HG12	21:I:302:CDL:H401	1.88	0.56
7:R:85:MET:HA	7:R:88:THR:HG22	1.86	0.56
5:J:149:LEU:HD22	21:L:601:CDL:H851	1.87	0.56
7:L:320:ALA:CB	8:X:253:ASN:O	2.54	0.56
1:O:230:PRO:HD3	15:O:302:HEC:HBC3	1.87	0.56
7:L:310:VAL:HG22	7:L:329:MET:HB3	1.88	0.56
7:L:313:HIS:HA	7:L:316:TYR:CE1	2.41	0.56
6:T:72:ASP:HA	7:R:535:ARG:HH12	1.70	0.56
3:H:239:PRO:HB3	4:I:10:LEU:HD22	1.88	0.56
7:R:43:MET:O	7:R:126:PHE:CE1	2.59	0.56
23:R:603:HEA:O11	23:R:603:HEA:HHC	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:269:ALA:HB3	1:O:270:PRO:HD3	1.88	0.55
8:Q:276:MET:H	8:Q:281:HIS:CE1	2.24	0.55
2:M:133:GLY:HA3	3:N:277:GLY:HA3	1.88	0.55
3:H:265:PHE:CE2	16:H:607:MQ9:H252	2.39	0.55
21:I:301:CDL:H131	21:L:607:CDL:HB4	1.89	0.55
3:N:367:PRO:HB2	21:N:603:CDL:HA62	1.88	0.55
3:N:239:PRO:HB3	4:P:10:LEU:HD22	1.88	0.55
7:R:384:LEU:HD13	8:Q:50:TRP:CD1	2.42	0.55
23:R:603:HEA:HA	23:R:603:HEA:CBD	2.37	0.55
3:N:464:PRO:HB3	3:N:474:PRO:HB3	1.89	0.55
7:R:40:ILE:HA	7:R:43:MET:HE2	1.89	0.55
6:K:26:THR:HG21	6:K:35:GLU:HB3	1.89	0.55
1:O:292:SER:OG	3:N:36:THR:O	2.25	0.55
3:H:312:ILE:HG12	3:H:333:VAL:HG21	1.88	0.55
21:R:605:CDL:H521	21:R:605:CDL:OB9	2.07	0.54
3:H:68:MET:HE3	3:H:204:ILE:H	1.71	0.54
7:L:459:ARG:HG3	7:L:460:ARG:HG3	1.89	0.54
11:b:143:ILE:HD12	11:b:166:ILE:HD11	1.90	0.54
3:N:68:MET:HE3	3:N:204:ILE:H	1.73	0.54
7:R:398:PHE:HA	7:R:401:VAL:HG12	1.90	0.54
3:H:213:LEU:HD11	16:H:608:MQ9:H502	1.90	0.54
21:H:606:CDL:HB62	21:H:606:CDL:C52	2.34	0.54
1:O:139:ASP:OD1	1:O:142:GLN:NE2	2.40	0.54
3:N:213:LEU:HD21	20:H:603:HEM:HBC1	1.89	0.54
7:L:402:LEU:HD13	23:L:603:HEA:HH1	1.89	0.54
2:G:256:ARG:HH11	2:G:269:MET:HB2	1.73	0.54
10:V:50:VAL:HG12	10:V:144:ILE:CD1	2.38	0.53
23:R:603:HEA:HBC1	23:R:603:HEA:HMC3	1.88	0.53
8:X:130:VAL:HG22	8:X:222:GLU:HG3	1.90	0.53
8:Q:243:ARG:NH1	8:Q:255:ASP:O	2.41	0.53
7:L:320:ALA:HB2	8:X:253:ASN:O	2.08	0.53
11:b:87:LYS:H	11:b:156:GLU:HG2	1.73	0.53
7:L:479:VAL:HG22	9:Z:10:ILE:HA	1.89	0.53
6:T:72:ASP:HB3	7:R:537:ARG:HH12	1.72	0.53
7:R:22:GLY:H	21:R:605:CDL:HA22	1.74	0.53
21:N:603:CDL:HA4	21:N:604:CDL:H512	1.90	0.53
7:R:40:ILE:HG12	7:R:43:MET:CE	2.36	0.53
3:N:42:LEU:HD13	3:N:122:VAL:HG12	1.91	0.52
3:N:212:ILE:HD11	3:H:212:ILE:HD11	1.91	0.52
3:N:238:PHE:CE2	3:N:364:LEU:HB3	2.44	0.52
2:G:313:MET:HG3	2:G:344:LYS:HG3	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:502:PHE:O	5:S:100:ARG:HD2	2.10	0.52
10:V:74:GLY:HA3	10:V:103:GLN:OE1	2.08	0.52
3:N:22:PRO:HB3	21:H:604:CDL:HA62	1.90	0.52
3:N:370:VAL:HG22	4:P:39:GLY:HA3	1.91	0.52
7:R:265:PRO:O	7:R:269:ILE:HG13	2.09	0.52
7:R:80:ASN:HA	7:R:83:PHE:CE1	2.45	0.52
7:R:159:ASP:OD1	7:R:162:HIS:ND1	2.42	0.52
7:R:553:ARG:HH12	8:Q:83:GLU:HG3	1.75	0.52
1:C:273:MET:HE3	16:C:303:MQ9:H111	1.91	0.52
2:M:362:ARG:HD3	2:M:381:ILE:HD11	1.92	0.52
3:H:370:VAL:HG12	4:I:39:GLY:HA3	1.91	0.52
4:P:96:ARG:HE	4:P:98:TRP:HE1	1.57	0.52
8:X:223:PHE:O	8:X:257:VAL:HA	2.09	0.52
20:N:602:HEM:HBC1	3:H:213:LEU:HD21	1.92	0.51
8:Q:231:ILE:HG23	8:Q:246:LEU:HD23	1.92	0.51
10:V:73:LEU:HD23	10:V:73:LEU:H	1.75	0.51
3:H:154:GLU:HG2	20:H:603:HEM:HBB2	1.91	0.51
7:L:265:PRO:O	7:L:269:ILE:HG13	2.10	0.51
3:H:489:ASN:HD22	6:K:132:TYR:C	2.18	0.51
21:N:604:CDL:HA62	6:T:90:TRP:CZ2	2.41	0.51
21:H:604:CDL:OA7	21:H:604:CDL:H131	2.11	0.51
8:Q:137:GLN:HB3	8:Q:138:TRP:CE3	2.46	0.51
8:Q:231:ILE:HG22	8:Q:275:GLU:HG2	1.93	0.51
7:R:40:ILE:HA	7:R:43:MET:HG2	1.93	0.51
16:C:303:MQ9:H28	7:L:135:ILE:CG2	2.40	0.51
3:H:367:PRO:HB2	21:H:605:CDL:HA62	1.92	0.51
7:R:402:LEU:HD21	23:R:603:HEA:HAC	1.93	0.51
8:Q:130:VAL:HA	8:Q:222:GLU:HB3	1.92	0.51
16:C:303:MQ9:H203	16:C:303:MQ9:C23	2.39	0.51
21:H:611:CDL:H112	6:K:127:GLY:HA2	1.91	0.51
7:L:420:LYS:NZ	7:L:521:THR:O	2.43	0.51
7:L:458:PRO:HB3	8:X:274:THR:HG22	1.93	0.51
20:N:607:HEM:HHA	20:N:607:HEM:CBD	2.40	0.50
5:S:147:HIS:CE1	5:S:192:TRP:HB2	2.46	0.50
11:W:29:ILE:HB	17:W:401:WUO:O09	2.10	0.50
11:W:154:THR:HG23	11:W:159:GLU:HB3	1.93	0.50
7:L:310:VAL:CG1	7:L:313:HIS:CE1	2.92	0.50
8:Q:299:TYR:HB2	8:Q:316:ILE:HD13	1.92	0.50
4:P:58:PHE:HA	4:P:61:VAL:HG12	1.92	0.50
3:H:68:MET:HE1	3:H:203:LEU:HB3	1.94	0.50
8:X:222:GLU:OE2	8:X:259:GLN:NE2	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:M:502:9YF:O3	2:G:112:TRP:HZ2	1.95	0.50
7:R:25:GLY:H	21:R:605:CDL:HB21	1.76	0.50
7:L:264:HIS:NE2	7:L:268:TYR:CZ	2.75	0.50
7:R:264:HIS:NE2	7:R:268:TYR:HE2	2.10	0.50
7:R:357:THR:OG1	7:R:358:PRO:HD3	2.12	0.50
1:C:290:ILE:HG12	2:G:148:VAL:HG21	1.93	0.50
7:R:288:LYS:NZ	8:Q:88:PHE:O	2.45	0.49
8:Q:163:ARG:NH2	8:Q:197:ASN:OD1	2.45	0.49
8:X:137:GLN:HG3	8:X:138:TRP:CD2	2.47	0.49
4:I:92:TRP:NE1	21:I:302:CDL:OB7	2.46	0.49
10:V:82:ARG:HG2	10:V:109:VAL:HG21	1.95	0.49
2:G:254:LEU:HD12	2:G:402:LEU:HB3	1.94	0.49
7:L:264:HIS:CE1	7:L:268:TYR:CE2	2.90	0.49
11:b:101:THR:HG22	11:b:134:THR:H	1.77	0.49
8:Q:215:LEU:HD22	8:Q:221:ILE:HD12	1.94	0.49
7:R:388:VAL:HG13	7:R:393:PHE:HB3	1.95	0.49
7:L:430:LEU:HD21	7:L:493:TRP:HD1	1.78	0.49
7:L:507:VAL:O	7:L:508:ASP:OD1	2.30	0.49
2:M:224:TRP:NE1	2:M:418:GLU:OE2	2.42	0.49
3:N:238:PHE:CE2	3:N:364:LEU:CB	2.96	0.49
7:R:264:HIS:O	7:R:267:VAL:HG22	2.13	0.49
7:R:225:PRO:HA	7:R:228:THR:HG22	1.94	0.49
7:R:284:VAL:HG22	7:R:514:GLY:HA2	1.95	0.49
7:R:206:MET:O	7:R:293:TYR:OH	2.23	0.49
7:R:264:HIS:HE2	7:R:268:TYR:HE2	1.61	0.49
9:U:54:PRO:O	10:V:65:ARG:NH2	2.45	0.49
7:R:420:LYS:HG3	7:R:421:MET:HE2	1.95	0.49
20:H:610:HEM:HBC2	20:H:610:HEM:HMC1	1.95	0.49
6:T:100:SER:OG	7:R:135:ILE:HD11	2.13	0.48
2:G:133:GLY:HA3	3:H:277:GLY:HA3	1.95	0.48
11:W:98:VAL:HG22	11:W:137:VAL:HG22	1.94	0.48
7:L:90:MET:HE2	23:L:603:HEA:HMC3	1.94	0.48
12:c:21:CYS:N	28:c:301:PLM:O2	2.46	0.48
7:R:159:ASP:OD2	7:R:161:ILE:HB	2.12	0.48
3:H:164:ASP:OD1	3:H:167:SER:OG	2.27	0.48
7:R:59:ALA:HA	7:R:62:MET:HE2	1.96	0.48
3:H:365:GLN:OE1	3:H:373:ARG:NH2	2.45	0.48
16:C:303:MQ9:H271	16:C:303:MQ9:H253	1.67	0.48
3:H:121:MET:HG2	16:H:602:MQ9:H272	1.96	0.48
16:H:609:MQ9:H172	16:H:609:MQ9:H153	1.65	0.48
9:Z:2:SER:O	9:Z:5:LEU:N	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:65:ASP:HB3	3:N:91:THR:HG21	1.95	0.48
2:M:319:PRO:HG3	11:W:165:PRO:HG3	1.96	0.48
21:P:301:CDL:H781	21:P:301:CDL:H611	1.95	0.48
7:R:384:LEU:HD13	8:Q:50:TRP:HD1	1.78	0.48
6:K:86:ALA:O	7:L:35:THR:HG21	2.14	0.48
7:L:18:PRO:O	7:L:20:ARG:NH2	2.45	0.48
3:N:159:TYR:HA	20:N:602:HEM:HAA2	1.96	0.48
20:N:607:HEM:HBA2	20:N:607:HEM:CMA	2.44	0.48
7:R:37:HIS:CE1	7:R:38:LYS:HG3	2.49	0.48
4:P:83:ILE:HG12	21:P:301:CDL:H731	1.96	0.47
7:R:336:PRO:HA	7:R:339:ILE:HD12	1.96	0.47
4:I:58:PHE:HA	4:I:61:VAL:HG12	1.95	0.47
8:X:275:GLU:H	8:X:281:HIS:HE1	1.61	0.47
16:N:605:MQ9:H453	16:N:605:MQ9:H471	1.43	0.47
7:R:65:GLU:HB2	7:R:73:PHE:CE1	2.48	0.47
7:R:557:GLU:HB3	8:Q:86:ARG:HE	1.78	0.47
8:Q:131:ILE:HD13	8:Q:215:LEU:HD21	1.96	0.47
2:G:58:LEU:HD12	2:G:61:LYS:HE3	1.95	0.47
29:O:418:HOH:O	8:Q:137:GLN:HG3	2.14	0.47
16:N:601:MQ9:H322	16:N:601:MQ9:H303	1.52	0.47
5:S:73:VAL:HG22	5:S:113:PHE:CD1	2.49	0.47
16:H:609:MQ9:H253	16:H:609:MQ9:H271	1.53	0.47
8:X:234:PHE:O	8:X:242:LYS:HA	2.15	0.47
16:N:601:MQ9:C31	16:N:601:MQ9:C35	2.93	0.47
8:Q:275:GLU:H	8:Q:281:HIS:CE1	2.31	0.47
7:L:90:MET:HE2	23:L:603:HEA:CMC	2.44	0.47
23:L:603:HEA:HMA	23:L:603:HEA:HBA2	1.97	0.47
8:Q:154:PHE:HZ	8:Q:300:ILE:HG21	1.80	0.47
11:W:93:SER:OG	11:W:94:ASP:N	2.48	0.47
3:H:413:ILE:HD12	19:b:201:9YF:C29	2.45	0.47
4:I:94:ARG:HD2	4:I:99:ILE:HG13	1.97	0.47
7:L:95:ALA:O	7:L:98:ILE:HG22	2.15	0.47
7:L:550:MET:HE1	8:X:84:LEU:HB2	1.97	0.47
7:R:65:GLU:O	7:R:65:GLU:HG3	2.14	0.47
4:I:93:LEU:HB3	4:I:99:ILE:HG12	1.97	0.47
7:L:264:HIS:O	7:L:268:TYR:HD2	1.97	0.47
3:H:489:ASN:ND2	6:K:132:TYR:HA	2.29	0.47
21:H:604:CDL:H112	21:H:604:CDL:H1	1.96	0.47
21:H:611:CDL:H862	21:H:611:CDL:H831	1.76	0.47
7:R:266:GLU:HA	7:R:269:ILE:HD12	1.96	0.47
3:H:189:MET:O	3:H:193:LEU:HG	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:L:330:THR:O	7:L:333:ILE:HG22	2.15	0.47
1:O:273:MET:HE2	17:O:304:WUO:C88	2.44	0.46
3:H:253:VAL:HA	3:H:257:PHE:HB3	1.97	0.46
3:N:454:PRO:HA	6:T:79:ALA:HB2	1.97	0.46
8:Q:33:LEU:HD12	8:Q:50:TRP:HH2	1.80	0.46
10:V:125:LEU:HD23	10:V:125:LEU:H	1.80	0.46
11:W:107:PRO:HG2	11:W:110:GLY:HA3	1.97	0.46
3:H:212:ILE:HB	20:H:603:HEM:HAC	1.97	0.46
8:X:335:LEU:HB2	11:b:28:GLN:HG3	1.97	0.46
1:O:179:ARG:NH1	1:O:244:ASP:OD2	2.41	0.46
7:R:395:ILE:HD13	23:R:603:HEA:HAA2	1.96	0.46
16:O:303:MQ9:H353	16:O:303:MQ9:H371	1.63	0.46
5:J:192:TRP:O	5:J:192:TRP:CG	2.68	0.46
21:H:605:CDL:OA7	21:H:605:CDL:H541	2.16	0.46
7:L:355:PHE:HE1	7:L:363:VAL:HG21	1.81	0.46
7:R:420:LYS:NZ	7:R:522:SER:O	2.44	0.46
16:G:501:MQ9:H222	16:G:501:MQ9:H203	1.79	0.46
3:H:58:VAL:O	3:H:61:THR:OG1	2.32	0.46
6:K:71:GLU:OE1	7:L:205:ARG:NH1	2.49	0.46
7:L:44:TYR:CE1	7:L:126:PHE:HD1	2.33	0.46
2:M:63:ASP:OD2	3:N:27:ARG:HD2	2.15	0.46
4:P:94:ARG:NH2	21:P:301:CDL:O1	2.48	0.46
5:S:23:ASN:HB3	5:S:26:SER:HB3	1.98	0.46
7:R:370:LEU:HD23	8:Q:65:TRP:CD1	2.51	0.46
16:H:608:MQ9:H5M3	16:H:608:MQ9:C8	2.46	0.46
19:M:502:9YF:O3	2:G:112:TRP:CZ2	2.69	0.46
1:C:90:CYS:HB2	15:C:301:HEC:C2C	2.43	0.46
5:J:161:LEU:O	5:J:165:THR:HG23	2.16	0.46
1:O:90:CYS:HB2	15:O:301:HEC:C2C	2.43	0.46
3:H:496:ALA:H	5:J:169:LYS:HB3	1.80	0.46
2:M:287:GLU:CD	2:M:287:GLU:N	2.72	0.45
8:Q:218:GLY:HA2	8:Q:262:GLU:HB2	1.98	0.45
16:H:608:MQ9:H403	16:H:608:MQ9:H421	1.37	0.45
4:I:64:ARG:HH21	12:c:21:CYS:HA	1.80	0.45
7:L:448:VAL:HB	7:L:473:LEU:HD22	1.98	0.45
3:N:116:PHE:O	3:N:120:ILE:HG13	2.15	0.45
8:Q:60:VAL:HA	8:Q:63:ILE:HG12	1.98	0.45
16:H:609:MQ9:H422	16:H:609:MQ9:H403	1.52	0.45
7:L:386:PHE:O	8:X:242:LYS:HG2	2.15	0.45
4:I:98:TRP:NE1	21:I:302:CDL:OB3	2.41	0.45
7:R:40:ILE:CG1	7:R:43:MET:HE2	2.38	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:I:302:CDL:H712	21:I:302:CDL:HA61	1.99	0.45
7:L:264:HIS:O	7:L:267:VAL:HG22	2.15	0.45
7:L:420:LYS:HA	7:L:420:LYS:HD2	1.79	0.45
7:L:445:THR:HG23	7:L:446:PHE:CD1	2.52	0.45
3:N:60:LEU:O	20:N:602:HEM:HMD1	2.16	0.45
7:R:355:PHE:HE1	7:R:363:VAL:HG21	1.81	0.45
16:G:501:MQ9:C8	16:G:501:MQ9:C5M	2.88	0.45
21:H:611:CDL:H842	21:H:611:CDL:H811	1.78	0.45
8:X:101:ILE:N	8:X:102:PRO:HD2	2.32	0.45
7:R:310:VAL:HG23	7:R:310:VAL:O	2.17	0.45
7:R:507:VAL:HG12	10:V:30:ALA:CB	2.44	0.45
21:R:601:CDL:HB61	21:R:601:CDL:HA4	1.97	0.45
3:H:152:MET:HE1	3:H:341:PHE:HZ	1.80	0.45
6:K:95:ILE:HG12	6:K:124:SER:HB3	1.99	0.45
7:L:388:VAL:HG13	7:L:388:VAL:O	2.16	0.45
3:N:29:GLN:HG3	3:N:231:TRP:HZ2	1.82	0.45
16:N:605:MQ9:H153	16:N:605:MQ9:H172	1.53	0.45
6:T:26:THR:O	6:T:30:ALA:HB3	2.17	0.45
16:C:303:MQ9:H5M3	16:C:303:MQ9:H72	1.75	0.45
3:H:162:PRO:HG3	20:H:603:HEM:O1D	2.16	0.45
5:J:43:LEU:HD23	5:J:143:ALA:HA	1.98	0.45
7:L:312:ALA:C	7:L:314:HIS:H	2.24	0.45
8:X:167:MET:O	8:X:194:THR:OG1	2.30	0.45
7:R:155:SER:HA	7:R:157:LEU:H	1.81	0.45
8:Q:225:LEU:HB3	8:Q:245:VAL:HG12	1.98	0.45
1:O:114:TYR:O	1:O:118:SER:OG	2.23	0.45
3:N:59:TRP:O	3:N:59:TRP:CE3	2.70	0.45
6:T:123:THR:HG23	21:T:201:CDL:H132	1.99	0.45
11:b:46:ALA:HA	11:b:160:THR:HB	1.98	0.45
3:N:61:THR:O	3:N:61:THR:HG23	2.16	0.44
5:S:159:VAL:HG12	22:S:402:7PH:H28	1.98	0.44
7:L:247:PRO:C	8:X:248:GLU:HG3	2.42	0.44
7:R:32:ILE:HG13	7:R:33:THR:HG23	1.99	0.44
7:R:377:VAL:CG2	23:R:602:HEA:H263	2.47	0.44
7:R:483:ILE:HD11	9:U:13:VAL:HG12	1.98	0.44
1:C:130:GLN:HA	1:C:227:GLN:HE22	1.82	0.44
8:X:163:ARG:NH1	8:X:199:ASP:O	2.48	0.44
2:M:173:HIS:ND1	3:H:27:ARG:NH2	2.65	0.44
21:T:201:CDL:H521	21:T:201:CDL:H152	1.98	0.44
16:H:608:MQ9:H203	16:H:608:MQ9:H221	1.42	0.44
7:L:44:TYR:CD1	7:L:126:PHE:HD1	2.35	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:L:312:ALA:C	7:L:314:HIS:N	2.75	0.44
3:N:379:MET:HG2	3:N:419:PRO:HB3	2.00	0.44
16:N:606:MQ9:H222	16:N:606:MQ9:H203	1.61	0.44
16:N:605:MQ9:H321	16:N:605:MQ9:H303	1.76	0.44
2:G:319:PRO:HB3	11:b:148:LEU:HD21	1.98	0.44
16:G:501:MQ9:H322	16:G:501:MQ9:H303	1.45	0.44
3:H:39:SER:OG	3:H:126:ARG:HG3	2.17	0.44
16:H:607:MQ9:H103	16:H:607:MQ9:H122	1.39	0.44
16:H:607:MQ9:H272	16:H:607:MQ9:H253	1.73	0.44
16:H:609:MQ9:H203	16:H:609:MQ9:H221	1.47	0.44
16:O:303:MQ9:H221	16:O:303:MQ9:H203	1.50	0.44
3:N:358:ASP:OD1	3:N:358:ASP:N	2.49	0.44
7:R:310:VAL:HB	7:R:313:HIS:CE1	2.53	0.44
2:M:344:LYS:HE3	2:M:354:SER:HB3	1.99	0.44
2:G:319:PRO:HG3	11:b:165:PRO:HG3	1.99	0.44
2:G:285:TRP:HZ2	2:G:290:GLY:HA3	1.83	0.44
3:H:48:TYR:CG	3:H:265:PHE:HD1	2.36	0.44
16:H:609:MQ9:H372	16:H:609:MQ9:H353	1.76	0.44
6:K:26:THR:O	6:K:30:ALA:HB3	2.18	0.44
8:X:134:THR:CG2	8:X:141:LYS:HE2	2.47	0.44
7:R:373:GLY:O	7:R:377:VAL:HG23	2.16	0.43
23:R:603:HEA:HBC1	23:R:603:HEA:CMC	2.48	0.43
22:S:402:7PH:H37	21:T:201:CDL:H181	2.01	0.43
7:R:154:TYR:HD2	7:R:255:TRP:HZ3	1.65	0.43
1:C:77:ARG:HH12	8:X:163:ARG:HG3	1.83	0.43
7:L:445:THR:HA	7:L:477:SER:HA	2.01	0.43
9:Z:35:THR:HA	10:a:42:PRO:O	2.18	0.43
7:R:149:PHE:HD2	7:R:153:ALA:HA	1.84	0.43
8:Q:264:GLN:OE1	8:Q:264:GLN:HA	2.19	0.43
3:H:40:PHE:O	20:H:610:HEM:O1A	2.37	0.43
3:N:253:VAL:HA	3:N:257:PHE:HB3	2.01	0.43
21:H:604:CDL:OA7	21:H:604:CDL:H321	2.18	0.43
16:H:608:MQ9:H103	16:H:608:MQ9:H122	1.62	0.43
5:J:147:HIS:CE1	5:J:192:TRP:HB2	2.54	0.43
7:L:373:GLY:O	7:L:377:VAL:HG23	2.17	0.43
3:N:160:SER:HA	3:N:167:SER:HB2	2.01	0.43
16:G:501:MQ9:H103	16:G:501:MQ9:H122	1.41	0.43
19:G:502:9YF:C17	19:G:502:9YF:C21	2.96	0.43
9:Z:69:VAL:HG11	10:a:91:PRO:HB2	2.01	0.43
3:N:215:ILE:N	3:N:216:PRO:HD2	2.34	0.43
9:U:73:GLY:HA3	10:V:110:TYR:CE1	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:362:ARG:HD3	2:G:371:GLN:HB3	2.01	0.43
1:O:207:ALA:HA	1:O:208:PRO:HD3	1.87	0.43
19:M:502:9YF:C34	3:N:188:TRP:HB3	2.49	0.43
3:N:68:MET:CE	3:N:203:LEU:HB3	2.49	0.43
11:W:37:PRO:HB2	11:W:39:VAL:HG13	2.01	0.43
2:M:295:VAL:HG22	2:G:295:VAL:HG12	2.01	0.43
7:R:430:LEU:HD21	7:R:493:TRP:HD1	1.84	0.43
8:Q:131:ILE:HD11	8:Q:223:PHE:CE1	2.54	0.43
3:H:471:HIS:HB2	3:H:473:HIS:CE1	2.54	0.43
2:M:370:SER:HA	2:M:382:PHE:O	2.19	0.43
3:N:75:GLY:O	3:N:81:ARG:NH2	2.51	0.43
11:W:51:LEU:HD22	11:W:153:PHE:HD2	1.84	0.43
2:G:409:VAL:HG12	2:G:409:VAL:O	2.19	0.43
7:L:418:PHE:N	7:L:419:PRO:HD2	2.34	0.43
1:O:277:ILE:HG23	1:O:278:ILE:HG13	2.01	0.42
8:Q:275:GLU:H	8:Q:281:HIS:HE1	1.65	0.42
16:H:608:MQ9:H322	16:H:608:MQ9:H303	1.44	0.42
20:H:610:HEM:HBA1	20:H:610:HEM:CHA	2.32	0.42
7:R:96:THR:HB	7:R:97:PRO:HD3	2.01	0.42
7:R:510:PRO:HA	10:V:32:THR:HG22	2.01	0.42
11:W:45:GLN:OE1	11:W:52:ARG:NH1	2.50	0.42
1:C:207:ALA:HA	1:C:208:PRO:HD3	1.90	0.42
7:L:377:VAL:CG2	23:L:602:HEA:H263	2.49	0.42
2:M:328:ARG:O	2:M:328:ARG:HG2	2.19	0.42
16:N:601:MQ9:H23	16:N:601:MQ9:H271	1.74	0.42
8:Q:40:THR:HG23	8:Q:43:ALA:H	1.85	0.42
3:H:183:PRO:O	3:H:185:ILE:N	2.52	0.42
7:L:90:MET:CE	23:L:603:HEA:HMC3	2.49	0.42
8:X:319:PRO:HA	8:X:320:PRO:HD3	1.88	0.42
16:G:501:MQ9:H253	16:G:501:MQ9:H272	1.76	0.42
3:H:306:MET:HE1	16:H:602:MQ9:H3B	2.00	0.42
21:N:604:CDL:H811	19:W:402:9YF:C43	2.49	0.42
5:S:120:GLU:OE1	5:S:200:TYR:OH	2.36	0.42
16:H:607:MQ9:H71	16:H:607:MQ9:H5M3	1.81	0.42
5:J:81:SER:OG	5:J:186:HIS:NE2	2.52	0.42
7:L:314:HIS:HE1	23:L:602:HEA:CHA	2.33	0.42
1:O:182:ASP:OD2	2:M:260:ARG:NH2	2.48	0.42
1:C:218:ILE:HG22	1:C:246:VAL:HG12	2.01	0.42
21:G:504:CDL:H771	21:G:504:CDL:H741	1.83	0.42
7:R:191:THR:HA	7:R:194:VAL:HG12	2.02	0.42
8:Q:294:ASN:OD1	8:Q:295:ASP:N	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:L:74:LEU:O	11:b:28:GLN:NE2	2.53	0.42
1:O:218:ILE:HG22	1:O:246:VAL:HG12	2.01	0.42
2:M:393:PRO:HB2	2:M:405:ASN:HB2	2.01	0.42
3:N:282:ASN:N	3:N:283:PRO:HD3	2.35	0.42
16:N:601:MQ9:H203	16:N:601:MQ9:H222	1.56	0.42
7:R:110:GLN:HG2	7:R:518:GLU:OE1	2.20	0.42
11:W:24:CYS:N	28:W:403:PLM:O2	2.51	0.42
1:C:277:ILE:HG23	1:C:278:ILE:HG13	2.02	0.42
7:L:107:LEU:HB3	7:L:108:PRO:HD3	2.01	0.42
7:L:272:LEU:N	7:L:273:PRO:HD2	2.34	0.42
8:X:249:PRO:HB2	8:X:256:ASN:OD1	2.20	0.42
3:N:59:TRP:CE3	3:N:105:VAL:HG11	2.55	0.42
16:N:601:MQ9:H72	16:N:601:MQ9:H5M3	1.80	0.42
5:S:38:MET:HE2	7:R:222:ILE:HG23	2.01	0.42
7:R:441:GLY:O	7:R:445:THR:HG22	2.20	0.42
1:C:114:TYR:O	1:C:118:SER:OG	2.24	0.42
3:H:164:ASP:OD1	3:H:164:ASP:N	2.44	0.42
3:H:165:LEU:O	3:H:169:THR:HG23	2.20	0.42
7:R:334:ALA:HB1	23:R:602:HEA:H262	2.01	0.42
16:H:607:MQ9:H153	16:H:607:MQ9:H171	1.38	0.42
7:L:96:THR:HB	7:L:97:PRO:HD3	2.02	0.42
2:G:59:GLY:HA2	2:G:62:ILE:HD12	2.02	0.41
10:a:46:MET:O	10:a:50:VAL:HG23	2.20	0.41
7:R:95:ALA:O	7:R:98:ILE:HG22	2.20	0.41
2:G:373:ASP:HB2	2:G:381:ILE:CG1	2.50	0.41
5:J:185:TRP:C	5:J:187:PHE:H	2.28	0.41
7:L:391:SER:HA	7:L:458:PRO:HA	2.01	0.41
7:L:402:LEU:HD22	23:L:603:HEA:HBC2	2.03	0.41
20:N:607:HEM:HBB2	20:N:607:HEM:CMB	2.50	0.41
8:Q:101:ILE:CG2	8:Q:102:PRO:HD3	2.49	0.41
11:W:54:VAL:HG22	11:W:75:PHE:HB2	2.02	0.41
21:H:604:CDL:H602	21:H:604:CDL:H571	1.73	0.41
16:H:608:MQ9:H171	16:H:608:MQ9:H153	1.53	0.41
7:L:253:LEU:HD12	8:X:252:ASN:HB3	2.01	0.41
7:R:452:LEU:HG	7:R:473:LEU:HD23	2.02	0.41
8:Q:235:TRP:HD1	8:Q:241:PHE:O	2.03	0.41
21:H:601:CDL:H792	21:H:601:CDL:H822	1.72	0.41
7:L:17:PHE:CD1	7:L:18:PRO:HD2	2.56	0.41
3:N:66:PRO:HG3	3:N:208:TYR:CD2	2.55	0.41
3:N:363:LEU:CD1	4:P:10:LEU:HD11	2.48	0.41
20:N:602:HEM:HHC	20:N:602:HEM:HBB2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:Q:335:LEU:HB2	11:W:28:GLN:HG3	2.03	0.41
21:H:604:CDL:H181	21:H:604:CDL:H151	1.80	0.41
7:L:260:TRP:O	7:L:311:TRP:HB2	2.21	0.41
7:L:437:LEU:HD23	7:L:437:LEU:HA	1.95	0.41
2:M:174:ARG:NH2	3:H:14:ASP:OD2	2.53	0.41
3:H:174:ALA:HB1	16:H:609:MQ9:C3C	2.50	0.41
3:H:399:LYS:HA	3:H:399:LYS:HE2	2.03	0.41
7:L:32:ILE:HG13	7:L:33:THR:HG23	2.02	0.41
7:L:62:MET:HB3	7:L:82:LEU:HD23	2.03	0.41
7:L:314:HIS:CE1	23:L:602:HEA:CHA	3.03	0.41
3:N:142:VAL:CG1	16:N:606:MQ9:C45	2.88	0.41
7:R:489:LEU:N	7:R:490:PRO:HD2	2.36	0.41
3:H:68:MET:CE	3:H:203:LEU:HB3	2.50	0.41
6:K:131:GLU:OE1	7:L:120:ARG:NH2	2.51	0.41
11:b:96:GLY:HA3	11:b:138:GLU:O	2.19	0.41
5:S:162:LEU:HD23	5:S:162:LEU:HA	1.96	0.41
1:C:242:LYS:O	1:C:246:VAL:HG13	2.21	0.41
2:G:164:ARG:NH2	3:H:235:HIS:O	2.54	0.41
2:G:204:LEU:HD23	2:G:204:LEU:HA	1.95	0.41
8:X:67:LEU:HD23	8:X:67:LEU:HA	1.93	0.41
1:O:242:LYS:O	1:O:246:VAL:HG13	2.21	0.41
2:M:329:LYS:HD3	2:M:329:LYS:O	2.21	0.41
3:N:182:ILE:HA	3:N:183:PRO:HD3	1.99	0.41
3:N:213:LEU:CD2	20:H:603:HEM:HBC1	2.50	0.41
16:N:601:MQ9:C35	16:N:601:MQ9:H311	2.51	0.41
9:U:73:GLY:HA3	10:V:110:TYR:CZ	2.56	0.41
1:C:226:PRO:HD2	1:C:229:MET:HB3	2.03	0.41
15:C:302:HEC:HMB3	15:C:302:HEC:HBB3	2.02	0.41
16:C:303:MQ9:H311	16:C:303:MQ9:H352	2.03	0.41
3:H:116:PHE:O	3:H:120:ILE:HG13	2.21	0.41
7:L:456:GLY:HA2	8:X:235:TRP:CH2	2.56	0.41
1:O:122:MET:HG3	15:O:301:HEC:C1B	2.50	0.41
1:O:193:ASN:OD1	1:O:194:PHE:N	2.45	0.41
7:R:384:LEU:HD22	8:Q:50:TRP:HD1	1.86	0.41
9:U:32:HIS:HA	9:U:33:PRO:HD3	1.96	0.41
21:H:605:CDL:H372	21:H:605:CDL:H172	2.03	0.41
16:H:607:MQ9:C3A	16:H:608:MQ9:H5M3	2.44	0.41
16:O:303:MQ9:H303	16:O:303:MQ9:H322	1.71	0.40
3:N:366:ARG:HB3	21:N:603:CDL:OA4	2.20	0.40
5:S:147:HIS:NE2	5:S:192:TRP:HB2	2.36	0.40
21:H:606:CDL:OA7	21:H:606:CDL:HA32	2.19	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:L:35:THR:HG23	7:L:119:PRO:HB2	2.03	0.40
7:L:483:ILE:HA	7:L:486:VAL:HG22	2.03	0.40
7:L:508:ASP:HA	7:L:523:CYS:SG	2.62	0.40
7:L:537:ARG:HD3	7:L:537:ARG:HA	1.89	0.40
2:M:69:PHE:CZ	2:M:71:GLU:HG2	2.57	0.40
3:N:424:PHE:HE1	21:R:605:CDL:HB62	1.85	0.40
10:V:141:ASP:O	10:V:144:ILE:HG22	2.21	0.40
16:C:303:MQ9:H8	16:C:303:MQ9:H121	1.93	0.40
2:G:136:PHE:CZ	16:H:607:MQ9:C31	3.03	0.40
3:H:179:THR:HG23	3:H:189:MET:HE3	2.02	0.40
5:J:195:LEU:HA	5:J:198:THR:HG22	2.02	0.40
7:L:105:LEU:HD22	7:L:421:MET:HE2	2.03	0.40
7:L:370:LEU:HD23	8:X:65:TRP:CD1	2.56	0.40
19:M:502:9YF:O7	19:M:502:9YF:P	2.79	0.40
3:N:238:PHE:CE2	3:N:364:LEU:HB2	2.57	0.40
3:N:254:MET:HA	3:N:255:PRO:HA	1.73	0.40
6:T:22:TYR:OH	6:T:35:GLU:OE1	2.29	0.40
5:J:44:PHE:HE2	5:J:198:THR:HG21	1.86	0.40
6:K:68:GLU:HG2	7:L:197:ARG:HB2	2.03	0.40
2:M:225:LYS:HA	2:M:226:PRO:HD3	1.95	0.40
5:S:58:TRP:HB3	5:S:59:PRO:HD3	2.04	0.40
11:W:150:ASP:HA	11:W:163:ALA:HA	2.04	0.40
8:Q:132:ASP:OD2	8:Q:145:GLN:NE2	2.55	0.40
8:Q:225:LEU:O	8:Q:256:ASN:ND2	2.48	0.40
1:C:271:GLU:CD	3:H:281:ILE:HG13	2.46	0.40
3:H:66:PRO:HG3	3:H:208:TYR:CD2	2.57	0.40
7:L:44:TYR:HE2	7:L:104:ASN:HD22	1.68	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%)	210 (95%)	11 (5%)	0	100	100
1	O	221/278 (80%)	209 (95%)	11 (5%)	1 (0%)	24	55
2	G	378/408 (93%)	358 (95%)	18 (5%)	2 (0%)	24	55
2	M	379/408 (93%)	360 (95%)	18 (5%)	1 (0%)	36	66
3	H	531/556 (96%)	511 (96%)	19 (4%)	1 (0%)	43	72
3	N	533/556 (96%)	504 (95%)	29 (5%)	0	100	100
4	I	82/100 (82%)	80 (98%)	2 (2%)	0	100	100
4	P	82/100 (82%)	79 (96%)	3 (4%)	0	100	100
5	J	184/203 (91%)	178 (97%)	6 (3%)	0	100	100
5	S	182/203 (90%)	180 (99%)	2 (1%)	0	100	100
6	K	137/139 (99%)	131 (96%)	6 (4%)	0	100	100
6	T	137/139 (99%)	132 (96%)	5 (4%)	0	100	100
7	L	549/575 (96%)	527 (96%)	22 (4%)	0	100	100
7	R	550/575 (96%)	514 (94%)	36 (6%)	0	100	100
8	Q	282/341 (83%)	260 (92%)	21 (7%)	1 (0%)	30	60
8	X	297/341 (87%)	277 (93%)	20 (7%)	0	100	100
9	U	62/79 (78%)	60 (97%)	2 (3%)	0	100	100
9	Z	64/79 (81%)	56 (88%)	8 (12%)	0	100	100
10	V	142/157 (90%)	134 (94%)	8 (6%)	0	100	100
10	a	141/157 (90%)	131 (93%)	10 (7%)	0	100	100
11	W	140/186 (75%)	130 (93%)	10 (7%)	0	100	100
11	b	142/186 (76%)	129 (91%)	13 (9%)	0	100	100
12	Y	24/236 (10%)	20 (83%)	4 (17%)	0	100	100
12	c	23/236 (10%)	20 (87%)	3 (13%)	0	100	100
All	All	5483/6516 (84%)	5190 (95%)	287 (5%)	6 (0%)	49	77

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	H	184	VAL
1	O	196	GLY
8	Q	162	GLU
2	G	292	GLY
2	M	116	PRO
2	G	116	PRO

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	163/206 (79%)	163 (100%)	0	100	100
1	O	163/206 (79%)	163 (100%)	0	100	100
2	G	311/333 (93%)	310 (100%)	1 (0%)	86	95
2	M	312/333 (94%)	307 (98%)	5 (2%)	55	83
3	H	428/448 (96%)	425 (99%)	3 (1%)	76	91
3	N	429/448 (96%)	427 (100%)	2 (0%)	81	93
4	I	71/83 (86%)	71 (100%)	0	100	100
4	P	71/83 (86%)	71 (100%)	0	100	100
5	J	148/161 (92%)	146 (99%)	2 (1%)	59	85
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%)	450 (99%)	3 (1%)	76	91
7	R	453/471 (96%)	451 (100%)	2 (0%)	84	94
8	Q	244/288 (85%)	243 (100%)	1 (0%)	84	94
8	X	257/288 (89%)	254 (99%)	3 (1%)	63	87
9	U	51/59 (86%)	51 (100%)	0	100	100
9	Z	52/59 (88%)	52 (100%)	0	100	100
10	V	106/114 (93%)	106 (100%)	0	100	100
10	a	105/114 (92%)	105 (100%)	0	100	100
11	W	114/146 (78%)	114 (100%)	0	100	100
11	b	119/146 (82%)	119 (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	4448/5164 (86%)	4426 (100%)	22 (0%)	78	93

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	M	288	SER
2	M	289	ASP
2	M	293	THR
2	M	301	LEU
2	M	420	LYS
3	N	61	THR
3	N	392	MET
7	R	507	VAL
7	R	509	ASP
8	Q	162	GLU
2	G	420	LYS
3	H	184	VAL
3	H	185	ILE
3	H	345	ILE
5	J	81	SER
5	J	189	ASP
7	L	315	MET
7	L	388	VAL
7	L	389	THR
8	X	243	ARG
8	X	255	ASP
8	X	257	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

Mol	Chain	Res	Type
2	M	331	GLN
2	M	369	GLN
2	M	405	ASN
3	N	233	GLN
3	N	511	HIS
3	N	532	HIS
4	P	90	ASN
7	R	110	GLN
7	R	434	HIS
8	Q	137	GLN
10	V	87	ASN
10	V	138	ASN
11	W	55	HIS
1	C	81	GLN
1	C	227	GLN
2	G	115	GLN
2	G	331	GLN

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Mol	Chain	Res	Type
2	G	371	GLN
3	H	237	GLN
3	H	300	GLN
3	H	405	ASN
3	H	511	HIS
3	H	532	HIS
4	I	90	ASN
5	J	85	GLN
5	J	186	HIS
7	L	239	HIS
7	L	256	GLN
7	L	314	HIS
7	L	449	GLN
8	X	122	HIS
8	X	285	ASN

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 69 ligands modelled in this entry, 10 are monoatomic - leaving 59 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
23	HEA	L	603	7	67,67,67	3.84	30 (44%)	81,103,103	2.42	33 (40%)
16	MQ9	H	602	-	59,59,59	1.59	7 (11%)	73,75,75	1.26	9 (12%)
16	MQ9	N	606	-	59,59,59	0.35	0	73,75,75	0.41	1 (1%)
19	9YF	W	402	-	58,58,58	0.86	4 (6%)	68,71,71	1.06	2 (2%)
23	HEA	R	603	7	67,67,67	2.45	25 (37%)	81,103,103	2.51	32 (39%)
17	WUO	I	303	-	99,99,99	1.37	6 (6%)	122,125,125	1.25	16 (13%)
21	CDL	I	302	-	76,76,99	0.30	0	82,88,111	0.36	0
21	CDL	I	301	-	76,76,99	1.04	7 (9%)	82,88,111	1.11	4 (4%)
21	CDL	N	604	-	78,78,99	0.29	0	84,90,111	0.34	0
16	MQ9	C	303	-	59,59,59	0.50	0	73,75,75	0.67	1 (1%)
21	CDL	N	603	-	76,76,99	0.29	0	82,88,111	0.35	0
15	HEC	C	302	1	46,50,50	1.95	8 (17%)	58,82,82	1.58	7 (12%)
21	CDL	H	606	-	78,78,99	0.29	0	84,90,111	0.34	0
17	WUO	C	304	-	99,99,99	1.46	13 (13%)	122,125,125	1.40	16 (13%)
16	MQ9	G	501	-	44,44,59	0.38	0	55,57,75	0.47	1 (1%)
18	FES	G	503	2	0,4,4	-	-	-	-	-
21	CDL	H	605	-	76,76,99	0.29	0	82,88,111	0.35	0
16	MQ9	N	605	-	59,59,59	0.36	0	73,75,75	0.41	1 (1%)
21	CDL	R	605	-	76,76,99	0.30	0	82,88,111	0.40	0
21	CDL	H	611	-	78,78,99	1.05	8 (10%)	84,90,111	1.10	5 (5%)
27	9XX	b	202	-	31,31,41	1.11	4 (12%)	34,34,44	1.33	3 (8%)
20	HEM	H	610	3	50,50,50	2.07	15 (30%)	67,82,82	1.79	17 (25%)
19	9YF	G	502	-	58,58,58	0.86	4 (6%)	68,71,71	1.06	2 (2%)
23	HEA	L	602	-	67,67,67	2.23	24 (35%)	81,103,103	2.42	35 (43%)
23	HEA	R	602	-	67,67,67	2.23	23 (34%)	81,103,103	2.43	35 (43%)
15	HEC	C	301	1	46,50,50	1.92	9 (19%)	58,82,82	1.80	6 (10%)
21	CDL	L	607	-	76,76,99	0.30	0	82,88,111	0.35	0
16	MQ9	H	608	-	59,59,59	0.36	0	73,75,75	0.41	1 (1%)
27	9XX	R	608	-	41,41,41	1.10	3 (7%)	44,44,44	1.62	8 (18%)
16	MQ9	H	609	-	59,59,59	0.37	0	73,75,75	0.43	1 (1%)
16	MQ9	N	601	-	59,59,59	0.44	0	73,75,75	0.71	2 (2%)
15	HEC	O	302	1	46,50,50	1.95	8 (17%)	58,82,82	1.58	8 (13%)
22	7PH	S	401	-	37,37,37	0.31	0	40,42,42	0.34	0
28	PLM	W	403	-	9,10,17	0.38	0	8,9,17	0.36	0
17	WUO	W	401	-	99,99,99	1.37	6 (6%)	122,125,125	1.25	16 (13%)
20	HEM	N	602	3	50,50,50	1.74	12 (24%)	67,82,82	1.98	19 (28%)
16	MQ9	H	607	-	44,44,59	0.39	0	55,57,75	0.48	1 (1%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
21	CDL	H	604	-	73,73,99	0.30	0	79,85,111	0.36	0
27	9XX	Y	302	-	31,31,41	1.10	4 (12%)	34,34,44	1.25	2 (5%)
27	9XX	H	612	-	31,31,41	1.10	4 (12%)	34,34,44	1.36	3 (8%)
20	HEM	N	607	3	50,50,50	2.10	18 (36%)	67,82,82	1.60	15 (22%)
17	WUO	O	304	-	99,99,99	1.37	6 (6%)	122,125,125	1.26	15 (12%)
19	9YF	b	201	-	58,58,58	0.86	4 (6%)	68,71,71	1.05	2 (2%)
21	CDL	L	601	-	78,78,99	1.08	7 (8%)	84,90,111	0.95	2 (2%)
28	PLM	L	608	-	9,10,17	0.36	0	8,9,17	0.36	0
20	HEM	H	603	3	50,50,50	1.55	8 (16%)	67,82,82	1.61	13 (19%)
21	CDL	R	601	-	76,76,99	0.29	0	82,88,111	0.35	0
21	CDL	P	301	-	76,76,99	0.30	0	82,88,111	0.35	0
22	7PH	J	401	-	37,37,37	0.31	0	40,42,42	0.34	0
18	FES	M	501	2	0,4,4	-	-	-	-	-
16	MQ9	O	303	-	59,59,59	0.52	0	73,75,75	0.51	1 (1%)
28	PLM	c	301	-	9,10,17	0.36	0	8,9,17	0.36	0
15	HEC	O	301	1	46,50,50	1.92	9 (19%)	58,82,82	1.80	6 (10%)
21	CDL	G	504	-	78,78,99	1.04	6 (7%)	84,90,111	1.04	4 (4%)
22	7PH	S	402	-	37,37,37	0.31	0	40,42,42	0.34	0
28	PLM	Y	301	-	9,10,17	0.43	0	8,9,17	0.41	0
19	9YF	M	502	-	58,58,58	0.86	4 (6%)	68,71,71	1.04	2 (2%)
21	CDL	H	601	-	73,73,99	0.43	0	79,85,111	0.66	2 (2%)
21	CDL	T	201	-	78,78,99	0.29	0	84,90,111	0.35	0

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
23	HEA	L	603	7	-	12/36/76/76	-
16	MQ9	H	602	-	-	13/53/73/73	0/2/2/2
16	MQ9	N	606	-	-	22/53/73/73	0/2/2/2
19	9YF	W	402	-	-	29/54/78/78	0/1/1/1
23	HEA	R	603	7	-	16/36/76/76	-
17	WUO	I	303	-	-	43/84/148/148	0/3/3/3
21	CDL	I	302	-	-	39/87/87/110	-
21	CDL	I	301	-	-	43/87/87/110	-
21	CDL	N	604	-	-	56/89/89/110	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	MQ9	C	303	-	-	23/53/73/73	0/2/2/2
21	CDL	N	603	-	-	50/87/87/110	-
15	HEC	C	302	1	-	8/14/54/54	-
21	CDL	H	606	-	-	55/89/89/110	-
17	WUO	C	304	-	-	41/84/148/148	0/3/3/3
16	MQ9	G	501	-	-	20/35/55/73	0/2/2/2
21	CDL	H	605	-	-	42/87/87/110	-
18	FES	G	503	2	-	-	0/1/1/1
16	MQ9	N	605	-	-	21/53/73/73	0/2/2/2
21	CDL	R	605	-	-	49/87/87/110	-
21	CDL	H	611	-	-	42/89/89/110	-
27	9XX	b	202	-	-	15/33/33/43	-
20	HEM	H	610	3	-	4/14/54/54	-
19	9YF	G	502	-	-	27/54/78/78	0/1/1/1
23	HEA	L	602	-	-	9/36/76/76	-
23	HEA	R	602	-	-	9/36/76/76	-
15	HEC	C	301	1	-	7/14/54/54	-
21	CDL	L	607	-	-	43/87/87/110	-
16	MQ9	H	608	-	-	31/53/73/73	0/2/2/2
27	9XX	R	608	-	-	23/43/43/43	-
16	MQ9	H	609	-	-	28/53/73/73	0/2/2/2
16	MQ9	N	601	-	-	27/53/73/73	0/2/2/2
15	HEC	O	302	1	-	8/14/54/54	-
22	7PH	S	401	-	-	18/39/39/39	-
28	PLM	W	403	-	-	3/8/8/15	-
17	WUO	W	401	-	-	45/84/148/148	0/3/3/3
20	HEM	N	602	3	-	6/14/54/54	-
16	MQ9	H	607	-	-	20/35/55/73	0/2/2/2
21	CDL	H	604	-	-	41/84/84/110	-
27	9XX	Y	302	-	-	15/33/33/43	-
27	9XX	H	612	-	-	20/33/33/43	-
20	HEM	N	607	3	-	6/14/54/54	-
17	WUO	O	304	-	-	44/84/148/148	0/3/3/3
19	9YF	b	201	-	-	24/54/78/78	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	CDL	L	601	-	-	43/89/89/110	-
28	PLM	L	608	-	-	4/8/8/15	-
20	HEM	H	603	3	-	8/14/54/54	-
21	CDL	R	601	-	-	37/87/87/110	-
21	CDL	P	301	-	-	45/87/87/110	-
22	7PH	J	401	-	-	20/39/39/39	-
18	FES	M	501	2	-	-	0/1/1/1
16	MQ9	O	303	-	-	23/53/73/73	0/2/2/2
28	PLM	c	301	-	-	0/8/8/15	-
15	HEC	O	301	1	-	7/14/54/54	-
21	CDL	G	504	-	-	51/89/89/110	-
22	7PH	S	402	-	-	14/39/39/39	-
28	PLM	Y	301	-	-	1/8/8/15	-
19	9YF	M	502	-	-	26/54/78/78	0/1/1/1
21	CDL	H	601	-	-	34/84/84/110	-
21	CDL	T	201	-	-	40/89/89/110	-

All (286) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	L	603	HEA	C3B-C2B	8.04	1.53	1.34
23	L	603	HEA	CHD-C1D	7.57	1.53	1.38
23	L	603	HEA	FE-NB	7.55	2.18	1.94
15	O	302	HEC	CAC-C3C	7.33	1.58	1.35
23	L	603	HEA	C3D-C2D	7.33	1.52	1.36
15	C	302	HEC	CAC-C3C	7.32	1.58	1.35
15	C	301	HEC	CAC-C3C	7.29	1.58	1.35
15	O	301	HEC	CAC-C3C	7.27	1.58	1.35
23	L	603	HEA	CHA-C1A	7.17	1.52	1.38
15	C	302	HEC	CAB-C3B	7.09	1.58	1.35
15	O	302	HEC	CAB-C3B	7.08	1.58	1.35
23	L	603	HEA	FE-ND	7.06	2.16	1.94
23	L	603	HEA	C3A-C2A	7.04	1.53	1.37
23	L	603	HEA	C1A-NA	6.89	1.52	1.39
23	L	603	HEA	CHC-C4B	6.83	1.52	1.38
23	L	603	HEA	CHB-C4A	6.80	1.51	1.38
15	O	301	HEC	CAB-C3B	6.69	1.56	1.35
15	C	301	HEC	CAB-C3B	6.67	1.56	1.35
16	H	602	MQ9	C6-C5	6.60	1.47	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	R	603	HEA	FE-NB	6.45	2.14	1.94
23	L	603	HEA	CHD-C4C	6.19	1.53	1.39
23	L	603	HEA	FE-NC	6.15	2.15	1.95
23	L	603	HEA	C4A-NA	6.02	1.51	1.39
23	L	603	HEA	CHA-C4D	5.96	1.52	1.39
17	O	304	WUO	P52-O51	5.91	1.77	1.59
17	I	303	WUO	P52-O51	5.88	1.77	1.59
20	N	602	HEM	FE-NB	5.86	2.12	1.94
17	W	401	WUO	P52-O51	5.84	1.77	1.59
23	L	603	HEA	CHC-C1C	5.83	1.52	1.39
23	L	603	HEA	C1A-C2A	5.79	1.55	1.45
23	L	603	HEA	C4D-C3D	5.51	1.54	1.45
23	R	602	HEA	FE-NB	5.38	2.11	1.94
23	L	602	HEA	FE-NB	5.36	2.11	1.94
23	R	603	HEA	FE-ND	5.31	2.11	1.94
20	H	603	HEM	FE-NB	5.14	2.10	1.94
23	L	603	HEA	CHB-C1B	5.11	1.50	1.39
20	H	610	HEM	FE-NB	5.06	2.10	1.94
23	L	603	HEA	C4B-C3B	5.01	1.53	1.44
17	W	401	WUO	C50-C37	5.01	1.62	1.52
17	O	304	WUO	C50-C37	4.96	1.62	1.52
17	C	304	WUO	P52-O51	4.96	1.74	1.59
17	I	303	WUO	C50-C37	4.90	1.62	1.52
20	N	607	HEM	C1B-NB	-4.81	1.31	1.40
23	L	602	HEA	CHD-C1D	4.78	1.48	1.38
23	R	602	HEA	CHD-C1D	4.77	1.48	1.38
23	L	602	HEA	FE-ND	4.76	2.09	1.94
23	R	602	HEA	FE-ND	4.76	2.09	1.94
20	N	607	HEM	FE-NB	4.73	2.09	1.94
23	R	603	HEA	FE-NC	4.69	2.10	1.95
20	H	610	HEM	C1B-NB	-4.67	1.32	1.40
23	L	602	HEA	FE-NC	4.66	2.10	1.95
23	R	602	HEA	FE-NC	4.66	2.10	1.95
23	R	603	HEA	C1D-ND	-4.62	1.32	1.40
23	L	603	HEA	C1B-C2B	4.57	1.53	1.44
20	H	610	HEM	C4D-ND	-4.54	1.32	1.40
23	R	603	HEA	CHC-C4B	4.53	1.47	1.38
23	L	603	HEA	C1D-C2D	4.51	1.53	1.44
23	L	602	HEA	C3B-C2B	4.50	1.45	1.34
23	R	602	HEA	C3B-C2B	4.49	1.44	1.34
23	R	603	HEA	C3B-C2B	4.48	1.44	1.34
17	O	304	WUO	P52-O55	4.45	1.76	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	I	303	WUO	P52-O55	4.43	1.76	1.59
17	W	401	WUO	P52-O55	4.41	1.76	1.59
20	H	610	HEM	C1C-C2C	-4.37	1.36	1.45
20	N	602	HEM	FE-NC	4.34	2.09	1.95
20	H	610	HEM	FE-NC	4.30	2.09	1.95
23	R	603	HEA	CHD-C1D	4.29	1.47	1.38
20	N	607	HEM	FE-NC	4.28	2.09	1.95
23	L	603	HEA	C1C-C2C	4.27	1.53	1.43
23	R	602	HEA	C1A-NA	4.23	1.47	1.39
23	L	602	HEA	C1A-NA	4.23	1.47	1.39
23	R	603	HEA	C4A-NA	4.19	1.47	1.39
20	N	607	HEM	C4D-ND	-4.18	1.33	1.40
23	R	603	HEA	C3D-C2D	4.17	1.45	1.36
23	R	603	HEA	C4C-NC	-4.12	1.31	1.39
23	L	602	HEA	C3D-C2D	4.11	1.45	1.36
23	R	602	HEA	C3D-C2D	4.11	1.45	1.36
20	H	603	HEM	FE-NC	4.06	2.08	1.95
23	R	603	HEA	CHA-C1A	3.95	1.46	1.38
23	L	603	HEA	C3A-C4A	3.95	1.52	1.46
27	b	202	9XX	O1-C17	-3.94	1.40	1.47
27	H	612	9XX	O1-C17	-3.93	1.40	1.47
23	L	602	HEA	CHA-C1A	3.92	1.46	1.38
23	R	602	HEA	CHA-C1A	3.91	1.46	1.38
23	R	603	HEA	CHD-C4C	3.85	1.48	1.39
27	Y	302	9XX	O1-C17	-3.83	1.40	1.47
17	C	304	WUO	C50-C01	3.79	1.60	1.52
17	C	304	WUO	C50-C37	3.78	1.60	1.52
23	R	603	HEA	C1A-NA	3.76	1.46	1.39
23	R	603	HEA	CHB-C4A	3.69	1.45	1.38
20	N	607	HEM	C3C-C4C	-3.68	1.39	1.46
23	L	603	HEA	C3C-C4C	3.67	1.53	1.42
23	R	603	HEA	C11-C3B	-3.65	1.46	1.51
23	R	602	HEA	C3A-C2A	3.60	1.45	1.37
23	R	602	HEA	C4A-NA	3.60	1.46	1.39
23	L	602	HEA	C3A-C2A	3.60	1.45	1.37
23	R	603	HEA	CHC-C1C	3.58	1.47	1.39
23	L	602	HEA	C4A-NA	3.58	1.46	1.39
20	H	610	HEM	C4B-NB	-3.52	1.31	1.38
23	R	602	HEA	C4B-NB	-3.52	1.34	1.40
23	L	602	HEA	C4B-NB	-3.52	1.34	1.40
20	N	602	HEM	C1C-C2C	-3.50	1.38	1.45
20	N	607	HEM	C1C-C2C	-3.49	1.38	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	H	610	HEM	FE-ND	-3.49	1.84	1.94
23	R	603	HEA	C3A-C2A	3.47	1.45	1.37
23	L	602	HEA	CHD-C4C	3.46	1.47	1.39
23	R	602	HEA	CHD-C4C	3.46	1.47	1.39
15	C	302	HEC	CBC-CAC	-3.45	1.36	1.49
15	O	302	HEC	CBC-CAC	-3.45	1.36	1.49
16	H	602	MQ9	C2-C1	3.41	1.54	1.48
15	O	301	HEC	CBC-CAC	-3.37	1.37	1.49
15	C	301	HEC	CBC-CAC	-3.37	1.37	1.49
20	N	602	HEM	C1B-NB	-3.35	1.34	1.40
20	H	603	HEM	C1B-NB	-3.29	1.34	1.40
20	N	602	HEM	C4D-ND	-3.28	1.34	1.40
23	R	602	HEA	CHC-C4B	3.28	1.45	1.38
23	R	603	HEA	C1C-NC	-3.26	1.33	1.39
20	N	607	HEM	C1D-ND	-3.25	1.32	1.38
20	N	607	HEM	C1A-C2A	-3.23	1.38	1.44
23	L	602	HEA	CHB-C4A	3.23	1.44	1.38
23	L	602	HEA	CHC-C4B	3.22	1.44	1.38
20	N	607	HEM	C4B-NB	-3.22	1.32	1.38
17	C	304	WUO	C76-C57	3.22	1.60	1.50
23	R	602	HEA	CHB-C4A	3.21	1.44	1.38
23	L	603	HEA	CMA-C3A	3.19	1.52	1.45
20	H	603	HEM	C4D-ND	-3.17	1.34	1.40
23	R	602	HEA	CHA-C4D	3.15	1.46	1.39
23	L	602	HEA	CHA-C4D	3.15	1.46	1.39
20	N	607	HEM	O2D-CGD	-3.13	1.20	1.30
23	R	602	HEA	CHB-C1B	3.06	1.46	1.39
23	L	602	HEA	CHB-C1B	3.05	1.46	1.39
23	L	603	HEA	C3C-C2C	3.04	1.51	1.41
16	H	602	MQ9	O1-C1	-3.00	1.17	1.23
16	H	602	MQ9	C3-C4	2.99	1.53	1.48
21	L	601	CDL	OA6-CA4	-2.98	1.39	1.46
21	L	601	CDL	OB6-CB4	-2.98	1.39	1.46
23	L	602	HEA	C1C-NC	-2.98	1.34	1.39
20	H	610	HEM	O2D-CGD	-2.96	1.21	1.30
21	L	601	CDL	OB8-CB7	2.96	1.42	1.33
23	R	602	HEA	C1C-NC	-2.95	1.34	1.39
20	N	607	HEM	C4A-NA	-2.92	1.34	1.39
23	R	603	HEA	C4B-NB	-2.89	1.35	1.40
21	G	504	CDL	OB8-CB7	2.89	1.41	1.33
20	H	610	HEM	C1D-ND	-2.89	1.33	1.38
21	H	611	CDL	OB6-CB5	2.86	1.42	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	R	608	9XX	O1-C18	2.86	1.42	1.34
21	H	611	CDL	OA6-CA4	-2.82	1.40	1.46
23	R	603	HEA	O2D-CGD	-2.81	1.21	1.30
20	N	607	HEM	C3D-C2D	-2.79	1.30	1.36
21	I	301	CDL	OA6-CA4	-2.79	1.40	1.46
21	H	611	CDL	OB8-CB7	2.77	1.41	1.33
23	R	603	HEA	C4D-ND	-2.75	1.33	1.38
21	I	301	CDL	OB6-CB5	2.74	1.42	1.34
20	N	602	HEM	C4B-NB	-2.74	1.33	1.38
16	H	602	MQ9	O4-C4	-2.70	1.17	1.23
21	L	601	CDL	OB6-CB5	2.70	1.41	1.34
27	R	608	9XX	O-C15	2.67	1.41	1.33
20	H	610	HEM	C1C-NC	-2.67	1.34	1.39
19	b	201	9YF	O9-C	-2.66	1.40	1.46
17	W	401	WUO	C50-C01	2.65	1.57	1.52
20	N	607	HEM	O2A-CGA	-2.65	1.22	1.30
20	H	603	HEM	FE-ND	-2.63	1.86	1.94
17	C	304	WUO	O55-C56	-2.63	1.34	1.44
19	W	402	9YF	O9-C	-2.63	1.40	1.46
20	H	610	HEM	C1B-C2B	-2.62	1.39	1.44
19	M	502	9YF	O9-C	-2.61	1.40	1.46
19	G	502	9YF	O9-C	-2.60	1.40	1.46
21	G	504	CDL	OB6-CB4	-2.59	1.40	1.46
21	I	301	CDL	OB8-CB7	2.59	1.40	1.33
17	C	304	WUO	C61-C59	2.57	1.58	1.50
21	G	504	CDL	OB6-CB5	2.57	1.41	1.34
20	H	610	HEM	C3C-C4C	-2.54	1.41	1.46
23	R	602	HEA	C1B-NB	-2.54	1.33	1.38
27	b	202	9XX	O-C15	2.54	1.40	1.33
21	G	504	CDL	OA8-CA7	2.52	1.40	1.33
27	Y	302	9XX	O-C15	2.52	1.40	1.33
17	I	303	WUO	C50-C01	2.52	1.57	1.52
23	L	602	HEA	C1B-NB	-2.51	1.33	1.38
27	R	608	9XX	O1-C17	-2.49	1.42	1.47
17	C	304	WUO	P52-O55	2.49	1.69	1.59
21	L	601	CDL	OA8-CA7	2.48	1.40	1.33
15	C	302	HEC	CBB-CAB	-2.48	1.40	1.49
15	O	302	HEC	CBB-CAB	-2.48	1.40	1.49
16	H	602	MQ9	C7-C8	2.47	1.54	1.50
23	R	602	HEA	O2D-CGD	-2.47	1.22	1.30
23	R	602	HEA	C1D-ND	-2.47	1.36	1.40
23	L	602	HEA	C1D-ND	-2.47	1.36	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	L	602	HEA	O2D-CGD	-2.45	1.22	1.30
17	O	304	WUO	C50-C01	2.44	1.57	1.52
23	L	603	HEA	CMD-C2D	2.43	1.55	1.50
23	R	603	HEA	CHA-C4D	2.43	1.44	1.39
19	b	201	9YF	O11-C25	2.43	1.40	1.33
21	G	504	CDL	OA6-CA4	-2.42	1.40	1.46
19	G	502	9YF	O11-C25	2.41	1.40	1.33
21	G	504	CDL	OA6-CA5	2.41	1.41	1.34
19	M	502	9YF	O11-C25	2.41	1.40	1.33
20	H	610	HEM	O2A-CGA	-2.41	1.22	1.30
23	R	603	HEA	CHB-C1B	2.41	1.44	1.39
20	N	607	HEM	C4C-NC	-2.40	1.35	1.39
27	H	612	9XX	O-C15	2.40	1.40	1.33
19	W	402	9YF	O11-C25	2.40	1.40	1.33
17	C	304	WUO	O11-C06	-2.39	1.37	1.43
20	H	610	HEM	C2A-C3A	-2.38	1.32	1.38
17	C	304	WUO	C56-C57	2.37	1.58	1.50
17	C	304	WUO	O09-C08	-2.37	1.37	1.43
21	I	301	CDL	OA8-CA7	2.36	1.40	1.33
15	C	301	HEC	CBB-CAB	-2.36	1.40	1.49
15	O	301	HEC	CBB-CAB	-2.35	1.40	1.49
23	L	603	HEA	CMB-C2B	2.34	1.55	1.50
20	N	607	HEM	FE-ND	-2.34	1.87	1.94
21	I	301	CDL	OA8-CA6	-2.33	1.40	1.45
23	R	602	HEA	CHC-C1C	2.32	1.44	1.39
23	L	602	HEA	CHC-C1C	2.32	1.44	1.39
23	L	602	HEA	O2A-CGA	-2.32	1.23	1.30
21	H	611	CDL	OA8-CA6	-2.32	1.40	1.45
23	L	603	HEA	FE-NA	2.31	2.02	1.95
23	R	602	HEA	C11-C3B	-2.31	1.48	1.51
23	L	602	HEA	C11-C3B	-2.31	1.48	1.51
27	Y	302	9XX	O1-C18	2.31	1.40	1.34
21	H	611	CDL	OB6-CB4	-2.30	1.41	1.46
23	R	602	HEA	O2A-CGA	-2.30	1.23	1.30
17	O	304	WUO	C56-C57	2.30	1.58	1.50
15	O	301	HEC	CMD-C2D	2.30	1.55	1.50
15	O	301	HEC	C3D-C2D	-2.30	1.32	1.38
17	I	303	WUO	C56-C57	2.29	1.58	1.50
20	H	603	HEM	C1C-C2C	-2.29	1.40	1.45
15	C	301	HEC	CMD-C2D	2.29	1.55	1.50
15	C	301	HEC	C3D-C2D	-2.28	1.33	1.38
20	N	602	HEM	C3C-C4C	-2.27	1.42	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	C	304	WUO	O45-C44	-2.27	1.37	1.43
21	I	301	CDL	OB6-CB4	-2.26	1.41	1.46
15	C	302	HEC	CMB-C2B	2.25	1.55	1.50
17	W	401	WUO	C56-C57	2.25	1.57	1.50
20	N	607	HEM	C1C-NC	-2.24	1.35	1.39
20	N	607	HEM	C2A-C3A	-2.23	1.33	1.38
19	M	502	9YF	O9-C8	2.23	1.40	1.34
17	C	304	WUO	C06-C05	2.22	1.57	1.53
15	O	302	HEC	CMB-C2B	2.22	1.55	1.50
21	L	601	CDL	OA6-CA5	2.22	1.40	1.34
21	I	301	CDL	OA6-CA5	2.21	1.40	1.34
19	G	502	9YF	O11-C24	-2.20	1.40	1.45
20	N	602	HEM	C3D-C2D	-2.20	1.32	1.36
21	H	611	CDL	OA6-CA5	2.19	1.40	1.34
21	H	611	CDL	OA8-CA7	2.19	1.39	1.33
23	L	603	HEA	CAD-C3D	2.19	1.57	1.51
20	H	603	HEM	C1D-ND	-2.19	1.34	1.38
19	W	402	9YF	O9-C8	2.18	1.40	1.34
15	O	302	HEC	CMD-C2D	2.18	1.55	1.50
15	C	302	HEC	CMD-C2D	2.17	1.55	1.50
19	b	201	9YF	O9-C8	2.17	1.40	1.34
20	N	607	HEM	C1B-C2B	-2.17	1.40	1.44
27	b	202	9XX	O1-C18	2.16	1.40	1.34
19	b	201	9YF	O11-C24	-2.15	1.40	1.45
19	M	502	9YF	O11-C24	-2.14	1.40	1.45
19	W	402	9YF	O11-C24	-2.13	1.40	1.45
21	H	611	CDL	OB8-CB6	-2.13	1.40	1.45
23	R	603	HEA	O2A-CGA	-2.13	1.23	1.30
27	H	612	9XX	O1-C18	2.13	1.40	1.34
19	G	502	9YF	O9-C8	2.13	1.40	1.34
27	H	612	9XX	O-C16	-2.12	1.40	1.45
21	L	601	CDL	OB8-CB6	-2.12	1.40	1.45
23	R	603	HEA	C4B-C3B	2.11	1.48	1.44
15	C	301	HEC	C3C-C2C	-2.11	1.34	1.41
27	b	202	9XX	O-C16	-2.11	1.40	1.45
15	C	301	HEC	CMA-C3A	2.10	1.55	1.50
15	C	301	HEC	CMB-C2B	2.10	1.55	1.50
20	N	602	HEM	C3B-C4B	2.10	1.49	1.44
20	N	602	HEM	C4D-C3D	2.10	1.48	1.45
15	C	302	HEC	C3D-C2D	-2.10	1.33	1.38
20	N	602	HEM	C1A-NA	-2.09	1.35	1.39
15	O	302	HEC	C3D-C2D	-2.09	1.33	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	O	301	HEC	C3C-C2C	-2.09	1.34	1.41
15	C	302	HEC	CMA-C3A	2.09	1.55	1.50
15	O	301	HEC	CMB-C2B	2.08	1.55	1.50
15	O	301	HEC	CMA-C3A	2.07	1.55	1.50
15	O	302	HEC	CMA-C3A	2.07	1.55	1.50
16	H	602	MQ9	C26-C24	2.06	1.55	1.51
27	Y	302	9XX	O-C16	-2.06	1.40	1.45
20	H	603	HEM	C4B-NB	-2.04	1.34	1.38
20	H	610	HEM	C4C-NC	-2.04	1.35	1.39
23	L	602	HEA	C4C-NC	-2.04	1.35	1.39
17	W	401	WUO	O51-C50	-2.02	1.37	1.44
17	O	304	WUO	O51-C50	-2.01	1.37	1.44
17	C	304	WUO	C31-C01	2.01	1.57	1.52
17	I	303	WUO	O51-C50	-2.01	1.37	1.44
20	N	602	HEM	C1C-NC	-2.01	1.35	1.39

All (349) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	C	301	HEC	CBB-CAB-C3B	-8.60	110.24	127.43
15	O	301	HEC	CBB-CAB-C3B	-8.59	110.26	127.43
23	R	602	HEA	C3B-C4B-NB	6.85	117.71	109.84
23	R	603	HEA	C2B-C1B-NB	6.83	117.80	109.90
23	L	602	HEA	C3B-C4B-NB	6.81	117.67	109.84
15	C	301	HEC	CBC-CAC-C3C	-6.73	113.98	127.43
15	O	301	HEC	CBC-CAC-C3C	-6.72	114.01	127.43
17	C	304	WUO	O58-C59-C61	6.62	125.81	111.48
23	R	603	HEA	C3D-C4D-ND	6.10	116.24	110.35
23	R	603	HEA	C3B-C4B-NB	5.84	116.55	109.84
15	O	302	HEC	CBC-CAC-C3C	-5.83	115.79	127.43
20	N	602	HEM	CAD-C3D-C4D	5.82	134.84	124.70
15	C	302	HEC	CBC-CAC-C3C	-5.81	115.83	127.43
23	L	603	HEA	C3B-C4B-NB	5.70	116.40	109.84
20	N	602	HEM	CAD-C3D-C2D	-5.69	117.22	127.87
23	R	603	HEA	C13-C12-C11	5.56	123.28	114.39
23	L	603	HEA	C3D-C4D-ND	5.56	115.72	110.35
23	L	603	HEA	C2B-C1B-NB	5.53	116.29	109.90
23	R	602	HEA	C3C-C2C-C1C	-5.26	100.96	107.17
23	L	602	HEA	C3C-C2C-C1C	-5.25	100.98	107.17
27	R	608	9XX	O1-C18-C19	5.22	122.76	111.48
20	N	602	HEM	CHD-C1D-ND	5.20	130.01	124.42
23	R	602	HEA	C2B-C1B-NB	5.18	115.90	109.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	R	602	HEA	C3D-C4D-ND	5.18	115.36	110.35
23	L	602	HEA	C2B-C1B-NB	5.18	115.89	109.90
23	L	602	HEA	C3D-C4D-ND	5.18	115.36	110.35
23	L	602	HEA	C2D-C1D-ND	5.01	115.60	109.84
23	L	603	HEA	C2D-C1D-ND	5.00	115.59	109.84
15	C	302	HEC	CBB-CAB-C3B	-4.99	117.46	127.43
15	O	302	HEC	CBB-CAB-C3B	-4.99	117.46	127.43
23	R	602	HEA	C2D-C1D-ND	4.97	115.55	109.84
23	L	602	HEA	O11-C11-C3B	-4.93	102.22	111.26
23	R	602	HEA	O11-C11-C3B	-4.93	102.23	111.26
20	H	610	HEM	CHD-C1D-ND	4.89	129.69	124.42
21	H	611	CDL	OB6-CB5-C51	4.87	122.01	111.48
23	R	603	HEA	C3C-C2C-C1C	-4.82	101.49	107.17
27	R	608	9XX	C17-O1-C18	4.76	124.65	117.78
17	C	304	WUO	O58-C59-O60	-4.68	112.76	123.70
23	L	603	HEA	C26-C15-C16	4.60	123.22	115.23
23	L	603	HEA	C3C-C2C-C1C	-4.60	101.75	107.17
23	L	602	HEA	C3C-C4C-NC	4.59	113.66	109.80
23	R	602	HEA	C3C-C4C-NC	4.58	113.66	109.80
23	R	602	HEA	C2C-C1C-NC	4.57	117.47	110.14
23	L	602	HEA	C2C-C1C-NC	4.54	117.42	110.14
23	L	603	HEA	C26-C15-C14	-4.53	111.99	123.63
17	C	304	WUO	C03-O04-C05	4.49	122.49	113.72
20	H	610	HEM	CHC-C4B-NB	4.41	129.17	124.42
23	R	603	HEA	O11-C11-C3B	-4.38	103.23	111.26
20	N	607	HEM	CHC-C4B-NB	4.31	129.06	124.42
20	H	603	HEM	CHC-C4B-NB	4.29	129.04	124.42
17	O	304	WUO	O54-P52-O53	4.28	132.37	112.44
17	I	303	WUO	O54-P52-O53	4.27	132.30	112.44
17	W	401	WUO	O54-P52-O53	4.27	132.29	112.44
23	L	603	HEA	CHB-C1B-NB	-4.26	119.84	124.42
23	L	603	HEA	C27-C19-C20	4.23	122.58	115.23
20	H	610	HEM	CHA-C4D-ND	4.18	129.54	124.37
23	R	603	HEA	C17-C18-C19	-4.17	118.08	127.62
23	L	602	HEA	C1D-C2D-C3D	-4.13	102.64	106.98
23	R	602	HEA	C1D-C2D-C3D	-4.12	102.64	106.98
23	L	603	HEA	C1D-C2D-C3D	-4.06	102.71	106.98
21	I	301	CDL	OA6-CA5-C11	4.01	120.16	111.48
20	H	603	HEM	C1B-NB-C4B	3.99	109.93	105.21
27	H	612	9XX	O1-C18-C19	3.95	120.03	111.48
21	G	504	CDL	OB6-CB5-C51	3.93	119.99	111.48
23	L	603	HEA	C3C-C4C-NC	3.93	113.11	109.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	I	301	CDL	OB6-CB5-C51	3.91	119.94	111.48
19	G	502	9YF	O9-C8-C9	3.91	119.94	111.48
21	G	504	CDL	OA6-CA5-C11	3.91	119.94	111.48
20	N	602	HEM	CHD-C4C-NC	3.91	128.71	124.45
19	b	201	9YF	O9-C8-C9	3.91	119.94	111.48
23	R	603	HEA	CMD-C2D-C1D	3.91	131.14	125.03
27	b	202	9XX	O1-C18-C19	3.90	119.93	111.48
19	W	402	9YF	O9-C8-C9	3.89	119.89	111.48
23	R	602	HEA	C4B-C3B-C2B	-3.87	100.94	107.44
23	L	602	HEA	C4B-C3B-C2B	-3.85	100.96	107.44
20	H	603	HEM	CHD-C1D-ND	3.84	128.56	124.42
23	R	603	HEA	CAD-C3D-C4D	3.84	131.38	124.70
20	N	602	HEM	C4C-CHD-C1D	-3.83	117.89	126.02
19	M	502	9YF	O9-C8-C9	3.82	119.74	111.48
23	R	603	HEA	C4D-C3D-C2D	-3.80	101.36	106.89
23	R	603	HEA	C4B-NB-C1B	-3.78	100.73	105.21
20	N	607	HEM	CHD-C1D-ND	3.76	128.47	124.42
23	R	603	HEA	C2D-C1D-ND	3.76	114.16	109.84
23	L	603	HEA	C1B-C2B-C3B	-3.72	102.48	106.80
27	Y	302	9XX	O1-C18-C19	3.69	119.46	111.48
20	H	610	HEM	CAA-C2A-C1A	3.65	132.07	124.94
23	R	603	HEA	O11-C11-C12	-3.64	99.50	109.14
23	L	602	HEA	CAD-CBD-CGD	-3.63	104.05	113.67
20	N	602	HEM	CHD-C1D-C2D	-3.62	119.31	125.03
17	I	303	WUO	O77-C76-C57	3.62	118.83	108.40
23	R	602	HEA	CAD-CBD-CGD	-3.62	104.07	113.67
17	W	401	WUO	O77-C76-C57	3.61	118.81	108.40
20	N	607	HEM	C1B-NB-C4B	3.61	109.48	105.21
17	O	304	WUO	O77-C76-C57	3.58	118.72	108.40
23	R	603	HEA	C1B-C2B-C3B	-3.54	102.70	106.80
16	C	303	MQ9	C7-C6-C5	-3.50	118.88	124.89
23	L	603	HEA	CHA-C4D-ND	-3.47	120.69	124.42
23	R	603	HEA	CHB-C1B-C2B	-3.45	119.58	125.03
16	N	601	MQ9	C7-C6-C5	-3.44	118.99	124.89
23	L	602	HEA	CMD-C2D-C1D	3.31	130.20	125.03
23	L	603	HEA	C16-C17-C18	3.31	128.37	112.02
20	H	610	HEM	CAA-C2A-C3A	-3.29	119.69	127.07
23	R	603	HEA	C3C-C4C-NC	3.28	112.56	109.80
23	R	602	HEA	CMD-C2D-C1D	3.28	130.15	125.03
20	H	603	HEM	C3B-C4B-NB	-3.27	107.12	109.47
17	O	304	WUO	C03-O02-C01	3.25	125.67	117.98
23	R	603	HEA	CHC-C4B-NB	-3.25	120.35	124.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	N	607	HEM	CHD-C1D-C2D	-3.21	119.96	125.03
17	W	401	WUO	C03-O02-C01	3.19	125.55	117.98
21	H	611	CDL	OA6-CA5-C11	3.19	118.38	111.48
20	N	602	HEM	CHC-C1C-NC	3.19	127.93	124.45
23	L	603	HEA	C2C-C1C-NC	3.19	115.25	110.14
17	I	303	WUO	O04-C05-C12	3.16	112.96	106.69
17	O	304	WUO	O04-C05-C12	3.15	112.94	106.69
21	L	601	CDL	OB6-CB5-C51	3.15	118.29	111.48
17	I	303	WUO	C03-O02-C01	3.15	125.44	117.98
21	H	601	CDL	OA6-CA5-C11	3.11	118.21	111.48
23	R	603	HEA	C4B-C3B-C2B	-3.10	102.22	107.44
23	L	603	HEA	C4B-C3B-C2B	-3.10	102.22	107.44
23	L	603	HEA	C12-C13-C14	-3.09	104.04	112.16
17	W	401	WUO	O04-C05-C12	3.08	112.79	106.69
23	R	602	HEA	CMC-C2C-C1C	3.06	130.07	125.42
27	R	608	9XX	O1-C17-C16	3.04	113.21	106.21
20	H	603	HEM	CHA-C4D-ND	3.03	128.12	124.37
20	H	610	HEM	CMA-C3A-C4A	3.03	130.03	125.42
23	R	603	HEA	C2A-C1A-NA	3.03	113.24	110.32
23	L	602	HEA	CMC-C2C-C1C	3.02	130.02	125.42
17	C	304	WUO	C57-O58-C59	3.02	125.03	117.80
17	C	304	WUO	O38-C37-C50	3.02	115.08	107.42
15	O	302	HEC	O1D-CGD-CBD	-3.00	113.57	123.09
20	H	610	HEM	C4D-ND-C1D	3.00	108.76	105.21
15	C	302	HEC	O1D-CGD-CBD	-2.99	113.60	123.09
23	R	603	HEA	C1D-C2D-C3D	-2.99	103.83	106.98
27	R	608	9XX	O-C15-C14	2.98	120.93	111.83
23	L	603	HEA	CHD-C1D-ND	-2.98	120.68	124.37
17	O	304	WUO	C03-O04-C05	2.96	119.50	113.72
15	O	301	HEC	O1D-CGD-CBD	-2.96	113.71	123.09
23	R	602	HEA	C13-C14-C15	-2.95	120.86	127.62
23	L	602	HEA	C13-C14-C15	-2.95	120.87	127.62
15	C	301	HEC	O1D-CGD-CBD	-2.95	113.74	123.09
17	C	304	WUO	C39-O40-C41	2.94	119.46	113.72
23	R	602	HEA	C4B-NB-C1B	-2.92	101.75	105.21
23	L	602	HEA	C4B-NB-C1B	-2.90	101.77	105.21
23	L	603	HEA	C20-C19-C18	-2.89	114.67	121.17
23	L	603	HEA	CMB-C2B-C1B	2.88	129.53	125.03
17	W	401	WUO	O40-C41-C42	2.87	114.88	109.70
20	N	607	HEM	CHA-C4D-ND	2.87	127.92	124.37
20	N	602	HEM	O2A-CGA-O1A	-2.87	115.96	123.33
17	C	304	WUO	O77-C78-C80	2.86	120.56	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	H	602	MQ9	C15-C14-C16	2.86	120.19	115.23
23	R	602	HEA	C12-C11-C3B	2.86	116.59	112.12
23	L	602	HEA	C12-C11-C3B	2.86	116.59	112.12
23	L	603	HEA	C4D-C3D-C2D	-2.84	102.76	106.89
21	L	601	CDL	OA6-CA5-C11	2.84	117.62	111.48
16	H	602	MQ9	C25-C24-C26	2.83	120.14	115.23
20	N	602	HEM	CAD-CBD-CGD	-2.83	106.16	113.67
17	O	304	WUO	O55-P52-O53	-2.83	97.74	108.94
17	I	303	WUO	C03-O04-C05	2.81	119.20	113.72
17	W	401	WUO	O55-P52-O53	-2.80	97.83	108.94
17	I	303	WUO	O55-P52-O53	-2.80	97.84	108.94
17	O	304	WUO	O40-C41-C42	2.79	114.73	109.70
23	R	603	HEA	C17-C16-C15	-2.79	103.94	113.19
16	H	602	MQ9	C45-C44-C46	2.78	120.06	115.23
20	H	603	HEM	CHB-C1B-NB	2.78	127.81	124.37
15	O	302	HEC	CMB-C2B-C1B	-2.77	121.19	125.42
15	C	302	HEC	CMB-C2B-C1B	-2.77	121.20	125.42
20	H	610	HEM	CHD-C1D-C2D	-2.77	120.66	125.03
17	I	303	WUO	O40-C41-C42	2.76	114.68	109.70
20	H	603	HEM	C4D-ND-C1D	2.76	108.48	105.21
20	N	602	HEM	C4C-C3C-C2C	2.75	109.20	106.81
23	R	603	HEA	C2C-C1C-NC	2.74	114.53	110.14
20	N	607	HEM	C3B-C4B-NB	-2.73	107.51	109.47
21	I	301	CDL	OA8-CA7-C31	2.72	120.14	111.83
23	L	603	HEA	CHC-C4B-NB	-2.71	121.02	124.37
21	H	601	CDL	OB6-CB5-C51	2.70	117.32	111.48
19	G	502	9YF	O11-C25-C26	2.70	120.06	111.83
20	N	607	HEM	CMD-C2D-C1D	2.69	129.24	125.03
23	R	602	HEA	C1B-C2B-C3B	-2.69	103.69	106.80
23	L	602	HEA	C1B-C2B-C3B	-2.69	103.69	106.80
19	b	201	9YF	O11-C25-C26	2.69	120.03	111.83
15	O	301	HEC	CBD-CAD-C3D	2.67	119.92	112.53
15	C	301	HEC	CBD-CAD-C3D	2.67	119.92	112.53
19	M	502	9YF	O11-C25-C26	2.67	119.97	111.83
23	R	602	HEA	CAD-C3D-C4D	2.67	129.35	124.70
19	W	402	9YF	O11-C25-C26	2.67	119.97	111.83
23	L	602	HEA	CAD-C3D-C4D	2.66	129.34	124.70
27	H	612	9XX	O-C15-C14	2.65	119.93	111.83
17	W	401	WUO	O58-C57-C76	2.65	117.85	108.34
17	O	304	WUO	O58-C57-C76	2.65	117.84	108.34
23	R	602	HEA	CHC-C1C-C2C	-2.65	119.75	127.43
27	b	202	9XX	C17-O1-C18	-2.64	113.97	117.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	L	602	HEA	CHC-C1C-C2C	-2.64	119.75	127.43
23	R	602	HEA	O2A-CGA-CBA	2.63	122.33	114.00
23	L	602	HEA	O2A-CGA-CBA	2.63	122.31	114.00
17	I	303	WUO	O58-C57-C76	2.62	117.75	108.34
17	W	401	WUO	C03-O04-C05	2.62	118.83	113.72
27	R	608	9XX	C37-C17-C16	-2.60	105.39	112.69
27	H	612	9XX	C17-O1-C18	-2.59	114.04	117.78
21	H	611	CDL	OB8-CB7-C71	2.59	119.72	111.83
17	O	304	WUO	O38-C37-C50	2.58	113.98	107.42
27	R	608	9XX	O1-C18-O2	-2.58	117.68	123.70
16	H	609	MQ9	C7-C6-C5	-2.58	120.47	124.89
27	Y	302	9XX	O-C15-C14	2.57	119.68	111.83
23	L	603	HEA	CBA-CAA-C2A	2.56	119.61	112.53
16	H	602	MQ9	C10-C9-C11	2.56	119.67	115.23
23	L	602	HEA	C2A-C1A-NA	2.55	112.78	110.32
23	L	603	HEA	C17-C18-C19	2.55	133.46	127.62
23	R	603	HEA	C4A-NA-C1A	-2.54	101.68	105.82
23	R	602	HEA	C2A-C1A-NA	2.53	112.77	110.32
23	R	603	HEA	CBA-CAA-C2A	-2.51	105.58	112.53
20	N	602	HEM	C4C-NC-C1C	2.51	109.91	105.82
16	N	605	MQ9	C7-C6-C5	-2.50	120.60	124.89
21	G	504	CDL	OB8-CB7-C71	2.50	119.46	111.83
27	b	202	9XX	O-C15-C14	2.50	119.46	111.83
23	L	603	HEA	CMC-C2C-C1C	2.50	129.22	125.42
16	H	607	MQ9	C7-C6-C5	-2.49	120.62	124.89
16	O	303	MQ9	C7-C6-C5	-2.48	120.64	124.89
23	L	603	HEA	CMD-C2D-C1D	2.47	128.90	125.03
20	H	603	HEM	C1C-CHC-C4B	-2.47	120.77	126.02
16	N	606	MQ9	C7-C6-C5	-2.46	120.68	124.89
23	L	603	HEA	CAD-C3D-C4D	2.46	128.98	124.70
20	H	610	HEM	CAD-CBD-CGD	-2.45	107.17	113.67
16	G	501	MQ9	C7-C6-C5	-2.45	120.69	124.89
17	I	303	WUO	O38-C37-C50	2.45	113.64	107.42
15	O	302	HEC	CMD-C2D-C1D	-2.45	121.69	125.42
15	C	301	HEC	O1A-CGA-CBA	-2.45	115.33	123.09
15	O	301	HEC	O1A-CGA-CBA	-2.44	115.35	123.09
23	L	602	HEA	CHB-C1B-NB	-2.44	121.80	124.42
23	R	602	HEA	CHB-C1B-NB	-2.44	121.80	124.42
15	C	302	HEC	CMD-C2D-C1D	-2.44	121.71	125.42
16	H	608	MQ9	C7-C6-C5	-2.44	120.72	124.89
17	W	401	WUO	O38-C37-C50	2.43	113.58	107.42
23	R	602	HEA	CMB-C2B-C1B	2.41	128.79	125.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	L	602	HEA	CMB-C2B-C1B	2.40	128.79	125.03
23	L	602	HEA	C4D-C3D-C2D	-2.39	103.41	106.89
23	L	602	HEA	C27-C19-C20	2.39	119.38	115.23
23	R	602	HEA	C4D-C3D-C2D	-2.39	103.41	106.89
23	R	602	HEA	CBA-CAA-C2A	-2.39	105.93	112.53
23	R	602	HEA	C27-C19-C20	2.38	119.37	115.23
20	H	603	HEM	C1A-CHA-C4D	-2.38	120.64	126.25
23	L	602	HEA	CBA-CAA-C2A	-2.38	105.95	112.53
23	R	603	HEA	C27-C19-C18	-2.38	117.52	123.63
15	O	302	HEC	O1A-CGA-CBA	-2.37	115.57	123.09
15	C	302	HEC	O1A-CGA-CBA	-2.37	115.57	123.09
15	O	302	HEC	CMB-C2B-C3B	2.36	132.11	126.55
20	N	602	HEM	CHC-C4B-NB	2.36	126.96	124.42
17	C	304	WUO	O77-C78-O79	-2.35	117.75	123.63
17	O	304	WUO	C39-O40-C41	2.35	118.31	113.72
15	C	302	HEC	CMB-C2B-C3B	2.35	132.07	126.55
20	N	602	HEM	CMD-C2D-C1D	2.34	128.70	125.03
20	N	607	HEM	O2D-CGD-O1D	-2.34	117.31	123.33
27	R	608	9XX	O-C16-C17	2.34	115.02	108.35
23	L	603	HEA	O1D-CGD-CBD	-2.34	115.67	123.09
21	I	301	CDL	OB8-CB7-C71	2.33	118.95	111.83
17	C	304	WUO	C03-O02-C01	2.33	123.49	117.98
17	C	304	WUO	O77-C76-C57	2.32	115.09	108.40
17	C	304	WUO	O13-C12-C05	2.32	113.30	108.41
23	R	603	HEA	C16-C15-C14	2.31	126.34	121.17
20	H	603	HEM	C4A-CHB-C1B	-2.30	120.84	126.25
23	L	602	HEA	C3A-C2A-C1A	-2.30	104.87	107.05
23	L	603	HEA	C3A-C2A-C1A	-2.29	104.88	107.05
23	R	602	HEA	C3A-C2A-C1A	-2.29	104.88	107.05
23	R	603	HEA	OMA-CMA-C3A	-2.29	120.46	125.62
20	N	602	HEM	CMB-C2B-C1B	2.28	128.59	125.03
23	R	603	HEA	CAA-CBA-CGA	-2.28	107.62	113.67
23	R	603	HEA	CHA-C4D-C3D	-2.28	121.46	124.77
21	G	504	CDL	OA8-CA7-C31	2.27	118.77	111.83
17	C	304	WUO	O11-C06-C07	-2.27	105.03	110.38
20	H	610	HEM	C2A-C1A-NA	-2.26	107.65	110.15
23	R	603	HEA	CHD-C1D-ND	-2.25	121.58	124.37
17	O	304	WUO	O51-C50-C01	2.25	113.55	108.76
23	R	603	HEA	C13-C14-C15	-2.25	122.47	127.62
20	H	610	HEM	O2A-CGA-CBA	2.25	121.11	114.00
23	L	602	HEA	CHD-C1D-C2D	-2.25	120.56	126.95
23	R	602	HEA	CHD-C1D-C2D	-2.25	120.56	126.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	R	602	HEA	CHA-C4D-C3D	-2.25	121.50	124.77
17	W	401	WUO	O51-C50-C01	2.24	113.53	108.76
23	L	602	HEA	CHA-C4D-C3D	-2.24	121.51	124.77
17	I	303	WUO	O40-C41-C48	2.23	111.97	106.44
16	H	602	MQ9	C16-C14-C13	-2.23	116.17	121.17
17	I	303	WUO	O51-C50-C01	2.23	113.50	108.76
20	H	610	HEM	C4B-C3B-C2B	-2.22	105.24	107.28
20	H	610	HEM	CHD-C4C-C3C	2.21	128.94	125.21
17	W	401	WUO	O13-C12-C05	2.21	113.08	108.41
17	I	303	WUO	O13-C12-C05	2.21	113.08	108.41
20	N	602	HEM	CHB-C1B-NB	2.21	127.10	124.37
16	H	602	MQ9	C20-C19-C21	2.20	119.05	115.23
23	R	602	HEA	C4A-NA-C1A	-2.20	102.23	105.82
23	L	603	HEA	C4B-NB-C1B	-2.20	102.60	105.21
20	N	607	HEM	C4C-CHD-C1D	-2.20	121.34	126.02
23	L	602	HEA	C4A-NA-C1A	-2.20	102.23	105.82
17	O	304	WUO	O13-C12-C05	2.20	113.05	108.41
17	W	401	WUO	O40-C41-C48	2.20	111.89	106.44
20	H	610	HEM	C1B-NB-C4B	2.19	107.80	105.21
17	O	304	WUO	O40-C41-C48	2.19	111.86	106.44
20	H	610	HEM	C1A-CHA-C4D	-2.18	121.13	126.25
20	N	607	HEM	O2D-CGD-CBD	2.17	120.85	114.00
20	N	602	HEM	CHB-C4A-NA	2.17	127.79	123.86
21	H	611	CDL	OB6-CB5-OB7	-2.16	118.65	123.70
20	N	607	HEM	CAD-C3D-C4D	2.15	128.44	124.70
23	R	602	HEA	O11-C11-C12	-2.15	103.45	109.14
23	R	602	HEA	CBC-CAC-C3C	-2.15	116.80	127.53
23	L	602	HEA	CBC-CAC-C3C	-2.15	116.80	127.53
16	H	602	MQ9	C35-C34-C33	-2.14	118.13	123.63
16	H	602	MQ9	C22-C23-C24	-2.14	122.72	127.62
16	N	601	MQ9	C5M-C5-C6	-2.14	120.93	124.45
23	L	602	HEA	O11-C11-C12	-2.14	103.47	109.14
20	H	603	HEM	C4C-CHD-C1D	-2.14	121.47	126.02
23	L	603	HEA	C20-C21-C22	2.14	122.58	112.02
17	C	304	WUO	O04-C05-C12	2.13	110.92	106.69
17	C	304	WUO	O13-C14-C16	2.13	118.32	111.83
16	H	602	MQ9	C30-C29-C31	2.13	118.92	115.23
20	H	610	HEM	CHB-C1B-NB	2.13	127.00	124.37
20	N	607	HEM	C1A-CHA-C4D	-2.12	121.26	126.25
20	N	602	HEM	O2A-CGA-CBA	2.12	120.69	114.00
20	H	603	HEM	CHD-C4C-NC	2.12	126.76	124.45
23	R	602	HEA	CHC-C4B-C3B	-2.11	120.49	125.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	N	607	HEM	CHD-C4C-NC	2.11	126.75	124.45
20	N	602	HEM	C2A-C1A-NA	-2.10	107.82	110.15
20	N	607	HEM	CAD-C3D-C2D	-2.10	123.93	127.87
23	L	602	HEA	CHC-C4B-C3B	-2.10	120.50	125.80
15	C	301	HEC	CHC-C4B-NB	2.10	126.74	124.45
17	I	303	WUO	O45-C44-C39	-2.10	105.07	110.08
21	H	611	CDL	CB6-CB4-CB3	-2.10	106.89	111.78
23	R	603	HEA	CAD-CBD-CGD	-2.09	108.12	113.67
17	O	304	WUO	O45-C44-C39	-2.08	105.11	110.08
27	R	608	9XX	O1-C17-C37	2.08	112.61	107.96
23	R	602	HEA	CHC-C4B-NB	-2.08	121.80	124.37
17	W	401	WUO	O45-C44-C39	-2.06	105.16	110.08
17	I	303	WUO	C39-O40-C41	2.06	117.75	113.72
15	O	301	HEC	CHC-C4B-NB	2.06	126.69	124.45
23	L	602	HEA	CHC-C4B-NB	-2.05	121.83	124.37
17	W	401	WUO	C39-O40-C41	2.05	117.72	113.72
23	L	603	HEA	CHC-C1C-NC	-2.05	120.14	123.86
23	R	602	HEA	C21-C20-C19	-2.05	106.40	113.19
20	N	607	HEM	O2A-CGA-O1A	-2.04	118.08	123.33
23	L	602	HEA	C21-C20-C19	-2.04	106.42	113.19
17	W	401	WUO	O09-C08-C03	-2.04	105.22	110.08
15	O	302	HEC	CHC-C4B-NB	2.03	126.67	124.45
20	H	610	HEM	O2D-CGD-O1D	-2.03	118.11	123.33
17	O	304	WUO	O58-C59-C61	2.03	115.86	111.48
20	N	602	HEM	CHB-C1B-C2B	-2.02	121.20	126.95
17	C	304	WUO	O10-C07-C08	-2.02	105.61	110.38
23	L	603	HEA	C13-C12-C11	2.02	117.62	114.39
17	W	401	WUO	O58-C59-C61	2.02	115.85	111.48
20	H	603	HEM	C4C-NC-C1C	2.02	109.11	105.82
17	I	303	WUO	O09-C08-C03	-2.01	105.28	110.08
17	C	304	WUO	O34-C33-C31	-2.01	105.64	110.38
17	I	303	WUO	O58-C59-C61	2.01	115.82	111.48

There are no chirality outliers.

All (1450) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
15	O	302	HEC	C2B-C3B-CAB-CBB
15	O	302	HEC	C4B-C3B-CAB-CBB
15	O	302	HEC	C4C-C3C-CAC-CBC
15	C	302	HEC	C2B-C3B-CAB-CBB
15	C	302	HEC	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
15	C	302	HEC	C4C-C3C-CAC-CBC
16	O	303	MQ9	C17-C18-C19-C21
16	O	303	MQ9	C32-C33-C34-C35
16	O	303	MQ9	C32-C33-C34-C36
16	O	303	MQ9	C42-C43-C44-C45
16	O	303	MQ9	C42-C43-C44-C46
16	N	601	MQ9	C5-C6-C7-C8
16	N	601	MQ9	C1-C6-C7-C8
16	N	601	MQ9	C7-C8-C9-C10
16	N	601	MQ9	C7-C8-C9-C11
16	N	601	MQ9	C20-C19-C21-C22
16	N	601	MQ9	C28-C29-C31-C32
16	N	601	MQ9	C30-C29-C31-C32
16	N	601	MQ9	C31-C32-C33-C34
16	N	601	MQ9	C42-C43-C44-C45
16	N	601	MQ9	C42-C43-C44-C46
16	N	601	MQ9	C47-C48-C49-C51
16	N	605	MQ9	C7-C8-C9-C10
16	N	605	MQ9	C7-C8-C9-C11
16	N	605	MQ9	C37-C38-C39-C40
16	N	605	MQ9	C37-C38-C39-C41
16	N	605	MQ9	C47-C48-C49-C51
16	N	606	MQ9	C12-C13-C14-C15
16	N	606	MQ9	C12-C13-C14-C16
16	N	606	MQ9	C18-C19-C21-C22
16	N	606	MQ9	C20-C19-C21-C22
16	N	606	MQ9	C22-C23-C24-C25
16	N	606	MQ9	C22-C23-C24-C26
16	N	606	MQ9	C27-C28-C29-C30
16	N	606	MQ9	C27-C28-C29-C31
16	N	606	MQ9	C42-C43-C44-C45
16	N	606	MQ9	C42-C43-C44-C46
16	N	606	MQ9	C47-C48-C49-C50
16	C	303	MQ9	C5-C6-C7-C8
16	C	303	MQ9	C1-C6-C7-C8
16	C	303	MQ9	C7-C8-C9-C10
16	C	303	MQ9	C7-C8-C9-C11
16	C	303	MQ9	C15-C14-C16-C17
16	C	303	MQ9	C22-C23-C24-C25
16	C	303	MQ9	C22-C23-C24-C26
16	G	501	MQ9	C17-C18-C19-C20
16	G	501	MQ9	C17-C18-C19-C21

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Mol	Chain	Res	Type	Atoms
16	H	607	MQ9	C9-C11-C12-C13
16	H	607	MQ9	C27-C28-C29-C30
16	H	607	MQ9	C27-C28-C29-C31
16	H	607	MQ9	C32-C33-C34-C36
16	H	608	MQ9	C7-C8-C9-C10
16	H	608	MQ9	C7-C8-C9-C11
16	H	608	MQ9	C32-C33-C34-C35
16	H	608	MQ9	C32-C33-C34-C36
16	H	608	MQ9	C37-C38-C39-C41
16	H	609	MQ9	C7-C8-C9-C11
16	H	609	MQ9	C22-C23-C24-C25
16	H	609	MQ9	C22-C23-C24-C26
16	H	609	MQ9	C40-C39-C41-C42
16	H	609	MQ9	C42-C43-C44-C45
16	H	609	MQ9	C42-C43-C44-C46
16	H	609	MQ9	C47-C48-C49-C51
17	O	304	WUO	C56-C57-O58-C59
17	O	304	WUO	C61-C59-O58-C57
17	C	304	WUO	O60-C59-O58-C57
17	C	304	WUO	C50-O51-P52-O55
17	I	303	WUO	C06-C05-C12-O13
19	M	502	9YF	C7-C2-O2-P
19	W	402	9YF	C1-O-P-O2
19	W	402	9YF	C1-O-P-O8
19	G	502	9YF	C1-O-P-O1
19	G	502	9YF	C1-O-P-O2
19	G	502	9YF	C1-O-P-O8
19	G	502	9YF	C26-C25-O11-C24
19	G	502	9YF	O12-C25-O11-C24
19	b	201	9YF	C1-O-P-O1
19	b	201	9YF	C1-O-P-O2
19	b	201	9YF	O10-C8-O9-C
20	N	602	HEM	C2D-C3D-CAD-CBD
20	N	602	HEM	C4D-C3D-CAD-CBD
20	H	603	HEM	C2B-C3B-CAB-CBB
20	H	603	HEM	C2D-C3D-CAD-CBD
20	H	610	HEM	C1A-C2A-CAA-CBA
20	H	610	HEM	C3A-C2A-CAA-CBA
21	N	603	CDL	CA2-OA2-PA1-OA3
21	N	603	CDL	CA2-OA2-PA1-OA4
21	N	603	CDL	CA2-OA2-PA1-OA5
21	N	603	CDL	CA3-OA5-PA1-OA3

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Mol	Chain	Res	Type	Atoms
21	N	603	CDL	CB2-OB2-PB2-OB3
21	N	603	CDL	CB2-OB2-PB2-OB4
21	N	603	CDL	CB2-OB2-PB2-OB5
21	N	603	CDL	CB3-OB5-PB2-OB3
21	N	603	CDL	CB3-OB5-PB2-OB4
21	N	604	CDL	CA2-OA2-PA1-OA4
21	N	604	CDL	CA2-OA2-PA1-OA5
21	N	604	CDL	CA3-OA5-PA1-OA2
21	N	604	CDL	CA3-OA5-PA1-OA3
21	N	604	CDL	C11-CA5-OA6-CA4
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	P	301	CDL	CA2-C1-CB2-OB2
21	P	301	CDL	CA2-OA2-PA1-OA3
21	P	301	CDL	CA2-OA2-PA1-OA4
21	P	301	CDL	CA2-OA2-PA1-OA5
21	P	301	CDL	CA3-OA5-PA1-OA2
21	P	301	CDL	CB2-OB2-PB2-OB4
21	P	301	CDL	CB2-OB2-PB2-OB5
21	P	301	CDL	CB3-OB5-PB2-OB3
21	T	201	CDL	CA2-OA2-PA1-OA3
21	T	201	CDL	CA2-OA2-PA1-OA4
21	T	201	CDL	CB2-OB2-PB2-OB3
21	T	201	CDL	CB2-OB2-PB2-OB4
21	T	201	CDL	CB2-OB2-PB2-OB5
21	T	201	CDL	CB3-OB5-PB2-OB2
21	R	601	CDL	CA2-C1-CB2-OB2
21	R	601	CDL	CA2-OA2-PA1-OA3
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	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	OA6-CA4-CA6-OA8
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

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Mol	Chain	Res	Type	Atoms
21	R	605	CDL	CB3-OB5-PB2-OB4
21	G	504	CDL	CA2-C1-CB2-OB2
21	G	504	CDL	CA2-OA2-PA1-OA5
21	G	504	CDL	CA3-OA5-PA1-OA3
21	G	504	CDL	OA5-CA3-CA4-OA6
21	G	504	CDL	C11-CA5-OA6-CA4
21	G	504	CDL	CB2-OB2-PB2-OB3
21	G	504	CDL	CB2-OB2-PB2-OB4
21	G	504	CDL	CB2-OB2-PB2-OB5
21	G	504	CDL	CB3-OB5-PB2-OB3
21	G	504	CDL	C51-CB5-OB6-CB4
21	H	601	CDL	CA3-OA5-PA1-OA2
21	H	601	CDL	CB3-OB5-PB2-OB2
21	H	601	CDL	CB3-OB5-PB2-OB3
21	H	604	CDL	CA3-OA5-PA1-OA2
21	H	604	CDL	CA3-OA5-PA1-OA4
21	H	604	CDL	CB3-OB5-PB2-OB2
21	H	604	CDL	CB3-OB5-PB2-OB3
21	H	605	CDL	CA2-OA2-PA1-OA3
21	H	605	CDL	CA2-OA2-PA1-OA4
21	H	605	CDL	CA2-OA2-PA1-OA5
21	H	605	CDL	CA3-OA5-PA1-OA2
21	H	605	CDL	CA3-OA5-PA1-OA3
21	H	605	CDL	CB2-OB2-PB2-OB3
21	H	605	CDL	CB2-OB2-PB2-OB4
21	H	605	CDL	CB2-OB2-PB2-OB5
21	H	606	CDL	CB2-C1-CA2-OA2
21	H	606	CDL	CA2-OA2-PA1-OA5
21	H	606	CDL	CA3-OA5-PA1-OA4
21	H	606	CDL	CB2-OB2-PB2-OB4
21	H	606	CDL	CB3-OB5-PB2-OB2
21	H	606	CDL	CB3-OB5-PB2-OB4
21	H	611	CDL	CA2-OA2-PA1-OA3
21	H	611	CDL	CA2-OA2-PA1-OA4
21	H	611	CDL	CA2-OA2-PA1-OA5
21	H	611	CDL	CB2-OB2-PB2-OB3
21	H	611	CDL	CB2-OB2-PB2-OB4
21	H	611	CDL	CB2-OB2-PB2-OB5
21	I	301	CDL	CA2-OA2-PA1-OA3
21	I	301	CDL	CA2-OA2-PA1-OA4
21	I	301	CDL	CA2-OA2-PA1-OA5
21	I	302	CDL	CA2-OA2-PA1-OA3

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Mol	Chain	Res	Type	Atoms
21	I	302	CDL	CA2-OA2-PA1-OA4
21	I	302	CDL	CA2-OA2-PA1-OA5
21	L	601	CDL	O1-C1-CA2-OA2
21	L	601	CDL	CA2-OA2-PA1-OA3
21	L	601	CDL	CA2-OA2-PA1-OA5
21	L	601	CDL	OA7-CA5-OA6-CA4
21	L	601	CDL	C11-CA5-OA6-CA4
21	L	601	CDL	CB2-OB2-PB2-OB4
21	L	601	CDL	CB2-OB2-PB2-OB5
21	L	601	CDL	CB3-OB5-PB2-OB2
21	L	601	CDL	CB3-OB5-PB2-OB3
21	L	607	CDL	CA2-OA2-PA1-OA3
21	L	607	CDL	CA2-OA2-PA1-OA4
21	L	607	CDL	CA2-OA2-PA1-OA5
21	L	607	CDL	CB2-OB2-PB2-OB4
21	L	607	CDL	CB3-OB5-PB2-OB2
21	L	607	CDL	CB3-OB5-PB2-OB3
22	J	401	7PH	C1-O11-P-O12
22	J	401	7PH	C1-O11-P-O13
22	J	401	7PH	O22-C21-O21-C2
23	R	602	HEA	C2A-C3A-CMA-OMA
23	R	602	HEA	C3B-C11-C12-C13
23	R	602	HEA	O11-C11-C12-C13
23	R	603	HEA	C3B-C11-C12-C13
23	R	603	HEA	O11-C11-C12-C13
23	R	603	HEA	C15-C16-C17-C18
23	L	602	HEA	C2A-C3A-CMA-OMA
23	L	602	HEA	C3B-C11-C12-C13
23	L	602	HEA	O11-C11-C12-C13
23	L	603	HEA	C1A-C2A-CAA-CBA
23	L	603	HEA	C3A-C2A-CAA-CBA
23	L	603	HEA	C3B-C11-C12-C13
27	R	608	9XX	O2-C18-O1-C17
27	Y	302	9XX	O-C16-C17-C37
27	H	612	9XX	O-C16-C17-O1
27	b	202	9XX	C19-C18-O1-C17
27	b	202	9XX	O2-C18-O1-C17
17	O	304	WUO	C06-C05-C12-O13
17	W	401	WUO	O04-C03-O02-C01
16	O	303	MQ9	C47-C48-C49-C51
16	N	601	MQ9	C47-C48-C49-C50
16	N	605	MQ9	C47-C48-C49-C50

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Mol	Chain	Res	Type	Atoms
16	N	606	MQ9	C47-C48-C49-C51
16	C	303	MQ9	C47-C48-C49-C51
16	H	607	MQ9	C32-C33-C34-C35
16	H	609	MQ9	C47-C48-C49-C50
17	W	401	WUO	O79-C78-O77-C76
21	N	604	CDL	OA9-CA7-OA8-CA6
21	R	601	CDL	OA9-CA7-OA8-CA6
21	R	605	CDL	OB9-CB7-OB8-CB6
21	I	301	CDL	OB9-CB7-OB8-CB6
21	I	302	CDL	OB9-CB7-OB8-CB6
27	R	608	9XX	O6-C15-O-C16
27	H	612	9XX	O6-C15-O-C16
17	O	304	WUO	O60-C59-O58-C57
21	N	604	CDL	OA7-CA5-OA6-CA4
21	G	504	CDL	OA7-CA5-OA6-CA4
21	G	504	CDL	OB7-CB5-OB6-CB4
16	O	303	MQ9	C47-C48-C49-C50
17	W	401	WUO	C80-C78-O77-C76
21	N	604	CDL	C31-CA7-OA8-CA6
21	R	601	CDL	C31-CA7-OA8-CA6
21	H	605	CDL	C71-CB7-OB8-CB6
21	I	301	CDL	C71-CB7-OB8-CB6
21	I	302	CDL	C71-CB7-OB8-CB6
17	C	304	WUO	C61-C59-O58-C57
19	b	201	9YF	C9-C8-O9-C
21	H	611	CDL	C51-CB5-OB6-CB4
22	J	401	7PH	C22-C21-O21-C2
27	R	608	9XX	C19-C18-O1-C17
16	O	303	MQ9	C20-C19-C21-C22
16	O	303	MQ9	C35-C34-C36-C37
16	N	601	MQ9	C12-C11-C9-C10
16	N	605	MQ9	C15-C14-C16-C17
16	N	605	MQ9	C20-C19-C21-C22
16	G	501	MQ9	C12-C11-C9-C10
16	H	607	MQ9	C25-C24-C26-C27
16	H	608	MQ9	C12-C11-C9-C10
16	H	608	MQ9	C15-C14-C16-C17
16	H	608	MQ9	C30-C29-C31-C32
16	H	609	MQ9	C15-C14-C16-C17
16	H	609	MQ9	C20-C19-C21-C22
16	H	609	MQ9	C25-C24-C26-C27
16	H	609	MQ9	C45-C44-C46-C47

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Mol	Chain	Res	Type	Atoms
16	O	303	MQ9	C18-C19-C21-C22
16	O	303	MQ9	C33-C34-C36-C37
16	N	601	MQ9	C12-C11-C9-C8
16	N	601	MQ9	C18-C19-C21-C22
16	N	605	MQ9	C13-C14-C16-C17
16	N	605	MQ9	C18-C19-C21-C22
16	C	303	MQ9	C13-C14-C16-C17
16	H	608	MQ9	C13-C14-C16-C17
16	H	609	MQ9	C13-C14-C16-C17
16	H	609	MQ9	C18-C19-C21-C22
16	H	609	MQ9	C23-C24-C26-C27
16	H	609	MQ9	C38-C39-C41-C42
23	R	603	HEA	C2D-C3D-CAD-CBD
21	L	601	CDL	OA9-CA7-OA8-CA6
17	W	401	WUO	C16-C14-O13-C12
17	C	304	WUO	C80-C78-O77-C76
17	I	303	WUO	C16-C14-O13-C12
21	N	603	CDL	C71-CB7-OB8-CB6
21	R	605	CDL	C71-CB7-OB8-CB6
21	I	302	CDL	C31-CA7-OA8-CA6
27	R	608	9XX	C14-C15-O-C16
27	H	612	9XX	C14-C15-O-C16
16	O	303	MQ9	C17-C18-C19-C20
16	O	303	MQ9	C37-C38-C39-C40
16	N	601	MQ9	C27-C28-C29-C30
16	N	605	MQ9	C27-C28-C29-C30
16	C	303	MQ9	C17-C18-C19-C20
16	H	607	MQ9	C7-C8-C9-C10
16	H	607	MQ9	C12-C13-C14-C15
16	H	607	MQ9	C17-C18-C19-C20
16	H	608	MQ9	C27-C28-C29-C30
16	H	608	MQ9	C37-C38-C39-C40
16	H	608	MQ9	C42-C43-C44-C45
16	H	609	MQ9	C7-C8-C9-C10
16	O	303	MQ9	C37-C38-C39-C41
16	N	601	MQ9	C27-C28-C29-C31
16	N	605	MQ9	C27-C28-C29-C31
16	C	303	MQ9	C17-C18-C19-C21
16	H	607	MQ9	C7-C8-C9-C11
16	H	607	MQ9	C12-C13-C14-C16
16	H	607	MQ9	C17-C18-C19-C21
16	H	608	MQ9	C27-C28-C29-C31

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Mol	Chain	Res	Type	Atoms
16	H	608	MQ9	C42-C43-C44-C46
17	O	304	WUO	O40-C41-C48-O49
17	W	401	WUO	O15-C14-O13-C12
17	C	304	WUO	O79-C78-O77-C76
21	N	603	CDL	OB9-CB7-OB8-CB6
21	L	607	CDL	OA9-CA7-OA8-CA6
20	H	603	HEM	C4D-C3D-CAD-CBD
23	R	603	HEA	C4D-C3D-CAD-CBD
21	R	605	CDL	OA7-CA5-OA6-CA4
17	I	303	WUO	C21-C22-C23-C24
17	I	303	WUO	O04-C05-C12-O13
21	P	301	CDL	O1-C1-CB2-OB2
21	L	601	CDL	O1-C1-CB2-OB2
19	b	201	9YF	C26-C25-O11-C24
21	G	504	CDL	C71-CB7-OB8-CB6
17	I	303	WUO	O15-C14-O13-C12
21	H	605	CDL	OB9-CB7-OB8-CB6
21	R	605	CDL	C11-CA5-OA6-CA4
21	H	605	CDL	C51-CB5-OB6-CB4
21	L	607	CDL	C11-CA5-OA6-CA4
21	I	302	CDL	OA9-CA7-OA8-CA6
16	H	608	MQ9	C47-C48-C49-C51
17	O	304	WUO	C80-C78-O77-C76
21	L	601	CDL	C31-CA7-OA8-CA6
21	L	607	CDL	C31-CA7-OA8-CA6
16	N	605	MQ9	C45-C44-C46-C47
16	G	501	MQ9	C30-C29-C31-C32
16	H	609	MQ9	C30-C29-C31-C32
23	L	603	HEA	C26-C15-C16-C17
16	N	605	MQ9	C43-C44-C46-C47
16	G	501	MQ9	C12-C11-C9-C8
16	G	501	MQ9	C28-C29-C31-C32
16	H	607	MQ9	C13-C14-C16-C17
16	H	607	MQ9	C23-C24-C26-C27
16	H	608	MQ9	C12-C11-C9-C8
16	H	608	MQ9	C18-C19-C21-C22
16	H	609	MQ9	C28-C29-C31-C32
16	H	609	MQ9	C33-C34-C36-C37
16	H	609	MQ9	C43-C44-C46-C47
23	L	603	HEA	C14-C15-C16-C17
21	G	504	CDL	OB9-CB7-OB8-CB6
16	O	303	MQ9	C14-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
16	O	303	MQ9	C34-C36-C37-C38
16	O	303	MQ9	C39-C41-C42-C43
16	N	601	MQ9	C24-C26-C27-C28
16	N	605	MQ9	C34-C36-C37-C38
16	N	606	MQ9	C19-C21-C22-C23
16	N	606	MQ9	C34-C36-C37-C38
16	N	606	MQ9	C39-C41-C42-C43
16	N	606	MQ9	C44-C46-C47-C48
16	C	303	MQ9	C14-C16-C17-C18
16	G	501	MQ9	C9-C11-C12-C13
16	G	501	MQ9	C29-C31-C32-C33
16	H	602	MQ9	C29-C31-C32-C33
16	H	602	MQ9	C34-C36-C37-C38
16	H	602	MQ9	C39-C41-C42-C43
16	H	607	MQ9	C14-C16-C17-C18
16	H	608	MQ9	C19-C21-C22-C23
16	H	608	MQ9	C24-C26-C27-C28
16	H	608	MQ9	C29-C31-C32-C33
16	H	608	MQ9	C39-C41-C42-C43
16	H	609	MQ9	C39-C41-C42-C43
23	R	602	HEA	C19-C20-C21-C22
23	R	603	HEA	C19-C20-C21-C22
23	L	602	HEA	C19-C20-C21-C22
16	C	303	MQ9	C47-C48-C49-C50
19	b	201	9YF	O12-C25-O11-C24
17	I	303	WUO	C64-C65-C66-C67
21	H	601	CDL	C79-C80-C81-C82
27	R	608	9XX	C3-C4-C5-C6
16	G	501	MQ9	C27-C28-C29-C30
17	O	304	WUO	O79-C78-O77-C76
17	C	304	WUO	C06-C05-C12-O13
17	O	304	WUO	C21-C22-C23-C24
17	C	304	WUO	C64-C65-C66-C67
16	G	501	MQ9	C32-C33-C34-C35
27	b	202	9XX	C18-C19-C20-C21
17	O	304	WUO	C42-C41-C48-O49
17	W	401	WUO	C22-C23-C24-C25
21	H	611	CDL	OB7-CB5-OB6-CB4
21	L	607	CDL	OA7-CA5-OA6-CA4
21	H	605	CDL	CB2-C1-CA2-OA2
21	I	301	CDL	CB2-C1-CA2-OA2
21	L	601	CDL	CB2-C1-CA2-OA2

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Mol	Chain	Res	Type	Atoms
21	L	601	CDL	CA2-C1-CB2-OB2
19	M	502	9YF	C26-C25-O11-C24
17	O	304	WUO	C65-C66-C67-C68
17	W	401	WUO	C24-C25-C26-C27
17	I	303	WUO	C68-C69-C70-C71
27	R	608	9XX	C10-C11-C12-C13
17	O	304	WUO	O04-C05-C12-O13
16	N	605	MQ9	C30-C29-C31-C32
16	G	501	MQ9	C20-C19-C21-C22
16	H	607	MQ9	C12-C11-C9-C10
16	H	607	MQ9	C15-C14-C16-C17
16	H	607	MQ9	C20-C19-C21-C22
16	H	608	MQ9	C20-C19-C21-C22
16	H	608	MQ9	C40-C39-C41-C42
16	H	609	MQ9	C35-C34-C36-C37
16	N	605	MQ9	C28-C29-C31-C32
16	G	501	MQ9	C18-C19-C21-C22
16	H	607	MQ9	C12-C11-C9-C8
16	H	607	MQ9	C18-C19-C21-C22
16	H	608	MQ9	C28-C29-C31-C32
16	H	608	MQ9	C38-C39-C41-C42
16	H	608	MQ9	C47-C48-C49-C50
17	I	303	WUO	C89-C88-C90-C91
19	M	502	9YF	C31-C32-C33-C34
19	M	502	9YF	C34-C33-C35-C36
21	R	605	CDL	CB5-C51-C52-C53
21	L	607	CDL	CA5-C11-C12-C13
21	R	601	CDL	O1-C1-CB2-OB2
21	G	504	CDL	O1-C1-CB2-OB2
21	H	601	CDL	O1-C1-CB2-OB2
17	W	401	WUO	C71-C72-C73-C74
21	H	604	CDL	C57-C58-C59-C60
21	N	604	CDL	C51-CB5-OB6-CB4
21	H	606	CDL	C51-CB5-OB6-CB4
16	N	601	MQ9	C17-C18-C19-C20
16	H	609	MQ9	C27-C28-C29-C30
21	R	601	CDL	CA5-C11-C12-C13
21	H	604	CDL	CB5-C51-C52-C53
21	I	302	CDL	CA5-C11-C12-C13
21	H	605	CDL	OB7-CB5-OB6-CB4
16	N	605	MQ9	C44-C46-C47-C48
16	C	303	MQ9	C9-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
19	M	502	9YF	C11-C10-C9-C8
21	N	604	CDL	CA7-C31-C32-C33
21	N	604	CDL	CB5-C51-C52-C53
21	P	301	CDL	CA5-C11-C12-C13
21	R	601	CDL	CB7-C71-C72-C73
21	H	604	CDL	CB7-C71-C72-C73
21	H	611	CDL	CA7-C31-C32-C33
21	L	601	CDL	CA5-C11-C12-C13
21	L	607	CDL	CA7-C31-C32-C33
27	R	608	9XX	C12-C13-C14-C15
27	H	612	9XX	C18-C19-C20-C21
19	M	502	9YF	O12-C25-O11-C24
22	S	402	7PH	C22-C21-O21-C2
19	W	402	9YF	C33-C35-C36-C37
20	N	602	HEM	C3D-CAD-CBD-CGD
20	H	603	HEM	C3D-CAD-CBD-CGD
17	C	304	WUO	C85-C86-C87-C88
19	G	502	9YF	C30-C31-C32-C33
17	W	401	WUO	C59-C61-C62-C63
17	W	401	WUO	C78-C80-C81-C82
21	T	201	CDL	CA7-C31-C32-C33
21	H	604	CDL	CA7-C31-C32-C33
21	H	606	CDL	CB7-C71-C72-C73
21	H	611	CDL	CA5-C11-C12-C13
21	I	301	CDL	CA7-C31-C32-C33
17	C	304	WUO	C42-C41-C48-O49
17	W	401	WUO	C85-C86-C87-C88
21	R	605	CDL	O1-C1-CA2-OA2
21	H	605	CDL	O1-C1-CA2-OA2
21	H	606	CDL	O1-C1-CA2-OA2
21	H	606	CDL	C71-CB7-OB8-CB6
21	I	301	CDL	CA5-C11-C12-C13
21	L	607	CDL	CB7-C71-C72-C73
21	N	604	CDL	OB7-CB5-OB6-CB4
21	H	606	CDL	OB7-CB5-OB6-CB4
21	H	601	CDL	C77-C78-C79-C80
17	W	401	WUO	C88-C90-C91-C92
16	H	602	MQ9	C15-C14-C16-C17
16	H	602	MQ9	C13-C14-C16-C17
21	N	603	CDL	CA7-C31-C32-C33
21	N	603	CDL	C51-CB5-OB6-CB4
21	H	601	CDL	C11-CA5-OA6-CA4

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Mol	Chain	Res	Type	Atoms
19	W	402	9YF	C11-C10-C9-C8
21	G	504	CDL	CB5-C51-C52-C53
21	H	601	CDL	CB7-C71-C72-C73
22	J	401	7PH	C31-C32-C33-C34
27	b	202	9XX	C27-C28-C29-C30
17	C	304	WUO	O40-C41-C48-O49
21	H	601	CDL	C56-C57-C58-C59
21	H	601	CDL	OA7-CA5-OA6-CA4
22	S	402	7PH	O22-C21-O21-C2
21	R	605	CDL	CB2-C1-CA2-OA2
17	O	304	WUO	C16-C14-O13-C12
21	N	604	CDL	C71-CB7-OB8-CB6
21	G	504	CDL	C31-CA7-OA8-CA6
21	H	604	CDL	C15-C16-C17-C18
22	S	402	7PH	C21-C22-C23-C24
19	M	502	9YF	C30-C31-C32-C33
19	W	402	9YF	C30-C31-C32-C33
19	b	201	9YF	C33-C35-C36-C37
16	O	303	MQ9	C25-C24-C26-C27
16	G	501	MQ9	C32-C33-C34-C36
21	N	603	CDL	C11-CA5-OA6-CA4
21	R	605	CDL	C51-CB5-OB6-CB4
21	L	607	CDL	C51-CB5-OB6-CB4
22	S	401	7PH	C22-C21-O21-C2
21	N	603	CDL	OA7-CA5-OA6-CA4
21	N	603	CDL	OB7-CB5-OB6-CB4
21	R	605	CDL	OB7-CB5-OB6-CB4
21	L	607	CDL	OB7-CB5-OB6-CB4
22	J	401	7PH	C35-C36-C37-C38
21	H	604	CDL	O1-C1-CB2-OB2
21	H	605	CDL	O1-C1-CB2-OB2
21	I	301	CDL	O1-C1-CA2-OA2
15	O	302	HEC	C2A-CAA-CBA-CGA
15	C	302	HEC	C2A-CAA-CBA-CGA
27	Y	302	9XX	C24-C25-C26-C27
22	S	401	7PH	O22-C21-O21-C2
21	P	301	CDL	C11-CA5-OA6-CA4
21	T	201	CDL	C51-CB5-OB6-CB4
21	H	604	CDL	C11-CA5-OA6-CA4
21	I	302	CDL	C11-CA5-OA6-CA4
23	L	603	HEA	O11-C11-C12-C13
16	C	303	MQ9	C26-C27-C28-C29

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Mol	Chain	Res	Type	Atoms
17	C	304	WUO	C16-C14-O13-C12
21	I	302	CDL	CB5-C51-C52-C53
27	R	608	9XX	C18-C19-C20-C21
17	O	304	WUO	O15-C14-O13-C12
21	N	604	CDL	OB9-CB7-OB8-CB6
17	W	401	WUO	C26-C27-C28-C29
21	N	603	CDL	C53-C54-C55-C56
21	R	601	CDL	C11-C12-C13-C14
17	O	304	WUO	C61-C62-C63-C64
17	W	401	WUO	C64-C65-C66-C67
21	N	604	CDL	C14-C15-C16-C17
21	N	604	CDL	C22-C23-C24-C25
21	T	201	CDL	C34-C35-C36-C37
21	H	605	CDL	C53-C54-C55-C56
21	H	605	CDL	C55-C56-C57-C58
21	H	611	CDL	C34-C35-C36-C37
21	I	301	CDL	C17-C18-C19-C20
22	S	401	7PH	C33-C34-C35-C36
17	C	304	WUO	C63-C64-C65-C66
21	P	301	CDL	C75-C76-C77-C78
21	H	606	CDL	OB9-CB7-OB8-CB6
19	W	402	9YF	C18-C19-C20-C21
19	G	502	9YF	C26-C27-C28-C29
21	N	603	CDL	C55-C56-C57-C58
21	N	604	CDL	C73-C74-C75-C76
21	I	301	CDL	C53-C54-C55-C56
21	I	302	CDL	C15-C16-C17-C18
21	L	607	CDL	C55-C56-C57-C58
22	J	401	7PH	C25-C26-C27-C28
27	R	608	9XX	C11-C12-C13-C14
21	P	301	CDL	OA7-CA5-OA6-CA4
17	O	304	WUO	C82-C83-C84-C85
17	C	304	WUO	C19-C20-C21-C22
17	I	303	WUO	C91-C92-C93-C94
19	W	402	9YF	C13-C14-C15-C16
19	b	201	9YF	C12-C13-C14-C15
21	P	301	CDL	C52-C53-C54-C55
22	J	401	7PH	C33-C34-C35-C36
22	J	401	7PH	C34-C35-C36-C37
21	H	611	CDL	CB5-C51-C52-C53
21	R	601	CDL	C31-C32-C33-C34
16	N	601	MQ9	C17-C18-C19-C21

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Mol	Chain	Res	Type	Atoms
16	G	501	MQ9	C27-C28-C29-C31
21	N	604	CDL	C75-C76-C77-C78
21	G	504	CDL	C74-C75-C76-C77
21	H	601	CDL	C71-C72-C73-C74
21	H	601	CDL	C76-C77-C78-C79
27	b	202	9XX	C11-C12-C13-C14
21	I	301	CDL	C51-CB5-OB6-CB4
19	M	502	9YF	C39-C40-C41-C42
21	P	301	CDL	C12-C13-C14-C15
19	G	502	9YF	C15-C16-C17-C18
21	H	606	CDL	C56-C57-C58-C59
21	H	606	CDL	C74-C75-C76-C77
21	L	601	CDL	C80-C81-C82-C83
21	R	601	CDL	CB5-C51-C52-C53
21	H	601	CDL	CB5-C51-C52-C53
22	S	401	7PH	C21-C22-C23-C24
17	O	304	WUO	C19-C20-C21-C22
17	O	304	WUO	C20-C21-C22-C23
17	O	304	WUO	C62-C63-C64-C65
17	C	304	WUO	C23-C24-C25-C26
17	I	303	WUO	C26-C27-C28-C29
21	N	604	CDL	C54-C55-C56-C57
21	P	301	CDL	C59-C60-C61-C62
21	T	201	CDL	C12-C13-C14-C15
21	H	606	CDL	C75-C76-C77-C78
17	W	401	WUO	C19-C20-C21-C22
21	N	604	CDL	C74-C75-C76-C77
21	H	604	CDL	C52-C53-C54-C55
21	H	606	CDL	C77-C78-C79-C80
21	N	603	CDL	C13-C14-C15-C16
21	G	504	CDL	C32-C33-C34-C35
19	b	201	9YF	C30-C31-C32-C33
21	G	504	CDL	OA9-CA7-OA8-CA6
19	G	502	9YF	C13-C14-C15-C16
21	I	301	CDL	C75-C76-C77-C78
21	I	302	CDL	OA7-CA5-OA6-CA4
17	C	304	WUO	C69-C70-C71-C72
21	H	611	CDL	C12-C13-C14-C15
16	H	609	MQ9	C19-C21-C22-C23
17	W	401	WUO	C25-C26-C27-C28
17	W	401	WUO	C66-C67-C68-C69
17	W	401	WUO	C67-C68-C69-C70

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Mol	Chain	Res	Type	Atoms
19	b	201	9YF	C9-C10-C11-C12
21	N	604	CDL	C56-C57-C58-C59
21	H	606	CDL	C18-C19-C20-C21
21	H	611	CDL	C55-C56-C57-C58
21	I	302	CDL	C36-C37-C38-C39
27	b	202	9XX	C21-C22-C23-C24
17	W	401	WUO	C14-C16-C17-C18
21	H	606	CDL	CB5-C51-C52-C53
21	L	601	CDL	CB7-C71-C72-C73
17	O	304	WUO	C91-C92-C93-C94
17	I	303	WUO	C20-C21-C22-C23
19	G	502	9YF	C37-C38-C39-C40
21	R	605	CDL	C52-C53-C54-C55
21	G	504	CDL	C73-C74-C75-C76
21	H	604	CDL	C77-C78-C79-C80
21	H	605	CDL	C37-C38-C39-C40
21	I	302	CDL	C34-C35-C36-C37
21	L	601	CDL	C31-C32-C33-C34
21	L	607	CDL	C73-C74-C75-C76
27	R	608	9XX	C22-C23-C24-C25
17	C	304	WUO	O15-C14-O13-C12
21	L	601	CDL	C53-C54-C55-C56
21	G	504	CDL	C55-C56-C57-C58
21	H	604	CDL	C56-C57-C58-C59
21	H	611	CDL	C57-C58-C59-C60
21	I	302	CDL	C17-C18-C19-C20
16	C	303	MQ9	C27-C28-C29-C30
17	W	401	WUO	C61-C62-C63-C64
19	b	201	9YF	C11-C12-C13-C14
21	P	301	CDL	C13-C14-C15-C16
21	L	601	CDL	C71-C72-C73-C74
17	W	401	WUO	C61-C59-O58-C57
19	G	502	9YF	C28-C29-C30-C31
21	N	604	CDL	C55-C56-C57-C58
21	L	601	CDL	C78-C79-C80-C81
17	C	304	WUO	C16-C17-C18-C19
17	C	304	WUO	C93-C94-C95-C96
21	H	601	CDL	C54-C55-C56-C57
21	H	604	CDL	C78-C79-C80-C81
21	H	605	CDL	C31-C32-C33-C34
21	N	603	CDL	CB5-C51-C52-C53
27	Y	302	9XX	C9-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
27	H	612	9XX	C23-C24-C25-C26
28	W	403	PLM	C3-C4-C5-C6
19	G	502	9YF	C9-C10-C11-C12
21	T	201	CDL	OB7-CB5-OB6-CB4
21	H	604	CDL	OA7-CA5-OA6-CA4
21	I	301	CDL	OB7-CB5-OB6-CB4
16	G	501	MQ9	C25-C24-C26-C27
17	W	401	WUO	C21-C22-C23-C24
19	M	502	9YF	C28-C29-C30-C31
21	N	603	CDL	C17-C18-C19-C20
21	N	603	CDL	C52-C53-C54-C55
21	P	301	CDL	C34-C35-C36-C37
21	R	605	CDL	C54-C55-C56-C57
21	G	504	CDL	C33-C34-C35-C36
22	S	401	7PH	C32-C33-C34-C35
27	R	608	9XX	C20-C21-C22-C23
21	H	606	CDL	C73-C74-C75-C76
21	I	301	CDL	C57-C58-C59-C60
21	L	601	CDL	C32-C33-C34-C35
19	M	502	9YF	C29-C30-C31-C32
19	b	201	9YF	C14-C15-C16-C17
21	G	504	CDL	C31-C32-C33-C34
21	H	605	CDL	C54-C55-C56-C57
21	H	611	CDL	C82-C83-C84-C85
21	I	301	CDL	C73-C74-C75-C76
27	b	202	9XX	C11-C10-C9-C8
21	P	301	CDL	C72-C73-C74-C75
21	R	605	CDL	C37-C38-C39-C40
22	S	401	7PH	C27-C28-C29-C2A
19	b	201	9YF	C28-C29-C30-C31
21	P	301	CDL	C14-C15-C16-C17
21	G	504	CDL	C54-C55-C56-C57
21	H	606	CDL	C76-C77-C78-C79
22	J	401	7PH	C36-C37-C38-C39
27	H	612	9XX	C9-C10-C11-C12
17	O	304	WUO	C64-C65-C66-C67
21	R	605	CDL	C33-C34-C35-C36
21	H	604	CDL	C17-C18-C19-C20
19	G	502	9YF	C9-C8-O9-C
21	T	201	CDL	C11-CA5-OA6-CA4
21	H	605	CDL	C11-CA5-OA6-CA4
21	L	607	CDL	C56-C57-C58-C59

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Mol	Chain	Res	Type	Atoms
20	N	607	HEM	C4D-C3D-CAD-CBD
21	H	605	CDL	OA7-CA5-OA6-CA4
17	W	401	WUO	C82-C83-C84-C85
21	R	605	CDL	C74-C75-C76-C77
21	H	611	CDL	C15-C16-C17-C18
21	L	607	CDL	C38-C39-C40-C41
17	I	303	WUO	C94-C95-C96-C97
17	C	304	WUO	C84-C85-C86-C87
21	H	611	CDL	C51-C52-C53-C54
21	R	605	CDL	CA7-C31-C32-C33
17	O	304	WUO	C16-C17-C18-C19
17	W	401	WUO	C80-C81-C82-C83
21	N	604	CDL	C11-C12-C13-C14
21	N	604	CDL	C18-C19-C20-C21
20	N	607	HEM	C2D-C3D-CAD-CBD
17	O	304	WUO	C67-C68-C69-C70
22	S	402	7PH	C35-C36-C37-C38
22	J	401	7PH	C28-C29-C2A-C2B
19	b	201	9YF	C13-C14-C15-C16
16	N	606	MQ9	C15-C14-C16-C17
16	C	303	MQ9	C40-C39-C41-C42
21	G	504	CDL	C35-C36-C37-C38
21	H	605	CDL	C17-C18-C19-C20
21	I	301	CDL	C51-C52-C53-C54
21	I	301	CDL	C71-C72-C73-C74
21	G	504	CDL	C52-C53-C54-C55
21	H	604	CDL	C73-C74-C75-C76
21	G	504	CDL	C51-C52-C53-C54
16	C	303	MQ9	C19-C21-C22-C23
20	H	603	HEM	C4B-C3B-CAB-CBB
21	P	301	CDL	C38-C39-C40-C41
19	b	201	9YF	C35-C36-C37-C38
21	T	201	CDL	C76-C77-C78-C79
21	H	604	CDL	C13-C14-C15-C16
22	S	402	7PH	C38-C39-C3A-C3B
21	H	605	CDL	CA7-C31-C32-C33
27	H	612	9XX	C12-C13-C14-C15
17	O	304	WUO	C70-C71-C72-C73
17	I	303	WUO	C18-C19-C20-C21
17	I	303	WUO	C80-C81-C82-C83
21	L	607	CDL	C13-C14-C15-C16
17	W	401	WUO	C62-C63-C64-C65

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Mol	Chain	Res	Type	Atoms
17	W	401	WUO	C92-C93-C94-C95
21	R	605	CDL	C32-C33-C34-C35
21	G	504	CDL	C77-C78-C79-C80
21	L	607	CDL	C75-C76-C77-C78
27	b	202	9XX	C7-C8-C9-C10
17	C	304	WUO	O04-C05-C12-O13
22	S	401	7PH	C32-C31-O31-C3
21	R	601	CDL	C37-C38-C39-C40
19	M	502	9YF	C13-C14-C15-C16
21	R	605	CDL	C75-C76-C77-C78
21	H	601	CDL	C53-C54-C55-C56
21	H	611	CDL	C11-C12-C13-C14
21	N	604	CDL	C77-C78-C79-C80
21	R	601	CDL	C13-C14-C15-C16
21	H	606	CDL	C19-C20-C21-C22
21	H	606	CDL	C1-CB2-OB2-PB2
21	N	604	CDL	C53-C54-C55-C56
21	R	605	CDL	C34-C35-C36-C37
21	R	605	CDL	C51-C52-C53-C54
21	I	301	CDL	C31-C32-C33-C34
19	M	502	9YF	C17-C18-C19-C20
16	C	303	MQ9	C38-C39-C41-C42
21	T	201	CDL	OA7-CA5-OA6-CA4
21	N	604	CDL	C71-C72-C73-C74
21	T	201	CDL	C52-C53-C54-C55
21	H	605	CDL	C51-C52-C53-C54
21	N	603	CDL	C56-C57-C58-C59
21	H	604	CDL	C75-C76-C77-C78
22	S	402	7PH	C27-C28-C29-C2A
19	b	201	9YF	C29-C30-C31-C32
21	R	605	CDL	C13-C14-C15-C16
21	H	605	CDL	C56-C57-C58-C59
17	O	304	WUO	C22-C23-C24-C25
27	b	202	9XX	C10-C11-C12-C13
21	H	611	CDL	C76-C77-C78-C79
21	L	607	CDL	C71-C72-C73-C74
21	R	605	CDL	C15-C16-C17-C18
19	M	502	9YF	C20-C21-C22-C23
21	I	301	CDL	C72-C73-C74-C75
19	M	502	9YF	C35-C36-C37-C38
21	R	601	CDL	C53-C54-C55-C56
19	W	402	9YF	C24-C-C1-O

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Mol	Chain	Res	Type	Atoms
21	G	504	CDL	OA5-CA3-CA4-CA6
21	H	605	CDL	OB5-CB3-CB4-CB6
21	I	301	CDL	OA5-CA3-CA4-CA6
17	W	401	WUO	O60-C59-O58-C57
19	G	502	9YF	O10-C8-O9-C
21	R	605	CDL	C11-C12-C13-C14
22	J	401	7PH	C37-C38-C39-C3A
21	I	301	CDL	C14-C15-C16-C17
17	C	304	WUO	C59-C61-C62-C63
21	T	201	CDL	CB7-C71-C72-C73
21	H	611	CDL	CB7-C71-C72-C73
21	H	604	CDL	C79-C80-C81-C82
21	I	302	CDL	C31-C32-C33-C34
21	T	201	CDL	C51-C52-C53-C54
21	H	611	CDL	C52-C53-C54-C55
21	I	302	CDL	C35-C36-C37-C38
17	W	401	WUO	C86-C87-C88-C89
17	C	304	WUO	C90-C91-C92-C93
21	I	301	CDL	C56-C57-C58-C59
21	I	302	CDL	C56-C57-C58-C59
21	T	201	CDL	CB5-C51-C52-C53
19	M	502	9YF	C27-C28-C29-C30
21	G	504	CDL	C82-C83-C84-C85
17	W	401	WUO	C16-C17-C18-C19
19	G	502	9YF	C18-C19-C20-C21
17	I	303	WUO	C85-C86-C87-C88
21	N	603	CDL	CA3-CA4-CA6-OA8
21	N	603	CDL	CB3-CB4-CB6-OB8
21	P	301	CDL	CA3-CA4-CA6-OA8
21	G	504	CDL	CB3-CB4-CB6-OB8
21	H	601	CDL	CB3-CB4-CB6-OB8
21	H	605	CDL	CA3-CA4-CA6-OA8
21	H	606	CDL	CB3-CB4-CB6-OB8
19	G	502	9YF	C29-C30-C31-C32
19	G	502	9YF	C36-C37-C38-C39
21	L	607	CDL	C57-C58-C59-C60
21	H	606	CDL	C53-C54-C55-C56
22	S	402	7PH	C33-C34-C35-C36
22	J	401	7PH	C23-C24-C25-C26
21	H	604	CDL	C51-C52-C53-C54
21	H	606	CDL	C72-C73-C74-C75
21	L	601	CDL	C13-C14-C15-C16

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Mol	Chain	Res	Type	Atoms
17	I	303	WUO	C92-C93-C94-C95
21	L	601	CDL	C76-C77-C78-C79
21	N	604	CDL	C19-C20-C21-C22
17	I	303	WUO	C19-C20-C21-C22
21	N	604	CDL	C12-C13-C14-C15
22	S	401	7PH	O32-C31-O31-C3
16	N	601	MQ9	C13-C14-C16-C17
19	G	502	9YF	C14-C15-C16-C17
17	I	303	WUO	C93-C94-C95-C96
17	O	304	WUO	C68-C69-C70-C71
17	C	304	WUO	C81-C82-C83-C84
17	I	303	WUO	C62-C63-C64-C65
19	W	402	9YF	C36-C37-C38-C39
21	R	601	CDL	C12-C13-C14-C15
21	H	606	CDL	C51-C52-C53-C54
21	I	302	CDL	C32-C33-C34-C35
27	R	608	9XX	C5-C6-C7-C8
22	J	401	7PH	C1-O11-P-O14
21	N	603	CDL	C12-C13-C14-C15
21	T	201	CDL	C31-C32-C33-C34
27	R	608	9XX	C28-C29-C30-C31
27	H	612	9XX	C6-C7-C8-C9
21	R	601	CDL	C16-C17-C18-C19
17	W	401	WUO	C76-C57-O58-C59
21	N	604	CDL	CA6-CA4-OA6-CA5
21	L	607	CDL	CA3-CA4-OA6-CA5
19	W	402	9YF	C38-C39-C40-C41
21	T	201	CDL	C78-C79-C80-C81
21	R	601	CDL	C75-C76-C77-C78
21	R	605	CDL	C17-C18-C19-C20
21	L	601	CDL	C52-C53-C54-C55
17	C	304	WUO	C88-C90-C91-C92
19	G	502	9YF	C33-C35-C36-C37
19	G	502	9YF	C12-C13-C14-C15
21	T	201	CDL	C57-C58-C59-C60
21	H	601	CDL	C13-C14-C15-C16
21	I	302	CDL	C73-C74-C75-C76
19	b	201	9YF	C10-C11-C12-C13
21	G	504	CDL	C83-C84-C85-C86
21	H	605	CDL	CA2-C1-CB2-OB2
21	T	201	CDL	OB5-CB3-CB4-OB6
21	R	601	CDL	OB5-CB3-CB4-OB6

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Mol	Chain	Res	Type	Atoms
19	b	201	9YF	C19-C20-C21-C22
21	I	301	CDL	C31-CA7-OA8-CA6
17	W	401	WUO	C20-C21-C22-C23
19	M	502	9YF	C9-C10-C11-C12
21	T	201	CDL	C53-C54-C55-C56
21	I	302	CDL	C12-C13-C14-C15
27	Y	302	9XX	C19-C20-C21-C22
16	C	303	MQ9	C25-C24-C26-C27
17	I	303	WUO	C63-C64-C65-C66
21	P	301	CDL	C51-C52-C53-C54
21	R	601	CDL	C17-C18-C19-C20
27	H	612	9XX	C20-C21-C22-C23
19	W	402	9YF	C37-C38-C39-C40
28	L	608	PLM	C5-C6-C7-C8
21	G	504	CDL	C36-C37-C38-C39
21	N	604	CDL	O1-C1-CB2-OB2
21	N	603	CDL	C57-C58-C59-C60
21	H	604	CDL	C31-C32-C33-C34
27	H	612	9XX	C10-C11-C12-C13
21	L	607	CDL	C71-CB7-OB8-CB6
21	L	601	CDL	C72-C73-C74-C75
21	I	301	CDL	C60-C61-C62-C63
19	G	502	9YF	C17-C18-C19-C20
21	H	611	CDL	C78-C79-C80-C81
21	N	603	CDL	C39-C40-C41-C42
17	W	401	WUO	C65-C66-C67-C68
21	H	601	CDL	C15-C16-C17-C18
21	H	604	CDL	C59-C60-C61-C62
16	O	303	MQ9	C29-C31-C32-C33
16	H	609	MQ9	C24-C26-C27-C28
21	I	302	CDL	C11-C12-C13-C14
21	I	302	CDL	C75-C76-C77-C78
19	W	402	9YF	C26-C25-O11-C24
27	H	612	9XX	C19-C18-O1-C17
16	H	609	MQ9	C17-C18-C19-C20
17	C	304	WUO	C91-C92-C93-C94
21	N	604	CDL	C24-C25-C26-C27
21	R	605	CDL	C60-C61-C62-C63
21	H	605	CDL	C39-C40-C41-C42
16	H	602	MQ9	C25-C24-C26-C27
21	R	601	CDL	C39-C40-C41-C42
21	P	301	CDL	C33-C34-C35-C36

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Mol	Chain	Res	Type	Atoms
21	I	301	CDL	C33-C34-C35-C36
17	I	303	WUO	C82-C83-C84-C85
17	O	304	WUO	C89-C88-C90-C91
17	C	304	WUO	C89-C88-C90-C91
19	b	201	9YF	C31-C32-C33-C34
21	R	601	CDL	C72-C73-C74-C75
21	I	301	CDL	CA4-CA3-OA5-PA1
21	L	607	CDL	C76-C77-C78-C79
21	I	301	CDL	C38-C39-C40-C41
22	J	401	7PH	C22-C23-C24-C25
27	R	608	9XX	C4-C5-C6-C7
27	H	612	9XX	C19-C20-C21-C22
17	O	304	WUO	C69-C70-C71-C72
17	O	304	WUO	C83-C84-C85-C86
21	N	603	CDL	C37-C38-C39-C40
21	P	301	CDL	C17-C18-C19-C20
21	H	605	CDL	C13-C14-C15-C16
21	L	607	CDL	C16-C17-C18-C19
27	Y	302	9XX	C21-C22-C23-C24
17	O	304	WUO	O55-C56-C57-C76
21	R	601	CDL	OB5-CB3-CB4-CB6
21	I	301	CDL	OB5-CB3-CB4-CB6
21	R	601	CDL	C51-C52-C53-C54
17	W	401	WUO	C27-C28-C29-C30
17	C	304	WUO	C87-C88-C90-C91
21	N	604	CDL	C79-C80-C81-C82
21	G	504	CDL	CA7-C31-C32-C33
17	I	303	WUO	C27-C28-C29-C30
21	L	601	CDL	C17-C18-C19-C20
17	I	303	WUO	C16-C17-C18-C19
17	C	304	WUO	C67-C68-C69-C70
22	S	402	7PH	C39-C3A-C3B-C3C
21	L	607	CDL	C31-C32-C33-C34
21	H	605	CDL	C60-C61-C62-C63
27	H	612	9XX	C27-C28-C29-C30
21	H	604	CDL	C18-C19-C20-C21
27	Y	302	9XX	C10-C11-C12-C13
17	W	401	WUO	C23-C24-C25-C26
19	W	402	9YF	C12-C13-C14-C15
21	N	604	CDL	C17-C18-C19-C20
21	H	606	CDL	C34-C35-C36-C37
21	H	606	CDL	CA2-C1-CB2-OB2

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Mol	Chain	Res	Type	Atoms
21	I	302	CDL	C39-C40-C41-C42
21	H	601	CDL	C71-CB7-OB8-CB6
19	b	201	9YF	C36-C37-C38-C39
21	H	606	CDL	C17-C18-C19-C20
17	O	304	WUO	C56-C57-C76-O77
19	G	502	9YF	C1-C-C24-O11
19	b	201	9YF	C1-C-C24-O11
21	T	201	CDL	CB3-CB4-CB6-OB8
21	H	604	CDL	CB3-CB4-CB6-OB8
21	H	605	CDL	CB3-CB4-CB6-OB8
21	R	605	CDL	C18-C19-C20-C21
17	W	401	WUO	C91-C92-C93-C94
21	N	604	CDL	C15-C16-C17-C18
21	H	604	CDL	C11-C12-C13-C14
21	H	604	CDL	C72-C73-C74-C75
21	G	504	CDL	C12-C13-C14-C15
21	H	611	CDL	C14-C15-C16-C17
21	L	607	CDL	C58-C59-C60-C61
16	N	601	MQ9	C15-C14-C16-C17
21	N	603	CDL	CA5-C11-C12-C13
27	Y	302	9XX	O-C16-C17-O1
17	I	303	WUO	C69-C70-C71-C72
19	W	402	9YF	O9-C-C1-O
21	H	611	CDL	OA5-CA3-CA4-OA6
19	M	502	9YF	C37-C38-C39-C40
21	N	603	CDL	C73-C74-C75-C76
21	N	604	CDL	C1-CB2-OB2-PB2
27	R	608	9XX	C-C1-C2-C3
21	I	301	CDL	OA9-CA7-OA8-CA6
22	S	402	7PH	C32-C33-C34-C35
17	O	304	WUO	O58-C57-C76-O77
17	C	304	WUO	O58-C57-C76-O77
19	b	201	9YF	O9-C-C24-O11
17	I	303	WUO	C14-C16-C17-C18
16	G	501	MQ9	C23-C24-C26-C27
28	L	608	PLM	C7-C8-C9-CA
17	O	304	WUO	C31-C01-O02-C03
19	M	502	9YF	C15-C16-C17-C18
21	P	301	CDL	C56-C57-C58-C59
19	M	502	9YF	C40-C41-C42-C43
21	G	504	CDL	CB7-C71-C72-C73
19	G	502	9YF	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
21	H	601	CDL	C75-C76-C77-C78
27	Y	302	9XX	C36-C27-C28-C29
19	W	402	9YF	C29-C30-C31-C32
21	L	607	CDL	C54-C55-C56-C57
17	O	304	WUO	C90-C91-C92-C93
17	I	303	WUO	C17-C18-C19-C20
17	I	303	WUO	C81-C82-C83-C84
21	N	603	CDL	C54-C55-C56-C57
19	W	402	9YF	C40-C41-C42-C43
17	I	303	WUO	C90-C91-C92-C93
21	L	601	CDL	C34-C35-C36-C37
16	O	303	MQ9	C44-C46-C47-C48
16	N	605	MQ9	C9-C11-C12-C13
16	C	303	MQ9	C24-C26-C27-C28
21	R	601	CDL	C71-C72-C73-C74
21	L	607	CDL	C36-C37-C38-C39
21	H	611	CDL	C17-C18-C19-C20
21	I	301	CDL	C12-C13-C14-C15
21	N	603	CDL	CB2-C1-CA2-OA2
21	R	601	CDL	CB2-C1-CA2-OA2
21	R	605	CDL	CA2-C1-CB2-OB2
21	H	606	CDL	C13-C14-C15-C16
27	H	612	9XX	C22-C23-C24-C25
22	S	401	7PH	C34-C35-C36-C37
21	N	604	CDL	OA5-CA3-CA4-CA6
21	T	201	CDL	OA5-CA3-CA4-CA6
21	G	504	CDL	OB5-CB3-CB4-CB6
21	H	611	CDL	OA5-CA3-CA4-CA6
22	S	401	7PH	O11-C1-C2-C3
22	S	402	7PH	O11-C1-C2-C3
21	H	601	CDL	C72-C73-C74-C75
17	I	303	WUO	C87-C88-C90-C91
27	Y	302	9XX	C26-C27-C28-C29
27	b	202	9XX	C26-C27-C28-C29
21	I	302	CDL	CB7-C71-C72-C73
28	W	403	PLM	C4-C5-C6-C7
21	H	605	CDL	C73-C74-C75-C76
21	H	611	CDL	C72-C73-C74-C75
21	L	607	CDL	C52-C53-C54-C55
21	P	301	CDL	C18-C19-C20-C21
16	G	501	MQ9	C5-C6-C7-C8
16	H	608	MQ9	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
21	I	302	CDL	C38-C39-C40-C41
27	R	608	9XX	C27-C28-C29-C30
21	T	201	CDL	C13-C14-C15-C16
21	P	301	CDL	C35-C36-C37-C38
21	L	601	CDL	C79-C80-C81-C82
16	H	608	MQ9	C35-C34-C36-C37
19	W	402	9YF	O12-C25-O11-C24
21	N	603	CDL	CB7-C71-C72-C73
21	I	301	CDL	C39-C40-C41-C42
22	S	401	7PH	C26-C27-C28-C29
21	R	605	CDL	CA3-CA4-OA6-CA5
21	L	607	CDL	OB9-CB7-OB8-CB6
22	J	401	7PH	C2B-C2C-C2D-C2E
22	S	401	7PH	C37-C38-C39-C3A
27	H	612	9XX	O2-C18-O1-C17
21	P	301	CDL	OA5-CA3-CA4-OA6
21	T	201	CDL	OA5-CA3-CA4-OA6
21	G	504	CDL	OB5-CB3-CB4-OB6
21	I	301	CDL	OB5-CB3-CB4-OB6
21	L	601	CDL	OB5-CB3-CB4-OB6
21	L	607	CDL	OB5-CB3-CB4-OB6
22	S	401	7PH	O11-C1-C2-O21
22	S	402	7PH	O11-C1-C2-O21
16	H	602	MQ9	C14-C16-C17-C18
21	N	604	CDL	CA3-CA4-CA6-OA8
21	R	605	CDL	CA3-CA4-CA6-OA8
21	H	604	CDL	C14-C15-C16-C17
21	H	606	CDL	C12-C13-C14-C15
23	R	603	HEA	C26-C15-C16-C17
16	O	303	MQ9	C23-C24-C26-C27
16	N	606	MQ9	C13-C14-C16-C17
16	G	501	MQ9	C1-C6-C7-C8
16	H	608	MQ9	C1-C6-C7-C8
21	H	605	CDL	C76-C77-C78-C79
19	G	502	9YF	O9-C-C24-O11
21	H	601	CDL	OB6-CB4-CB6-OB8
21	H	605	CDL	OA6-CA4-CA6-OA8
21	H	605	CDL	OB6-CB4-CB6-OB8
21	H	606	CDL	OB6-CB4-CB6-OB8
21	I	301	CDL	OA6-CA4-CA6-OA8
19	W	402	9YF	C31-C32-C33-C34
27	b	202	9XX	C36-C27-C28-C29

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Mol	Chain	Res	Type	Atoms
17	I	303	WUO	C22-C23-C24-C25
17	O	304	WUO	C23-C24-C25-C26
21	T	201	CDL	C54-C55-C56-C57
21	T	201	CDL	C75-C76-C77-C78
21	T	201	CDL	C83-C84-C85-C86
21	G	504	CDL	C78-C79-C80-C81
17	C	304	WUO	C31-C01-O02-C03
19	W	402	9YF	C2-O2-P-O8
17	C	304	WUO	C26-C27-C28-C29
21	H	601	CDL	CA2-C1-CB2-OB2
21	H	604	CDL	CA2-C1-CB2-OB2
17	W	401	WUO	C70-C71-C72-C73
21	G	504	CDL	C71-C72-C73-C74
21	L	607	CDL	C18-C19-C20-C21
28	L	608	PLM	C1-C2-C3-C4
21	R	601	CDL	C51-CB5-OB6-CB4
19	W	402	9YF	C39-C40-C41-C42
17	O	304	WUO	C50-C01-O02-C03
16	H	602	MQ9	C20-C19-C21-C22
17	C	304	WUO	C92-C93-C94-C95
21	N	604	CDL	C16-C17-C18-C19
21	N	603	CDL	C76-C77-C78-C79
21	H	611	CDL	C33-C34-C35-C36
21	P	301	CDL	CA7-C31-C32-C33
21	T	201	CDL	OB5-CB3-CB4-CB6
21	I	302	CDL	OB5-CB3-CB4-CB6
21	L	607	CDL	OB5-CB3-CB4-CB6
21	I	302	CDL	C51-CB5-OB6-CB4
21	R	601	CDL	OB7-CB5-OB6-CB4
21	I	302	CDL	OB7-CB5-OB6-CB4
21	R	605	CDL	C53-C54-C55-C56
17	W	401	WUO	C42-C41-C48-O49
17	W	401	WUO	C87-C88-C90-C91
27	R	608	9XX	C25-C26-C27-C28
27	H	612	9XX	C26-C27-C28-C29
21	H	606	CDL	O1-C1-CB2-OB2
21	I	301	CDL	C52-C53-C54-C55
21	P	301	CDL	CA4-CA3-OA5-PA1
21	P	301	CDL	C71-C72-C73-C74
22	J	401	7PH	C26-C27-C28-C29
15	O	301	HEC	C4B-C3B-CAB-CBB
15	O	301	HEC	C4C-C3C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
15	C	301	HEC	C4B-C3B-CAB-CBB
15	C	301	HEC	C4C-C3C-CAC-CBC
21	H	611	CDL	C81-C82-C83-C84
21	N	604	CDL	OA5-CA3-CA4-OA6
21	H	605	CDL	OB5-CB3-CB4-OB6
21	I	301	CDL	OA5-CA3-CA4-OA6
21	N	604	CDL	C52-C53-C54-C55
23	R	602	HEA	C4A-C3A-CMA-OMA
23	R	603	HEA	C4A-C3A-CMA-OMA
23	L	602	HEA	C4A-C3A-CMA-OMA
17	O	304	WUO	C24-C25-C26-C27
21	N	604	CDL	C51-C52-C53-C54
22	J	401	7PH	C29-C2A-C2B-C2C
23	L	603	HEA	C4D-C3D-CAD-CBD
21	G	504	CDL	C81-C82-C83-C84
21	N	603	CDL	OA6-CA4-CA6-OA8
21	N	604	CDL	OA6-CA4-CA6-OA8
21	T	201	CDL	OB6-CB4-CB6-OB8
21	R	605	CDL	OB6-CB4-CB6-OB8
21	H	604	CDL	OB6-CB4-CB6-OB8
21	I	302	CDL	OB6-CB4-CB6-OB8
21	I	302	CDL	C59-C60-C61-C62
17	C	304	WUO	C56-C57-C76-O77
21	H	611	CDL	CB3-CB4-CB6-OB8
21	I	301	CDL	CA3-CA4-CA6-OA8
21	I	302	CDL	CB3-CB4-CB6-OB8
19	M	502	9YF	C12-C13-C14-C15
21	H	601	CDL	OB9-CB7-OB8-CB6
21	I	301	CDL	C36-C37-C38-C39
21	L	601	CDL	CA7-C31-C32-C33
27	Y	302	9XX	C12-C13-C14-C15
17	I	303	WUO	C50-C37-O38-C39
19	G	502	9YF	C16-C17-C18-C19
17	I	303	WUO	C88-C90-C91-C92
15	O	301	HEC	C2B-C3B-CAB-CBB
15	O	302	HEC	C2C-C3C-CAC-CBC
15	C	301	HEC	C2B-C3B-CAB-CBB
15	C	302	HEC	C2C-C3C-CAC-CBC
19	M	502	9YF	C1-O-P-O8
19	W	402	9YF	C1-O-P-O1
21	N	603	CDL	CA3-OA5-PA1-OA2
21	N	603	CDL	CA3-OA5-PA1-OA4

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Mol	Chain	Res	Type	Atoms
21	N	603	CDL	CB3-OB5-PB2-OB2
21	N	604	CDL	CA3-OA5-PA1-OA4
21	N	604	CDL	CB3-OB5-PB2-OB2
21	P	301	CDL	CA3-OA5-PA1-OA3
21	T	201	CDL	CA2-OA2-PA1-OA5
21	R	601	CDL	CB2-OB2-PB2-OB4
21	H	601	CDL	CA3-OA5-PA1-OA3
21	H	601	CDL	CB3-OB5-PB2-OB4
21	H	604	CDL	CA2-OA2-PA1-OA3
21	H	604	CDL	CA3-OA5-PA1-OA3
21	H	604	CDL	CB3-OB5-PB2-OB4
21	H	605	CDL	CA3-OA5-PA1-OA4
21	H	606	CDL	CA2-OA2-PA1-OA3
21	H	606	CDL	CA3-OA5-PA1-OA2
21	H	606	CDL	CA3-OA5-PA1-OA3
21	H	606	CDL	CB2-OB2-PB2-OB3
21	H	606	CDL	CB2-OB2-PB2-OB5
21	H	611	CDL	CB3-OB5-PB2-OB2
21	H	611	CDL	CB3-OB5-PB2-OB3
21	H	611	CDL	CB3-OB5-PB2-OB4
21	L	601	CDL	CA2-OA2-PA1-OA4
21	L	601	CDL	CB2-OB2-PB2-OB3
21	L	607	CDL	CB2-OB2-PB2-OB3
21	L	607	CDL	CB2-OB2-PB2-OB5
21	L	607	CDL	CB3-OB5-PB2-OB4
27	Y	302	9XX	C16-C17-O1-C18
27	H	612	9XX	C16-C17-O1-C18
16	N	606	MQ9	C12-C11-C9-C10
22	S	401	7PH	C24-C25-C26-C27
16	H	602	MQ9	C23-C24-C26-C27
21	H	606	CDL	C52-C53-C54-C55
21	P	301	CDL	C1-CB2-OB2-PB2
21	P	301	CDL	CB4-CB3-OB5-PB2
21	H	611	CDL	CB4-CB3-OB5-PB2
21	R	605	CDL	CA5-C11-C12-C13
21	I	302	CDL	CA7-C31-C32-C33
21	H	604	CDL	C12-C13-C14-C15
21	H	604	CDL	C80-C81-C82-C83
21	G	504	CDL	C76-C77-C78-C79
21	G	504	CDL	C79-C80-C81-C82
22	S	402	7PH	C29-C2A-C2B-C2C
17	I	303	WUO	C83-C84-C85-C86

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Mol	Chain	Res	Type	Atoms
17	C	304	WUO	C50-C01-O02-C03
21	H	611	CDL	C71-C72-C73-C74
21	H	604	CDL	O1-C1-CA2-OA2
17	C	304	WUO	C76-C57-O58-C59
21	R	605	CDL	CB6-CB4-OB6-CB5
21	H	606	CDL	CA3-CA4-OA6-CA5
21	H	606	CDL	CB6-CB4-OB6-CB5
21	L	607	CDL	CB3-CB4-OB6-CB5
21	P	301	CDL	OA5-CA3-CA4-CA6
21	H	604	CDL	OA5-CA3-CA4-CA6
21	L	601	CDL	OB5-CB3-CB4-CB6
21	T	201	CDL	C58-C59-C60-C61
27	H	612	9XX	C36-C27-C28-C29
19	W	402	9YF	C9-C10-C11-C12
21	N	604	CDL	CA2-C1-CB2-OB2
21	L	601	CDL	C51-C52-C53-C54
19	M	502	9YF	C38-C39-C40-C41
17	O	304	WUO	O58-C59-C61-C62
16	C	303	MQ9	C23-C24-C26-C27
16	H	609	MQ9	C27-C28-C29-C31
21	N	603	CDL	OB6-CB4-CB6-OB8
21	P	301	CDL	OA6-CA4-CA6-OA8
21	G	504	CDL	OB6-CB4-CB6-OB8
21	L	601	CDL	C77-C78-C79-C80
17	C	304	WUO	O77-C78-C80-C81
21	N	604	CDL	C31-C32-C33-C34
21	H	604	CDL	CA5-C11-C12-C13
21	R	605	CDL	CB3-CB4-CB6-OB8
21	I	301	CDL	C15-C16-C17-C18
22	S	402	7PH	C36-C37-C38-C39
16	N	606	MQ9	C12-C11-C9-C8
21	G	504	CDL	C15-C16-C17-C18
21	I	302	CDL	C76-C77-C78-C79
21	N	603	CDL	C35-C36-C37-C38
19	M	502	9YF	C25-C26-C27-C28
27	Y	302	9XX	C6-C7-C8-C9
23	R	603	HEA	C3D-CAD-CBD-CGD
21	H	606	CDL	C31-CA7-OA8-CA6
16	N	601	MQ9	C40-C39-C41-C42
17	I	303	WUO	C35-C37-O38-C39
21	L	601	CDL	C12-C13-C14-C15
28	L	608	PLM	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
17	W	401	WUO	O55-C56-C57-C76
16	N	606	MQ9	C24-C26-C27-C28
21	T	201	CDL	C79-C80-C81-C82
21	R	601	CDL	C73-C74-C75-C76
21	H	606	CDL	OA9-CA7-OA8-CA6
17	I	303	WUO	O40-C41-C48-O49
21	H	606	CDL	C78-C79-C80-C81
21	I	301	CDL	C37-C38-C39-C40
21	L	601	CDL	C54-C55-C56-C57
19	W	402	9YF	O10-C8-O9-C
21	H	606	CDL	C31-C32-C33-C34
16	N	605	MQ9	C32-C33-C34-C35
17	I	303	WUO	C25-C26-C27-C28
21	T	201	CDL	C11-C12-C13-C14
16	C	303	MQ9	C31-C32-C33-C34
21	L	607	CDL	C37-C38-C39-C40
23	R	603	HEA	CAD-CBD-CGD-O1D
15	O	302	HEC	CAA-CBA-CGA-O1A
15	C	302	HEC	CAA-CBA-CGA-O1A
19	W	402	9YF	C16-C17-C18-C19
21	H	606	CDL	C14-C15-C16-C17
17	C	304	WUO	C24-C25-C26-C27
21	H	606	CDL	C16-C17-C18-C19
23	L	603	HEA	C2D-C3D-CAD-CBD
16	G	501	MQ9	C15-C14-C16-C17
20	N	607	HEM	C3D-CAD-CBD-CGD
23	L	603	HEA	C3D-CAD-CBD-CGD
19	M	502	9YF	C16-C17-C18-C19
21	R	605	CDL	O1-C1-CB2-OB2
16	N	601	MQ9	C19-C21-C22-C23
21	H	601	CDL	C51-C52-C53-C54
21	H	601	CDL	C19-C20-C21-C22
19	G	502	9YF	C38-C39-C40-C41
21	I	301	CDL	CB3-CB4-OB6-CB5
21	I	301	CDL	CB6-CB4-OB6-CB5
21	N	603	CDL	C14-C15-C16-C17
21	H	601	CDL	C52-C53-C54-C55
21	L	601	CDL	C74-C75-C76-C77
19	b	201	9YF	C20-C21-C22-C23
19	W	402	9YF	C9-C8-O9-C
20	N	607	HEM	CAA-CBA-CGA-O1A
16	O	303	MQ9	C30-C29-C31-C32

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Mol	Chain	Res	Type	Atoms
21	L	601	CDL	OA5-CA3-CA4-CA6
16	N	601	MQ9	C38-C39-C41-C42
23	R	603	HEA	C14-C15-C16-C17
23	R	603	HEA	CAD-CBD-CGD-O2D
17	I	303	WUO	C86-C87-C88-C90
19	G	502	9YF	C31-C32-C33-C35
21	H	611	CDL	OB6-CB4-CB6-OB8
21	I	302	CDL	OA6-CA4-CA6-OA8
15	O	301	HEC	CAD-CBD-CGD-O2D
15	C	301	HEC	CAD-CBD-CGD-O2D
23	R	603	HEA	C27-C19-C20-C21
28	Y	301	PLM	C5-C6-C7-C8
16	G	501	MQ9	C13-C14-C16-C17
16	H	602	MQ9	C18-C19-C21-C22
22	S	401	7PH	C25-C26-C27-C28
17	W	401	WUO	C94-C95-C96-C97
21	N	604	CDL	C20-C21-C22-C23
21	R	605	CDL	C12-C13-C14-C15
21	G	504	CDL	C16-C17-C18-C19
21	H	605	CDL	C74-C75-C76-C77
16	N	601	MQ9	C45-C44-C46-C47
22	S	401	7PH	C36-C37-C38-C39
16	H	608	MQ9	C33-C34-C36-C37
21	H	601	CDL	CA5-C11-C12-C13
23	L	603	HEA	CAD-CBD-CGD-O1D
21	T	201	CDL	C71-C72-C73-C74
22	J	401	7PH	C27-C28-C29-C2A
20	N	607	HEM	CAA-CBA-CGA-O2A
21	H	611	CDL	C83-C84-C85-C86
21	N	603	CDL	C15-C16-C17-C18
22	S	401	7PH	C2A-C2B-C2C-C2D
21	H	606	CDL	C57-C58-C59-C60
17	I	303	WUO	O55-C56-C57-O58
21	N	603	CDL	OA5-CA3-CA4-OA6
21	R	605	CDL	OA5-CA3-CA4-OA6
21	R	605	CDL	C71-C72-C73-C74
20	H	603	HEM	CAD-CBD-CGD-O2D
17	O	304	WUO	C84-C85-C86-C87
19	M	502	9YF	C36-C37-C38-C39
21	H	611	CDL	C84-C85-C86-C87
21	R	601	CDL	C52-C51-CB5-OB6
23	L	603	HEA	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
21	T	201	CDL	C72-C73-C74-C75
21	N	603	CDL	CA2-C1-CB2-OB2
17	O	304	WUO	C92-C93-C94-C95
22	J	401	7PH	C38-C39-C3A-C3B
23	R	602	HEA	CAD-CBD-CGD-O2D
23	L	602	HEA	CAD-CBD-CGD-O2D
19	M	502	9YF	C18-C19-C20-C21
21	I	302	CDL	C37-C38-C39-C40
21	H	611	CDL	C1-CB2-OB2-PB2
22	S	402	7PH	C26-C27-C28-C29
23	R	602	HEA	CAD-CBD-CGD-O1D
23	L	602	HEA	CAD-CBD-CGD-O1D
19	W	402	9YF	C26-C27-C28-C29
17	O	304	WUO	C94-C95-C96-C97
17	C	304	WUO	C27-C28-C29-C30
21	R	601	CDL	O1-C1-CA2-OA2
17	W	401	WUO	C83-C84-C85-C86
17	W	401	WUO	C84-C85-C86-C87
21	H	611	CDL	C13-C14-C15-C16
21	H	606	CDL	C21-C22-C23-C24
22	S	401	7PH	C31-C32-C33-C34
15	O	302	HEC	CAA-CBA-CGA-O2A
15	C	302	HEC	CAA-CBA-CGA-O2A
16	N	601	MQ9	C43-C44-C46-C47
21	H	606	CDL	C33-C34-C35-C36
21	I	302	CDL	C18-C19-C20-C21
21	L	607	CDL	C14-C15-C16-C17
20	H	603	HEM	CAD-CBD-CGD-O1D
21	H	604	CDL	C53-C54-C55-C56
21	L	601	CDL	C73-C74-C75-C76
20	N	602	HEM	CAA-CBA-CGA-O2A
21	P	301	CDL	C74-C75-C76-C77
20	N	602	HEM	CAA-CBA-CGA-O1A
17	I	303	WUO	C61-C62-C63-C64
21	R	605	CDL	C36-C37-C38-C39
17	I	303	WUO	C65-C66-C67-C68
27	R	608	9XX	C29-C30-C31-C32
16	N	605	MQ9	C40-C39-C41-C42
19	W	402	9YF	O9-C8-C9-C10
15	O	301	HEC	CAA-CBA-CGA-O1A
15	O	301	HEC	CAD-CBD-CGD-O1D
15	C	301	HEC	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
15	C	301	HEC	CAD-CBD-CGD-O1D
21	N	604	CDL	C78-C79-C80-C81
27	R	608	9XX	C13-C14-C15-O
17	C	304	WUO	C94-C95-C96-C97
21	H	611	CDL	C58-C59-C60-C61
17	W	401	WUO	C89-C88-C90-C91
27	R	608	9XX	C25-C26-C27-C36
27	H	612	9XX	C5-C6-C7-C8
23	R	603	HEA	C18-C19-C20-C21
21	G	504	CDL	C14-C15-C16-C17
21	H	606	CDL	C12-C11-CA5-OA6
27	Y	302	9XX	C13-C14-C15-O
21	I	301	CDL	C58-C59-C60-C61
21	H	606	CDL	C58-C59-C60-C61
27	R	608	9XX	C32-C33-C34-C35
21	P	301	CDL	C52-C51-CB5-OB6
17	O	304	WUO	C50-O51-P52-O54
17	C	304	WUO	C50-O51-P52-O53
17	C	304	WUO	C50-O51-P52-O54
19	b	201	9YF	C2-O2-P-O8
20	N	607	HEM	C2A-CAA-CBA-CGA
21	P	301	CDL	C73-C74-C75-C76
21	H	601	CDL	C32-C31-CA7-OA8
21	L	601	CDL	C84-C85-C86-C87
27	b	202	9XX	O1-C18-C19-C20
21	R	605	CDL	OB5-CB3-CB4-OB6
28	W	403	PLM	C1-C2-C3-C4
21	H	605	CDL	C75-C76-C77-C78
19	W	402	9YF	C7-C2-O2-P
27	Y	302	9XX	C11-C10-C9-C8
21	R	601	CDL	C34-C35-C36-C37
23	R	602	HEA	CAA-CBA-CGA-O1A
23	L	602	HEA	CAA-CBA-CGA-O1A
21	L	607	CDL	C39-C40-C41-C42
27	b	202	9XX	C20-C21-C22-C23
21	I	302	CDL	C57-C58-C59-C60
21	G	504	CDL	C52-C51-CB5-OB6
21	P	301	CDL	C36-C37-C38-C39
21	N	604	CDL	O1-C1-CA2-OA2
21	I	302	CDL	CA3-CA4-CA6-OA8
16	H	602	MQ9	C35-C34-C36-C37
17	O	304	WUO	O77-C78-C80-C81

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Mol	Chain	Res	Type	Atoms
16	H	602	MQ9	C31-C32-C33-C34
20	H	610	HEM	CAA-CBA-CGA-O2A
21	N	604	CDL	C52-C51-CB5-OB6
21	T	201	CDL	C12-C11-CA5-OA6
17	I	303	WUO	C70-C71-C72-C73
21	H	605	CDL	CA5-C11-C12-C13
21	N	603	CDL	C36-C37-C38-C39
17	I	303	WUO	C31-C01-O02-C03
19	W	402	9YF	C35-C36-C37-C38
21	N	603	CDL	C74-C75-C76-C77
17	O	304	WUO	C66-C67-C68-C69
17	W	401	WUO	C72-C73-C74-C75
21	N	603	CDL	C60-C61-C62-C63
21	H	601	CDL	C72-C71-CB7-OB8
21	P	301	CDL	C31-C32-C33-C34
21	H	606	CDL	CA7-C31-C32-C33
21	P	301	CDL	C37-C38-C39-C40
21	L	601	CDL	CA6-CA4-OA6-CA5
21	N	603	CDL	O1-C1-CA2-OA2
21	N	603	CDL	O1-C1-CB2-OB2
16	N	606	MQ9	C29-C31-C32-C33
15	O	301	HEC	CAA-CBA-CGA-O2A
15	C	301	HEC	CAA-CBA-CGA-O2A
23	R	602	HEA	CAA-CBA-CGA-O2A
23	L	602	HEA	CAA-CBA-CGA-O2A
21	G	504	CDL	C13-C14-C15-C16
16	O	303	MQ9	C12-C11-C9-C10
21	R	601	CDL	CA7-C31-C32-C33
27	H	612	9XX	O-C16-C17-C37
15	O	302	HEC	CAD-CBD-CGD-O2D
15	C	302	HEC	CAD-CBD-CGD-O2D
27	b	202	9XX	C25-C26-C27-C36
27	R	608	9XX	C13-C14-C15-O6
21	P	301	CDL	C53-C54-C55-C56
21	H	606	CDL	C20-C21-C22-C23
27	R	608	9XX	C19-C20-C21-C22
17	O	304	WUO	O79-C78-C80-C81
21	P	301	CDL	C52-C51-CB5-OB7
21	H	606	CDL	C12-C11-CA5-OA7
27	b	202	9XX	O2-C18-C19-C20
21	H	601	CDL	OB7-CB5-OB6-CB4
21	H	604	CDL	OB7-CB5-OB6-CB4

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Mol	Chain	Res	Type	Atoms
20	N	602	HEM	CAD-CBD-CGD-O2D
23	R	603	HEA	CAA-CBA-CGA-O1A
23	L	603	HEA	CAA-CBA-CGA-O2A
17	I	303	WUO	O77-C78-C80-C81
20	H	610	HEM	CAA-CBA-CGA-O1A
21	G	504	CDL	C52-C51-CB5-OB7
16	H	602	MQ9	C45-C44-C46-C47
20	H	603	HEM	C2C-C3C-CAC-CBC
17	W	401	WUO	C44-C39-O38-C37
21	N	604	CDL	C52-C51-CB5-OB7
27	Y	302	9XX	C20-C21-C22-C23
23	R	603	HEA	O11-C11-C3B-C4B
21	T	201	CDL	C12-C11-CA5-OA7
21	H	601	CDL	C32-C31-CA7-OA9
16	H	608	MQ9	C26-C27-C28-C29
21	R	601	CDL	C55-C56-C57-C58
21	N	604	CDL	C34-C35-C36-C37

There are no ring outliers.

50 monomers are involved in 235 short contacts:

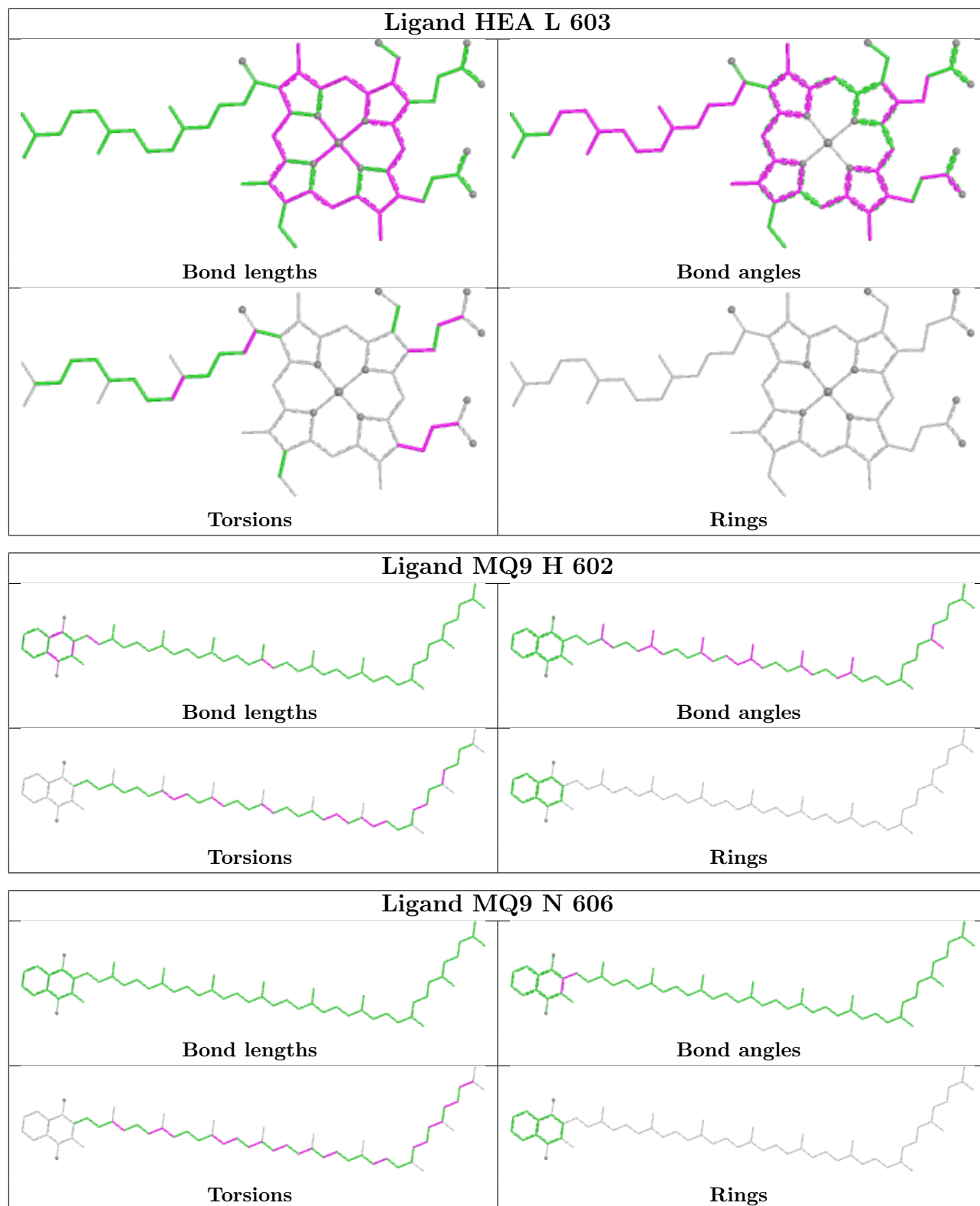
Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	L	603	HEA	6	0
16	H	602	MQ9	3	0
16	N	606	MQ9	9	0
19	W	402	9YF	3	0
23	R	603	HEA	15	0
17	I	303	WUO	2	0
21	I	302	CDL	5	0
21	I	301	CDL	4	0
21	N	604	CDL	7	0
16	C	303	MQ9	16	0
21	N	603	CDL	4	0
15	C	302	HEC	3	0
21	H	606	CDL	4	0
16	G	501	MQ9	6	0
21	H	605	CDL	3	0
16	N	605	MQ9	10	0
21	R	605	CDL	5	0
21	H	611	CDL	4	0
20	H	610	HEM	5	0
19	G	502	9YF	2	0

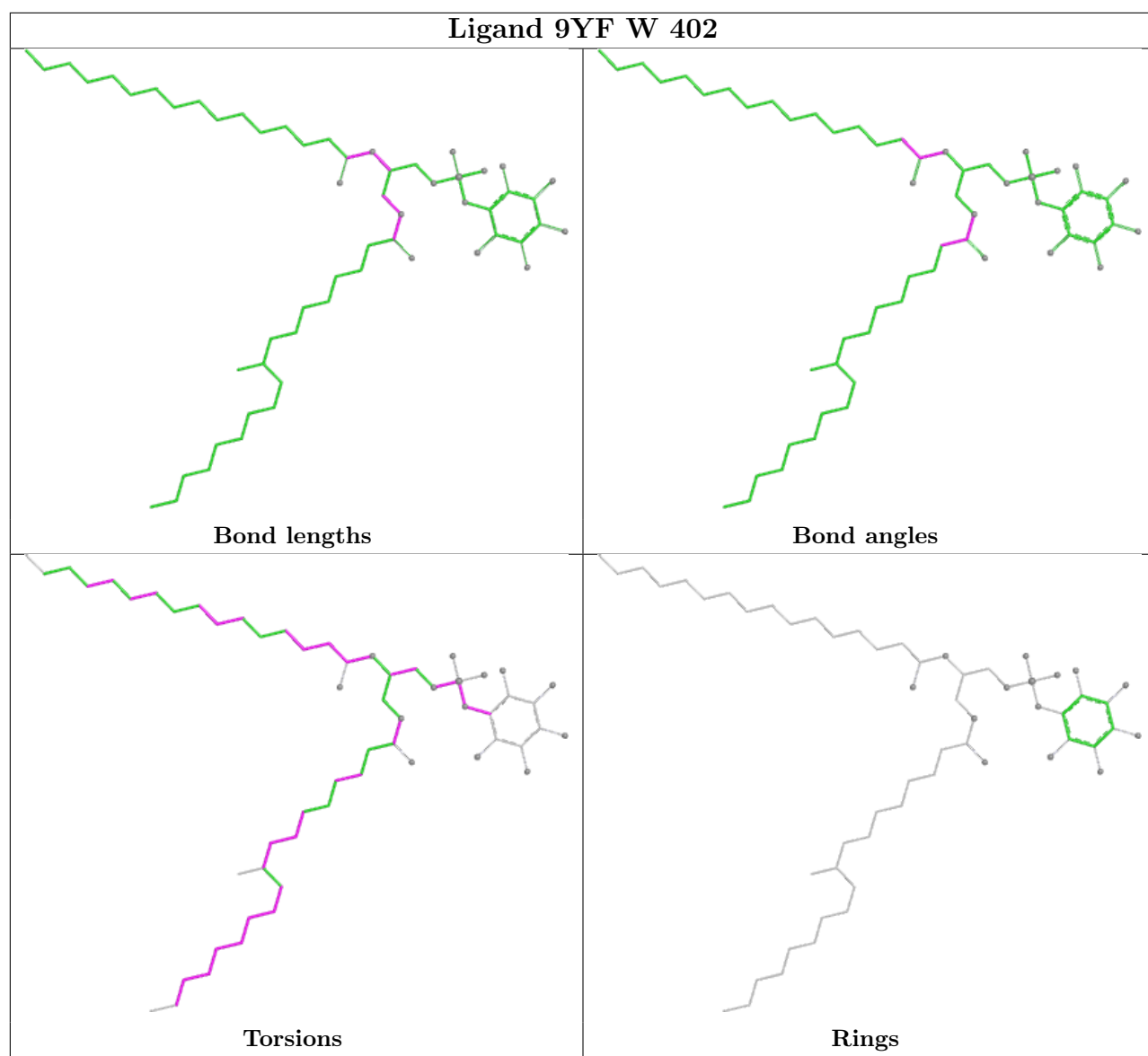
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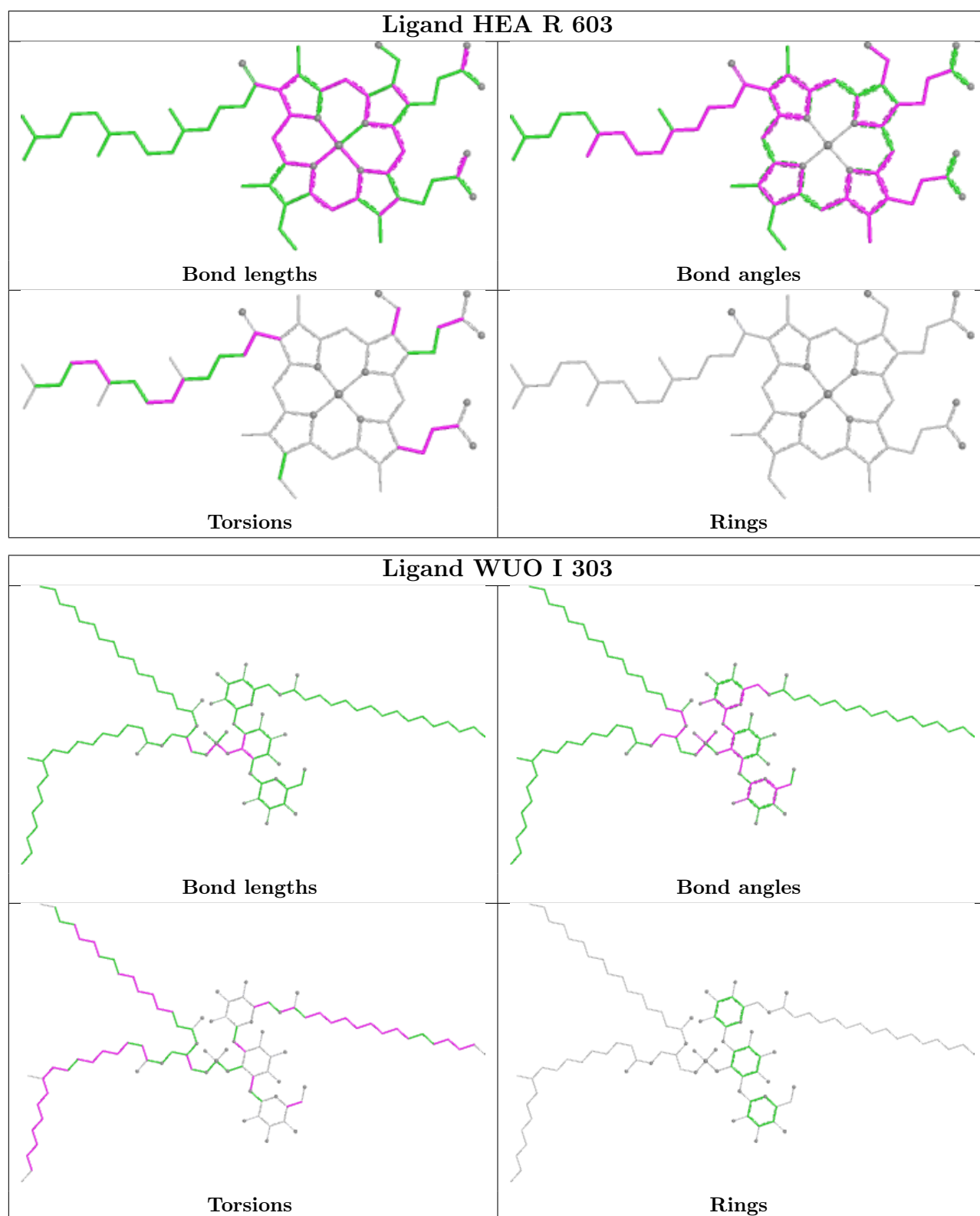
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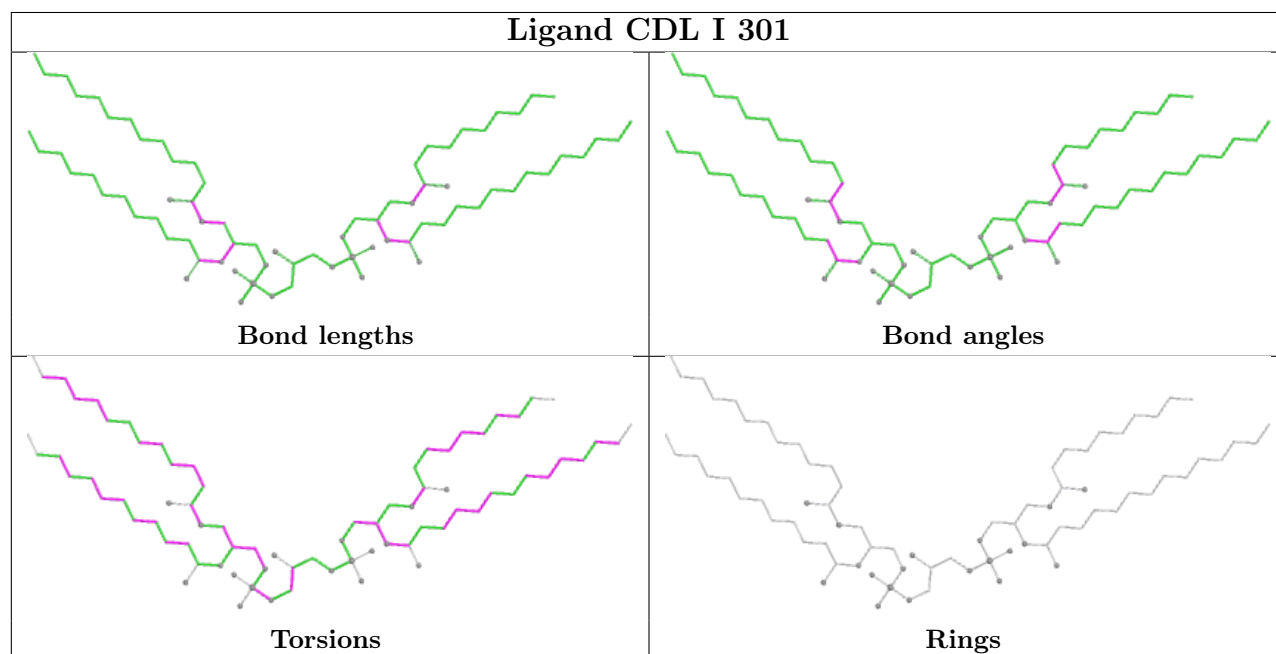
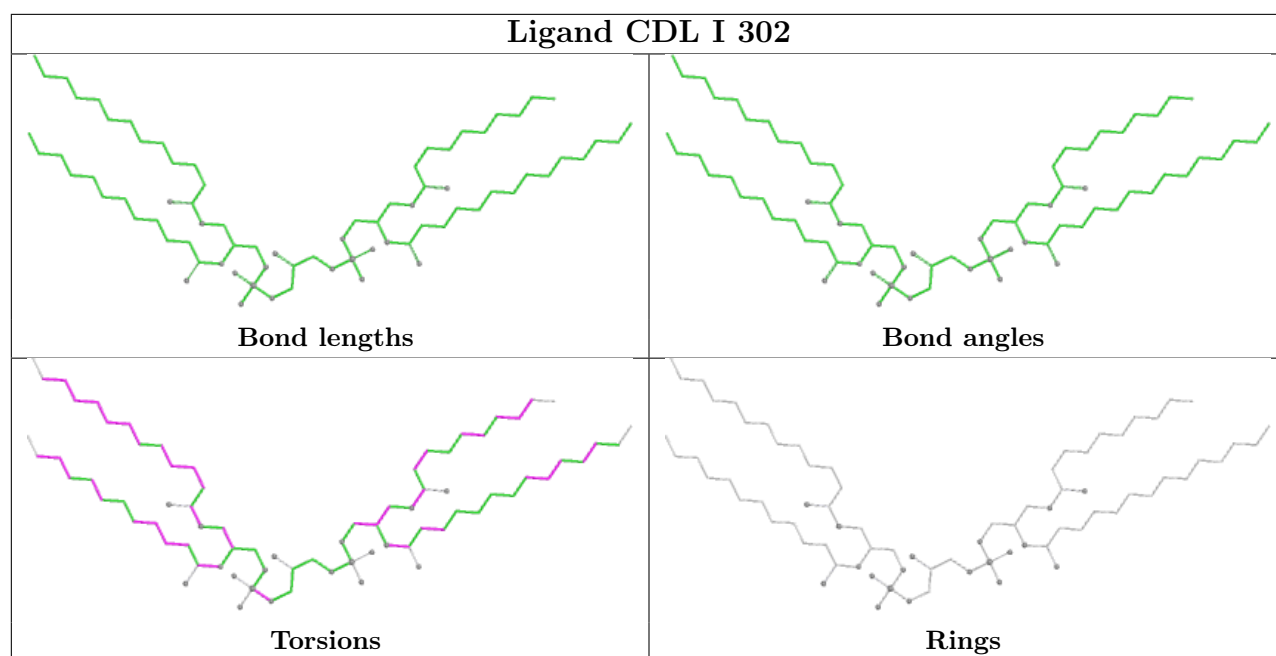
Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	L	602	HEA	7	0
23	R	602	HEA	7	0
15	C	301	HEC	1	0
21	L	607	CDL	2	0
16	H	608	MQ9	17	0
27	R	608	9XX	1	0
16	H	609	MQ9	7	0
16	N	601	MQ9	9	0
15	O	302	HEC	2	0
22	S	401	7PH	1	0
28	W	403	PLM	2	0
17	W	401	WUO	1	0
20	N	602	HEM	6	0
16	H	607	MQ9	22	0
21	H	604	CDL	9	0
20	N	607	HEM	4	0
17	O	304	WUO	1	0
19	b	201	9YF	3	0
21	L	601	CDL	1	0
20	H	603	HEM	10	0
21	R	601	CDL	1	0
21	P	301	CDL	3	0
16	O	303	MQ9	5	0
28	c	301	PLM	1	0
15	O	301	HEC	4	0
21	G	504	CDL	2	0
22	S	402	7PH	2	0
19	M	502	9YF	7	0
21	H	601	CDL	4	0
21	T	201	CDL	4	0

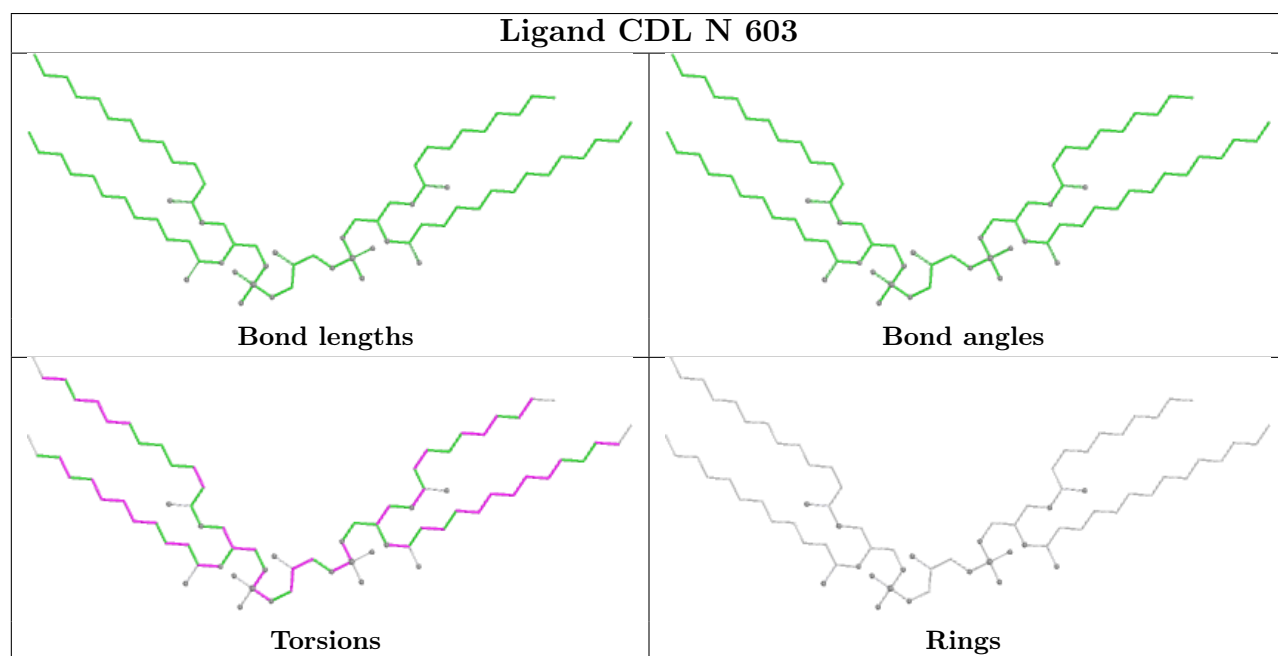
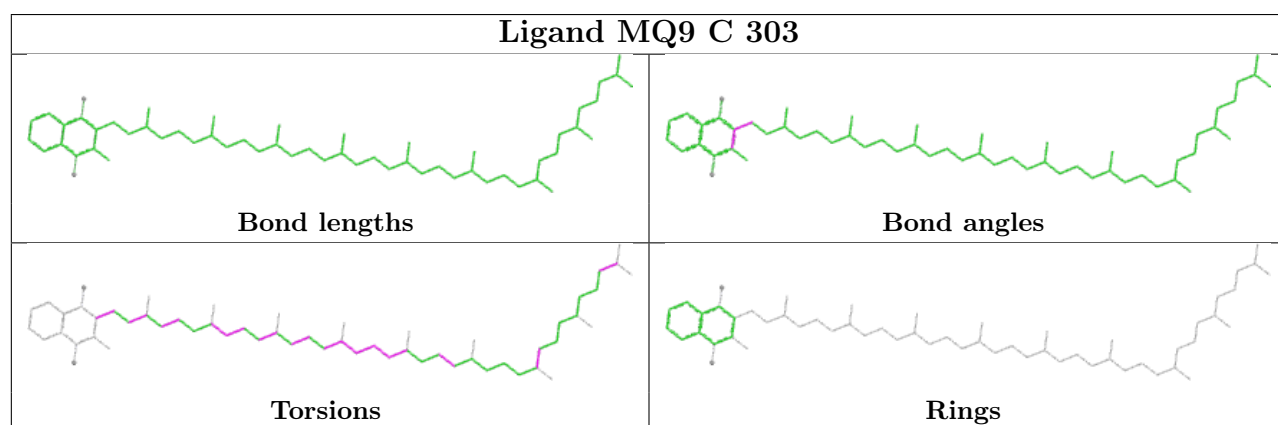
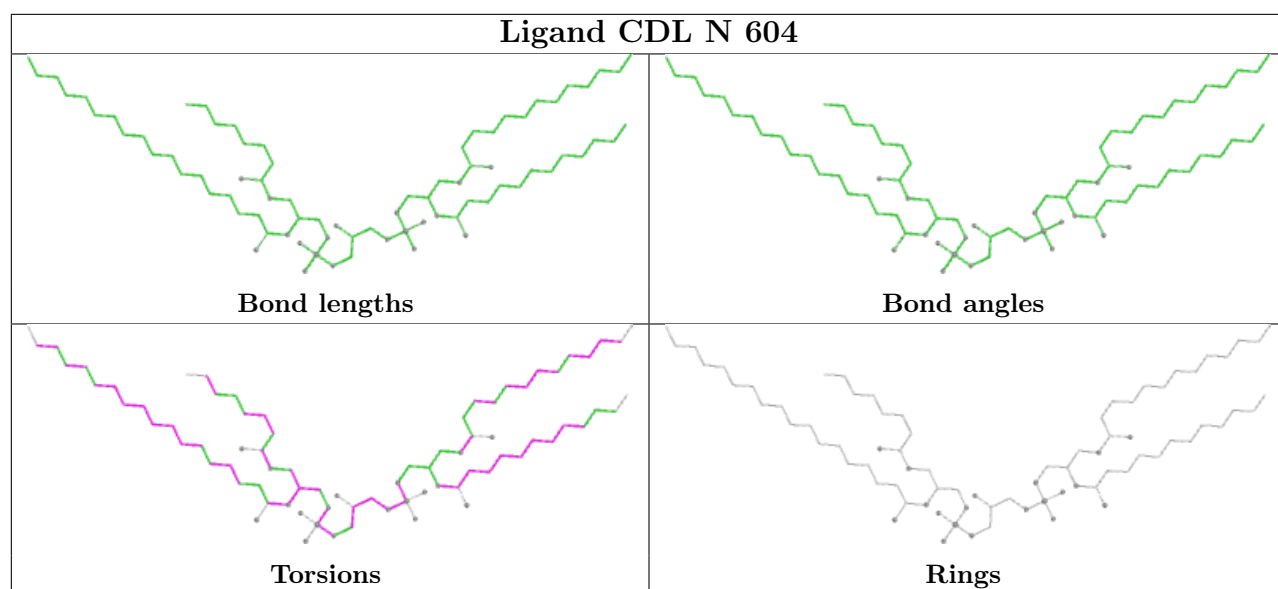
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



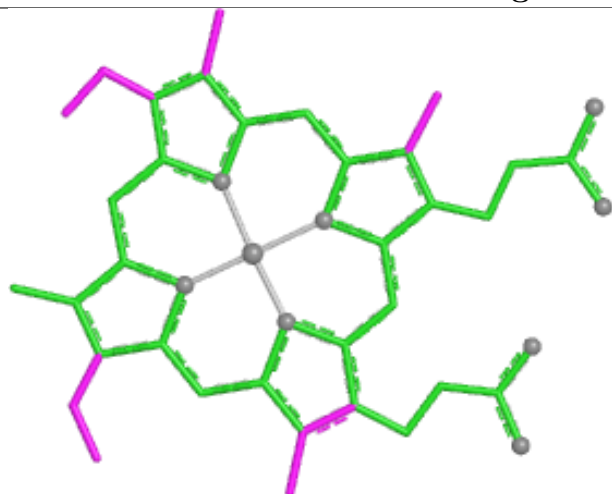




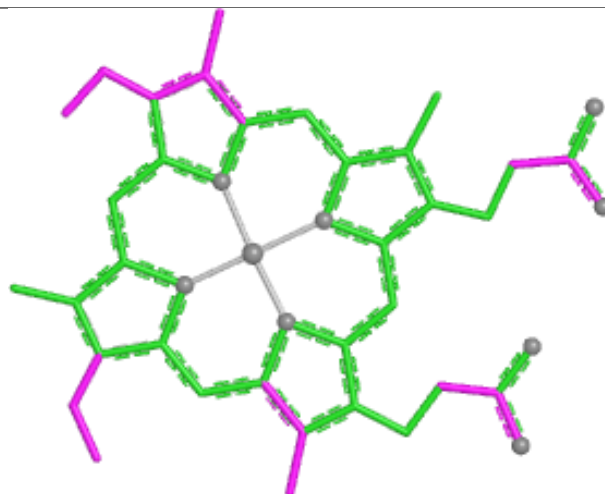




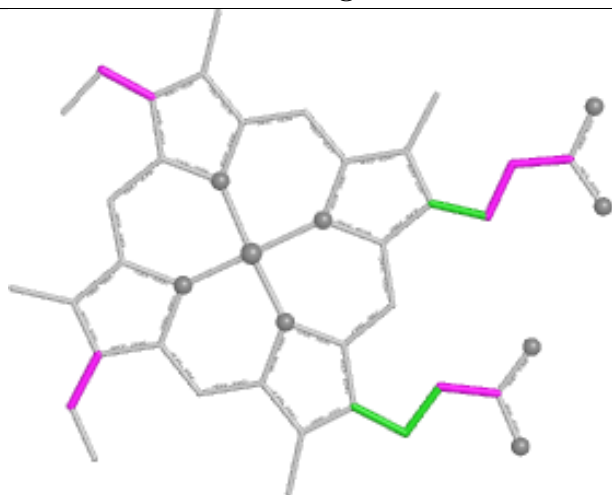
Ligand HEC C 302



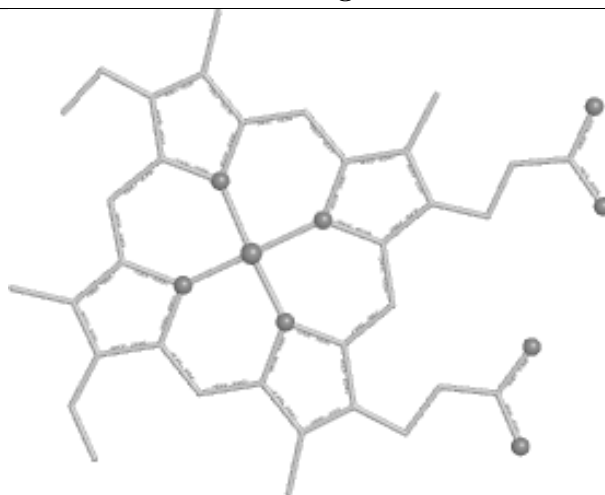
Bond lengths



Bond angles

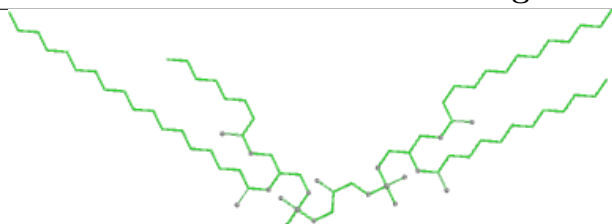


Torsions

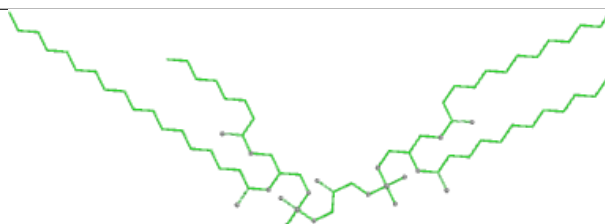


Rings

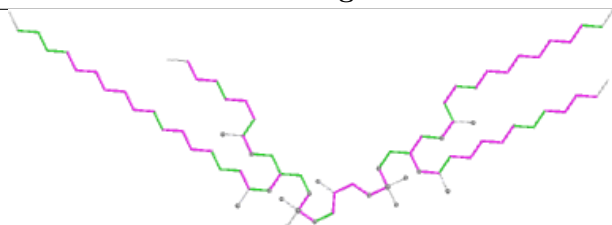
Ligand CDL H 606



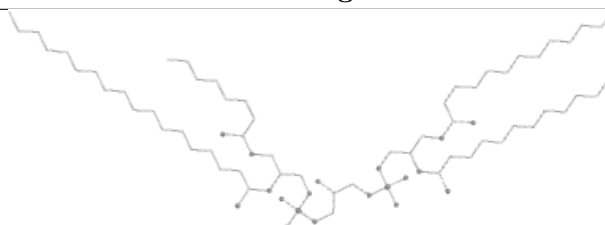
Bond lengths



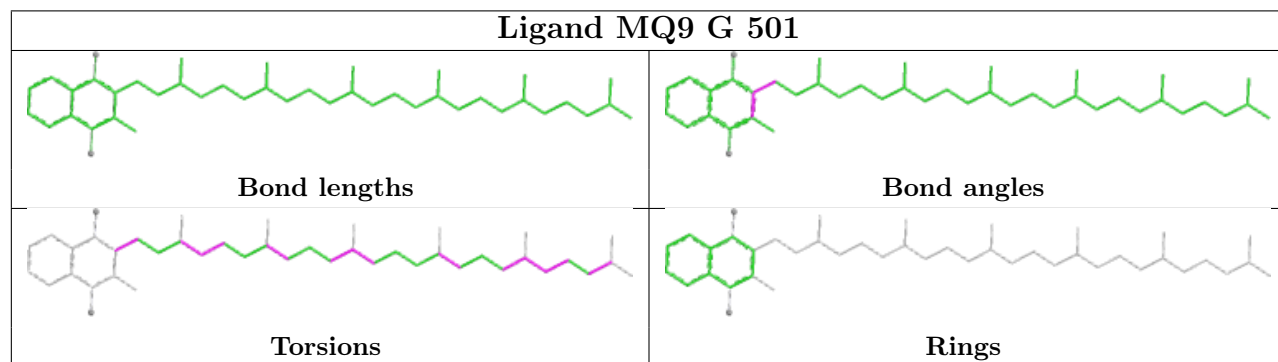
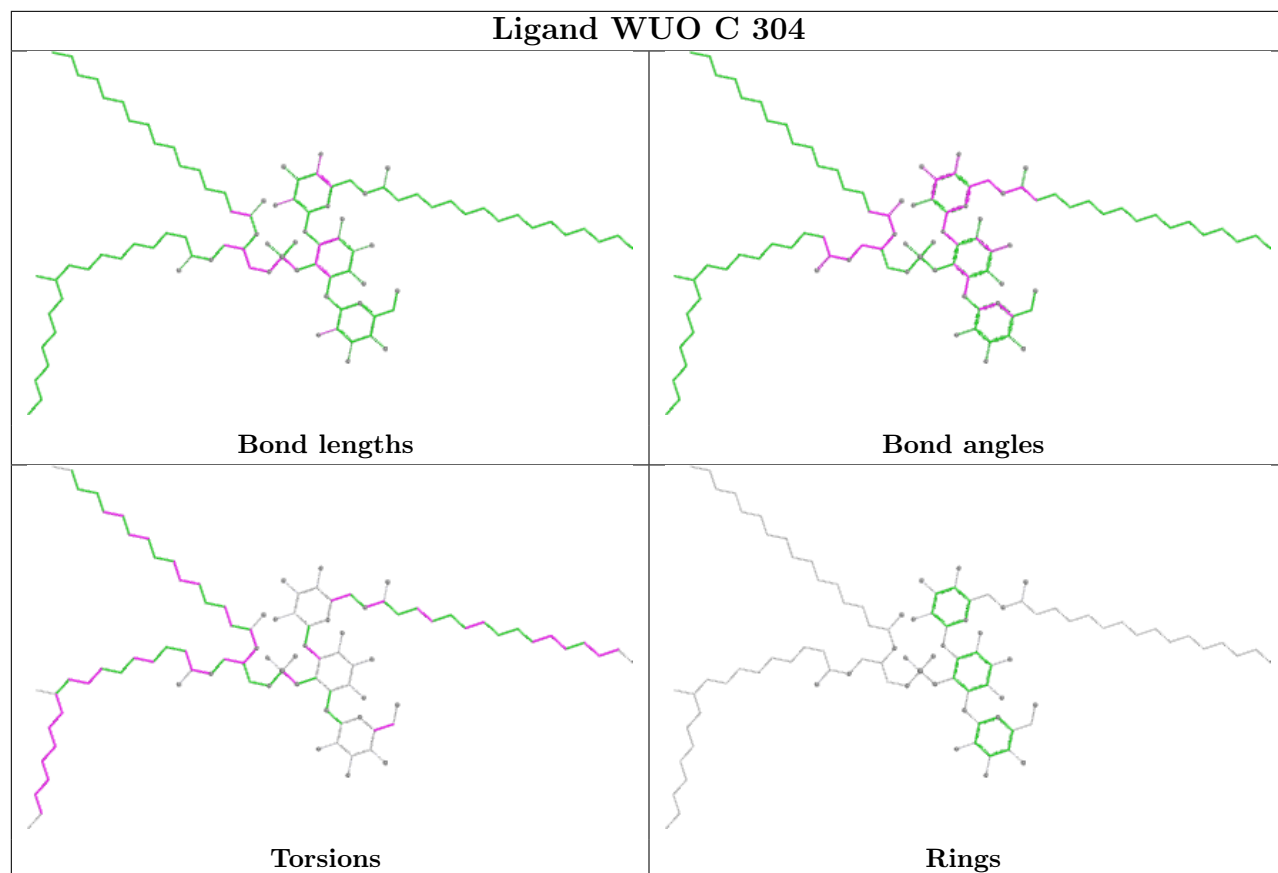
Bond angles

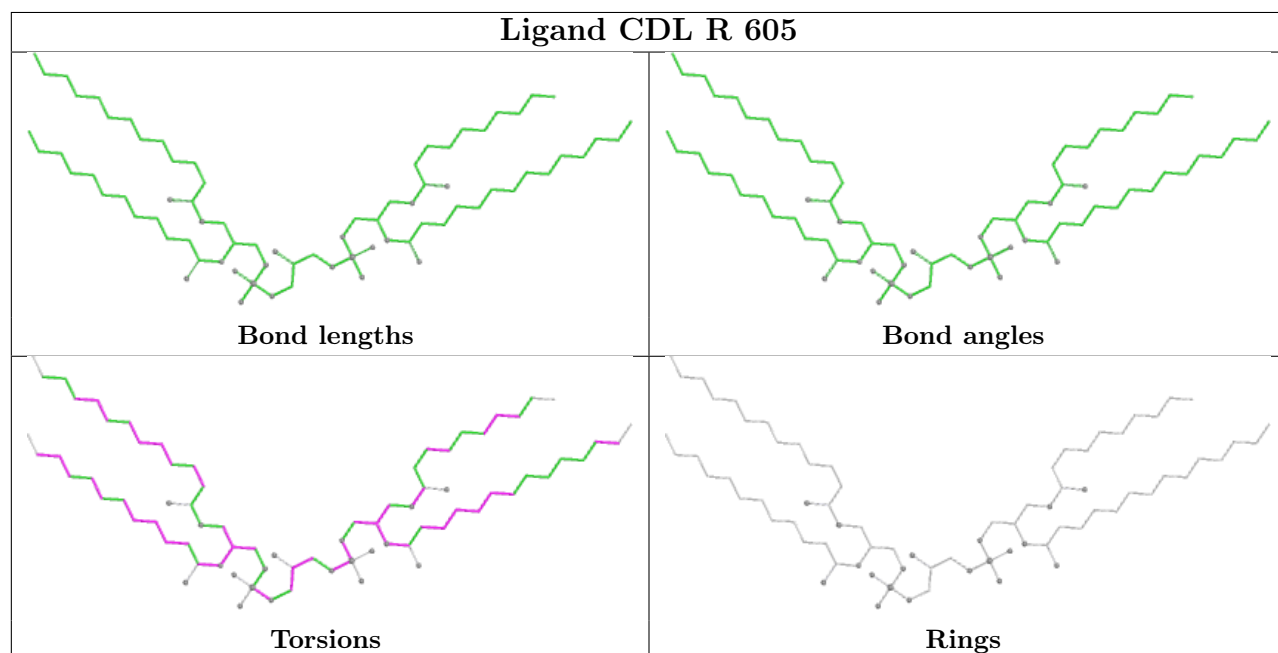
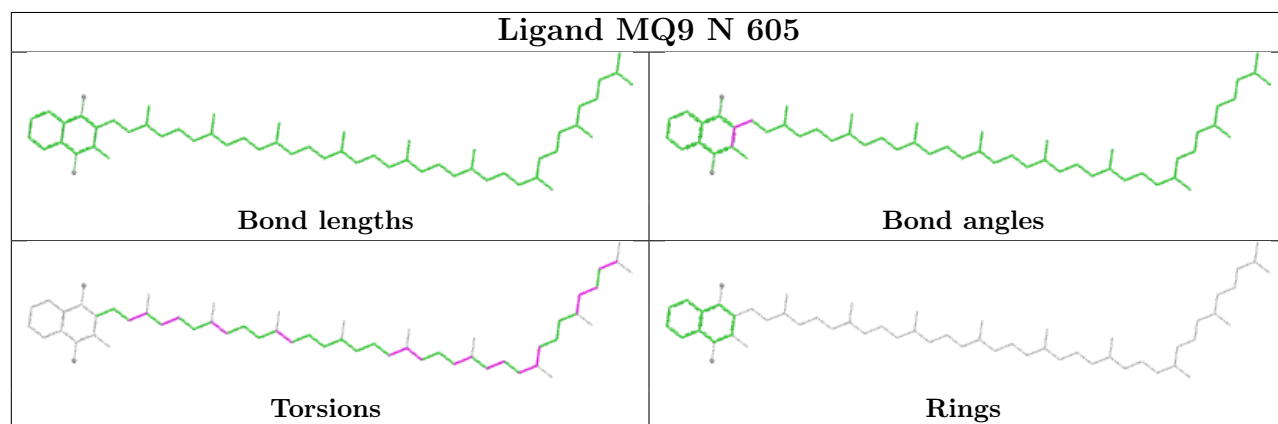
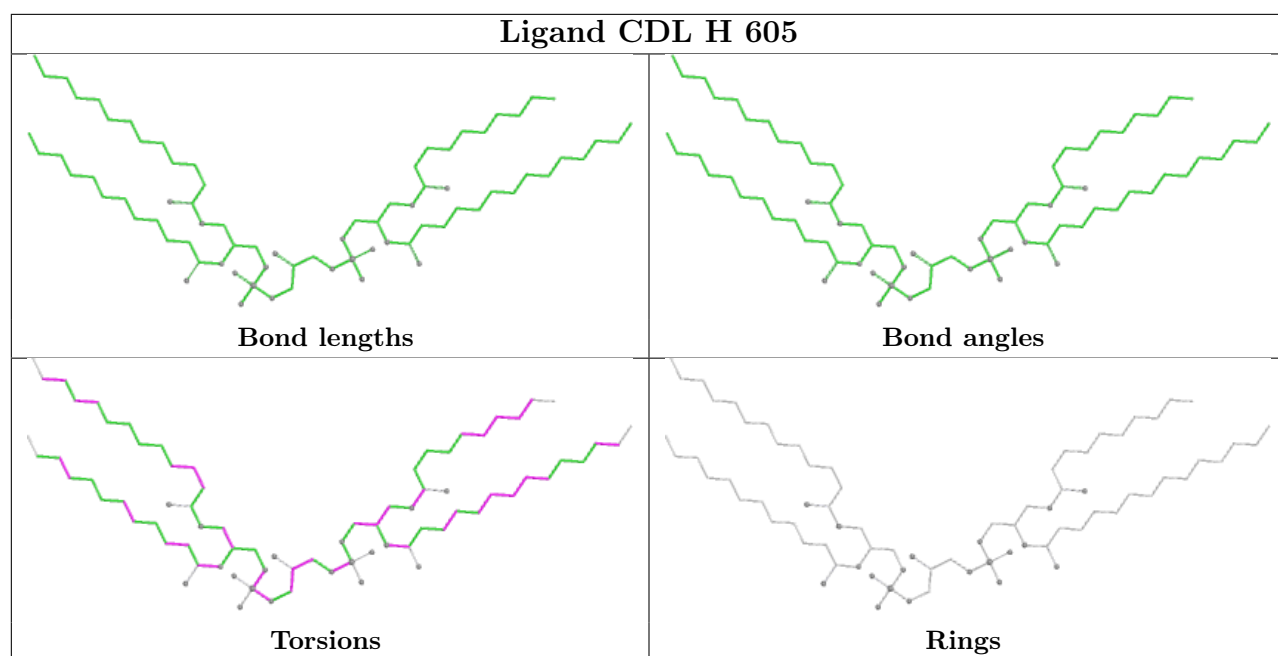


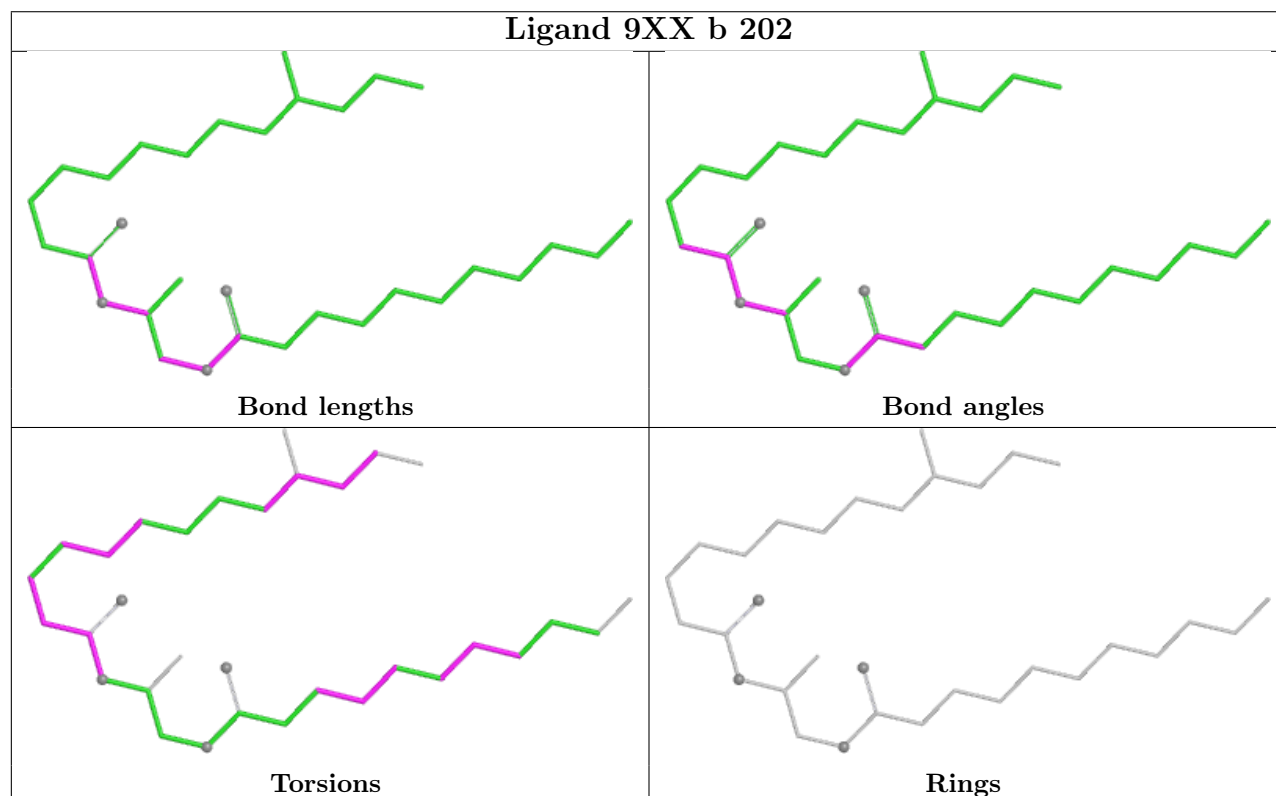
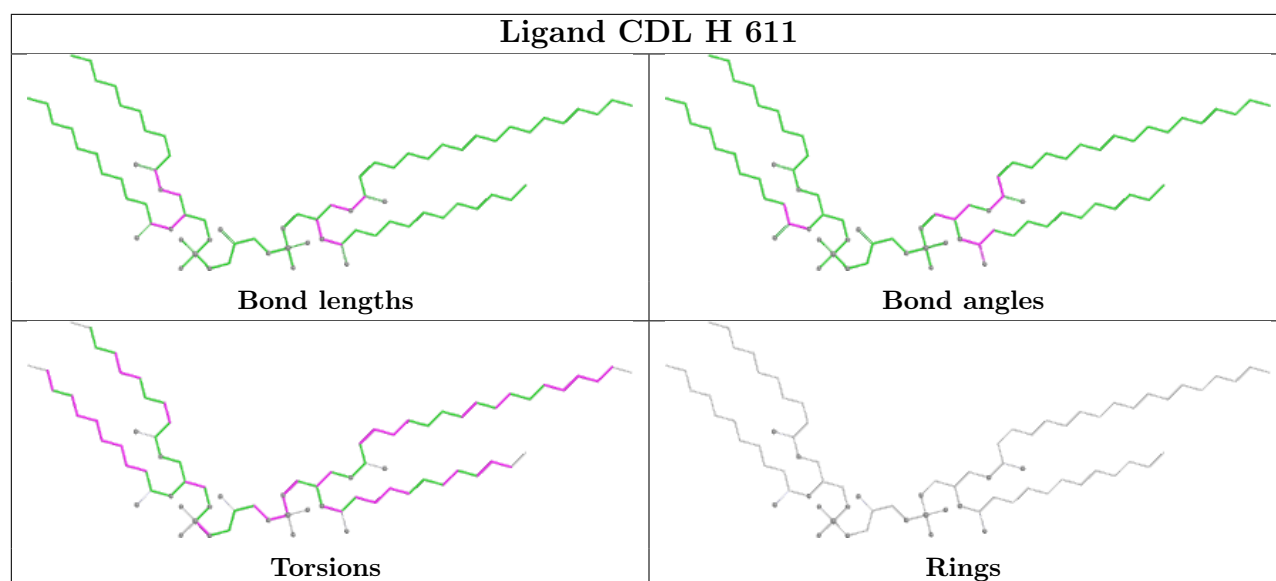
Torsions

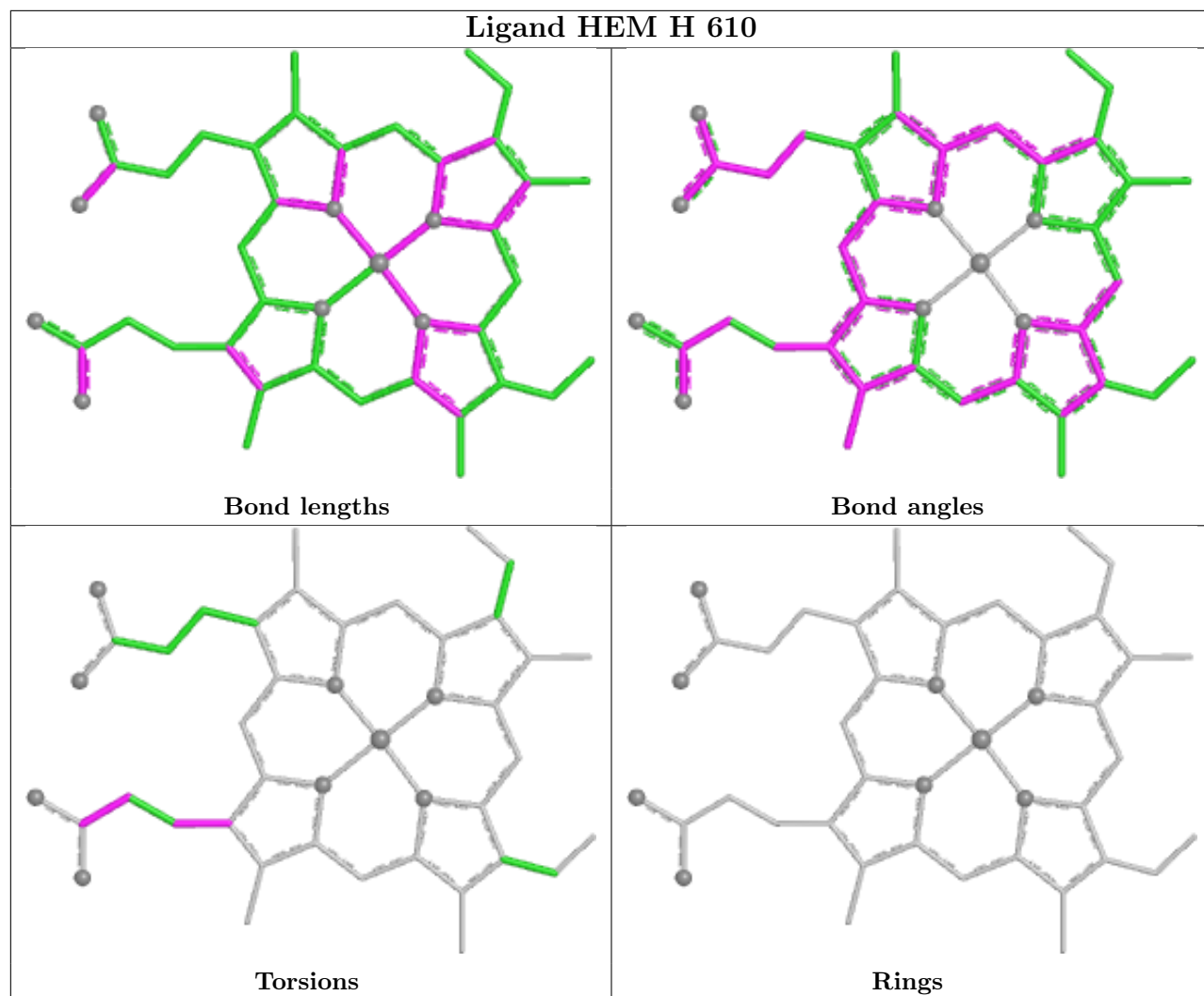


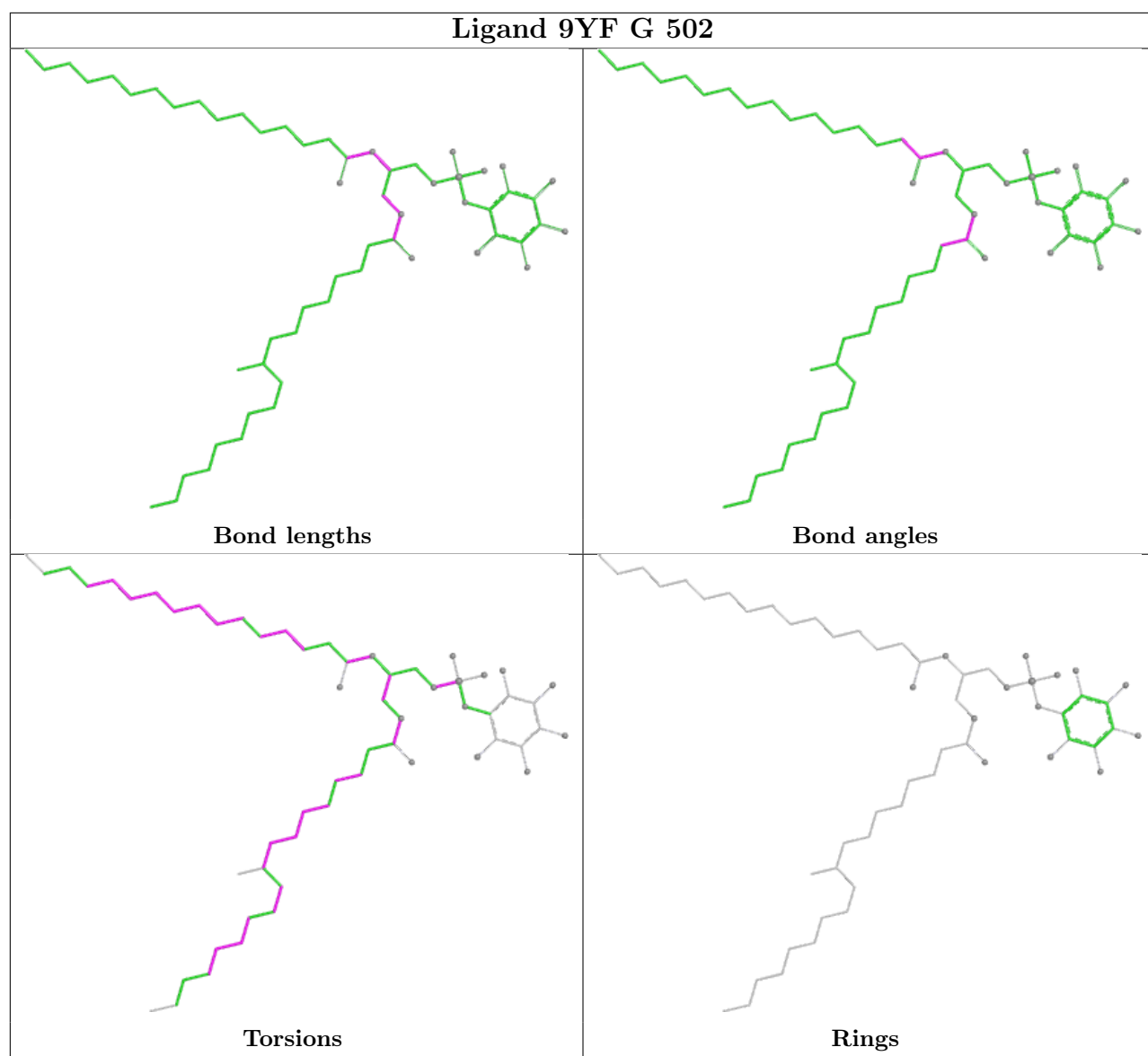
Rings

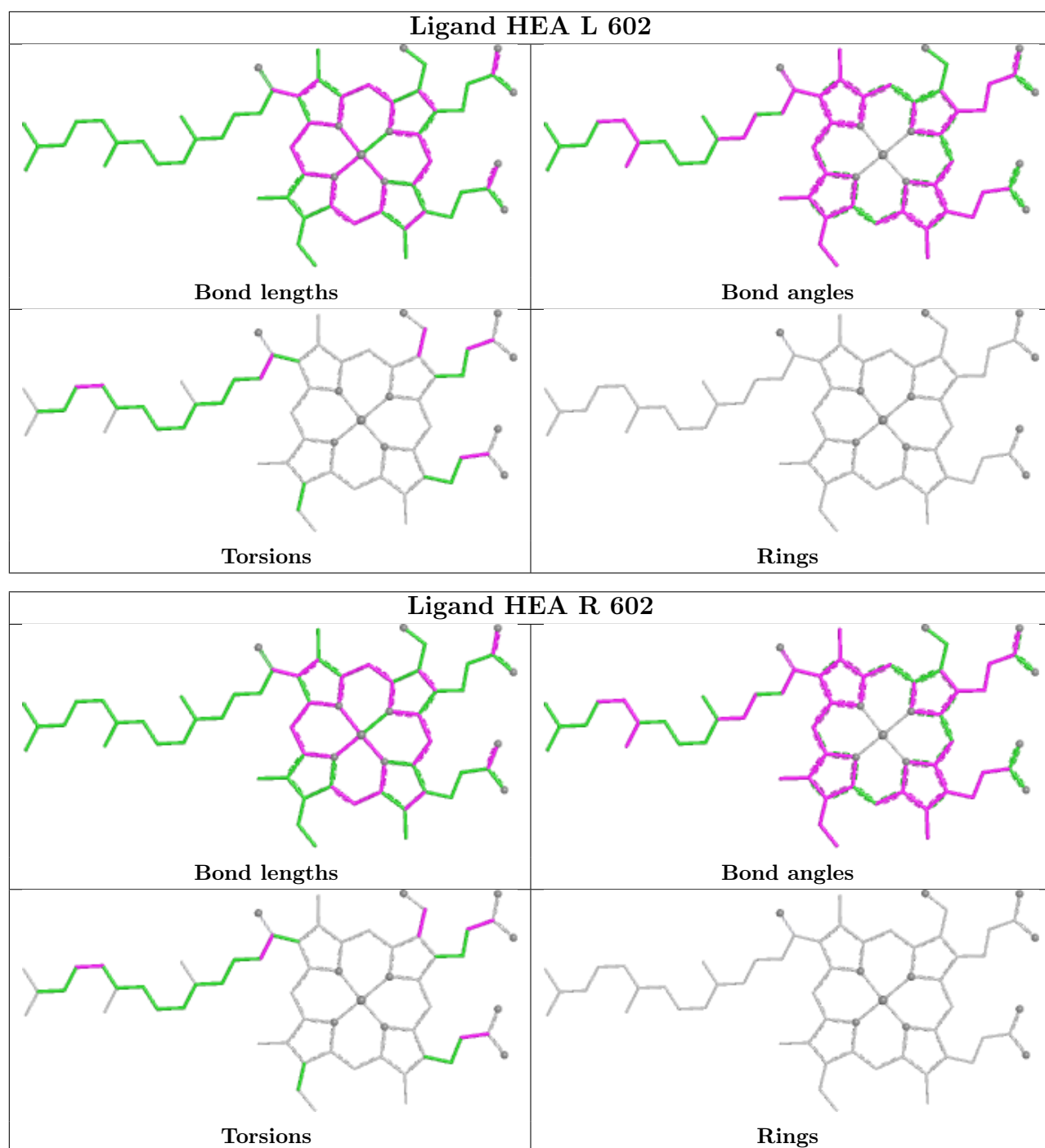




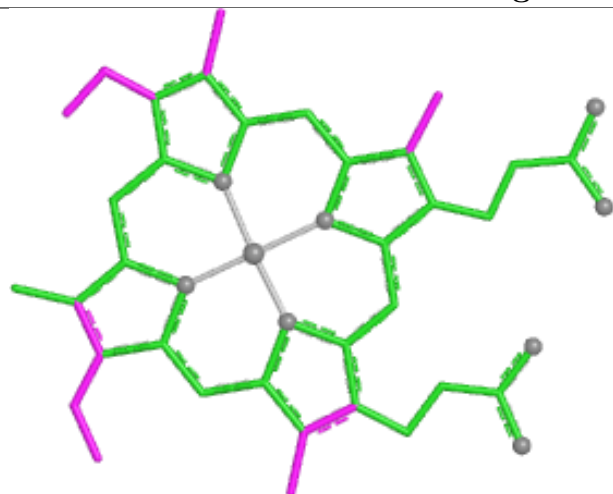




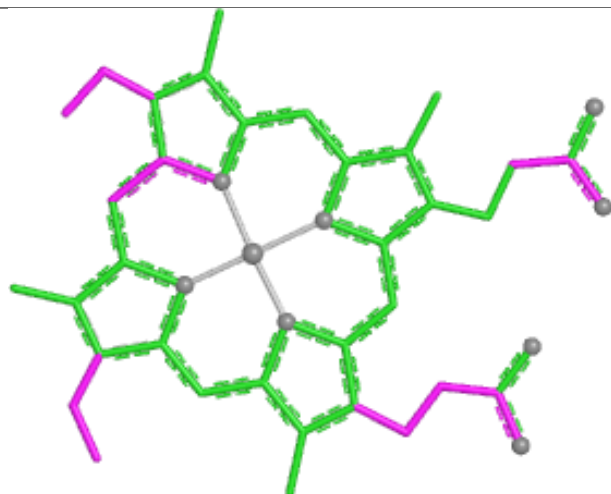




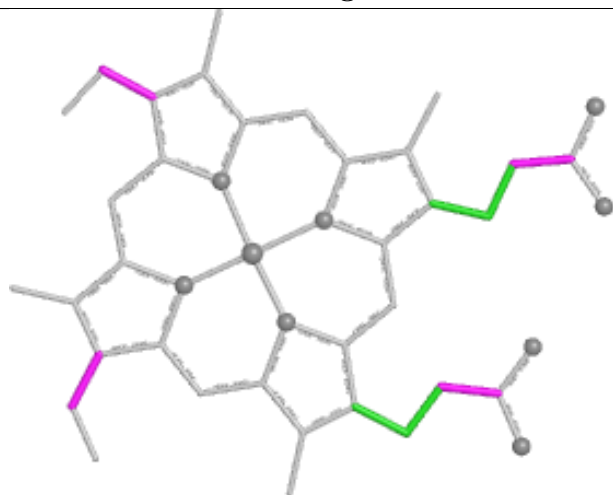
Ligand HEC C 301



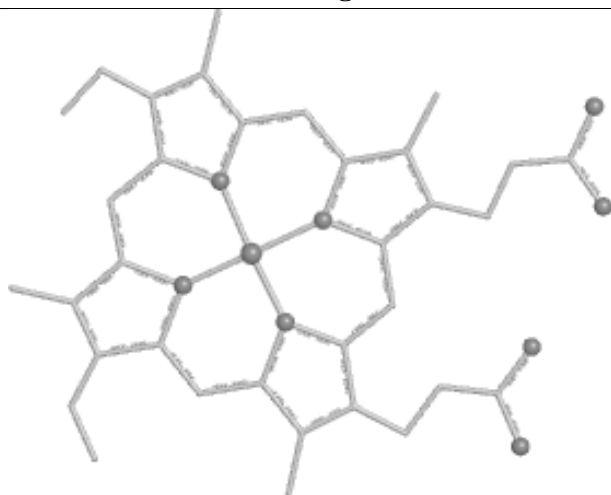
Bond lengths



Bond angles

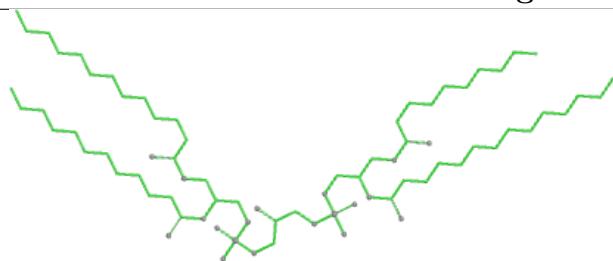


Torsions

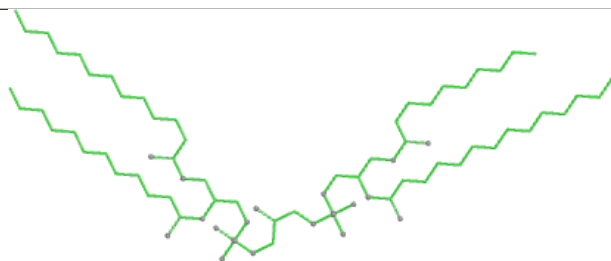


Rings

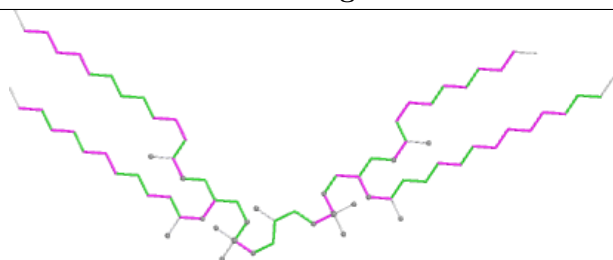
Ligand CDL L 607



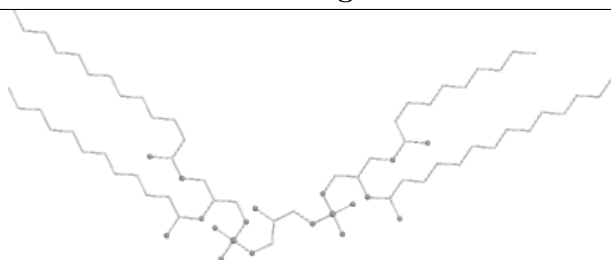
Bond lengths



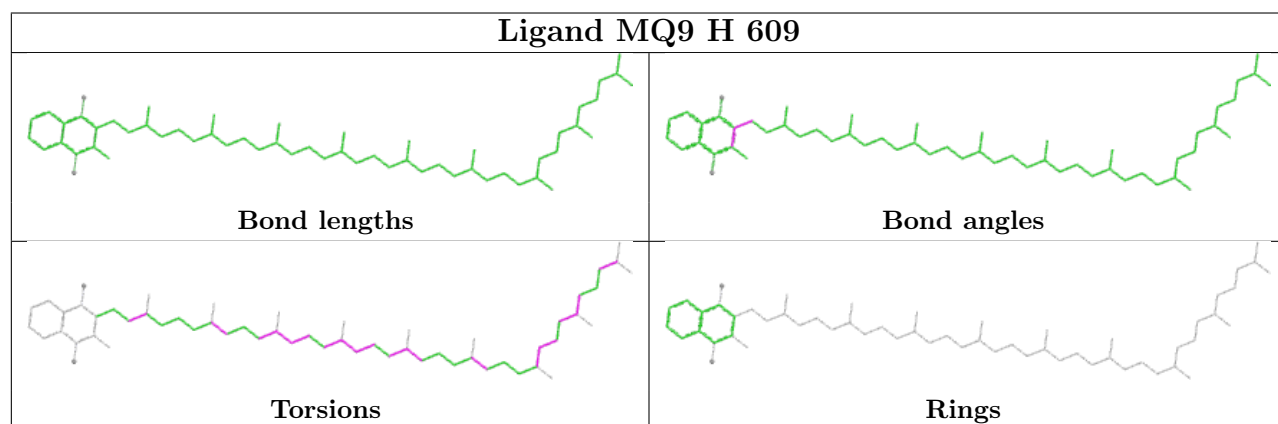
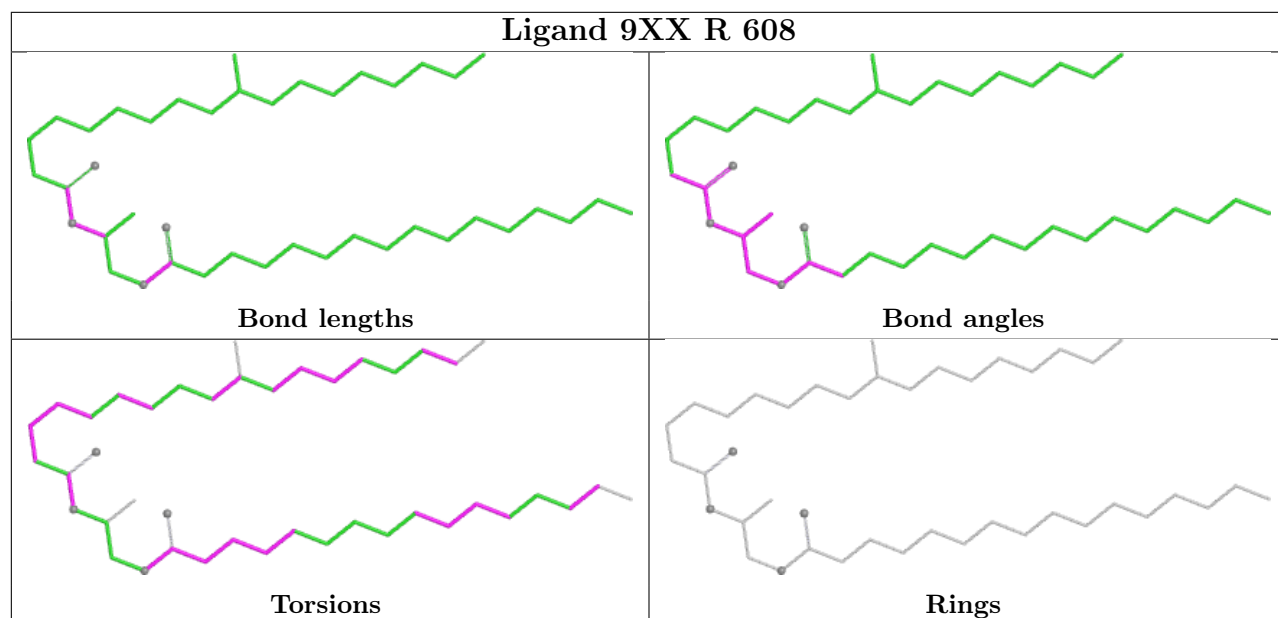
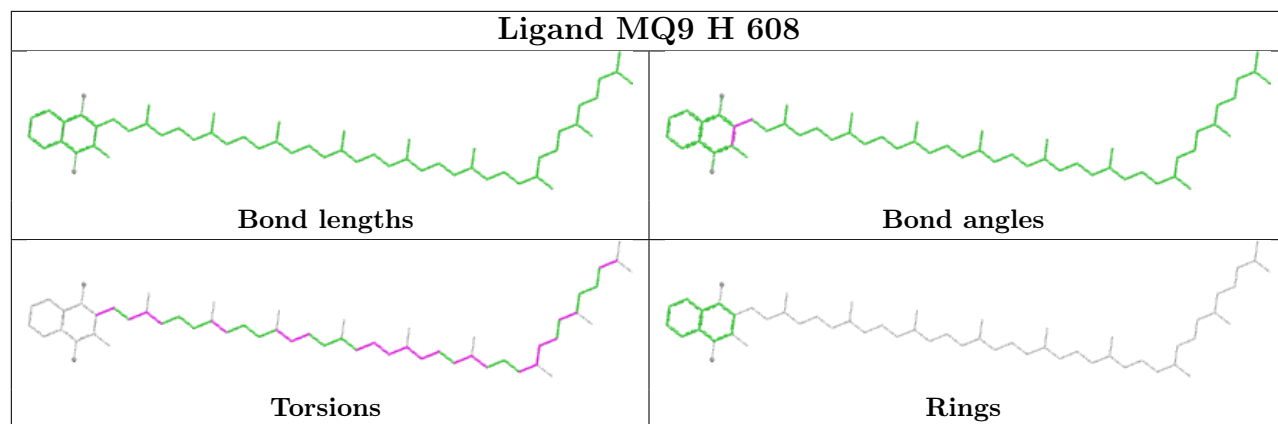
Bond angles

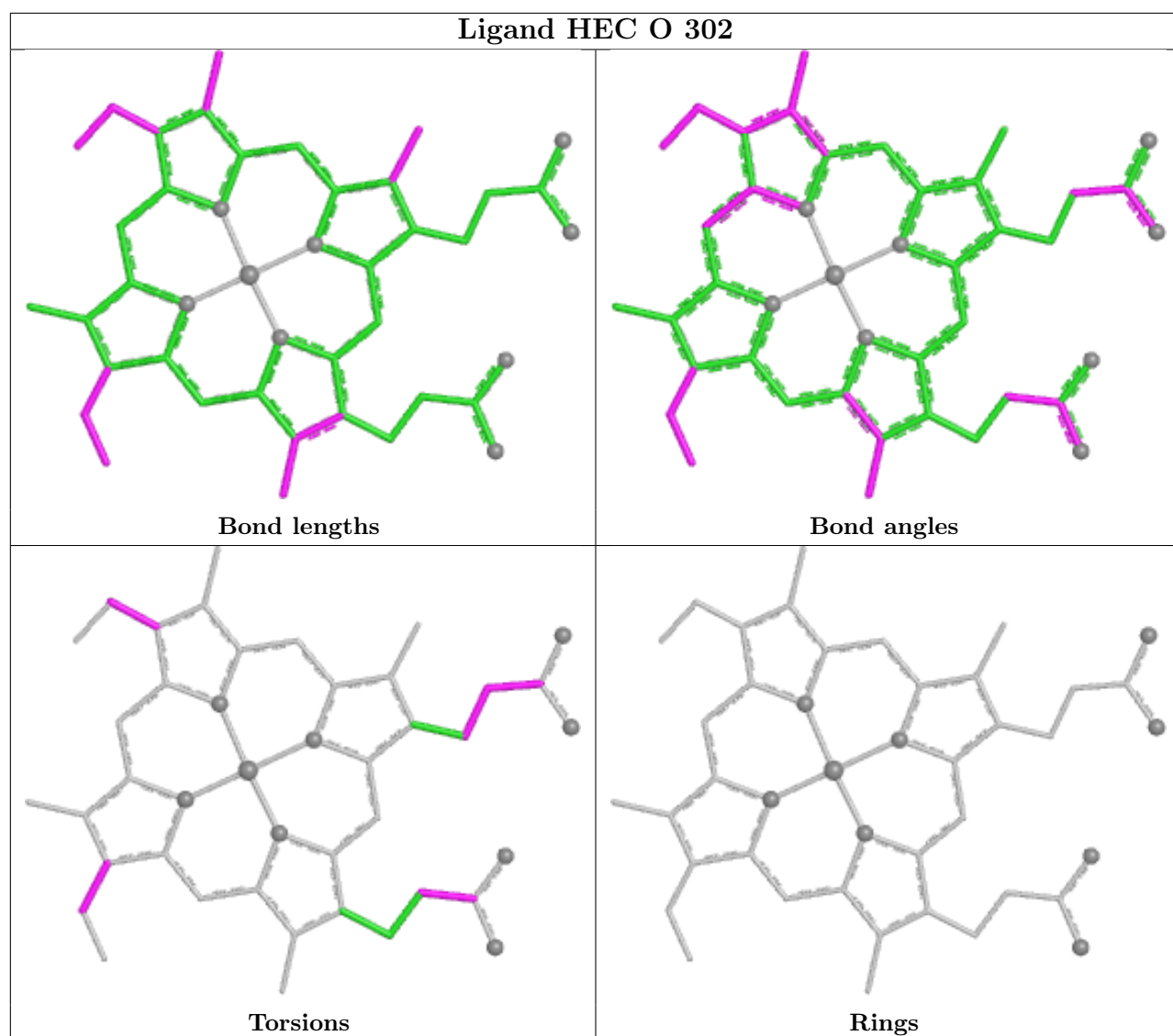
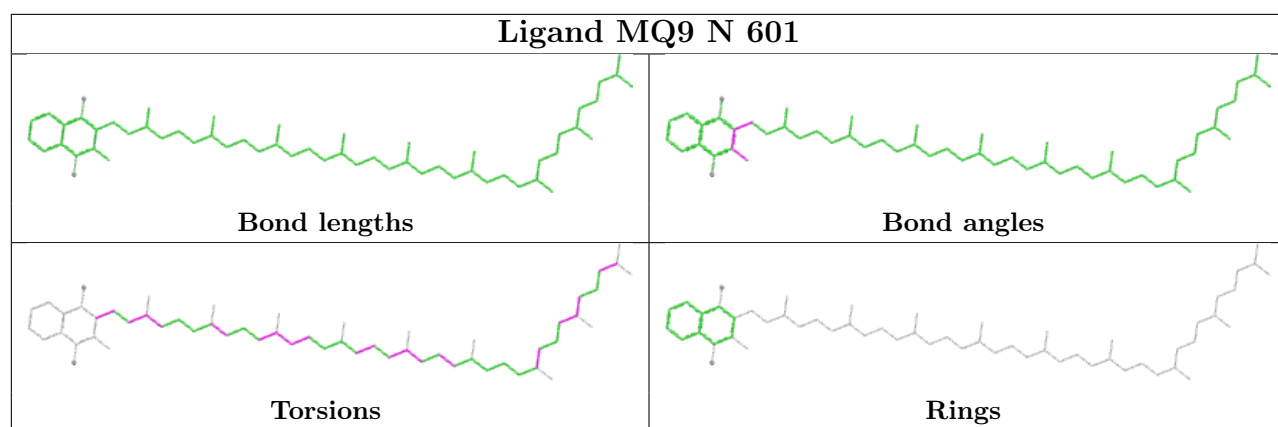


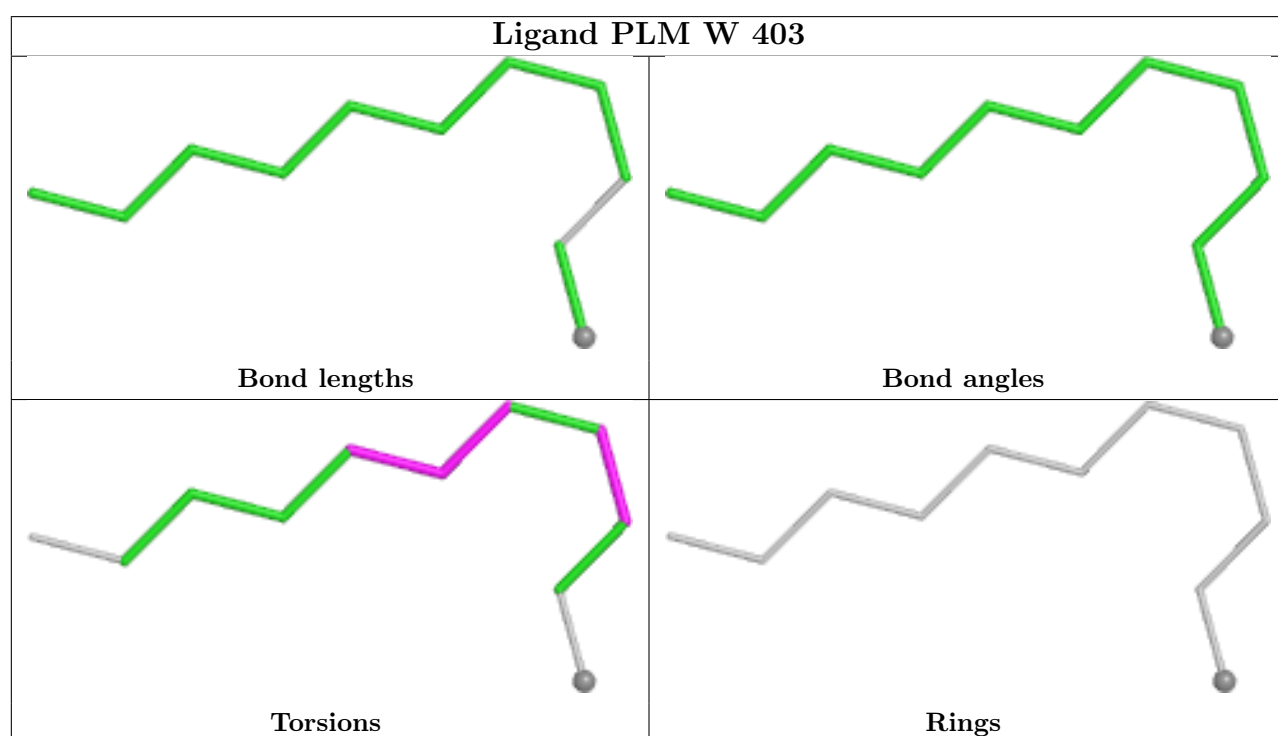
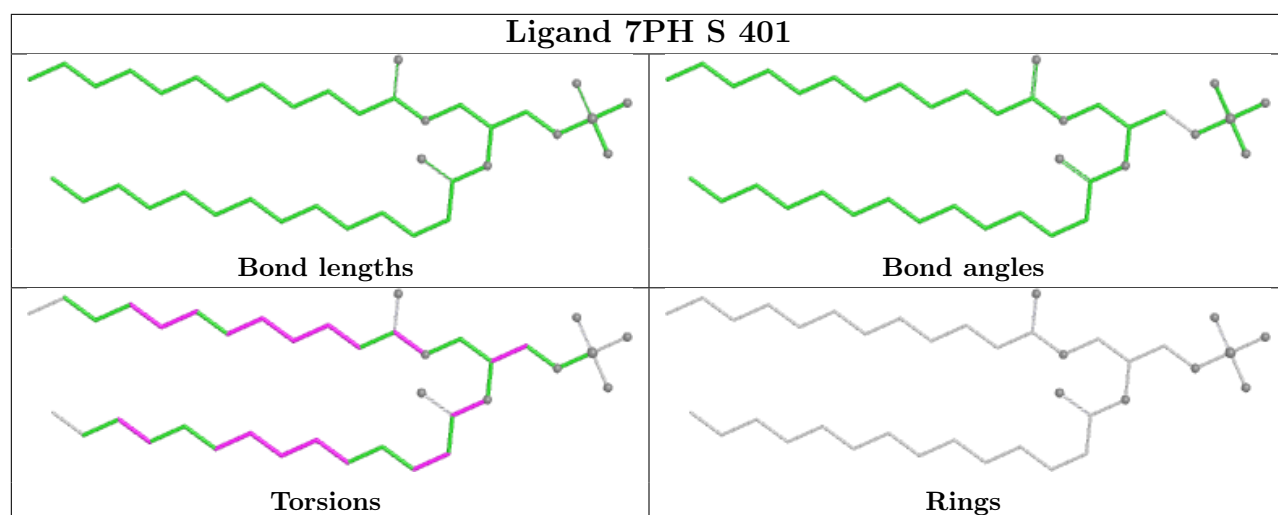
Torsions

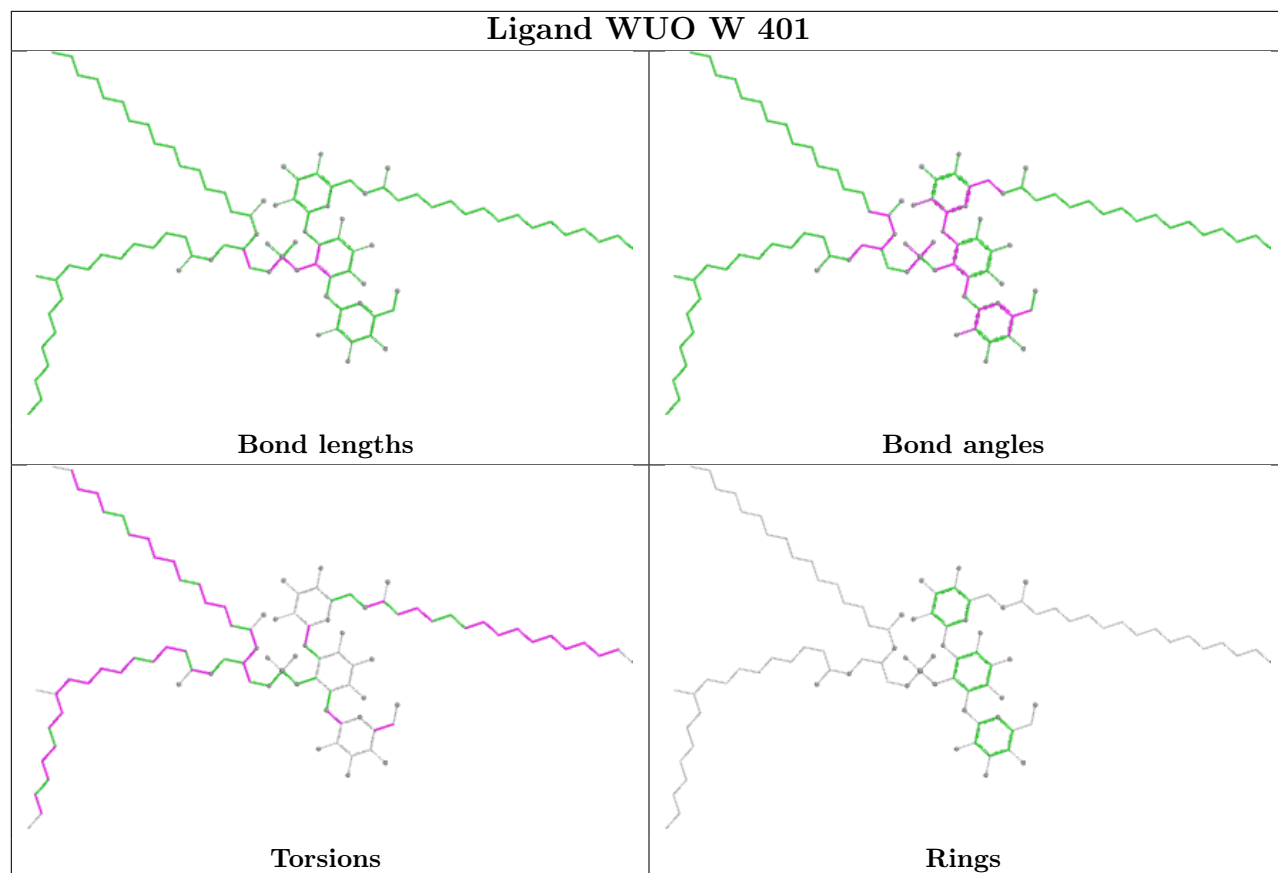


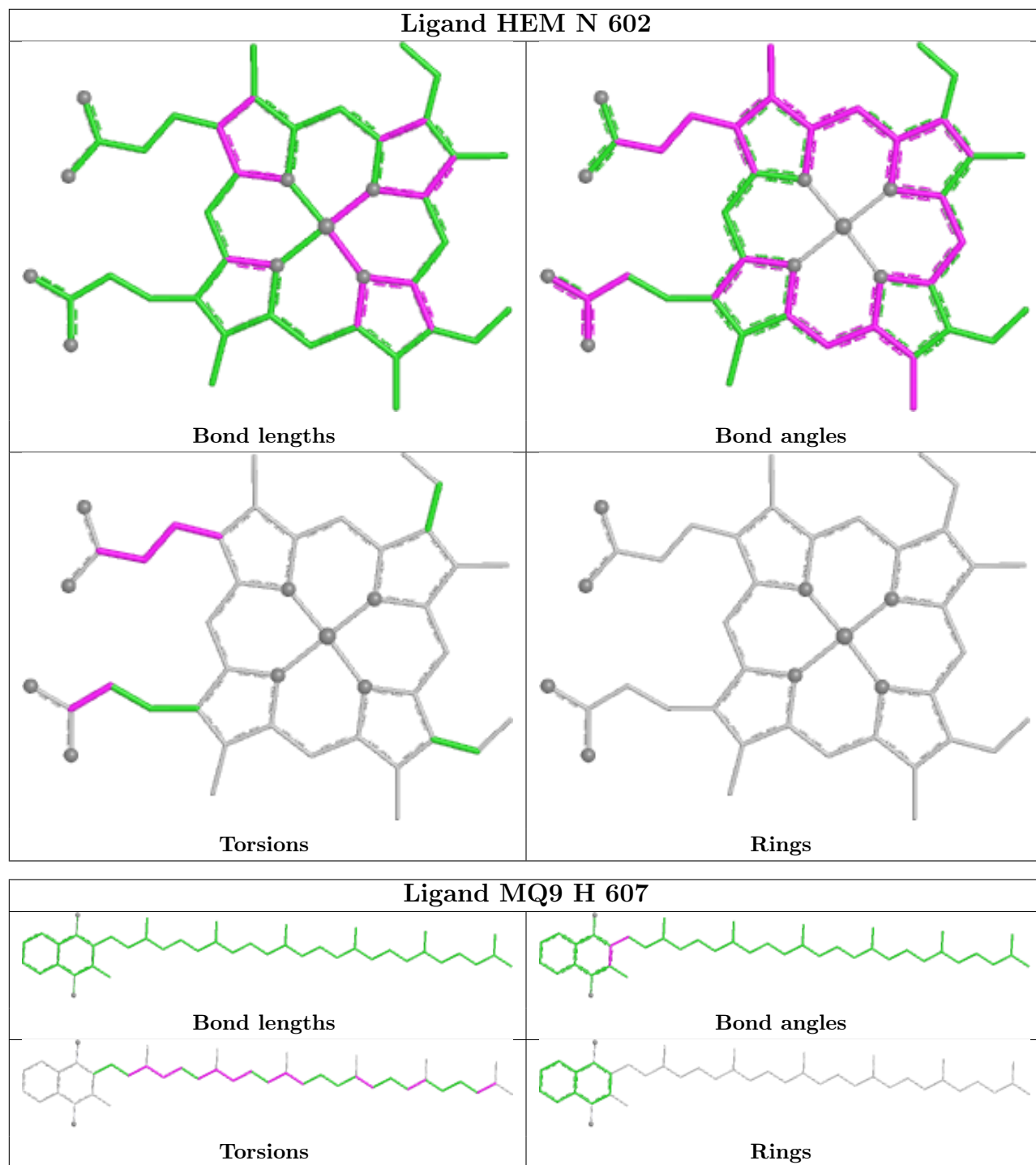
Rings

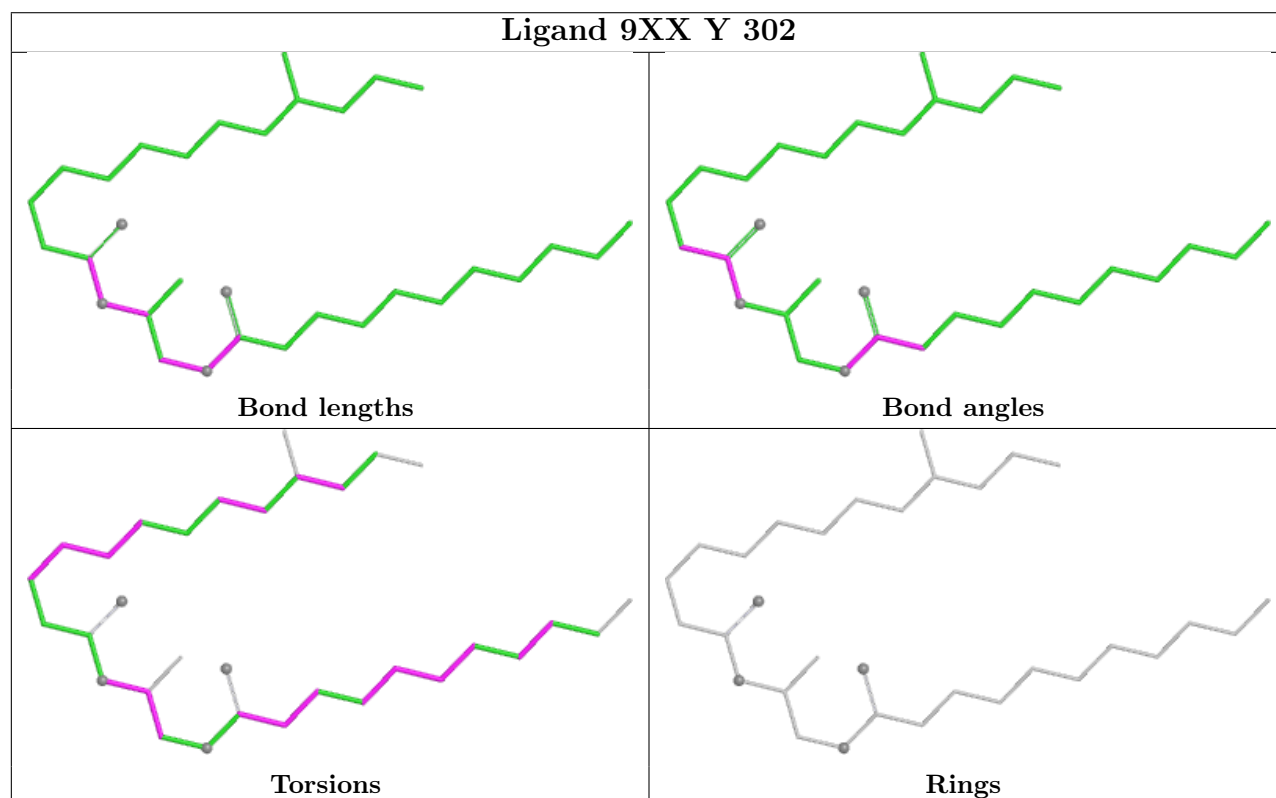
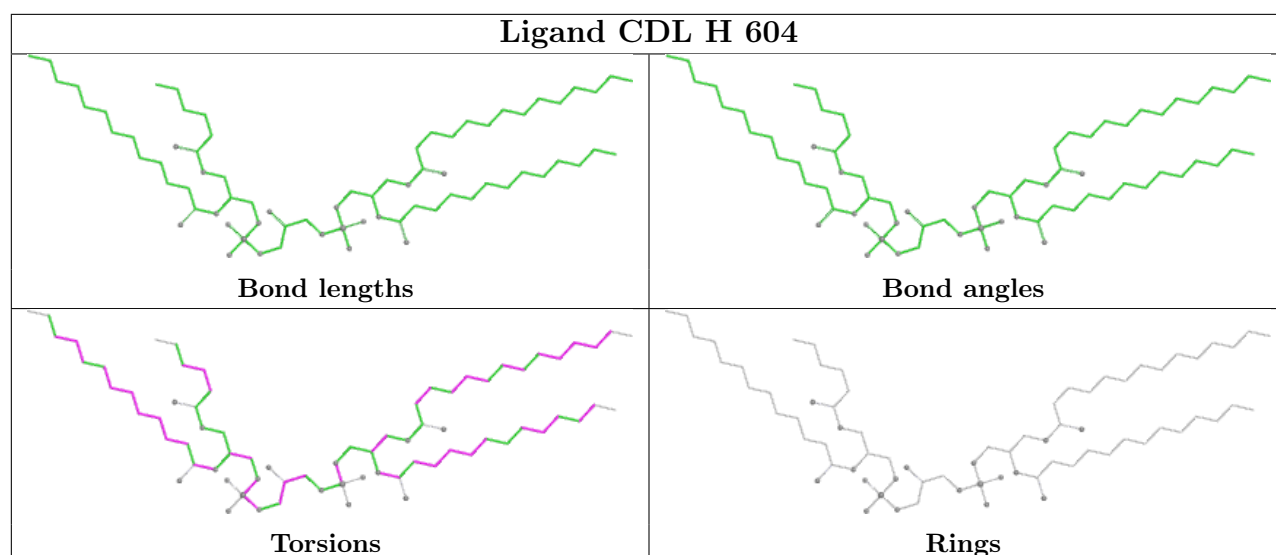


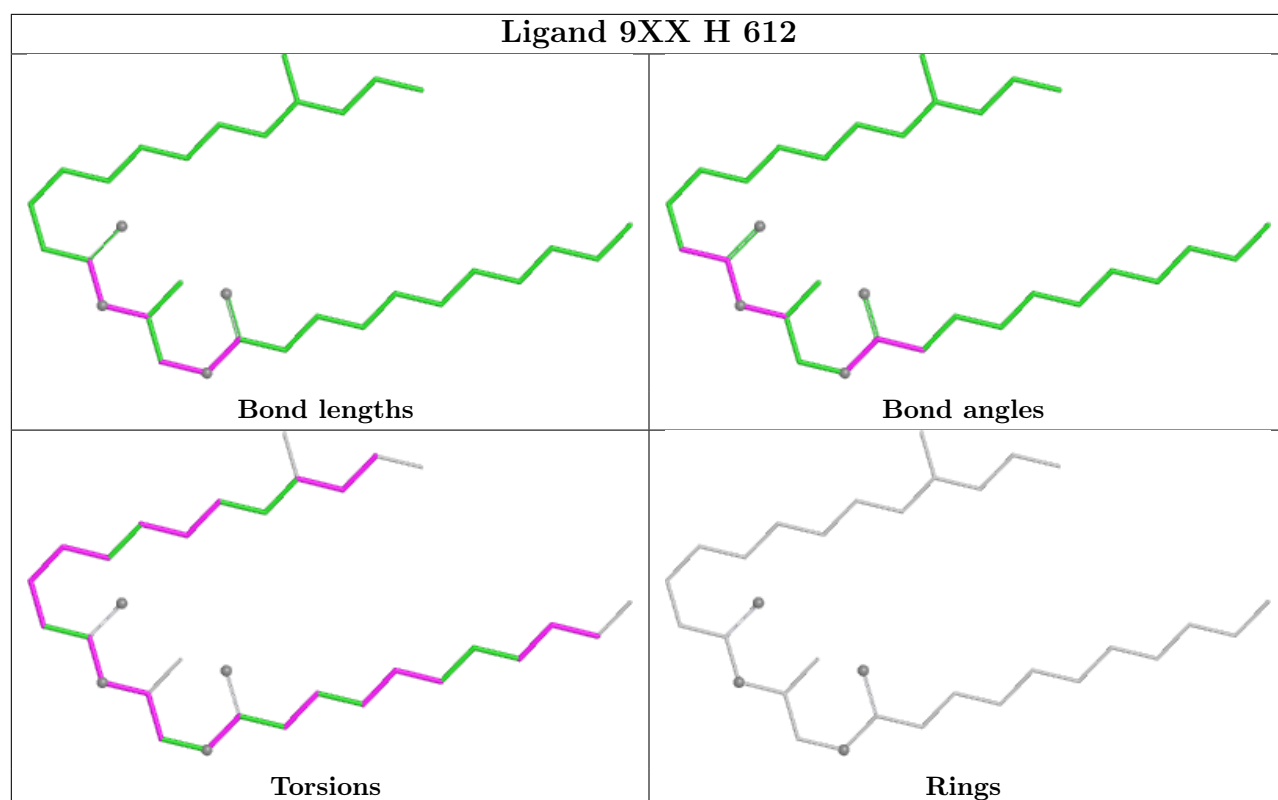


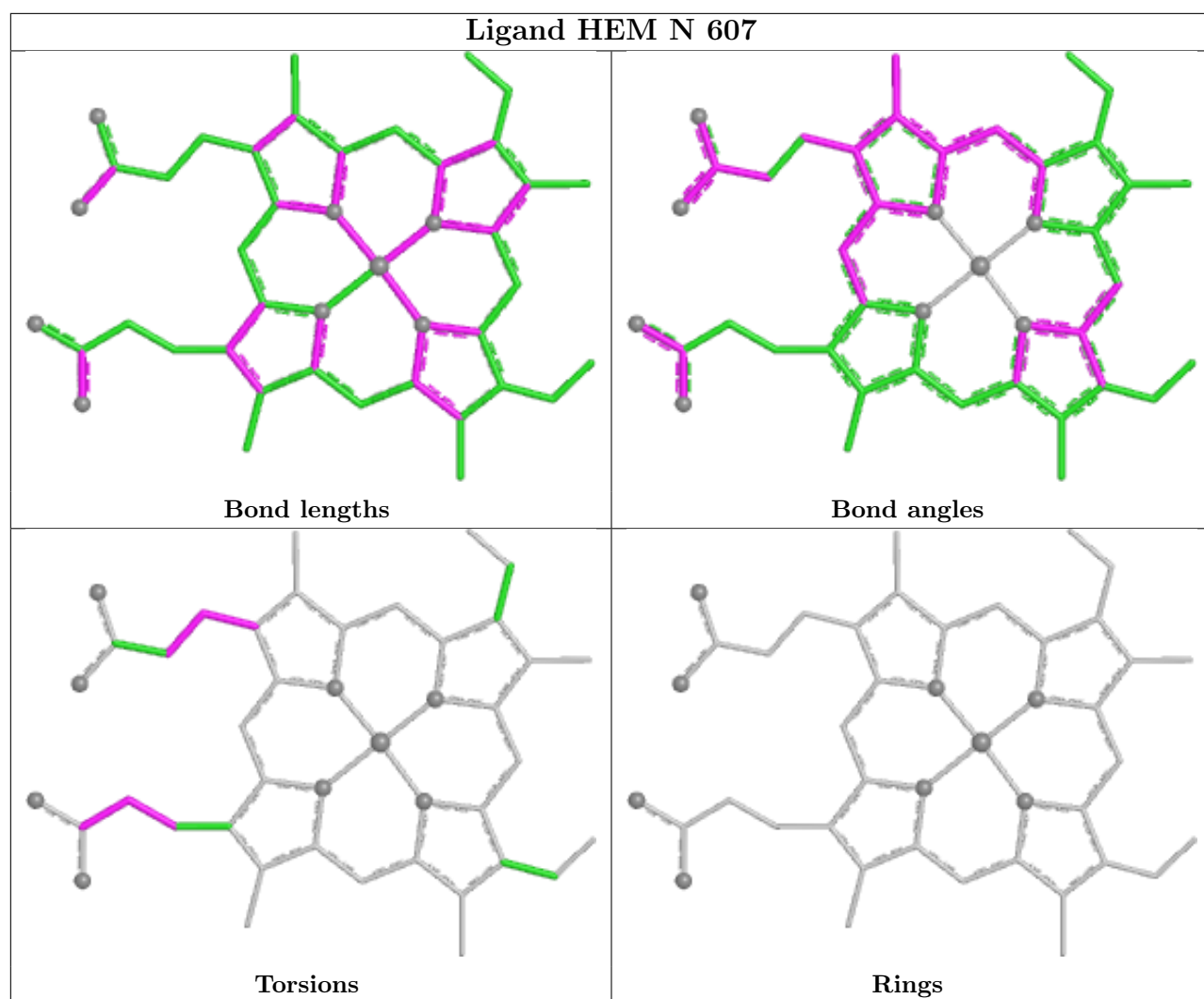


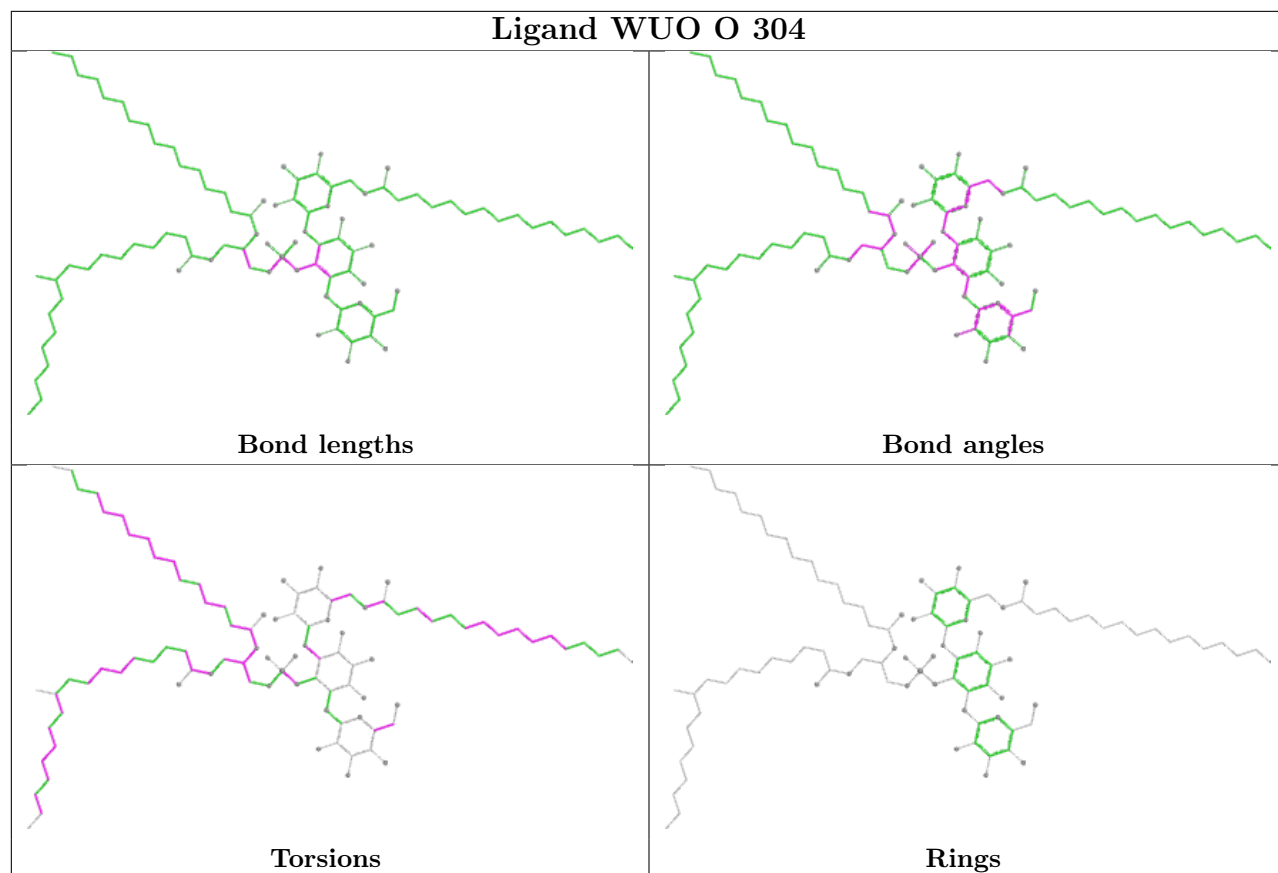


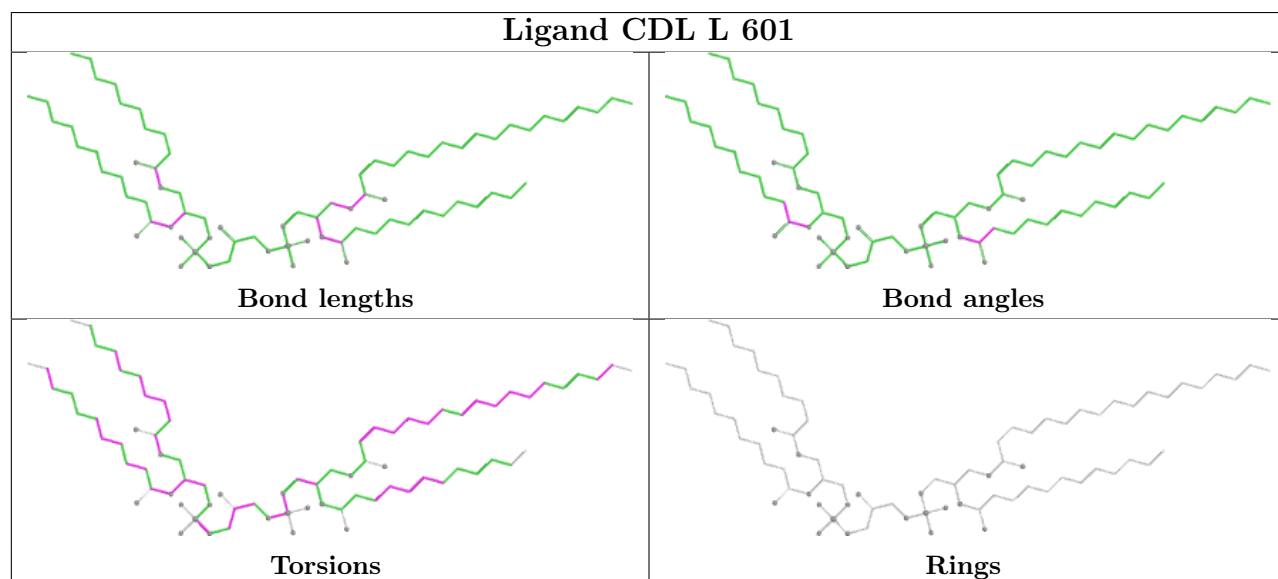
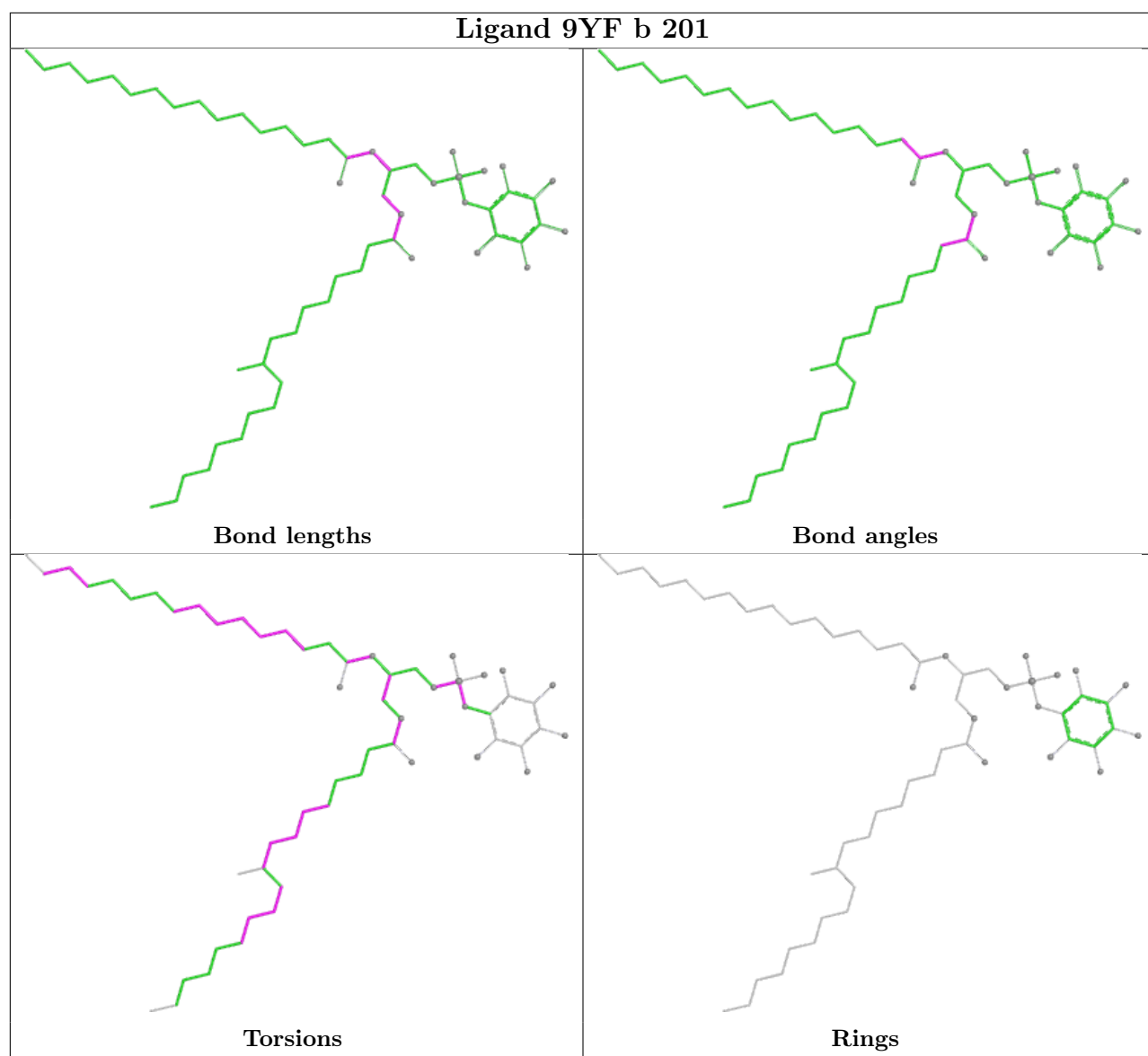


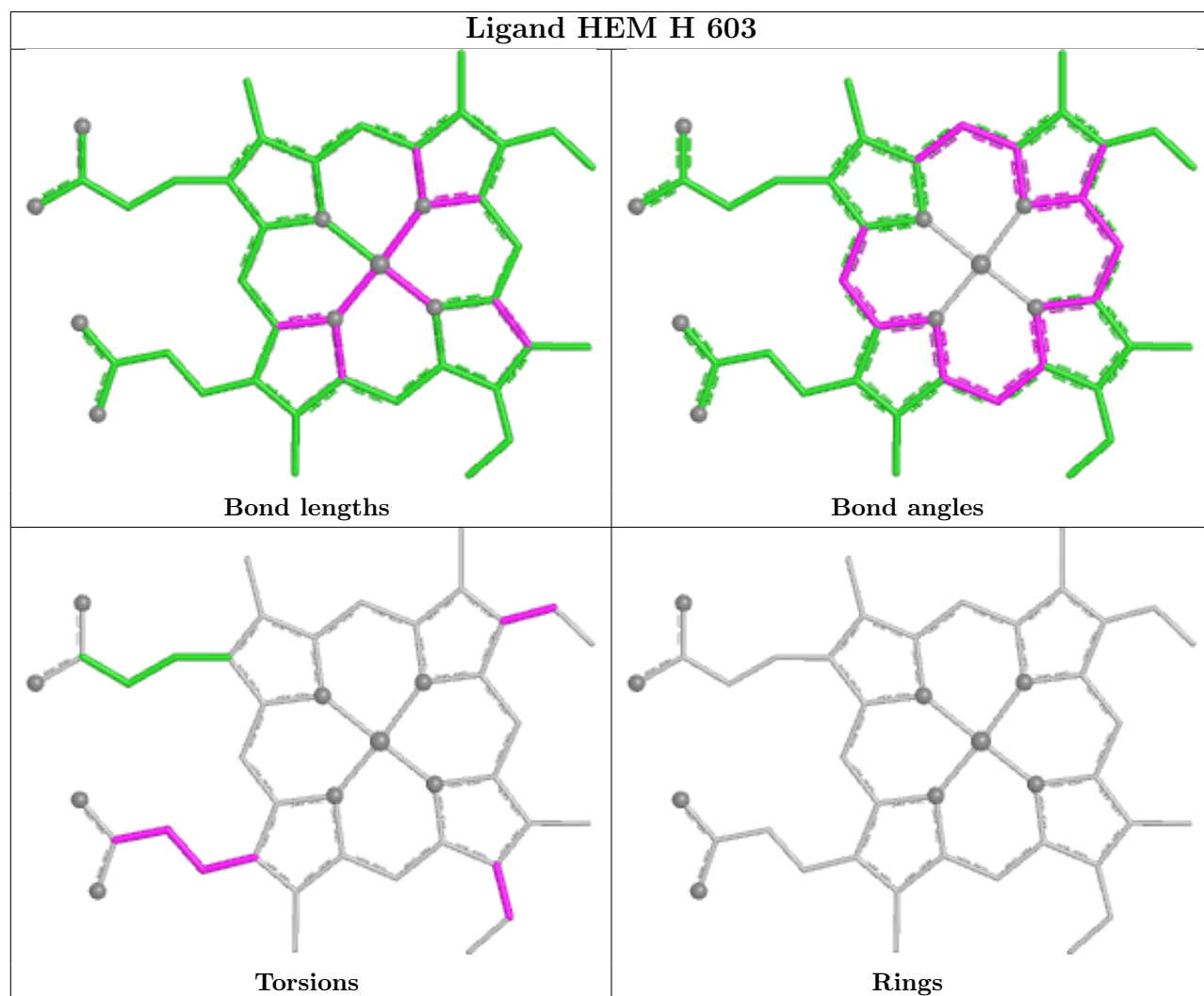
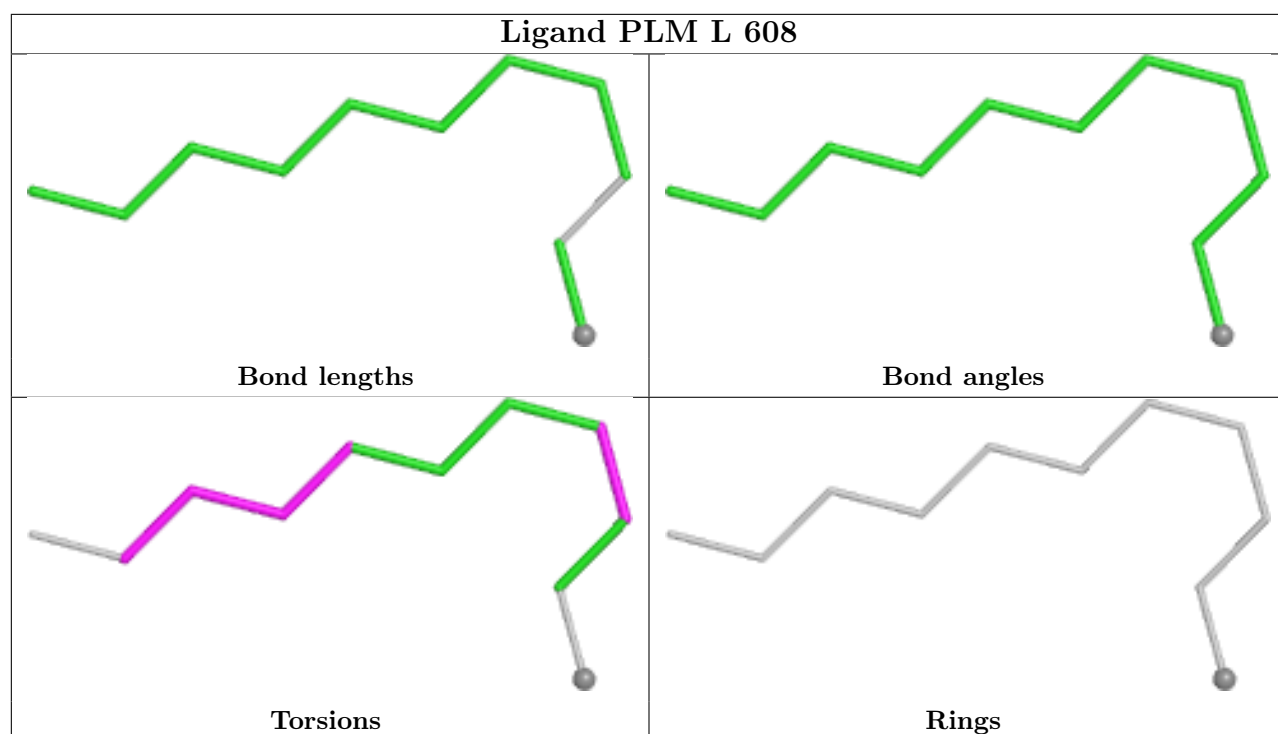


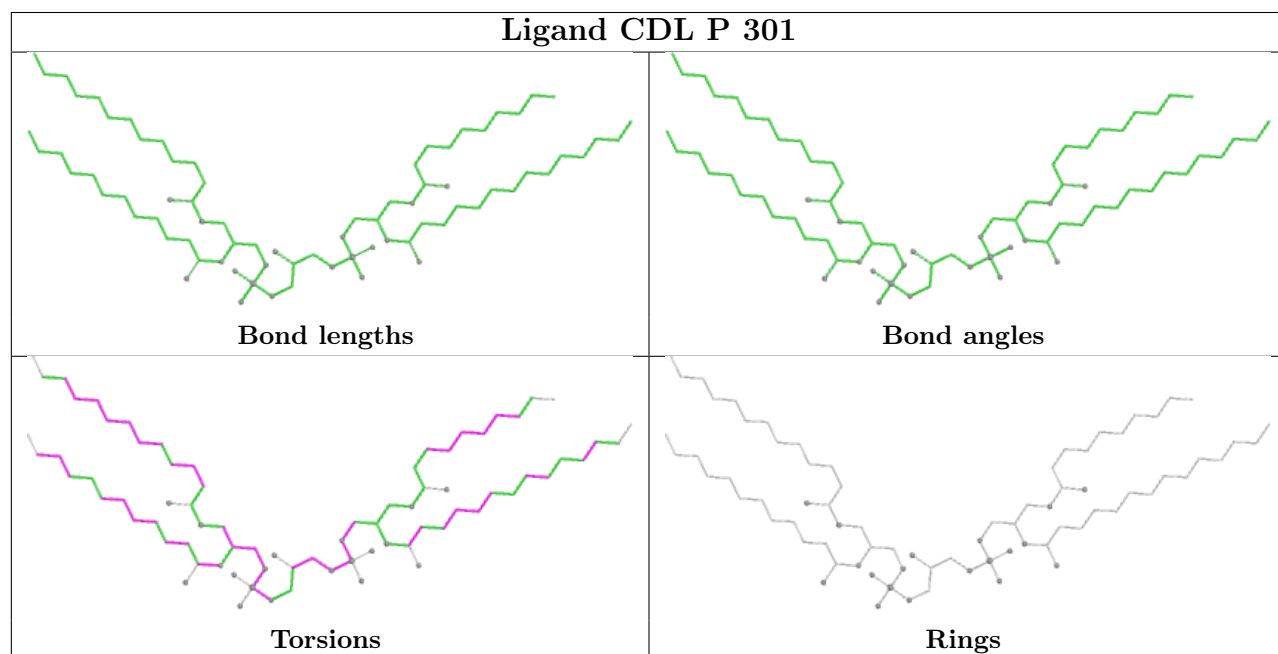
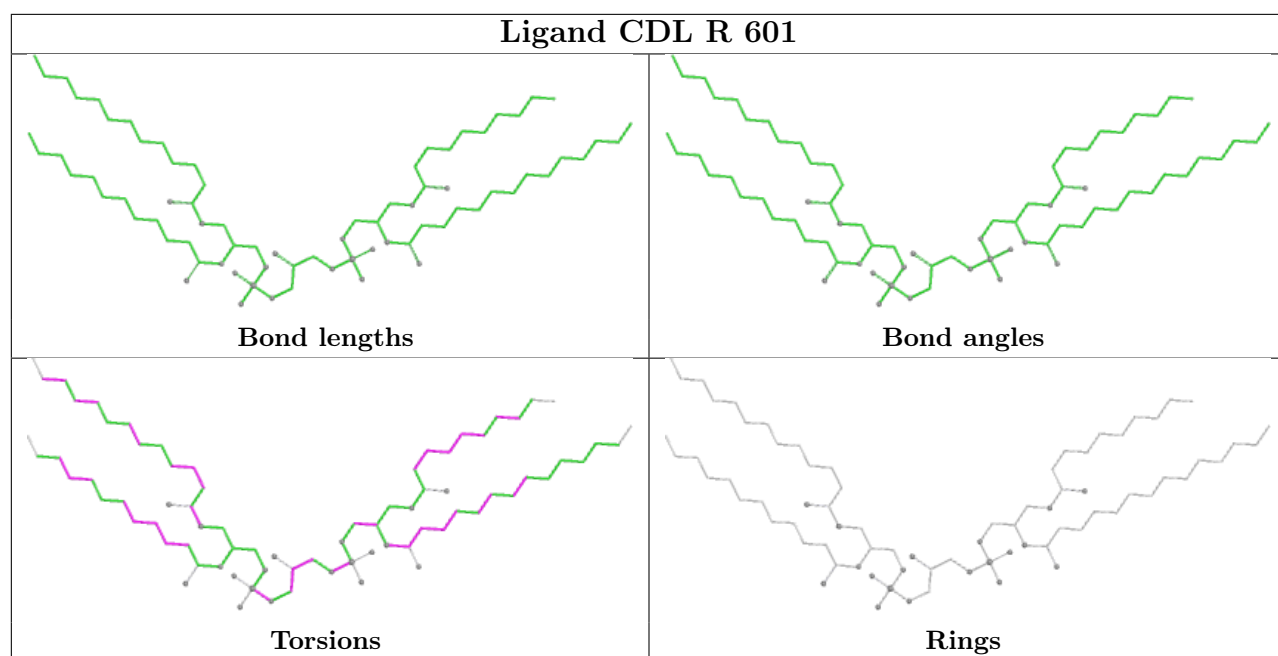


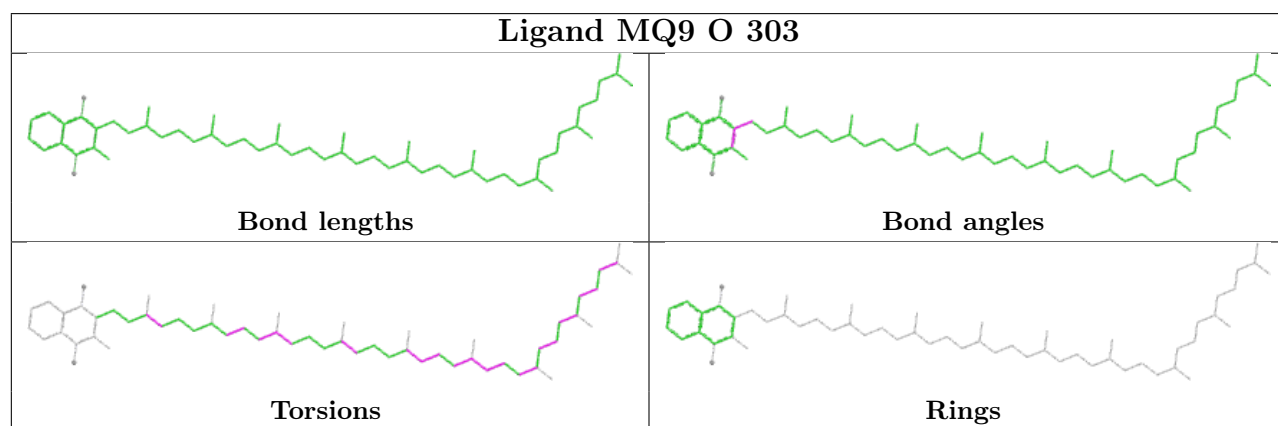
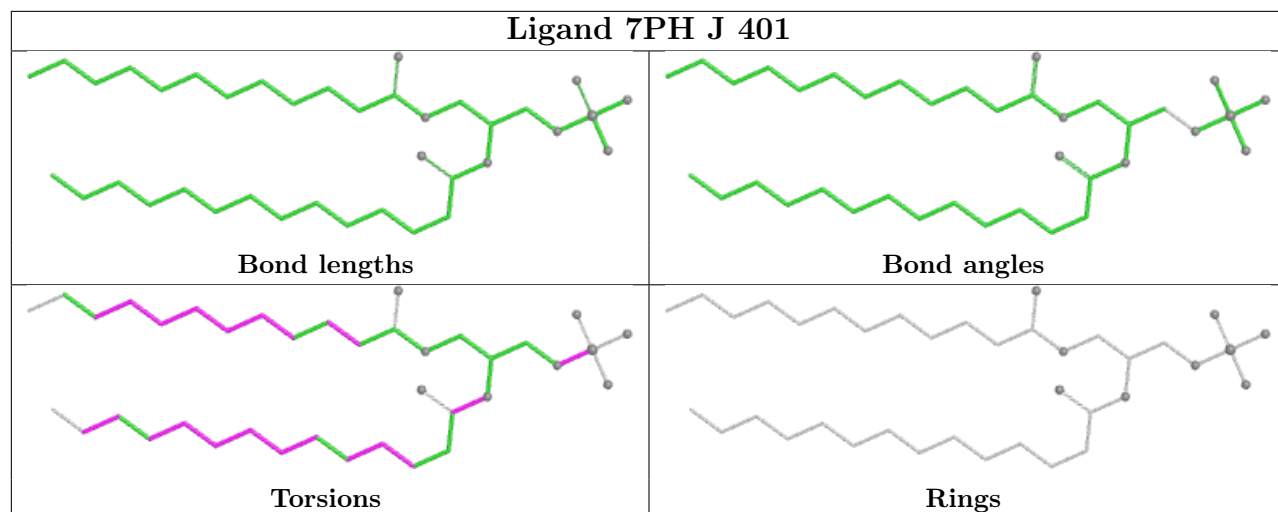




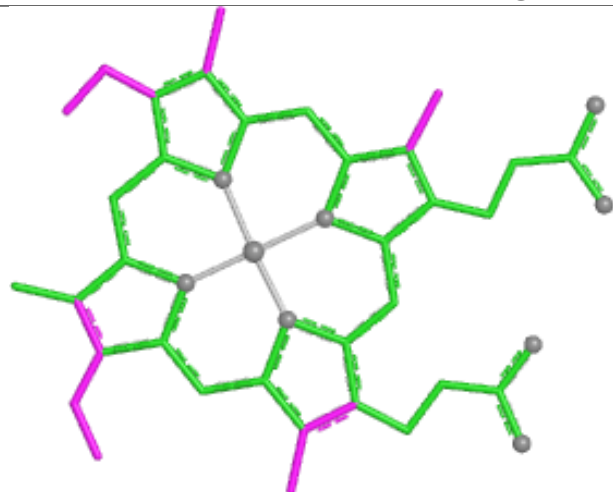




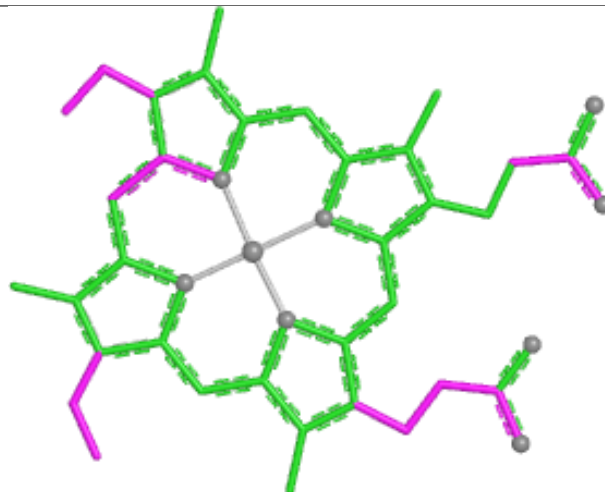




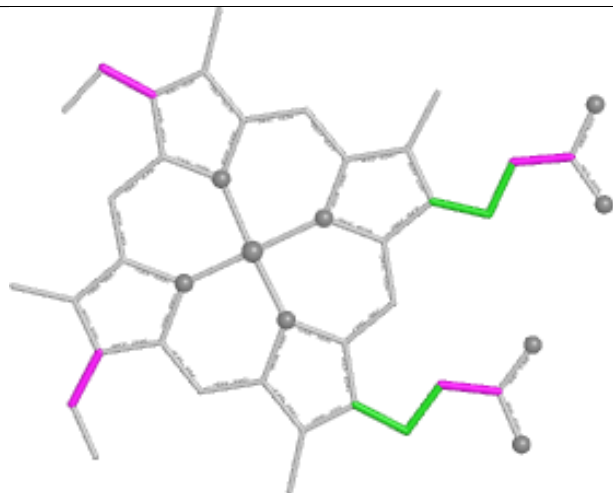
Ligand HEC O 301



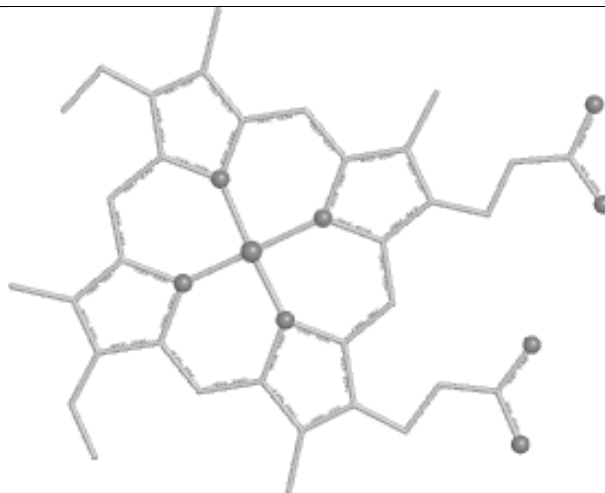
Bond lengths



Bond angles

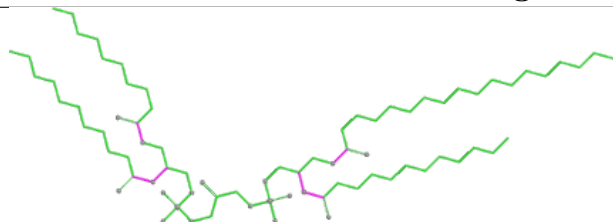


Torsions

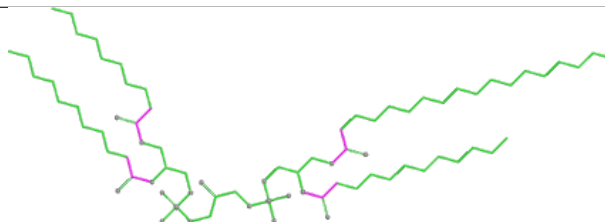


Rings

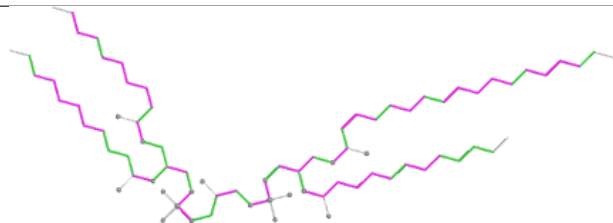
Ligand CDL G 504



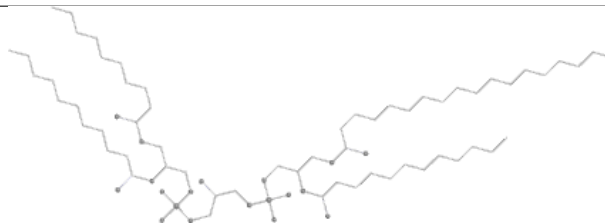
Bond lengths



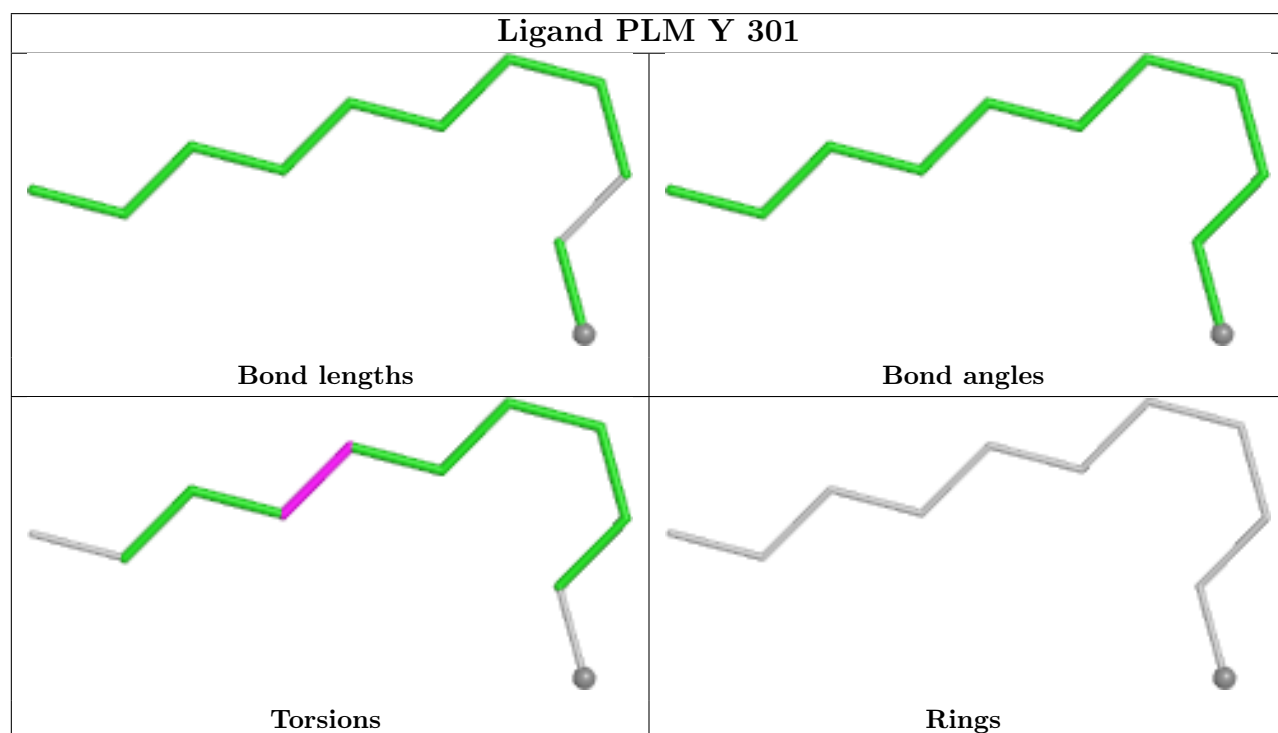
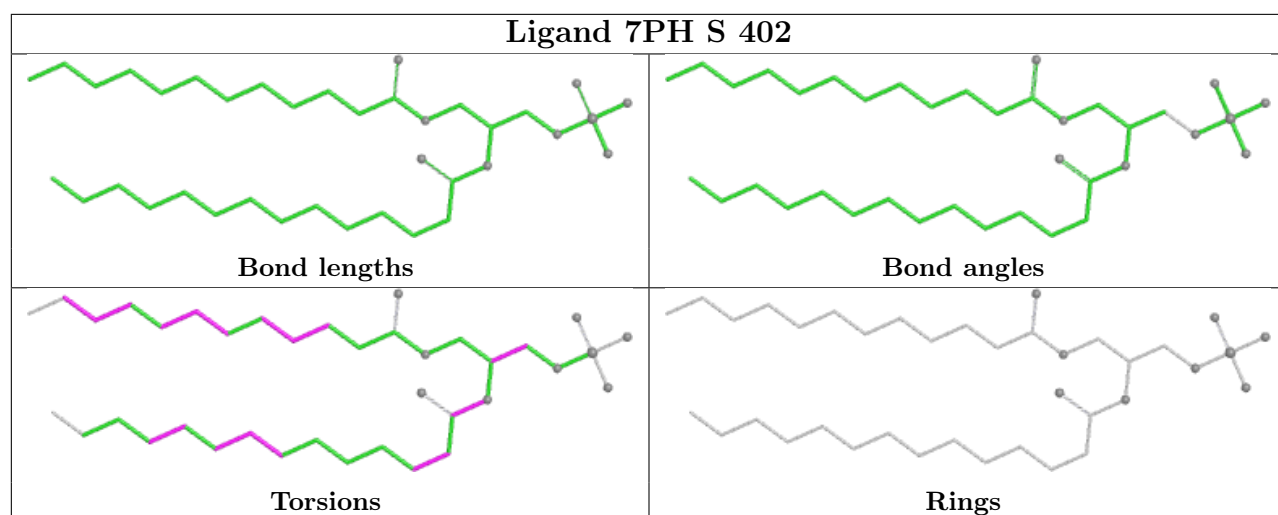
Bond angles

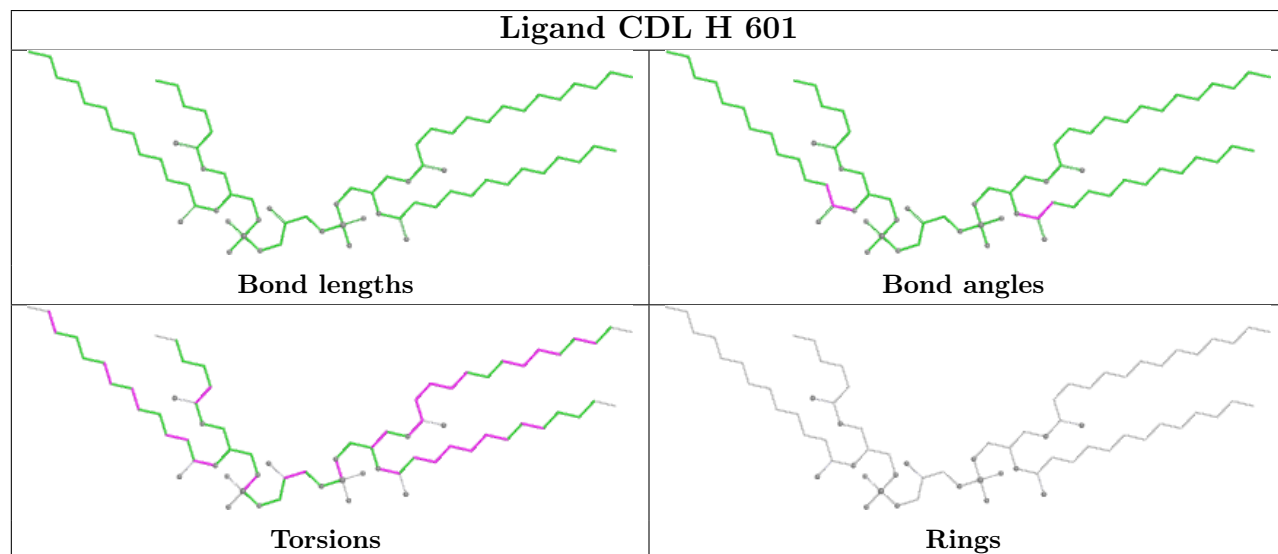
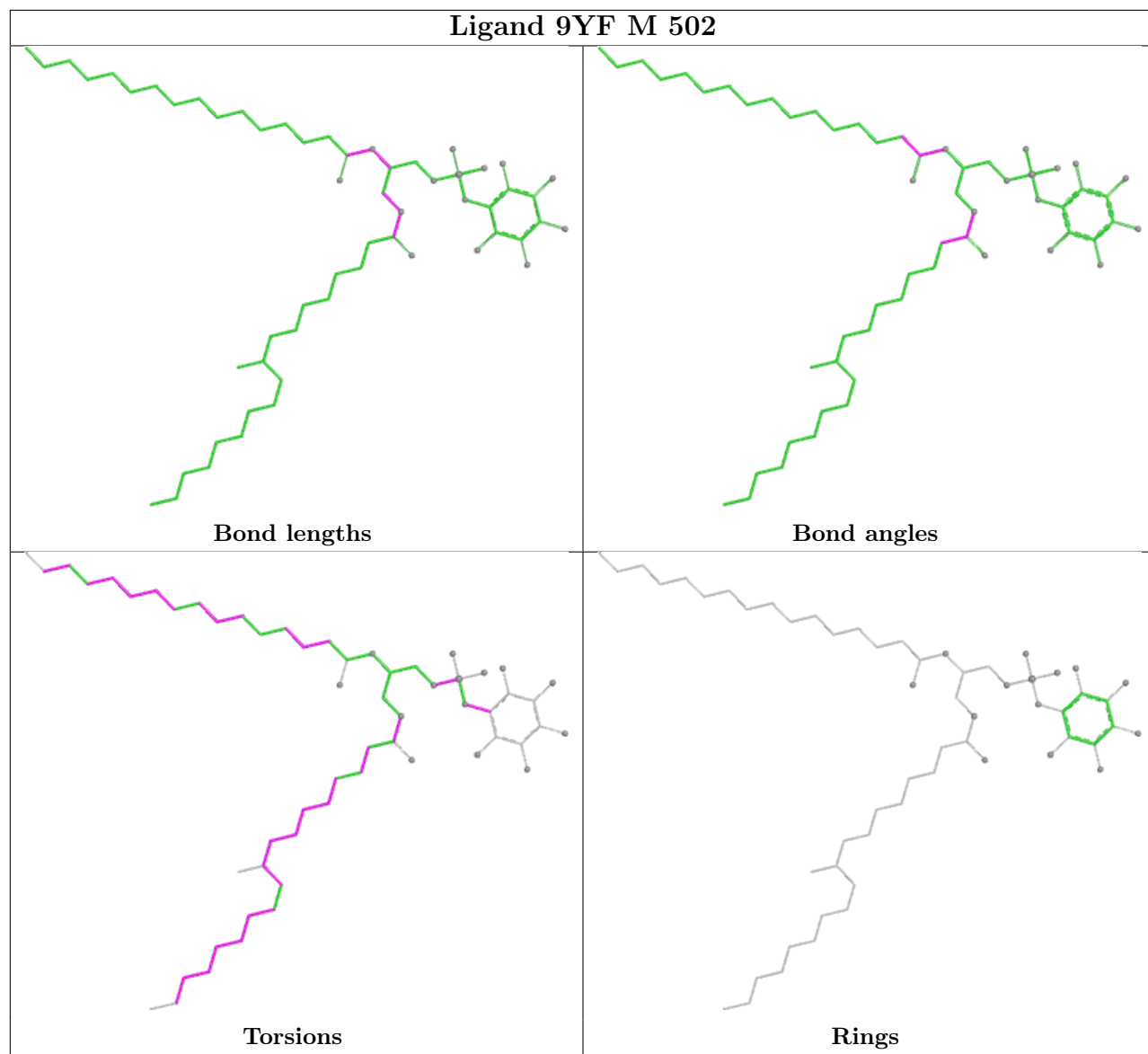


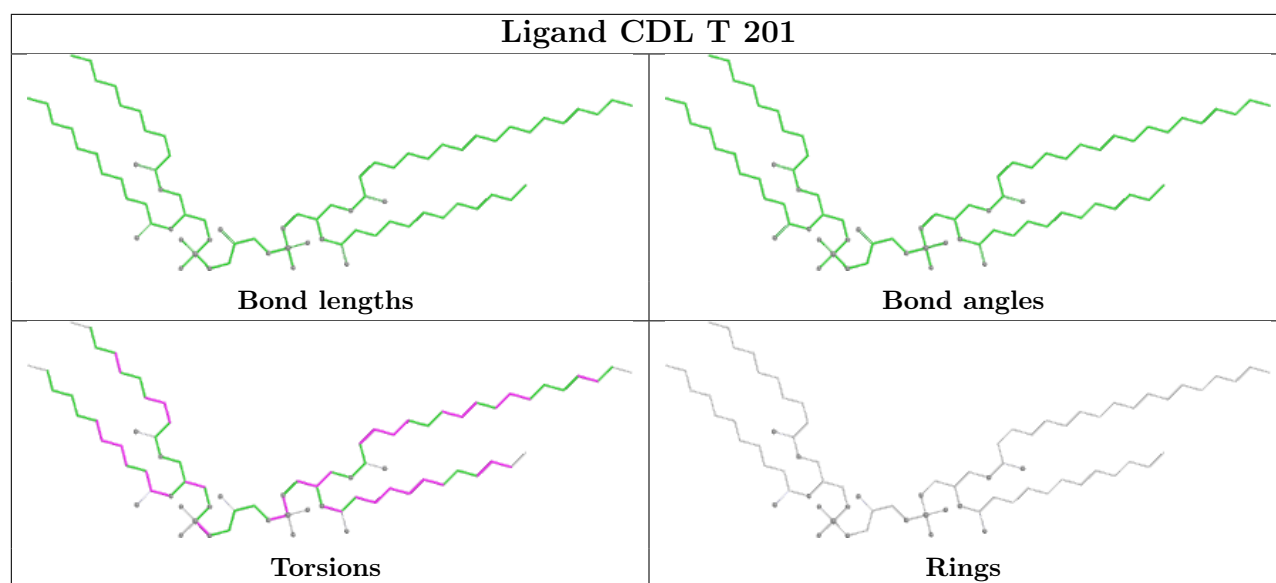
Torsions



Rings







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

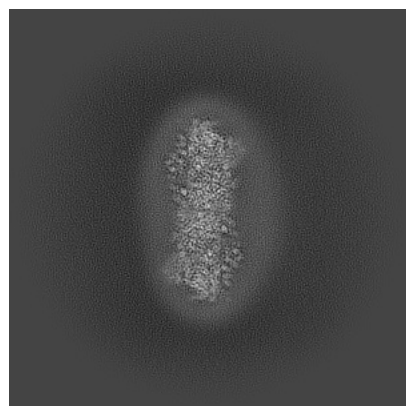
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-17210. These allow visual inspection of the internal detail of the map and identification of artifacts.

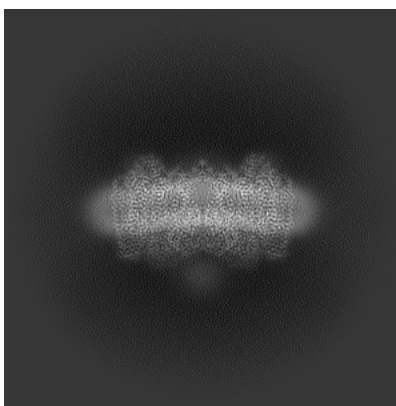
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

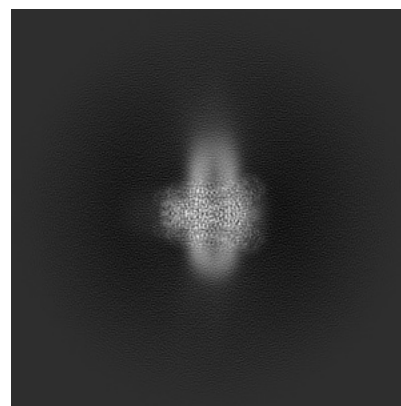
6.1.1 Primary map



X

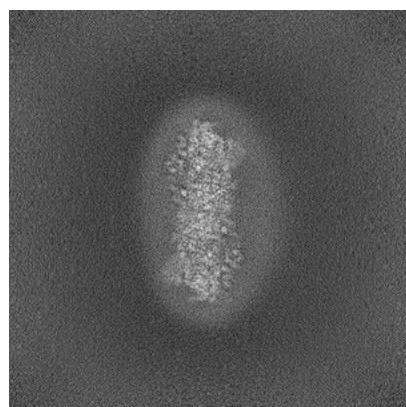


Y

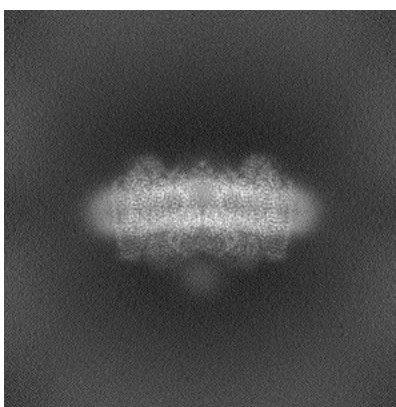


Z

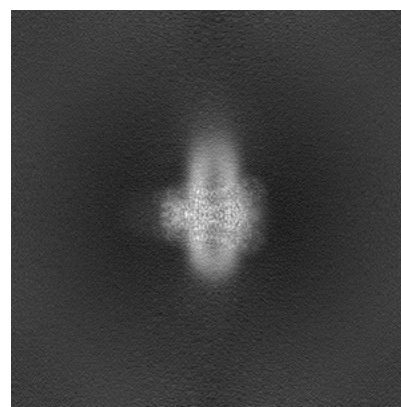
6.1.2 Raw map



X



Y

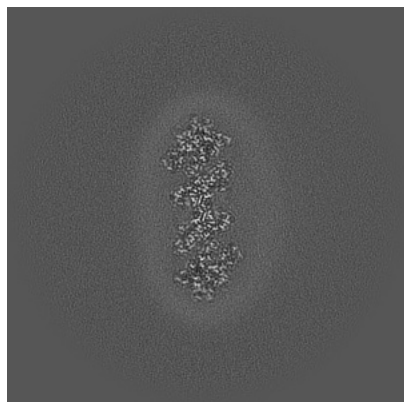


Z

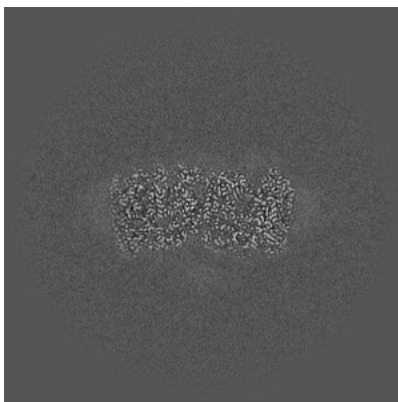
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

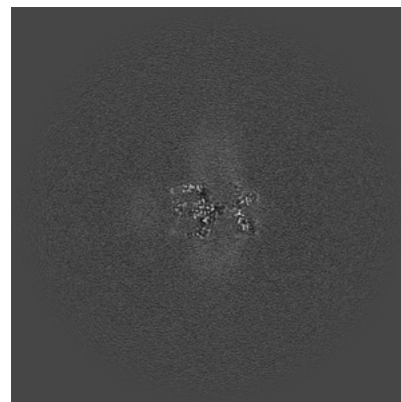
6.2.1 Primary map



X Index: 270

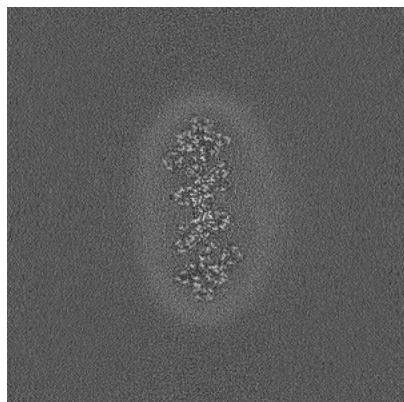


Y Index: 270

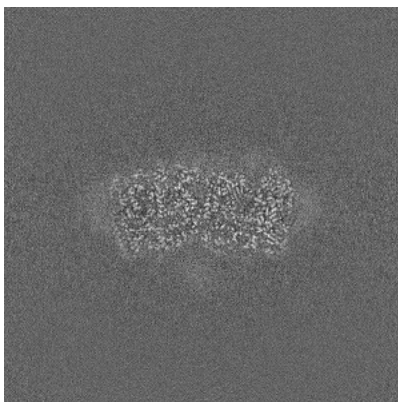


Z Index: 270

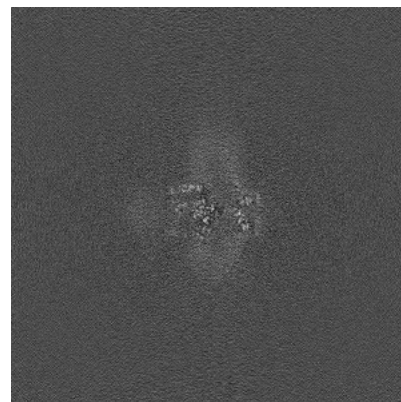
6.2.2 Raw map



X Index: 270



Y Index: 270

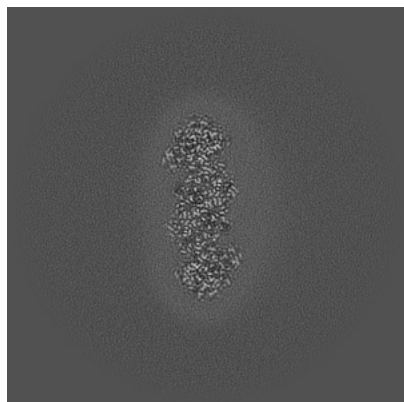


Z Index: 270

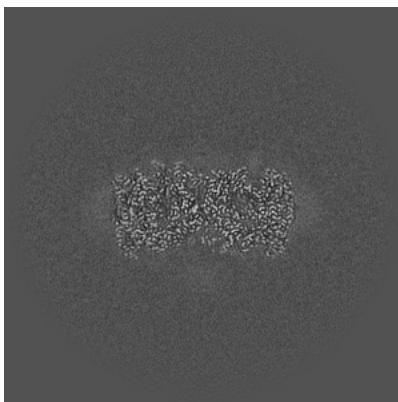
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

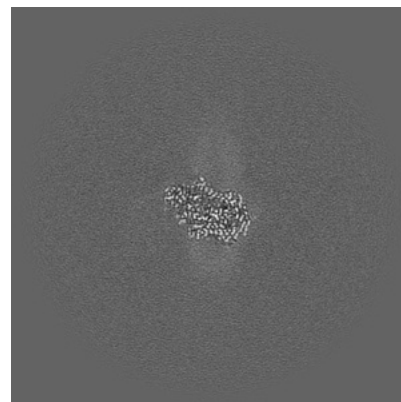
6.3.1 Primary map



X Index: 255

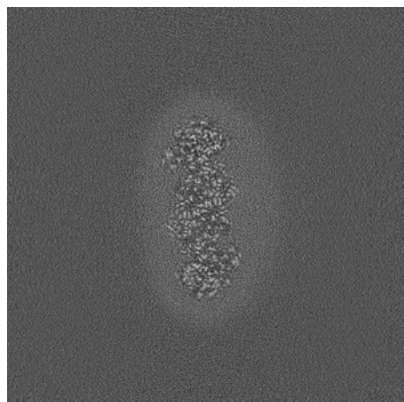


Y Index: 267

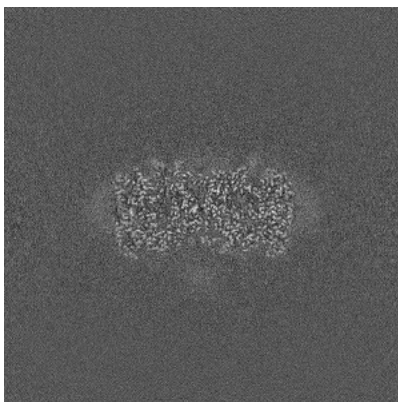


Z Index: 293

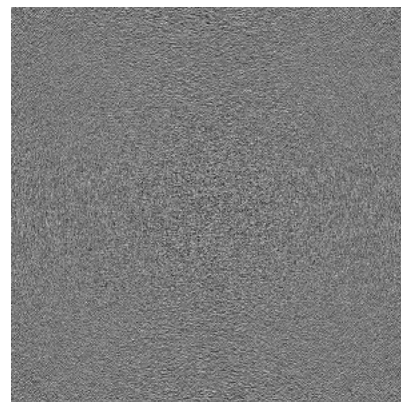
6.3.2 Raw map



X Index: 255



Y Index: 267

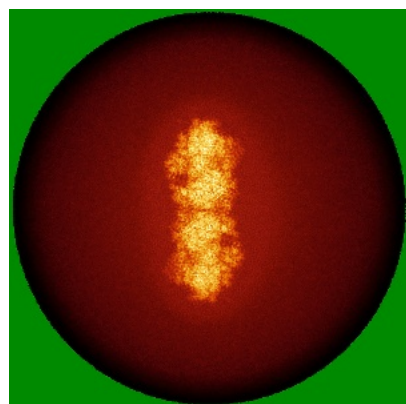


Z Index: 0

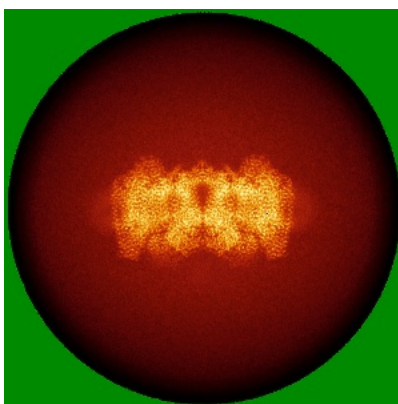
The images above show the largest variance slices of the map in three orthogonal directions.

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

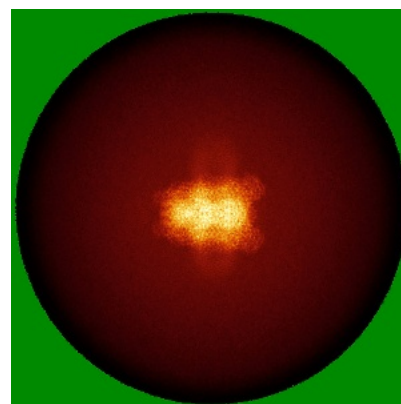
6.4.1 Primary map



X

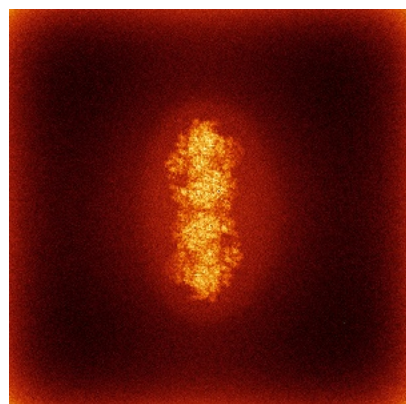


Y

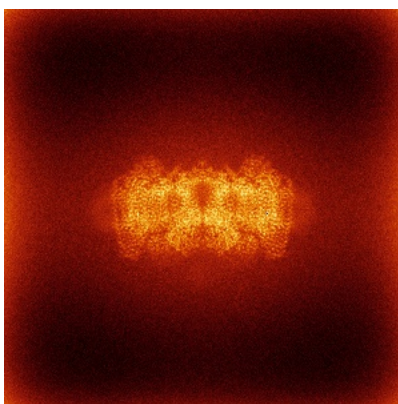


Z

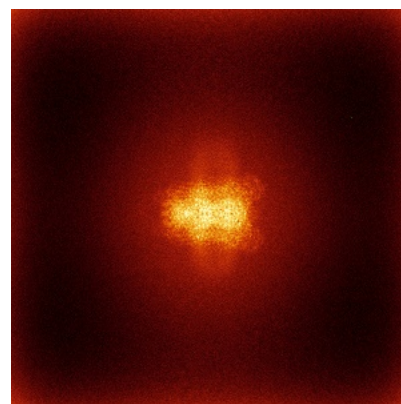
6.4.2 Raw map



X



Y

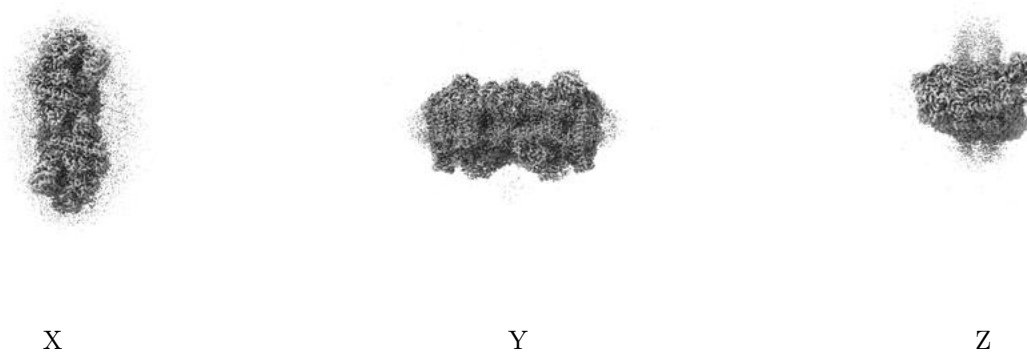


Z

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.

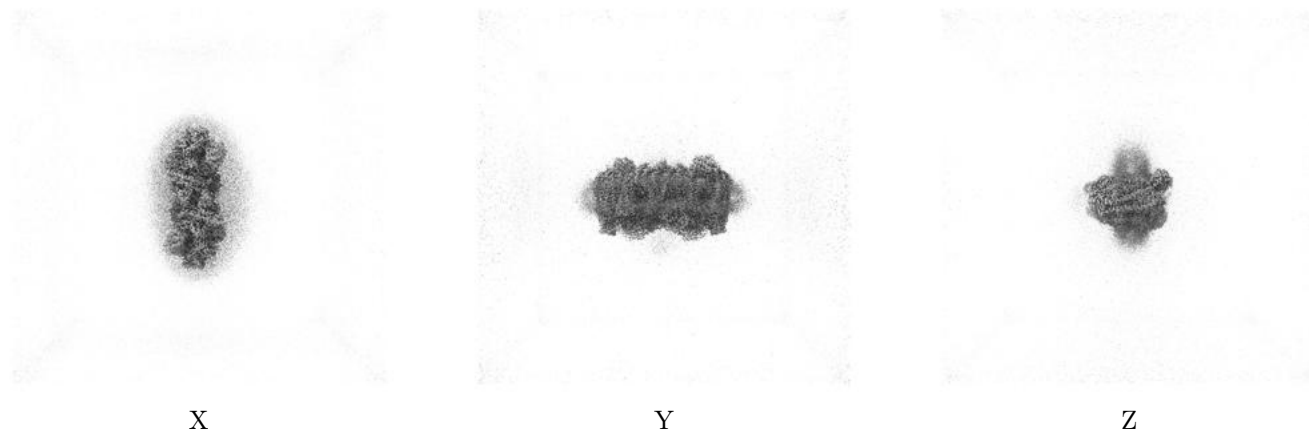
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.194. 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.

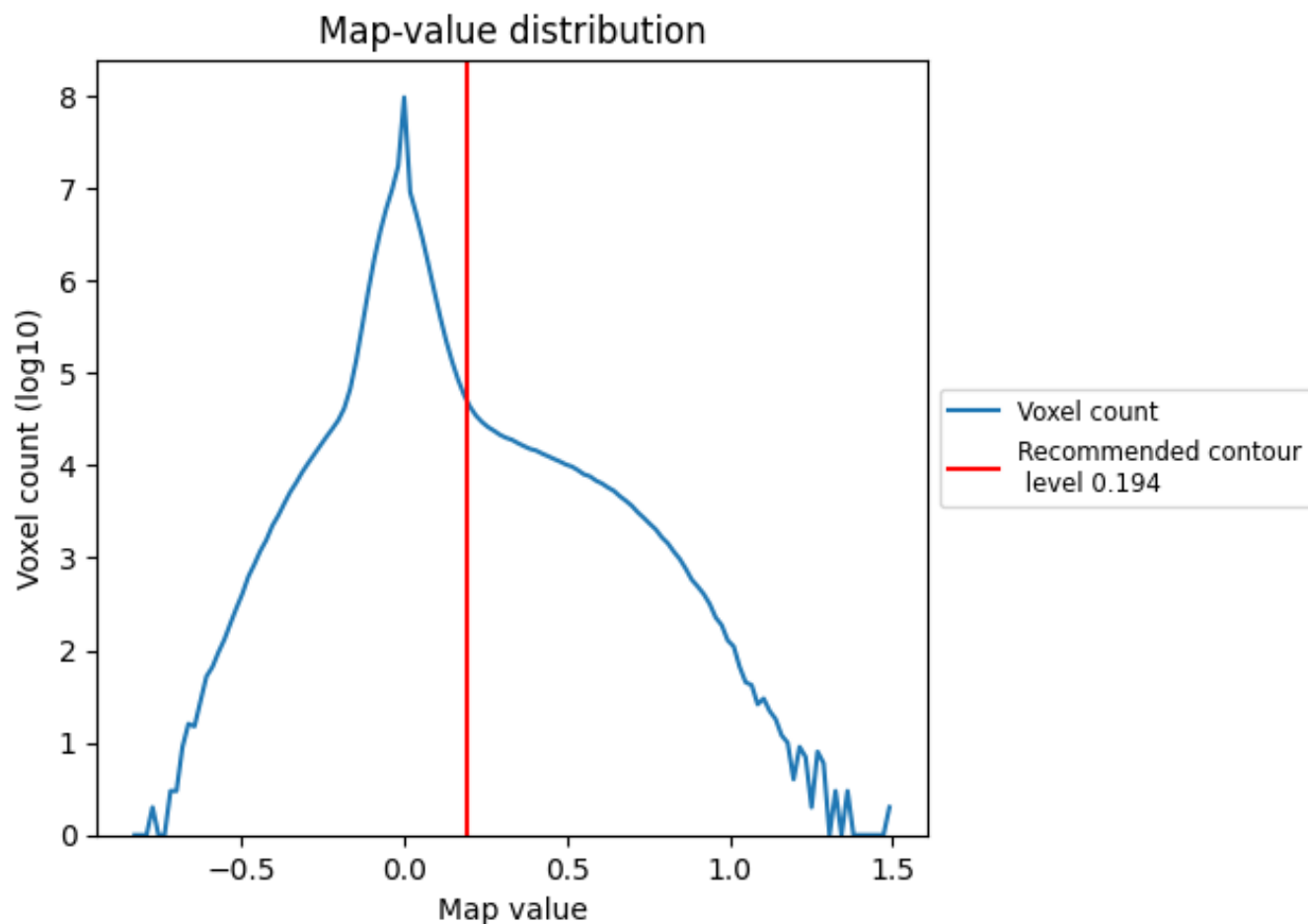
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

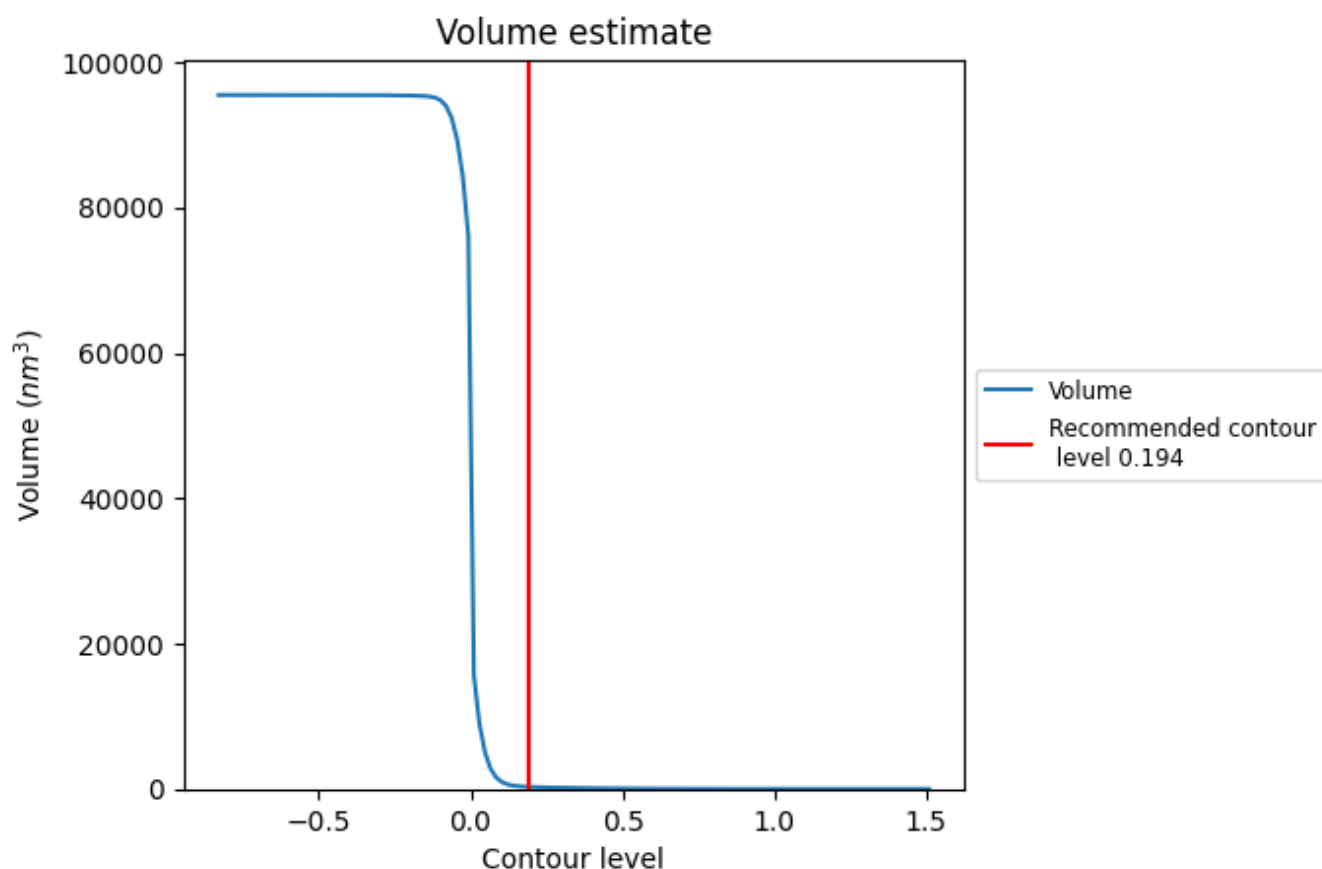
This section contains the results of statistical analysis of the map.

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.

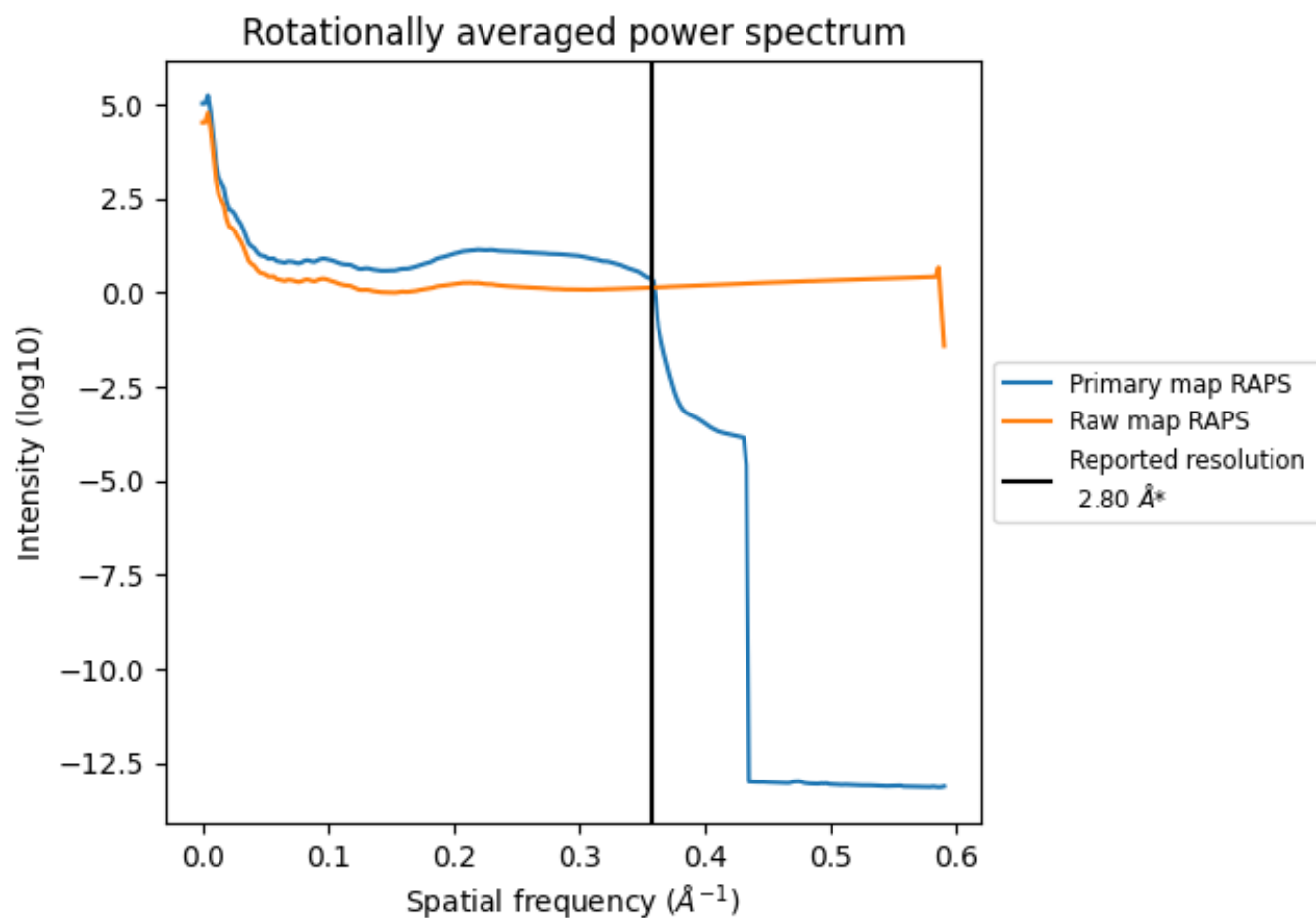
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 274 nm^3 ; this corresponds to an approximate mass of 247 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 ⓘ

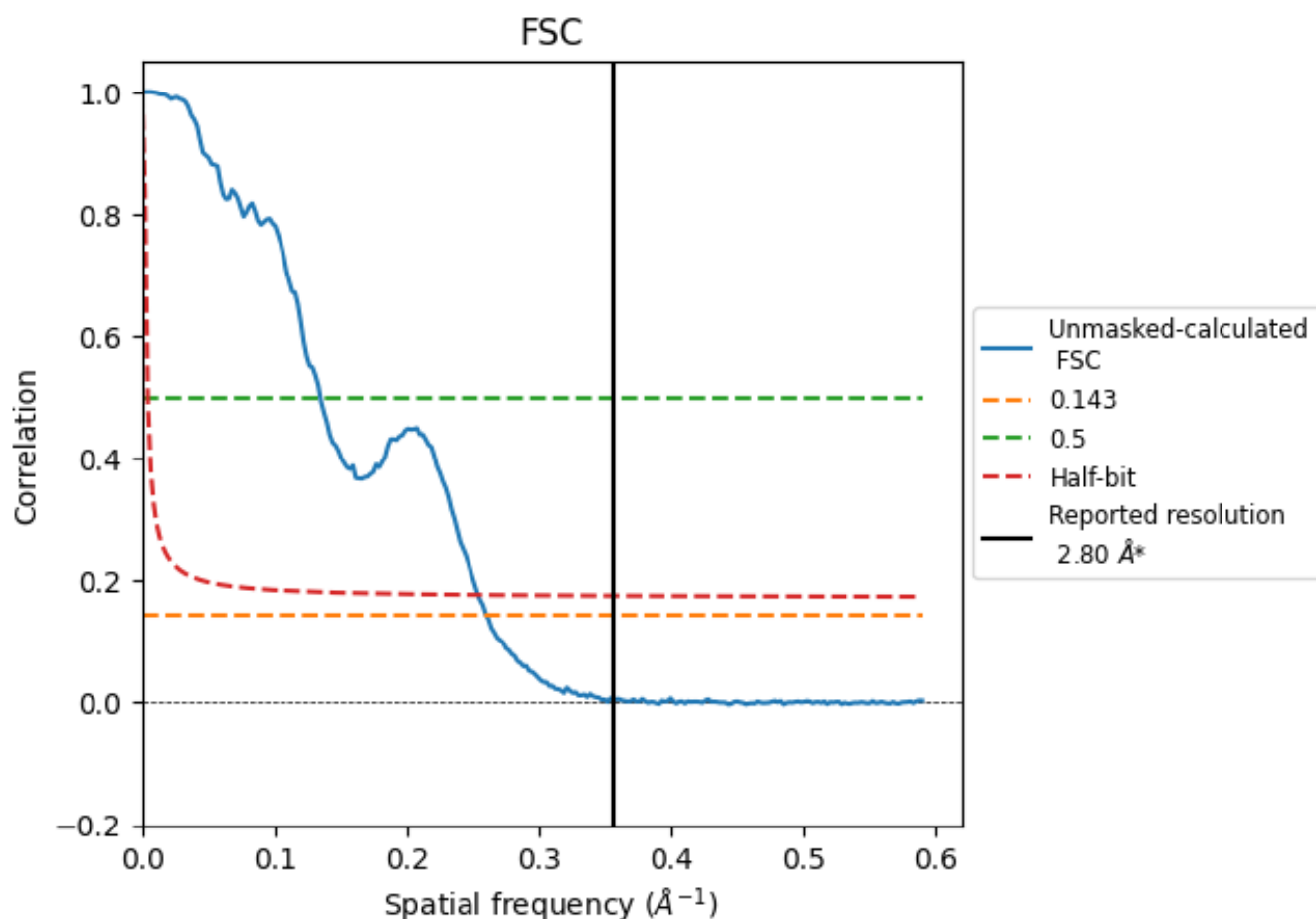


*Reported resolution corresponds to spatial frequency of 0.357 $\text{\AA}^{-1}$

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 0.357 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

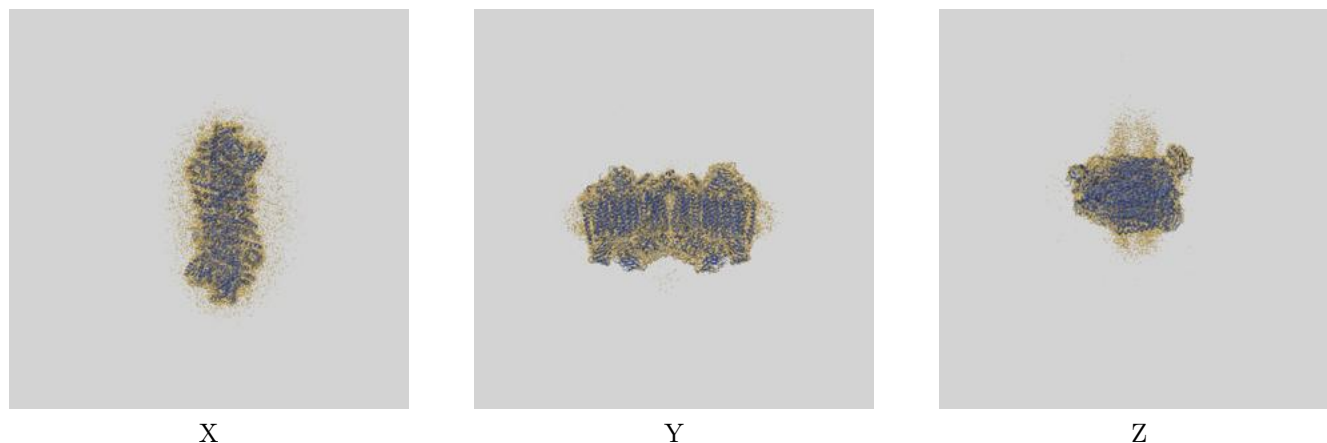
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.80	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.83	7.41	3.93

*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 3.83 differs from the reported value 2.8 by more than 10 %

9 Map-model fit [i](#)

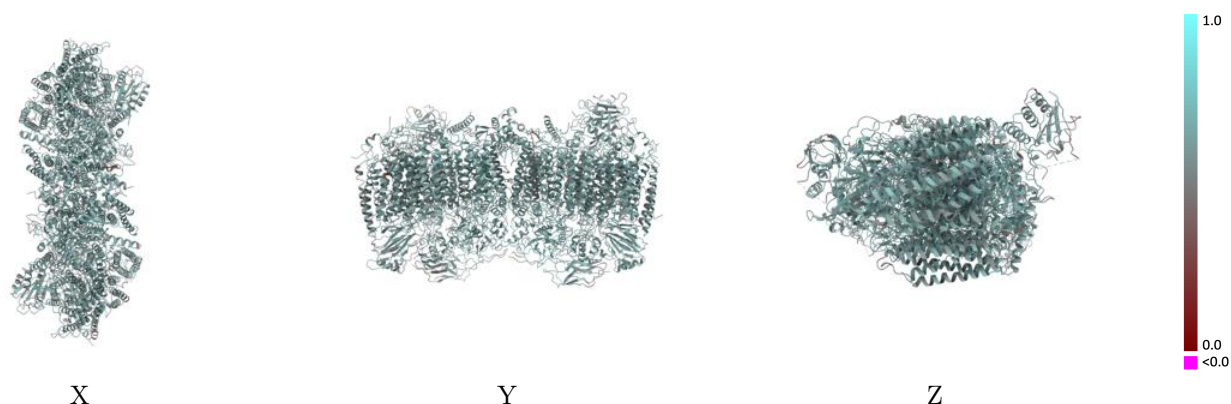
This section contains information regarding the fit between EMDB map EMD-17210 and PDB model 8OVC. Per-residue inclusion information can be found in section [3](#) on page [19](#).

9.1 Map-model overlay [i](#)



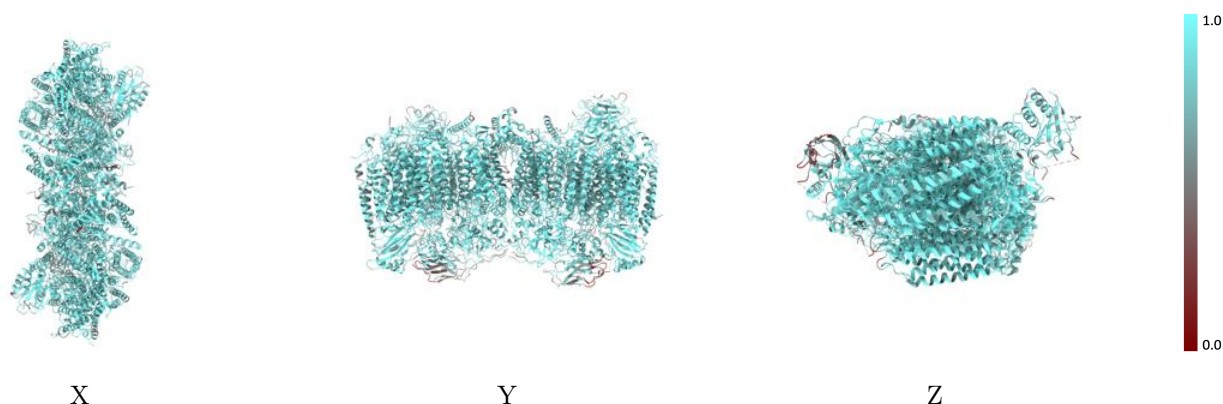
The images above show the 3D surface view of the map at the recommended contour level 0.194 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



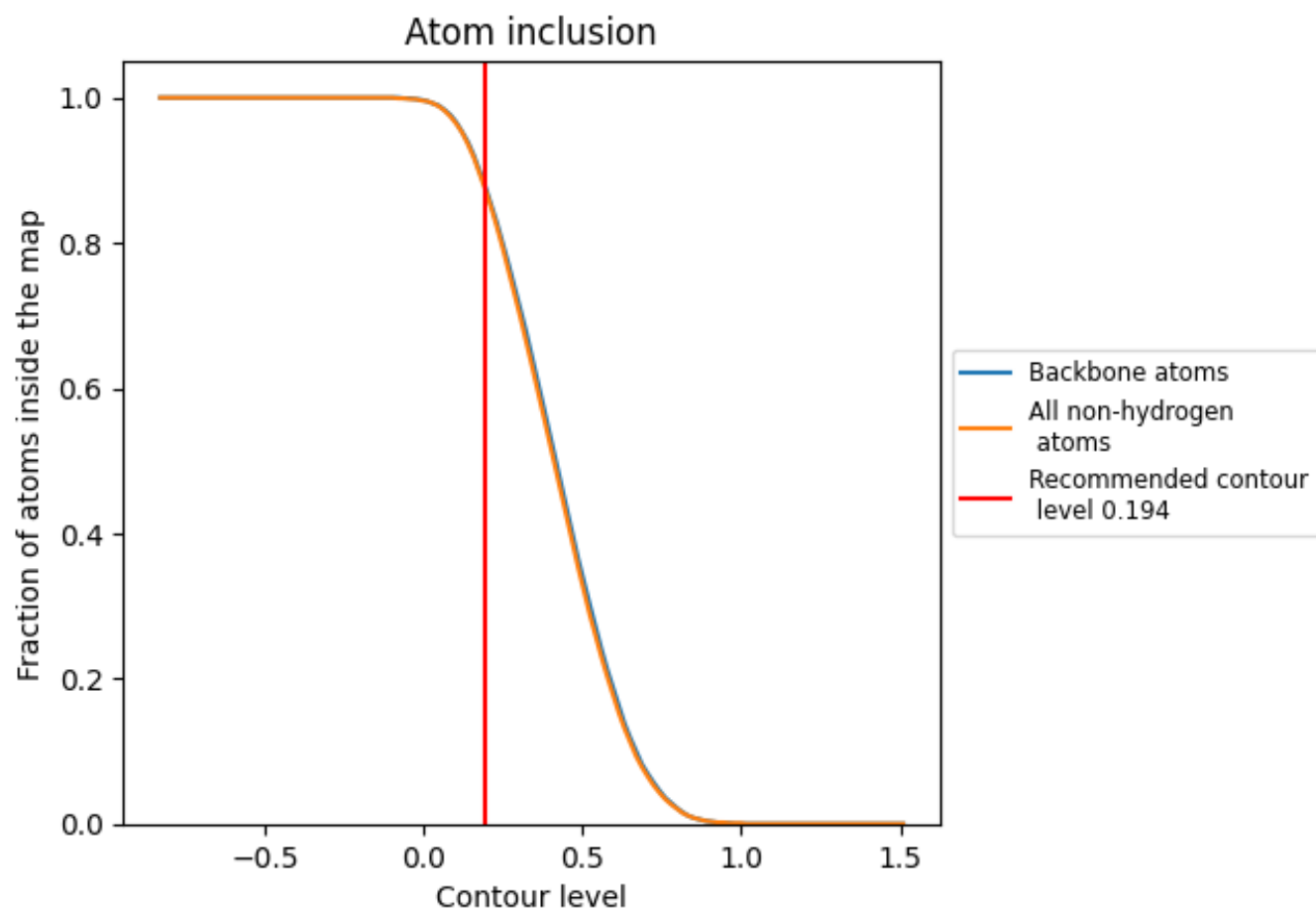
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.194).

9.4 Atom inclusion [i](#)



At the recommended contour level, 88% of all backbone atoms, 87% 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 (0.194) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8730	 0.5980
C	 0.9220	 0.6240
E	 0.7430	 0.5400
F	 0.6870	 0.4700
G	 0.9030	 0.6170
H	 0.9180	 0.6210
I	 0.8380	 0.5910
J	 0.8960	 0.5980
K	 0.9010	 0.5940
L	 0.9340	 0.6130
M	 0.9030	 0.6120
N	 0.9170	 0.6200
O	 0.9050	 0.6100
P	 0.8560	 0.5920
Q	 0.8200	 0.5570
R	 0.9160	 0.6010
S	 0.8800	 0.5940
T	 0.8790	 0.5820
U	 0.7920	 0.5560
V	 0.7780	 0.5480
W	 0.5380	 0.5340
X	 0.8420	 0.5850
Y	 0.7350	 0.5530
Z	 0.7890	 0.5610
a	 0.8360	 0.5730
b	 0.6010	 0.5630
c	 0.8430	 0.5760
e	 0.7390	 0.4720
f	 0.8290	 0.5120

